

**The Spectrum and Term Analysis of Nd III
and
Hyperfine Structure of Energy Levels in Co II**

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I declare that the work presented within this thesis comes from my original research, all else is appropriately referenced and acknowledged.

14th of March, 2024

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I dedicate this thesis to my mother Xiaomei

‘The miracle of the appropriateness of the language of mathematics for the formulation of the laws of physics is a wonderful gift which we neither understand nor deserve.’

Eugene Paul Wigner

Abstract

Developments in observational astrophysics are producing higher-quality data at increasingly immense volumes. As a result, the requirements for reference data on the properties of atoms in astrophysics are no longer met. This thesis aims to address this problem, primarily through high-resolution Fourier transform spectroscopy of laboratory atomic plasmas of elements of urgent astrophysical needs, which include the rare-earth and iron-group elements that are of particular interest in nucleosynthesis and stellar structure investigations, owing to their complex spectra and intriguing cosmic relative abundances. The spectrum and atomic structure of the second ionisation stage of the rare-earth element neodymium (Nd III, 60 protons) were very poorly known experimentally. Spectra of Nd were recorded in the region 11 500–54 000 cm⁻¹ (870–185 nm) using resolving powers up to 10⁶ and measured wavenumbers were accurate to a few parts in 10⁸. Analysis of the Nd spectra was supplemented by grating spectroscopy and semi-empirical atomic structure calculations. Overall, 258 energy levels and 957 transitions of Nd III have been identified, where 219 energy levels were identified for the first time. The high-resolutions of modern astrophysical spectra can also observe the hyperfine structure of atomic energy levels, which cause distortion and broadening of spectral lines and must be considered in stellar spectral line modelling. For the first ionisation stage of the iron-group element cobalt (Co II, 27 protons), hyperfine structure constants of only 28 of the ~500 experimentally known energy levels were previously investigated. The analysis of Co Fourier transform spectra led to the determination of the magnetic dipole interaction constants for 298 energy levels of Co II, 264 of which were determined for the first time. The order of magnitude increase in the available atomic reference data for Nd III energy levels and Co II hyperfine structure will enable wider and more reliable applications of these elements in astrophysical investigations.

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Contents

Abstract	5
Acknowledgements	6
Table of Contents	15
List of Figures	20
List of Tables	22
Abbreviations	23
1 Introduction	24
1.1 Astrophysics and Atomic Data	25
1.1.1 Spectroscopy in Astrophysics	25
1.1.2 Developments in Astronomical Spectroscopy	27
1.1.3 Properties of Atomic Transitions	29
1.2 Rare-earth and Iron-group Elements in Astrophysics	31
1.2.1 Relative Abundance and Spectra Complexity	31
1.2.2 Gravitational Wave Detection, Kilonovae, and REEs	33

1.2.3	Stellar Astrophysics and Absorption Spectra Modelling	36
1.3	Objectives	38
1.4	Previous Investigations in the Literature	40
1.4.1	Nd III Energy Levels and Transitions	40
1.4.2	Co II Hyperfine Structure Constants	44
1.5	Summary and Thesis Structure	45
2	Theory of Atomic Structure and Spectra	47
2.1	Introduction	47
2.2	Solving the Schrödinger Equation	48
2.2.1	Central Field Approximation and Electronic Configuration	49
2.2.2	Residual Electrostatic Repulsion	51
2.2.3	Relativistic Corrections and Spin-orbit Interaction	52
2.2.4	Matrix Method for the Hamiltonian and its Eigenstates	53
2.2.5	Angular Momentum Coupling and Term Symbols	54
2.2.6	Labelling Energy Levels	58
2.2.7	Configuration Interaction	59
2.2.8	Nd III Atomic Structure and Coupling Conditions	60
2.3	Electric Dipole (E1) Transitions	63
2.3.1	Transition Probabilities	64
2.3.2	Selection Rules and Theoretical Line Strengths	66
2.4	Perturbations to Energy Levels	68
2.4.1	Hyperfine Structure	68

2.4.2	Isotope Shifts	70
2.4.3	Zeeman Splitting	70
2.5	Plasma Thermodynamic and Radiative Properties	71
2.5.1	Atomic Partition Function and the Boltzmann Distribution	71
2.5.2	Saha Equilibrium and Ion Fractions	72
2.5.3	Spectral Line Profiles	73
2.5.4	Self-absorption	74
2.5.5	Meaning of ‘Strong’ and ‘Weak’ Lines	76
3	Principles of Fourier Transform Spectroscopy	78
3.1	Introduction	78
3.2	Ideal Fourier Transform Spectrometer	79
3.2.1	The Michelson Interferometer	79
3.2.2	Example Interferograms and Spectra	80
3.3	Real Fourier Transform Spectrometer	83
3.3.1	Interferogram Asymmetry and Phase Correction	83
3.3.2	Spectral Range and Digital Interferogram Sampling	85
3.3.3	Spectral Resolution and the Instrumental Profile	87
3.3.4	Aperture Size and the Instrumental Profile	90
3.3.5	Interferogram Modulation Efficiency	94
3.3.6	Photomultiplier Tubes and Spectral Intensity Response	95
3.4	Sources of Noise and Error	96
3.4.1	Noise in Interferograms and Spectra	96

3.4.2	Systematic Errors	98
3.5	Why Choose Fourier Transform Spectroscopy?	101
4	Laboratory Measurements of Nd Spectra	103
4.1	Introduction	103
4.2	The Imperial College VUV Fourier Transform Spectrometer	104
4.2.1	Design of the Imperial College VUV FT Spectrometer	105
4.2.2	Interferogram Sampling System	107
4.3	Experimental Set-up and Operation	109
4.3.1	Vacuum Pumping	110
4.3.2	Light Source Set-up	111
4.3.3	Spectrometer and Light Source Alignment	112
4.3.4	Photomultiplier Tube Detectors and Optical Filters	113
4.3.5	Measuring Interferograms	116
4.4	Nd Discharge Sources	117
4.4.1	Hollow Cathode Discharge Lamp	117
4.4.2	Penning Discharge Lamp	119
4.4.3	Nd Metal Handling and Lamp Maintenance	120
4.5	Optimisation of Lamp Running Conditions	126
4.5.1	HCL Optimal Conditions	127
4.5.2	PDL Optimal Conditions	131
4.6	Final Measurements of Nd Spectra	133
4.7	Nd Vacuum Spark and Stellar Grating Spectra	135

4.8	Summary of the Laboratory Measurements of Nd Spectra	137
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5 Nd Fourier Transform Spectra and Calibration 138

5.1	Introduction	138
5.2	Fourier Transform of Interferograms	139
5.2.1	Co-adding Interferograms	139
5.2.2	Phase Correction	146
5.2.3	Interferogram Apodisation	147
5.2.4	Noise Level Determination	148
5.3	Spectral Line Fitting and Line List Creation	149
5.3.1	Voigt Profile Fitting and Statistical Wavenumber Uncertainty	150
5.3.2	Line Profiles due to Nd Isotope Shifts	151
5.3.3	Centre-of-gravity Fitting	151
5.3.4	Asymmetric Voigt Profile Fitting	153
5.3.5	Challenges in Fitting the Nd-Ar FT PDL Spectral Lines	156
5.3.6	Custom Line Fitting Program	157
5.4	Absolute Wavenumber Calibration	159
5.4.1	Calibration Factor	160
5.4.2	Wavenumber Uncertainty	161
5.4.3	Line Selection for Calibration and Results	163
5.5	Relative Intensity Calibration	166
5.5.1	Spectral Intensity Response Functions	167
5.5.2	Relative Intensity Calibration of All Spectra	169

5.5.3	Relative Intensity Uncertainty Estimation	172
5.6	Merging Line Lists	174
5.7	Summary of the Nd FT Spectra and their Calibration	174
6	Analysis of the Atomic Structure and Spectrum of Nd III	177
6.1	Introduction	177
6.2	Species in the Nd-Ar Spectra	178
6.3	Nd III Line Classification and Energy Level Identification	180
6.3.1	Principal Methods to Establish New Energy Levels	180
6.3.2	Line Classification Assistance from Nd III Isotope Structure	187
6.3.3	Line Classification Assistance from Nd-Ar Hollow Cathode FT Spectra .	189
6.4	Energy Level Optimisation and Ritz Wavenumber Uncertainties	191
6.4.1	Optimum Energies and Energy Uncertainties	191
6.4.2	Effects of Systematic Shifts on Uncertainties	192
6.5	Term Analysis Methodology for Nd III	194
6.6	Confirmation and Revision of Known Nd III Levels	194
6.6.1	H. M. Crosswhite's Identifications - NIST ASD Energy Levels	196
6.6.2	Confirmation of Energy Levels by Ryabchikova et al. (2006)	199
6.6.3	Revision of $4f^3(^4I^\circ)5d\ ^5H^\circ_3$ by Ryabchikova et al. (2006)	199
6.7	Searching for Unknown Energy Levels of Nd III	201
6.7.1	Completing the $4f^3(^4I^\circ)5d$ and $4f^3(^4I^\circ)6p$ Sub-configurations	202
6.7.2	Completing the $4f^3(^4I^\circ)6s$ Sub-configuration	203
6.7.3	Locating the $4f^3(^4G^\circ)5d$ Sub-configuration	204

6.7.4	New Cowan Code Nd III Atomic Structure Calculations	205
6.7.5	Configuration Mixing between $4f^35d$ and $4f^36s$ in $4f^3(^4G^\circ)5d\ ^5I^\circ_7$	206
6.7.6	Zeeman Splitting and J Values of 34994 cm^{-1} and 35154 cm^{-1}	207
6.7.7	The Singlets $^1H^\circ_5$ and $^1I^\circ_6$ of $4f^3(^2H2^\circ)5d$	209
6.7.8	Higher-lying $4f^36p$ Energy Levels	210
6.7.9	Challenges in Finding Unknown $4f^4$ Energy Levels	210
6.7.10	Finding the $4f^4\ ^5G_5$ Energy Level	211
6.7.11	Finding the $4f^4\ ^3K_{27}$ Energy Level	212
6.7.12	Finding the $4f^4\ ^3K_{26}$ Energy Level	214
6.7.13	Finding the $4f^4\ ^5F_5$ Energy Level	215
6.7.14	Finding the $4f^4\ ^3K_{28}$ Energy Level	215
6.7.15	Finding the $4f^4\ ^5F_{2,3,4}$, $4f^3(^4F^\circ)5d\ ^5F^\circ$, and $4f^3(^4S^\circ)5d\ ^5D^\circ$ Energy Levels	216
6.7.16	Finding the $4f^4\ ^5G_{3,4}$ and $4f^4\ ^3H_{45}$ Energy Levels	219
6.7.17	Levels of the $4f^3(^4I^\circ)7s$ and $4f^3(^4I^\circ)6d$ Sub-configurations	219
6.7.18	Levels of the $4f^35f$ Configuration	220
6.8	Term Analysis Results	221
6.8.1	List of Identified Energy Levels	221
6.8.2	Transitions Classified from Laboratory Sources	222
6.9	Summary of the Term Analysis of Nd III	224
7	Outlook from the Analysis of Nd III Atomic Structure	225
7.1	Introduction	225
7.2	Applications to Astrophysical Spectra	225

7.3	Ongoing Work	232
7.4	Nd Discharge Lamp Thermal Conditions	233
7.5	Possible Experimental Strategies for Future Nd III Term Analyses	238
7.5.1	Experimentally Unknown Configurations of Interest	239
7.5.2	Resonance Plasma Collisional Cross-sections	240
7.6	Remarks on Key Strategies in the Analysis of Complex Atomic Structure	240
7.6.1	Variety of Light Source Thermal Conditions	241
7.6.2	Wide Spectral Range and High Spectral Resolution	242
7.6.3	Accurate and Complete Line Lists	242
7.6.4	Accurate Atomic Structure and Transition Probability Calculations . . .	243
8	Hyperfine Structure Analysis of Co II Energy Levels	244
8.1	Introduction	244
8.2	Fourier Transform Spectra of Cobalt	245
8.3	Custom Analysis Program - <i>hfs_fit</i>	246
8.3.1	Initial Parameter Determination	246
8.3.2	Least-squares Fit by Simulated Annealing	248
8.3.3	Treating Instrumental Ringing	250
8.4	Considerations for Self-Absorption	252
8.5	Parameter Constraints	253
8.5.1	Well-constrained Parameters	253
8.5.2	Poorly Constrained and Most Significant Parameters	254
8.5.3	Parameter Mean and Uncertainty Estimation	259

8.6	Strategy of Analysis	261
8.7	Summary of Results	262
8.8	Comparisons with More Recent Literature	264
8.8.1	Laser Spectroscopy by Koszorús et al. (2023)	264
8.8.2	Independent Analysis of Archival FT Spectra by Fu et al. (2021)	264
8.8.3	Semi-empirical Calculations of Co II HFS	266
8.9	Summary of the Analysis of Co II HFS	271
9	Conclusions	273
9.1	Energy Levels and Transitions of Nd III	273
9.2	Hyperfine Structure Interaction Constants of Co II Energy Levels	274
9.3	Impacts and Future Work	275
	Bibliography	295
	Appendix A Nd III Cowan Code Parameters	296
	Appendix B Custom Spectral Line Fitting Program Functionalities	302
	Appendix C Nd III Energy Levels Experimentally Identified	305
	Appendix D Nd III Transitions Classified from Laboratory Plasmas	312
	Appendix E Unclassified Nd III Line List of Dr H. M. Crosswhite	343
	Appendix F Co II Magnetic Interaction Hyperfine Structure Constants	367
	Appendix G Nd-Ar PDL FT Spectra Plots	377

List of Figures

1.1	A Section of the UV Absorption Spectrum of χ Lupi	26
1.2	Solar Elemental Abundance	31
1.3	Atomic Complexity Measure	33
1.4	AT2017gfo Spectrum Observed by X-shooter and HST	34
1.5	Model Kilonova Spectra with Various REE Abundances	35
1.6	Radial Velocity Variations of γ Equulei	37
1.7	Radial Velocity Variations of a Nd III Line in γ Equulei	37
1.8	LTE and NLTE Modelling of a Co II Stellar Absorption Line	39
1.9	Nd III Transitions Predicted with the Highest Weighted Oscillator Strengths . .	43
2.1	Gross Atomic Structure of the 4f-excited System of Nd III	62
2.2	Model Self-Absorption of a Voigt Profile	76
3.1	Schematic Diagram of the Michelson Interferometer	79
3.2	Comparisons between Types of Spectra and their Interferograms	82
3.3	Spectra of Continuously and Discretely Sampled Interferograms	86
3.4	Spectrum of an Insufficiently Discretely Sampled Interferogram	86
3.5	Sampling in the Second Alias	87

3.6	Finite Path Difference Instrumental Sinc Function	88
3.7	Cosine Bell Apodisation and Instrumental Ringing	89
3.8	Imaging a Finite Aperture Size Interferogram	91
4.1	Exterior of the IC VUV FT Spectrometer	106
4.2	Optics Layout within the IC VUV FT Spectrometer	107
4.3	He-Ne Laser and Light Source Beam Positions in the IC VUV FT Spectrometer	108
4.4	Nd FT Spectroscopy Experimental Set-up	110
4.5	Hamamatsu R11568 PMT Quantum Efficiency and Sensitivity	114
4.6	SCHOTT GG475 Long-pass Optical Filter Transmittance	115
4.7	Diagram of Components of the HCL	118
4.8	Diagram of Components of the PDL	119
4.9	Depleted Nd Hollow Cathode	122
4.10	Photographs of New and Depleted PDL Cathodes	123
4.11	Photographs of PDL Anode Rings	125
4.12	Damaged HCL O-ring	126
4.13	Annotated Photo of the HCL Set-up	127
5.1	Co-added Interferogram vs. Single Interferogram	140
5.2	Co-added Interferogram vs. Single Interferogram with Brief Fluctuations	141
5.3	Co-added Interferogram vs. Single Interferogram at a Small Fluctuation	142
5.4	Spectra of Co-added Interferogram with and without Co-adding Interferogram with a Small Fluctuation	143
5.5	Inconsistent Interferogram Centres	144

5.6	Spectra of Co-adding Interferograms with Inconsistent Centres	145
5.7	<i>XGREMLIN</i> Phase Correction Interface	147
5.8	Complex Spectrum after Phase Correction	148
5.9	Isotope Line Profiles of Two Nd Lines	152
5.10	Asymmetric Voigt Fit Example	155
5.11	Number of lines observed per 100 cm^{-1} in the Penning Lamp	156
5.12	Observed Nd-Ar spectra between $19659\text{-}19669\text{ cm}^{-1}$	157
5.13	Line Fitting Program GUI	158
5.14	Wavenumber Calibration Spectrum Order	160
5.15	Total Systematic Uncertainties	163
5.16	Nd-Ar PDL FT Spectral Lines Selected for Wavenumber Calibration	165
5.17	Nd-Ar HCL FT Spectral Lines Selected for Wavenumber Calibration	166
5.18	Intensity Calibration Lamp Spectrum Filtering	168
5.19	Intensive Response Curves	170
5.20	Relative Intensity Calibration Factors	171
5.21	Determination of Wavenumber Boundaries for Merging Line Lists	175
5.22	Spectrum of the Nd-Ar Penning Lamp	176
6.1	Grotrian Diagram of four Energy Levels	180
6.2	Grotrian Diagram of three Known Levels and one New Level	182
6.3	Example Output of <i>LEVHAMD</i>	183
6.4	Isotope Shifts in Nd III Lines	188
6.5	Width against Wavenumber for the Nd-Ar FT Spectra	189

6.6	Self-absorption of Nd II in the Penning Discharge Lamp	190
6.7	Flow Chart Summarising the Empirical Spectrum Analysis of Nd III	195
6.8	Classified Transitions from $4f^3(4I^\circ)5d\ ^5I^\circ$ and $4f^3(4I^\circ)5d\ ^5H^\circ$ to the Ground Term	197
6.9	Blend of $4f^4\ ^5I_6 - 4f^3(4I^\circ)5d\ ^5I^\circ_6$ and $4f^4\ ^5I_4 - 4f^3(4I^\circ)5d\ ^5H^\circ_3$ at 19593 cm^{-1} . .	200
6.10	Spectral Synthesis of $4f^4\ ^3K2_6 - 34994.015\text{ cm}^{-1}$ of HD 144897	208
6.11	Identifications of $4f^3(^2H2^\circ)5d\ ^1H^\circ_5$ and $4f^3(^2H2^\circ)5d\ ^1I^\circ_6$ by Dr Ryabstev	209
6.12	Classifications of five Transitions to $4f^4\ ^5G_5$ in Stars	212
6.13	The Level Search for $4f^4\ ^3K2_7$	213
6.14	The Level Search for $4f^4\ ^5F_{2,3,4}$	216
6.15	Two False Classifications Identified by Stellar Spectroscopy	218
6.16	Summary of Identified Nd III Energy Levels	222
6.17	Transitions used to Optimise Nd III Level Energies	223
7.1	Synthesis of three Nd III Lines in three Different Stars	227
7.2	Pulsational Characteristics Observed in Classified Nd III Lines	228
7.3	Ritz Wavelength $17400.13\text{ \AA}$ of $4f^4\ ^5G_5 - 4f^3(4I)\ ^5H_6$ Observed in γ Equulei . . .	229
7.4	Nd Abundance Analysis of HD 170973	231
7.5	Predicted Nd III Spectrum using Temperature of 7300 K and 20000 K	234
7.6	Boltzmann Plot of Nd III Transitions in Spectrum E	235
7.7	Nd Vacuum Spark Temperature Estimation	237
7.8	Enhancement of Nd III Lines through the Duffendack-Penning Reaction	241
8.1	Unsatisfactory Initial HFS Parameters Example	247
8.2	Satisfactory Initial HFS Parameters Example	248

8.3	Fitting Instrumental Ringing in HFS Analysis	251
8.4	Unresolved Co II HFS with Correct A Constants	256
8.5	Unresolved Co II HFS with Incorrect A Constants	257
8.6	HFS Analysis with Same J Values for Both Levels	258
8.7	Doppler Width of Co II Hyperfine Transitions	261
8.8	Co II Transition Observed with Resolved Hyperfine Component Transition . . .	263
8.9	Fitting Blended Line for HFS of $3d^7(a^2D)5s\ ^3D_1$	269
8.10	Example of Questionable A_{calc}	270
B.1	Line Fitting Program GUI shown again	302
E.1	Difference between Observed and Dr Crosswhite's Nd III Wavenumbers	344
G.1	Nd-Ar PDL FT Spectra Part 1	378
G.2	Nd-Ar PDL FT Spectra Part 2	379
G.3	Nd-Ar PDL FT Spectra Part 3	380
G.4	Nd-Ar PDL FT Spectra Part 4	381
G.5	Nd-Ar PDL FT Spectra Part 5	382
G.6	Nd-Ar PDL FT Spectra Part 6	383
G.7	Nd-Ar PDL FT Spectra Part 7	384
G.8	Nd-Ar PDL FT Spectra Part 8	385
G.9	Nd-Ar PDL FT Spectra Part 9	386
G.10	Nd-Ar PDL FT Spectra Part 10	387
G.11	Nd-Ar PDL FT Spectra Part 11	388
G.12	Nd-Ar PDL FT Spectra Part 12	389

List of Tables

4.1	Summary of Parameters of the IC VUV FT Spectrometer	105
4.2	Nd-Ne HCL Optimal Condition Search	129
4.3	Nd-Ar HCL Optimal Condition Search	130
4.4	Nd-Ar PDL Optimal Condition Search	132
4.5	Nd HCL FT Spectra Parameters	134
4.6	Nd-Ar PDL FT Spectra Parameters	134
4.7	Nd sliding VS Spectra Parameters	136
5.1	Summary of Nd-Ar PDL FT Spectra Noise Determination	149
5.2	Relative Abundance of Naturally Occurring Nd Isotopes	151
5.3	Summary of Wavenumber Calibration	164
5.4	Summary of Intensity Calibration	172
6.1	Non-Nd III Species and Lines Identified in Nd PDL FT Spectrum Merged Line List	178
6.2	Theoretical $g_u A$ Values from Configuration Mixing of $4f^3(^4G^\circ)5d\ ^5I^\circ_7$	206
6.3	Predicted and Observed $4f^4\ ^5F_J - 4f^35d(^4S^\circ)\ ^5D^\circ_{J-1}$ Transitions	217
8.1	Inconsistent HFS A Constants with Fu et al. (2021)	265

8.2	Inconsistent HFS A Constants with Recent Calculations	268
A.1	Nd III Cowan Code Parameters	297
C.1	Observed Nd III Energy Levels	306
D.1	Nd III Transitions Classified from the Nd-Ar PDL FT Spectra	314
D.2	Classified Nd III Transitions Observed Only from the Nd VS Spectra	334
E.1	Unclassified Nd III Line List of Dr H. M. Crosswhite Compared with the Penning Lamp Line List	345
F.1	HFS A Constants of Even Energy Levels of Co II	368
F.2	HFS A Constants of Odd Energy Levels of Co II	372

Abbreviations

COG	Centre-of-gravity
FT	Fourier Transform
FWHM	Full Width at Half Maximum
HCL	Hollow Cathode Lamp
HFS	Hyperfine Structure
IR	Infrared
NIST ASD	National Institutes of Standards and Technology Atomic Spectra Database
PDL	Penning Discharge Lamp
PMT	Photomultiplier Tube
REE	Rare-earth Elements
RMS	Root-mean-square
SNR	Signal-to-noise Ratio
UV	Ultraviolet
VUV	Vacuum Ultraviolet
VS	Vacuum Spark

Chapter 1

Introduction

Out of the four fundamental forces in the current standard model of particle physics, the electromagnetic force is arguably the most common type of force we experience day to day. Aside from counteracting the gravitational force pulling us into the centre of the Earth, it is accountable for what we see through our eyes, how we feel through direct contact with other objects, and when we make movements through electric impulses. The particle responsible for the electromagnetic force is the photon, also known as electromagnetic radiation and more loosely referred to as light. Photons are both particles and waves, this is a well-known physical principle and will be applied throughout this thesis.

Interactions between light and matter are key considerations in almost all theoretical and/or experimental investigations in physics. One of the most important methods is to investigate the relative energy contributions of the wavelengths of the detected light, analogous to how one observes the brightness of different colours by eye. This is referred to as spectroscopy and this thesis focuses on the spectroscopy of interactions between light and atoms in gaseous or plasma states. Each atom (and ion) of the elements of the periodic table in the gaseous or plasma state interacts with light uniquely, absorbing and emitting unique wavelengths of light. This fingerprint-like property is called the spectrum of the atom. The spectrum of an atom can change depending on the surrounding environment of the atom, observing such changes in the spectrum provides observers with information about the environment.

The atoms investigated in this thesis belong to the elements of neodymium and cobalt, both of which are metals if placed on Earth. However, they can be in the gaseous or plasma state

if the temperature is high enough, such temperatures are naturally found in the atmospheres of stars or remnants of stars. Not all stars or stellar remnants are the same, and so their environments for their atoms also differ from one another. The differences in the environments are observable from the atomic spectra of the astrophysical objects, which one can use to deduce properties such as elemental abundances, temperatures, densities, magnetic fields, and stages of stellar evolution. When this information is obtained for many stars of a galaxy, the history and evolution of the galaxy could also be gauged. One of the ultimate goals of this field of astrophysical research is to understand the origins of the elements and how everything came to be. It is expected that many more discoveries are required along the way to answer this question, which will greatly impact our knowledge of the universe and improve our daily lives when applied by the hands of the right people.

1.1 Astrophysics and Atomic Data

1.1.1 Spectroscopy in Astrophysics

The work of this thesis aims to advance observational astrophysics by measuring previously unknown and less accurate reference atomic data in the laboratory. The scope of atomic data concerned the spectral properties of bound-to-bound transitions of electrons within atoms, which often produce very detailed and sharp spectral features, composing complex spectra requiring high-resolution instrumentation to observe accurately. Atomic data characterising inter-atomic interactions, such as collisions or free-electron captures, and nuclear reactions, such as nuclear stabilities or decay mechanisms, are also important in the theories and modelling of astrophysical objects, but they were beyond the scope of the present work. All atomic transitions mentioned in this thesis correspond to bound-to-bound electron transitions unless specified otherwise.

As there are so many elements on the periodic table, spectral lines of their neutral atoms and ions of the first few ionisation stages can all appear together in spectra of stellar atmospheres. The atoms and ions in stellar atmospheres absorb continuum radiation emitted from the surface of stars, and re-emit the absorbed photons into different directions, causing a reduction of the number of observed photons at the absorption wavelengths. The result is an absorption

atmosphere. Many lines are identified but some remained unknown, as can be seen in lines of the observed spectrum with significantly lower flux compared to the modelled spectrum, showing apparent absorption of unknown origin. To resolve this problem, one must identify and measure the unknown absorption transition wavelengths to an accuracy equal to or higher than the accuracy achievable in telescopes, which typically involves laboratory spectroscopy of the species of interest at higher resolving powers.

Space and ground-based telescopes achieved resolving powers and signal levels to distinguish individual atomic transitions observed from stellar spectra decades ago. However, many transition wavelengths remain unknown and require investigation of the electronic structures (quantum states) of the corresponding atoms and ions. Furthermore, the high resolving powers, $\sim 10^5$, of these telescopes are even able to observe small perturbations from external or internal electromagnetic fields of the atoms and ions, which can change the shapes of the corresponding transitions and must also be characterised. This thesis aims to address the incompleteness of atomic data. More specific and detailed discussions of how atomic data influences spectroscopy in astrophysics are discussed in the rest of this chapter, with a particular focus on motivations for the atoms (neodymium and cobalt ions) investigated in the present work.

1.1.2 Developments in Astronomical Spectroscopy

Over the years, countless astronomical spectra have been recorded and archived. Further investigations using these archival spectra when better reference atomic data become available are not unexpected. At the same time, telescopes with higher resolution and larger collecting areas were also built, since resolutions and signal strengths are also primary limitations aside from reference atomic data. While even better telescopes are being built, the limitations of incomplete atomic data must also be addressed; developments in atomic reference data ideally should not lag behind the developments of new telescopes.

Examples of current telescopes capable of high-resolution spectroscopy include: the Hubble Space Telescope using its Space Telescope Imaging Spectrograph (STIS) instrument to observe in the range 115 to 1000 nm, with resolving powers between 30 000 and 114 000 in the ultraviolet (UV) and up to 17 000 for other spectral regions [2], high-resolution UV spectra (unavailable for ground-based telescopes) recorded using this instrument are catalogued and intended for

investigations for decades to come (e.g. [3,4]); the Gaia-ESO survey [5–7] combines observations between the space telescope Gaia and the Very Large Telescope (VLT) of the European Southern Observatory, the VLT contains the Ultraviolet and Visual Echelle Spectrograph (UVES) [8], capable of resolving powers between 40 000 and 110 000 in the spectral range between 300 and 1100 nm, and spectra of several stars recorded using this instrument were used in the analysis of the present work (see section 4.7); the Apache Point Observatory Galactic Evolution Experiment (APOGEE) [9], part of the Sloan Digital Sky Survey III [10], collected spectra for 146 000 stars in the near infrared (IR) between 1510 and 1700 nm using the Sloan 2.5 m telescope at resolving powers of 22 500, to investigate the evolution of galaxies; similarly, the High Efficiency and Resolution Multi-element Spectrograph (HERMES) of the 3.9 m Anglo-Australian Telescope has a spectral range between 470 and 790 nm and resolving powers of either 28 000 or 50 000 [11], the instrument can record high-resolution spectra for 400 stars simultaneously and is involved in the Galactic Archaeology Survey [12], with spectra of 600 000 nearby stars in the most recent data release [13].

Examples of planned telescopes capable of high-resolution spectroscopy include: the Large Ultraviolet Optical Infrared Surveyor [14] is a space telescope mission under planning, it aims to provide orders of magnitude improvement in sensitivity compared to the Hubble Space Telescope, while observing at similar spectral resolving powers; the Willian Herschel Telescope’s Enhanced Area Velocity Explorer [15] is under construction and aims to perform galactic surveys in the spectral range between 366 to 975 nm at resolving powers of 20 000; and the Extremely Large Telescope (ELT) [16] of the European Southern Observatory is under construction and plans to use the ArmazoNes high Dispersion Echelle Spectrograph [17] with planned resolving power of 100 000 and spectral range between 400 and 1800 nm.

Evidently, the amount of data produced by the telescopes is (and will be) enormous, and detailed analyses will require high-quality atomic data. While the signal strength and resolving powers are designed to be sufficient, the availability of atomic data is currently lagging behind [18], as was the case for the χ Lupi spectral analysis (Figure 1.1) and for the analyses that will be discussed in subsection 1.2.2 and subsection 1.2.3.

Astrophysicists query databases when they require atomic data. Popular atomic transition databases include: Kurucz’s atomic spectral line database [19], the National Institute of Standards and Technology Atomic Spectra Database (NIST ASD) [20], the Vienna atomic line

database [21], and the Atomic Database on Rare Earths at Mons University (Belgium) [22]. Generally, experimental results for atomic spectral data are the most reliable. Theoretical or semi-empirical atomic data are used when experimental data are unavailable. The atomic spectral databases include results from experimental, theoretical, and/or semi-empirical investigations. The most important parameters of the spectrum of an atom in astrophysical spectroscopy will be discussed in the next subsection.

1.1.3 Properties of Atomic Transitions

To model and investigate astrophysical spectra, such as in the analysis of Figure 1.1, one requires various information on the atomic transitions. The following is a list of the most significant properties of atomic transitions in the context of stellar spectroscopy.

Wavelength

The wavelength of each transition must be known, with uncertainties better than a few parts in 10^7 for resolving powers $\sim 10^5$. Each wavelength λ is related to the energy separation E between the two energy levels (or energy degenerate quantum states) of an atom involved in the transition through the Planck relation $E = hc/\lambda$. The energy levels are referred to as fine structure energy levels. The word ‘fine structure’ expresses the degree of accuracy and detail of the description of atomic structure that is determined by relativistic effects and the possible total electron angular momenta of the atom (see section 2.2). Within the context of Figure 1.1, the transition wavelengths correspond to energy separations between atomic fine structure energy levels.

Transition Probabilities

The transition probability (also referred to as the $\log(gf)$, oscillator strength, or line strength, see section 2.3) of each transition must be known. The transition probability determines the likelihood of a transition and therefore the intensity of the transition. It applies to both the absorption and emission of photons and partly contributes to the lifetime of the spontaneous de-excitation of its upper energy level. The intensity of a transition is also affected by the number

of atoms in the associated energy levels of the transition, so if the transition probability is known, the relative abundance of the atoms in the astronomical object could be determined.

Whether differences in relative elemental abundance could be observed depends on the accuracy of the transition probabilities. Typical uncertainties in transition probabilities are on the order of 10%; a few percent is the achievable accuracy of experimental measurements [23] and 10% is around the minimum for theoretical calculations of many-electron atoms [24]. The 10% uncertainty is sufficient to observe elemental abundance differences, e.g., it corresponds to approximately ± 0.04 dex on the log y -scale of Figure 1.2.

Small Perturbations - Hyperfine Structure, Isotope Shifts, and Zeeman Splitting

More accurate descriptions of the energy levels than those of the fine structure description are required in some cases. This is because the aforementioned small perturbations from external or internal electromagnetic fields can produce significant deviations from fine structure energies that are observable in high-resolution stellar absorption spectra. Examples include hyperfine structure (HFS), isotope shifts, and Zeeman splitting (see section 2.4), all of which cause line distortion, broadening, or splitting, which must be included to correctly model stellar spectra and stellar environments [25]. The effects of the small perturbations depend on the energy levels, they are characterised by measurable and calculable constants for each energy level.

The accuracy requirements for the small perturbation constants of energy levels become higher with increasing telescope spectral resolving power. Generally, the constants are measured in the laboratory at resolving powers significantly above those of the telescopes, so the measured constants are sufficiently accurate. Theoretical calculations of these constants are less accurate, but still offer good estimations when perturbations are small under a relatively lower resolving power, e.g., when the perturbation patterns are not fully resolved.

Energy Levels

The experimental measurements and theoretical calculations of transition wavelengths, transition probabilities, HFS constants, isotope shifts, and Zeeman splitting constants (Landé g -factors) all require knowledge of the energy levels involved in the transitions of interest, because the energy levels represent wavefunctions that physically determine electron distributions

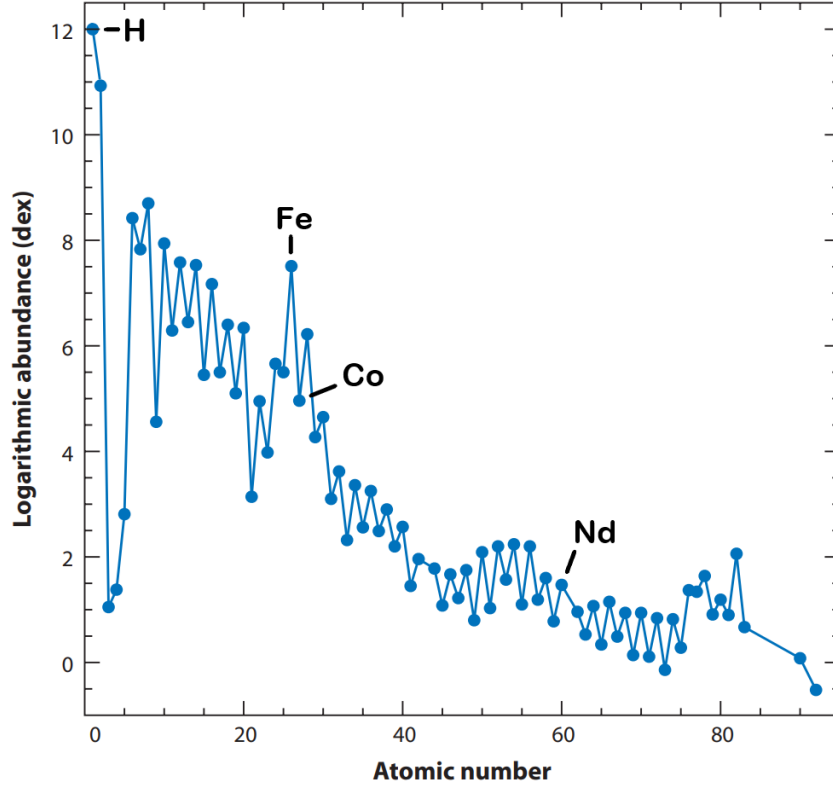


Figure 1.2: Solar elemental abundance relative to the abundance of hydrogen in units of dex (one dex is one order of magnitude). Figure adapted from Asplund et al. (2009) [27].

within the atom. As the observation of a spectral line is only an energy separation between two energy levels, it does not inform us about absolute level energies of the transition relative to the ground (lowest) energy or ionisation (zero binding) energy. This is one of the main challenges in the investigation of atomic structures, which involves identifying absolute level energies unique to each atom, such an analysis is referred to as an empirical spectrum analysis or term analysis [26].

1.2 Rare-earth and Iron-group Elements in Astrophysics

1.2.1 Relative Abundance and Spectra Complexity

As the thesis title suggests, the present work is dedicated to identifying energy levels of the Nd^{2+} ion (Nd III, atomic number $Z = 60$) and determining HFS constants of the Co^{1+} ion (Co II, $Z = 27$). Nd belongs to the group of elements known as the rare-earth elements (REEs, used in

this thesis to refer to the lanthanides, $57 \leq Z \leq 71$) and Co belongs to the iron-group elements ($24 \leq Z \leq 28$). Their importance to astrophysics is illustrated by the relative solar abundance of the elements, as shown in [Figure 1.2](#). The nuclear stability of iron (Fe) causes a high relative abundance of the iron-group elements. Therefore, the spectra of the iron-group elements appear in spectra of most stars in the universe. In the Sun, the relative abundance of the REEs is among the lowest. However, some stars contain orders of magnitude higher relative abundance of REEs compared to the Sun. For example, Nd abundance in the famous Przybylski’s star was estimated at 5.48 ± 0.40 dex using Nd III transitions¹ [28], whereas the solar Nd abundance ([Figure 1.2](#)) was estimated to be 10^4 times lower at 1.42 ± 0.04 dex [27]. Apart from the four orders of magnitude difference, the abundance pattern of the REEs within Przybylski’s star was found to follow that of the Sun ([Figure 1.2](#)), but the abundance differences in lighter elements did not follow such a uniform shift [28]. Investigating the elemental abundance of stars gives key insights into their predecessors, galactic environment, and history. Przybylski’s star was likely a remnant of a nucleosynthesis event that produced a much larger number of heavy elements compared to the event that created the Sun. Due to lower binding energies of nuclei heavier than those of the iron-group elements, the production of heavy elements such as the REEs is not energetically favourable and hence the origin of the elements heavier than those of the iron-group is unsettled.

The REEs and iron-group elements are also important in astrophysics because of their complex spectra. This means photons are more likely to be absorbed by their atoms, which have many possible transitions compared to atoms with much simpler spectra. In other words, the REEs and iron-group elements contribute most of the opacities of stellar atmospheres. The complexity can be inferred from the number of possible quantum states in an atom. Valence electrons of an atom rearrange into possible quantum states when excited under a hot environment such as a star, and the number of possible arrangements for the REEs and iron-group elements is greater than most other elements. The measure of complexity for each element is illustrated in [Figure 1.3](#). The iron-group elements and REEs are the most abundant atoms in the green and red bands (open-d and open-f shells), respectively. Therefore, the abundance and complexity of the two groups of elements imply that one can seldom avoid their complex spectra in stellar or galactic abundance analyses. This is emphasised by the title of one of Przybylski’s original

¹Results using Nd I and Nd II transitions are also within this range.

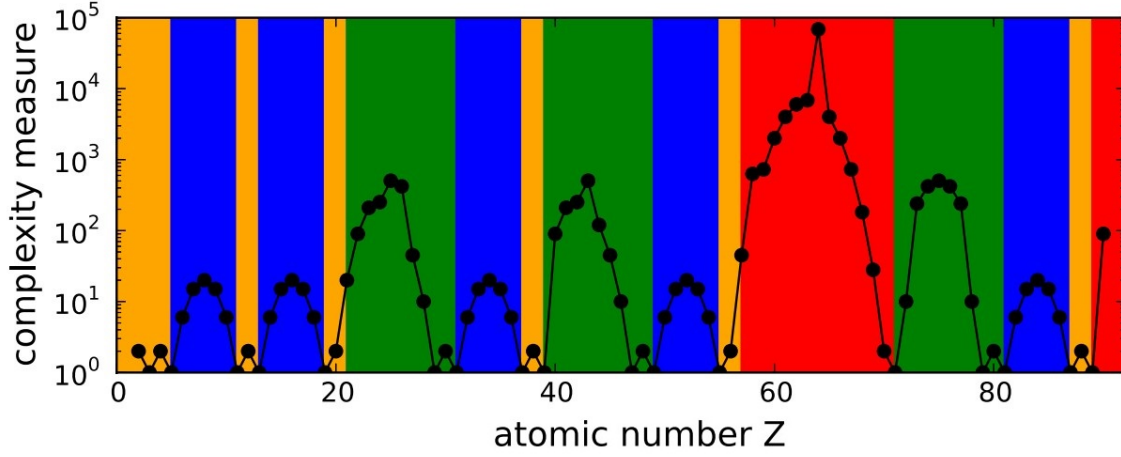


Figure 1.3: Complexity of the elements measured using the number of quantum states in the ground configuration of the corresponding singly ionised species. The coloured bands represent valence shell orbitals, yellow for s, blue for p, green for d, and red for f. See subsection 2.2.1 for the meaning of configuration and orbitals. Figure from Kasen et al. (2013) [30].

papers on his star: ‘Is iron present in the atmosphere of HD 101065?’ [29].

The extent of atomic data for atoms with complex spectra is never fully complete and this thesis will be an example of why this is the case (e.g. limitations of the methods). The atomic (ionic) species investigated in my work of the thesis were selected to be of urgent astrophysical needs, which will be discussed in the next two subsections.

1.2.2 Gravitational Wave Detection, Kilonovae, and REEs

In 2017, the gravitational waves of a neutron star merger event were detected by large laser interferometers (GW170817 [31]). This was the first neutron star merger event detected with an electromagnetic counterpart (AT2017gfo, e.g. [32, 33]) and was a hallmark in multi-messenger astronomy. The electromagnetic counterpart of a neutron star merger is a kilonova, AT2017gfo was recorded by space and ground-based telescopes worldwide. Examples of the spectrum of AT2017gfo are shown in Figure 1.4. The heat of the radioactive decay of ejecta material was expected to have produced the kilonova continuum emission spectrum, which was absorbed by atoms in the ejecta where the largest source of absorption is expected to be from the REEs (e.g. [30, 34–39]). Therefore, neutron star mergers are currently good candidates as a source of heavy elements in the universe, shedding light on the long-standing question of where elements heavier than the iron-group elements come from.

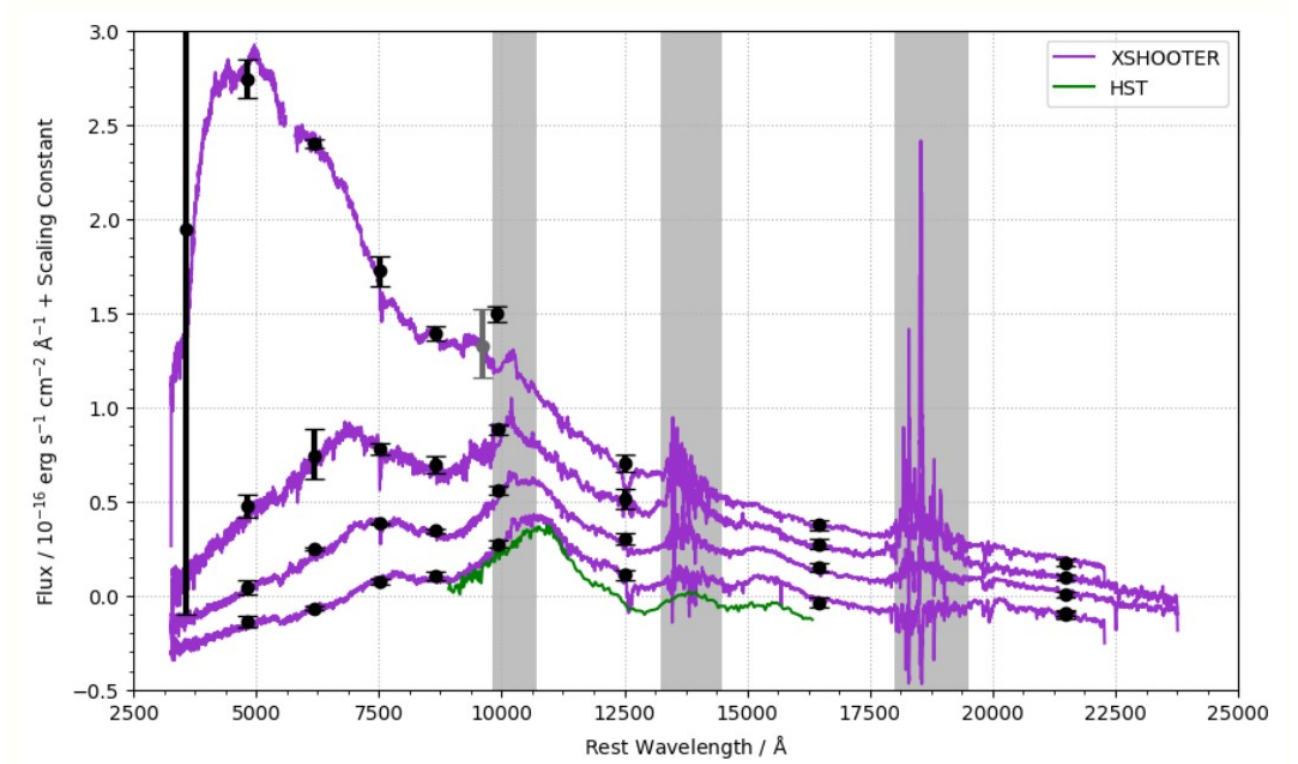


Figure 1.4: Spectrum of AT2017gfo observed by X-shooter [40] of the Very Large Telescope (VLT) in purple and the Hubble Space Telescope in green. The data show four snapshots between 1.4 and 4.4 days after the merger event, where the reduction in flux is forward in time. The black data points are photometry for intensity measurements and the shaded regions are regions of significant Earth atmospheric absorption with high noise. Figure from the AT2017gfo Data Release [35, 36, 41, 42].

Compared to the resolving power used for the stellar spectrum of Figure 1.1, the resolving powers used to record AT2017gfo were very low, because the spectral lines were broadened and merged together due to the rapid expansion of the ejecta material (e.g. see [43]). This means the accuracy requirements for wavelengths are not as stringent compared to the analysis of Figure 1.1. However, the requirements for the extent of wavelength and transition probability data are much bigger as the entire continuum spectrum must be modelled from the UV to the microwave wavelengths to investigate the physical environment of the kilonova, as opposed to modelling individual spectral lines to investigate stellar atmospheres. In recent years, much effort has been made to address the incompleteness in atomic transition data in kilonovae analyses through large-scale atomic structure calculations of the first few ionisation stages of the heavy elements, with REEs as the focus (e.g. [30, 44, 45]). An example of elemental abundance analysis using large-scale atomic structure calculations by Kasen et al. (2017) [46] is shown in Figure 1.5. These results show a large dependence on the kilonova spectral features on the relative abundance of the REEs in the ejecta material.

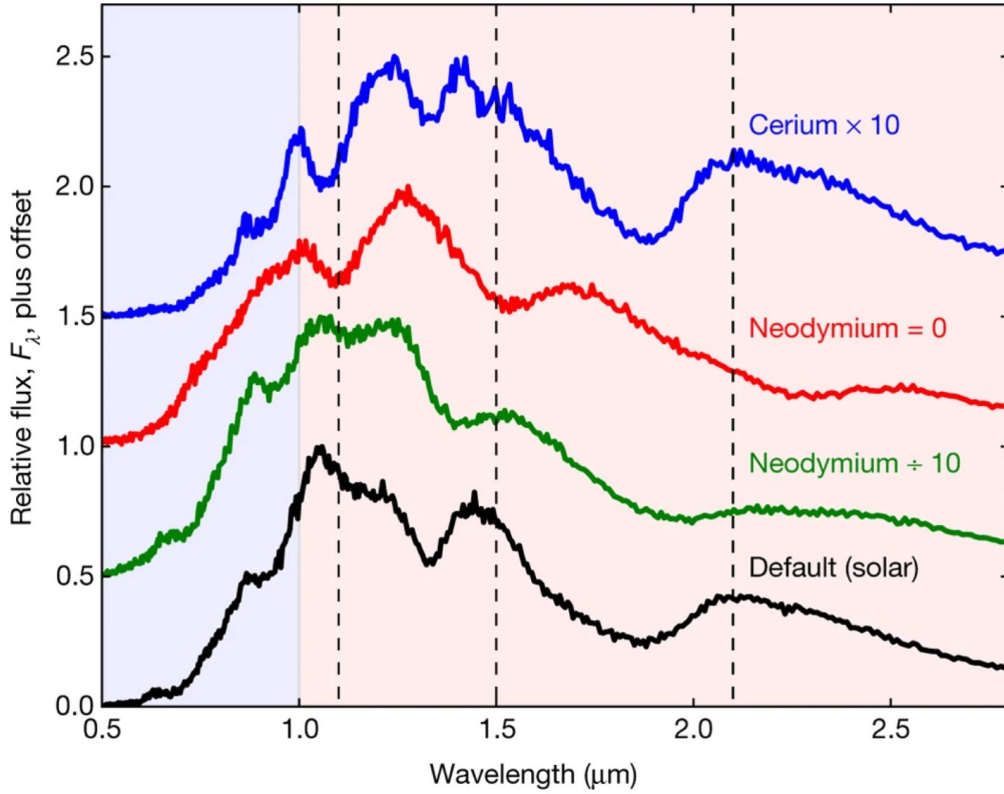


Figure 1.5: Modelled kilonova spectra of different REE abundances. The black spectrum is from solar elemental abundances, coloured spectra are the results from changing specific REE abundances relative to solar abundances. Large spectral features using solar abundance are marked by vertical dashed lines, which differ significantly from the other REE abundance models. Figure from Kasen et al. (2017) [46].

Since the detection of AT2017gfo, reliable identifications of kilonova spectral features were always hindered by the incompleteness and inaccuracies in atomic data, e.g., [45, 47, 48]. The authors of Tanaka et al. (2020) [45] and Kasen et al. (2017) [46] acknowledged the limitations in their atomic structure calculations, where the lack of accuracy in theoretical transition data hindered meaningful comparison between observed and modelled kilonova spectral features. Similarly, the review article by Cowan et al. (2021) [47] emphasised the requirement for atomic energy level data and calibration of theoretical atomic structure models to experimental atomic energy levels due to the challenges in many-body quantum mechanics of atoms of the heavy elements. In this thesis, the importance of such a calibration to experimental energy levels in theoretical calculations will be demonstrated. Lastly, another kilonova was detected recently in 2023 through observation of gamma-ray bursts [48]. The new James Webb Space Telescope [49] observed the kilonova between 29 and 61 days after the merger event, and REEs and the heavy element of tellurium were concluded to be within the ejecta. Still, the authors of Levan et al. (2023) [48] stated challenges they faced when modelling spectra of the late epochs of a kilonova,

such as the breakdown of local thermodynamic equilibrium and fundamental uncertainties in the atomic physics of the heavy elements.

Gravitational wave astronomy is still in its early stages. Existing laser interferometers for gravitational wave detection (e.g. LIGO [50], Virgo [51], and Kagra [52]) are being improved and more laser interferometer facilities are being planned around the world (e.g. the Einstein Telescope [53] and Cosmic Explorer [54]) and planned for space-based operation (e.g. LISA [55], DECIGO [56], TianQin [57], and Taiji [58]), all of which could work together to further improve detection sensitivities to gravitational wave sources and their locations. The number of kilonova detections is only expected to increase and the continued observation of the electromagnetic counterpart of neutron star merger events will supplement the testing of physical theories in the environments currently unachievable on Earth, provided that the needs for reference atomic data are met.

1.2.3 Stellar Astrophysics and Absorption Spectra Modelling

REEs and roAp Stars

In chemically peculiar stars, abundances of the REEs can be orders of magnitude above those observed in the Sun. Some of these stars also exhibit strong magnetic fields with rapidly expanding and contracting atmospheres. These stars are classed as rapidly oscillating chemically peculiar A-type (roAp) stars. Przybylski’s Star was the first star of this type and a list of roAp stars can be found in Table 1 of Kurtz et al. (2006) [59]. The roAp stars have extreme environments that offer good opportunities to investigate theories of stellar formation and structure, which are yet to be fully understood.

In roAp stars, REE spectral lines experience Doppler shifts from the atmospheric expansion and contraction, examples are shown in Figure 1.6 and Figure 1.7. In contrast, radial velocity variations for iron and barium lines were found to be negligible. Nd III and Pr III lines tend to show strong radial velocity amplitudes in roAp stars (e.g. [60,61]) and this is expected to be due to species-dependent stratification of elemental abundance in their atmospheres [60,62]. When the REE abundance of the Ap star HD 144897 was investigated [63], spectral line modelling for all species was successful except for half of the lines of Nd III, which failed to agree with

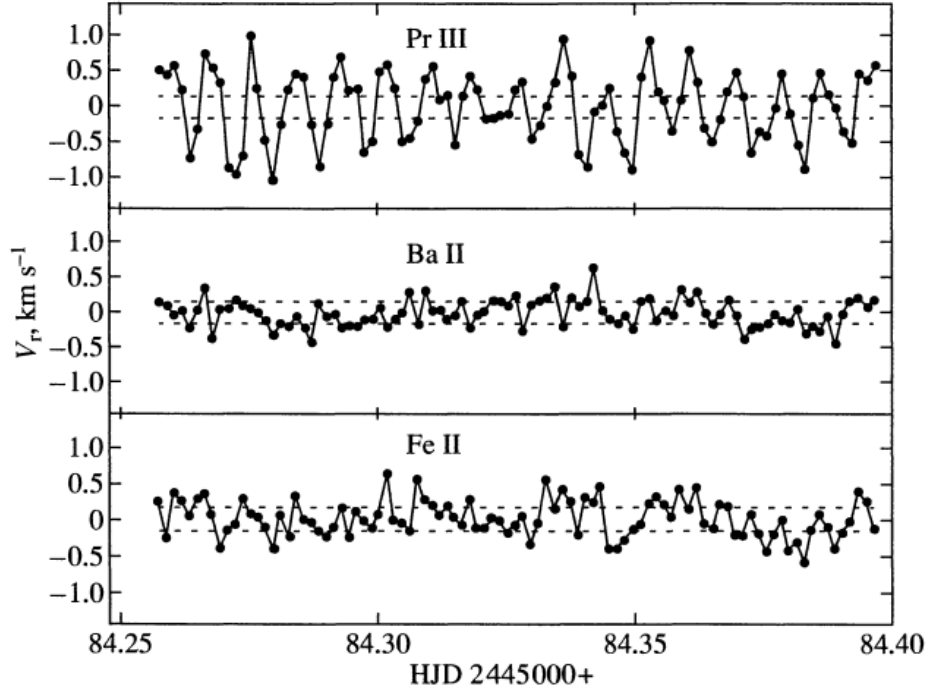


Figure 1.6: Radial velocity variations against time observed for absorption lines of γ Equulei against time, where an HJD (Heliocentric Julian Date) interval of 0.05 is 72 minutes. The species shown are: doubly ionised praseodymium (top), singly ionised barium (middle), and singly ionised iron (bottom). Figure taken from Savanov et al. (1999) [60].

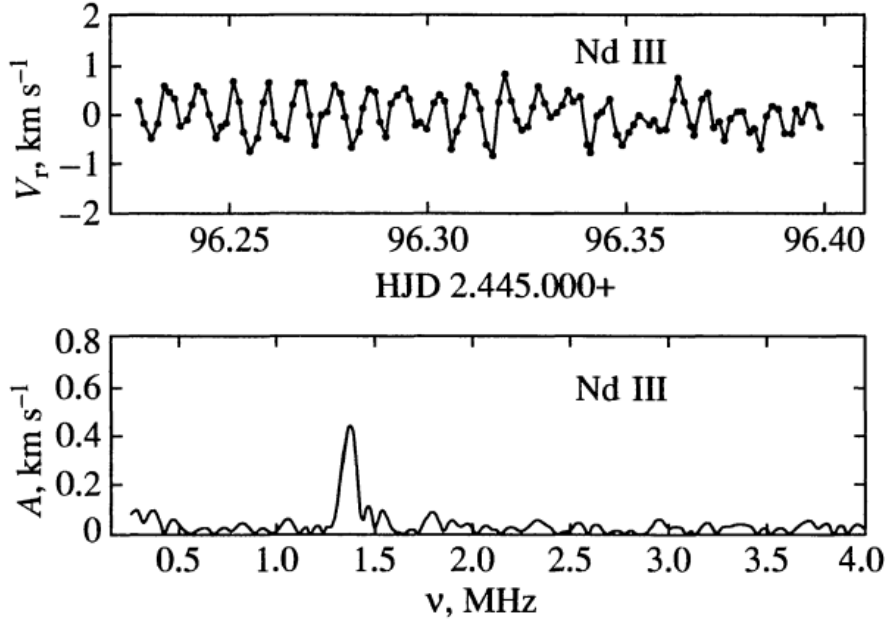


Figure 1.7: Radial velocity variations for the Nd III line at 614.507 nm of γ Equulei against time (top), where an HJD (Heliocentric Julian Date) interval of 0.05 is 72 minutes. The power spectrum (bottom) shows the oscillation period to be 13 minutes (MHz was chosen in Savanov et al. (1999) [60] to represent 10^{-3} Hz, a possible misprint). Figure edited from Savanov et al. (1999) [60].

observations. A revision of the Nd III atomic energy levels and transitions was performed with the aid of the stellar spectra, but the need for more accurate laboratory confirmations of these was stated.

Hyperfine Structure Seen in Stellar Absorption Lines

The HFS of an atom mostly arises from magnetic dipole interaction between the magnetic dipoles induced by electron and nucleus angular momenta (section 2.4). The energy shifts from this interaction are very small but can be comparable to Doppler line widths (explained in subsection 2.5.3) in a plasma of a few thousand Kelvin, typical near stellar surfaces. The HFS effects on stellar absorption line profiles were once thought to be insignificant [25]. This was proven wrong with the advancement of high-resolution stellar spectroscopy with resolving powers up to 10^5 .

To keep up with the higher quality stellar spectra from newer telescopes, stellar spectra models have evolved to consider non-local thermodynamic equilibrium effects, such as inclusions of particle collisions for energy level populations and radiative transfer between hyperfine structure energy levels, which resulted in higher requirements for atomic data. However, without accurate HFS data, significant abundance differences of order 0.1 dex or more can arise regardless of the sophistication of the models [64]. An example is shown in Figure 1.8, where the two narrow model line profiles assumed no HFS and the widest line profile assumed incorrect HFS. The abundance discrepancy obtained from inaccurate Co II HFS data can be more than 0.5 dex [64], an order of magnitude greater than the typical abundance uncertainties (± 0.05 dex) quoted for elements in the Sun (e.g. [65–67]).

1.3 Objectives

The available atomic data for all elements vary. The task of completely fulfilling astrophysical atomic data requirements is an immense task and too big an objective for one postgraduate research degree. Therefore, the present work prioritised the measurement and analysis of atomic reference data of the REEs and iron-group elements with the most poorly known atomic data, especially those in urgent need. The choices are also influenced by the feasibility of the available

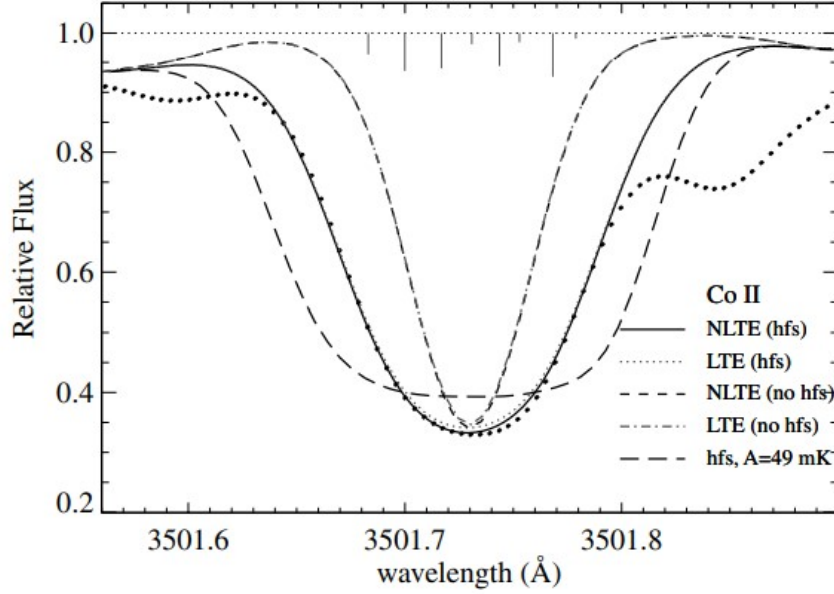


Figure 1.8: Modelling of a solar Co II absorption line. Observed flux values are the black circles. Results using local thermodynamic equilibrium (LTE) and non-local thermodynamic equilibrium (NLTE) models with or without HFS are shown. The wide curve with long dashed lines results from NLTE modelling using incorrect HFS constant value for one energy level of the transition, 49 mK as opposed to the correct value of 40 mK (1 mK is 10^{-3} cm^{-1}). Figure from Bergemann et al. (2010) [64].

laboratory equipment, such as whether the majority of the spectrum of the atom is within the spectral range of the laboratory spectrometer or if the spectrum of the atom could be produced reliably.

The present work aimed to experimentally identify energy levels and transitions of Nd III and determine magnetic dipole HFS constants of energy levels of Co II. The motivations for these choices were based on their astrophysical interest (discussed in the previous section), extreme lack of atomic data (discussed in the next section), correspondence of producible Nd III spectrum with the spectral range of the available instruments, and readily available Co II experimental spectra for analysis. The methodology used primarily high-resolution Fourier transform (FT) spectroscopy of emission spectra of laboratory plasmas at resolving powers around one order of magnitude above the highest available to modern telescopes, using the Imperial College Vacuum-UV (VUV) FT Spectrometer [68], and pure Nd cathodes in a hollow cathode discharge lamp (HCL, e.g. [69]) and a Penning discharge lamp (PDL, e.g. [70, 71]). Observed transition wavenumbers were ultimately calibrated against the caesium standard for frequency (e.g. [72]) and observed transition relative intensities were calibrated using tungsten and deuterium stan-

dard continuum lamps. Analysis of the spectra was performed using existing and newly created software, mainly by comparing experimental spectra with theoretical predictions and spectra observed from different plasma environments.

1.4 Previous Investigations in the Literature

1.4.1 Nd III Energy Levels and Transitions

Motivation

As discussed in [section 1.2](#), the REE Nd is important in kilonova and roAp stellar spectral modelling. The spectra of its atom and ions are complex and contribute much more opacity compared to atoms with simpler spectra, such as those with valence electrons in the s, p, or d orbitals. The high complexity of the REEs is also responsible for the difficulty in conducting experimental energy level identifications of their atoms [\[26\]](#), which has been a primary cause for the lack of atomic data for the REEs in the first place. A literature search of known experimental energy levels of the REEs (e.g. starting from the NIST ASD [\[20\]](#) and the compilation of Martin et al. (1978) [\[73\]](#)) showed that the number of experimentally known energy levels of Nd III is amongst the lowest, with only 40 identified [\[63\]](#). For comparison, the number of known experimental energy levels for Nd I, Nd II, Nd IV, and Nd V are around 740 [\[20, 74\]](#), 840 [\[20, 74–76\]](#), 360 [\[77, 78\]](#), and 150 [\[79, 80\]](#), respectively. The number of theoretically calculated energy levels depends on the configuration interaction space (see [subsection 2.2.7](#)). For context, the theoretical number of energy levels for Nd I-IV is on the order of a few 10^3 [\[30, 81, 82\]](#) used in kilonovae investigations.

The reliable experimental production of the Nd III spectrum was also expected to be feasible as Maria Aldenius (2001) [\[83\]](#) at Lund University had used laboratory instruments similar to those available for the present work: an FT spectrometer and an HCL. Furthermore, strong transitions of Nd III were estimated to lie within the spectral range of the FT spectrometer at Imperial College (see later discussions regarding [Figure 1.9](#)). Therefore, an extensive experimental investigation of Nd III atomic structure was expected to produce significant advancements in the accurate knowledge of its energy level and transition data.

A much more extensive experimental knowledge of Nd III atomic structure will allow more reliable stellar elemental abundance analyses involving Nd III spectral lines and allow benchmarking or calibration of theoretical atomic structure calculations of Nd III, which is especially important in transition probability calculations for spectral investigations of roAp stars and kilonovae. Transition probabilities can also be measured once the level energies are experimentally established.

Previous Experimental Investigations of Nd III Atomic Structure

The first experimental investigations of Nd III atomic structure were performed by Dieke, Crosswhite, and Dunn (1961) [84] and Dieke & Crosswhite (1963) [85] using Nd spark discharges and grating spectroscopy, which resulted in the identification of 29 energy levels by Dr Hannah M. Crosswhite. The 29 levels are in the compilation of Martin et al. (1978) [73] and currently listed on the NIST ASD [20]. The transitions she had classified belong to the lowest-lying levels of the ground and excited configurations, $4f^4$ and $4f^35d$ (see [subsection 2.2.1](#) and [subsection 2.2.8](#)). Dieke, Crosswhite, and Dunn identified transitions of Nd III by comparing grating spectra recorded at a range of discharge currents [84]. Dr Crosswhite’s line list of 643 transitions was particularly useful for my analysis and has been circulating unofficially within the astrophysical community [63], but was not published. I have included this line list of Dr Crosswhite at the end of [Appendix E](#) for the convenience of others. Experimental level lifetimes (see [subsection 2.3.1](#)) of Nd III are known for only five energy levels of Nd III [86]. No measurements of branching fractions (see [subsection 2.3.1](#) for explanation) or absolute transition probabilities of Nd III were found in the literature.

In the abundance analysis of the Ap star HD 144897, Ryabchikova et al. (2006) [63] revised 13 energy levels of Nd III and classified 11 previously unknown levels, totaling 40. This was done using Fourier transform spectroscopy of a Nd-Ne hollow cathode discharge by Maria Aldenius (2001) [83] and stellar spectroscopy of Nd.

Theoretical Investigations of Nd III Atomic Structure

Theoretical calculations of atomic structure and transitions provide invaluable information for experimental energy level investigations, as will be discussed in [Chapter 2](#) and [Chapter 6](#).

The first extensive theoretical investigations of the spectrum and energy levels of Nd III [63, 86–88] were made using the Cowan atomic structure code (e.g. [24, 89–91]), which uses the Hartree-Fock method for the Schrödinger equation with relativistic corrections and includes configuration interactions with one set of single-electron radial wavefunctions per configuration. Eigenvector compositions in the pure LS -coupling basis (see subsection 2.2.5) were published by Zhang et al. (2002) [86] and Ryabchikova et al. (2006) [63] for energy levels of the lowest excited configuration $4f^35d$ up to $33\,000\text{ cm}^{-1}$. Recently, calculations including many more configurations of Nd III were published using the GRASP2K [81, 92, 93], FAC [82, 93, 94], and HULLAC [93, 95] atomic structure codes, all of which consider the Dirac equation to fully include relativistic effects, in an effort to provide atomic data for kilonovae investigations. Only Gaigalas et al. (2019) [81] published extended lists of energy levels and transitions, and these have proved to be useful for the present analysis of Nd III atomic structure.

Eigenvector compositions [63, 86] and theoretical energy levels and transitions data [81] were particularly useful for the present term analysis of Nd III. The strongest transitions predicted for Nd III by Gaigalas et al. (2019) [81] are shown in Figure 1.9. This information greatly influenced the choice of Nd III as the objective of my work, along with the spectral ranges of the Imperial College FT spectrometer (see Chapter 4) that were ideal for this study. The gf of the $4f^4 - 4f^35d$ transitions in blue are relatively small in Figure 1.9, they are nevertheless transitions between the lowest even and odd configurations (e.g. transitions to the ground level), expected to have relatively much higher level populations. Therefore, the $4f^4 - 4f^35d$ transitions were expected to be the strongest transitions. Experimentally identifying levels of these two configurations is crucial to the identification of levels higher up in the Nd III system using the strongest transitions shown in Figure 1.9, because every level must be relative to the ground level, which can only be determined through a sequence of observed transitions between known levels to the ground level.

Previous atomic structure and transition calculations for Nd III were insufficiently accurate for the later stages of the present Nd III term analysis. New calculations were therefore made using the Cowan code, adjusting energy parameters to fit my newly identified experimental level energies (Appendix A). This will be explained in Chapter 2 and the records of incremental improvements to the calculations will be described in section 6.7. The new calculations were performed by Dr Alexander Ryabtsev as a collaboration, who was also a co-author of the most

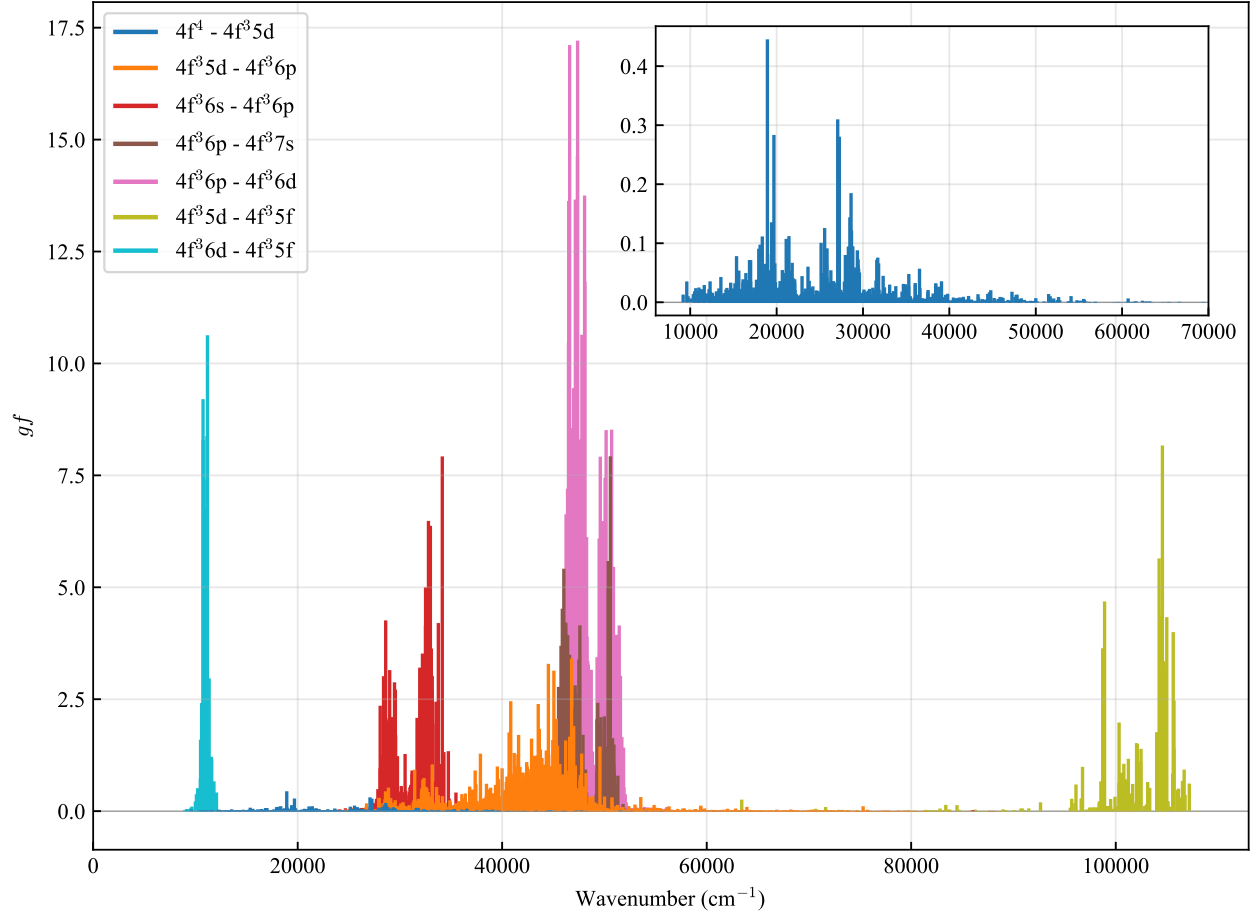


Figure 1.9: Nd III transitions calculated to have the highest weighted oscillator strengths gf [81] and separated into groups of upper and lower configurations (see subsection 2.2.1 for explanation).

recent term analysis of Nd III [63] in 2006. Details of this calculation can be found in our first results paper for Nd III [96].

1.4.2 Co II Hyperfine Structure Constants

As discussed in section 1.2, the iron-group element Co is important in stellar spectral modelling due to its complex atomic spectra and high cosmic relative abundance, contributing much more opacity compared to atoms with simpler spectra, such as those with valence electrons in the s or p orbitals. Due to advancements in high-resolution stellar spectroscopy, the small HFS effects on spectral lines have become significant factors in stellar modelling, mostly arising from the magnetic dipole interaction A constant of each energy level of the atoms.

Theoretical calculations and highly accurate laser spectroscopic measurements of Co II HFS were not found in the literature. The first measurements of Co II HFS were by FT spectroscopy by Prof. J. C. Pickering as published in Bergemann et al. (2010) [64], who determined HFS A constants six energy levels of Co II. A further set of HFS A constants for 22 other levels of the low-lying configurations were determined by Lawler et al. (2018) [97] using FT spectroscopy as part of their measurements of Co II transition probabilities. Similar to the conclusions of Bergemann, Pickering, and Gehren [64], Lawler et al. [97] showed that the inclusion of laboratory Co II HFS A constants created differences of order 0.1 dex in Co abundances in a metal-poor star HD 84937 compared to investigations neglecting the A constants [98, 99]. The 0.1 dex deviation was more than three times the uncertainty ± 0.027 dex of Co abundance obtained using Co II lines by Lawler et al. (2015) [98].

As will be discussed in Chapter 8, experimental FT spectra were used to determine Co II HFS constants. All of these spectra originate from the most recent term analysis of Co II led by Prof. J. C. Pickering at Imperial College [100–102], some of which were also used in the previous studies of Co II HFS [64, 97]. Therefore, an extensive investigation of Co II HFS using these spectra was expected to be feasible, which could solve the problem of the lack of HFS constants for Co II energy levels, because the spectra were already available and contained essentially all experimentally observed transitions that were used to determine the known Co II energy levels (about 500 in total). This was particularly fortuitous because of the enforced closure of Imperial College and our laboratory due to the COVID-19 pandemic when the Co II HFS

analysis was undertaken in 2020.

1.5 Summary and Thesis Structure

Developments in observational astronomy have led to higher requirements for atomic energy level and transition data. In many cases, the atomic data requirements for the atoms and ions of the REE and iron-group elements are not met, such as for the data needed to interpret spectra of kilonovae, chemically peculiar stars, and high-resolution stellar absorption spectra showing HFS. The present work aims to significantly improve the experimental knowledge of the energy levels and transitions of Nd III and HFS of the energy levels of Co II, primarily by high-resolution FT spectroscopy of emission spectra of the ions in spectral ranges between the IR and VUV.

In this thesis:

[Chapter 2](#) describes the theory of atomic structure employed in the Cowan code used to calculate level energies, eigenvector compositions, and transition probabilities, followed by theories in thermodynamics and radiative transfer which affect the intensities and shapes of atomic spectral lines observed in the present work. Many experimental parameters, instrumental design, and analysis strategies of my work were based on the theories in this chapter.

[Chapter 3](#) is the second theory chapter and describes the principles of FT spectroscopy. Similarly, many experimental parameters, instrumental design, and analysis strategies were also based on the theories in this chapter. The ideal FT spectrometer is presented, and then considerations for a real-world FT spectrometer, such as finite spectral range, finite resolution, and finite aperture sizes, are discussed. Lastly, the most significant sources of noise and systematic errors are discussed.

[Chapter 4](#) describes how experimental emission spectra of Nd were obtained. The Imperial College VUV FT Spectrometer is presented with discussions of how it was originally designed and operated in the present work. Then the design and operation of the light sources used to produce the Nd plasma are discussed, followed by descriptions of how the light source conditions were optimised for Nd III transitions. A list of experimental Nd spectra are presented in tables at the end of this chapter.

Chapter 5 documents how experimental emission spectra of Nd were Fourier transformed, how information such as wavenumbers and intensities of the spectral lines were obtained through spectrum fitting, and how the list of fitted spectral lines was wavenumber and intensity calibrated. Uncertainties of observed wavenumbers and intensities are discussed in detail.

Chapter 6 first explains how experimental atomic transition spectra could be used to identify energy levels and give the best estimates of level energies, within the context of the Nd spectra obtained in the present work. This chapter then contains a history of how each Nd III energy level was identified, primarily for demonstration of methodology and future references. This chapter ends with a summary of the identified energy levels and classified transitions of Nd III.

Chapter 7 is an extended conclusion chapter with retrospective comments for the term analysis of Nd III, such as examples of newly enabled astrophysical spectral analyses, ongoing work, strategies for future work, and emphasis on the effectiveness of the methodologies employed in the present work.

Chapter 8 describes how the Co II HFS analysis was carried out, including brief information on the spectra used, discussions on the multi-parameter optimisation method, considerations for self-absorption and parameter constraints, the overall strategy employed, and a summary of results at the end.

Chapter 9 is the final chapter with the summaries of results and thesis conclusion.

Chapter 2

Theory of Atomic Structure and Spectra

2.1 Introduction

This chapter summarises the theories including atomic structure, atomic transitions, plasma thermodynamics, and spectral line profiles. Expressions mostly follow those from Cowan's book [24] and units of quantities are either standard or atomic units, the expressions and units are only for theoretical discussion and not for the construction of computational models.

The first part of this chapter, [section 2.2](#), concerns theoretical calculations of atomic structure, which are indispensable in experimental energy level analyses. In previous experimental investigations of Nd III [63, 86], atomic structure calculations of Nd III were carried out using variations of the Cowan code [24, 89]. The theory for atomic structure in the Cowan codes is based on the Slater-Condon theory [103, 104], where radial wavefunctions are determined from a central field potential using the Hartree-Fock method (e.g. [105–107]), angular wavefunctions are constructed to be the eigenstates of the total angular momentum operator, and relativistic effects are approximated. Semi-empirical atomic structure calculations of Nd III in the present work were made by Dr Ryabtsev, which are the continuation of his work [63]. The semi-empirical parameters of the Cowan code that are determinable from experimental level energies are described in [subsection 2.2.1](#), [subsection 2.2.2](#), [subsection 2.2.3](#), and [subsection 2.2.7](#). Lastly, an overview of the calculated Nd III atomic structure is discussed in [subsection 2.2.8](#).

The second part of this chapter includes [section 2.3](#), [section 2.4](#), and [section 2.5](#), which contain theories required to interpret observed spectra in my thesis. The Nd III energy level analysis requires observation of transitions between Nd III energy levels. Only the electric dipole (E1) transition was considered since these are most likely and account for the majority of the observed transitions. Electric dipole transitions are observed at different intensities, which are based on transition selection rules and transition probabilities. Definitions of transition probabilities, theoretical calculations of transition probabilities, and applicable transition selection rules are discussed in [section 2.3](#). The consideration of theoretically predicted line profiles is the basis for spectral line fitting, which I used to measure transition wavenumbers (see [section 5.3](#)). Transitions between energy levels may be observed as several closely grouped transitions due to small perturbations, such as hyperfine structure due to the magnetic dipole moment of the nucleus, isotope shifts from the finite mass and volume of the nucleus, and/or Zeeman splitting from weak external magnetic fields, these effects and their relevance to the present work are discussed in [section 2.4](#). Lastly, observed spectral line intensities and line profiles are also affected by the thermodynamic properties (that determine energy level populations) and radiative transfer within the light source, these are discussed in [section 2.5](#).

2.2 Solving the Schrödinger Equation

The quantum states and quantum energies arising from non-relativistic interactions of particles within an atom are governed by the time-independent Schrödinger equation

$$\hat{H}\Psi = E\Psi, \quad (2.1)$$

where E is the energy, Ψ is the wavefunction, and under the approximation where protons and neutrons of the nucleus are stationary and have negligible volume, the Hamiltonian is

$$\hat{H} = \sum_{i=1}^N \left(-\frac{\hbar^2}{2m_e} \nabla_i^2 - \frac{Ze^2}{4\pi\epsilon_0|\hat{\mathbf{r}}_i|} \right) + \sum_{i=1}^N \sum_{j<i}^N \left(\frac{e^2}{4\pi\epsilon_0|\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j|} \right) \quad (2.2)$$

for atomic number Z and N electrons, each with index i and position $\mathbf{r}_i$ relative to the centre of the nucleus. The wavefunction is

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_N). \quad (2.3)$$

The eigenfunctions (stationary states) and energy eigenvalues of the Hamiltonian $\hat{H}$ describe the energy levels of an atom, and the energy separations between energy levels determine wavelengths (wavenumbers) of atomic transitions. This N -body problem will require drastic approximations, and this section describes the approach taken in the Slater-Condon theory [103, 104].

2.2.1 Central Field Approximation and Electronic Configuration

The many-electron atom Schrödinger equation is solved using the central field approximation, where the Hamiltonian is approximated using a linear sum of kinetic and potential energies of each electron $\hat{V}(|\hat{\mathbf{r}}_i|)$,

$$\hat{H}_c = \sum_{i=1}^N \left(-\frac{\hbar^2}{2m_e} \nabla_i^2 + \hat{V}(|\hat{\mathbf{r}}_i|) \right). \quad (2.4)$$

The central field approximation Hamiltonian $\hat{H}_c$ includes only the radial electron-nucleus and electron-electron interactions, this is applicable as the separations between electrons close to the nucleus and electrons in outer shells are mostly radial (i.e. electron screening effects). The central potential Schrödinger equation $\hat{H}_c \Psi = E \Psi$ is separable for each electron and the wavefunction for all electrons can be expressed as a product of individual electron wavefunctions [24]

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_N) = \prod_{i=1}^N \psi_i(\mathbf{r}_i) = \prod_{i=1}^N \frac{1}{r_i} \cdot P_{n_i l_i}(r_i) \cdot Y_{l_i m_{l_i}}(\theta_i, \phi_i) \cdot \sigma_{m_{s_i}}(s_{i_z}), \quad (2.5)$$

where $r_i = |\mathbf{r}_i|$, $P_{n_i l_i}(r_i)$ is the radial part of the one-electron wavefunction, $Y_{l_i m_{l_i}}(\theta_i, \phi_i)$ is spherical harmonic angular part of the one-electron wavefunction, and $\sigma_{m_{s_i}}(s_{i_z})$ is the spin vector. The one-electron wavefunctions $\psi(\mathbf{r}_i)$ are eigenfunctions of the angular momentum operators $\hat{\mathbf{l}}_i^2$, $\hat{l}_{z_i}$, $\hat{\mathbf{s}}_i^2$, and $\hat{s}_{z_i}$ with quantum numbers l_i , m_{l_i} , s_{i_z} , and m_{s_i} , respectively. The quantum number n of the radial wavefunction is the principal quantum number and a positive non-zero integer, l_i is an integer between 0 and $n-1$, $m_{l_i} = -l_i, -l_i+1, \dots, l_i-1, l_i$, $s_{i_z} = 1/2$, and $m_{s_i} = \pm 1/2$. The quantum numbers n_i and l_i are used to describe the orbital (or subshell)

of electron i , and the electronic configuration of an atom is written as a product of the orbitals,

$$(n_1 l_1)^{w_1} (n_2 l_2)^{w_2} (n_3 l_3)^{w_3} \dots (n_q l_q)^{w_q}, \quad (2.6)$$

where $\sum_{m=1}^q w_m$ is equal to N for N electrons in the atom. While the principal quantum numbers n_i are labelled using integers in this representation, the angular momentum quantum number l_i is labelled using the letters s, p, d, f, g, h, i, k, l, m, n, ... for $l_i = 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, \dots$, respectively. For example, the ground state configuration of the carbon atom (C I, $Z = 6$, and $N = 6$) is $1s^2 2s^2 2p^2$ and the ground state configuration of doubly ionised neodymium (Nd III, $Z = 60$, and $N = 58$) is $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 4f^4$ or $[\text{Xe}]4f^4$ from summarising full shells using the configuration of the noble gas xenon. The configuration of an atom can change upon excitation, for example, $[\text{Xe}]4f^4$ is the ground configuration of Nd III (it contains the ground energy level), and an electron in the 4f orbital may be excited to the 5d orbital, producing the excited configuration of Nd III of $[\text{Xe}]4f^3 5d$.

Since Pauli's exclusion principle applies to the electrons, the maximum number of electrons $w_{q,\text{max}}$ in an orbital q is $2(2l_q + 1)$, as shown in the example configurations of C I and Nd III. Additionally, the multi-electron product wavefunction (Equation 2.5) is anti-symmetrised, where the anti-symmetrised wavefunction is a normalised linear combination of the product wavefunction satisfying anti-symmetry with respect to the exchange of quantum states between any two electrons.

In Cowan's codes used during the present work [24, 91], the radial functions $P_{n_i l_i}(r_i)$ are determined using the Hartree-Fock (previously called self-consistent field) method, where the (Hartree-Fock) equations set by the central potential and the radial functions are solved numerically from minimising the average energy of each configuration. In Cowan's codes, only one set of $P_{n_i l_i}(r_i)$ is determined per configuration to reduce computational complexity, this will be assumed for the remaining discussions of the thesis. The configuration average energy is the summation of the expectation values of the Hamiltonian between all quantum states within a configuration divided by the number of quantum states within the configuration. In semi-empirical atomic structure calculations, the configuration average energies can be parameters determined using experimental level energies instead. For example, configuration average energies are the E_{av} parameters of Table A.1.

2.2.2 Residual Electrostatic Repulsion

The energy of the residual electrostatic repulsion between the electrons is

$$\hat{H} - \hat{H}_c = \hat{H}_r = \sum_{i=1}^N \left(-\frac{Ze^2}{4\pi\epsilon_0|\hat{\mathbf{r}}_i|} - \hat{V}(|\hat{\mathbf{r}}_i|) \right) + \sum_{i=1}^N \sum_{j<i}^N \left(\frac{e^2}{4\pi\epsilon_0|\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j|} \right), \quad (2.7)$$

which can be estimated for each product wavefunction Ψ determined from the central field approximation using time-independent perturbation theory, i.e., the expected change in energy due to repulsion is $\langle \Psi | \hat{H}_r | \Psi \rangle$. In this evaluation, the two-electron operator $(\Delta r_{ij})^{-1} = 2/|\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j|$ requires two integrals for anti-symmetrised wavefunctions for each pair of electrons [24],

$$\left\langle \Psi \left| \sum_{i=1}^N \sum_{j<i}^N (\Delta r_{ij})^{-1} \right| \Psi \right\rangle = \sum_{i=1}^N \sum_{j<i}^N \left[\langle \psi_i \psi_j | (\Delta r_{ij})^{-1} | \psi_i \psi_j \rangle - \langle \psi_i \psi_j | (\Delta r_{ij})^{-1} | \psi_j \psi_i \rangle \right], \quad (2.8)$$

where ψ_i and ψ_j are one-electron wavefunctions of Equation 2.5. The positive and negative terms within the summation are referred to as the direct and exchange integrals, respectively. The direct integral represents the energy increase from electron repulsion, and the exchange integral represents a minimum spatial separation between electrons with the same spin due to Pauli's exclusion principle.

The configuration average contribution from electrostatic repulsion (the second term in Equation 2.7) is obtained using Equation 2.8 if the summation is carried out over all quantum states of a configuration. Since the angular parts of the one-electron wavefunctions are spherical harmonics, the angular integrals of the direct and exchange integrals are not subject to the shape of the central field. On the other hand, the radial integrals depend on the radial wavefunctions of the central field and vary between configurations and atoms, these radial integrals are referred to as Slater integrals and are significant semi-empirical energy parameters in semi-empirical Hartree-Fock atomic structure calculations. For example, Slater integrals are the F^k (direct) and G^k (exchange) Cowan code parameters of Table A.1, their integral expressions are [24]:

$$F^k(ij) = \int_0^\infty \int_0^\infty \frac{2(r_<)^k}{(r_>)^{k+1}} |P_{n_i l_i}(r_i)|^2 |P_{n_j l_j}(r_j)|^2 dr_i dr_j, \quad (2.9)$$

$$G^k(ij) = \int_0^\infty \int_0^\infty \frac{2(r_<)^k}{(r_>)^{k+1}} P_{n_i l_i}^*(r_i) P_{n_j l_j}^*(r_j) P_{n_j l_j}(r_i) P_{n_i l_i}(r_j) dr_i dr_j, \quad (2.10)$$

where $r_<$ and $r_>$ are respectively the lesser and greater of r_i and r_j . The direct and exchange

integrals of Equation 2.8 are linear summations of $F^k(ij)$ and $G^k(ij)$, respectively, from the multipole expansion of $(\Delta r_{ij})^{-1}$ into Legendre polynomials. In this expansion, the summation is over non-zero (or legal) values of rank k with coefficients that are functions of the angular coordinates, all of which depend on l_i and l_j .

2.2.3 Relativistic Corrections and Spin-orbit Interaction

The shortcomings of non-relativistic quantum mechanics must be considered. Relativistic effects are much more significant in atoms with large electrostatic potentials, such as highly ionised atoms. However, due to the large electron screening found in the cases of the neutral and low ionisation stages of transition metals and REEs (e.g. Co II and Nd III), only the most significant relativistic effects are considered as additional terms in the Hamiltonian $\hat{H}$ of Equation 2.1. The list of these includes the mass-velocity, Darwin, and spin-orbit terms. The mass-velocity term is the correction to relativistic kinetic energy, this term depends on n_i and l_i . The Darwin term is due to the relativistically induced electric moment of the electron, it is dependent on n_i and only affects electrons with $l_i = 0$. Lastly, the spin-orbit term arises from the magnetic dipole interaction between the induced magnetic dipole of the relativistic orbital motion of the electrons and the intrinsic magnetic dipole of electron spins.

The spin-orbit interaction is the most important relativistic contribution to the energy level structure, fine structure levels arise from considering the electrostatic repulsion and spin-orbit interaction together. The spin-orbit contribution to the Hamiltonian is [24]

$$\hat{H}_{\text{SO}} = \sum_{i=1}^N \frac{1}{r_i} \frac{d\hat{V}(r_i)}{dr_i} (\hat{\mathbf{l}}_i \cdot \hat{\mathbf{s}}_i), \quad (2.11)$$

for $r = |\hat{\mathbf{r}}_i|$. Unlike the electrostatic repulsion, the spin-orbit interaction does not shift the configuration average energy since $n_i l_i m_{l_i}$ are in pairs of m_{s_i} , each with $m_{s_i} = \pm 1/2$ and so the summation over all states is zero. Configuration average energy¹ are split depending on electron spins s_i and angular momenta l_i , calculated using $\langle \Psi | \sum_i \xi_i(\hat{\mathbf{r}}_i) (\hat{\mathbf{l}}_i \cdot \hat{\mathbf{s}}_i) | \Psi \rangle$. Similar to the electrostatic repulsion, the radial part of the integral $\langle \Psi | \sum_i \xi_i(\hat{\mathbf{r}}_i) (\hat{\mathbf{l}}_i \cdot \hat{\mathbf{s}}_i) | \Psi \rangle$ is dependent on the central potential and its radial wavefunctions. The radial integral is referred to as the

¹Or term energy, depending on the coupling scheme, see subsection 2.2.5.

spin-orbit parameter, it is calculated for each orbital of each configuration of the wavefunction Ψ , but can also be fitted using experimental energy levels in semi-empirical calculations. For example, the spin-orbit parameters are the ζ of [Table A.1](#) and its integral expression for orbital $n_i l_i$ is [\[24\]](#)

$$\zeta_{n_i l_i} = \frac{\alpha^2}{2} \int_0^\infty \frac{1}{r_i} \frac{d\hat{V}(r_i)}{dr_i} |P_{n_i l_i}(r_i)|^2 dr_i, \quad (2.12)$$

where α is the fine-structure constant.

2.2.4 Matrix Method for the Hamiltonian and its Eigenstates

In Slater-Condon theory, the Hamiltonian $\hat{H}$ with relativistic corrections can be determined for a set of basis functions [\[24\]](#). Since the goal is to find energy eigenvalues E^k and eigenstates Ψ^k using the Schrödinger equation $\hat{H} |\Psi^k\rangle = E^k |\Psi^k\rangle$, a set of M basis functions Ψ_b is used to approximately represent the space spanned by the eigenstates,

$$|\Psi^k\rangle = \sum_{b=1}^M y_b^k |\Psi_b\rangle. \quad (2.13)$$

Applying $\langle \Psi_b |$ to the Schrödinger equation gives

$$\sum_{b'=1}^M y_{b'}^k \langle \Psi_b | \hat{H} | \Psi_{b'} \rangle = E^k y_b^k, \quad (2.14)$$

which is an eigenvector matrix equation with the eigenvector components y_b^k . The solution involves numerically diagonalising the Hamiltonian matrix $\langle \Psi_b | \hat{H} | \Psi_{b'} \rangle$ and choosing orthonormality of the basis functions Ψ_b such that $\langle \Psi_b | \Psi_{b'} \rangle = \delta_{bb'}$ and $\sum_{b=1}^M |y_b^k|^2 = 1$. The quantity $|y_b^k|^2$ is referred to as the eigenvector percentage of Ψ_b , examples for Nd III levels can be seen in [Table C.1](#).

The eigenstates Ψ^k and basis functions Ψ_b are separated into two symmetry groups, one for each parity and indicated by whether $\sum_i l_i$ is even or odd in the product wavefunction of [Equation 2.5](#). The radial parts of the basis functions are those calculated using the central field for each configuration (in Cowan's codes), but the choice of the angular parts of the basis functions Ψ_b is not trivial. Generally, the basis functions Ψ_b are chosen to minimise M to reduce computational complexity and with as much completeness as possible for the real eigenstates

of interest, i.e., to have linear combinations of Ψ_b that most resemble the real eigenfunctions Ψ^k .

For example, Ψ_b of configurations with energies near or above the ionisation energy are not very representative for the lowest real eigenstates that are of interest in Nd III, e.g., electron densities too far from nucleus. Therefore, Ψ_b constructed from $[\text{Xe}]4f^4$ and $[\text{Xe}]4f^35d$ (lowest even and odd configurations of Nd III, respectively) are expected to much more significantly represent the lower energy level structure compared to very highly excited configurations that are likely above ionisation energy, such as $[\text{Xe}]4f^25f^2$ and $[\text{Xe}]4f5d^3$. Therefore, one may decide to neglect Ψ_b constructed from the $[\text{Xe}]4f^25f^2$ and $[\text{Xe}]4f5d^3$ configurations in the energy level structure analysis of Nd III to reduce computational complexity. While energy level structure and branching fractions may not be affected by the neglect of these so-called far configurations, transition probabilities may be affected from their neglect (see related discussions in [section 7.3](#)). The central field approximation is often not very good for the heavy elements, where configuration interaction between multiple configurations ([subsection 2.2.7](#)) becomes essential considerations.

Another important consideration when choosing Ψ_b is that the total angular momentum (quantum number J) of an isolated atom is expected to be constant, therefore, the Hamiltonian $\hat{H}$ is expected to commute with the total atomic angular momentum operator $\hat{\mathbf{J}}^2$, implying that the two operators share the same eigenstates. Not only does this hint at suitable basis functions, but the Hamiltonian matrix can also be separated into smaller matrices corresponding to each possible value of J and diagonalised individually, reducing computational complexity.

2.2.5 Angular Momentum Coupling and Term Symbols

In the product wavefunction of [Equation 2.5](#), the radial parts are calculated using the central potential for each configuration, which can be used as the radial parts of the basis functions Ψ_b of each configuration. However, the product of the angular wavefunctions of all electrons in an atom is not an eigenstate of the total angular momentum operator $\hat{\mathbf{J}}^2$. To address this, orbital (l_i) and spin (s_i) angular momenta of all electrons in a configuration are coupled into the total angular momentum J .

Angular Momentum Coupling

The coupling between two angular momentum states $|j_1 m_1 j_2 m_2\rangle$ into the coupled state $|j_1 j_2 j m\rangle$ (eigenstate of $\hat{\mathbf{J}}^2 = \hat{\mathbf{J}}_1^2 + \hat{\mathbf{J}}_2^2 + 2\hat{\mathbf{J}}_1 \cdot \hat{\mathbf{J}}_2$) is the transformation

$$|j_1 j_2 j m\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} C(j_1 j_2 m_1 m_2; j m) |j_1 m_1 j_2 m_2\rangle \quad (2.15)$$

where j_i, m_i, j, m are angular momentum quantum numbers of $\hat{\mathbf{J}}_i^2, \hat{\mathbf{J}}_{z_i}, \hat{\mathbf{J}}^2$, and $\hat{\mathbf{J}}_z$, respectively, $C(j_1 j_2 m_1 m_2; j m)$ are the Clebsch-Gordon coefficients, and $j = |j_1 - j_2|, |j_1 - j_2| + 1, \dots, j_1 + j_2 - 1, j_1 + j_2$. The radial parts of the product wavefunction are independent of the summation and hence independent of angular momentum coupling. In the case of equivalent electrons, where multiple electrons in a configuration are in the same orbital, Pauli's exclusion principle forbids certain possible coupled angular momenta, the corresponding Clebsch-Gordon coefficients are set to zero and the resulting truncated basis is then normalised. Full orbitals (closed subshells) are spherically symmetric and contribute no angular momentum to the atom, hence, great simplifications can be made for larger atoms by reducing the number of basis functions by only coupling electrons in open subshells.

According to [Equation 2.15](#), there are different coupling orders (routes) to reach the total atomic angular momentum J . Each order gives a different set of basis functions Ψ_b , but the total number of basis functions constructed from a given configuration and J is the same, regardless of the coupling order. Therefore, there are multiple ways to represent the eigenfunctions of $\hat{\mathbf{J}}^2$ and therefore multiple possible angular momentum coupling bases for the eigenstates $|\Psi^k\rangle$ of the Hamiltonian $\hat{H}$.

The angular momentum coupling order, also known as the coupling condition, is generally chosen to produce basis functions that best resemble the physical environment (Hamiltonian eigenfunctions) of the electrons of the atom of interest, primarily for intuition. This means coupling electrons in the order of decreasing contribution to the diagonal of the Hamiltonian matrix and minimising off-diagonal contributions, before the diagonalisation of the Hamiltonian. The choice involves consideration of the relative sizes between the repulsion and spin-orbit terms of the Hamiltonian between all electrons, but it does not require consideration of the electronic kinetic and electron-nucleus potential energy terms because these two terms contribute only

to the diagonal of the Hamiltonian [24]. Three coupling conditions and their significance in the analyses of the present work are discussed in the remaining parts of this subsection, the coupling conditions that were applied to Nd III will be discussed in [subsection 2.2.8](#).

LS-Coupling

In *LS*-coupling, electron orbital angular momenta l_i are coupled together for a total orbital angular momentum L and electron spins s_i are coupled into a total spin S . The L and S then couple into the total angular momentum J . The basis functions resulting from the *LS*-coupling scheme give purely diagonal contributions to the Hamiltonian matrix if the spin-orbit matrix elements are negligible when electron repulsion interactions dominate. Therefore, the most significant perturbation from the configuration average energy, in this case, is the calculation of the repulsion term ([Equation 2.8](#)). The angular integrals depend on L and S , and the exchange contribution from Pauli's exclusion principle splits states of opposite exchange symmetries (same L but different S). Each L and S pair is referred to as the term of a configuration written in the form

$$^{2S+1}L \tag{2.16}$$

where $2S + 1$ is the multiplicity of the term labelled using integers and L is labelled using capital letters corresponding to the lowercase letters used in configuration labels for individual electron orbital angular momenta l . The words singlet, doublet, triplet, quartet, quintet, $\dots$, are often used to describe multiplicities of $2S + 1 = 1, 2, 3, 4, 5, \dots$, respectively for the term. The term symbol can repeat within a configuration (but with different l_i and s_i), in which case the repeating terms are given extra labels (e.g. γ or the seniority number) to distinguish between them.

The multiplicity is the number of possible total angular momentum J values, which have different energies relative to the term energy when including the much smaller perturbation from the spin-orbit term in the Hamiltonian. If the configuration closely resembles *LS*-coupling conditions, the spin-orbit perturbation splits terms of the configuration into fine structure energy levels labelled by the possible J values of each term,

$$(E_{\gamma LSJ} - E_{\gamma LS}) = \frac{1}{2} [J(J+1) - L(L+1) - S(S+1)] \cdot \zeta(\gamma LS), \tag{2.17}$$

where the energy separation between consecutive J values of each term is given by the Landé interval rule

$$(E_{\gamma LSJ} - E_{\gamma LS(J-1)}) = J \cdot \zeta(\gamma LS), \quad (2.18)$$

where the term is labelled using γ and ^{2S+1}L and the effective splitting proportionality factor $\zeta(\gamma LS)$ results from integrating for the expectation value of the spin-orbit Hamiltonian of the coupled wavefunctions and is in units of energy.

If LS -coupling basis functions closely resemble eigenstates of the Hamiltonian, relative separations of energy levels would correspond to those of LS -coupled terms, which could be gauged in an experimental energy level analysis using the above relations. Hund's rules could be also applicable: the term of the maximum multiplicity is lowest in energy, the largest L has the lowest energy of a particular multiplicity, and level energies increase with J if the outermost orbital is half-filled or less. The energy separation rules for LS -coupled terms were approximately observed for low-lying Nd III levels that roughly correspond to LS -coupling conditions. A similar discussion on transition selection rules and relative intensities for transitions between energy levels with approximate LS -coupling conditions will be in [subsection 2.3.2](#).

***jj*-Coupling**

In jj -coupling, each electron orbital angular momentum is coupled with electron spin first, and then the total angular momentum of the individual electrons j are coupled with each other. The basis functions resulting from the jj -coupling scheme contribute purely to the diagonal of the Hamiltonian matrix if the electron repulsion matrix elements are negligible compared to those of the spin-orbit interaction. The spin-orbit integral $\langle \Psi | \sum_i \xi_i(\mathbf{r}_i) (\hat{\mathbf{l}}_i \cdot \hat{\mathbf{s}}_i) | \Psi \rangle$ then dominates perturbations from the configuration average energy, where term splitting is determined by coupling of the j values.

The term symbol of jj -coupling between two electrons conveniently uses the total single-electron angular momentum quantum numbers in brackets (j, j) , and the possible J values can result from the successive coupling with the j values of any other electrons. Examples can be found for the $4f^3ns$ levels in [Table C.1](#). The splitting of the term energy depends on J and is from the much smaller electron repulsion. Similarly, exclusive transition selection rules, relative intensities, and energy separations apply between pure jj -coupled states, but they were not

considered in the Nd III energy level analysis due to the very small number of Nd III energy level described by this coupling scheme (see [subsection 2.2.8](#)).

J_cK -Coupling

The J_cK -coupling condition can apply to configurations with a lone electron that is highly excited and/or has high orbital angular momenta, good examples are the $3d^74f$ and $3d^75g$ configurations of Co II (e.g. [100–102]). The order of decreasing interaction strength in these two configurations of Co II is as follows: spin-orbit interaction of the $3d^7$ electrons splits their term energies² according to their total angular momentum J_c , then the repulsion from the direct (spin-independent) Slater integral between 3d and 4f or 5g orbitals splits energies according to K from coupling J_c with orbital angular momentum l of the excited electron, and lastly the spin-orbit interaction of the 4f or 5g orbitals and their exchange (spin-dependent) Slater integral with the 3d orbital splits energies into fine structure levels determined by the total atomic angular momentum J from coupling K with the spin s of the excited electron.

Term symbols of J_cK -coupling are in the form $J_c[K]$ (see the end of [Table F.2](#)). Similar to other coupling schemes, J_cK -coupled terms have special transition rules and fine structure patterns. No energy levels of Nd III were labelled using the J_cK -coupling scheme.

2.2.6 Labelling Energy Levels

Fine structure energy levels are labelled using the configuration, the term (with any repeated term identifier γ), and the J value, where the J value is often a subscript following the term symbol and a $^\circ$ symbol is sometimes used as a superscript following a term symbol to indicate terms of odd configurations. When a new energy level is identified empirically from experiments, the approach is to use the highest eigenvector percentage of the most suitable coupling scheme to assign it the most appropriate label.

²The term energies are energies of the LS -coupled terms of the $3d^7$ electrons because the repulsion between the 3d electrons is the largest interaction, much larger than the spin-orbit interactions of the 3d electrons. Therefore, it is the J_c values of the LS -coupled terms of the $3d^7$ electrons being considered for J_cK -coupling with the orbital and spin angular momenta of the lone excited electron. A similar situation exists for Nd III, see [subsection 2.2.8](#) for details.

Most eigenstates of heavy atoms such as those of the REEs with many electrons in open shells do not resemble any coupling scheme, due to the similar strengths of the electron repulsion and spin-orbit interaction. This means the basis functions $|\Psi^b\rangle$ with the largest percentages $|y_b^k|^2$ in any coupling scheme do not represent the majority of the calculated eigenstates $|\Psi^k\rangle$. In such cases, the leading percentage of the *LS*-coupling basis function is commonly used, for a few reasons. The *LS*-coupling scheme is the most common and understood coupling scheme; using *LS*-coupling to label energy levels provides efficient communication of intuition, such as expectations for the Landé interval rule, Hund’s rules, and *LS*-coupling transition selection rules and relative intensities (see [subsection 2.3.2](#)). When the leading percentage in the *LS*-coupling scheme becomes smaller (e.g. $\lesssim 50\%$), one would begin to expect deviations from *LS*-coupling level structure and common violations of the *LS*-coupling transition selection rules and relative intensities. The lowest-lying energy levels of an atom in both parities tend to approximate *LS*-coupling conditions reasonably well, and the lowest-lying levels are also usually involved in the strongest observed transitions and are most often discussed in spectral analyses. Due to these reasons, the preference for *LS*-coupling labels is not unexpected.

It is found that in calculations several energy levels can have the same leading percentage eigenvector, in which case the level with the largest leading percentage is prioritised for the assignment of the level label, and labels of candidate levels with smaller leading percentages are assigned using their eigenvector with the second highest percentage contribution. If conflicts persist, this procedure is iterated until all levels found from experimental spectra in an energy level analysis have unique labels. Generally, one must keep in mind that in any case of large ‘mixing’ (leading percentage $\lesssim 50\%$), the nature of the energy level, e.g., splitting patterns of the assigned terms and branching fractions (see [subsection 2.3.2](#)), must be gauged from its eigenvector composition. The coupling conditions of Nd III will be discussed in [subsection 2.2.8](#).

2.2.7 Configuration Interaction

As discussed in [subsection 2.2.4](#), the set of basis functions $|\Psi_b\rangle$ is chosen to be as complete as possible. Therefore, there is no reason to restrict basis functions to belong to only one configuration when calculating the energy levels (eigenstates) of said configuration, since basis functions from another configuration with the same parity and J value can also be included. This is particularly important when energies of the basis functions of the same parity and

J value are similar but belong to different configurations, because the real eigenstate of the Hamiltonian could be better represented by a combination of the basis functions of the differing configurations.

Configuration interaction means the inclusion of basis functions of more than one configuration to calculate matrix elements of the Hamiltonian of a specific parity and a particular J value. In configuration interaction, the size of the Hamiltonian matrix for the parity and the J value is extended from $M \times M$ to $(\sum_c M_c) \times (\sum_c M_c)$, where the set of basis functions for configuration c has size M_c for the parity and J value of interest. This induces extra off-diagonal matrix elements that are from radial integrals determined between orbitals of differing configurations, which can also be semi-empirical parameters, e.g., RD^k and RE^k of Table A.1, their integral expressions are the same as those of Equation 2.9 and Equation 2.10, respectively, except the radial wavefunctions are from the two interacting configurations. The spin-orbit matrix contributions from configuration interaction are generally negligible [24]. The diagonalisation of the configuration interaction Hamiltonian, with size $(\sum_c M_c) \times (\sum_c M_c)$ for a particular J , determines energies and eigenvectors for all levels of the J value and interacting configurations, this is the approach used in Nd III atomic structure calculations of the present work (see next subsection).

Lastly, it is worth mentioning additional effective parameters for each configuration within the Cowan code. These are the α , β , and γ parameters (e.g. [24, 108]). They can be understood as empirical radial integrals describing higher-order perturbations in single-configuration electrostatic interactions [24].

2.2.8 Nd III Atomic Structure and Coupling Conditions

Details of the atomic structure calculations for Nd III can be found in [96]. The calculations guided the search for new energy levels and were improved iteratively as new levels were identified. All calculations were performed by Dr Alexander Ryabtsev using the Cowan atomic structure code (e.g. [24, 89–91]) and the list of parameters are in Table A.1.

The basis functions were constructed using single-electron wavefunctions of the $4f^3(4f + 5d + 6s + 6p + 7s + 7d + 5f)$ and $4f^25d(5d + 6p)$ configurations and configuration interactions between all configurations of the same parity were included. This set of configuration have energies with

the greatest overlap with the experimental energy levels identified and aimed to be identified, which are the most significant contributions to eigenvector compositions and hence branching fractions crucial to classification through comparing with observed relative line intensities and level energy separations. Less significant configurations were neglected to simplify theoretical and computational complexity.

Semi-empirical energy parameters, i.e., the radial integrals described in [subsection 2.2.1](#), [subsection 2.2.2](#), [subsection 2.2.3](#), and [subsection 2.2.7](#) were fitted using experimental level energies for each configuration. However, the number of radial integrals was very large and could not be constrained using the number of known experimental level energies. Empirically determining the most significant parameters for each configuration was prioritised: the configuration average energy, the leading few terms of the Slater integrals, and the spin-orbit parameters. For the parameters not determined fully using the experimental level energies, configuration interaction radial integrals were fixed at a ratio of 0.7 compared to their ab initio values, some Slater integrals were mostly fixed at ratios between 0.75 (doubly-excited configurations) and 0.85 (singly-excited configurations during ab initio calculations) compared to their ab initio values, and some the other Slater integrals (e.g. $4f - 4f$ direct radial integrals) were fixed using corresponding ratios values obtained for configurations with well-constrained parameters (e.g. $4f^3 5d$ with many known levels). The $0.7 \sim 0.85$ factors are commonly required to improve ab initio Cowan code calculations [24].

A diagram illustrating the energy level structure of Nd III arising from the excitation of one electron of the ground configuration $4f^4$ is shown in [Figure 2.1](#). Electrons of the [Xe] core are not discussed as they are a part of the central potential and do not contribute to the atomic angular momentum J . In [Figure 2.1](#), the columns are sub-configurations representing the possible LS -coupling terms for the three in the $4f$ orbital, referred to as parent terms. Within each column of [Figure 2.1](#), the energies of all possible levels of a sub-configuration from coupling the parent term with the excited electron angular momenta are specified using boxes.

The reason to separate the excited configurations into sub-configurations with different parent LS -coupling terms arises from comparing the relative strengths of electrostatic repulsion between different orbitals (see [Table A.1](#)). Specifically, the Slater integrals between the $4f$ orbitals of the $4f^3$ electrons were an order of magnitude greater than the Slater integrals between orbitals of the excited electron nl and the $4f$ orbital. This is understood by the fact that the three

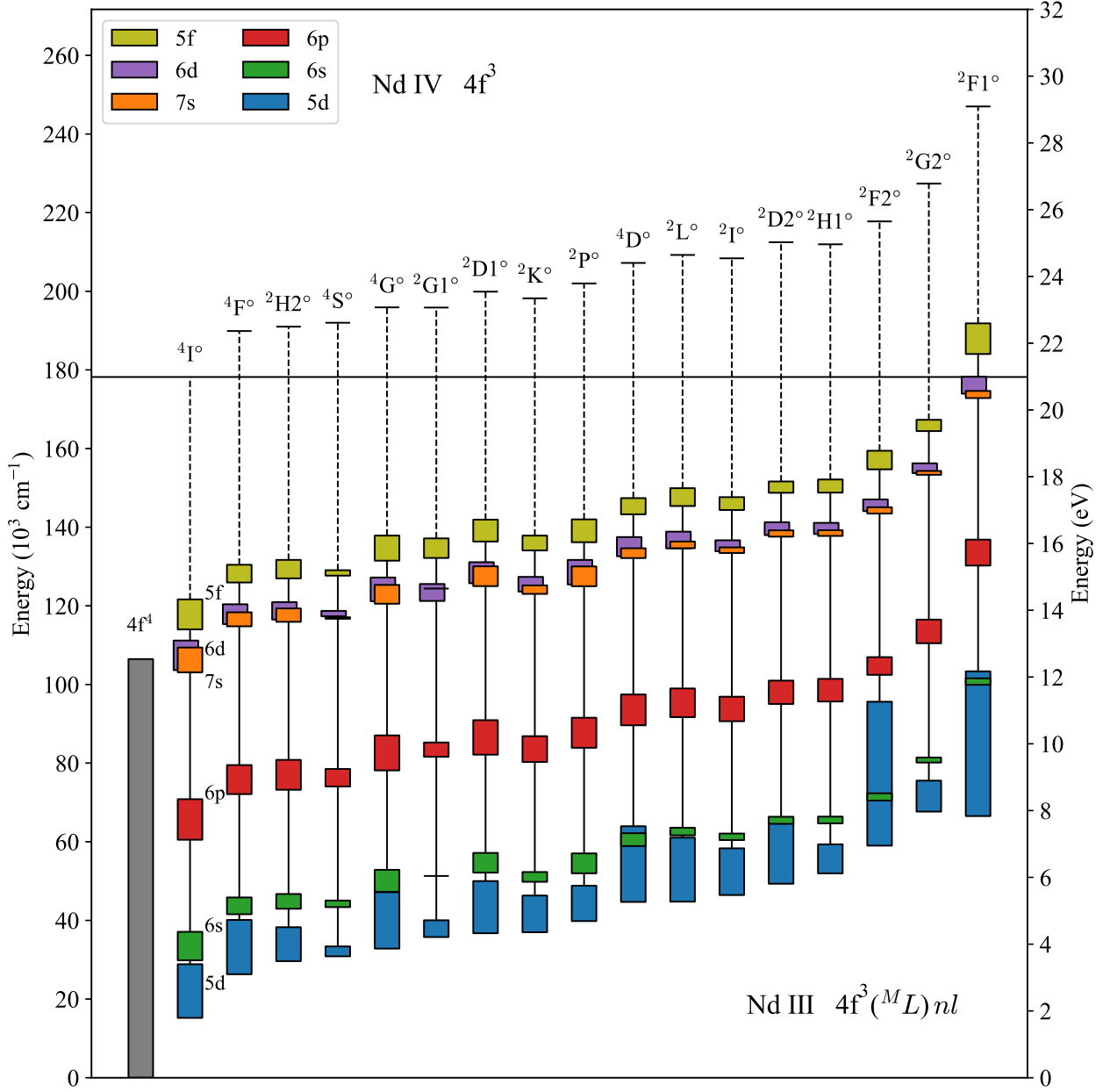


Figure 2.1: Gross atomic structure of Nd III arising from the excitation of one 4f electron, $4f^3(^M L)nl$ up to $nl = 5f$ in relation with the LS terms [77] of the Nd IV ground configuration $4f^3$. All levels are labeled according to the configurations and parent terms of their leading eigenvector components calculated in the present work using the Cowan code. The extent of each box shows the range of level energies within a given $4f^3(^M L)nl$ sub-configuration. The Nd III ionisation potential [109] is shown by the black horizontal line. Figure from Ding et al. (2024) [96].

4f electrons are closer together while the excited electron nl is on average much further away. The spin-orbit parameters $\zeta(4f)$ and $\zeta(nl)$ are also around one or two orders of magnitude smaller than the Slater integrals between the 4f orbitals. Therefore, the largest splitting of the configuration average energy of each $4f^3nl$ configuration was expected to be from the repulsion between the $4f^3$ electrons, which approximately corresponds to LS -coupling conditions between the $4f^3$ electrons.

The leading percentages (purities) of the lowest-lying levels of the $4f^4$ and $4f^35d$ configurations under the pure LS -coupling scheme were almost 100% (see [Table C.1](#) or [63,86]). However, the average purities of higher-lying levels are low ($\lesssim 50\%$), and were also low under other coupling schemes. This is because of the much higher level densities for higher-lying levels, meaning levels are closer in energy and more likely to be mixed. Furthermore, Slater integrals between orbitals of the excited electron nl and the 4f orbital were similar in size to the spin-orbit parameters of the 4f and nl orbitals, which is a situation that follows neither LS -coupling nor jj -coupling conditions. The exceptions are levels identified within the $4f^3ns$ configurations (more details in [section 6.7](#) and [Table C.1](#)), which have approximate jj -coupling conditions for jj -coupling between the excited ns electron and the LS -coupled $4f^3$ electrons due to much smaller contributions of Slater integrals between the 4f and ns orbitals that are similar in size to the spin-orbit parameters of the 4f orbital. The ns levels could also be classed as having J_cK -coupling conditions because the orbital angular momentum of the excited electron is zero.

The diagram of [Figure 2.1](#) illustrating the approximate Nd III atomic structure was particularly useful in the Nd III energy level analysis and will provide context for the readers of this thesis during discussions of any energy level or configuration of Nd III. All experimental energy levels identified in the present work belong to the configurations presented in [Figure 2.1](#).

2.3 Electric Dipole (E1) Transitions

Atoms at any energy level above ground can spontaneously decay to a lower level, emitting single or multiple photons. This is sometimes understood as the interaction between excited electrons of the atom and the zero-point energy of the quantised electromagnetic field (vacuum fluctuations). Therefore, the transition can occur from electric and magnetic dipole (E1, M1), quadrupole (E2, M2), octupole (E3, M3) interactions, and so on. The E1 transitions are orders

of magnitude more likely compared to other interactions and make up most of the observed spectra of atomic electron transitions. The transitions considered in this thesis will only be E1 transitions.

2.3.1 Transition Probabilities

The Einstein spontaneous transition probability [110] is defined as the total decay rate A_{ji} (s^{-1}) from a specific degenerate state j of the upper energy level to any of the $g_i = 2J_i + 1$ degenerate states of the lower energy level i with total angular momentum quantum number J_i [24]. The number of atoms in the specific degenerate state j of the upper energy level, $N_j(t)$, at time t is given by the rate equation

$$\frac{dN_j(t)}{dt} = - \sum_i A_{ji} N_j(t), \quad (2.19)$$

where the summation is over all possible lower levels of spontaneous de-excitation. There are $g_j = 2J_j + 1$ degenerate states in the energy level j with total angular momentum quantum number J_j , and one would expect them to be equally populated when small perturbations lifting the degeneracy of the fine structure levels (examples in [section 2.4](#)) could be ignored. Therefore, the intensity (units of Js^{-1}) of the spectral line with transition probability A_{ji} is

$$I(t) \propto hc\sigma_{ji}g_jA_{ji}N_j(t), \quad (2.20)$$

where $hc\sigma_{ji} = E_j - E_i$ and σ_{ji} is the wavenumber of the transition. In my work, the proportionality depends on the spectrometer intensity response, throughput, and detector (e.g. see [subsection 3.3.6](#)). The lifetime τ_j of an energy level is $(\sum_i A_{ji})^{-1}$ (including non-E1 decay channels), and the ratio $A_{ji}/\sum_i A_{ji}$ is referred to as the branching fraction or ratio, measurable as relative intensity. Experimentally determined lifetimes and branching fractions allow measurements of absolute transition probabilities. My work considers only relative intensities, which are measurable by FT spectroscopy (see [Chapter 3](#) and [section 5.5](#)). Without experimentally measured τ_j , assumptions of the level population $N_j(t)$ would be required to determine absolute transition probabilities (e.g. see [Equation 2.33](#) and [section 7.4](#)).

Various forms of the transition probability A_{ji} are used. Firstly, the quantity g_jA_{ji} is referred to as the weighted transition probability and is helpful in comparing relative intensities of

lines originating from energy levels with different statistical weights; $g_j A_{ji}$ will be repeatedly mentioned throughout [Chapter 6](#). Secondly, the oscillator strength f is related to the transition probability through [\[24\]](#)

$$gA = \frac{8\pi^2 e^2}{m_e c} \sigma^2 g f, \quad (2.21)$$

where g is the statistical weight of the initial level. Upper level weight g_u is used for g for $A = A_{ji}$ and emission oscillator strength f_{emission} . Lower level weight g_l is used for absorption oscillator strength $f_{\text{absorption}}$. The distinction is not often stated because $g_l f_{\text{absorption}} = g_u f_{\text{emission}}$ [\[110\]](#). Strong lines have f of order unity (e.g. [Figure 1.9](#)). The weighted absorption oscillator strength is often in discussions of absorption of continuum spectra, e.g., in stellar atmosphere spectroscopy the quantity $\log(gf)$ is nearly always used. Lastly, a more fundamental quantity is the line strength S , related to A through [\[24\]](#)

$$gA = \frac{64\pi^4 e^2 a_0^2}{3h} \sigma^3 S, \quad (2.22)$$

where a_0 is the Bohr radius. The line strength S is directly dependent on the wavefunctions of the two quantum states of the transition. This relationship is used in theoretical calculations of transition probabilities using the wavefunctions, determined from methods such as those discussed in [section 2.2](#).

The line strength S can arise from the consideration of the energy decay rate a of a classical electron oscillator as an analogue to the energy loss of the rate of spontaneous transition from an excited state $|\gamma' J' M'\rangle$ to the lower energy state $|\gamma J M\rangle$ (γ is used to distinguish repeated terms, J and M are the total angular momentum and its alignment) [\[24\]](#),

$$a = \frac{64\pi^4 e^2 a_0^2 \sigma^3}{3h} \sum_{q=-1}^1 |\langle \gamma J M | \hat{\mathbf{P}}_q | \gamma' J' M' \rangle|^2, \quad (2.23)$$

where

$$\hat{\mathbf{P}}_q = \sum_i^N |\hat{\mathbf{r}}_i| \sqrt{\frac{4\pi}{3}} Y_{1q}(\theta_i, \phi_i) \quad (2.24)$$

is the classical dipole moment of all N electrons in units of $-ea_0$. Efficient evaluation of the summations is enabled by the Wigner-Eckart theorem, which applies to the irreducible tensor

operator form of the position vector operator shown in [Equation 2.24](#):

$$\langle \gamma JM | \hat{\mathbf{P}}_q | \gamma' J' M' \rangle = (-1)^{J-M} \begin{pmatrix} J & 1 & J' \\ -M & q & M' \end{pmatrix} \langle \gamma J || \hat{\mathbf{P}} || \gamma' J' \rangle, \quad (2.25)$$

where the line strength S is the square of the absolute value of the reduced matrix element, $|\langle \gamma J || \hat{\mathbf{P}} || \gamma' J' \rangle|^2$, which is independent of M, M' and q .

2.3.2 Selection Rules and Theoretical Line Strengths

Selection rules indicate which transitions can occur. This is crucial information in classifying transitions between energy levels. For example, the electric dipole operator is odd in parity, therefore, the radial integral of $\langle \gamma JM | \hat{\mathbf{P}}_q | \gamma' J' M' \rangle$ is zero if $|\gamma' J' M' \rangle$ and $|\gamma JM \rangle$ have the same parity, i.e., E1 transitions can only occur between states opposite in parity. The Wigner 3- j symbol of [Equation 2.25](#) also restricts E1 transitions to obey $\Delta J = J' - J = 0, \pm 1$ and forbids $J = J' = 0$, otherwise the line strength S would be zero. Additionally, $\Delta M = 0, \pm 1$ which are the three possible polarisations of the radiation corresponding to the unit angular momentum quantum number of a photon. For an isolated atom, the parity and ΔJ selection rules are most reliable because they are independent of the coupling scheme and eigenvector composition of the upper and lower energy levels.

Theoretical calculations of transition probabilities are evaluations of the reduced matrix element $\langle \gamma J || \hat{\mathbf{P}} || \gamma' J' \rangle$ for the line strength S using computed wavefunctions. The reduced matrix elements $\langle \gamma J || \hat{\mathbf{P}} || \gamma' J' \rangle$ are in the basis of the real eigenfunctions of the Hamiltonian, which, in the calculation of atomic structure ([section 2.2](#)), are expanded into the basis of anti-symmetrised product wavefunctions between radial wavefunctions of the central potential (from different configurations in configuration interaction) and angular momentum coupled wavefunctions of $\hat{\mathbf{J}}^2$. Therefore, in the basis of a specific angular momentum coupling scheme $|\gamma J \rangle = \sum_{\beta} y_{\beta J}^{\gamma} |\beta J \rangle$, the reduced matrix element is

$$\langle \gamma J || \hat{\mathbf{P}} || \gamma' J' \rangle = \sum_{\beta} \sum_{\beta'} y_{\beta J}^{\gamma} \langle \beta J || \hat{\mathbf{P}} || \beta' J' \rangle y_{\beta' J'}^{\gamma'}, \quad (2.26)$$

where the upper-level basis is labelled using primes. The LS -coupling scheme is the most

convenient choice for evaluating the summation³, as the dipole operator does not operate on spin states. If β, β' are pure LS -coupling bases [24],

$$\langle \beta J || \hat{\mathbf{P}} || \beta' J' \rangle = \delta_{SS'} (-1)^{L+S+J'+1} \sqrt{(2J+1)(2J'+1)} \begin{Bmatrix} L & S & J \\ J' & 1 & L' \end{Bmatrix} \langle \beta LS || \hat{\mathbf{P}} || \beta' L' S' \rangle. \quad (2.27)$$

This has two important implications when $|\gamma J\rangle$ of levels of the two terms (βLS and $\beta L'S'$) correspond to pure LS -coupling conditions where the largest $|y_{\beta J}^\gamma|^2$ are almost unity. Firstly, additional LS selection rules apply according to the Wigner 6- j symbol and the Kronecker delta, where $\Delta S = 0$, $\Delta L = 0, \pm 1$, and $L = L' = 0$ is not allowed. Secondly, relative line strengths of transitions between the levels of the two LS terms are dominated by the square of the matrix element $\langle \beta J || \hat{\mathbf{P}} || \beta' J' \rangle$, where the strongest lines are those with $\Delta J = \Delta L$ (referred to as main or principal lines) and with largest J and J' . As discussed in subsection 2.2.8, the lowest-lying terms of the even and odd parities of Nd III are relatively pure in the LS -coupling scheme, transitions between these terms follow the intensity pattern predicted by Equation 2.27 and transitions violating the LS selection rules are relatively very weak.

Complications arise when energy levels are not pure, e.g., where the largest $|y_{\beta J}^\gamma|^2$ are only around 0.5 or less. Equation 2.26 is a sum of amplitudes, which could destructively interfere and become sensitive to the eigenvector compositions. This is usually quantified using the cancellation factor [24]. Weaker transitions are more sensitive to the compositions due to interference and are generally less accurately calculated. Furthermore, the radial integral of the dipole matrix element depends on radial wavefunctions of two or more configurations depending on the configuration interaction space, which also induces sensitivity to the radial wavefunctions and the central potential. Therefore, accurate atomic structure calculations are prerequisites to accurate line strength (transition probability) calculations. Examples of improved agreement between observed and theoretical line intensities from improved atomic structure calculations will be discussed throughout Chapter 6. In ideal situations, the uncertainty of theoretical transition probabilities is about 10% [24], which was the order of uncertainty used to gauge minimum theoretical transition probabilities uncertainties between relatively pure levels of Nd III.

³The choice of coupling scheme can affect the evaluation of the reduced matrix element due to limited basis, especially with significant configuration interaction [111].

2.4 Perturbations to Energy Levels

This section describes small perturbations to fine structure energy levels that are observable with high-resolution spectroscopy. Generally, the perturbations cause distortions in observed spectral lines and must be considered to accurately measure fine structure transition energies and intensities and carry out reliable spectral analyses.

2.4.1 Hyperfine Structure

The hyperfine interaction is the interaction between the magnetic dipole moment of the nucleus and the magnetic field at the nucleus produced by the electrons, plus the interaction between the electric quadrupole moment of the nucleus and the electric field gradient at the nucleus produced by the electrons. The dipole interaction is generally dominant and this is the case for Co II ([Chapter 8](#)), and its perturbing Hamiltonian has the same form as the spin-orbit term of [Equation 2.11](#), in the sense that it is proportional to a dot product between the two angular momentum operators $\hat{\mathbf{J}} \cdot \hat{\mathbf{I}}$:

$$\hat{H}_{\text{HFS}} = -\mu_{\text{B}} \frac{m_e}{m_p} g_{\text{I}} \frac{\mathbf{B}(0) \cdot \hat{\mathbf{J}}}{\hat{\mathbf{J}}^2} \hat{\mathbf{J}} \cdot \hat{\mathbf{I}}, \quad (2.28)$$

where $\hat{\mathbf{J}}$ is the total angular momentum operator of the electrons, $\hat{\mathbf{I}}$ is the total angular momentum operator of the nucleus, μ_{B} is the Bohr magneton, g_{I} is the g -factor of the nucleus, and $\mathbf{B}(0)$ is the average magnetic flux density of the electrons at the nucleus. The size of HFS splitting is affected by electron densities of the radial wavefunctions, where hyperfine interactions are strongest for electrons closest to the nucleus, such as the ns electrons.

In HFS, the total angular momentum of the nucleus, I , couples with the total electronic angular momentum, J , which induces a splitting of the fine structure levels into HFS levels described using the total atomic angular momentum quantum number F where

$$F = |I - J|, |I - J| + 1, \dots, I + J - 1, I + J.$$

Energy shifts for different values of F in the hyperfine magnetic dipole interaction are generally three orders of magnitude smaller than shifts from the spin-orbit interaction between the electrons themselves, and effects from the electric quadrupole interaction are generally even

smaller. By perturbation theory, the change in energy from a fine structure level with J to one of its HFS levels with F is given by [112]

$$\Delta E_{FJ} = \frac{1}{2}AK + B \frac{(3/4)K(K+1) - J(J+1)I(I+1)}{2I(2I-1)J(2J-1)}, \quad (2.29)$$

where

$$K = F(F+1) - J(J+1) - I(I+1),$$

A and B are magnetic dipole and electric quadrupole hyperfine interaction constants respectively. The first term $AK/2$ is identical to fine structure splitting in the pure LS -coupling condition (Equation 2.17) because both are magnetic dipole interactions. The fine structure transition becomes a group of hyperfine transitions with relative intensities, $R_{JFJ'F'}$, between the hyperfine levels with quantum numbers JF and $J'F'$ given by

$$R_{JFJ'F'} = \frac{(2F+1)(2F'+1)}{(2I+1)} \left\{ \begin{matrix} J & I & F \\ F' & 1 & J' \end{matrix} \right\}^2, \quad (2.30)$$

where the squared factor is a Wigner 6- j symbol, which includes the selection rules: $\Delta F = 0, \pm 1$ but not $F = 0 \leftrightarrow F' = 0$ [24, 113]. The relative intensities are identical to the LS -coupling relative intensities of Equation 2.27 (with a normalisation of the line strength by $(2I+1)$), again because both are magnetic dipole interactions. The HFS splitting does not shift the configuration and fine structure level average energies, also similar to the spin-orbit interaction. This is important as the fine structure transition wavenumber is the wavenumber of the average intensity of the hyperfine transitions between two fine structure levels, this average wavenumber is referred to as the centre-of-gravity (COG) wavenumber and is a parameter from line fitting (see subsection 5.3.3). The hyperfine angular momentum coupled states with total angular momentum F are almost always very pure due to orders of magnitude smaller perturbation compared to other terms of the Hamiltonian. Significantly mixed hyperfine structure states were not observed in Co II, therefore, Equation 2.29 and Equation 2.30 could be used to produce theoretical hyperfine structure line profiles in the Co II HFS analysis.

2.4.2 Isotope Shifts

Isotope shifts are differences in level energies between different isotopes, which come from two effects: finite nuclear mass and finite nuclear volume. This means that the spectral lines of different isotopes of the same atom will appear as a group of transitions with relative intensities corresponding to their relative isotopic abundances.

For larger atoms such as those of Nd, the effects of finite nuclear volume are more prominent [24]. The isotope shift to an energy level from the finite nuclear volume is referred to as the field shift and can be understood using a reduced nuclear potential near the origin, where non-negligible electron density within the nucleus increases the level energy (decreases the electron binding energy). Therefore, the size of isotope field shifts is also configuration-dependent and more prominent in *ns* electrons. This provides very useful hints in classifying the configurations of levels of a transition because transitions between two configurations are expected to have the same line profiles arising from isotope field shifts, except for levels with significant configuration mixing. Isotope shifts were always considered in the energy level analysis of Nd III when they were observed, which will be discussed in [Chapter 6](#). Examples of isotope shifts observed in spectra of Nd III can be seen from [Figure 6.4](#). The wavenumber order of the isotope component transitions depends on both the isotope shifts of the upper and lower energy levels; if the field shift is larger for the upper level of a transition, the transition wavenumber increases with increasing atomic mass, and vice versa.

2.4.3 Zeeman Splitting

Significant effects of external fields were not expected for the light sources of the experiments. However, the effects of an external magnetic field are observable in magnetic stars (e.g. [63]). Observations of the Zeeman splitting of energy levels in magnetic Nd-rich stars have contributed to the energy level analysis of Nd III (see [Figure 6.10](#) and [Chapter 7](#)). The Zeeman splitting of fine structure levels can be treated with perturbation theory, $\hat{H}_Z = -\hat{\mu} \cdot \hat{\mathbf{B}}$, which shifts level energies by

$$\Delta E_Z = \mu_B g_J |\mathbf{B}| M_J, \quad (2.31)$$

were μ_B is the Bohr magneton, g_J is the Landé g -factor, and M_J is magnetic quantum number of the atom.

2.5 Plasma Thermodynamic and Radiative Properties

The spectra of atoms vary depending on the plasma conditions, for example within the stars and laboratory light sources. This is a complex subject within the field of microscopic plasma physics and radiative transfer research, so only the most simple and widely used approximations regarding energy level and ion populations will be discussed here which are useful in understanding the observed relative line intensities. Plasma conditions also affect the spectral line profiles of individual atomic transitions, which is important in fitting spectral lines for transition wavenumbers and intensities, which will be discussed in the final parts of this section.

2.5.1 Atomic Partition Function and the Boltzmann Distribution

Under thermal equilibrium and in the approximation where the atoms, ions, and free electrons within a plasma are non-interacting, the partition function for a particular atom with N electrons is

$$u_N = \sum_j g_j e^{-E_j/k_B T}, \quad (2.32)$$

where E_j and $g_j = 2J_j + 1$ are the energy and statistical weight of the j^{th} energy level of the atom. The partition function is usually defined over the states which contribute significantly to the summation, e.g., a principal quantum number n beyond which the energy levels have negligible populations under temperature T , or a truncation of the infinite number of bound states due to neighbouring charged particles in a plasma changing the nuclear Coulomb potential at large radii.

Consequently, the number density n_N^j of atoms in the energy level E_j is in the Boltzmann distribution

$$\frac{n_N^j}{n_N} = \frac{g_j e^{-E_j/k_B T}}{u_N}, \quad (2.33)$$

where n_N is the total number density of the atomic species. The statistical weight does not need to be considered in [Equation 2.20](#) if this quantity is used for level population, here the relative populations already consider the statistical weight. The Boltzmann distribution is used to roughly estimate relative intensities of Nd III transitions observed in the experimental spectra of the present work during the energy level analysis ([section 7.4](#)).

2.5.2 Saha Equilibrium and Ion Fractions

Under thermal and ionisation equilibrium, i.e., a constant number of electrons and atoms in each ionisation stage, the fraction of the number densities between the ionisation state n_{N-1} with $N - 1$ electrons and neutral state n_N with N electrons is given by the Saha equation [[114](#)]

$$\frac{n_{N-1}}{n_N} = \frac{2}{n_e} \left(\frac{2\pi m_e k_B T}{h^2} \right)^{\frac{3}{2}} \frac{u_{N-1}}{u_N} e^{-I_N/k_B T}, \quad (2.34)$$

where I_N is the first ionisation energy of the element with atomic number $Z = N$, u_{N-1} and u_N are the partition functions of the ion and neutral atom respectively. This formula can be applied iteratively for higher ionisations if the successive ionisation energies are known, where the electron number density contribution from all ionisation stages is

$$\sum_{N=0}^{N=Z} (Z - N) n_N, \quad (2.35)$$

where the n_N here is the number density of ions with N electrons. This, together with [Equation 2.33](#) and [Equation 2.34](#), will therefore offer a first-order estimation of the relative occupancies of all energy levels of all ions at a given n_e or pressure. Hence, higher temperatures, lower pressures or densities, and lower ionisation energies promote ionisation.

The Saha equilibrium is frequently used in stellar astrophysics and kilonovae modelling [[93,115](#)]. When paired with the Boltzmann distribution, the Saha equilibrium can also provide qualitative guidance and explanation for ionisation and energy level populations in laboratory light sources, such as in comparisons between the hollow cathode and Penning discharge lamps used in the present work to produce Nd spectra ([section 4.4](#) and [section 4.5](#)).

2.5.3 Spectral Line Profiles

The transition between two fine structure or two hyperfine structure levels is not monochromatic. Instead, the transition wavenumber varies over some normalised distribution function $P(\sigma)$ where $\int_{-\infty}^{\infty} P(\sigma) d\sigma = 1$. The functional form of the line profile is required in fitting spectral lines for transition wavenumbers of observed transitions (see [section 5.3](#) and [Chapter 8](#)).

Natural Line Profile

The Heisenberg uncertainty principle, $\Delta E \Delta \tau \simeq \hbar$ implies an uncertainty in the energy of a level due to the uncertainty in the natural lifetime of the level, where the probability distribution of an atom staying in an excited state is exponential due to spontaneous decay. The Fourier transform of an exponential distribution in time is a Lorentzian distribution in energy (e.g. wavenumber), which is the natural line profile

$$P(\sigma) = \frac{\Gamma/\pi}{(\sigma - \sigma_0)^2 + \Gamma^2}, \quad (2.36)$$

where σ_0 is the mean wavenumber and 2Γ is the full width at half maximum (FWHM) which decreases with increasing $\Delta\tau$. Typical lifetimes of neutral atoms are about 10^{-8} s, which gives $\Gamma \simeq 5 \times 10^{-4} \text{ cm}^{-1}$ [24]. This is negligible compared to other broadening effects that exist in the discharge lamps used for experiments in this project.

Resonance and Collision (Pressure) Broadening

In resonance broadening, the radiation field within a plasma may induce absorption of the appropriate lower level or stimulated emission of the appropriate upper level, both effects reduce the natural lifetime and broaden spectral lines. In collision or pressure broadening, excitation or de-excitation could be caused by collisions with electrons or other atoms/ions in a plasma, which also reduces the natural lifetime of energy levels. The two broadening mechanisms result in the increase of Γ in [Equation 2.36](#) usually by one or more orders of magnitude without changing the Lorentzian shape.

Doppler Broadening

Under the assumption of Maxwell-Boltzmann velocity distribution for the atoms, the application of the Doppler frequency shift between the moving atoms and the stationary detector leads to a Gaussian profile for $P(\sigma)$, where the full width at half maximum (FWHM) of this profile at wavenumber σ is given by

$$FWHM = \sigma \sqrt{\frac{8k_B T \ln(2)}{mc^2}}, \quad (2.37)$$

where m is the mass of the atomic species in question. For heavy atoms in temperatures of a few 10^3 K, this FWHM could be of the order of 0.1 cm^{-1} (3000 MHz).

Voigt Profile

Generally, all previously mentioned broadening effects exist within a plasma and combine through convolution between their individual profiles $P(\sigma)$. The resulting profile is the convolution between a Lorentzian distribution and a Gaussian distribution called the Voigt distribution. The Gaussian width component contributes relatively more to the line width near the centre of the spectral line, and the Lorentzian width component contributes relatively more to the size and extension of the wings of a spectral line, because the Gaussian function drops to zero sharply compared to a Lorentzian function. An example of a Voigt profile can be seen for the $p = 0$ curve in [Figure 2.2](#).

The line profile of a transition between two fine structure levels therefore follows the Voigt profile convolved with the instrumental profile (see [Chapter 3](#)). When internal or external perturbations exist, e.g., nuclear effects or Zeeman splitting ([section 2.4](#)), the transitions between each pair of hyperfine, isotope, or Zeeman-split levels are individual Voigt profiles convolved with the instrumental profile.

2.5.4 Self-absorption

[Equation 2.19](#) and [Equation 2.20](#) assume the plasma to be optically thin, however, this is never completely true, as photons from spontaneous emission will be absorbed from traversing through the finitely sized plasma. This effect, known as self-absorption, was reviewed in detail

by [116] and a suitable model to explain affected line profiles was given by

$$I(\sigma) = I_0 P(\sigma) e^{-p \frac{P(\sigma)}{P(\sigma_0)}}, \quad (2.38)$$

where $I(\sigma)$ and $I_0 P(\sigma)$ are the intensity profiles with ($p > 0$) and without ($p = 0$) self-absorption respectively, and

$$p = h\sigma_0 B P(\sigma_0) \int n_a(x) dx, \quad (2.39)$$

where B is the total probability of absorption [110], and $n_a(x)$ is the number density of all (degenerate) states absorbing σ_0 . This model assumes one-dimensional photon traversal along the x direction, $P(\sigma)$ to be independent of x and the same for both emission and absorption line profiles, and the spectral energy density $\rho(\sigma)$ to be constant over the range at which σ_0 is absorbed (across the line shape), i.e., the absorption rate is $BN\rho(\sigma_0)$ for N atoms in the lower levels absorbing σ_0 .

Various values of p for a Voigt profile are shown in Figure 2.2. ‘Self-reversal’ is often used to describe spectral lines with a dip at the original peak wavenumber, e.g., as seen for $p = 2$ in Figure 2.2 and the line in Figure 6.6. A Voigt profile would be a poor fit for $p > 0$, as the fitted FWHM of the spectral line would be larger than it would be for $p = 0$. This can be deduced from Figure 2.2 from considering the normalisation of the peak intensity of all p values. Thus, self-absorption can be identified from anomalously large line widths found during the fitting of Voigt profiles to observed spectral lines, compared to widths of nearby non-self-absorbed lines. Additionally, the residuals (observed line profile minus fitted line profile) of a Voigt fit for $p > 0$ will also resemble an up-side-down ‘W’, where the peak and width are overestimated in the fit, e.g., see the fitted line and its residual at 19660.25 cm^{-1} of Figure 5.12).

Consideration of self-absorption is important in the analysis of spectral lines of transitions between fine structure energy levels, especially those perturbed by internal or external fields when the size of perturbation is comparable with or larger than the line width. Under these conditions, line profiles are unique to each component transition between pairs of perturbed/split levels [116]. For example, a more intense hyperfine transition would contribute more to the spectral energy density at its wavenumber, causing itself to be more self-absorbed compared to less intense hyperfine transitions. This would cause wavenumber shifts and uncertainties when determining its fine structure level energies through COG fitting (subsection 5.3.3). Such a line

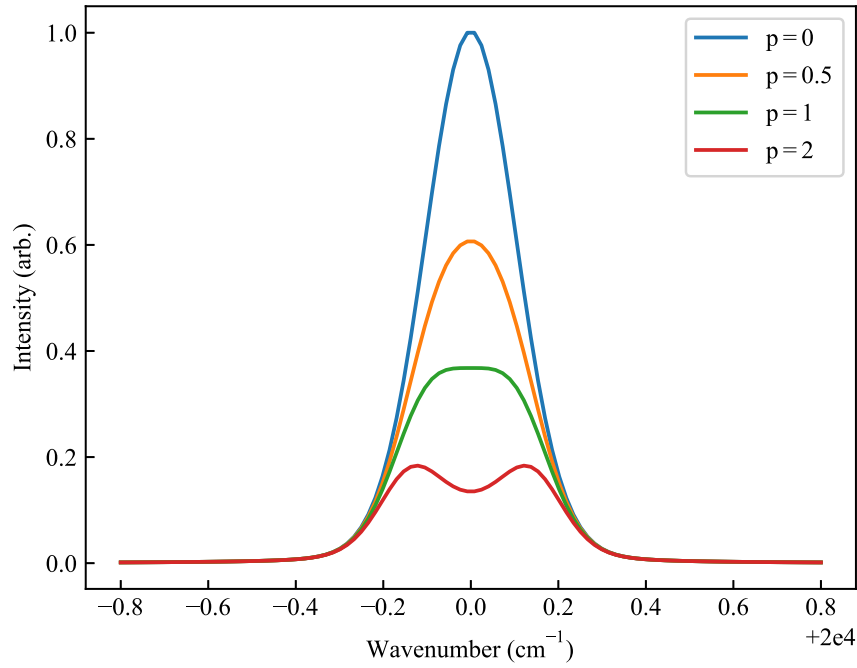


Figure 2.2: Modelled self-absorption of a Voigt profile for a line centered at $20\,000\text{ cm}^{-1}$ with Gaussian standard deviation and Lorentzian half width and half maximum at 0.1 and 0.01 cm^{-1} respectively.

would also be unsuitable for wavenumber or intensity calibration as other lines may not have the wavenumber shift or reduced intensity from self-absorption. Therefore, the requirement of line profile symmetry and small Voigt profile fit residuals are crucial in the selection of lines for wavenumber calibration ([subsection 5.4.3](#)). Furthermore, the determination of hyperfine structure constants in energy levels would be greatly hindered if there is self-absorption due to the resulting line profile distortion (see [section 8.4](#)).

Generally, experimental conditions are chosen to avoid self-absorption in the spectral lines of interest. However, analysis involving self-absorbed lines is seldom avoidable. Most commonly self-absorbed lines in emission spectra involve lower energy levels with the highest populations, such as the ground term levels or levels with very long lifetimes.

2.5.5 Meaning of ‘Strong’ and ‘Weak’ Lines

Throughout my thesis and in the literature, observed and theoretical atomic transitions are often loosely described using the two words ‘strong’ and ‘weak’ in similar but varying contexts. Generally, whether a transition is strong or weak is described by the signal-to-noise (SNR)

ratio. Within the expected spectral range, strong lines will almost certainly show up in most spectra and far above the noise level, whereas weak lines describe lines around or below the noise level. Lines lying somewhere in between these two extreme cases are sometimes described as having intermediate SNRs.

The SNR of a spectral line depends on many factors such as its transition probability (line strength), level populations, the instrumental response, and the noise level. For instance, resonance transitions involving ground term levels of an atom could have orders of magnitude lower transition probabilities compared to transitions between higher-lying configurations of that atom, but these resonance transitions are often observed as the highest SNR transitions because of much higher level populations. Therefore in this context, the resonance transitions are referred to as strong compared to the higher transition probability transitions between higher-lying configurations. In another example, two lines may have the same transition probability and level populations, but they are observed in different spectral regions with significantly different noise levels or instrumental intensity response.

Chapter 3

Principles of Fourier Transform Spectroscopy

3.1 Introduction

This chapter contains fundamental information on how the spectrum of a light source could be obtained using an FT spectrometer to the accuracy required for detailed atomic structure analyses. All experimental parameters described in [Chapter 4](#) were chosen considering the instrumental theory, and the analysis of the experimental data and their conclusions in later chapters are also inseparable from considering the physics of the apparatus. The depth of information within this chapter is sufficient to undertake the projects of the present work but is insufficient to construct a state-of-the-art FT spectrometer. More theory of FT spectroscopy can be obtained from sources such as [\[117–119\]](#), which are the primary sources of literature for this chapter. The units used for wavelengths and energies in this thesis are most often the wavenumber $\sigma = 1/\lambda$ in cm^{-1} for convenience, due to the use of FT spectroscopy.

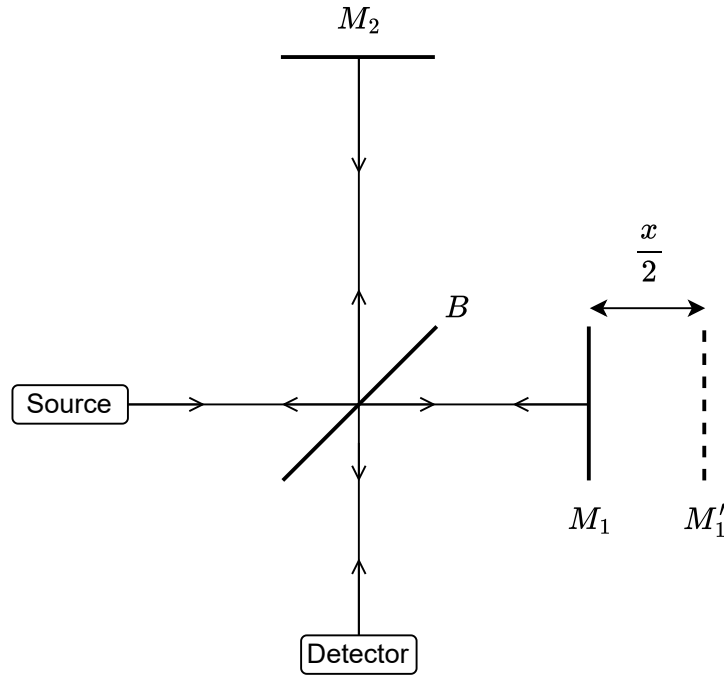


Figure 3.1: Schematic diagram of the Michelson interferometer, where B is a 50/50 beam-splitter, M_1 is the moving mirror, M_2 is the stationary mirror, and M'_1 is the position of the moving mirror at zero optical path difference, $x = 0$.

3.2 Ideal Fourier Transform Spectrometer

3.2.1 The Michelson Interferometer

The Fourier transform spectrometer is an application of the Michelson interferometer, which is shown schematically in Figure 3.1. In the Michelson interferometer, a light source is incident on a 50/50 beamsplitter B at a 45-degree angle, the split and transmitted beams are reflected by two mirrors, which recombine at the beamsplitter and are detected by the detector. The mirror M_1 can move and the mirror M_2 is stationary, moving M_1 changes the optical path difference between the split beams and induces interference in the recombined beams. Intensities recorded by the detector vary as a function of optical path difference x , this function is referred to as the interferogram.

For a plane wave, monochromatic source with wavenumber σ_0 and Dirac delta function intensity spectrum $2a^2\delta(\sigma - \sigma_0)$, the phase difference of the two combining beams is $2\pi\sigma_0x$ and the amplitude $A(x)$ of the recombined beam is the sum of the equal amplitude a of the two split beams,

$$A(x) = a + ae^{i2\pi\sigma_0x}, \quad (3.1)$$

which gives the intensity of the combined beam

$$I(x) = A(x)\overline{A(x)} = a^2 + a^2 e^{i2\pi\sigma_0 x} + a^2 + a^2 e^{-i2\pi\sigma_0 x} = 2a^2(1 + \cos(2\pi\sigma_0 x)). \quad (3.2)$$

The intensity $I(x)$ is the interferogram, where the constant term $2a^2$ is the average intensity and information regarding the spectrum is contained within the cosine modulation term $2a^2 \cos(2\pi\sigma_0 x)$. The monochromatic interferogram without the constant offset term can be expressed as a cosine transform of the monochromatic spectrum

$$I(x) = \int_0^\infty 2a^2 \delta(\sigma - \sigma_0) \cos(2\pi\sigma x) d\sigma, \quad (3.3)$$

the input monochromatic spectrum can therefore be recovered from the reverse cosine transform of the interferogram $I(x)$. However, since half of the recombined beam is directed towards the detector, and the other half is directed towards the source, the detector sees an average intensity of a^2 . This means that the measured interferogram (without average intensity offset) amplitudes are halved, $I_{\text{meas}}(x) = I(x)/2 = a^2 \cos(2\pi\sigma_0 x)$, which has a reverse cosine transform of $a^2 \frac{1}{2} [\delta(\sigma + \sigma_0) + \delta(\sigma - \sigma_0)]$ when recovering the spectrum. The positive part of the recovered spectrum $a^2 \frac{1}{2} \delta(\sigma - \sigma_0)$ is at 1/4 of the intensity of the input spectrum $2a^2 \delta(\sigma - \sigma_0)$, which is also reflected about $\sigma = 0$. It follows that if the input spectrum is polychromatic $B(\sigma)$, the cosine transform of its measured interferogram

$$B_{\text{meas}}(\sigma) = \int_{-\infty}^\infty I_{\text{meas}}(x) \cos(2\pi\sigma x) dx \quad (3.4)$$

would be $B(\sigma)$ reflected about $\sigma = 0$ and scaled by a factor of 1/4. In practical FT spectroscopy, the polychromatic interferogram is never symmetric about $x = 0$ (see [subsection 3.3.1](#)), the spectrum is recovered using the Fourier transform instead, hence the name for FT spectroscopy.

3.2.2 Example Interferograms and Spectra

Due to the FT relation between the spectrum $B(\sigma)$ and the interferogram $I(x)$, one can gauge the widths of the distributions within the two relevant representations using the bandwidth theorem, e.g.,

$$\sigma_1 \sigma_2 = \frac{1}{2\pi}, \quad (3.5)$$

where $\sigma_{1,2}$ are standard deviations of a pair of normalised Gaussian distributions that are FTs of each other. For example, the interferogram of a laser line or an atomic transition spectral line is expected to be many orders of magnitude wider (have information that is observable far from $x = 0$) compared to the interferogram of a tungsten lamp which has a continuum spectrum.

Qualitative comparisons between different types of spectra observed in the present work and their corresponding interferograms are shown in [Figure 3.2](#). The single Voigt profile representing one atomic emission line produces an interferogram modulated by the FT of the Voigt profile, where interference is no longer observed beyond 7.5 cm of optical path difference x . The change in interference amplitude with respect to x is negligible unless x differs by hundreds of wavelengths (see plot on the top right of [Figure 3.2](#)). Therefore, the zero optical path difference position (frequently referred to as the centre burst) is not obvious at all for a near-monochromatic interferogram. On the other hand, the continuum spectrum has a much larger spectral range, corresponding to an interferogram with a well-defined and narrow centre burst at zero optical path difference. Lastly, the interferogram of the synthetic complex atomic emission spectrum contains characteristics from both the interferogram of the single emission line spectrum and the interferogram of the continuum spectrum. The different spectral lines of the complex atomic emission spectrum interfere with each other and enhance the centre burst as it is the only optical path difference position where all wavelengths are in phase. Since all lines in the spectrum are narrow (a small fraction of a nm), interference remains observable up to an optical path difference of around 7.5 cm, which is similar to the single line interferogram and orders of magnitude higher compared to the continuum spectrum with a spectral range of a few hundred nm. Although the noise levels are the same in the complex and single-line spectra, the SNR of the interferogram of the complex line spectrum is much higher due to additive signals from all lines at the zero optical path difference point.

All results shown on [Figure 3.2](#) are theoretical, hence the interferograms are perfectly symmetric about zero optical path difference. The constant noise levels and the maximum optical path difference are typical for the FT spectrometer used in the present work. The intensity axis is subject to the normalisation of the FT algorithm, but spectra are generally represented as SNR per unit wavenumber after determining the noise level (see [subsection 5.2.4](#)).

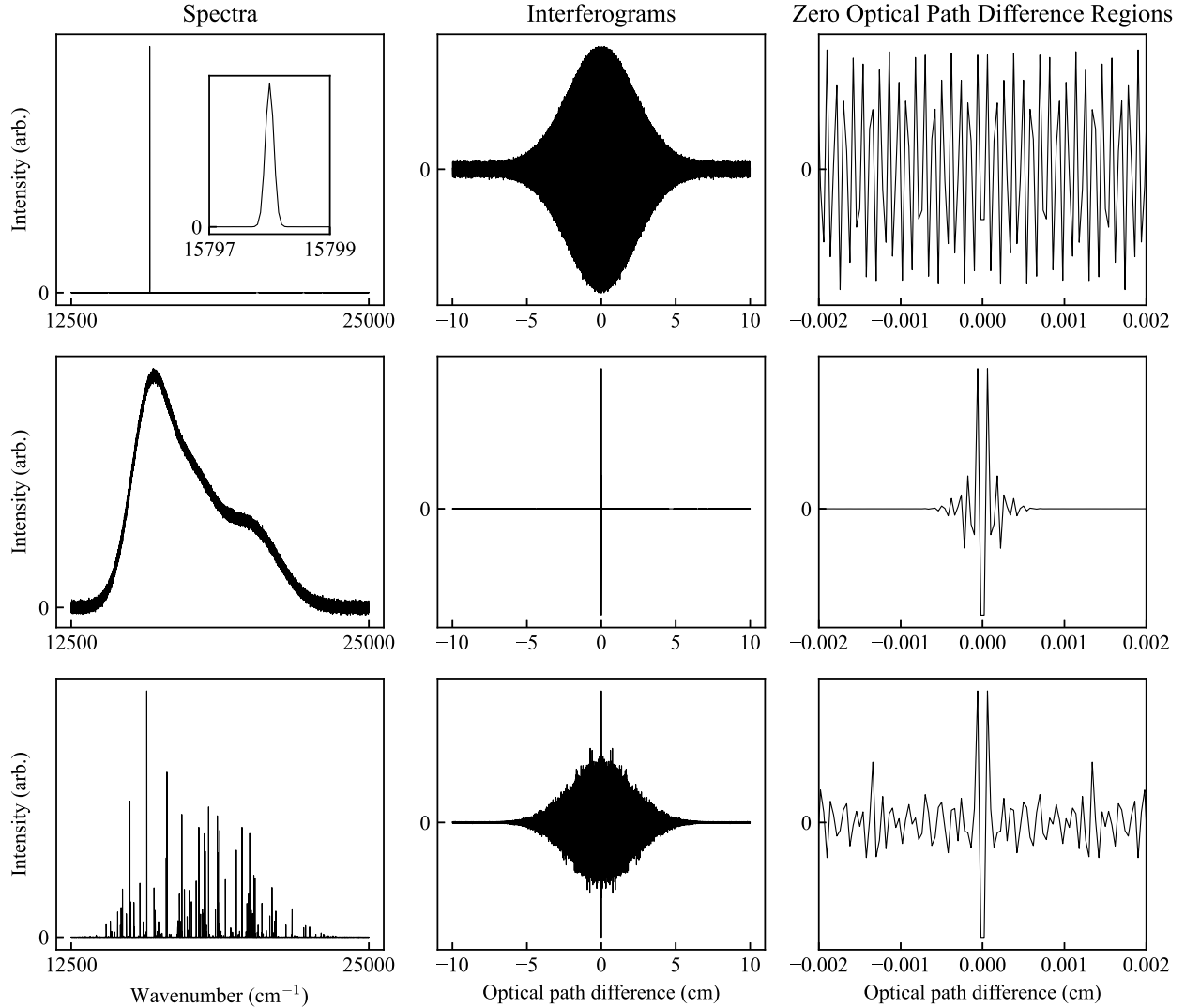


Figure 3.2: Comparisons between three types of spectra between 800 and 400 nm and their interferograms in the context of FT spectroscopy of complex atomic emission spectra: (top) spectrum of a single atomic transition emission line represented by a Voigt profile with a typical width produced in the light sources, approximately 0.15 cm^{-1} (4.5 GHz) in FWHM and a zoom is shown; (middle) spectrum of a continuum light source spanning the visible spectral range, similar to spectra observed for intensity calibration lamps such as a tungsten lamp; and (bottom) spectrum of 10^3 lines each with the typical width of the single line of the top spectrum. Interferograms in this figure are modelled to be undersampled at spatial intervals above the Nyquist (half-wavelength) interval, this is evident from the apparent modulation of the cosine waveform on the top right panel and the absence of a single highest interferogram intensity point at 0 cm. In practice, undersampling can be advantageous (see [subsection 3.3.2](#)).

3.3 Real Fourier Transform Spectrometer

There exist important differences between ideal and non-ideal (real) interferometers. Effects of asymmetric interferograms, finite sampling interval, finite mirror displacement, finite aperture size, and instrumental spectral intensity response will be discussed in this section, all of which are crucial considerations when designing and operating an FT spectrometer.

3.3.1 Interferogram Asymmetry and Phase Correction

Many factors affect the position of the zero optical path difference for each wavenumber and affect the symmetry of the interferogram about $x = 0$. For example, detection systems will have wavenumber-dependent time delays, the stationary and moving mirrors cannot be aligned to be exactly equidistant from the beamsplitter, the moving mirror cannot precisely start and end at equal optical path differences about $x = 0$, real light sources will have variations in intensity, the beamsplitter thickness cannot be precisely equal for the two paths taken through the beamsplitter, and the optical components will induce wavenumber-dependent phase shifts when the beams are reflected from or transmitted through them. Phase shifts from instrumental limitations are referred to as phase errors and must be corrected.

Due to the inevitable asymmetry in the interferogram $I(x)$, the spectrum $B(\sigma)$ need to be recovered using the FT of $I(x)$, transforming the even and odd parts of $I(x)$ about $x = 0$,

$$B(\sigma) = \int_{-\infty}^{\infty} I(x)e^{-i2\pi\sigma x}dx = \int_{-\infty}^{\infty} I(x)[\cos(2\pi\sigma x) - i\sin(2\pi\sigma x)]dx. \quad (3.6)$$

The goal is to observe the real spectrum without instrumental wavenumber-dependent phase errors $\phi(\sigma)$ of the zero optical path difference position for each σ in the interferogram. This is achieved through a procedure known as phase correction, where $\phi(\sigma)$ is determined using the resulting complex spectrum of the transform as

$$\phi(\sigma) = \arctan\left(\frac{\text{Im}[B(\sigma)]}{\text{Re}[B(\sigma)]}\right), \quad (3.7)$$

and the real spectrum of the light source is then given by the quantity $e^{-i\phi(\sigma)}B(\sigma)$. There are advantages of applying phase correction to the complex spectrum compared to taking the

absolute value of the complex spectrum $|B(\sigma)|$. For example, phase correction provides clear distinctions between positive and negative spectral features (instrumental effects typically cause negative features, e.g. see [subsection 3.3.3](#) and [subsection 3.4.2](#)), and the noise in the absolute value spectrum is $\sqrt{2}$ higher than the phase-corrected spectrum. The reason for the latter is that taking the absolute value combines the noise in both the real and imaginary spectrum, whereas in phase correction the phase information is obtained from spectrum signals significantly above the noise level.

For atomic emission spectra the phase curve $\phi(\sigma)$ is obtained by fitting a smooth curve (e.g. polynomial) through its sampled values at all spectral lines above a certain SNR threshold, usually around 10. For continuum spectra, the curve can also be obtained from regions with significant SNR. The phase curve $\phi(\sigma)$ is a slowly varying function of wavenumber, which would be factored into requirements for the optics when designing an FT spectrometer, e.g., there should be no significant absorption features in the wavelength range of interest. Since phase is defined using zero optical path difference position, this position must be found in a measured interferogram and specified. Although this position cannot be specified exactly, ideally it should be as close as possible. This is because the imaginary spectrum becomes larger with more asymmetry; an increase in the useful information within the imaginary spectrum would require a more accurate phase curve $\phi(\sigma)$. In other words, specifying zero optical path difference position far from the true value would directly increase the influence of uncertainties of the phase curve $\phi(\sigma)$ on the phase-corrected real spectrum [\[119–121\]](#). In practice, the zero optical path difference position is chosen as the sampled position which gives the flattest phase curve $\phi(\sigma)$, since the gradient of this curve increases with increased offset of the zero optical path difference for each wavenumber. An example will be shown in a later chapter during the phase correction of a spectrum of the present work ([Figure 5.7](#)).

As discussed above, the increase in the amount of asymmetry in an interferogram increases the requirement for the accuracy of the determined phase curve $\phi(\sigma)$. For this reason, interferograms are measured to be double-sided (equal distance from $x = 0$), and therefore as symmetric as possible in the FT spectroscopy of atomic spectra to provide the highest accuracy in phase correction and atomic transition wavenumbers. Furthermore, slowly varying intensities of light sources, such as a linear drift in intensity as the interferogram is recorded, will be an odd function about $x = 0$ for the double-sided interferogram and be averaged out in the real part

of the FT spectrum [117, 119].

3.3.2 Spectral Range and Digital Interferogram Sampling

In FT spectroscopy digital samples of $I(x)$ are acquired as integrated intensity samples at discrete optical path differences as the mirror moves. Therefore, discrete FT (the FFT algorithm) and the Nyquist theorem apply. The Nyquist theorem states that the minimum wavelength $\lambda_{\min}$ observable from an optical path difference sampling interval of Δx is $2\Delta x$. Therefore, the maximum observable wavenumber $\sigma_{\max} = 1/\lambda_{\min}$ for a given sampling interval Δx is

$$\sigma_{\max} = \frac{1}{2\Delta x}. \quad (3.8)$$

Generally, the optical path difference spanned by three consecutive interferogram samples, $2\Delta x$, is slightly less than $\lambda_{\min}$ to avoid coincidental sampling at zero interference amplitude positions.

Intensities can be sampled at intervals where $\sigma_{\max}$ is smaller than the highest observable wavenumber of the spectrum. This is referred to as undersampling and complications often arise. To illustrate these, one can consider the discretely sampled interferogram $I_s(x)$ to be a multiplication between the continuous interferogram $I(x)$ and a Dirac delta comb function with period Δx

$$I_s(x) = I(x) \cdot \left[\Delta x \sum_{n=-\infty}^{\infty} \delta(x - n\Delta x) \right]. \quad (3.9)$$

By the convolution theorem, the spectrum $B_s(\sigma)$ from the FT of $I_s(x)$ would be a convolution between $B(\sigma)$ and the FT of the comb function, which is

$$B_s(\sigma) = B(\sigma) * \left[\frac{1}{\Delta x} \sum_{n=-\infty}^{\infty} \delta\left(\sigma - \frac{n}{\Delta x}\right) \right], \quad (3.10)$$

that is, the spectrum $B(\sigma)$ including its reflection about $\sigma = 0$ is repeated infinitely with period $1/\Delta x$. A comparison between $B(\sigma)$ and $B_s(\sigma)$ is illustrated in Figure 3.3, where $\sigma_{\max}$ is slightly larger than the highest wavenumber of the spectrum. If $\sigma_{\max}$ is much larger than the highest observable wavenumber of the spectrum $B(\sigma)$, the gaps between the repetitions of $B(\sigma)$ would be much larger, but the shape and absolute wavenumber of the spectrum of interest (between 0 and $\sigma_{\max}$), would be unaffected. However, if $\sigma_{\max}$ is smaller than the highest wavenumber

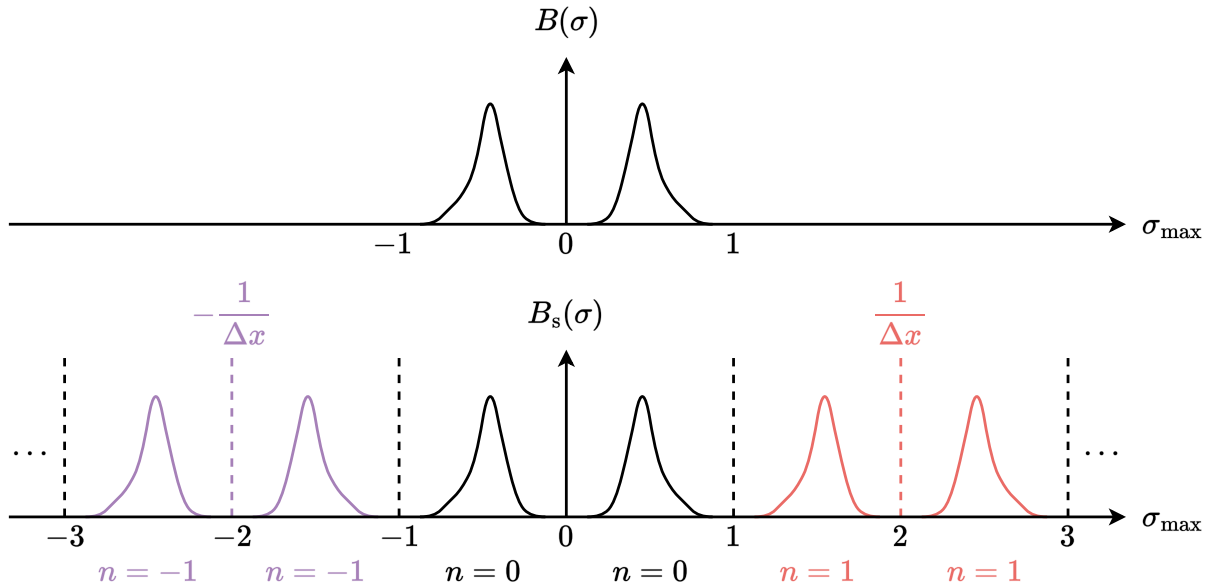


Figure 3.3: Comparison between the spectra of continuously and discretely sampled interferogram, where the $\sigma_{\max}$ of the sampling interval Δx is larger than the highest wavenumber of the real spectrum.

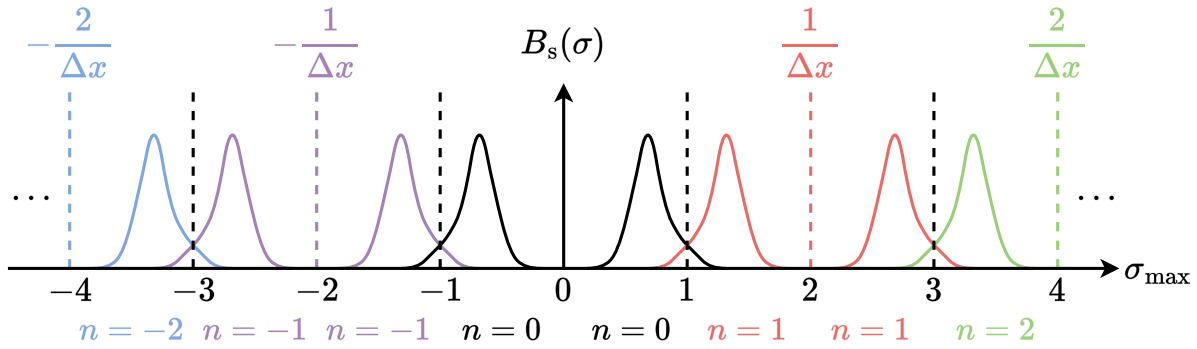


Figure 3.4: Spectrum of an undersampled interferogram, where the $\sigma_{\max}$ of the sampling interval Δx is smaller than the highest wavenumber in the real spectrum.

of $B(\sigma)$, i.e., if the spectrum is undersampled, overlaps between the repeated spectra will occur, this is illustrated in Figure 3.4. This situation must be avoided in order to obtain the true spectrum of the light source, as the overlapping components add and are at incorrect wavenumbers.

Undersampling is in fact common practice, this is because the lower number of intensity samples from using a larger Δx induce less noise in the spectrum (see section 3.4), when no more useful information is obtained from sampling denser points [119]. To avoid overlaps, the real spectrum must lie within the spectral range spanned between $m\sigma_{\max}$ and $(m+1)\sigma_{\max}$ for integer m , in which case Δx can be up to $m+1$ times larger than the Nyquist interval set by the highest

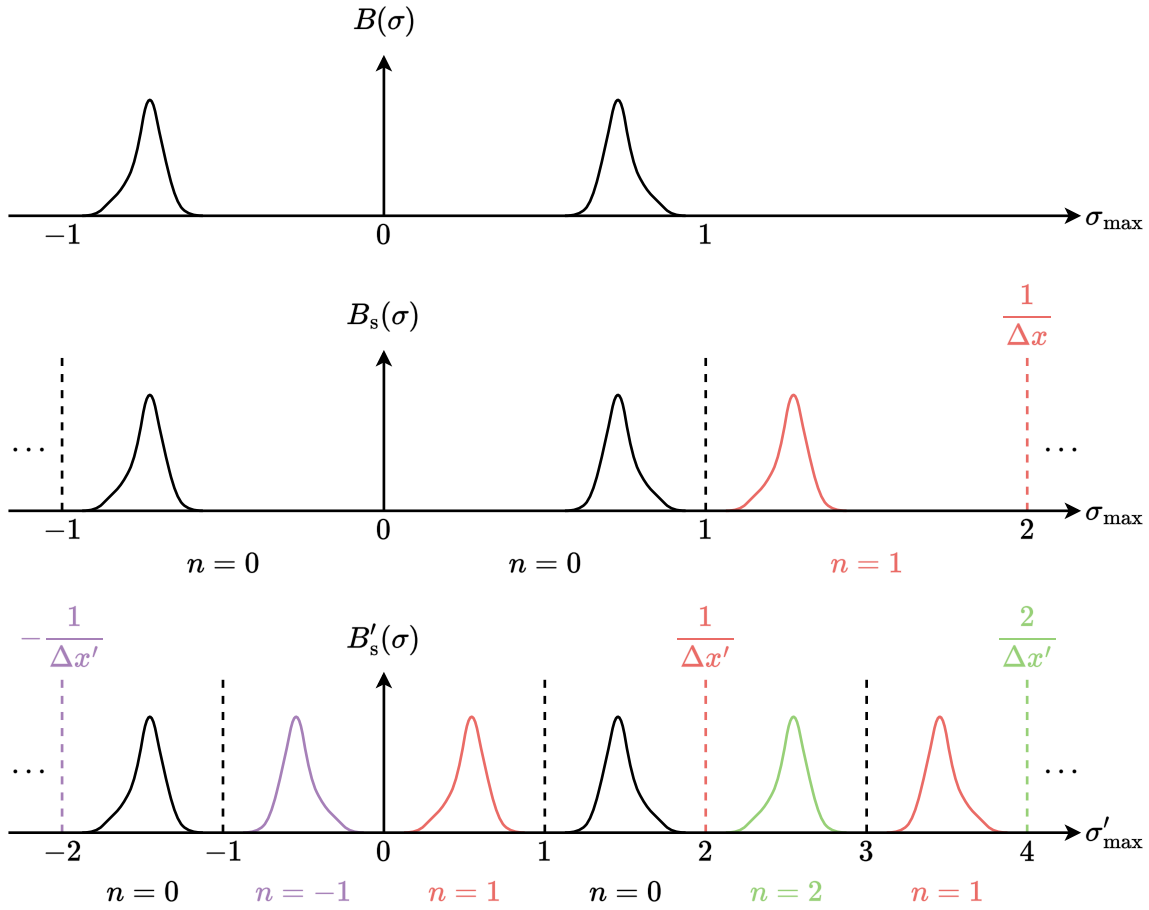


Figure 3.5: Spectra from (top) continuous interferogram, (middle) sampling at the Δx Nyquist interval set by the highest wavenumber in the real spectrum, and (bottom) sampling at the half of the Δx Nyquist interval set by the highest wavenumber in the real spectrum.

wavenumber in the spectrum. Figure 3.5 illustrates a scenario where $m = 0$ in the middle plot and $m = 1$ in the bottom plot, where $\Delta x' = 2\Delta x$ and $2\sigma'_{\max} = \sigma_{\max}$. The integer $m + 1$ is referred to as the order of the alias. All except one spectrum measured in the present work (Table 4.5 and Table 4.6) were measured in the second alias, with the exception being a VUV spectrum (51 000 to 68 000 cm^{-1}) measured in the fourth alias with spectral range 17 000 cm^{-1} .

3.3.3 Spectral Resolution and the Instrumental Profile

The discussion so far has assumed infinite mirror displacement, as was shown in the limits of summations and integrals, which is not possible for a real FT spectrometer. If the maximum optical path difference is L on both sides of the zero optical path difference position, the interferogram is effectively multiplied, or apodised, by a box function of height unity and width $2L$ centered around the zero optical path difference position. Using Equation 3.6 and the

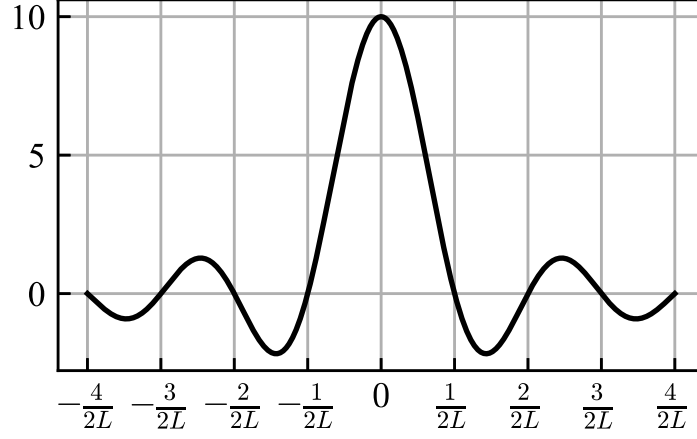


Figure 3.6: Sinc function convolved with the spectrum due to maximum finite optical path difference L .

convolution theorem, the spectrum is therefore convolved with the normalised sinc function of wavenumber,

$$\frac{\sin(2\pi\sigma L)}{\pi\sigma} = 2L \operatorname{sinc}(2\pi\sigma L), \quad (3.11)$$

which is the FT of the unit height box function of width $2L$ centred around $x = 0$. The sinc function is shown in Figure 3.6 and first reaches zero at $\sigma = \pm 1/(2L)$, which is the measure of spectral resolution. Normalisation of the discrete FT relationship between $I_s(x)$ and $B_s(\sigma)$, together with the relationship between the total optical path difference $2L$ and sampling interval Δx ($2L = N\Delta x$ for N samples), define that $1/(2L)$ is the wavenumber separation between consecutive points $\Delta\sigma$ in the discrete spectrum $B_s(\sigma)$.

The sinc function from finite optical path difference is a part of the instrumental spectral profile that is convolved with the spectrum. For example, when the spectral line width of each atomic transition is much narrower than the sinc function instrumental profile, all observed spectral lines will have the sinc profile. This potential instrumental broadening is not ideal as the width of observed lines determines the accuracy of the measured transition wavenumbers. Furthermore, the sinc function has oscillations about zero, decaying with $1/\sigma$, usually referred to as instrumental ringing. The ringing can distort spectral lines in close enough proximity and is particularly troublesome when the high-intensity lines possess ringing significantly above the noise level for an extended region of the spectrum, masking weaker lines. An example of a small amount of ringing can be seen in Figure 8.3 from the analysis of Co II HFS discussed in Chapter 8.

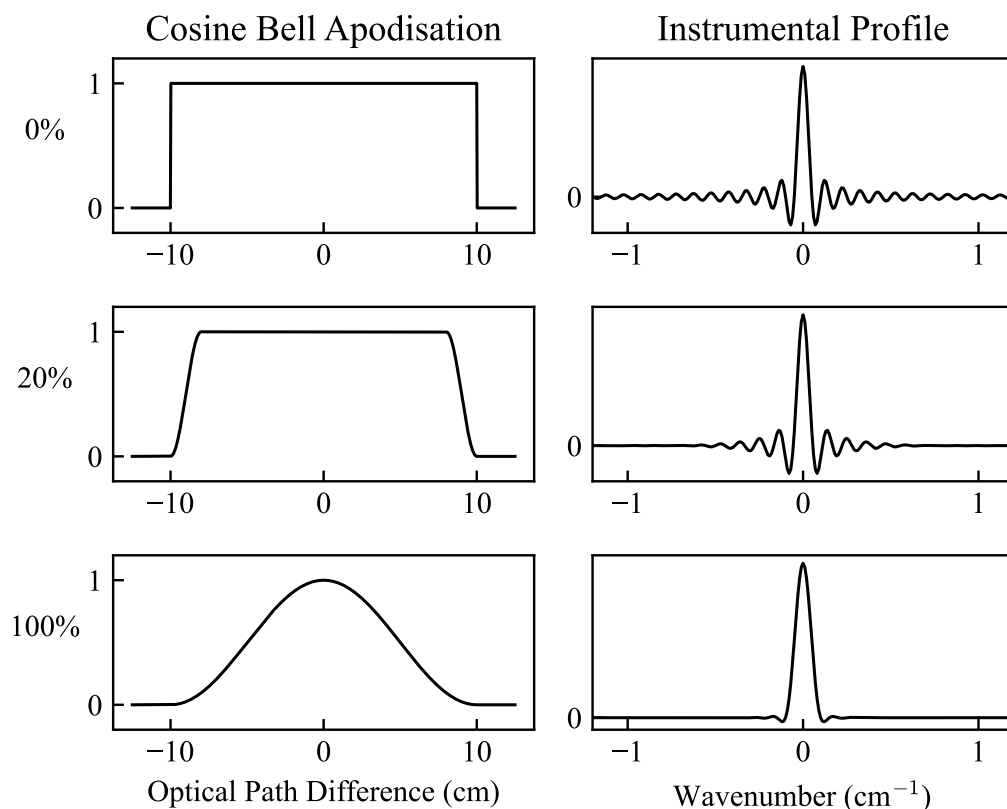


Figure 3.7: Unit height box function with width 20 cm and various cosine bell apodisations (left) and corresponding instrumental profiles (right). Each percentage (row) is the percentage of the number of points within each end of the interferogram to be apodised with the cosine bell, where 0% means the ideal interferogram is apodised only by the box function of the finite optical path difference, and 100% implies the ideal interferogram is apodised by a full cosine bell instead.

When designing an FT spectrometer, the resolution and the maximum optical path difference are chosen such that the width of the sinc function is much smaller than the widths of spectral lines from the light sources of interest. In the interferogram domain, this corresponds to a box function width that is much larger than the width of the interferograms of interest, i.e., the moving mirror can traverse to optical path differences where interference is no longer observed. If the width of the sinc function is comparable to the width of the spectral lines, the observed lines will be broadened and distorted so wavenumber measurements will be less accurate. However, this can be alleviated by considering the convolution with the sinc function in the spectral line fitting, and by bringing down the interferogram edges more slowly to reduce ringing, using another apodising function such as the bell of a cosine as opposed to the sudden discontinuity of the box function [119, 122]. Examples of additional cosine bell apodisation and reduced instrumental ringing are shown in Figure 3.7. As seen from the figure, increased cosine

bell apodisation width increases the width of the instrumental function, the trade-off to reduce ringing is therefore reducing the spectral resolution. This increased width of the instrumental profile may also become non-negligible compared to the spectral line widths of the lamp, which may invalidate the assumption of Voigt profiles for spectral line fitting. In the present work, a small percentage of points within both ends of the interferograms were always apodised using cosine bells. This is because the spectral range of instrumental ringing without cosine bell apodisation (0% in [Figure 3.7](#)) is significantly wider than slight cosine bell apodisation (e.g. at most 20%), which induced only a small loss of spectral resolution but separated many weak lines in the vicinity of strong lines from ringing distortion.

In the interest of maximising SNR, it is not always beneficial to maximise the resolution of a measurement. For example, the interferograms in the top and bottom rows of [Figure 3.2](#) contain only noise at optical path differences beyond 7.5 cm, this data will only add noise to the spectrum and the resolution is more than enough to resolve spectral line profiles ([subsection 2.5.3](#)) of the light source. For this reason, a compromise must be reached between SNRs and resolutions of FT spectra for the accuracy of measured transition wavenumbers, the resolution is generally chosen such that the FWHM of the atomic spectral lines contain three or four statistically independent samples separated by $\Delta\sigma$ [119], typically $\Delta\sigma \sim 0.05 \text{ cm}^{-1}$ (150 MHz) for the light sources used in this thesis. Even more unnecessary data points are in the interferogram of the continuum spectrum of [Figure 3.2](#) (middle row). The continuum light sources are used for purposes of intensity calibration as standard lamps, the resolution of a measurement of continuum light sources is chosen to be higher than or to match resolutions of the calibration certificates of the continuum intensity.

3.3.4 Aperture Size and the Instrumental Profile

In addition to the finite optical path difference, the finite input aperture size is another major contributing factor to the instrumental profile. The entrance input aperture ideally needs to be as big as possible to increase throughput and SNR, however, this is not always beneficial when high resolution is sought.

In an FT spectrometer, input light from the aperture is collimated, it is passed through the interferometer and then focused onto the detector. For an extended light source at the size of

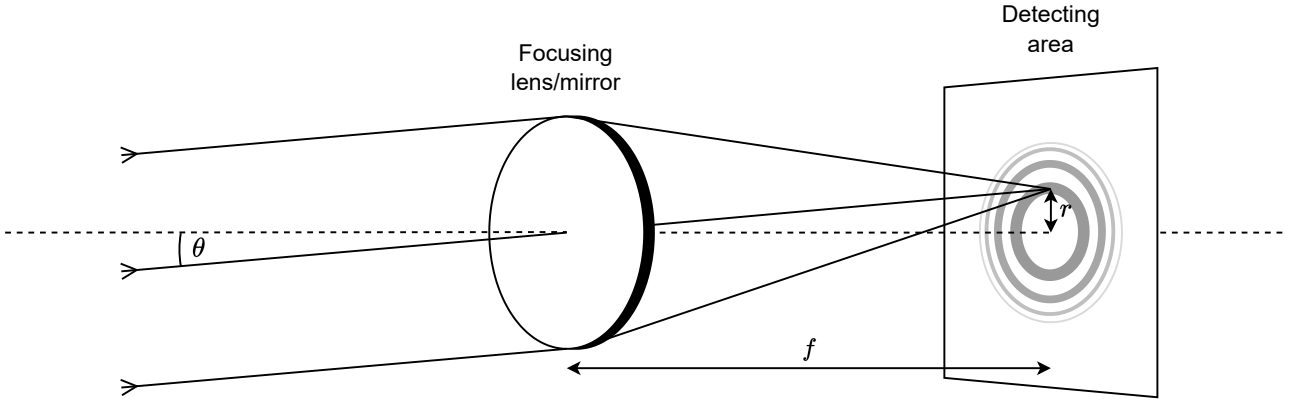


Figure 3.8: Diagram illustrating the image produced by a circular aperture at the focal plane of the focusing lens or mirror with focal length f . In this case, the alignment is ideal with uniform illumination of the aperture, photons of the entire bull's eye pattern is also measured by the detector's detecting area. The intensity contribution of the off-axis beam at θ is shown at radius r from the centre of the bull's eye pattern. Neighbouring rings show consecutive orders of interference. Figure adapted from [119].

the aperture, the set-up results in collimated beams with a range of off-angle axes, each with an angle θ relative to the on-axis beam and with optical path difference $x \cos \theta$, where θ is within the solid angle subtended by the aperture as viewed from the centre of the collimating mirror [117]. In typical set-ups, a collimating mirror is used and a focusing mirror focuses all collimated beams onto the detector's detecting area for maximum throughput. The situation is illustrated in Figure 3.8. Therefore, the contribution to the measured interferogram from a monochromatic source ($\sigma = \sigma_0$) with unit amplitude from an infinitesimal solid angle of the circular aperture $d\Omega$ at θ is

$$dI(x) = \cos(2\pi\sigma_0 x \cos \theta) d\Omega. \quad (3.12)$$

Using cylindrical symmetry and small angle approximation,

$$d\Omega = 2\pi \sin \theta d\theta \approx 2\pi \theta d\theta, \quad (3.13)$$

where

$$\Omega = \int_0^\theta 2\pi \theta' d\theta' = \pi \theta^2 \quad (3.14)$$

and

$$\cos \theta = 1 - \frac{\theta^2}{2} = 1 - \frac{\Omega}{2\pi}. \quad (3.15)$$

So the interferogram $I(x)$ is then

$$\int_0^{\Omega_{\max}} \cos\left(2\pi\sigma_0x\left(1 - \frac{\Omega}{2\pi}\right)\right) d\Omega = \Omega_{\max} \text{sinc}\left(\frac{\sigma_0x\Omega_{\max}}{2}\right) \cos\left(2\pi\sigma_0x\left(1 - \frac{\Omega_{\max}}{4\pi}\right)\right), \quad (3.16)$$

integrated to the solid angle subtended by the aperture $\Omega_{\max}$ viewed from the centre of the on-axis collimating mirror [117]. Evaluation of the integral is found in Appendix 1 of [123].

Compared to the ideal monochromatic interferogram, $I(x) = \cos(2\pi\sigma_0x)$, two effects are introduced by the circular aperture in Equation 3.16. Firstly, a linear scaling factor independent of wavenumber is applied to the x axis of the interferogram and the σ axis of the spectrum, this is significant and addressed through wavenumber calibration (see section 5.4). Secondly, the monochromatic interferogram is multiplied by a sinc function. This implies that on top of the box function interferogram apodisation from the finite optical path difference, the interferogram is additionally apodised by a sinc function; the total instrumental line profile is a convolution between a sinc function from finite optical path difference and a box function from finite aperture diameter. The width of the box function of this instrumental profile depends on the size of the aperture, where a larger $\Omega_{\max}$ corresponds to a wider box function. Therefore, source spectral lines are broadened with increasing aperture size and the ability to resolve them is limited by the aperture size.

The sinc function in the interferogram domain due to finite aperture reaches zero when

$$\frac{\sigma_0x\Omega_{\max}}{2\pi} > 1, \quad (3.17)$$

so sampling interferograms at the optical path differences beyond the point where the sinc function has reached zero reduces signal and increases noise. The highest observable wavenumber $\sigma_0 = \sigma_{\max}$ will exceed this limit first at the longest optical path difference $x = L$. These two quantities are used in the above inequality to estimate the suitable $\Omega_{\max}$ under the maximum resolving power, $R_{\max} = \sigma_{\max}/\Delta\sigma = 2L\sigma_{\max}$, required during a measurement. Generally, the arguments of the sinc function are chosen such that its amplitude at L is the maximum [119], where the argument of the sine function is $\pi/2$, i.e.,

$$\frac{\sigma_{\max}L\Omega_{\max}}{2\pi} = \frac{R_{\max}\Omega_{\max}}{4\pi} = \frac{1}{2}. \quad (3.18)$$

The $1/2$ has a physical meaning and explains why the signal is reduced when sampling beyond where the sinc function has reached zero. One can consider that for [Figure 3.8](#), $\theta \approx r/f$, the optical path difference between the on-axis and the off-axis beams of wavenumber $\sigma_{\max}$ is

$$x - x \cos \theta \approx x - x \left(1 - \frac{r^2}{2f^2} \right) = \frac{xr^2}{2f^2} = \frac{m}{\sigma_{\max}}, \quad (3.19)$$

where this difference is an m number of wavelengths for m number of fringes contained within r . Since the optical path difference scales with r^2 , the fringes become thinner and denser as r increases, as illustrated on [Figure 3.8](#). From [Equation 3.14](#) and [Equation 3.19](#),

$$\Omega_{\max} = \pi \theta_{\max}^2 = \frac{\pi r_{\max}^2}{f^2} = \frac{2\pi m}{L\sigma_{\max}} = \frac{4\pi m}{R_{\max}}, \quad (3.20)$$

or

$$\frac{R_{\max}\Omega_{\max}}{4\pi} = m. \quad (3.21)$$

Therefore, maximising the sinc function amplitude at $\sigma_{\max}$ and L is equivalent to limiting the maximum number of fringes of $\sigma_{\max}$ observed within the detector area to be $1/2$. For the case in [Figure 3.8](#), $m = 4$ and the detector would sample multiple bright and dark fringes at once, decreasing signal for a particular fringe of interest, to avoid this, one would need to reduce the size of the aperture, the maximum optical path difference, or the photon collecting area to reduce m .

[Equation 3.20](#) can be converted to the maximum aperture diameter formula generally used in FT spectroscopy, which is

$$d_{\max} = f \sqrt{\frac{8}{R_{\max}}}, \quad (3.22)$$

for a collimating mirror of focal length f . The apertures used in the experiments of the present work were always maximised using this formula. The maximum resolving power $R_{\max}$ does not need to be calculated using $\sigma_{\max}$ of the alias. Generally, the maximum observable wavenumber of the light source is selected to be significantly smaller than $\sigma_{\max}$ of the alias to avoid overlaps (e.g. [Figure 3.4](#)). Therefore, the maximum observable wavenumber of the spectrum can be used instead of using $\sigma_{\max}$ of the alias for a larger maximum aperture diameter $d_{\max}$.

The effects of misalignment of optical components are non-trivial mathematically. Qualitatively, one can consider the case where the centre of the bull's eye pattern of [Figure 3.8](#) is shifted away

from the optical axis, resulting in a reduced number of fringes on one side and an increased number of fringes on the other side of the bull's eye, since the image is cropped by the circular aperture. The additionally detected fringes effectively increase m and therefore reduce the achievable resolving power at a fixed aperture size. Furthermore, the asymmetry in the amount of photons detected per fringe would cause shifts in wavenumber. Non-uniform illumination of the aperture is yet another complexity, however, the apertures used in the present work are around 1 mm in diameter and were used for plasma discharges with diameters of around 10 mm, so the effects from non-uniform illumination were assumed negligible.

Misalignment and non-uniform illumination will contribute to the instrumental profile and make it very difficult to be fully defined. In the literature, unwanted artefacts in the spectrum are referred to as ghosts (e.g. [124]), and many of such ghosts can be due to the instrumental profile (two more examples in [subsection 3.4.2](#)). As discussed, the finite aperture and finite optical path difference are the main contributors to the instrumental profile in the context of high-resolution atomic emission FT spectroscopy. Consideration of these two effects was sufficient in the present work as the design and operation of the Imperial College VUV FT spectrometer produced no other significant or characterisable instrumental profile contributions.

3.3.5 Interferogram Modulation Efficiency

In the ideal interferogram of a monochromatic light source, the average intensity (the constant term in [Equation 3.2](#)) is equal to the interferogram amplitude. However, complete interference is prevented by a variety of instrumental limitations in practice, and the measure of the efficiency of interference is the modulation efficiency, defined as

$$\frac{I_{\max} - I_{\min}}{I_{\max} + I_{\min}}, \quad (3.23)$$

for the maximum and minimum intensity of the interferogram (most likely at the zero optical path difference position) $I_{\max}$ and $I_{\min}$, respectively. The modulation efficiency is 100% for the ideal interferogram. In practice, the measured SNR is proportional to this ratio and the ratio is affected by the reflection and transmission coefficients of the optical components interacting with the two beams, the ratio of the intensity of the split beams, flatness and parallelism of the component surfaces, and misalignment of the components, all preventing complete interference

[119]. Factors affecting the modulation efficiency are also wavelength-dependent. In the daily operation of the Imperial College VUV FT spectrometer, the modulation efficiency is maximized by re-aligning the stationary and moving mirrors using a Hg lamp in the UV region. Modulation efficiency was typically $\sim 54\%$. This created a reference for good optical alignment and could serve as a benchmark for possible indications of degradation of the optical components. The tolerance for imperfections of the optics is much tighter for measurements of UV and VUV wavelengths compared to the IR and visible wavelengths since the size of any imperfections need to be significantly smaller than the wavelengths of interest to produce interference at an acceptable modulation efficiency [125].

3.3.6 Photomultiplier Tubes and Spectral Intensity Response

Photomultiplier tubes (PMTs) are common detectors in high-resolution Fourier transform spectroscopy and were used in the present work. Small apertures are required for high spectral resolutions, so the amount of light throughput for high-resolution is very low, requiring highly sensitive detectors and PMTs were good candidates.

When a PMT absorbs photons, photo-electrons are ejected at the photocathode by the photo-electric effect at quantum efficiencies (ratio of emitted electrons to incident photons) dependent on photon energy. These ejected electrons are accelerated and focused onto a chain of dynodes which amplify the number of ejected electrons by many orders of magnitude to produce detectable currents. Since the ejected electron energy is negligible to the gain in electron energy during the initial acceleration, photocurrents produced by PMTs are dependent on photon energy only through the quantum efficiency dependence on energy. Therefore, the intensities of interferograms and their corresponding FT spectra are proportional to units of photon flux (s^{-1}).

In addition to the quantum efficiency, photons are lost through imperfect collimations, reflections, and transmissions when they interact with the optical components of the instrument as a whole, contributing to a spectral intensity response function as a function of wavenumber. The response function is the fraction of transmitted photons at a particular wavenumber and can be obtained using standard continuum lamps such as tungsten and deuterium lamps (see [section 5.5](#)). In designing an FT spectrometer for a particular wavenumber range, the variation

of the intensity response with respect to wavenumber is aimed to be smooth, which is to allow reliable intensity calibrations and phase corrections.

3.4 Sources of Noise and Error

Effects that induce phase errors, reduce signal, or increase noise have been parts of the discussions of [section 3.3](#). This section discusses more sources of noise and error that are crucial considerations in the high-resolution FT spectroscopy of atomic spectra.

3.4.1 Noise in Interferograms and Spectra

As briefly mentioned in [subsection 3.3.2](#) and [subsection 3.3.3](#), sampling interferogram points that do not contribute more information to the spectrum increases noise. With the assumption of white noise, the local $(SNR)_\sigma$ of the spectrum is related to the $(SNR)_x$ of the interferogram by [\[119\]](#)

$$(SNR)_\sigma = \sqrt{\frac{2}{N}} \cdot \frac{B(\sigma)}{\overline{B(\sigma)}} \cdot (SNR)_x, \quad (3.24)$$

where $(SNR)_x$ is defined as the SNR of the interferogram centre burst, N is the number of sampled points, and $\overline{B(\sigma)}$ is the mean signal strength of the spectrum. In addition to the $\sqrt{N}$ increase in the noise level, the mean signal strength is also proportional to the noise level. The three most significant sources of noise in the present work are photon noise, source noise, and digitising noise, and are together most significantly in the form of white noise.

The photon noise is fundamental to the detection of photons, where the mean number of photons n detected is the mean of a Poisson distribution. Given the large number of photons detected per integration period, the distribution is Gaussian by the central limit theorem, with a mean of n , a standard deviation of $\sqrt{n}$, and a SNR of $\sqrt{n}$. The photon noise is equal to the square root of the average interferogram intensity (neglecting other sources of noise) and is essentially constant over the optical path differences of the interferogram, because $\sqrt{n}$ changes very little with change in n for large n . The photon noise in the interferogram is, therefore, a form of white noise and remains as white noise in the FT spectrum, directly proportional to $\sqrt{n}$. To improve the photon noise limited SNR, $\sqrt{n}$, one would either increase the number of photons

detected within the spectral range of interest (a brighter light source) or reduce the spectral range, provided that the spectral lines of interest are still within the reduced spectral range. Limiting spectral range to improve SNR of relatively weaker lines of interest is an important consideration in practice, e.g., I aimed to maximise the SNR of all Nd III when recording Nd spectra ([Chapter 4](#)). Since the photon noise is fundamental, FT spectroscopy aims to produce spectrum noise limited by or comparable to the photon noise.

The source noise comes in two parts, additive or multiplicative [119]. Additive noise is due to random source intensity fluctuations occurring at the sampling frequency and directly raises the noise level of the spectrum. The size of the additive noise follows the inverse of the frequency, which is observable in the spectrum at wavenumbers close to $\sigma = 0$. The high sampling frequencies of modern FT spectrometers mean that additive noise is seldom significant, however, significant additive source noise was observed at the lowest pressures of a discharge source in the present work (see [subsection 4.5.2](#)). Multiplicative noise affects the interferogram modulation, i.e., fluctuations of source intensity between samples are correlated and not random, which may occur at the power line frequency. Modulation of the interferogram inevitably alters the instrumental profile, for this reason, multiplicative source noise is minimised using sufficiently stable light sources (see [Chapter 4](#)). Effects of multiplicative noise are further discussed in [subsection 3.4.2](#) and e.g. [124].

The digitising noise [119] arises from rounding error during analogue-to-digital conversion and is dependent on the converter. This noise is white noise and becomes more significant with more strong lines in a spectrum, and even more significant in continuum or absorption spectra.

Noise can be reduced through the process of co-adding interferograms, i.e., detecting more photons at the same optical path differences. In weak light sources, where photon noise is dominant, this can improve SNR by $\sqrt{N}$ for N co-adds. However, the Nd spectra observed in the visible region are very line-rich and the SNR improvement from co-adding was observed to be significantly below $\sqrt{N}$, indicating the significance of source or digitising noise in these spectral regions with many strong lines (see [subsection 5.2.1](#)).

Except for the negligible multiplicative source noise in the present work, all above mentioned sources of noise contributed to white noise in the spectrum. Therefore, the noise level of each spectrum was determined as a constant value independent of wavenumber, this can be seen from the figures of [section 5.2](#). Variations of the constant noise level with wavenumber were observed

within the visible regions of Nd spectra, but could not be characterised due to small significance and a large number of weak lines within the spectral regions hindering the determination of the noise level (see [subsection 5.2.4](#)).

3.4.2 Systematic Errors

Effects of systematic errors in the measured interferogram can be summarised by considering three additional parameters $\epsilon_{1,2,3}$ in the FT of a monochromatic double-sided interferogram of unit amplitude with maximum optical path difference L and wavenumber σ_0 [117],

$$B(\sigma) = \int_{-L}^L \left[(1 + \epsilon_1) \cos(2\pi\sigma_0(x + \epsilon_2)) + \epsilon_3 \right] e^{-i2\pi\sigma x} dx. \quad (3.25)$$

The parameters $\epsilon_{1,2,3}$ in their simplest forms are either random noise, constant offsets, or single spatial frequency oscillations as a function of x , all of which form a basis for any systematic variation in the interferogram.

Background Radiation

The most convenient of the three factors to analyse is ϵ_3 . If ϵ_3 is random, it would be additional white noise, which could come from the noise of background light sources that arrived at the detector without traversing through the interferometer, i.e. when ϵ_3 is a constant. For a constant ϵ_3 , the spectrum $B(\sigma)$ contains a non-zero value at $\sigma = 0$ and would not affect the spectrum of interest, but the background will contribute noise. If ϵ_3 is periodic, a spectral line will appear at its spatial frequency, which would cause unwanted spectral features. This could be periodic changes in the background radiation. In the present work, effects from the background are negligible as the laboratory lights were switched off during measurements and there was no significant light scattering.

However, there exists one significant background which is the frequency-stabilised He-Ne laser for calibration of the sampling system of the Imperial College VUV FT spectrometer (see [subsection 4.2.1](#)). It is observed despite taking a different path through the interferometer due to its scattered light, when the observing spectral region contains its wavelength 632.8 nm. The laser intensity was dampened through neutral density filters but its interferogram signal

was still significant and recorded simultaneously with the light source interferogram. Since the optical path of the laser is different from that of the light source (see [subsection 4.2.1](#)), the phase curve for correction of phase errors of the light source interferogram applied to the laser interferogram is incorrect, which rendered spectral regions a few hundred wavenumbers around the laser wavenumber unreliable (see 15800 cm^{-1} of [Figure G.1](#)). However, one strong Nd III resonance transition was still observable at 632.9 nm, 0.1 nm (20 cm^{-1}) away from the laser in this region at 400 SNR, despite laser ringing of around 100 SNR. The laser background was thus an almost negligible issue as only a small spectral region around 15798 cm^{-1} was unreliable.

Sampling Errors

The question is, what is the accuracy of the optical path difference measurement when the interferogram intensity is sampled during a scan? If ϵ_2 of [Equation 3.25](#) is a small value dependent on σ , it would be a part of phase errors and be treated using phase correction (see [subsection 3.3.1](#)). Random errors in optical path difference measurements are also part of ϵ_2 , these cause random errors in their corresponding intensity values and contribute to the white noise of the interferogram and spectrum.

However, if ϵ_2 changes periodically with x , significant changes to the instrumental function are at stake and ghosts would appear. Periodic changes in x measurement are generally caused by electrical fluctuations and mechanical vibrations. To see their effects on the spectrum, one can consider $\epsilon_2 = \epsilon_{21} \sin(2\pi\epsilon_{22}x)$ for

$$B(\sigma) = \int_{-L}^L \left[\cos(2\pi\sigma_0(x + \epsilon_{21} \sin(2\pi\epsilon_{22}x))) \right] e^{-i2\pi\sigma x} dx. \quad (3.26)$$

Assuming ϵ_{21} is small, the real part of this transform yields, after Taylor's expansion,

$$L \operatorname{sinc}(2\pi(\sigma - \sigma_0)) + L\pi\sigma_0\epsilon_{21} \operatorname{sinc}(2\pi(\sigma - (\sigma_0 + \epsilon_{22}))) - L\pi\sigma_0\epsilon_{21} \operatorname{sinc}(2\pi(\sigma - (\sigma_0 - \epsilon_{22}))), \quad (3.27)$$

for $\sigma > 0$ [117]. The expected sinc instrumental profile centered around σ_0 with finite optical path difference L is the first term, but it is followed by two of the same sinc profile at $\sigma_0 \pm \epsilon_{22}$ with a small fraction $\pi\sigma_0\epsilon_{21}$ of the amplitude, the one at $\sigma_0 - \epsilon_{22}$ is also upside down. This means that all spectral lines will contain two equidistant ghosts with the same line profile with the ghost at the lower wavenumber being inverted. If ϵ_2 is symmetric about $x = 0$, i.e., using

cosine instead of sine to describe ϵ_2 , the two ghosts are both positive and are in the imaginary spectrum instead.

For complex atomic spectra, periodic sampling errors would be detrimental as the ghosts and the lines will essentially be guaranteed to distort each other and induce unnecessary spectral lines and blending. In designing an FT spectrometer, dampening of mechanical and electrical oscillations is implemented. Furthermore, the sampling rate is high enough to sample above the typical frequency of these oscillations, enabling corrections to systematic errors in sampling x . This is the design approach used for the Imperial College VUV FT spectrometer used in the present work to minimise sampling errors (see [subsection 4.2.2](#) for more details).

Multiplicative Source Noise

The apodisation of the interferogram from finite optical path difference and finite aperture size can be described by a (approximately) wavenumber-independent but x -dependent ϵ_1 . Random ϵ_1 is also white noise, and a constant ϵ_1 implies either a higher or lower intensity of the detected photons or different detector gains. The variation in ϵ_1 as a function of x is of most interest, and reducing such variation in ϵ_1 to be negligible is another important requirement for FT spectroscopy since ϵ_1 is directly related to the stability of the intensity of the light source. To explain the importance of a stable light source, one can consider the periodic variation $\epsilon_1 = \epsilon_{11} \cos(2\pi\epsilon_{12}x)$ and its spectrum

$$B(\sigma) = \int_{-L}^L \left[(1 + \epsilon_{11} \cos(2\pi\epsilon_{12}x)) \cos(2\pi\sigma_0x) \right] e^{-i2\pi\sigma x} dx. \quad (3.28)$$

The real part of this transform yields, for $\sigma > 0$,

$$L \operatorname{sinc}(2\pi(\sigma - \sigma_0)) + L \frac{\epsilon_{11}}{2} \operatorname{sinc}(2\pi(\sigma - (\sigma_0 + \epsilon_{12}))) + L \frac{\epsilon_{11}}{2} \operatorname{sinc}(2\pi(\sigma - (\sigma_0 - \epsilon_{12}))). \quad (3.29)$$

As opposed to periodic sampling errors, both ghosts are positive in the real spectrum at $\pm\epsilon_{12}$ around the line with the same line profile, and if ϵ_1 was asymmetric about $x = 0$ the ghosts would appear in the imaginary spectrum with the higher wavenumber ghost negative. In the experiments of the present work, the light sources used were sufficiently stable such that no ghosts from light source intensity variations were observed.

In poorly designed FT spectrometers, the quality of alignment can also change as the mirror is moved, which inevitably reduces the modulation efficiency and would be a part of ϵ_1 . This was negligible in the Imperial College VUV FT spectrometer, which uses retroreflectors as mirrors to minimise sensitivity to alignment (see [subsection 4.2.1](#) for more information on the design of the instrument).

3.5 Why Choose Fourier Transform Spectroscopy?

Fabry-Pérot spectrometers and laser spectroscopic techniques provide higher resolutions compared to FT spectroscopy. Particularly, Doppler-free spectroscopy is capable of resolutions one order of magnitude higher than those of FT spectroscopy, because FT resolving powers are limited by the Doppler widths of the spectral lines [118]. However, these high-resolution methods have much smaller spectral ranges, which would be detrimental to a large-scale energy level analysis if a large fraction of the transitions, e.g., those for Nd III across IR and UV ([Figure 1.9](#)), are unobserved because they lie outside of the spectral range.

In the field of the analysis of atomic structure, (diffraction) grating spectroscopy is another widely used technique [126]. Compared to FT spectroscopy, grating spectroscopy has its advantages and disadvantages. For the primary goals of the present work, the disadvantages of using grating spectroscopy outweigh the advantages one would gain from using grating spectroscopy.

Grating spectroscopy is more effective in short wavelength ranges. Below ~ 200 nm, FT spectrometer VUV beamsplitters and mirrors are difficult to manufacture due to tight tolerances [125] (described in [subsection 3.3.5](#)) and to maintain due to absorption of higher energy photons, which hastens optical degradation. FT spectrometers of the type at Imperial College have not been constructed to measure wavelengths below ~ 135 nm¹, whereas grating spectrometers can measure tens of nanometres [118]. For Nd III, most of the strong lines interconnected to the ground level of Nd III are expected to be within the $12\,500\text{--}50\,000\text{ cm}^{-1}$ (200–800 nm) region (see [Figure 1.9](#)), within the spectral range limit of FT spectroscopy. Moreover, high-

¹There exists an FT spectrometer that does not use a beamsplitter, designed for absorption spectroscopy, and is capable of wavelengths shorter than 135 nm at a French synchrotron facility, e.g. [127, 128].

resolution FT spectrometers offer resolving powers generally one order of magnitude higher than those of high-resolution grating spectrometers, and FT spectra are free from overlapping diffraction orders. FT spectroscopy thus offers the advantage of higher resolution over almost the entire spectral range of interest.

Another advantage of grating spectroscopy is its ability to measure spectra of unstable discharges, often at much higher currents and containing relatively more ions in higher ionisation stages, which are also excited to higher-lying energy levels. As discussed in [subsection 3.4.2](#), a stable source is a requirement for FT spectroscopy. An HCL (see [subsection 4.4.1](#)) was able to produce a stable Nd plasma, and spectra of Nd III were recorded using an FT spectrometer [83]. Therefore, with the expectation of a stable source of Nd spectra being possible by using an HCL, the ideal choice was still FT spectroscopy for its higher resolving powers, lack of overlapping orders, and generally wider spectral range capability.

In practice, FT spectroscopy and grating spectroscopy are both employed to supplement each other. Aside from the shorter wavelength advantage of grating spectroscopy, many weaker transitions unobserved in the FT spectra of stable lamps are observable in grating spectra of unstable discharges with much higher currents and/or grating spectra with extended exposure durations. Observing weaker transitions can be invaluable information, and the term analysis of Nd III of this thesis contains many examples, where grating spectra of sliding vacuum sparks (VS) and Nd-rich stars supported the analysis using the measured FT spectra (see [Chapter 6](#) for details).

Chapter 4

Laboratory Measurements of Nd Spectra

4.1 Introduction

As discussed in [Chapter 1](#), Nd III atomic structure is experimentally largely unknown. Apart from five levels of the ground term, only 25 of the hundreds of possible energy levels of the $4f^35d$ configuration were previously identified. Therefore, the goal was to measure the emission spectra of Nd III under a variety of plasma conditions to maximise the number of Nd III transitions observed and to provide the best datasets for the subsequent energy level analysis. In this chapter, the light sources and instrumentation that were available for measuring Nd emission spectra at Imperial College will be described.

All laboratory spectra recorded during the present work were made using the Imperial College VUV FT spectrometer, and its design, set-up, and operation are discussed in [section 4.2](#) and [section 4.3](#). No modifications to the Imperial College VUV FT spectrometer were made during the present work, more details regarding the design of the Imperial College VUV FT spectrometer are available, e.g., [[68](#),[117](#)]. Design and detailed operation of the Nd light sources are discussed in [section 4.4](#), and the optimisation of light source running conditions for Nd III spectra is documented in [section 4.5](#). The sets of final spectra used for the Nd III energy level analysis are summarised in [section 4.6](#). Brief details of spectra used by collaborators are included in [section 4.7](#).

4.2 The Imperial College VUV Fourier Transform Spectrometer

Most of the strongest lines of Nd III are expected to be within the region $10\,000\text{--}60\,000\text{ cm}^{-1}$ (near IR to the VUV, see [Figure 1.9](#)), including the transitions to the ground term levels. Observing transitions to the ground term levels is crucial as the energies of all levels are determined relative to the ground level, i.e., level energies can only be determined using transitions to the ground level or transitions to/from levels that have transitions to the ground level, either directly or through transitions linking levels eventually to the ground level. Observing the strongest transitions between different configurations will provide the best information for the energy level analysis of Nd III, as they are the most likely transitions to be observed and observed with high accuracies. The spectral range of most transitions of interest coincides with the full spectral range of the Imperial College VUV FT spectrometer [\[68\]](#), which is also between the near IR to VUV.

The Imperial College VUV FT spectrometer has been extensively used to study atomic structures of the iron-group elements in the UV. The spectral resolution of the instrument is sufficient to resolve spectral lines of these elements in typical plasma light sources for FT spectroscopy. However, the relative atomic mass of the REEs is almost triple that of the iron-group elements. According to [Equation 2.37](#), the dominant Doppler line widths of REEs in the plasma sources are expected to be significantly narrower. Measurements are also required at IR-visible wavelengths, further reducing the Doppler line widths. The spectral resolution of the Imperial College VUV FT spectrometer was found to be sufficient for the light sources used to produce Nd spectra through my preliminary investigations. At the time, the maximum spectral resolution achievable by the spectrometer was 0.037 cm^{-1} (maximum optical path difference 13.5 cm), where typical FWHMs of the PDL (see [subsection 4.4.2](#)) Nd spectral lines used for the energy level analysis were between $0.1\text{--}0.25\text{ cm}^{-1}$ (see [Figure 6.5](#) for more details).

Parameters describing the Imperial College VUV FT spectrometer are listed in [Table 4.1](#).

Table 4.1: Parameters of the Imperial College VUV FT Spectrometer as of 2021.

Parameter	Imperial College VUV FT Spectrometer
Max. Optical Path Difference	13.5 cm
Min. Spectral Resolution	0.037 cm^{-1}
Max. Resolving Power	1.35×10^6 at 200 nm
Long Wavelength Limit	Observed at $\sim 11\,000 \text{ cm}^{-1}$ (910 nm)
Short Wavelength Limit	Expected at $\sim 71\,000 \text{ cm}^{-1}$ (140 nm)
Input Aperture Diameter	0.85-8 mm
Beamsplitter Material	MgF ₂
Tank Dimensions	$1.5 \times 0.25 \times 0.25 \text{ m}$

4.2.1 Design of the Imperial College VUV FT Spectrometer

A photograph of the exterior of the Imperial College VUV FT spectrometer is shown in [Figure 4.1](#). A schematic diagram of the optical components within the Imperial College VUV FTS is shown in [Figure 4.2](#). Not shown on the optical diagram is another output of $\sim 50\%$ of the input intensity composed of the transmission of the beam from C_1 through the top part of the beamsplitter and the reflection of the beam from C_2 at the top part of the beamsplitter. This second output is collected using the PMT housing on the left side of the tank on [Figure 4.1](#). The two outputs (each at half of the input intensity) are made possible by the retro-reflecting mirrors separating the optical paths between the incident and reflected beams. This offers advantages over the traditional Michelson interferometers ([Figure 3.1](#)) where half of the input intensity is reflected back onto the light source. For example, the total intensity can be measured to check for intensity variations, the SNR can be improved by recording essentially twice as many interferograms to reduce random noise, and two spectral regions could be recorded at the same time using different PMTs and optical filters, which is also useful for branching fraction measurements that require identical plasma conditions between different spectra [[117](#), [119](#)]. In the present work, interferogram measurements using only one detector at point P were sufficient for acquiring spectra for the Nd III energy level analysis as the Nd spectrum is very intense from the IR to the UV.

The slim and compact design of the main interferometer tank was partially motivated by

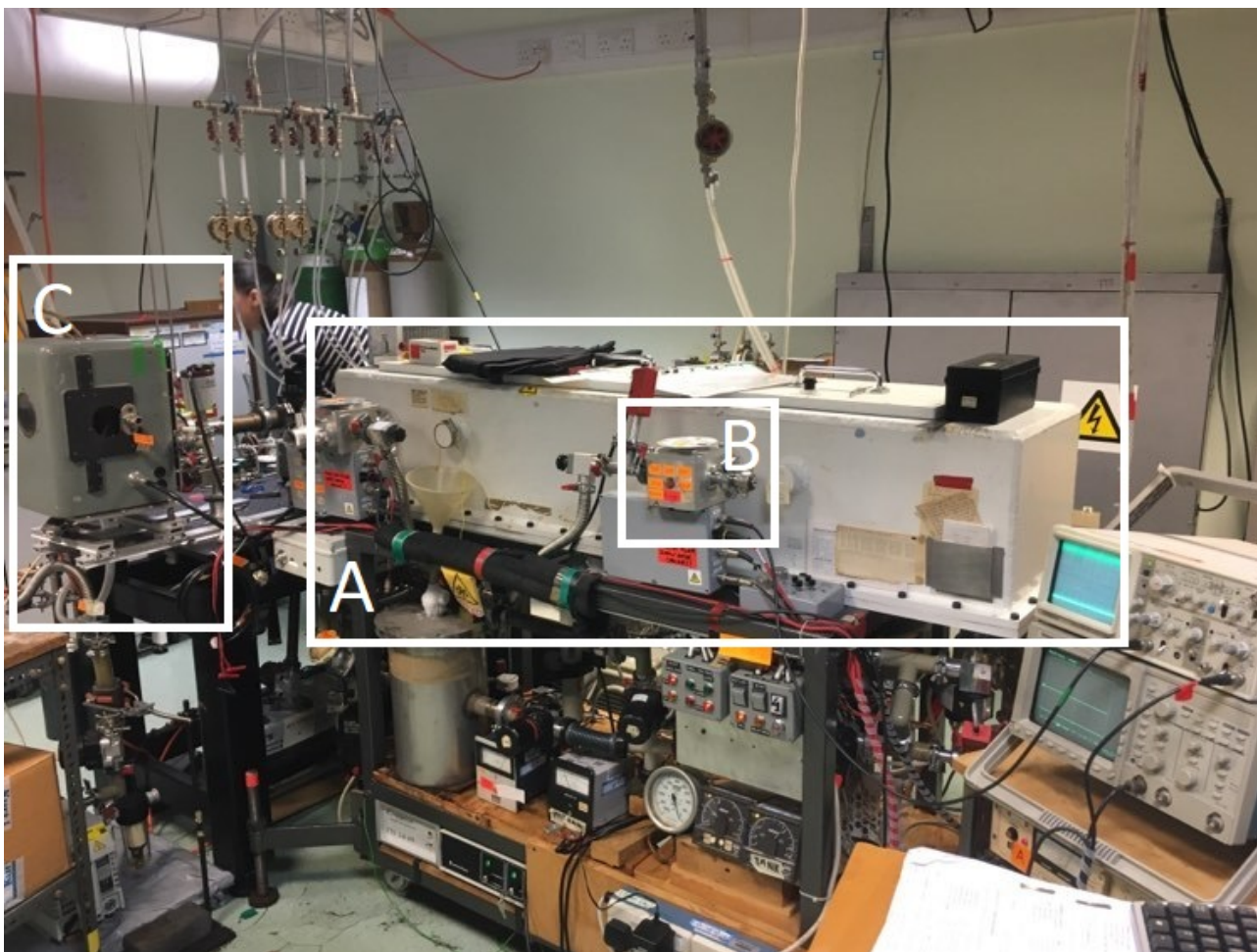


Figure 4.1: Exterior of the IC VUV FT spectrometer, showing A) main interferometer tank containing optical components kept under vacuum ($\sim 10^{-8}$ atmospheres), B) PMT and optical filter housing kept under vacuum for VUV measurements, and C) a glow discharge light source to be measured.

the ease of evacuation of air which also negates the use of more powerful pumps with more vibrations (more details on vacuum pumping in [section 4.3](#)). The long and compact design was also motivated by the use of shallow incident and reflection angles (5°) of the beams at the beamsplitter, as opposed to the 45° angle in the traditional Michelson interferometer ([Figure 3.1](#)). Using a larger area of the beamsplitter reduces the significance of unwanted polarisation or phase shift effects from imperfections in the beamsplitter. Complete interference of the recombining beams is prevented by imperfections in the optics, e.g., not perfectly flat or parallel. The tolerance for the size of such imperfections is limited by the wavelength of interest, this was one of the main challenges in designing the VUV FT spectrometer, as the longer wavelength IR or visible FT spectrometer tolerances are much easier to meet [\[125\]](#).

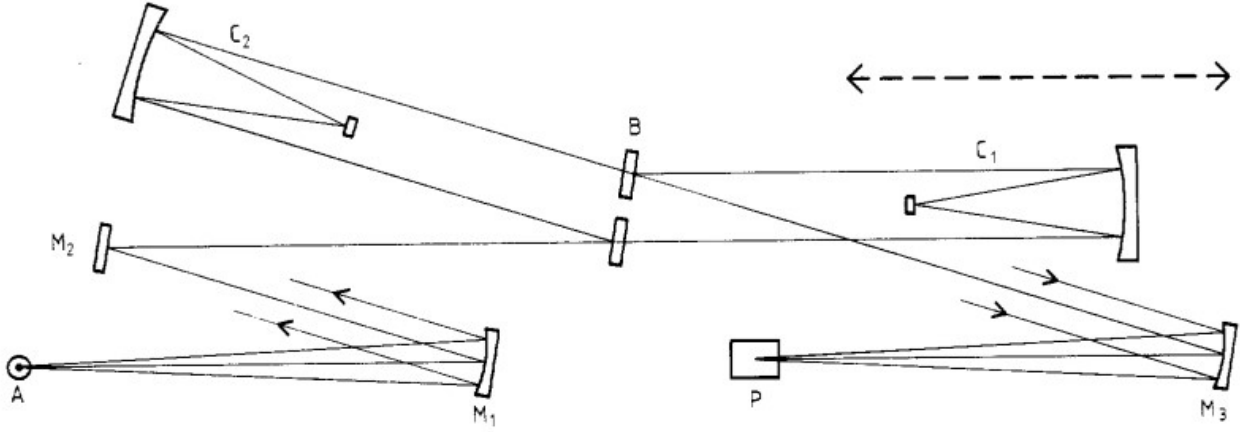


Figure 4.2: Schematic diagram of the optical components within the Imperial College VUV FT spectrometer [68], where A is the input aperture and P is the detector at the focal points of the collimating mirror M_1 and focusing mirror M_3 , respectively, M_2 is a folding mirror to direct the collimated beam towards the MgF_2 beamsplitter B , and $C_{1,2}$ are the moving and stationary catseye mirrors acting as retro-reflectors when paired with the smaller plane secondary mirrors at their focal points.

4.2.2 Interferogram Sampling System

As discussed in [Chapter 3](#), optical path difference measurements in the recording of interferograms set the wavenumber scale of FT spectra. In the Imperial College VUV FT spectrometer, relative optical path differences are determined by a frequency-stabilised He-Ne laser (632.8 nm at 4.5 mW, class IIIa) that enters through the bottom of the main interferometer tank and travels through the spectrometer in a path slightly different from the path taken by the light source. The beam positions on the beamsplitter and moving catseye mirror are shown in [Figure 4.3](#). The result of different optical paths between the laser and light source photons is a linear wavenumber scaling, which can be accounted for in spectra wavenumber calibration (see [section 5.4](#)). The laser interferogram is recorded separately using photodiode detectors and the monochromatic nature of the He-Ne laser causes its interferogram to be essentially a single cosine waveform, where the peak-to-peak distance corresponds to the optical path difference of one wavelength of the laser. This information is used to determine the precise optical path differences for successive samples of the interferogram of the light source of interest.

In performing the fast-Fourier transform of an interferogram, a constant optical path separation Δx between each intensity sample is imperative. Systematic variations in Δx due to electronic and mechanical imperfections can lead to ghosts in the resulting spectra (see [subsection 3.4.2](#)). Random noise in Δx corresponds to random noise in the interferogram signal, which leads

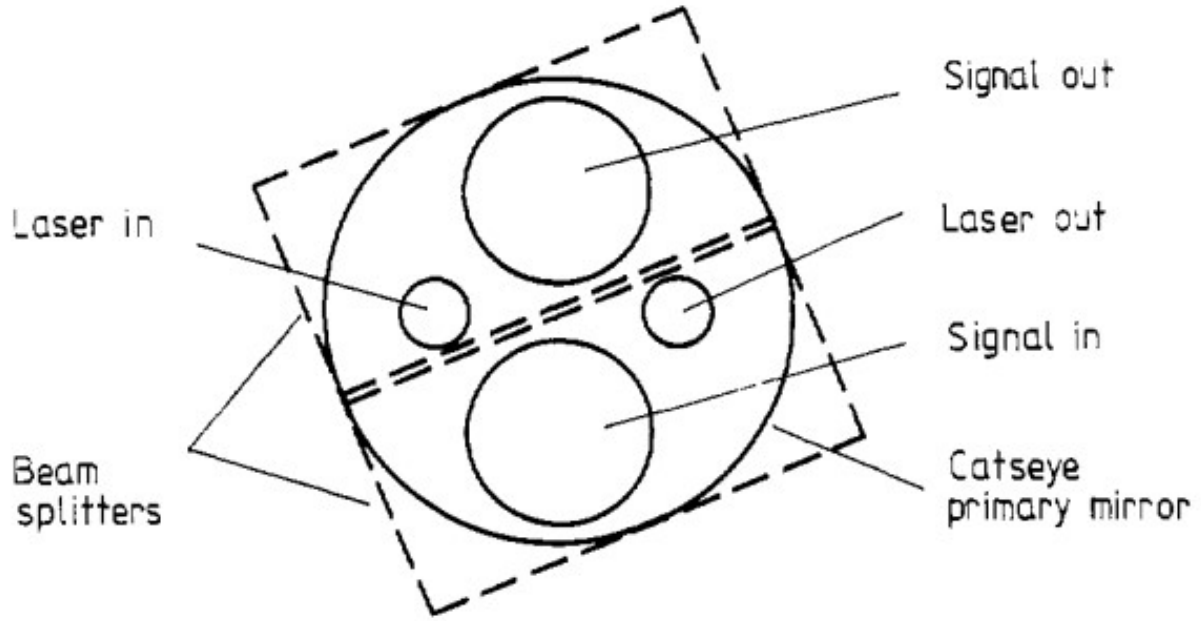


Figure 4.3: Beam positions of the He-Ne laser and the light source (signal in/out) on the beamsplitter and moving catseye mirror in the Imperial College VUV FT spectrometer [68]. The bottom half of the beamsplitter is the splitting component, the top half is the recombining component.

to white noise in the corresponding FT spectra. Sources of error in Δx measurement were minimised to satisfy the resolution and spectral range requirements for the investigation of complex atomic emission spectra using stable discharge light sources (e.g. see section 4.4). The sampling system used by the Imperial College VUV FT spectrometer was developed by Dr J. Brault [119, 129]. It uses the clock of an ADC to sync the timestamps of intensity measurements of the interferograms of the He-Ne laser and the light source, essentially placing the two interferograms onto the same time scale.

The clock of the ADC is 50 MHz, which can be used to gauge the uncertainty in Δx for a chosen mirror scan velocity. All interferograms were measured at a scan velocity of 2000 fringes/s, an optical path change of 2000 times the He-Ne laser wavelength per second. The sampling interval Δx at 50 MHz and 2000 laser fringes/s corresponds to $(2000 \times 632.8)/(50 \times 10^6) = 0.025$ nm and is more than three orders of magnitude lower than the Nyquist limit required to observe the shortest wavelength of the instrument, e.g., VUV limit $120/2 = 60$ nm. Therefore, under general observing conditions where the interferogram is required to be sampled at spatial frequencies comparable to the Nyquist limit, the relative uncertainty in Δx is of order 10^{-3} , which means SNRs of order 10^3 are achievable in the FT spectra.

The lower limit of the random noise in Δx is established by the 50 MHz ADC clock, but systematic variations in the scan velocity (and hence in Δx) require further treatment. For example, the power line frequency plus its first few harmonics and general mechanical resonance frequencies are in the 10^2 Hz range [129]. Such variations are measurable at the sampling rate of the ADC at $50 \text{ MHz} / 1024 = 50 \text{ kHz}$ (still below the VUV Nyquist limit at typical scan velocities), which is the rate at which the light source interferogram is sampled¹. For the He-Ne interferogram, a timestamp is made for every 632.8 nm change in the optical path and so the 2000 Hz fringe sampling rate can also measure systematic velocity variations in the 10^2 Hz range.

The exact optical path difference at which the intensities of the laser and light source interferograms were sampled can be obtained using the timestamps counting integer wavelengths of the laser interferogram. As discussed above, the velocity variations are slow compared to the sampling rates of the interferograms. Therefore, the laser fringe timestamps are interpolated for any conversion between time and optical path difference, i.e., the light source interferogram as a function of time can be converted to a function of optical path difference. Due to variations in velocity, the light source interferogram after conversion to the optical path difference axis does not possess a constant Δx , but this can be solved by interpolating the light source interferogram intensity samples at constant spatial intervals. Aside from achieving high accuracy in constant Δx (few parts in $\sim 10^{-3}$ of the laser wavelength) for fast-Fourier transform, this sampling method also allows the great advantage of the selection of any Δx based on the spectral region and alias of interest (see [subsection 3.3.2](#) for explanation).

4.3 Experimental Set-up and Operation

The experimental set-up for the Imperial College VUV FT spectrometer consists of the main interferometer tank, housings for the PMTs and optical filters, and light sources. A nose-piece component is used to select one of two light sources, consisting of a rotatable plane mirror and a lens at the half of the optical path between the source and the input aperture of the

¹The 1024 factor should be the decimation factor [130], where 1024 samples at the clock frequency are averaged at the 50 kHz sampling frequency to reduce noise.

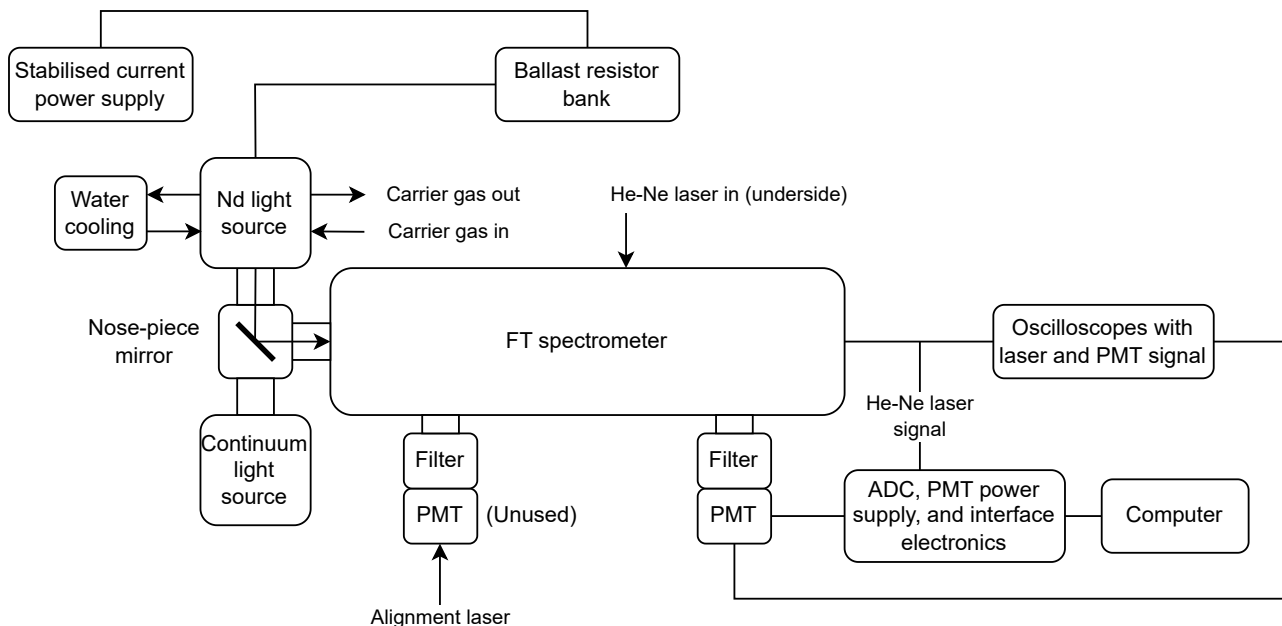


Figure 4.4: Diagram illustrating the experimental set-up and component arrangements for the FT spectroscopy of Nd emission spectra. Photographs of this set-up are in [Figure 4.1](#) and [Figure 4.13](#).

spectrometer to image the extended source at the aperture. The set-up and arrangement of components are illustrated in [Figure 4.4](#). This section describes the purpose and usage of the components shown on the diagram, details on the design and operation of the Nd discharge sources will be in [section 4.4](#).

4.3.1 Vacuum Pumping

To eliminate significant atmospheric absorption from molecular oxygen under 200 nm (above $50\,000\text{ cm}^{-1}$), the VUV FT spectrometer is kept under a vacuum of $\sim 3 \times 10^{-5}$ mbar when measuring spectra in the VUV. This is achieved through the use of a rotary and a diffusion pump (under the main interferometer tank) with a liquid nitrogen cold trap (metal cylinder next to the letter A in [Figure 4.1](#)), which condenses any vapour to aid the vacuum pumping and prevent contamination of the optical components. When measuring above 200 nm, absorption of radiation by air is much less significant, but pressure shifts (e.g. from vibrations) in the air could cause inhomogeneous refractive indices. For this reason, the tank was still evacuated, but only to ~ 0.05 mbar and without using the diffusion pump. The rotary pump was switched off during all measurements to avoid vibrations. The housing for the PMTs and filters, the nose-piece, and the connection to the light sources are also evacuated to $\sim 10^2$ mbar for VUV

measurements below 200 nm using the rotary pump outside of measurements and a sorption pump during measurements. The sorption pump does not produce vibrations and was sufficient for the small volume of vacuum required from the vacuum tubing, the nose-piece, and PMT housings. The optical path differences of the recombining beams occur in the vacuum within the main interferometer tank, therefore the measured wavenumbers are vacuum wavenumbers in all spectral regions. Any leaks could be easily detected if there was an anomalously large pressure that did not respond well to further pumping or any rapid pressure increases after switching off the rotary pump.

The Nd light sources (more details in [section 4.4](#)) were also vacuum pumped, this was achieved using a rotary pump for the HCL ([subsection 4.4.1](#)) and a turbomolecular pump for the PDL ([subsection 4.4.2](#)) to achieve a higher vacuum. Vacuums were required for these discharge lamps prior to filling them with low-pressure noble gases. Any leaks would lead to the production of complex molecular spectra and oxidation of the cathode material. Gas line connections up to the exits of the compressed gas cylinders were also pumped before flushing the lamps with pure noble gases. Between the rotary pump and the light sources, a liquid nitrogen cold trap was used to prevent any oil vapours from the rotary pump from reaching the lamp plasma. Any leaks could be detected following similar procedures taken for leak-testing the main interferometer tank, but the inability of the lamps to produce a stable discharge was an additional indicator of an air leak. For the lamp set-ups in the experiments of the present work, the HCL and PDL were pumped down to $\lesssim 10^{-3}$ mbar and $\lesssim 10^{-5}$ mbar respectively before flushing them with the noble gases, which took around an hour and longer if the lamps were previously disassembled. These pressure readings were taken using gauges attached to the lamp exits, as close to the plasma as possible.

4.3.2 Light Source Set-up

Light sources for FT spectroscopy are required to produce stable intensities throughout the interferogram scan duration, and any oscillations and random fluctuations in source intensity would cause ghosts and noise in the spectrum, respectively (see [section 3.4](#)). This stability is achieved through supplying the HCL and PDL with a stable direct current, paired with a set of ballast resistors. The ballast resistors are large and air-cooled, this was to achieve stable electrical resistance and hence stable lamp currents. In the case of lamp instabilities, e.g., arcs

between the anode and cathodes, shortages are also prevented by the ballast resistors.

The HCL and PDL are water-cooled and produce plasmas of a few 10^3 K, similar to the melting point of many metals. Watercooling of the cathodes reduces the Doppler widths, prevents low-melting point metals from melting, and prevents damage to the lamps from overheating. Without water cooling of the Nd cathode, the HCL was unable to operate using Nd cathodes. Nd magnets behind the cathodes in the PDL are also conveniently cooled by design (subsection 4.4.2).

To calibrate relative intensities of the observed atomic spectral lines, continuum light sources were used to determine the spectral response functions of the spectrometer for each combination of PMTs and optical filters (see section 5.5 for more details). For the measurements of Nd spectra between near IR and VUV, a tungsten lamp and a deuterium lamp were used as the calibration sources above and under 300 nm, respectively. The purpose of the nose-piece was for the light source and calibration source to use the same optical components without switching and re-aligning the lamps, which could take hours for the HCL and PDL, involving vacuum pumping.

4.3.3 Spectrometer and Light Source Alignment

The spectrometer optical components were aligned through motor adjustments of the cats-eye retro-reflectors of Figure 4.2 within the main interferometer tank. Adjustments to the retro-reflectors were required each day for their re-alignment, as vibrations, pressure changes, and thermal expansions can shift their positions [117]. This was carried out by adjusting the retro-reflectors to maximise interferogram modulation efficiency (Equation 3.23) of a Hg lamp interferogram at zero optical path difference each day using the same aperture diameter (1.5 mm) and PMT (Hamamatsu model R7154 serial no. TJQ5161) without optical filters. The modulation efficiency was determined using the observed PMT output voltages, i.e., intensity measurements, on the oscilloscope. Throughout the entire experimental stage of the project, the modulation efficiency remained $\sim 54\%$. Since interferograms are recorded for the optimisation of spectrometer alignment each morning, the re-alignment procedure also ensures the correct initialisation of the spectrometer, e.g., finding the correct position of the zero optical path difference for double-sided interferograms (advantages of double-sided interferograms are

explained in [subsection 3.3.1](#)). The Hg lamp is selectable and always attached to the spectrometer just before the entrance aperture.

The Nd light sources, intensity calibration sources, and the PMTs were aligned using the alignment laser shown in [Figure 4.4](#). A view through the HCL or the PDL into the spectrometer was possible, therefore, aligning the Nd light source was a matter of ensuring the laser passed through the central section of the lamp plasma with the highest intensity. Checking the highest intensity was also possible by altering lamp alignment to maximise the PMT output voltage.

Alignment of the intensity calibration lamps is important for comparing with the measurements made for their calibration certificates, which were recorded for the emitting parts of the lamps. The calibration lamps were placed at approximately the same distance from the nose-piece plane mirror compared to the Nd light source plasma, this was to maintain the wavelength-dependent throughput due to the wavelength-dependent focal length of the imaging lens within the nose-piece. The tungsten lamp was found to be too bright and easily saturated the PMT voltages, so an extra aperture was placed in front of the tungsten filament to reduce the intensity of the tungsten lamp at the spectrometer input. The deuterium lamp is relatively dim, has a small emitting volume, and is sensitive to alignment. Its position was adjusted to be at twice the focal length of the imaging lens within the nose-piece depending on the wavelength region of the measurement, which minimised magnification at the input aperture to maximise throughput of the dim source. Calibration spectra were recorded before and after the measurement of Nd spectra using the same aperture diameters to check for temporal changes in instrumental spectral relative intensity response (e.g. change in the vacuum). However, the rotation of the nose-piece mirror was set by screws with insufficient consistency. To address this, adjustments were made to these screws such that the PMT gain and readings were the same for the before and after Nd spectrum scans.

4.3.4 Photomultiplier Tube Detectors and Optical Filters

Spectral Range Selection

The spectral range of the Imperial College VUV FT spectrometer is from the NIR to VUV. However, the full spectral range is almost never used for a spectrum. This is because the noise

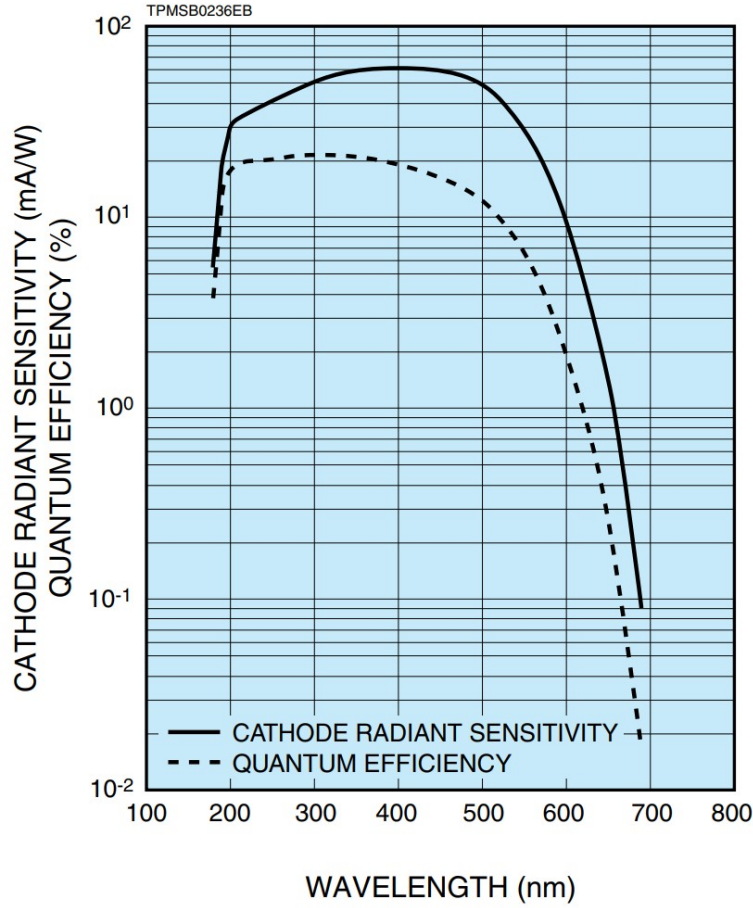


Figure 4.5: Quantum efficiency and radiant sensitivity of the Hamamatsu R11568 PMT [131].

in the recorded spectrum is most often dominated by photon noise (see [section 3.4](#)), where lower-intensity atomic spectral lines could be drowned out by the simultaneous detection of higher-intensity lines. PMTs and filters can be selected to limit the spectral range of detection. The Imperial College VUV FT spectrometer is used with side-on PMTs from Hamamatsu, and long-pass, short-pass, and bandpass filters from SCHOTT and Acton Optics. Example PMT quantum efficiency of the R11568 PMT model and the transmission curve of the long-pass GG475 optical filter are shown in [Figure 4.5](#) and [Figure 4.6](#), respectively. The wavelength range of the R11568 PMT is very broad, between 200 and 600 nm, using the GG475 long pass filter restricts the spectral range to be between 450 and 600 nm, this would reduce photon noise from unwanted photons in the 200 to 450 nm region, which instead can be measured in another PMT and filter combination. The spectral range between 200 and 600 nm would also require measuring in the first alias (see [subsection 3.3.2](#) for the definition of alias), which would be twice as many data points and induces a $\sim \sqrt{2}$ increase in noise compared to measuring in the second alias, which is possible for the 450 and 600 nm region.

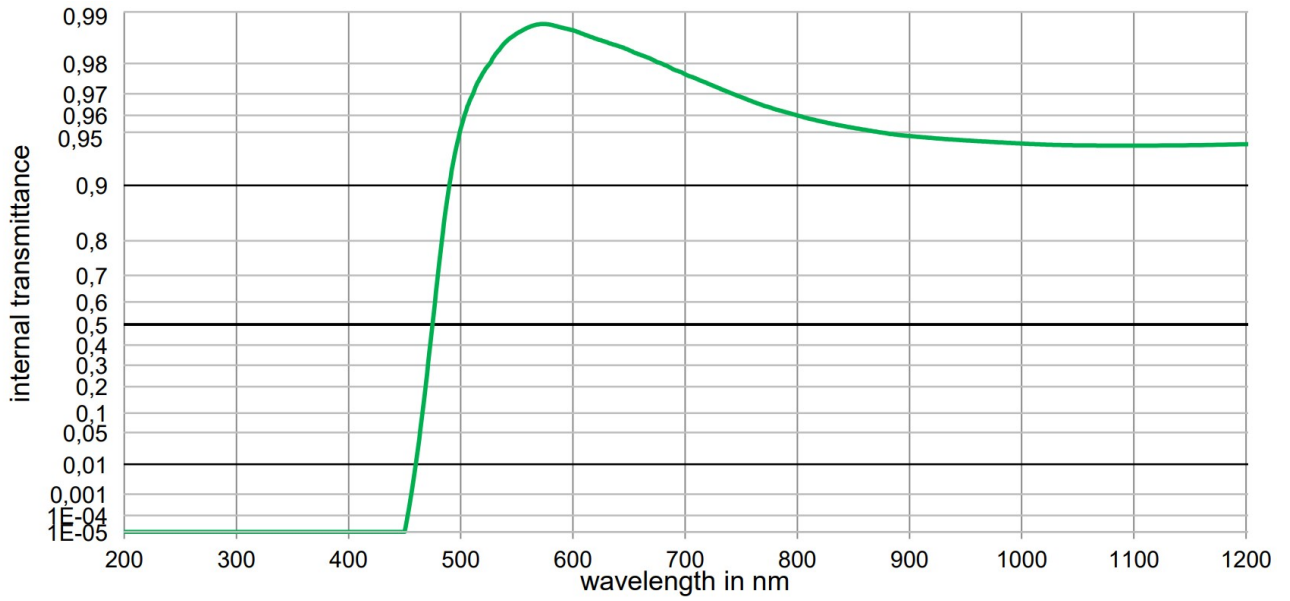


Figure 4.6: Transmittance of the SCHOTT GG475 Long-pass optical filter [132].

The PMT and optical filter combinations were chosen to minimise photon noise for the lines of interest, which involves maximising the relative contribution of photons from those transitions. In the case of Nd III, the combined instrumental intensity response functions due to PMT and filter combinations were chosen such that Nd III resonance lines lay near the peak of the response function, e.g., around the 500 nm region using the PMT of Figure 4.5 and the filter of Figure 4.6. Due to the lack of accurate knowledge of Nd III atomic structure, I decided to select PMT and filter combinations to maximise the SNRs and the number of lines observed within the entire spectral range of the Imperial College VUV FT spectrometer, while making sure the known Nd III transitions did not lay in low spectral response regions. For both the HCL and PDL, my preliminary measurements indicated line-rich and intense visible-UV regions above 300 nm and line-sparse and dim UV-VUV regions below 300 nm. In the regions above 300 nm, the spectral ranges selected were relatively smaller compared to those below 300 nm to reduce the photon noise by reducing the total number of photons detected for each spectrum.

All spectral ranges were chosen to be within the second alias. The spectral range of the PMT and filter combinations must be well within the maximum and minimum wavenumber of the spectral range of the alias. Otherwise, spectral lines exceeding the limits will appear as reflections in the spectrum, which would lie from the exceeded limit by the amount of wavenumber exceeded, causing incorrect wavenumber measurements and unnecessary line blending (see subsection 3.3.2). The possible spectral ranges using the available PMTs and filters were not

narrow enough to permit suitable measurement using the third alias in the IR-UV region. This was not an issue as splitting the spectrum into smaller regions is also not always the best option as it would increase systematic uncertainties in wavenumber calibration (see [section 5.4](#)), which may result in less accurate wavenumber measurements.

PMT Gain

When choosing the PMT gain, two conditions were required to be met. Firstly, any loss of signal to noise or saturation was to be avoided. Saturation was especially likely to occur at the zero optical path point where all wavelengths destructively or constructively interfere. This was of most concern for the tungsten calibration lamp in the IR-visible when the extra aperture was unused by mistake with the lowest PMT gain, saturation caused significant artefacts in the regions of the observed continuum spectrum where only noise was expected, i.e., outside the spectral range set by the PMT and filter. Secondly, the PMTs were required to operate under the linear gain regime, such that the output voltage is proportional to the number of photons detected (after applying the quantum efficiency), this is important for relative intensity measurements and calibration.

Two options were available for the Hamamatsu PMTs, where ten or five of the electron-multiplying dynodes (stages) could be used. In the IR-visible spectral region, the Nd discharge lamps were bright enough to cause saturation at the lowest appropriate gain using the ten-stage option, despite the deliberately reduced spectral ranges to reduce photon noise, the five-stage option was therefore used in these cases. Saturation of the ten-stage option had rarely been the case for the Imperial College VUV FT spectrometer, as it has been mostly used to investigate emission spectra of the iron-group elements. When recording interferograms, all PMT output voltages were between 0.35 and 0.7 V to avoid saturation, and gain voltages were set within 30–90 V per stage to operate in the PMT linear response regime.

4.3.5 Measuring Interferograms

Generally, multiple measurements of the same interferogram were recorded (co-adds) to reduce noise. Two or four co-adds were often used for preliminary measurements, such as when testing lamp conditions (see [section 4.5](#)). Final spectra were recorded with around 10 to 30

co-adds depending on whether measuring more co-adds offers diminishing returns on SNR (see [subsection 5.2.1](#)), which took at least two hours. To ensure the stability of the interferogram sampling system, vibrations and contacts with the main interferometer tank and its frame were minimised. Accidental mechanical perturbations may cause the system to lose count of the laser wavelengths, causing the scan of the interferogram or the ongoing multiple co-adds of an interferogram to fail. Interferograms of the intensity calibration lamps were also recorded in co-adds of 16, before and after the co-adds for the Nd lamp interferograms to check for any temporal variations in instrumental intensity response, e.g., due to changes in vacuum or alignment. Recording interferograms of the intensity calibration lamps was relatively quicker (~ 1 min per co-add) as the requirement for resolution for these continuum spectra was an order of magnitude lower, i.e., the mirror moved much shorter distances. In contrast, measuring one interferogram co-add of a Nd spectrum in the visible region took about 7 minutes.

4.4 Nd Discharge Sources

4.4.1 Hollow Cathode Discharge Lamp

With a stable current supply, the HCL can produce stable discharges with constant intensity, sufficiently constant to avoid inducing ghosts to the instrumental function ([subsection 3.4.2](#)). Transitions of Nd III were observed through FT spectroscopy using an HCL with Ne as the carrier gas [83]. This set-up was achieved using the custom HCL manufactured at Imperial College using the Hentzinger constant current power supply. A diagram of the lamp is shown in [Figure 4.7](#), the design was by Dr Matt Ruffoni and inspired by Danzmann et al. (1988) [69].

A plasma containing Nd and the carrier gas atoms and ions is produced within the cathode through the process of sputtering; the large negative potential applied to the Nd cathode creates an electric field with the anodes, capable of ionising the carrier gas and accelerates positively charged ions into the walls of the Nd hollow cathode. The impacts eject surface Nd atoms and the plasma is maintained through the constant gas flow and collisions between the atoms, ions, and electrons. The collisions also excite energy levels of the atoms, and emission spectra are therefore produced from spontaneous de-excitations. When recording IR-visible spectra, a silica window is used. For recording VUV spectra under 200 nm, a much more expensive MgF_2

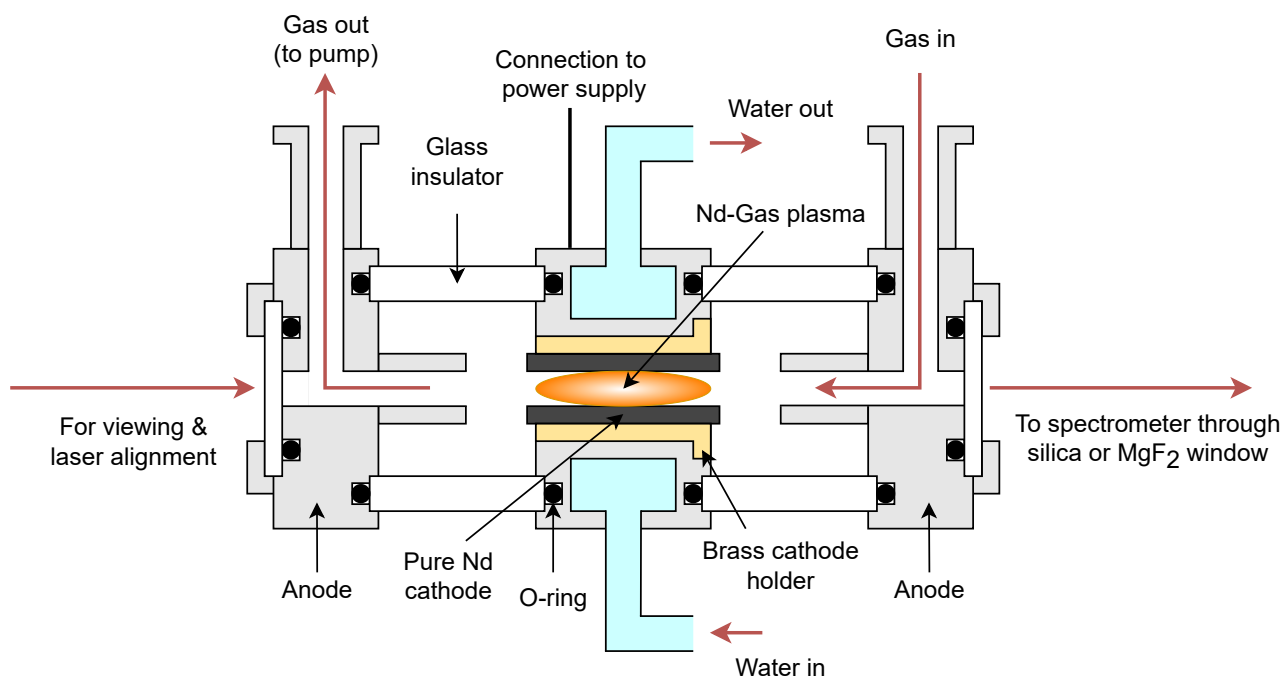


Figure 4.7: Diagram illustrating components of the custom HCL of Imperial College, showing a cross-section through the centre of the lamp.

window is used as the transmission of silica sharply declines under 200 nm.

The design shown in [Figure 4.7](#) enables convenient switching of components such as the output window without fully disassembling the lamp. The brass cathode holder is removable with the removal of only one anode piece, without disturbing the other anode and water connections. Another advantage of the small extent of disassembly is the lower probability of gas leakage due to the handling of the o-rings and their contact surfaces. Water cooling of the HCL prevented overheating and reduced Doppler broadening of spectral lines. The HCL was placed under a vacuum before filling with a noble gas to a pressure controlled by gas flow using valves and the rotary pump. Noble gases are used as carrier gases as they do not produce molecules with molecular spectra that would hinder analysis of the spectra of the atoms. In the present work, the use of He, Ne, and Ar were investigated (see [subsection 4.5.1](#) for more details). The glow at the centre of the plasma was white and very bright to the eye, which indicated high line densities and intensities throughout the visible spectrum.

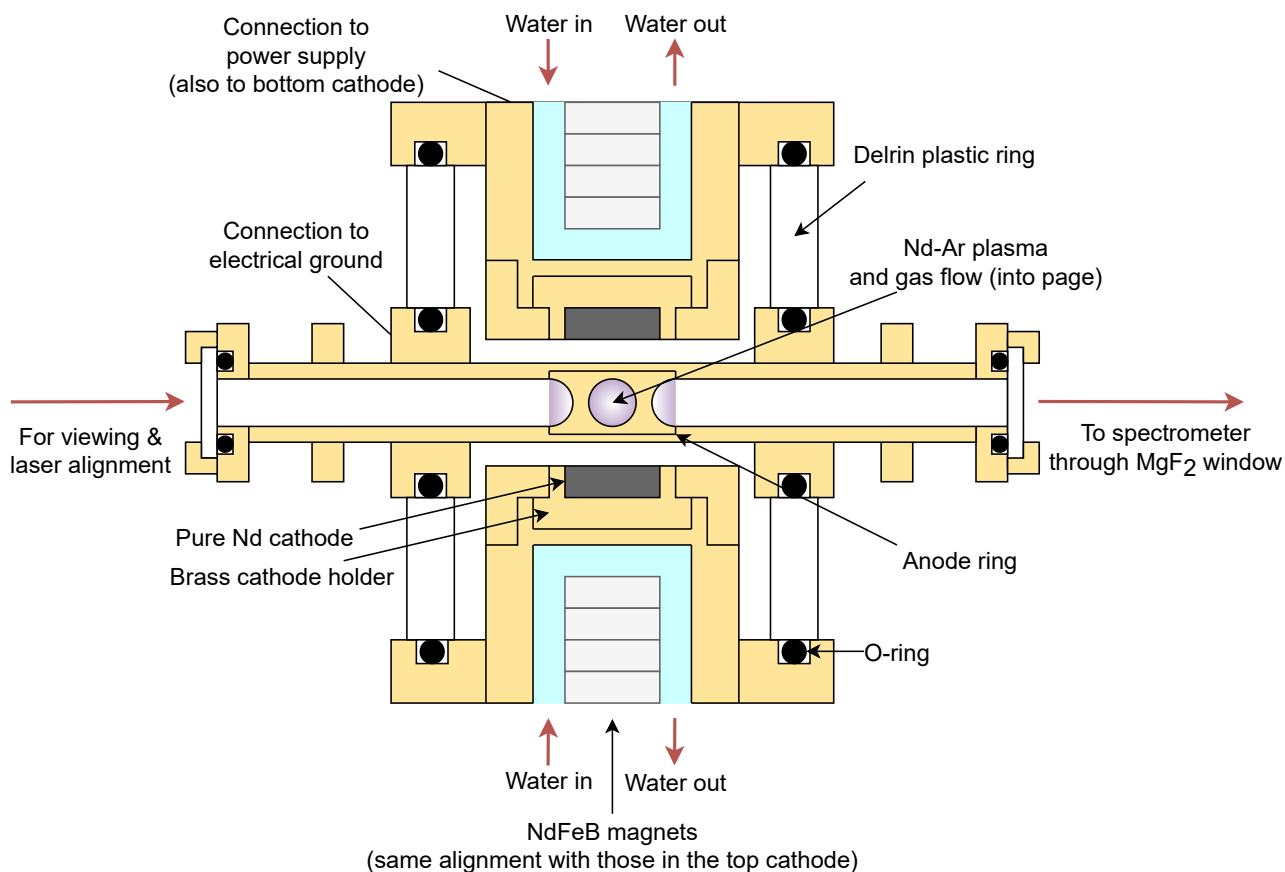


Figure 4.8: Diagram illustrating components of the custom PDL of Imperial College, showing a cross-section through the centre of the lamp.

4.4.2 Penning Discharge Lamp

The Penning discharge lamp is suitable for producing plasma containing doubly ionised iron group elements [133, 134]. For Nd, the first and second ionisation energies are expected to be lower than those of the iron-group elements due to larger electron screening. Therefore, the PDL was expected to be suitable for investigation of the spectrum of Nd III. A PDL built by the group of Prof. Manfred Kock [70, 71] was used in producing Nd emission spectra. A diagram illustrating the central cross-section of the PDL is shown in Figure 4.8.

Similar to the HCL, the plasma is produced by sputtering metal atoms using a noble gas, but with different electrode arrangements and an additional magnetic field along the axis of the electrodes. In Figure 4.8, two Nd cathodes face each other and the anode ring is situated in between, which contains the brightest part of the plasma. The curved surface of the anode ring has four equidistant holes facing its centre, two for gas flow, one for viewing plus alignment, and one for emission to the spectrometer. At the time of assembly, the field strength of the

NdFeB magnets at the centre of the anode ring measured 0.08 T, the field strength is known to decay over months due to water corrosion of the magnets, but experiments with the PDL lasted a month and the final disassembly and water drainage showed no signs of corrosion on the magnets. This magnetic field confines electrons emitted from the cathodes at their radial positions as their orbital radii are much smaller than the size of the discharge. The electrons therefore oscillate between the cathodes and create higher electron densities in the plasma (relative to atomic densities) compared to the HCL, ionising and exciting the atoms within. The ionised atoms are accelerated towards the cathodes, sputtering more metal atoms for the discharge. Therefore, the PDL enables plasma discharges at lower pressures, higher currents, higher voltages, and higher effective temperatures compared to the HCL, containing higher densities of ions at higher ionisation stages (e.g. see [Equation 2.34](#)).

Only the MgF_2 window was available for the PDL, as it was canonically used for UV-VUV investigations of the spectra of the doubly ionised iron-group elements. The transmission curve of MgF_2 is very similar to silica at the visible-IR regions, so comparisons with the HCL visible-IR spectra measured using silica windows were straightforward. The PDL was run using Ar as the carrier gas. The choice was made by investigating carrier gas sputtering efficiency of the He, Ne, and Ar in the HCL, where the noble gas with the highest atomic mass (Ar) produced the highest intensities of Nd lines. More details on optimising PDL running conditions for maximising Nd III transition intensities in the PDL are in [subsection 4.5.2](#). No previous publications or records were found in the literature on using a PDL with pure Nd cathodes to produce emission spectra of Nd. Similar to the HCL, the glow at the centre of the plasma was white, but slightly more blue. This was expected as the PDL produces higher densities of ions at higher ionisations, and transitions from ions of higher ionisations tend to be higher in energy due to larger energy level separations from less electron screening.

4.4.3 Nd Metal Handling and Lamp Maintenance

Cathode Properties

The pure Nd metal cathodes were manufactured by Goodfellow Materials Company based in Cambridge. The metal itself appeared tough and no signs of melting were observed during the experiments. For the HCL, the Nd metal was produced in the shape of a hollow cylinder

with a length of 40 ± 1 mm, an outer diameter of 10.0 ± 0.5 mm, and an inner diameter of 8.0 ± 0.5 mm. For the PDL, the Nd metal was produced in the shape of a disc with a diameter of 23.0 ± 0.1 mm and thickness of 8.0 ± 0.1 mm. The brass cathode holders of the PDL were manufactured by the Mechanical Instrumental Workshop of the Physics department at Imperial College. The Nd disc inserts were machined into the holders and their exposed surfaces were smoothed. The purities of all Nd cathodes were 99.5%, with 0.5% containing mostly Fe and Pr. Relatively small numbers of Fe transitions were observed in the spectra, but this did not hinder the analysis of Nd III transitions. No transitions of Pr were observed. Pr has one less proton compared to Nd and therefore would have spectra more similar to Nd, with strong transitions in the IR-visible. However, the strongest transitions of Pr I-III were not observed due to the low relative abundance of Pr in the cathodes and the photon noise from the overwhelming number of photons from Nd transitions in the IR-visible.

Nd Oxides

The colour of the Nd metal was dark grey and packaged by Goodfellow under a yellow-coloured oil. When taken out, the grey Nd metal was also stored under over-the-counter mineral oil, which allowed preservation for up to a year until the HCL Nd cathode was used again and depleted. Gashes of the metal revealed a shiny silver colour, implying the grey coating could be a form of Nd oxide layer. A photograph of the depleted Nd hollow cathode is shown in [Figure 4.9](#), a gash across the top² is visible. The exposed shiny surfaces look more gold than silver. This photograph was taken one year after the gash was made (originally silver in colour), so reactions with the brass cathode holder may have caused the colour change. No transitions of Cu and Zn (i.e. brass) were identified in the recorded spectra.

In the HCL and PDL, flakes of the grey compound were deposited in regions away from the discharges and were concluded to be the result of sputtering, where the oxide layer was removed in the process before the Nd metal was revealed for stable discharge. This was expected to have caused the instabilities (shorts and sparks) that always accompanied the warm-up periods of

²This gash was due to the tolerance of the manufactured outer diameter 10.0 ± 0.5 mm, where the Nd hollow cathode was slightly too thick for the HCL brass cathode holder. A small screw within the wall of the cathode holder for securing cathodes likely caused the gash when the cathode was inserted and removed by force. Therefore, a tolerance of 10.0 ± 0.1 mm should be recommended.



Figure 4.9: Photograph of the depleted Nd hollow cathode, where the broken section was the thinnest.

the lamps. Since the vacuum of the HCL is not perfectly kept because there was no vacuum pumping overnight, oxide layers would have formed to some extent before the HCL was run again. The production of these flakes during warm-up was visible through the glass insulators of the HCL. However, they did not prevent stable discharge from taking place after warming up the HCL and PDL.

Thinner flakes were reduced to light grey dust over the course of two days from exposure to the atmosphere, and their colour corresponded to that of Nd (III) oxide. Prolonged inhalation of this dust would cause lung damage [135, 136]. Similar to running any metal cathode in the HCL and PDL, the rotary pump was fitted with an air filter to catch fine particles to prevent such dust from contaminating the air in the lab. Nevertheless, the ease of production of this Nd (III) oxide dust is highlighted (e.g. relative to the rust of iron).

PDL and HCL Maintenance

As discussed in subsection 4.4.2, the PDL is more efficient at sputtering metal than the HCL. Over the three hours of running the Nd-Ar PDL, circular craters with depths similar to the cathode thickness formed on the Nd discs, see Figure 4.10. The missing Nd in these craters was deposited at various places within the PDL. While the sputtered flakes were easy to remove,

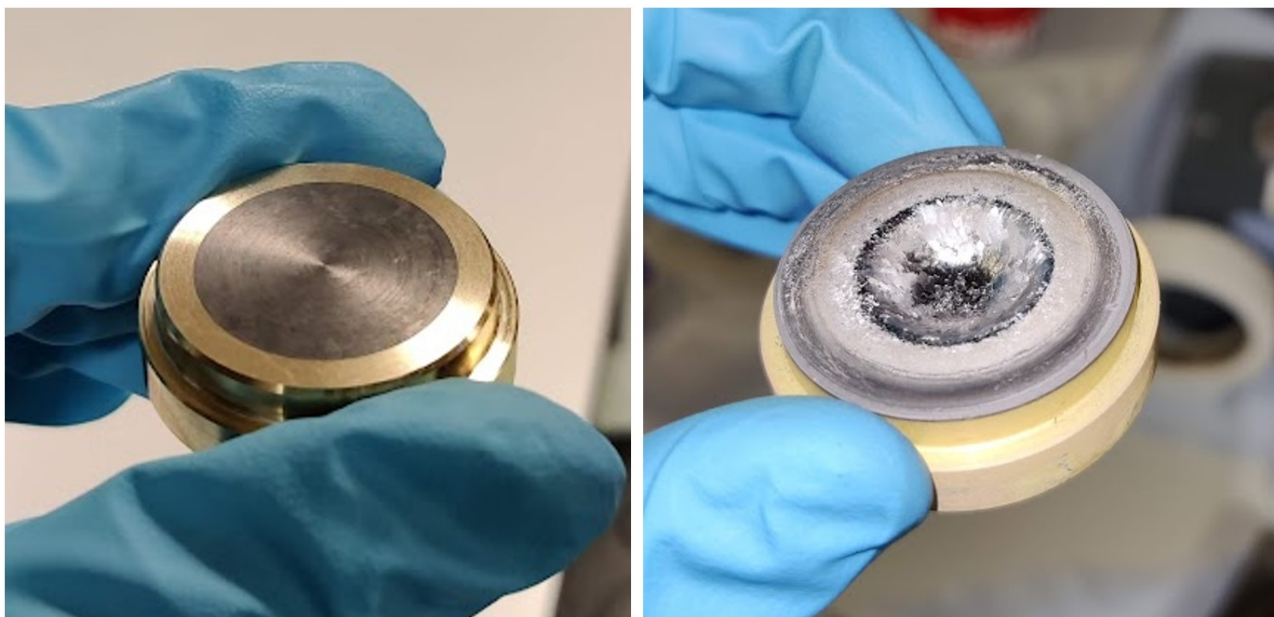


Figure 4.10: New (left) and depleted PDL (right) Cathodes. The shiny silver colour on the depleted cathodes was reduced to dark grey after months of storage in mineral oil (not shown).

most of the pure Nd was deposited as a coating over the brass surface of the anode ring and the surrounding surfaces. The layer of deposited Nd was thickest at the anode, sufficiently thick to change the shape of the anode. To prevent interference with the electric fields and the stable operating geometry within the PDL, the Nd deposits were removed after the use of each pair of Nd PDL cathodes. The common practice for cleaning metal off the brass components is carried out by grinding threaded rods through the holes of the anode ring to remove the thick layers and using sandpaper for thinner layers (with ethanol or acetone at the interface of friction to avoid combustion).

From experience, two important precautions for cleaning are recommended. First, Nd is flammable and is even more so when the Nd is in the form of thin flakes, especially when the PDL was opened from being in the vacuum where the sputtered Nd had yet to oxidise. Spontaneous combustion is possible and was observed. For this reason, the PDL, HCL, and their components after disassembly were placed inside a fire bucket over a night or two, away from flammable materials to oxidise slowly under the atmosphere. Grinding and sandpapering were then performed as gently as possible, inside the fire bucket as burning sparks were common. Secondly, the continued forced removal of sputtered Nd degrades the brass lamp surfaces, especially for the PDL anode ring and its edges of the four holes, where the highest amounts of Nd deposits were found, see [Figure 4.11](#) for comparisons. Removal of deposited

Nd from rougher surfaces was much more difficult and the anode edges deformed after a few cleans, which eventually induced dramatic lamp instabilities. This was verified when a brand new anode ring used in replacement of the worn anode produced highly stable discharges in the PDL. Therefore, gentle and careful removal of sputtered Nd is emphasised again, but spare anode rings should also be considered essential. A solution to dissolve Nd but not brass may also be viable.

The Nd deposits also occurred in the HCL but not to the extent where daily cleaning and grinding was required. The HCL ran until the cathode depleted after weeks of continued running. Two cleans were carried out and these were only from when disassembly was required. On one such occasion, a sputtered flake of Nd or Nd oxide fell out from the cathode in the stable HCL plasma when run at its highest operating current, hours after warm-up. This ejected piece was glowing, appeared to be burning, and laid in a corner between the front glass insulator and just under the cathode holder. The o-ring at this corner of the lamp was found to be damaged, presumably from the high temperatures of the glowing-hot flake. Surprisingly, the damaged o-ring was still able to keep the vacuum and experiments continued for weeks as no spares were immediately available. A photograph of the damaged section of the o-ring is in [Figure 4.12](#).

Initial Cathode Cleaning

Since the Nd metals were covered in oil on delivery, the oil and impurities in the packaging were removed. After the Nd discs were machined into their brass holders, they were also wrapped under towels fully soaked in over-the-counter mineral oil for a few weeks until they were used. For cleaning, the Nd cathodes were placed under acetone in a beaker, surrounded by warm water in an ultrasonic bath. The ultrasonic bath was run twice and for three minutes each time, the cathodes were washed using acetone before and after each ultrasonic clean. This did not remove the oxide layer but ensured fewer impurities in the spectra and better lamp stability. Due to the design of the PDL brass cathode holder, a hole is required on its reverse-side for the air to leave as the Nd disc had been pressed into place in the holder. The residual oil within this hole is observed after disassembly of the PDL but did not appear to affect the spectra. As the Nd was covered in the dark grey oxide layer already, exposure to the air of up to two hours did not show observable changes to the cathodes and did not hinder their usage, but exposures to the air were generally minimised. Nd reacts with water slowly and it was unknown whether



Figure 4.11: Photographs of PDL anode rings: (top-left) new anode ring and cleaned after a single use; (top-right) worn anode ring and cleaned after multiple uses, chipped corners are visible, Nd coating remaining within the holes were not removable by force, (bottom-left) anode ring taken out of the PDL immediately after an experiment, fully coated with Nd, and (bottom-right) anode ring taken out of the PDL after an experiment, but rested under the atmosphere for two days, very thin coatings of Nd were reduced to the light grey Nd oxide dust visible at the bottom hole, slightly thicker layers near the circumference at the top has reduced into curled flakes of dark grey colour.



Figure 4.12: Damaged HCL O-ring due to a sputtered glowing-hot Nd flake landing nearby.

Nd would react with ethanol, so these two liquids were not used for cleaning and acetone was used instead.

4.5 Optimisation of Lamp Running Conditions

The goal is to experimentally measure as many Nd III transitions as possible at the highest achievable SNRs and within a variety of Nd plasma conditions using the available instruments. Theoretical modelling of the plasma within the HCL and PDL (e.g. [137]) was beyond the scope of the present work. Therefore, the approach was to empirically determine the optimal discharge conditions while keeping in mind expectations for the lamps from previous theoretical and experimental studies. For example, the PDL is expected, and was indeed observed, to produce higher SNRs of Nd III transitions due to its capability of producing higher densities of doubly ionised metal atoms compared to the HCL. However, because of the lower effective temperatures in the HCL, its spectral lines are narrower due to smaller Doppler broadening, and allow higher resolution measurements compared to the PDL. In both the HCL and PDL, observed SNRs of the known Nd III transitions to the ground term levels were maximised from the experimental parameter search of varying carrier gas pressures and lamp currents of stable discharges. Although the pressure and current measurements may differ between the set-up of my work and possible future set-ups, e.g., pressure gauge sensitivities, gauge positioning, and ballast resistance, the overall trend for intensity dependence on pressure and current is still expected to be valuable information for any future experiments using the HCL, PDL, and similar experimental designs.

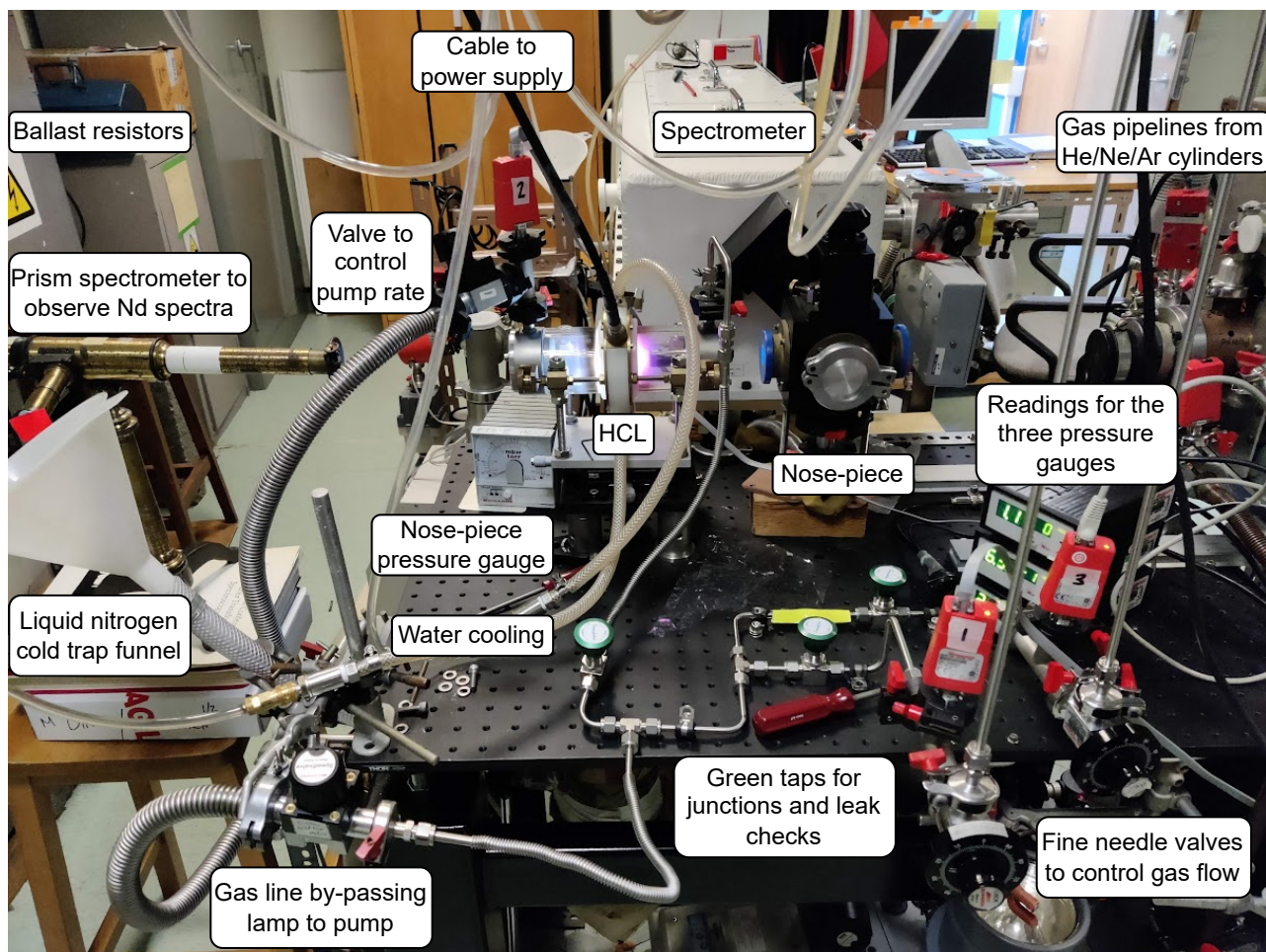


Figure 4.13: Annotated photograph of the set-up of the HCL. The lamp was running with Ar carrier gas, hence the purple glow, the glow would be orange with Ne.

The set-up of the HCL is shown in [Figure 4.13](#) and is also applicable to the PDL. The current was controlled using the power supply. In warming up the lamps, the current was slowly raised to the desired value for stability, this generally took at least 30 minutes. The lamp pressure could be controlled by the fine needle valves and the valve attached to the lamp connecting to the pump, the flow rate could in principle be controlled using these valves, but preliminary investigations showed no dependence of line intensities on how open these valves were. Therefore, the pressures in the lamps were only controlled by the fine needle valves closer to the gas cylinders and the valve on the lamp was always fully open.

4.5.1 HCL Optimal Conditions

Only one Nd hollow cathode was used with the HCL throughout the experiments. The noble gases used in the HCL as carrier gas were He, Ne, and Ar. No transitions of Nd atoms were

observed using He, and this was concluded to be the insufficient sputtering efficiency of the light He ions. The variation of SNR with currents and pressures was investigated for known Nd I-III transitions in the Nd-Ne and Nd-Ar HCL.

For the Nd-Ne HCL, the SNRs of all known Nd III transitions increased with increasing currents, but stable discharge could only be achieved up to between 0.4 and 0.45 A. Stable pressures of the Nd-Ne HCL were achieved between 1 and 3 mbar, measured by pirani gauge number two in [Figure 4.13](#) at the back of the HCL, and the highest SNRs of Nd III transitions were with 2 mbar pressure. Results of the pressure dependence of SNR in the Nd-Ne HCL are shown in [Table 4.2](#). Another set of measurements for Nd III transition SNRs was made at 1.0, 1.6, 1.8, 2.0, 2.2, and 2.4 mbar pressure and 0.45 A current, which indicated 1.8-2.0 mbar to produce the highest SNRs for the Nd III transitions. The final spectra of Nd-Ne HCL were recorded at 1.8 mbar and 0.45 A.

For the Nd-Ar HCL, the SNRs of Nd III transitions also increased with increasing currents but had a larger range of stable currents between 0.15 and 0.45 A. Stable pressures of the Nd-Ar HCL were between 0.2 and 0.6 mbar and the highest SNRs of Nd III transitions were from pressures of 0.6 mbar. Results of the pressure dependence of SNR in the Nd-Ar HCL are shown in [Table 4.3](#). While the Nd II-III transitions increased in SNR with increasing pressure up to 0.6 mbar, the Nd I transitions peaked at 0.4 mbar, suggesting relatively lower Nd I densities at higher pressures, similar to the Nd-Ne HCL. Another set of measurements for Nd III SNRs was made at 0.35, 0.40, 0.45, 0.50, 0.55, 0.50, and 0.65 mbar at 0.45 A, and similar SNR trends for Nd I-III were observed. Pressures above 0.45 mbar were found to only be stable for the short duration of the small number of co-adds (around 30 minutes) used for the results in [Table 4.2](#) and [Table 4.3](#). In the final measurements, up to 30 co-adds were recorded in the IR-visible region, which took around three hours. Therefore, the final spectra of Nd-Ar HCL were recorded at 0.45 A and 0.43 mbar, which was the highest pressure that was stable over a seemingly indefinite number of hours.

It is worth noting that in [Figure 4.13](#) the HCL discharge is brighter towards the back, this was also observed for the Nd-Ne discharge in the HCL. This was previously observed for other metal cathodes. Different electric fields between the two anodes and gas flow interaction with the plasma were suspected to be the cause. At the point of eventual final depletion of the HCL Nd cathode, the thinnest and broken section was around 2/3 of the length from the front of

Table 4.2: SNR of Nd transitions of the Nd-Ne HCL measured at 0.45 Å and pressures 1.0–3.0 mbar, using PMT R11568 (TQH7778) and filter GG475 with Ne carrier gas, 2 co-adds each.

Species	Line (cm ⁻¹)	Pressure (mbar)				
		1.0	1.5	2.0	2.5	3.0
Nd III	18883.7	249	297	342	300	165
Nd III	18988.2	164	194	220	193	107
Nd III	19210.9	312	361	423	378	224
Nd III	19251.2	104	124	140	128	71
Nd III	19499.0	249	293	343	304	170
Nd III	19593.1	290	333	391	334	184
Nd III	20288.7	132	160	185	165	93
Nd II	19179.8	243	312	378	341	211
Nd II	19630.1	345	451	546	497	306
Nd II	17513.6	52	58	63	58	30
Nd II	17574.4	36	54	65	63	39
Nd I	17613.3	1601	1504	1597	1361	682
Nd I	17449.4	1440	1368	1407	1213	610
Nd I	19209.3	2282	2119	2055	1752	854
Nd I	18892.4	326	334	344	291	146

Table 4.3: SNR of Nd transitions of the Nd-Ar HCL measured at 0.45 A and pressures 0.2–0.6 mbar, using PMT R11568 (TQH7778) and filter GG475 with Ar carrier gas, 4 co-adds each.

Species	Line (cm ⁻¹)	Pressure (mbar)				
		0.2	0.3	0.4	0.5	0.6
Nd III	18883.7	378	645	956	1238	1271
Nd III	18988.2	187	299	443	575	621
Nd III	19210.9	387	643	946	1226	1286
Nd III	19251.2	142	223	317	402	411
Nd III	19499.0	276	458	677	904	1010
Nd III	19593.1	352	561	810	1035	1095
Nd III	20288.7	137	215	311	411	446
Nd II	19179.8	268	420	631	837	938
Nd II	19630.1	380	605	905	1230	1404
Nd II	17513.6	56	73	93	110	113
Nd II	17574.4	35	61	99	147	194
Nd I	17613.3	2335	2666	2895	2692	1849
Nd I	17449.4	1913	2188	2300	2092	1378
Nd I	19209.3	3539	3803	3730	3097	1894
Nd I	18892.4	377	454	508	487	347

the cathode (see [Figure 4.9](#)).

4.5.2 PDL Optimal Conditions

For the HCL, the final Nd-Ar spectra under optimal conditions had significantly higher SNRs of Nd III lines compared to those of the Nd-Ne spectra. This was also expected for the PDL and so the PDL was run only using Ar as the carrier gas, in considering the available resources and time. The SNRs of Nd I-III transitions were recorded at 0.45 A at pressures 0.1, 0.5, 0.8, 1.0, 2.0, 3.0, and 10 μ bars, indicated by the Penning gauge sensitive down to 10^{-5} mbar attached to the turbomolecular pump of the PDL. Results are shown in [Table 4.4](#). The SNRs of Nd I-II transitions increased with increasing pressure and the Nd III transitions were observed to increase in SNR with decreasing pressure, until a sharp drop-off for pressures below 0.8×10^{-3} mbar. This drop-off was due to high source noise and was observable on the PMT output of the oscilloscope. Due to the repeated cleaning and re-assembly of the PDL each day, the optimal pressures and the drop-off pressure were found to differ between each day, and this is reflected in the running pressures given in [Table 4.6](#). The source noise and variability of the drop-off were suspected to be due to differing vacuum or leaks at the lowest PDL running pressures and the nonidentical electrodes of each day.

Similar to the HCL, the SNRs of Nd II-III transitions increased with increasing current. However, SNRs of Nd I transitions decreased with increasing current, suggesting lower Nd I densities at higher PDL currents. Furthermore, the SNRs of Nd I transitions were two orders of magnitude lower compared to the HCL. Comparisons between PDL and HCL spectra were therefore expected to be able to reliably identify lines originating from Nd I, which was useful later in the analysis of these spectra (see [subsection 6.3.3](#)). The stable currents were between 0.1 and 0.8 A. The widest range of running pressures in [Table 4.4](#) were only obtainable at 0.45 A, as the cathodes would deplete at higher currents before the full range of pressures was investigated. However, increasing the current also increased the SNR drop-off pressure, i.e., 0.8×10^{-3} mbar was noisy and unstable at 0.8 A. Based on further similar investigations, a compromise between running pressure and current was made for stability and SNRs, which was around 2.0×10^{-3} mbar (immediately above the SNR drop-off pressure) and 0.75 A, respectively.

Table 4.4: SNR of Nd transitions of the Nd-Ar PDL measured at 0.45 A, using PMT R11568 (TQH7778) and filter GG475 with Ar carrier gas, 2 co-adds each.

Species	Line (cm ⁻¹)	Pressure (10 ⁻³ mbar)						
		0.1	0.5	0.8	1.0	2.0	3.0	10
Nd III	18883.7	85	124	840	780	785	726	641
Nd III	18988.2	60	71	450	410	385	347	283
Nd III	19210.9	93	128	846	780	770	707	605
Nd III	19251.2	31	42	277	256	250	225	187
Nd III	19499.0	109	129	788	716	653	589	460
Nd III	19593.1	104	128	827	751	715	647	534
Nd III	20288.7	53	64	388	358	328	293	228
Nd II	19179.8	22	67	486	500	673	684	731
Nd II	19630.1	41	123	869	911	1160	1150	1170
Nd II	17513.6	5	10	72	73	91	90	97
Nd II	17574.4	7	21	137	140	169	171	181
Nd II	18439.8	6	17	118	120	158	156	148
Nd II	18561.9	14	33	223	231	282	278	261
Nd II	20616.8	22	61	405	416	519	514	496
Nd I	17613.3	-	77	67	77	150	164	200
Nd I	17449.4	-	58	50	58	115	120	145
Nd I	19209.3	3	57	50	57	105	111	122
Nd I	18892.4	-	30	27	30	52	54	59
Nd I	18589.9	-	48	43	48	97	105	123
Nd I	16103.2	3	8	5	8	10	9	10
Nd I	16180.5	-	7	5	7	11	11	10

4.6 Final Measurements of Nd Spectra

The full spectral range of the Imperial College VUV FT spectrometer was utilised in measuring Nd-Ne HCL, Nd-Ar HCL, and Nd-Ar PDL spectra at their respective running pressures and currents which maximised SNRs of the known Nd III resonance transitions. The PMT and filter combinations dividing the full spectral range were identical for the HCL and PDL. This was for convenient relative intensity comparisons between the spectra of the two lamps. The divided spectral ranges also overlap each other, to the extent where a sufficient number of lines are shared between two regions for wavenumber and intensity calibrations (see [section 5.4](#) and [section 5.5](#)). Resolutions of the spectra were chosen such that there were at least three data points across the FWHM of a spectral line and that no instrumental ringing was observed. This was not achievable at the highest resolution of the spectrometer (0.037 cm^{-1}) for the IR-visible spectra of the HCL, but the spectra were later proved very useful for the energy level analysis nonetheless (see [subsection 6.3.3](#)). At shorter wavelengths, larger Doppler broadening allowed resolutions to be reduced. The shorter optical path differences of lower resolutions allowed a shorter amount of time per co-add and lower noise. Therefore, spectra in the UV-VUV region were able to be recorded with significantly more co-adds than at longer wavelengths to further reduce noise.

The list of spectra recorded using the HCL and their experimental parameters are shown in [Table 4.5](#). For the shortest wavelength spectral region $51\,000\text{--}68\,000\text{ cm}^{-1}$, only Ar lines were observed with the Nd-Ar HCL, and no lines were observed with the Nd-Ne HCL. At the running conditions in [Table 4.5](#), the HCL was stable enough to maintain the discharge for several hours per day, without changing the optimal currents and pressures.

The list of Nd-Ar PDL FT spectra and their experimental parameters are in [Table 4.6](#), and their plots can be found in [Appendix G](#). These spectra were chosen for the measurements of Nd III transition wavenumbers since the known Nd III lines were highest in SNR in these spectra. The spectral ranges for the Nd-Ar PDL spectra are the same as [Table 4.5](#), where the uppercase letter of the names in [Table 4.6](#) corresponds to the first lowercase letter of the names in [Table 4.5](#). In [Table 4.6](#), the spectral ranges presented indicate which spectrum a line from [Table D.1](#) belongs to. Similar to the HCL, a negligible number of lines (about ten) were observed in the deeper VUV; the spectrum above $54\,000\text{ cm}^{-1}$ was thus neglected. As discussed

Table 4.5: Details of all 13 recorded Nd HCL spectra, measured at 0.45 A, 0.43 mbar for Ar and 1.8 mbar for Ne.

Spec.	Spec. Range (cm^{-1})	Res. (cm^{-1})	Gas	PMT	Filters	Window	Co-adds	Int. Calib. Lamp
aa	10500–21000	0.037	Ar	R928	OG530	Silica	25	W
an	10500–21000	0.037	Ne	R928	OG530	Silica	30	W
ba	12500–25000	0.037	Ar	R11568	GG475	Silica	17	W
bn	12500–25000	0.037	Ne	R11568	GG475	Silica	23	W
ca	15798–31596	0.037	Ar	R11568	SP500 + GG385	Silica	22	W
cn	15798–31596	0.037	Ne	R11568	SP500 + GG385	Silica	22	W
da	22700–45400	0.037	Ar	R11568	UG5-C	Silica	21	W
dn	22700–45400	0.037	Ne	R11568	UG5-C	Silica	23	W
ea	28500–57000	0.050	Ar	R7154	None	Silica	28	D ₂
en	28500–57000	0.050	Ne	R7154	None	Silica	23	D ₂
fa	31596–63192	0.080	Ar	R8486	180-B-1D	MgF ₂	64	D ₂
fn	31596–63192	0.080	Ne	R8486	180-B-1D	MgF ₂	53	D ₂
ga	51000–68000	0.100	Ar	R8487	None	MgF ₂	71	D ₂

Table 4.6: Nd-Ar PDL FT spectra parameters [96].

Spec.	Spec. Range (cm^{-1})	Res. (cm^{-1})	Press. (microbar)	Current (mA)	PMT	Filters	Co-adds	Int. Calib. Lamp
A	11890-17687	0.045	1.7	750	R928	OG530	8	W
B	17687-21300	0.050	2.2	750	R11586	GG475	7	W
C	21300-25369	0.050	2.3	650-750	R11586	GG385+SP500	19	W
D	25369-32480	0.055	2.4	750	R11586	UG5-C	21	W
E	32480-44422	0.070	1.7	750	R7154	-	23	D ₂
F	44422-53822	0.080	2.0	750	R8486	180-B-1D	32	D ₂

in [subsection 4.5.2](#), there exists source noise at the lower limit of the stable running pressures due to inconsistent vacuums and nonidentical electrodes. The Nd-Ar PDL was always run at the lowest stable pressure, but the effects of source noise are not always obvious and were in fact unknown during the measurements for spectra A and E, where major improvements to spectrum A (up to double the SNRs) and minor improvements to spectrum E (up 1.5 times increase in SNRs) could be expected using the same set-up. These improvements were not attempted in the interests of time and resources.

4.7 Nd Vacuum Spark and Stellar Grating Spectra

As discussed in [section 3.5](#), grating spectroscopy can supplement FT spectra greatly. The final parts of analysis of Nd III atomic structure (see [section 6.7](#)) were performed in collaboration with Dr Alexander Ryabtsev of the Institute of Spectroscopy of the Russian Academy of Sciences and Dr Tatiana Ryabchikova of the Institute of Astronomy of the Russian Academy of Sciences. Some details of the spectra they used are described in this section for the coherence of the thesis. Full details can be found in [\[96\]](#).

Grating Spectra of Nd Vacuum Sliding Sparks

The list of Nd VS grating photographic plates used by Dr Ryabtsev is listed in [Table 4.7](#). The spectral ranges indicate which spectrum a line from [Table D.2](#) belongs to. The plate serial number (No .514a, 522a, 522b) is according to the NIST grating plate archive classification. ISAN stands for the Institute of Spectroscopy of the Russian Academy of Sciences, Troitsk, Russia. NIVS stands for normal incidence spectrograph. The NIST plates were possibly recorded by Dr J.-F. Wyart [\[138\]](#) and were shared with Dr Ryabstev. The ISAN plates were recorded by Dr Ryabstev himself, and spectrum fitting was carried out by Dr Kononov. For the analysis of $4f^35f$ levels of Nd III involving transitions between $4f^35d$ and $4f^35f$ around 100 nm, another plate in the range 820-1169 Å was used by Dr Ryabtsev in combination with plate number 1 of [Table 4.7](#), which was likely also recorded by Dr J.-F. Wyart [\[138\]](#).

Relative intensity measurements of photographic plates differ from those using PMTs in FT spectroscopy. In response to radiation, photographic plates darken. The amount of darkening

Table 4.7: Nd sliding VS spectra parameters [96].

Spec. No.	Date; No.	Instrument	Spec. Range (Å)
1	November 10 2002	ISAN-NIVS 6.65 m	390-1525
2	November 28 2002	ISAN-NIVS 6.65 m	1904-2327
3	No. 514a Track No. 1	NIST-NIVS 10 m	2333-2570
4	No. 522a, b Track No. 5	NIST-NIVS 10 m	2651-3213

for a given incident intensity is determined by the exposure duration and energy flux sensitivity of the photographic plates, which also depends on wavelength. The sensitivity is generally determined experimentally (e.g. [139]). In the present work, approximate energy flux sensitivity curves that are assumed independent of wavelength were used to intensity calibrate the VS grating spectra, where calibrated relative intensities correspond to relative energy flux, which is proportional to relative photon flux multiplied by wavenumber. Due to large uncertainties of this intensity calibration and in the instrumental spectral response of the grating spectrometer, the differences between multiplying and not multiplying calculated weighted transition probabilities with wavenumber (see Equation 2.20) when analysing photographic plate relative intensities was negligible.

The uncertainties of relative intensity measurements using photographic plates are much larger compared to the relative intensity uncertainties achievable in FT spectroscopy using PMTs (see subsection 5.5.3), the low dynamic range of the plate darkening restricts observed intensities to have only a few distinguishable intensity values (e.g. see Table D.2 and Table E.1). Nevertheless, (calibrated) photographic plate intensity measurements were still found to be useful in the term analysis of Nd III, where intensity patterns of relative transition probabilities are generally followed.

Stellar Spectra

Dr Ryabchikova used mainly spectra of two stars HD 170973 and HD 144897 to observe transitions of Nd III, their absorption spectra were recorded at the Very Large Telescope of the European Southern Observatory at resolving power 80 000 between 3030 and 10400 Å. The two stars were chosen for their very high Nd abundances, about 4 orders of magnitude higher compared to the solar photosphere, and largely differing surface magnetic field strengths, HD 170973 with 392 ± 5 G and HD 144897 with 8.8 kG [96]. This meant that Nd III transitions could be observed at reasonable SNRs, with or without Zeeman splitting of energy levels, which offered more evidence for the correct classification of Nd III transitions using theoretical Landé g -factors of Equation 2.31.

4.8 Summary of the Laboratory Measurements of Nd Spectra

The full spectral range (11 000-70 000 cm^{-1} , NIR to VUV) and highest resolution (0.037 cm^{-1} , resolving power 1.3×10^6 at 200 nm) of the Imperial College VUV FT spectrometer were used in recording laboratory Nd emission spectra produced in the Nd-Ne HCL, the Nd-Ar HCL, and the Nd-Ar PDL. The currents and pressures of these light sources were chosen for their stability and to maximise the SNRs of the known Nd III transitions. The full spectral range was split into smaller regions using combinations of PMTs and optical filters to reduce photon noise, but with overlapping regions to allow wavenumber and intensity calibration (section 5.4 and section 5.5, respectively). Grating spectra recorded for other sources of Nd spectra became available during the later analysis of Chapter 6, and aided the Nd III energy level search greatly.

Chapter 5

Nd Fourier Transform Spectra and Calibration

5.1 Introduction

Raw interferograms recorded from the Nd-Ar PDL (Table 4.6), Nd-Ar HCL (Table 4.5), and Nd-Ne HCL (Table 4.5) in the experiments of Chapter 4 were Fourier transformed into spectra in preparation for the analysis of Nd III atomic structure. To maximise the SNRs of spectral lines, the interferograms were co-added to improve the SNR, transformed, and the resulting spectra were then phase corrected (section 5.2). After obtaining the spectra, individual spectral lines were fitted using model line profiles to extract data such as wavenumbers, wavenumber uncertainties, and relative intensities of the observed atomic transitions, creating a line list for each spectrum (section 5.3). Each line list was then wavenumber calibrated using Ar II wavenumber standards (section 5.4), intensity calibrated using tungsten and deuterium standard lamps (section 5.5), and combined with other line lists to create a merged line list containing all observed spectral lines (section 5.6).

The final merged line list only contains lines from spectra of the Nd-Ar PDL, which were the only spectra used for wavenumber measurements. This was because the Nd III lines in the Nd-Ar PDL FT spectra have the highest SNRs and many weaker Nd III lines were unobserved in the Nd-Ar and Nd-Ne HCL spectra. Nevertheless, the HCL spectra were still useful to compare the PDL spectra with, especially in analysing blended lines and relative line intensities emitted

from their different plasma conditions (see [section 6.3](#) for more details).

5.2 Fourier Transform of Interferograms

5.2.1 Co-adding Interferograms

Noise Reduction

Co-adding interferograms is the summation of interferogram intensity samples recorded at the same optical path differences. Co-adding photon-noise limited N interferograms enhances the SNR by $\sqrt{N}$ by reducing noise by a factor of $\sqrt{N}$ [119], which ultimately reduces measured wavenumber uncertainties and enhances weak lines. The $\sqrt{N}$ scaling and the existence of other sources of noise (e.g. digitising noise, see [section 3.4](#)), means co-adding ever more interferograms offers diminishing SNR returns. The number of co-adds for each measurement in [Table 4.6](#) was chosen to compromise between diminishing SNR returns and interferogram scan durations. As these were shorter for lower spectral resolution scans in the UV, the number of co-adds was greater in the UV.

An example of noise reduction by co-adding 23 interferograms is shown in [Figure 5.1](#), where the noise (clearly visible on both sides) of the interferogram was reduced by a factor of around $\sqrt{23} \sim 5$ compared to the peak signal. For interferograms recorded in the line-rich and intense visible regions, the SNR return for recording N interferograms diminished much quicker than $\sqrt{N}$ due to the relatively much higher number of strong lines, e.g., the enhancement of SNR between 4 co-adds and 16 co-adds was not the expected factor of 2, but observed to be around 1.3, potentially due to significant digitising noise (see [section 3.4](#)).

Effects of Small Intensity Fluctuations

The interferograms produced from each scan were inspected prior to co-adding. Interferograms that displayed large fluctuations in intensity due to significant lamp instabilities were not included in the co-add, e.g., when the stable discharge became pulsed sparks for an extended period of the scan, often requiring adjustment of lamp currents to reach stable discharge again.

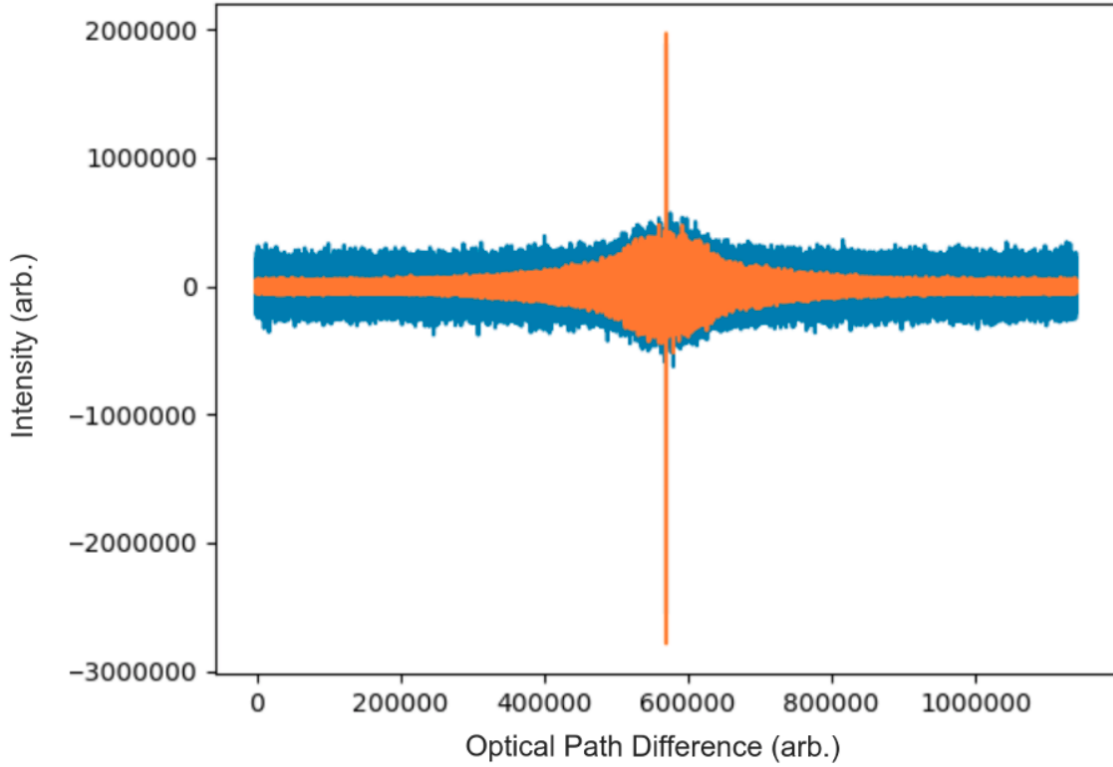


Figure 5.1: Comparison between a co-add of 23 interferograms (orange, divided by 23) and a single interferogram (blue) taken for the UV region of spectrum en of Table 4.5. The centre bursts of both interferograms are approximately the same in amplitude. This spectral region has low photon intensity compared to the visible regions.

On the other hand, small and brief intensity fluctuations were generally not accompanied by prolonged lamp instability. Interferograms with these small intensity fluctuations were still useful as the fluctuations average out during co-adding and contributed only a small amount of noise in their spectra, e.g., a small spike in the co-added interferogram is a small amplitude cosine in the final spectrum. An example of the co-added interferogram of spectrum C in the visible and a single interferogram with such small intensity fluctuations are shown in Figure 5.2, where after co-adding the intensity fluctuations are seen to be almost negligible.

To demonstrate that co-adding interferograms with small intensity fluctuations negligibly affects the spectrum, Figure 5.3 shows plots of a co-add of three interferograms and a single interferogram (included in the co-add of the three), plotted at the optical path differences containing a small intensity fluctuation. As expected in the co-added interferogram shown in orange, the fluctuation is at around one-third of its amplitude. The resulting FT spectra created with and without co-adding the single interferogram of Figure 5.3 are shown in Figure 5.4. In the top plot, no differences in line shapes between the two spectra were visible in the lines

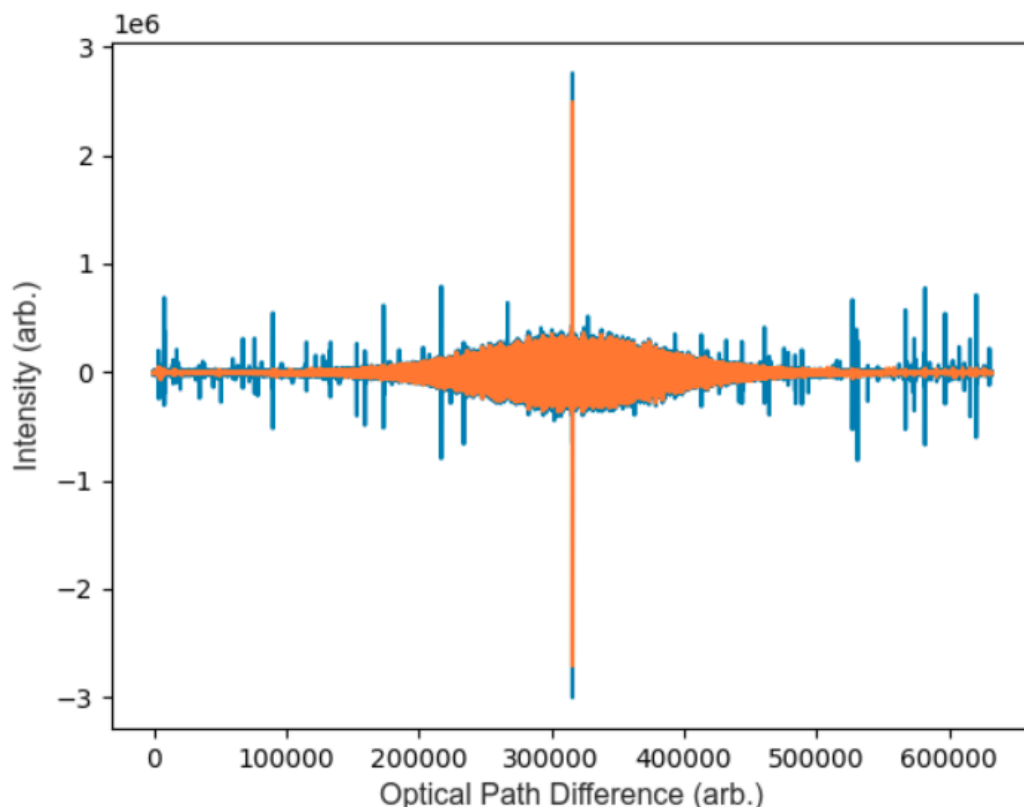


Figure 5.2: Comparison between a co-add of 19 interferograms (orange, divided by 19) and a single interferogram (blue) taken for the visible region of spectrum C of Table 4.6. This region has high intensity, and co-adding many interferograms is not as effective in reducing noise compared to the lower intensity UV region (see Figure 5.1 for comparison).

shown in this typical segment of the spectrum. In the bottom plot showing a region where there are no spectral lines, including the interferogram with the intensity fluctuation in the co-added interferograms reduced the noise as expected. Thus co-adding interferograms with small intensity fluctuations was concluded to be effective in reducing noise without significantly affecting the spectrum.

It should be noted that only spectrum C of the Nd-Ar PDL (orange interferogram of Figure 5.2) has many small intensity fluctuations in its co-added interferograms due to unstable lamp conditions. This was later found to be due to the worn anode ring where the brass edges were significantly deformed from repeated forced removal of sputtered Nd, see the top-right photograph of Figure 4.11. The small intensity fluctuations were rare in other Nd-Ar PDL FT spectra. In retrospect, identifying very weak lines and blended lines in spectrum C was slightly more difficult compared to doing this task in other spectra. Therefore, the number of small fluctuations in lamp intensity should still be minimised where possible.

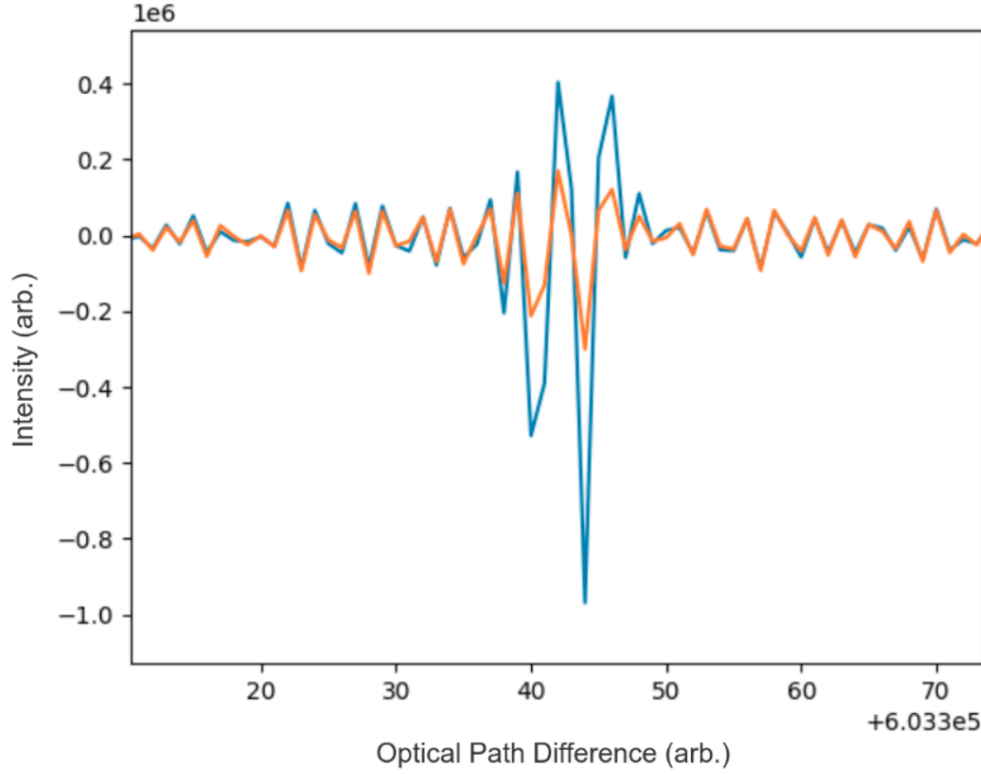


Figure 5.3: Comparison between a co-add of 3 interferograms (orange, divided by 3) and a single interferogram (blue) taken for the visible-UV region of spectrum da of [Table 4.5](#).

Effects of Significant Phase Errors

Ideally, only interferogram intensities sampled at the same optical path differences should be co-added, within tolerances allowed by the uncertainty in the measured optical path differences. There existed instrumental instabilities of the Imperial College VUV FT spectrometer [68] at the time of the experiments, where recorded intensities of repeated interferogram scans were sometimes shifted in optical path difference (shifted in phase) by more than allowed by the expected optical path difference accuracy of the instrument (i.e. from the sampling system [subsection 4.2.2](#)). This was most clearly observed when inspecting the centre bursts of the repeated scans of the interferograms to be co-added. For example, not all centre bursts of [Figure 5.5](#) were measured at the same optical path differences, which could not be due to noise as the interferograms were recorded in the intense visible spectral region.

Co-adding interferograms recorded at different optical path differences essentially causes destructive interference and reduces the SNR of observed spectral lines. This is clearly seen in [Figure 5.6](#), where the noise is essentially the same for co-adds of 3, but the SNRs of the

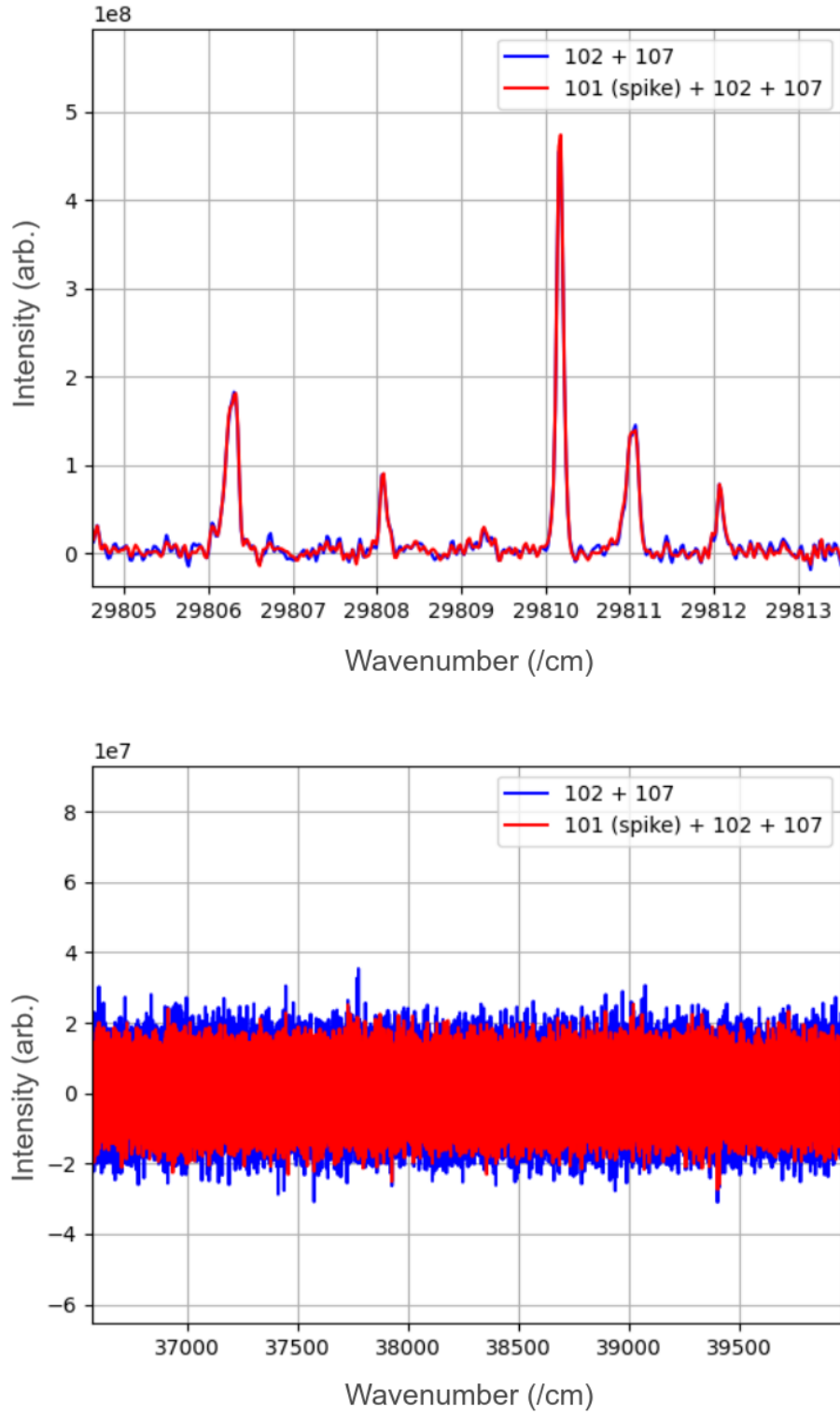


Figure 5.4: Comparison between the spectrum of the interferogram of 3 co-adds ($101 + 102 + 107$, orange curve from Figure 5.3) and the spectrum of the interferogram of 2 co-adds ($102 + 107$) without the interferogram 101 with the spike in intensity (blue curve in Figure 5.3). The co-adds were divided by the number of co-added interferograms to place spectrum intensities on the same scale. The top plot shows a section including several spectral lines and the bottom plot shows a region with no spectral lines where the spectrum noise alone can be seen.

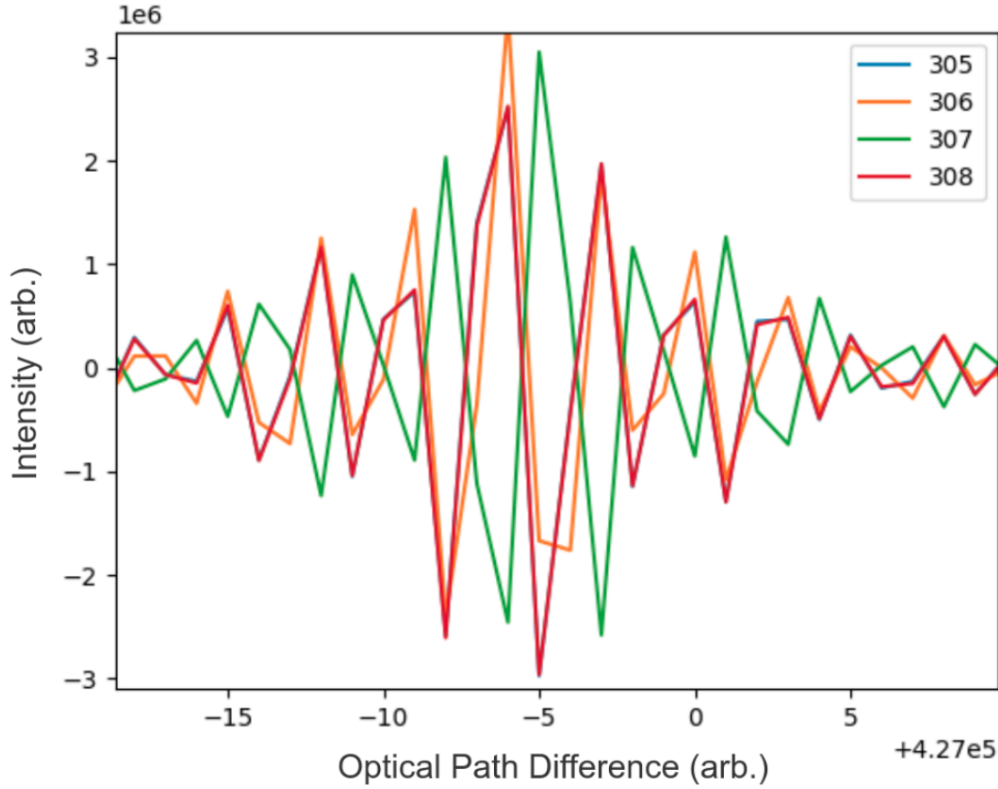


Figure 5.5: Plots of the centre bursts of four interferograms for the spectrum da of Table 4.5, where 305 and 308 match almost exactly, 306 is slightly out of phase from 305 and 308, and 307 is almost completely out of phase compared to 305 and 308.

lines are more than halved when the completely-out-of-phase interferogram 307 is co-added (red spectrum). Additionally, the resulting spectral line shapes varied between the different combinations of co-adds; there were visible shifts in the asymmetries of line profiles. This was expected as co-adding interferograms of different phases cause shifts in the phase correction curve (see subsection 3.3.1 and the next section), which ultimately affects the uncertainty in the measured wavenumber of the affected lines [120].

The majority (around 70%) of individual interferogram scans in a series had negligible differences in phase throughout their optical path difference ranges. Interferograms expected to negatively impact the co-add due to phase shifts were identified by inspecting centre bursts and the overall co-added interferograms for asymmetries in modulation due to destructive interference. Any interferograms that displayed these issues were removed from the co-add.

The shifts in phase were almost discontinuous in the interferograms, which could occur at any point during the scan, one or two times over the course of a few minutes, i.e., an interferogram could be in phase with the previous scans for the majority of its scan duration but then become

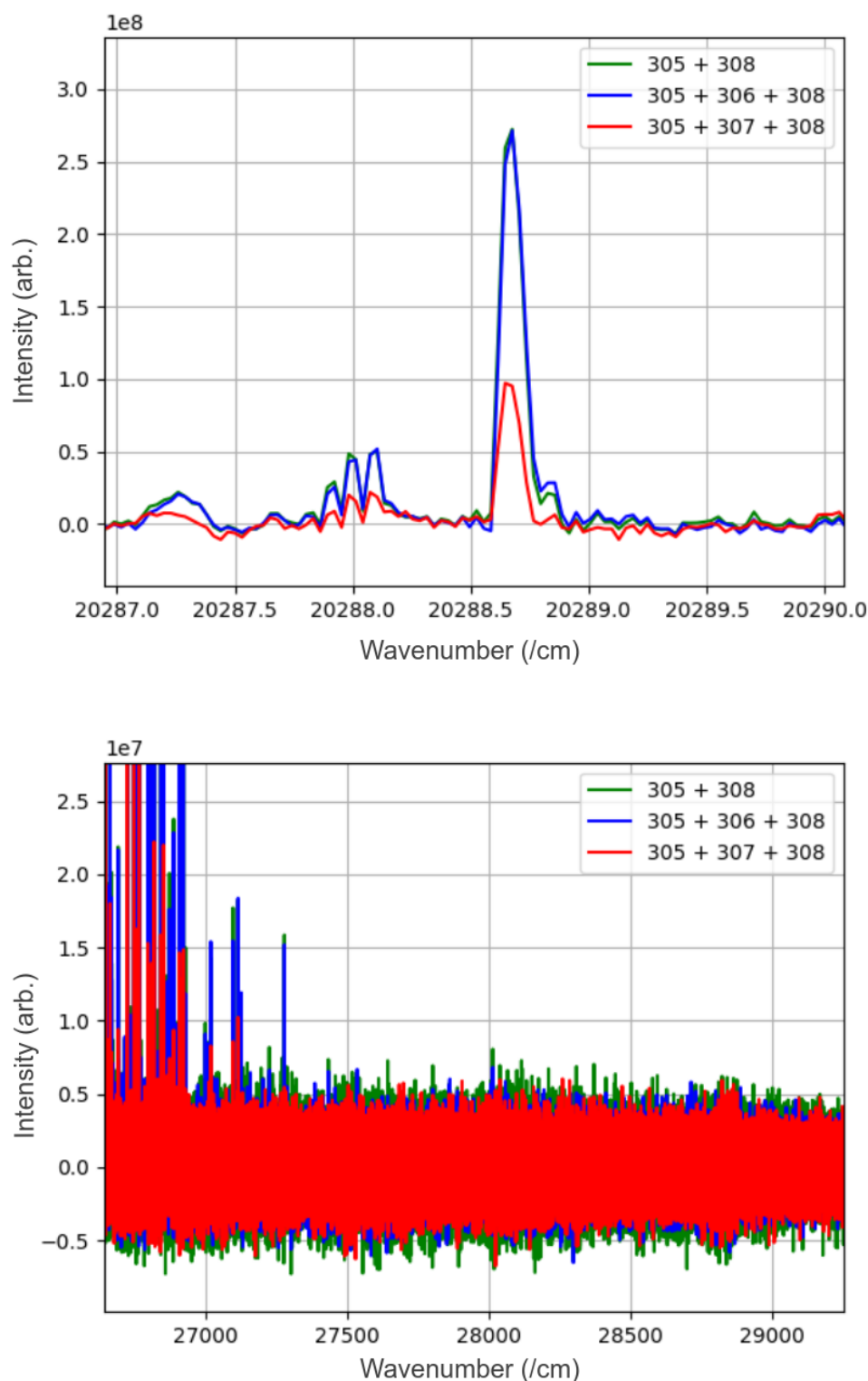


Figure 5.6: Plots of spectra of three co-add combinations of interferograms from Figure 5.5. The co-added interferograms were divided by the number of interferograms to place the spectra on the same intensity scale. The top plot shows a section with line shapes visible and the bottom plot shows an extended noise region.

out of phase. Their intermittent occurrence became more and more frequent over the course of a year, which also increased with the amount of time the instrument’s electronics were left switched on. The gradual increase in the frequency of these random occurrences was similar to problems that arose from the recently (2023) identified failure of the PMT power supply, but further investigation into this matter was not conducted.

After rejecting interferograms with significant phase shifts or excessive intensity spikes from lamp instabilities, the remaining ‘good’ interferograms were co-added, which are the numbers of co-adds listed on [Table 4.5](#) and [Table 4.6](#).

5.2.2 Phase Correction

Once the co-added interferograms were finalised, they were Fourier transformed. As discussed in [subsection 3.3.1](#), experimental interferograms are not expected to be symmetric about the zero optical path difference point, which results in non-zero imaginary components in their FTs and these cause distorted line shapes in the real spectra and signals to be lost to the imaginary spectra. Real spectra could of course be obtained by taking the absolute values of the resulting complex spectra of the FT, but this is not the best method in the interest of maximising SNR [119] since the noise is sampled twice, once in the real spectrum and once in the imaginary spectrum. Instead, a phase correction has to be applied to the FT of each set of co-added interferograms. This can be thought of as rotating each point in the complex spectrum onto the real number axis using a smooth and slow-varying phase function of wavenumber, leaving only noise in the imaginary component. This method differs from taking the absolute values of the complex spectrum as the phase curve is sampled from spectral lines significantly above the noise level, and so phase correction provides a $\sqrt{2}$ advantage in SNR compared to obtaining the spectrum using the absolute values.

The phase curve for each spectrum was sampled using spectral lines above a chosen SNR threshold. A point on the interferogram was carefully selected as the point closest to zero optical path difference interferogram centre burst, this minimises the slope of the phase curve, as the derivative of the phase curve contributes to errors in the phase curve [120]. The sampled phase curve was then fitted with a Chebyshev polynomial (up to order 2) to determine the phase angles throughout the complex spectrum. These procedures and the FT of interferograms were

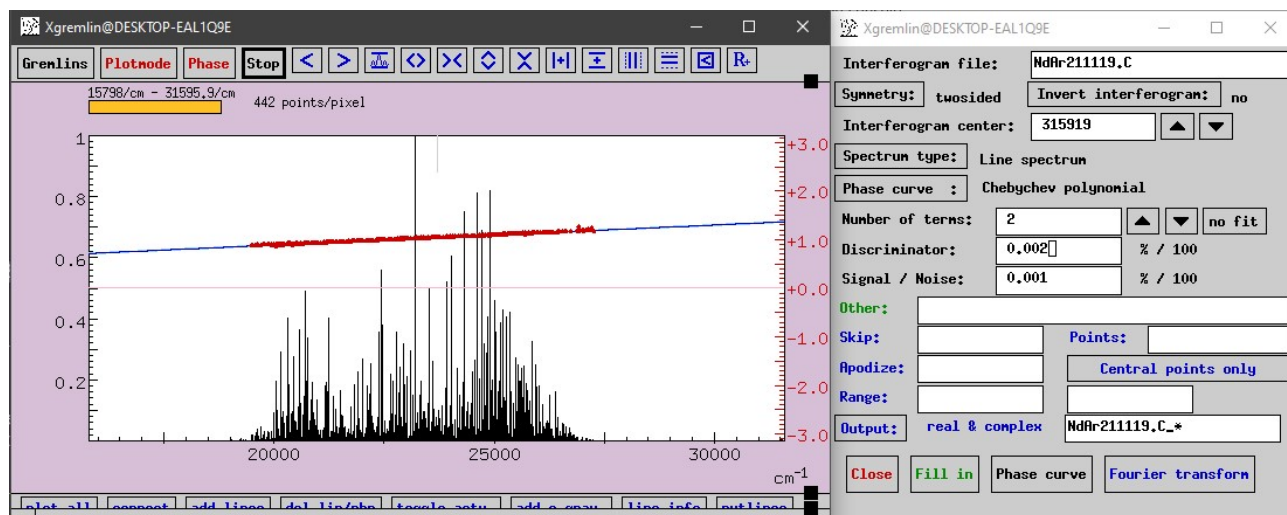


Figure 5.7: Phase correction interface in *XGREMLIN* [122] for spectrum C of Table 4.6. The red dots are phase curve values sampled from lines above twice the noise level, which was set at 0.001% of the maximum intensity value. The blue line shows the first-order Chebyshev polynomial fitted to the sampled phase points. The centre was chosen as the 315919th interferogram data point.

handled by the computer program *XGREMLIN* [122], and an example of a spectrum, its phase points, and fitted phase curve are shown in Figure 5.7. Figure 5.8 shows the residuals in the imaginary spectrum in blue. The residuals are mostly from the strongest lines, around 0.5% of the real spectrum SNR, and approximately at the noise level. These residuals result from the tiny uncertainties in the phase curve and partially set the wavenumber uncertainty limits (see discussion of Equation 5.1 later).

5.2.3 Interferogram Apodisation

It is worth noting that the ‘Apodize’ functionality of *XGREMLIN* [122] (bottom right of Figure 5.7) is useful in reducing instrumental ringing (subsection 3.3.3) of any under-resolved spectra. No ringing was observed in the PDL spectra and all PDL interferograms were apodised using the selected default value, which is 5% of the number of points within one side of the interferograms. This is the number of points on both ends of the interferogram that are brought down to zero smoothly using a cosine bell [122], thus reducing ringing that would result from a truncated interferogram due to its finite total optical path difference (see discussions of Figure 3.7). On the other hand, instrumental ringing was observed for the HCL spectra recorded in the IR-visible region due to the insufficient maximum resolution of the Imperial College VUV FT spectrometer for the narrower lines. The values entered in the ‘Apodize’ field of the

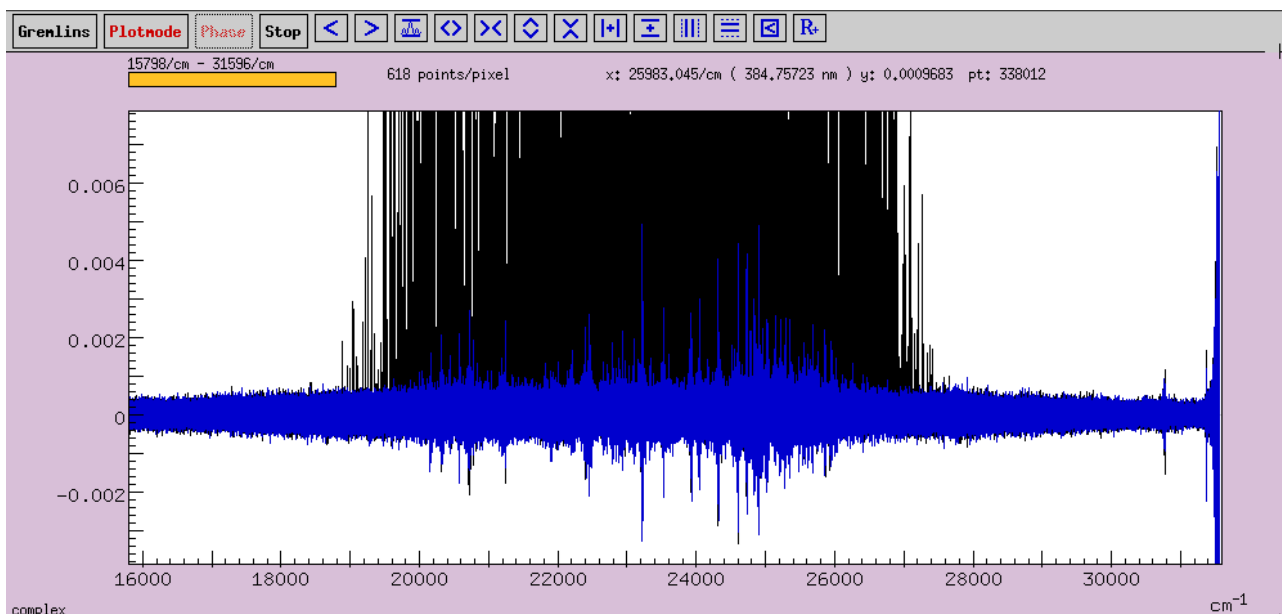


Figure 5.8: Plot of the complex spectrum after the phase correction process shown in Figure 5.7. The real and imaginary spectra are in black and blue respectively. The y -axis scale is the same as that of Figure 5.7, but has been expanded here to show the residuals in the imaginary spectrum (blue).

XGREMLIN window were 20% of the number of points within one side of the interferograms. The range of ringing for each spectral line was reduced significantly, but the ringing was still observable for strong and narrow lines in the HCL spectrum (see Figure 2.2).

5.2.4 Noise Level Determination

Each Nd-Ar PDL FT spectrum was divided by its noise level, i.e., a constant value independent of wavenumber, to represent the spectrum intensity scale in terms of SNR. The peak value of a spectral line was therefore its SNR. This SNR is used in the calculation of uncertainties associated with each spectral line. It can be seen from Figure 5.4, Figure 5.6, and Figure 5.8 that the noise of FT spectra within spectral regions with spectral lines is essentially white noise. However, in the vicinities of the strongest lines having significant residuals from phase correction, the local noise can be higher than the general white noise level of the spectrum. This meant that the SNRs of weak lines that were only a little above the spectrum noise level and were situated to the wings of strong lines were likely to be underestimated.

A noise level independent of wavenumber was determined for each of the six spectra of Table 4.6. This was estimated by averaging the RMS values (square root of the average squared deviation

Table 5.1: Summary of Nd-Ar PDL FT spectra noise determination. The numbers are in arbitrary units proportional to relative photon counts per wavenumber σ .

Spec.	Lower σ	Central σ	Higher σ	Average
A	8.79	12.50	9.70	10.30
B	2.75	4.74	2.69	3.39
C	6.19	6.64	6.33	6.39
D	5.84	11.20	7.92	8.32
E	3.93	3.82	3.89	3.88
F	1.65	1.58	1.58	1.60

from the mean) of each spectrum within three selected regions with no spectral lines. Two from the regions where instrumental intensity response reaches zero, e.g., for [Figure 5.8](#) this would be around 19 000 and 27 000 cm^{-1} , and one from the central region generally containing intense lines and high line-densities. The noise level estimation for the six Nd-Ar PDL FT spectra ([Table 4.6](#)) are summarised in [Table 5.1](#). The maximum variation of noise within a spectrum was found to be no more than a factor of two, and there were no variations in the noise levels across the UV regions of spectra E and F. There was difficulty in accurately estimating the noise level in line-rich spectra A, B, C, and D, where line-free regions were almost non-existent within the central portions of these spectra (see [subsection 5.3.5](#)). In contrast to spectra E and F, the noise levels within spectra A, B, C, and D were always higher in the central regions compared to the lower and higher wavenumber regions with zero instrumental intensity response, which was likely due to the inclusion of low SNR and very weak lines in the noise level estimation, this is particularly true for the most line-rich spectra B and D. Nevertheless, the potentially uncertain SNRs of spectral lines in spectra B and D did not cause significant disagreements between measured wavenumbers and Nd III level energies identified in the analysis.

5.3 Spectral Line Fitting and Line List Creation

The first step after obtaining the phase-corrected and noise normalised Nd-Ar PDL FT spectra was to fit each of the observed spectral lines using model line profiles for a set of parameters for each line to produce a ‘line list’ for each spectrum. This is generally a laborious process in the

analysis of complex atomic spectra and took many weeks to complete for the six Nd-Ar PDL FT spectra (Table 4.6). An advantage of inspecting the spectra line-by-line is that it helps the spectroscopists to familiarise themselves with the spectra, obtaining general information such as line profiles, locations of strong lines, and line densities. The spectral lines were first fitted using tools in the *XGREMLIN* [122] program and later adjustments to the line list were made through my custom line fitting program (see subsection 5.3.6). The primary parameters of interest for each line are the observed wavenumber, SNR, FWHM, and intensity which is the area under the line, proportional to photon flux. The observed wavenumbers and their uncertainties (calculated using SNR and FWHM) are the most important parameters to determine accurately since these are then used to establish accurate experimental level and transition energies, the aim of the Nd III term analysis.

5.3.1 Voigt Profile Fitting and Statistical Wavenumber Uncertainty

The Voigt profile was used to fit the spectral lines, which is the ideal profile considering all broadening effects discussed in subsection 2.5.3. The observed spectral lines were in general very well described by the Voigt profile, the statistical wavenumber uncertainty of line i fitted by a Voigt profile is given by [119, 120]

$$\delta\sigma_{\text{meas},i} \approx \frac{\sqrt{R_i \cdot FWHM_i}}{SNR_i}, \quad (5.1)$$

where R_i is the resolution of the spectrum containing line i . However, small deviations were evident from fit residuals peaking around 1% of the SNR of strong and symmetric lines with no obvious signs of self-absorption. A weak line may not be classified as observed if it is blended with a strong line (or with wings of a strong line due to phase errors and instrumental artefacts) with more than two orders of magnitude higher relative intensity, i.e., one cannot tell whether the weak line is in the fit residuals, in which case the wavenumber uncertainty of such a strong line would be considered unaffected and the line itself would not be classified as a blend.

Empirically, any SNR_i above 100 are reduced to 100 in the uncertainty calculation to prevent unrealistic uncertainties since there are generally non-noise related factors contributing to a minimum $\delta\sigma_{\text{meas}}$; the Voigt profile is not a perfect fit, e.g., deviations from the Maxwellian velocity distribution of atoms means deviation from the Gaussian profile due to Doppler broad-

ening, uncertainties in phase correction will affect the profile in the real spectrum, existence of self-absorption, unresolved small hyperfine or isotope structure, unknown blend with much weaker lines, and the observed profiles were convolved with the finitely wide instrumental function, which is difficult to fully define as was discussed throughout [Chapter 3](#).

5.3.2 Line Profiles due to Nd Isotope Shifts

Table 5.2: Relative Abundance of Naturally Occurring Nd Isotopes

Isotope	^{142}Nd	^{143}Nd	^{144}Nd	^{145}Nd	^{146}Nd	^{148}Nd	^{150}Nd
Relative Abundance (%)	27.15	12.17	23.80	8.29	17.19	5.76	5.64

Naturally occurring Nd contains 7 stable isotopes, and their relative abundances [140] are listed in [Table 5.2](#). As discussed in [section 2.4](#), fine structure atomic energy levels are perturbed by different isotopic nuclei, which were observable in Nd line profiles in the Nd-Ar FT spectra. Examples of Nd line profiles showing isotope shifts are shown in [Figure 5.9](#) and at 20288 cm^{-1} of [Figure 5.6](#). Although there are 7 isotopes, only five peaks are visible in [Figure 5.9](#) in the lines measured in the Nd-Ar HCL because the two isotopes ^{143}Nd and ^{145}Nd with odd nucleon numbers also have HFS in their energy levels. HFS spreads and redistributes intensities of the less abundant ^{143}Nd and ^{145}Nd lines into many more component lines, which were much weaker and were not possible to see in the FT spectra due to being either lost in the noise or insufficient spectral resolution. The lines of the five even nucleon number isotopes were very commonly observed as components of the fine structure transition line, which was actually useful in line classification (see [subsection 6.3.2](#)).

5.3.3 Centre-of-gravity Fitting

If one wanted to obtain information on HFS and isotope structure, a Voigt profile would be used to fit each fine structure transition of each Nd isotope and each hyperfine transition of each Nd isotope. The present work however aims to establish experimental level energies of fine structure levels and not to establish individual HFS or isotope shift components. Therefore, the isotope and hyperfine structure effects of affected lines were averaged to obtain unperturbed fine structure level energies. This averaging was performed by estimating the wavenumber of a fine

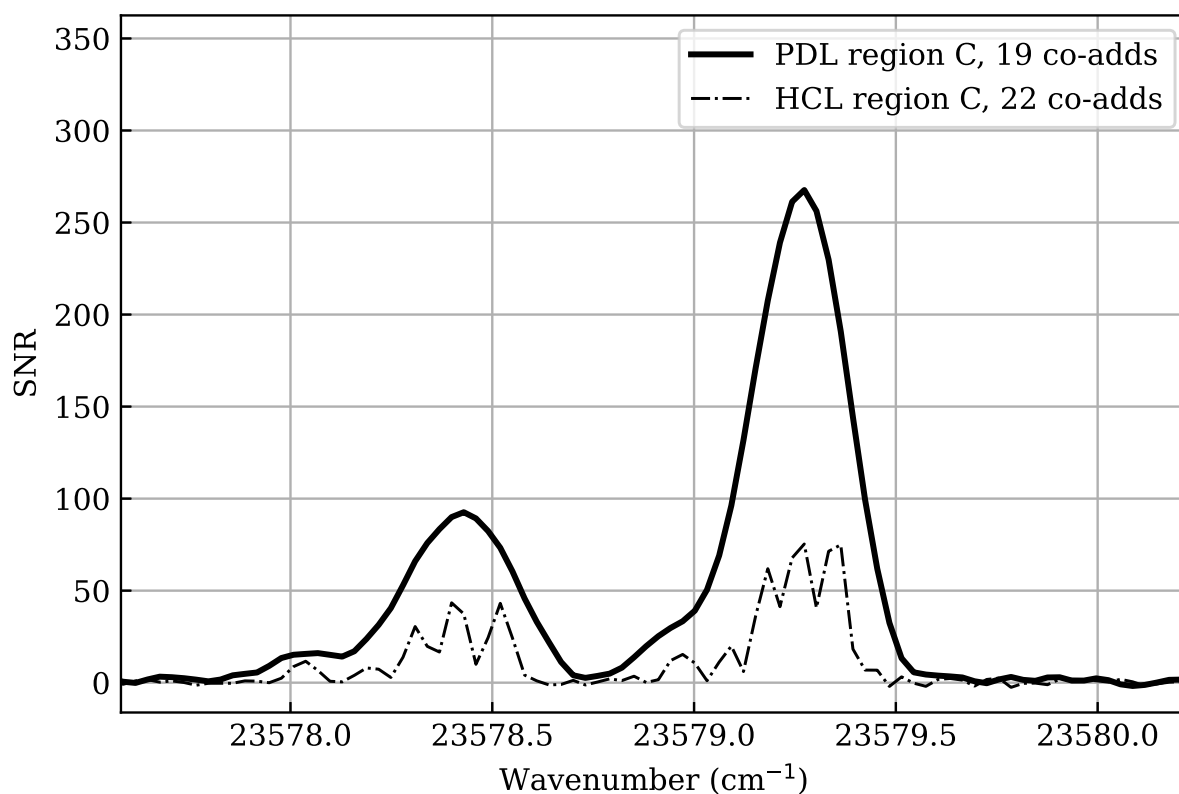


Figure 5.9: Two Nd lines showing the expected isotope line profile observed in the PDL and HCL FT spectra. The higher wavenumber line is from Nd II, the other is unclassified but also likely from Nd II due to enhanced SNR in the PDL and because all Nd III $4f^4 - 4f^35d$ profiles were found in this work to skew in the opposite direction (see [subsection 2.4.2](#) for explanation).

structure line to be its average photon wavenumber, i.e., $\sum_i \sigma_i I_i / \sum_i I_i$ where I_i is proportional to the photon flux per unit wavenumber, similar to how a centre-of-mass is calculated, hence the name centre-of-gravity (COG) fit. The area under the spectral line was obtained from the numerical integration of I_i over σ_i .

The choice of the wavenumber limits of a particular fine structure transition spectral line containing the wavenumbers σ_i will affect the resulting COG wavenumber. Typically, the wavenumber limits are where the line reaches the noise level, but this is especially difficult for noisy lines or slightly blended lines. Empirically, the observed wavenumber uncertainty (Equation 5.1) is doubled for a COG-fitted wavenumber [119]. Many non-blended spectral lines showing significant and recognisable isotope shift line profiles were fitted using the COG method.

5.3.4 Asymmetric Voigt Profile Fitting

Limitations of COG line fitting arise when an asymmetric line due to nuclear effects is not obvious to the eye or when a line is blended with one or more transitions. COG fitting is not applicable for the latter scenario. Every observed Nd spectral line should be in principle fitted using the COG method as isotope shifts and hyperfine structure exist for all levels. However, not all levels have significant enough nuclear perturbations to distort the fine structure line profile to require COG fitting. However, upon familiarisation with the Nd-Ar PDL FT spectra, I found a large fraction of spectral lines would require COG fitting, but I considered this laborious approach to be impractical due to the immense number of lines and blends in the Nd-Ar PDL FT spectra.

Recognising line profiles affected by nuclear effects was important as this could aid line classification (see subsection 6.3.2). For Nd line profiles in the Nd-Ar PDL FT spectra, many were ever so slightly asymmetric to the eye, noticed during the initial line list creation for each spectrum using *XGREMLIN*. To address this, to avoid performing COG fitting to tens of thousands of lines, and to more reliably fit asymmetric line profiles in blends, an asymmetric Voigt profile was employed to fit spectral lines to include small nuclear perturbations.

As expected, the line widths observed in the Nd-Ar PDL FT spectra were dominated by the Doppler width (Equation 2.37). This was deduced as the Lorentzian width component was

one order of magnitude lower than the Gaussian width component for the Voigt profile fits. Therefore, an asymmetric Voigt profile could be produced by varying the Gaussian width component as a function of wavenumber across a spectral line using one parameter. More specifically [141], the Gaussian width is

$$G_w(\sigma) = \frac{2G_{w0}}{1 + e^{a(\sigma-\sigma_0)}}, \quad (5.2)$$

where a is the asymmetry parameter, G_{w0} and σ_0 are the Gaussian width and wavenumber of the usual Voigt profile ($a = 0$) respectively. The wavenumber of the fitted line was estimated using the COG of this asymmetric Voigt profile.

This asymmetric Voigt profile was of course not an accurate physical description of isotope shifts, however, it approximated the line profiles extremely well, allowing ~ 6000 lines showing slight asymmetry to be fitted automatically, and thus overall improvements to wavenumber fitting and wavenumber accuracy were achieved. In the example shown in Figure 5.10, the choice of COG wavenumber limits was difficult due to slight blending with a second weaker line, the asymmetry was not obviously recognisable and only evident from Voigt fit residuals. When fitted using the Voigt profile, the observed wavenumber differed from Ritz¹ and asymmetric Voigt fit values by more than the wavenumber uncertainty. The example in Figure 5.10 was fitted with $a = -1.62$, and any spectral lines fitted using asymmetric Voigt profiles with $|a| > 1$ were visibly asymmetric, which indicated significant nuclear perturbations of the energy levels of the transition. The statistical wavenumber uncertainties (Equation 5.1) were there doubled for $|a| > 1$, similar to the uncertainty estimation of manual COG fitting. The asymmetry parameter a was fixed at 0 for lines with SNRs lower than 10 since asymmetry could come from the noise for these lines.

¹The Ritz wavenumber is the wavenumber separation between best estimates of level energies determined by the measured wavenumbers of all observed transitions, see section 6.4 for more information. In the case of Figure 5.10, a much stronger transition with 2000 SNR dominates the weighted estimation of the Ritz wavenumber, hence the symmetric Voigt fit was confidently less accurate.

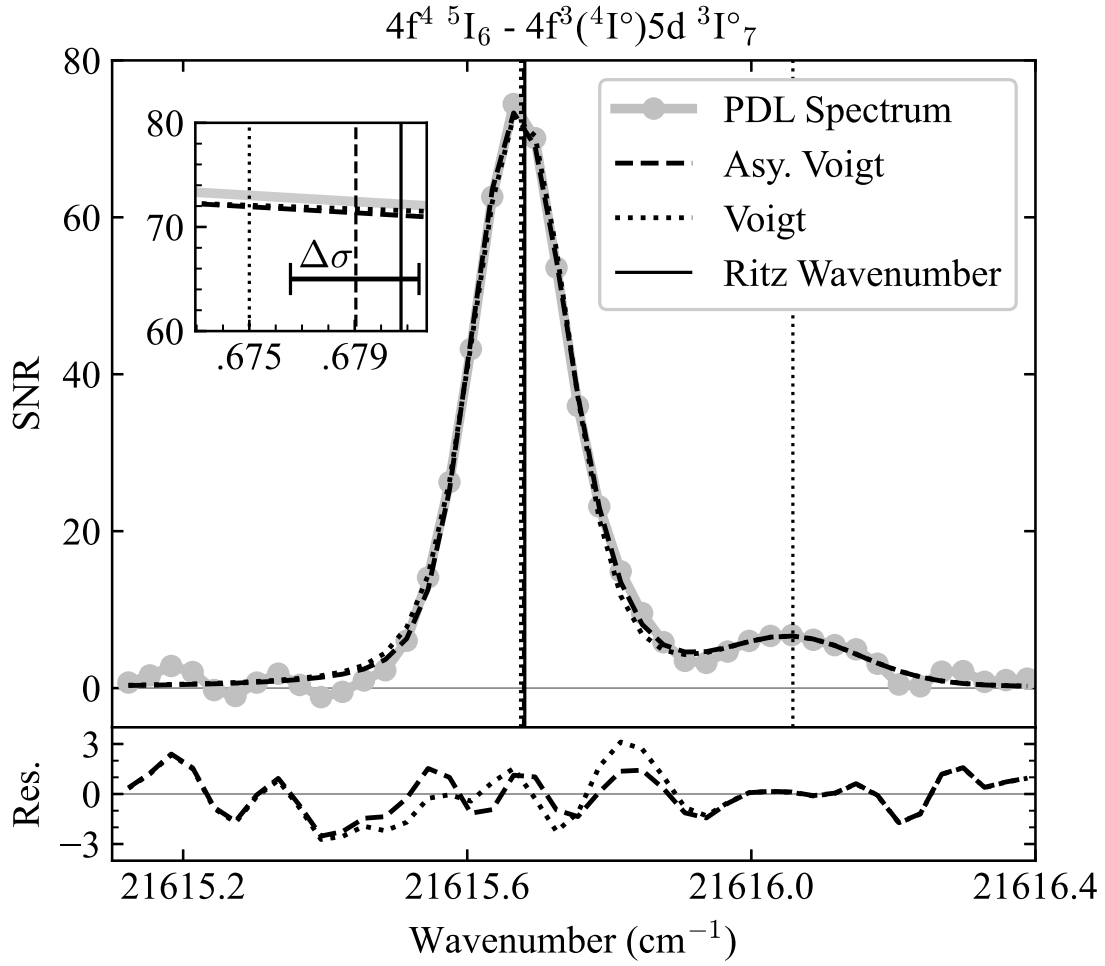


Figure 5.10: Nd III transition $4f^4 \ ^5I_6 - 4f^3(^4I^\circ)5d \ ^3I^\circ_7$ at $21615.679 \text{ cm}^{-1}$, slightly blended with an unclassified line at $21616.058 \text{ cm}^{-1}$. Fits using asymmetric Voigt and normal Voigt profiles are shown in dashed and dotted lines respectively, their residuals are shown in the lower plot and their fitted wavenumbers are shown by the vertical lines. The wavenumber uncertainty of the asymmetric Voigt fit $\Delta\sigma$ is shown in the zoomed section. The Ritz wavenumber is also shown as a solid black vertical line. Figure adapted from Ding et al. (2024) [96].

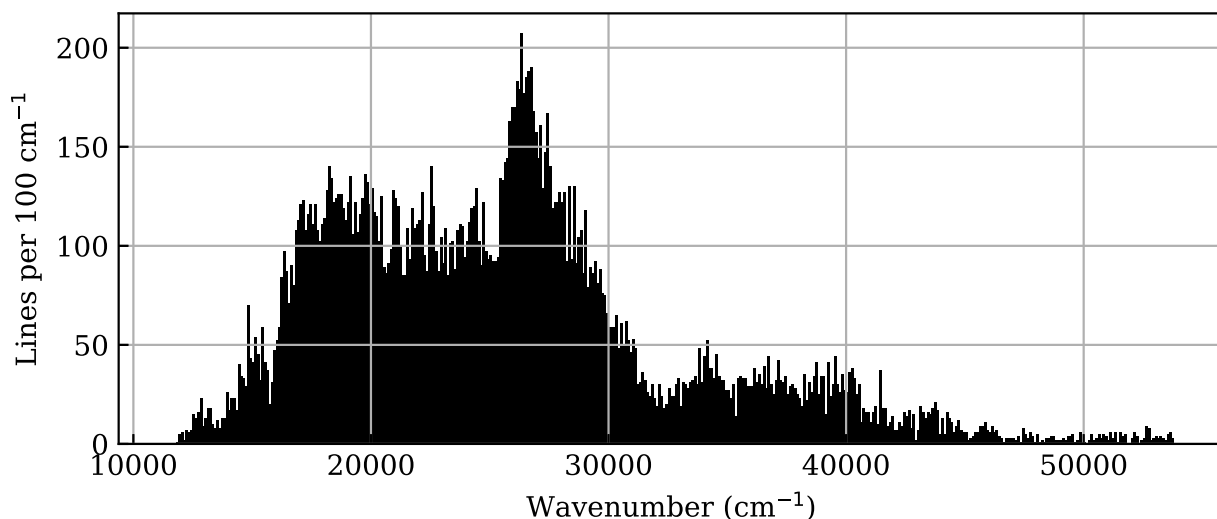


Figure 5.11: Histogram of the 21584 fitted lines of the Nd-Ar PDL FT spectra in bin widths of 100 cm^{-1} . This distribution is largely dependent on the experimental parameters (Table 4.6), e.g., instrumental response and discharge conditions.

5.3.5 Challenges in Fitting the Nd-Ar FT PDL Spectral Lines

As discussed in the Chapter 1, the REEs have very complex atomic spectra, and blended spectral lines are expected to be very common and had been the main limitation in the experimental analyses of their atomic structure in the past. Figure 5.11 shows the overall line densities of the Nd-Ar PDL spectra as a histogram of the number of lines per 100 cm^{-1} of the fitted lines. The high frequency of line-blending and difficulties in line fitting within the line-rich visible spectral region are demonstrated in Figure 5.12, where the HCL and PDL possessed different plasma environments with different intensities and line widths of Nd transitions. One may argue that the 13 fitted PDL lines were all blended to some extent and there could be unfitted weak lines in the PDL spectrum. However, the presence of significant blends could be detected in the residuals of the line fits and very minor blending was accounted for in the wavenumber uncertainties (e.g. doubled uncertainties for $|a| > 1$). Isotope shifts of Nd energy levels is another layer of complexity in line identification and fitting; in Figure 5.12, the unclassified line at 19667.9 cm^{-1} was possibly misidentified as an individual line rather than a part of the isotope structure of the Nd I line.

It is essentially not possible to produce a line list that perfectly describes the observed spectra. Ambiguities exist when one decides how to fit spectral lines, e.g., a weak line could be mistaken as noise and vice versa, a blend may not be obvious, where lines showing significant

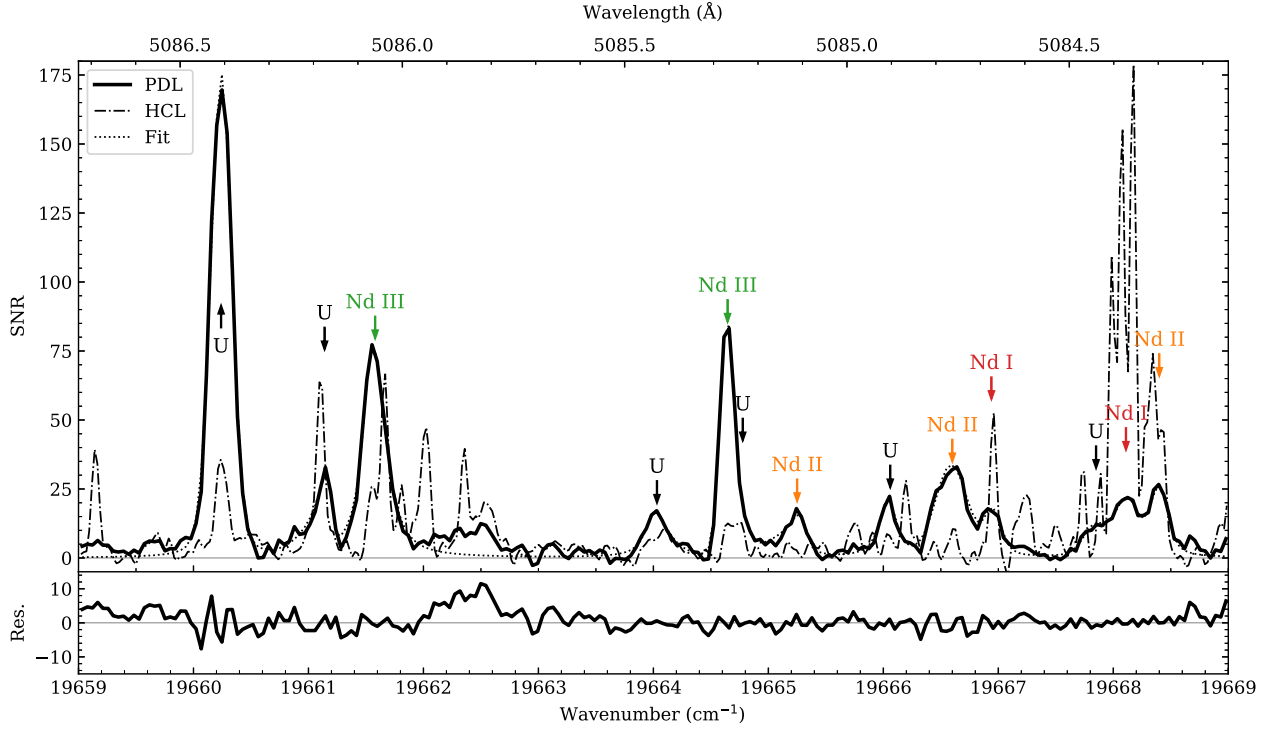


Figure 5.12: Observed Nd-Ar spectra between 19659-19669 cm^{-1} containing lines with intermediate signal-to-noise ratios and showing weak and uncertain blended lines. PDL and HCL spectra are the solid and dash-dotted lines respectively. The dotted line shows the fit to the PDL spectrum, residuals are shown at the bottom. Lines identified in the PDL spectrum are indicated by vertical arrows and labels, those with label U are unclassified. Figure from Ding et al. (2024) [96].

isotope/hyperfine structure or self-absorbed lines could be mistaken as blends. To resolve this, one would need information on the lines of interest, such as species of origin, level energies, level populations, level hyperfine structure constants, level isotope shifts, and transition probabilities, which, in the case of Nd, were often limited and is in fact the main motivation of the present work. Inaccuracies and incompleteness of the line list were expected at all stages of the analysis and in addressing the frequent changes required in the line list, I created a custom spectrum fitting program. Its importance is discussed in the next section and its functionalities are explained in [Appendix B](#).

5.3.6 Custom Line Fitting Program

The asymmetric Voigt profile ([subsection 5.3.4](#)) I used for spectral line fitting was not available in the FT spectrum fitting program *XGREMLIN* [122] and frequent alterations of the line list

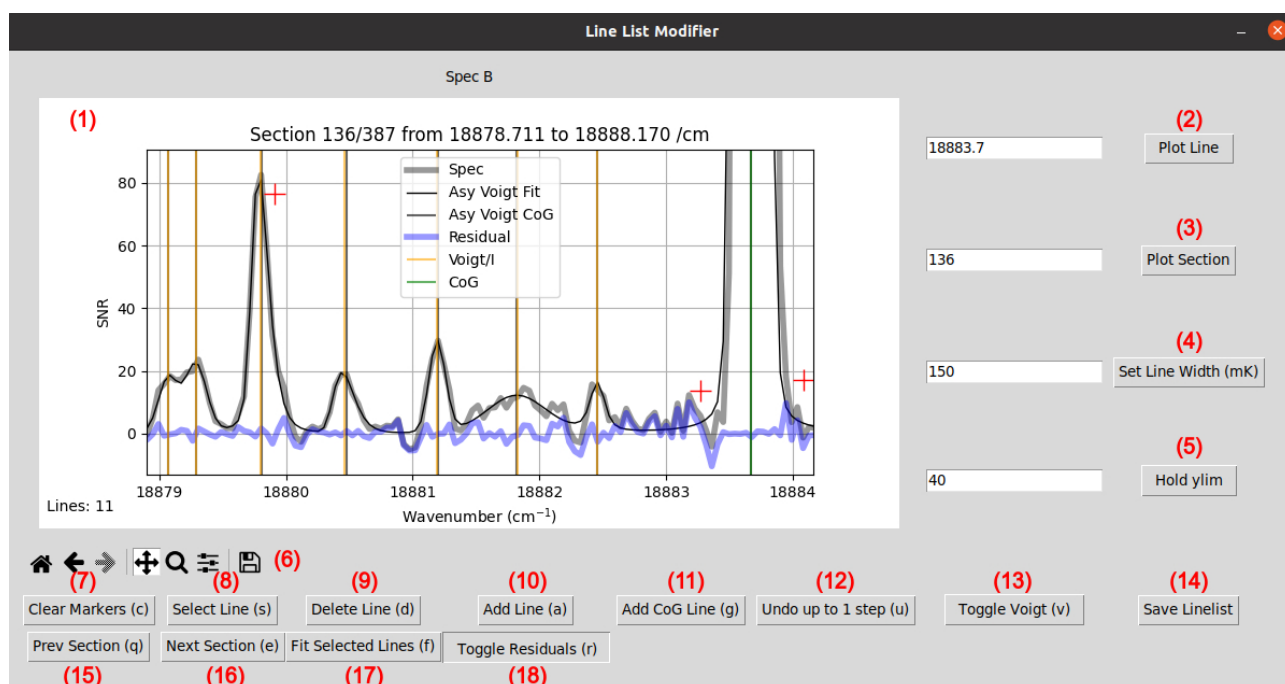


Figure 5.13: Graphical user interface of the line fitting program used to alter the line list during the analysis of Nd III atomic structure.

were also expected during the analysis of Nd III atomic structure (due to blends and weak lines, see subsection 5.3.5 and section 6.7). To accommodate these needs for the analysis, I developed a custom computer program, which allowed a streamlined workflow by automatically calibrating wavenumbers and intensities of the fitted lines, and producing inputs to other common computer programs I used for atomic structure analyses (more details in the discussion of Figure 6.7).

The custom line fitting computer program was written in *Python* using the *matplotlib*, *tkinter*, *scipy*, *numpy*, and *pandas* packages, with inspirations from *XGREMLIN* [122]. The graphical user interface is shown in Figure 5.13, and the functionalities (1) to (18) are explained in Appendix B. All three fitting methods, Voigt, COG, and asymmetric Voigt fitting were made possible. Wavenumbers fitted using Voigt profiles in *XGREMLIN* are shown as yellow vertical lines, vertical black lines are wavenumbers of asymmetric Voigt profile fitting, this presentation aided the identifications of asymmetric line profiles. A COG fit can be carried out by specifying two wavenumber limits by clicking on the plot, an example is shown by the two red crosses around a strong Nd III resonance transition.

After the initial line list creation using *XGREMLIN*, i.e., using a line detection threshold SNR of 10, manually adding weak lines for Voigt profile fitting, manually adding lines for COG fitting (around 500), and checking stronger lines and residuals, the entire line list was fitted

again in the custom program using the asymmetric Voigt profiles. Lines already fitted using the COG method were not fitted again, these lines showed very obvious and common isotope patterns (e.g. [Figure 5.9](#), [Figure 6.4](#)). The spectrum fitting using my custom program required another inspection to double-check the asymmetric Voigt fits, such as looking for unconsidered blends and extreme asymmetry parameters (e.g. $|a| > 5$). Newly fitted lines are automatically wavenumber and intensity calibrated. The methods for wavenumber and intensity calibrations are detailed in the next two sections.

5.4 Absolute Wavenumber Calibration

The six Nd-Ar PDL FT spectra of [Table 4.6](#) were calibrated onto an absolute wavenumber scale set by the caesium frequency standard (e.g. [\[72\]](#)). As discussed in [Chapter 3](#), the wavenumber axis of a FT spectrum is scaled linearly by a small calibration factor due to instrumental effects, e.g., finitely sized aperture, systematic offsets in optical path measurement. This is measured using a frequency stabilised He-Ne laser in the Imperial College VUV FT spectrometer and the laser takes a different path through the spectrometer compared to the PDL radiation.

The measured wavenumber σ_{meas} is related to the calibrated absolute wavenumber σ_{cal} by [\[142\]](#)

$$\sigma_{\text{cal}} = (1 + k_{\text{eff}})\sigma_{\text{meas}}, \quad (5.3)$$

where k_{eff} is the linear calibration factor to remove the instrumental wavenumber scaling of a FT spectrum, which can be obtained if σ_{cal} is known for at least one line in the spectrum. In practice, σ_{cal} for multiple lines across the widest possible spectral range is used for a weighted average of the calibration factor k_{eff} (see the next section). As each of the six Nd-Ar PDL FT spectra was measured under different instrumental conditions, a different k_{eff} was determined for each spectrum.

The suitable σ_{cal} were 28 Ar II transitions [\[143\]](#), measured by Whaling et al. (1995) [\[144\]](#) using FT spectroscopy. These Ar II lines are wavenumber calibration standards because their transition energies were found to be insensitive to pressure shifts [\[143\]](#) as their upper-levels are low-lying, tightly bound, and not easily affected by inter-atomic interactions. The Ar II wavenumber standards [\[144\]](#) were calibrated against CO wavelength standards from heterodyne

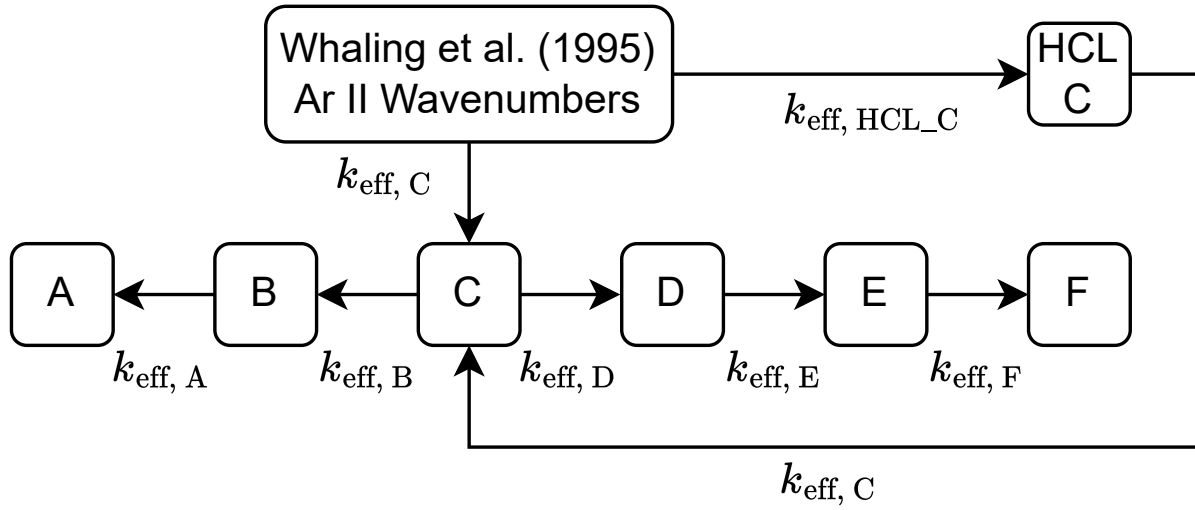


Figure 5.14: Diagram illustrating the order in which the spectra are calibrated starting from calibrating spectrum C using the Ar II wavenumber standards. The arrows indicate the determination and application of calibration factors $k_{\text{eff},j}$ for spectrum j . For example, $k_{\text{eff},B}$ is determined using lines in spectrum B that are also in spectrum C, where the line wavenumbers in spectrum C had been calibrated using $k_{\text{eff},C}$ previously. A second calibration route for spectrum C using the Nd-Ar HCL spectrum is also shown, this was to check consistency using a different set of Ar II reference lines.

frequency measurements [145] with accuracies less than one part in 10^9 , which in turn referred to the caesium standard (e.g. [72]).

The spectrum containing most of the 28 Ar II lines was spectrum C of Table 4.6. After the k_{eff} of spectrum C was determined using these Ar II lines, all lines in C were calibrated using Equation 5.3 to the absolute wavenumber scale. Wavenumbers of calibrated lines of spectrum C that were present in the overlapping spectral regions with spectra B and D then became suitable σ_{cal} for the calibration of spectra B and D. This process was iterated until the wavenumbers of all Nd-Ar PDL FT spectra were calibrated, see figure Figure 5.14 for an illustration of this calibration process.

5.4.1 Calibration Factor

Within a spectrum, the calibration factor $k_{\text{eff},i}$ of an individual line i is

$$k_{\text{eff},i} = \left(\frac{\sigma_{\text{cal},i}}{\sigma_{\text{meas},i}} \right) - 1 \quad (5.4)$$

using its calibrated wavenumber $\sigma_{\text{cal},i}$ and measured wavenumber $\sigma_{\text{meas},i}$. The k_{eff} of a spectrum is then the weighted average of $k_{\text{eff},i}$

$$k_{\text{eff}} = \frac{\sum_i w_i k_{\text{eff},i}}{\sum_i w_i}, \quad (5.5)$$

with weights $w_i = (\delta k_{\text{eff},i})^{-2}$ where²

$$\delta k_{\text{eff},i} = (1 + k_{\text{eff},i}) \sqrt{\left(\frac{\delta \sigma_{\text{cal},i}}{\sigma_{\text{cal},i}}\right)^2 + \left(\frac{\delta \sigma_{\text{meas},i}}{\sigma_{\text{meas},i}}\right)^2}. \quad (5.6)$$

The uncertainty in k_{eff} is given by [142, 146]

$$\delta k_{\text{eff}} = \frac{\sqrt{\sum_i [w_i + w_i^2 (k_{\text{eff}} - k_{\text{eff},i})^2]}}{\sum_i w_i}. \quad (5.7)$$

5.4.2 Wavenumber Uncertainty

To estimate $\delta k_{\text{eff},i}$, the statistical uncertainty of measured wavenumber $\delta \sigma_{\text{meas},i}$ and uncertainty of the calibrated wavenumber $\delta \sigma_{\text{cal},i}$ were needed.

The statistical uncertainty of line i is given by Equation 5.1. For the Ar II wavenumber standard lines in spectrum C, $\delta \sigma_{\text{cal},i}$ were their measurement uncertainties [144]. For other spectra, $\delta \sigma_{\text{cal},i}$ were the final wavenumber uncertainties of lines after calibration through the uncertainty propagation using Equation 5.3, where

$$\delta \sigma_{\text{cal},i} = \sqrt{(\delta \sigma_{\text{meas},i})^2 + [\delta(k_{\text{eff}} \sigma_{\text{meas},i})]^2} = \sqrt{(\delta \sigma_{\text{meas},i})^2 + (\delta \sigma_{\text{sys},i})^2}. \quad (5.8)$$

The uncertainty $\delta(k_{\text{eff}} \sigma_{\text{meas},i})$ is referred to as the systematic uncertainty, given by

$$\delta \sigma_{\text{sys},i} = k_{\text{eff}} \sigma_{\text{meas},i} \sqrt{\left(\frac{\delta k_{\text{eff}}}{k_{\text{eff}}}\right)^2 + \left(\frac{\delta \sigma_{\text{meas},i}}{\sigma_{\text{meas},i}}\right)^2} = \delta k_{\text{eff}} \sigma_{\text{meas},i}, \quad (5.9)$$

since the second term in the square root is negligible compared to the first in the Nd-Ar PDL FT spectra.

²The $(1 + k_{\text{eff},i})$ is often simplified to unity in the literature (e.g. [142]), because $k_{\text{eff},i}$ are a few orders magnitude smaller than unity.

The systematic uncertainty $\delta\sigma_{\text{sys},i}$ depends solely on δk_{eff} of the spectrum, which, from equation [Equation 5.7](#), depends on three factors: $\delta k_{\text{eff},i}$, variance of $k_{\text{eff},i}$, and the number of lines used for determining k_{eff} . $\delta k_{\text{eff},i}$ contains calibration uncertainty of the lines, but this quantity is used as the weightings. If the selection of lines has very low variance in $k_{\text{eff},i}$ and/or if a much larger number of lines were selected, $\delta\sigma_{\text{sys},i}$ for the spectrum to be calibrated can be lower than the $\delta\sigma_{\text{sys},i}$ of the neighbouring, already calibrated spectrum. This should not be possible since how well the reference wavenumbers were calibrated would be ignored, in other words, the systematic uncertainties of each spectrum are correlated. To take the previous systematic uncertainties into account, they were added linearly during wavenumber calibration for a total systematic uncertainty $\delta\sigma'_{\text{sys},i}$, since any potential systematic wavenumber shift in a calibrated spectrum will exist in spectra calibrated using the calibrated spectrum. So the final observed wavenumber uncertainties (in parentheses of column 5 of [Table D.1](#)) are

$$\delta\sigma_{\text{cal},i} = \sqrt{(\delta\sigma_{\text{meas},i})^2 + (\delta\sigma'_{\text{sys},i})^2}, \quad (5.10)$$

where

$$\delta\sigma'_{\text{sys},i} = \delta\sigma_{\text{sys},i} + \sum_j \delta\sigma_{\text{sys},j}, \quad (5.11)$$

where $\delta\sigma_{\text{sys},j}$ are mean total systematic uncertainties of the selected calibrated wavenumbers in spectrum j and the summation over j includes all previously calibrated and correlated spectra. The systematic uncertainties of the Ar II wavenumber standards in spectrum C were assumed zero.

The total systematic uncertainties $\delta\sigma'_{\text{sys},i}$ for all lines in the six Nd-Ar PDL FT spectra are illustrated in [Figure 5.15](#), these were added in quadrature with statistical uncertainties ([Equation 5.1](#)) to yield the final calibrated wavenumber uncertainties $\delta\sigma_{\text{cal},i}$ (in parentheses of column 5 of [Table D.1](#)). The linear relationship $\delta\sigma_{\text{sys},i} = \delta k_{\text{eff}}\sigma_{\text{meas},i}$ is clearly seen for each spectrum, $\delta\sigma'_{\text{sys},i}$ is the lowest in spectrum C (21300 to 25369 cm^{-1}), and the step changes in $\delta\sigma'_{\text{sys},i}$ are the linear accumulation of systematic uncertainties from correlated spectra.

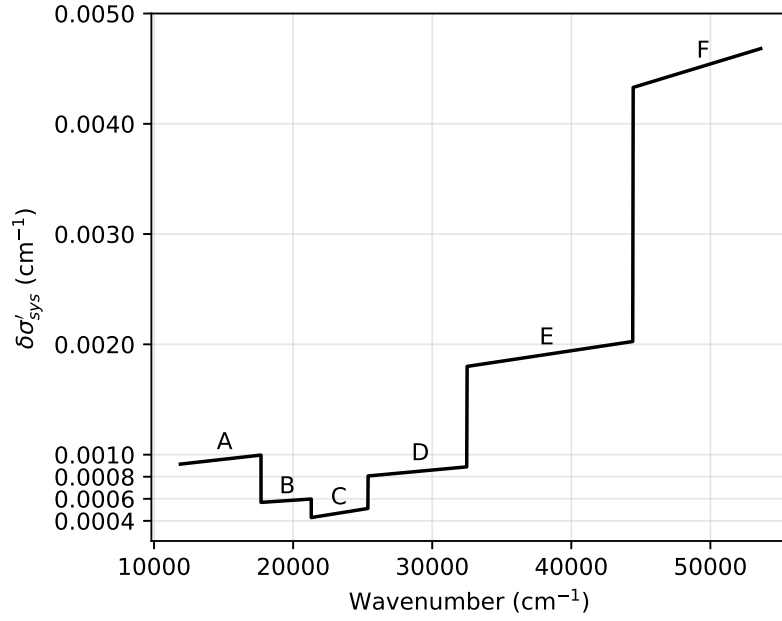


Figure 5.15: Total systematic wavenumber uncertainties as a function of wavenumber. The vertical lines show boundaries of the spectra in the merged line list (see [section 5.6](#)), no lines lie on these boundaries. The section with the lowest systematic wavenumber uncertainty belongs to spectrum C containing the Ar II wavenumber standards used for calibration.

5.4.3 Line Selection for Calibration and Results

Not all 28 Ar II wavenumber standard transitions [143, 144] were used to determine the calibration factor. Similarly, not all lines within overlapping regions of two spectra were used. For a line to be selected for use in calibration, it must resemble the fitting line profile, the Voigt profile, as much as possible for an accurate measurement of its wavenumber. This placed multiple requirements on lines selected for calibration: a minimum SNR, symmetric profile, not blended, fitted using Voigt profiles, minimal self-absorption, and residuals of fit that were at most 2 parts in 100. As lines used for determining calibration factors were shared between two spectra, these requirements must be satisfied in both spectra. After selection, their calibration factors $k_{\text{eff},i}$, the calibration factor of the spectrum k_{eff} , and associated uncertainties were determined. Occasionally, a few selected reference lines were found to have anomalous $k_{\text{eff},i}$ compared to the rest (outliers), which were then removed. The criteria for this removal was when the uncertainty in $k_{\text{eff},i}$ did not overlap with 2 standard deviations in $k_{\text{eff},i}$ from the value of k_{eff} . These could be due to unknown blends, unknown self-absorption, or issues with line fitting.

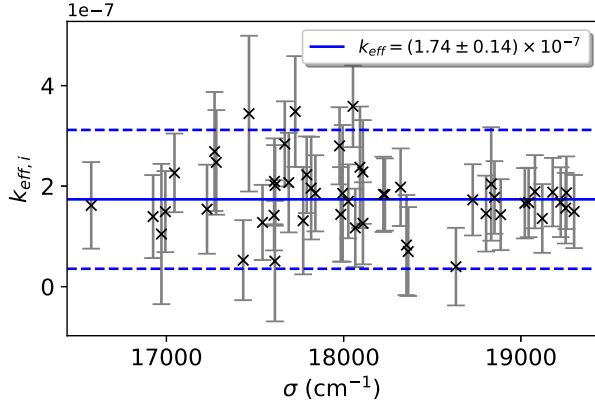
Table 5.3: Summary of wavenumber calibration.

Spec.	Origin of $\sigma_{\text{cal},i}$	No. of $\sigma_{\text{cal},i}$	Min. SNR	k_{eff} (10^{-7})	Mean $\delta\sigma'_{\text{sys},i}$ (10^{-3} cm^{-1})
A	B	51	50	1.74 ± 0.14	0.97
B	C	69	50	1.39 ± 0.09	0.58
C	Ar II	13	28	-3.10 ± 0.20	0.47
D	C	44	50	-2.95 ± 0.12	0.84
E	D	34	25	-2.88 ± 0.19	1.9
F	E	12	25	-4.32 ± 0.38	4.5

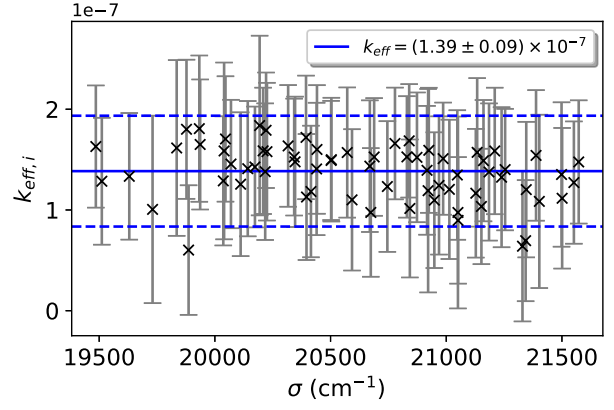
The final sets of lines selected for the determination of calibration factors in each Nd-Ar PDL FT spectrum are shown in Figure 5.16. After removing outliers, the uncertainties in individual $k_{\text{eff},i}$ factors roughly matched with the order of spread of $k_{\text{eff},i}$ evenly around k_{eff} . No significant deviation from the flat relation between $k_{\text{eff},i}$ and wavenumber was observed. Details for calibration line selection and resulting calibration factors k_{eff} of each spectrum are summarised in Table 5.3.

Based on the selection method, only 13 of the 28 Ar II lines were available for the determination of the calibration factor of spectrum C of the Nd-Ar PDL, and other spectra contained less or none of the 28 Ar II lines. To improve the confidence in this initial calibration, the Nd-Ar HCL spectrum containing these Ar II lines was also calibrated and was then used to calibrate spectrum C as a second route, as shown in Figure 5.14. Results are shown in Figure 5.17. In the Nd-Ar HCL FT spectrum C, 18 of the 28 Ar II wavenumber standards were available. The discrepancy in k_{eff} obtained for spectrum C between the two routes (i.e., Figure 5.16c and Figure 5.17b) was 6×10^{-9} , well within uncertainties of both k_{eff} . The discrepancy translates to 0.00012 cm^{-1} at $20\,000 \text{ cm}^{-1}$, which is one order of magnitude smaller than the mean statistical uncertainty $\delta\sigma_{\text{meas}}$ of wavenumbers in C with SNR greater than 50. Therefore, the discrepancy was negligible and the two calibration factors were concluded consistent. Again, no significant deviation from the horizontal relation between $k_{\text{eff},i}$ and wavenumber was observed, and so other systematic effects such as poor phase correction on the measured wavenumbers were concluded negligible.

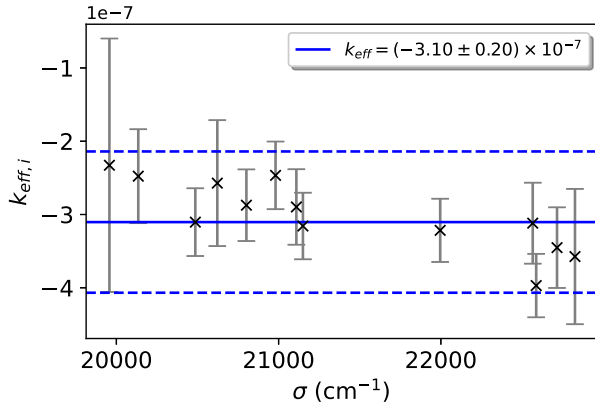
The uncertainty in k_{eff} for spectrum C was lower when calibrating using the Nd-Ar HCL spec-



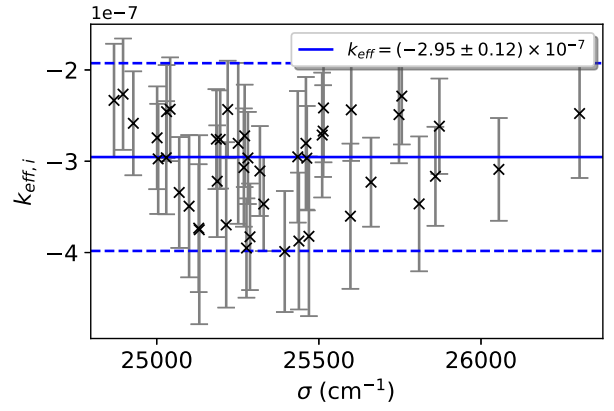
(a) $k_{\text{eff},i}$ of PDL spectrum A using calibration lines from PDL spectrum B



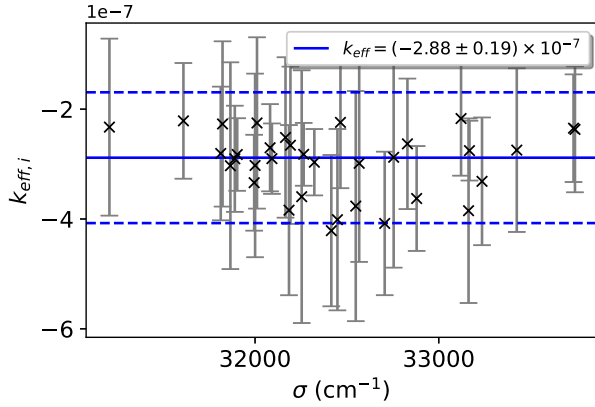
(b) $k_{\text{eff},i}$ of PDL spectrum B using calibration lines from PDL spectrum C



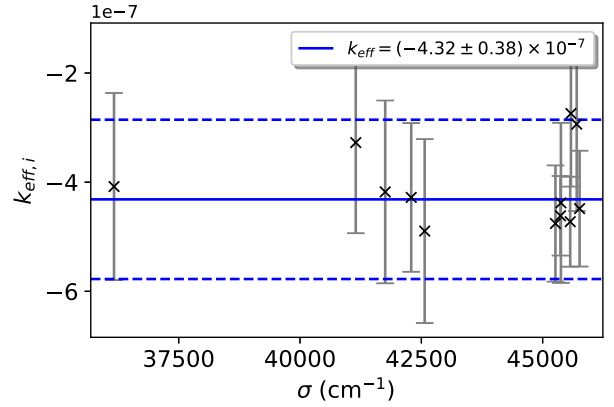
(c) $k_{\text{eff},i}$ of PDL spectrum C using Ar II wavenumber standards



(d) $k_{\text{eff},i}$ of PDL spectrum D using calibration lines from PDL spectrum C

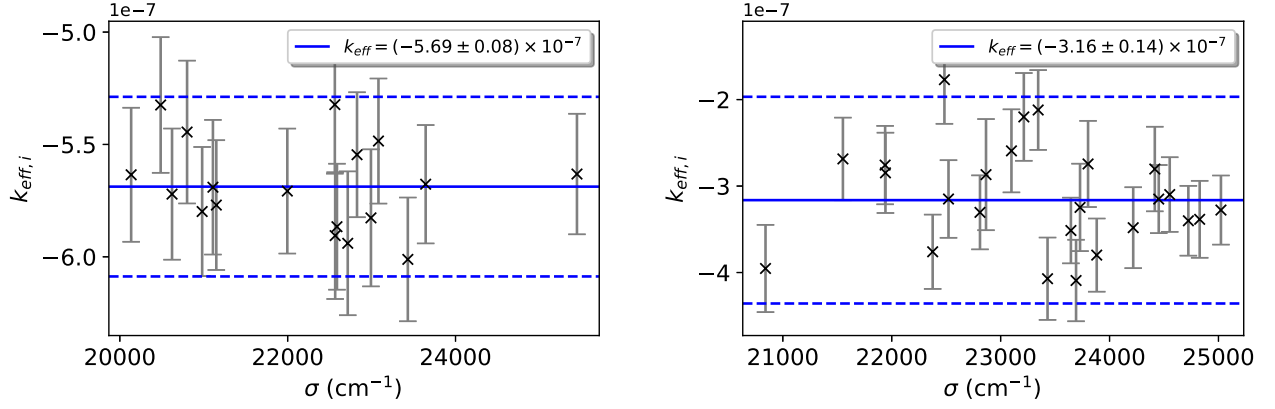


(e) $k_{\text{eff},i}$ of PDL spectrum E using calibration lines from PDL spectrum D



(f) $k_{\text{eff},i}$ of PDL spectrum F using calibration lines from PDL spectrum E

Figure 5.16: Plots of individual calibration factors $k_{\text{eff},i}$ determined from calibration lines in each spectrum against their respective wavenumbers. Error bars show uncertainties $\delta k_{\text{eff},i}$. The blue solid lines are the values of calibration factor k_{eff} for the spectra. The region between blue dashed lines is within two standard deviations in $k_{\text{eff},i}$ from k_{eff} .



(a) $k_{\text{eff},i}$ of HCL spectrum C using Ar II wavenumber standards

(b) $k_{\text{eff},i}$ of PDL spectrum C using calibration lines from HCL spectrum C

Figure 5.17: Plots of individual calibration factors $k_{\text{eff},i}$ determined for Ar II lines in the HCL and calibration lines in spectrum C against their respective wavenumbers. Error bars show uncertainties $\delta k_{\text{eff},i}$. The blue lines are the values of calibration factor k_{eff} for the spectra. The region between dashed blue lines is within two standard deviations in $k_{\text{eff},i}$ from k_{eff} .

trum since spectral lines were narrower in the HCL. However, this k_{eff} obtained from the HCL spectrum was unused for wavenumber calibration. While the Ar II wavenumber standards may be insensitive to pressure conditions, this may not be true for the Nd lines selected for the wavenumber calibration of spectrum C in the second route; the HCL and PDL plasma pressures differ significantly (measured at lamp exits, 0.43 mbar and 2.0×10^{-3} mbar respectively). Investigating whether the selected Nd lines are sensitive to pressure shifts was not feasible since the spectra of Nd I-III are poorly known as most observed lines have unknown upper and lower energy levels.

5.5 Relative Intensity Calibration

The six Nd-Ar PDL FT spectra of Table 4.6 were calibrated onto the same relative intensity scale. Intensity calibration aided the classification of transitions between atomic energy levels in my work by enabling comparisons between measured relative intensities and their theoretical values. The observed intensities in the FT spectra depend on the smoothly varying instrumental response function, the source-aperture geometry (throughput), and PMT gain, all of which differ for each of the six spectra and result in relative response functions defined over the wavenumber ranges of each of the six spectra. The PMT gains were within the linear response regime, so

the calibrated relative intensities are expected to be proportional to their absolute intensities, which were measured as photon fluxes.

Similar to wavenumber calibration, intensity calibration was carried over to neighbouring spectra. For convenience, intensities from all spectra were calibrated relative to intensities measured and calibrated in spectrum C, in the same iterative fashion described by the diagram from [Figure 5.14](#), and using the same calibration lines found in neighbouring spectra used in wavenumber calibration from [Table 5.3](#). The relative intensities post-calibration should only be considered rough estimates, with high uncertainties ($\sim 15\%$ or higher). However, this accuracy is sufficient when comparing with theoretical relative intensities during the energy level analysis since relative intensities of transitions of an energy level often differ by more than an order of magnitude.

5.5.1 Spectral Intensity Response Functions

To determine spectral intensity response functions, spectra of radiometrically calibrated tungsten and deuterium standard lamps were recorded before and after the recording of each of the six Nd-Ar PDL FT spectra from [Table 4.6](#), at 16 co-adds per spectrum. No dramatic variations were found between the before and after spectra. The variations were mostly in the UV at around 3% and were likely due to shifts in the vacuum over hours of recording interferograms. Absolute intensities were known for the standard lamps from their calibration certifications. These were in units of spectral radiance ($\text{Wcm}^{-2}\text{sr}^{-1}\text{nm}^{-1}$) as a function of wavelength $L^{\text{cert}}(\lambda)$, approximately at 5 nm intervals. The intensity per steradian emitted by the lamp within a wavelength interval $d\lambda$ is

$$dI = L^{\text{cert}}(\lambda)d\lambda = \sigma^{-2}L_{\lambda}^{\text{cert}}(\sigma)d\sigma, \quad (5.12)$$

where $L_{\lambda}^{\text{cert}}(\sigma)$ are the $L^{\text{cert}}(\lambda)$ values with wavenumber σ as the x -axis rather than λ . This intensity dI entered the FT spectrometer through the aperture, passed through the optical components and filters, and was measured in the spectrum $S^{\text{obs}}(\sigma)$ as temporally integrated PMT currents proportional to the photon flux, which is related to dI by

$$R(\sigma)dI \propto hc\sigma S^{\text{obs}}(\sigma)d\sigma, \quad (5.13)$$

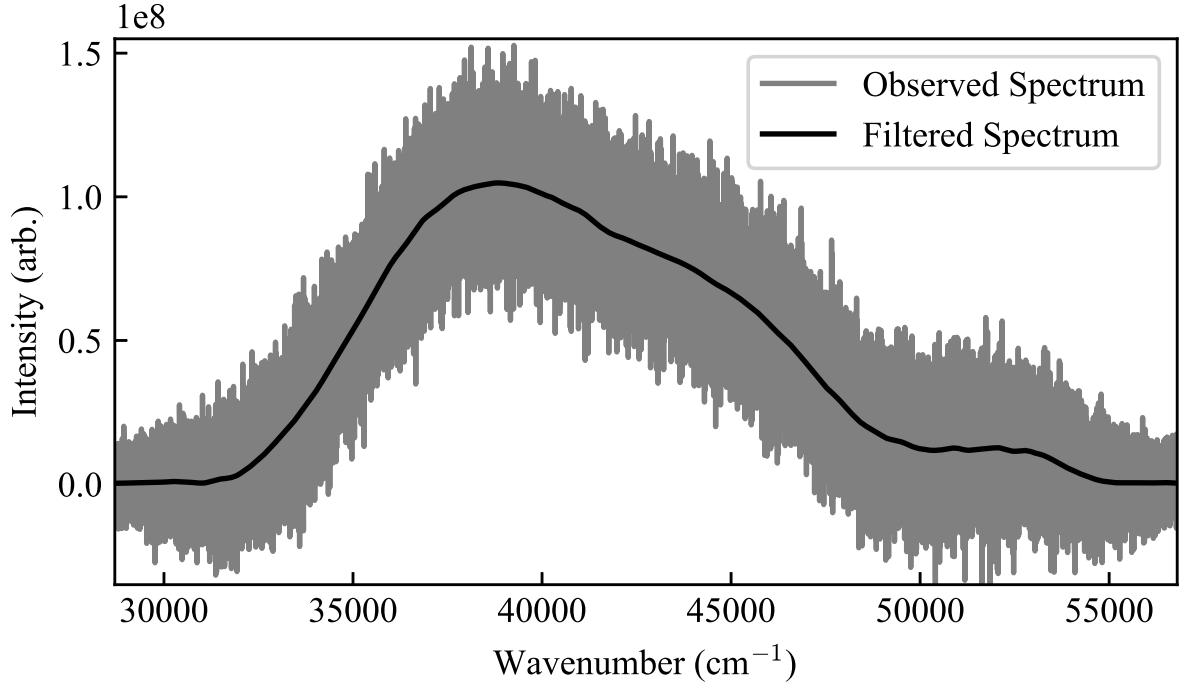


Figure 5.18: Observed and filtered spectrum of a deuterium lamp recorded in the region of spectrum E of Table 4.6. The smooth filtered spectrum is used with the lamp calibration certificate data to generate response function values for each line.

where the input intensity dI is multiplied by the response function $R(\sigma)$ and the proportionality includes experimental factors such as throughput and PMT gain. The relative intensity of a line prior to passing through the instruments is its observed relative intensity (area under the line) divided by $R(\sigma)$.

By equating the two expressions for dI , the response function $R(\sigma)$ is then defined as

$$R(\sigma) \propto \frac{\sigma^3 S^{\text{obs}}(\sigma)}{L_{\lambda}^{\text{cert}}(\sigma)}. \quad (5.14)$$

The proportionality constant is ignored as it is not required in relative intensity calibration; $R(\sigma)$ was normalised using its peak value. Before the determination of the response functions, the observed spectra $S^{\text{obs}}(\sigma)$ were first filtered by triangle functions, i.e., two equally weighted running averages of the same width, where the width was the resolution of the certificate divided by the resolution of $S^{\text{obs}}(\sigma)$. An example of this filtering process is shown in Figure 5.18. The reason for this filtering is to obtain the smoothly varying response function by removing noise and matching the low resolution provided on the calibration certificates that could not measure

sharper spectral features in the standard lamps. Response functions for all spectra are shown in [Figure 5.19](#). The response function values were interpolated using cubic splines at the wavenumber of each line in the line list. At the upper wavenumber limit of spectrum D, the response function suffers noise due to low tungsten lamp intensity in the UV, this was not problematic as no lines above 32480 cm^{-1} from spectrum D were in the line list (see [Table 4.6](#) and [section 5.6](#)).

5.5.2 Relative Intensity Calibration of All Spectra

All line intensities in a spectrum were divided by the normalised response function value for that spectrum at their respective wavenumbers. This gave an intensity-calibrated line list for each spectrum. All spectra were then placed on the same intensity scale set by spectrum C using spectral lines in the overlapping regions of successive spectra. Since the calibrated relative intensities of each spectrum are proportional to their absolute intensities, the relative intensities of each spectrum should also be proportional to the relative intensities in spectrum C. For the calibration of line i , a proportionality constant h_i is obtained from

$$h_i = \frac{I_{\text{cal},i}^C}{I_{\text{cal},i}}, \quad (5.15)$$

where $I_{\text{cal},i}^C$ is the relative line intensity from the spectrum already calibrated onto the scale set by spectrum C and $I_{\text{cal},i}$ is the relative line intensity from the spectrum to be calibrated onto the scale set by spectrum C, which is the measured intensity $I_{\text{meas},i}$ divided by the normalised response function of the spectrum to be calibrated $R(\sigma_i)$.

The h factor of a spectrum and its uncertainty δh was determined using the same weighted average method used for wavenumber calibration ([section 5.4](#)), with uncertainty in the measured intensity $I_{\text{meas},i}$ prior to division by the response function given by [\[119\]](#)

$$\frac{\delta I_{\text{meas},i}}{I_{\text{meas},i}} \approx \frac{2}{SNR_i} \sqrt{\frac{FWHM_i}{R_i}}, \quad (5.16)$$

similar to wavenumber statistical uncertainty, SNR_i above 100 were reduced for this calculation to a cap of 100. Results for h_i and h for all spectra are shown in [Figure 5.20](#). The h_i of spectrum B varied by up to a factor of 2, as opposed to around ten percent for other spectra, so the error

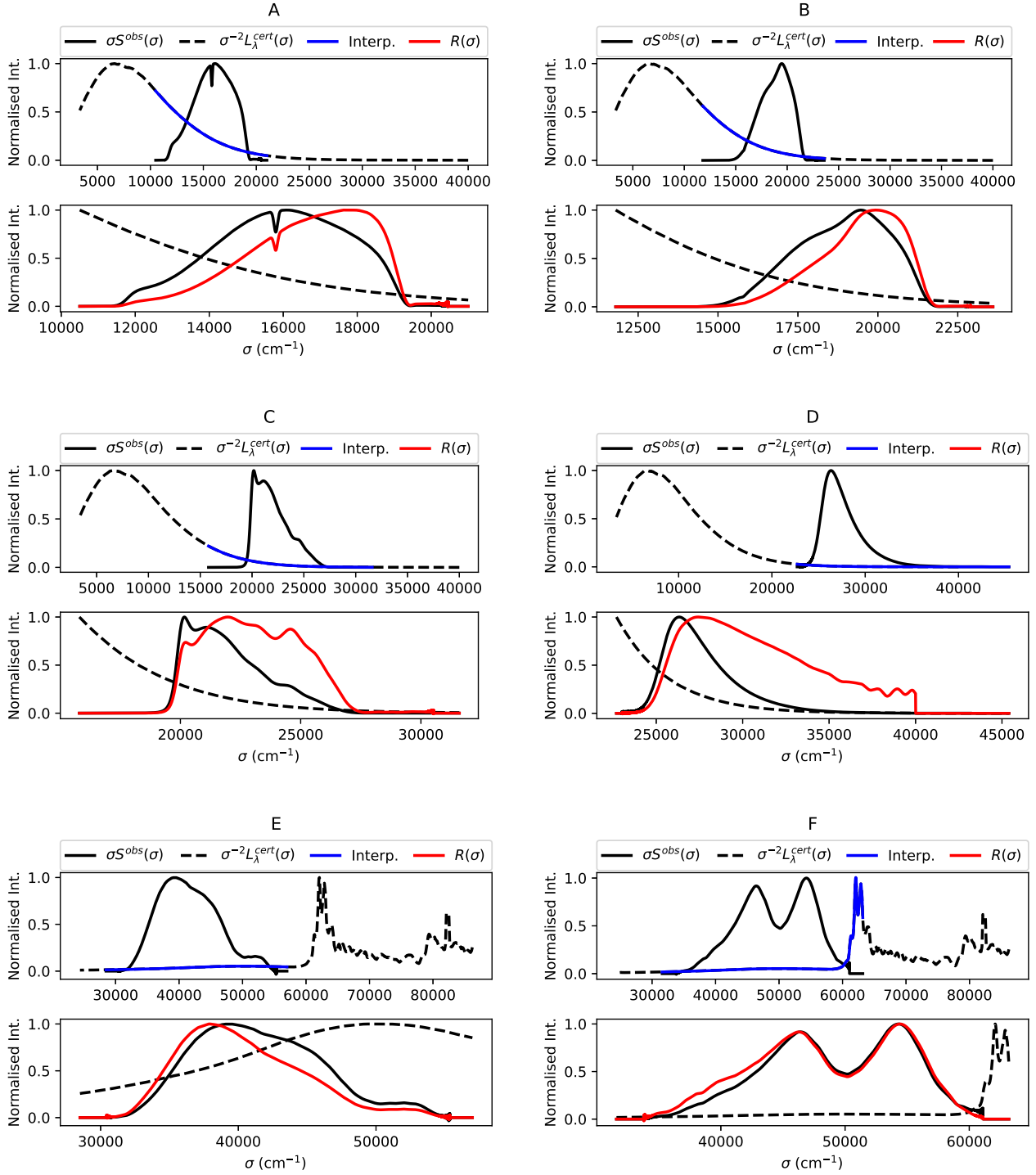
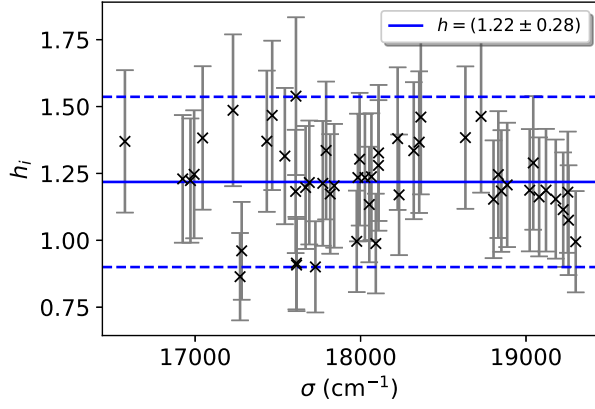
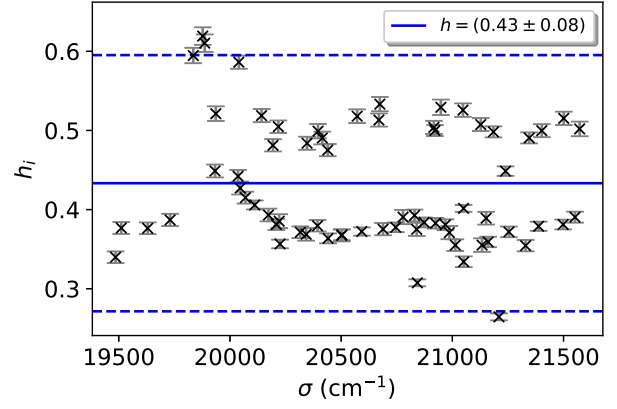


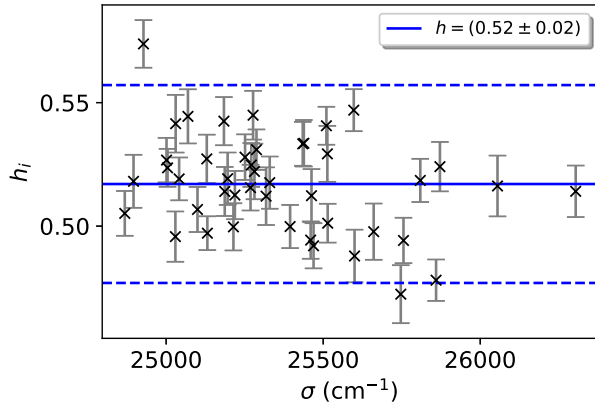
Figure 5.19: Plots showing determinations of the response function $R(\sigma)$ (red) for PDL spectra A to F. The black solid line shows the filtered observed spectra of calibration lamps weighted by σ (black solid), and the black dashed line shows certificate spectra, both in units of relative energy flux per unit wavenumber. The blue lines show sections of the certificate spectra that were interpolated using cubic splines to match the higher resolutions of $\sigma S^{obs}(\sigma)$ to obtain $R(\sigma)$. The dip in the middle of spectrum A is caused by the He-Ne laser, which has a different optical path in the instrument and hence a different phase curve. The certificate spectra between top and bottom panels are on different scales, their peak values within each plot are normalised for illustration and are accounted for in the normalised response curves.



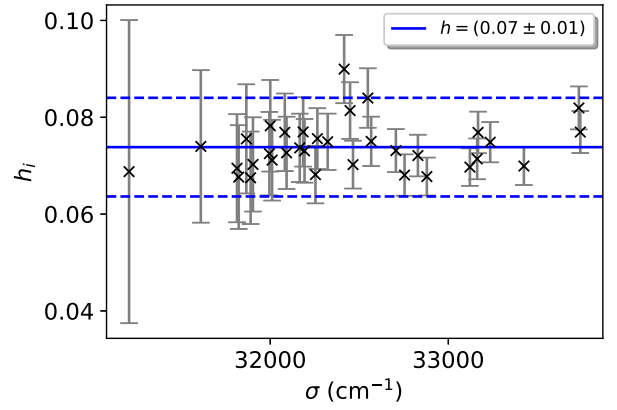
(a) h_i of PDL spectrum A using calibration lines from spectrum B



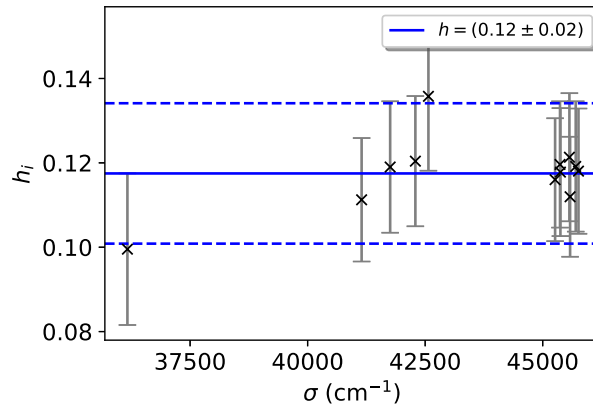
(b) h_i of PDL spectrum B using calibration lines from spectrum C



(c) h_i of PDL spectrum D using calibration lines from spectrum C.



(d) h_i of PDL spectrum E using calibration lines from spectrum D



(e) h_i of PDL spectrum F using calibration lines from spectrum E

Figure 5.20: Plots of individual intensity calibration factors h_i determined for all calibration lines in each spectrum against their respective wavenumbers. Error bars show uncertainties δh_i . The blue lines are the values of calibration factor h for the spectra. The region between dashed blue lines is within two standard deviations in h_i from h .

Table 5.4: Summary of relative intensity calibration using only previously known Nd III lines for spectra A, B, C, and D.

Spec.	$I_{\text{cal},i}^C$ from	No. of $I_{\text{cal},i}^C$	Min. SNR	h	h from σ calibration lines
A	B	8	11	1.03 ± 0.08	1.22 ± 0.28
B	C	5	20	0.31 ± 0.02	0.43 ± 0.08
C	-	-	-	1 ± 0	1 ± 0
D	C	4	8	0.48 ± 0.05	0.52 ± 0.02
E	D	5	30	0.07 ± 0.01	0.07 ± 0.01
F	E	5	15	0.12 ± 0.02	0.12 ± 0.02

bars of h_i of spectrum B look much smaller in comparison due to much larger y -axis extent. The h_i of A also varied more than spectra D, E, and F, but to a lesser extent compared to spectrum B. This could be explained by transitions/level population sensitivity to lamp conditions, as each spectrum was recorded on a different day and lamp conditions may not have been identical. For example, some level populations of Nd II were expected to be affected by the charge transfer reaction of ground state Nd I with Ar II ions [147], which could be sensitive to Ar pressure in the lamp.

The h of spectra A and B were unsatisfactory due to large variation in the values for different spectral lines. So a second attempt at determining the h factors was made using only Nd III lines (except for E and F as no Nd III were known within those regions); the Nd III level populations were not expected to be affected by the resonance charge transfer reaction with Ar II. Results are summarised in Table 5.4. Good consistency was observed between the two attempts for D, E, and F. For the h of A and B, the Nd III lines had lower bound values of h from using all of the wavenumber calibration lines. The relative intensities calibrated against spectrum C were eventually calibrated using the set of h determined in the second attempt only using previously known Nd III lines where possible. These are given in column 5 of Table 5.4, where uncertainties in h are from the standard deviations of h_i of the spectra.

5.5.3 Relative Intensity Uncertainty Estimation

To compare observed and theoretical relative intensities, the uncertainties in the observed relative intensities must be gauged. For line i with intensity $I_{\text{meas},i}$, its relative intensity calibrated

against the relative intensities of spectrum C was then

$$I_{\text{cal},i}^C = \frac{h_i I_{\text{meas},i}}{R(\sigma_i)}, \quad (5.17)$$

this is a product of three quantities, each with their own uncertainty, so the uncertainty in $I_{\text{cal},i}$ was estimated to be

$$\frac{\delta I_{\text{cal},i}^C}{I_{\text{cal},i}^C} = \sqrt{\left(\frac{\delta I_{\text{meas},i}}{I_{\text{meas},i}}\right)^2 + \left(\frac{\delta h_i}{h_i}\right)^2 + \left(\frac{\delta R(\sigma_i)}{R(\sigma_i)}\right)^2}. \quad (5.18)$$

The first term in the square root was determined by [Equation 5.16](#), the second term was determined from [Table 5.4](#), and the last term for the response function comes from several different uncertainties, e.g., continuum source certificate value uncertainties, PDL window transmission, instrumental conditions before and after Nd spectrum measurement (e.g. changes in vacuum or alignment), signal-to-noise of the measured continuum spectra, and alignment differences between the Nd-Ar PDL and standard lamps. From the literature [\[23\]](#), all mentioned effects contribute a few percent of fractional uncertainty, so the fractional uncertainty in $R(\sigma)$ was estimated as 10%. The maximum relative intensity uncertainty for lines with SNR greater than 100 was 20%, the minimum was 10%, and so 15% was recommended for the strongest Nd III lines in Ding et al. (2024) [\[96\]](#). The mean uncertainty for lines below 10 SNR was estimated at 30%.

The above estimation does not include uncertainties when comparing relative intensities from different spectra. The relative level populations cannot be assumed to be the same for all six spectra, due to different lamp conditions on different days. Regardless of whether a spectrum was intensity calibrated using Nd III lines, there was also no guarantee that the upper-level populations of the calibration lines were not sensitive to small changes in pressures and lamp conditions, only some reassurance can be obtained from the small spread of h_i around their weighted mean values since the h_i were sampled from different energy levels. Therefore, extra caution was still expected to be required when comparing relative intensities across different spectra, i.e., uncertainties could be much greater than estimated.

5.6 Merging Line Lists

After the absolute wavenumber and relative intensity calibrations of each of the six Nd-Ar PDL FT spectra (Table 4.6), the lines were merged into one line list. This was done by specifying wavenumber boundaries for each spectrum since lines within overlapping spectral regions were observed in two spectra. The selection of boundary wavenumbers was based on the difference in SNRs observed between two overlapping spectra. This analysis is shown in Figure 5.21. The determined boundaries were 17687, 21300, 25369, 32485, and 44438 cm^{-1} , with the exception that the 21300 cm^{-1} boundary between spectra B and C was chosen due to a slightly poor fit (21177 cm^{-1}) in the y -intercept found for the method shown in Figure 5.21. All wavenumbers in the merged line list are plotted in Figure 5.22, the height of each line is its relative intensity calibrated against the relative intensities of spectrum C. With the merged line list and the custom spectrum fitting program at hand, the analysis of the Nd-Ar PDL FT spectra and the atomic structure of Nd III was ready to commence.

5.7 Summary of the Nd FT Spectra and their Calibration

Interferograms recorded with the Nd-Ar PDL, Nd-Ar HCL, and Nd-Ne HCL were co-added, transformed, and phase corrected to produce emission spectra of the light sources. Spectra of the Nd-Ar PDL were fitted to obtain line wavenumbers and relative intensities of the observed atomic transitions, the uncertainties of these quantities were determined by the fitted SNRs and FWHMs. Transition wavenumbers and relative intensities and tabulated into a merged line list for the atomic structure analysis of Nd III. At the conclusion of the term analysis of Nd III, 21584 lines were fitted in total, of which 15002 lines were fitted using Voigt profiles, 6085 lines were fitted with the size of asymmetry parameter of Equation 5.2 greater than 1, and 497 were fitted using the COG method. Approximately 2000 spectral lines were fitted after the line list preparations described in this chapter, during the atomic structure analysis of Nd III discussed in the next chapter. The dynamic range of the Nd-Ar PDL FT spectra is about four orders of magnitude, with the maximum SNR at 8600. The mean total wavenumber uncertainty of lines above 100 SNR is 0.0015 cm^{-1} .

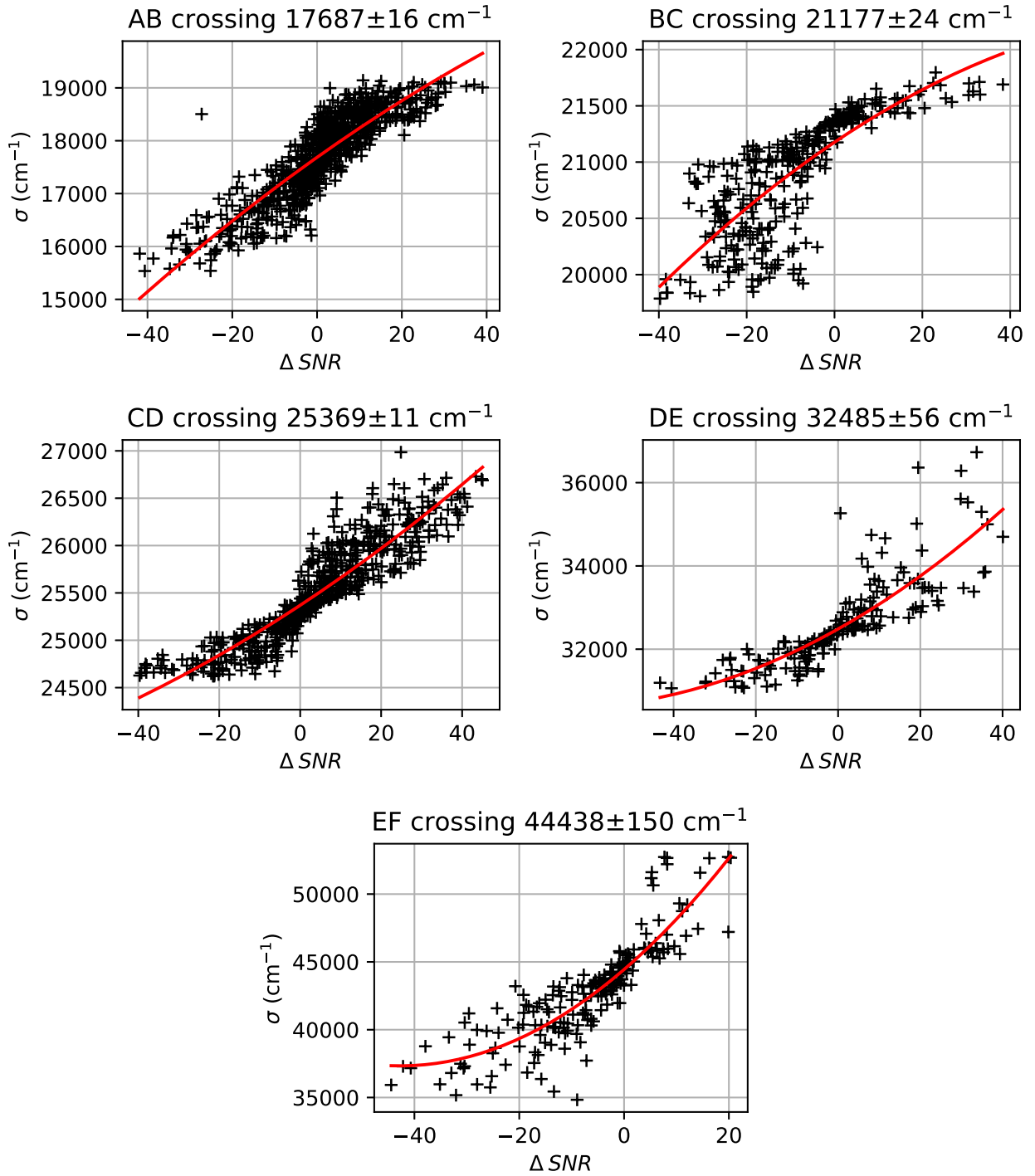


Figure 5.21: Plot of wavenumber of all lines in each overlap region of the six spectra against the difference between their SNRs. Red curves show a parabolic fit and the y -intercept value (crossing point between two spectra) is indicated at the top of each plot.

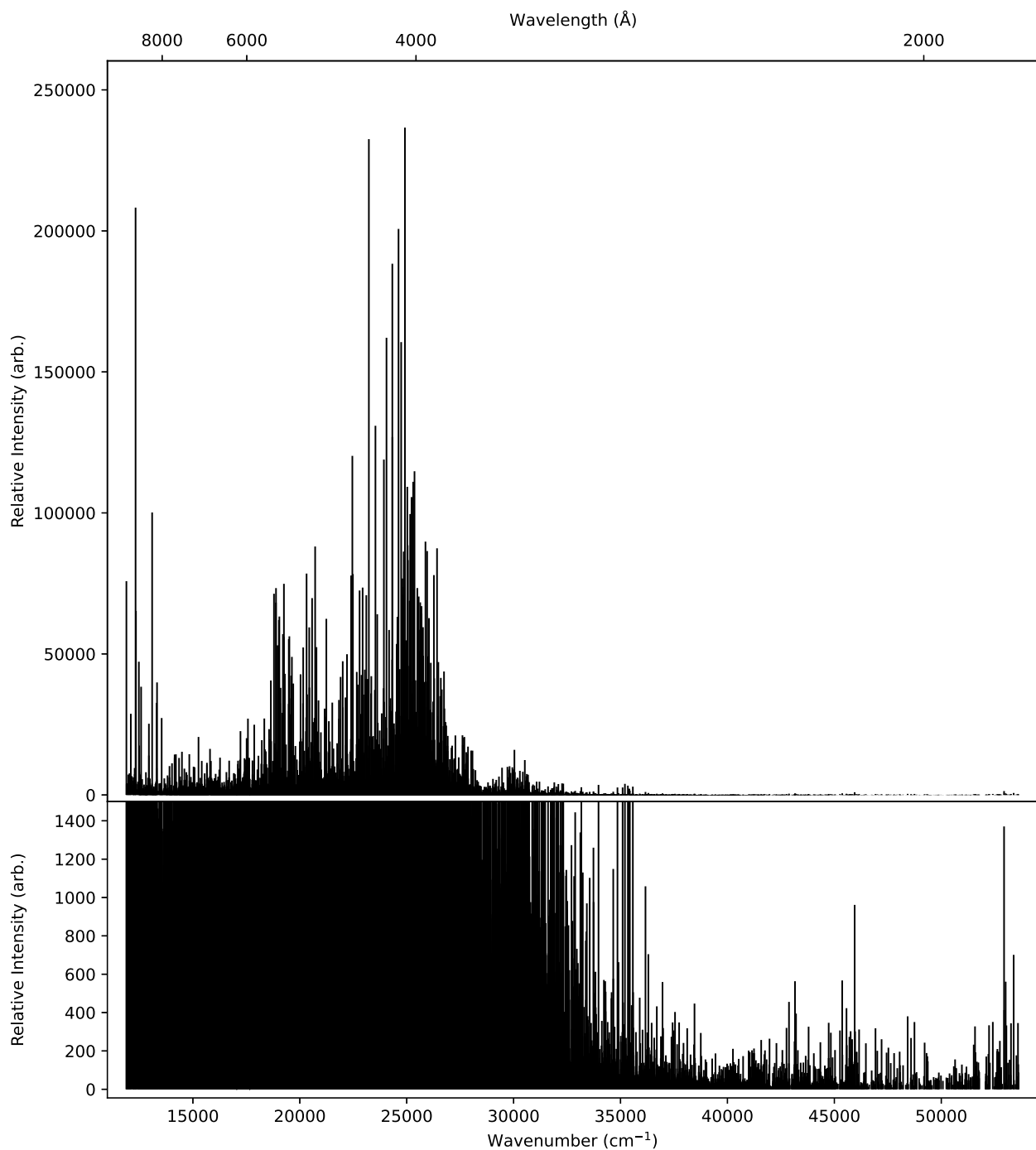


Figure 5.22: Relative intensity of all lines in the Nd-Ar PDL FT spectra line list. The bottom plot shows an expansion on the y -axis. The intensity scale is the same as the intensities in Table D.1.

Chapter 6

Analysis of the Atomic Structure and Spectrum of Nd III

6.1 Introduction

Energy levels are derived using observed spectral lines (energy level separations) in the empirical spectrum analysis of an atom, this is also often referred to as the term analysis [26] of the atom as the observed level energies are also assigned terms of eigenfunctions that best represent them. The methodology generally relies on theoretical atomic structure calculations as a guide to level energies and line intensities. In term analysis, observed transitions are said to be classified when they are assigned atomic species, upper and lower level energies, and upper and lower level J values that agree with experimental evidence. Consequently, the energy levels of the transitions are then derived if the levels connect to the ground level either directly or through at least one chain of transitions involving other levels.

The first step in classifying lines was to compare the extracted line list of the Nd-Ar PDL spectra with literature energy levels and line lists of atomic species expected to be observed (see [section 6.2](#)). Since the analysis is focused on Nd III, transitions of Nd III were carefully classified one by one, and transitions of other species were classified using spectral data from the literature. The methodology for the term analysis Nd III in this work will be discussed in [section 6.3](#), [section 6.4](#), and [section 6.5](#) of this chapter. The analysis itself is described in chronological order in [section 6.6](#) and [section 6.7](#), where specific classifications of transitions

Table 6.1: Non-Nd III Species and Lines Identified in Nd PDL FT Spectrum Merged Line List

Species	No. of Lines	Tolerance (cm^{-1})	Classified using lines from:
Nd I	1636	± 0.05	allowed E1 Ritz transitions [20]
Nd II	6574	± 0.05	allowed E1 Ritz transitions [20]
Nd IV	54	± 0.20	classified and observed wavenumbers [77]
Ar I	48	± 0.05	classified and observed wavenumbers [148]
Ar II	430	± 0.05	classified and observed wavenumbers [149]
Ar III	90	± 0.05	classified and observed wavenumbers [149]
Fe I	468	± 0.05	classified and observed wavenumbers [150]
Fe II	294	± 0.05	classified and observed wavenumbers [151]

and identifications of energy levels (and their labelling) will be discussed. Lastly, the lists of identified energy levels and classified transitions of Nd III are presented in [section 6.8](#).

6.2 Species in the Nd-Ar Spectra

Transitions of Nd I-IV, Ar I-III, Fe I-II were observed in the Nd-Ar PDL FT spectra. The presence of the first four ionisation stages of Nd was not surprising as the PDL is known to produce up to the third ionisation stage of the iron group elements (e.g. [133, 134]), which have higher ionisation potentials than the REEs due to decreased screening from their fewer number of core electrons. The number of lines classified in the final line list from each species is listed in [Table 6.1](#), with descriptions of how lines of each species were classified. For Nd I-II, no suitable line lists were found in the literature, and so allowed E1 transitions were produced using energy levels in the NIST ASD [20, 73–75]. If the wavenumber of a line from the line list lies within a tolerance of $\pm 0.05 \text{ cm}^{-1}$ of the Ritz wavenumber of an allowed E1 transition, then the species of that line was classified. For other species, observed wavenumbers of experimentally classified transitions in the literature [77, 148–151] were used instead. The wavenumber matching tolerance for Nd IV was chosen from the uncertainties of the compared literature line list [77]. The tolerances for other species were chosen as the largest wavenumber

uncertainty in the Nd-Ar PDL spectral line list.

For Nd I-II, critically evaluated energy levels in the NIST ASD [20] (mostly from the compilation by W. C. Martin [73] and the energy level analyses [74,75]) were used to compute Ritz wavenumbers of transitions allowed by the rigorous E1 selection rules $\Delta J = 0, \pm 1$, but not $J = 0 \leftrightarrow 0$ and change of parity. The allowed Ritz wavenumbers under these rules were produced using a very simple computer program *STRANS* and matched with observed wavenumbers.

The number of classified Nd I-II lines is uncertain. A large fraction of these levels have only configuration and J value assigned, with no data on predicted eigenvector compositions, which are crucial in calculating transition probabilities (see discussions regarding Equation 2.26). Classifications of lines involving such Nd I-II levels are therefore less reliable as correct classifications need to be confirmed in a detailed analysis of Nd I-II atomic structure with eigenvector composition calculations, which is not the focus of this work. The NIST ASD [20] does not contain the full list of classified transitions leading to the determination of the Nd I-II levels in the database. The level list for Nd I is also slightly outdated, where small extensions to the known levels have been published recently since 2018 [152–154]. But in the interest of time, the inaccuracies and incompleteness of Nd I-II data were concluded as insignificant for the empirical spectrum analysis of Nd III. This is because the classification of the Nd III transitions had to satisfy a set of criteria, which would essentially eliminate the possibility of lines being misclassified as belonging to other species (this will be discussed in section 6.3). The purpose of classifying lines of non-Nd III species is a part of the Nd III classification criteria; the correctly classified Nd III lines should likely not belong to Table 6.1, provided that any potential blends with these lines are analysed correctly.

The Ar I-III line lists in the literature are of much higher quality than those of Nd but are still likely to be incomplete (as with most atoms). This again did not significantly affect Nd III energy level analysis for the same reasons. A few transitions of the excited configurations $4f^25d$ and $4f^26p$ of Nd IV were classified using the extensive line list from Wyart et al. (2007) [77]. These lines appeared to have larger widths but were low in SNR (< 10), which suggested that Nd IV did not dominate the PDL spectra and would have minimal impact on the analysis of Nd III, since the resonance lines of Nd IV also lie below the VUV wavelength range of the recorded Nd-Ar FT spectra.

The PDL cathode impurities (0.5%) were primarily Fe and Pr. The strongest transitions, e.g.,

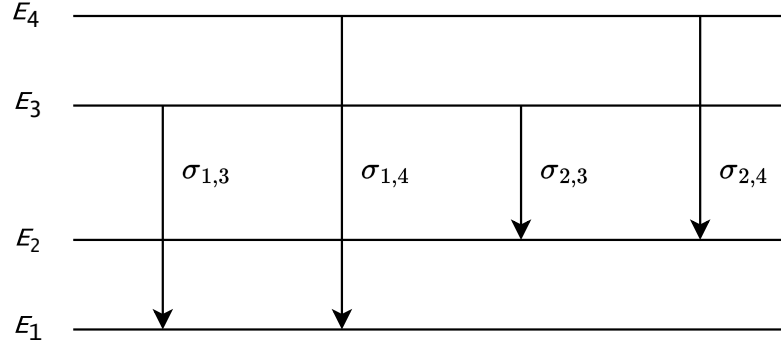


Figure 6.1: Grotrian diagram of four hypothetical energy levels and four transitions between them. Adapted from Cowan’s book [24].

resonance lines, of Fe I and Fe II lie in the UV [20, 150, 151], and were observed at intermediate SNRs due to relatively much fewer number and lower SNRs of Nd lines in the UV compared to the visible region. However, the strongest transitions of Pr I-III [20, 73] could not be reliably identified as they lie in the line-rich visible region and were likely masked by the high photon noise level in that region.

The classified Nd, Ar, and Fe transitions of Table 6.1 provided insight into the thermal conditions and line profiles of the Nd PDL and HCL spectra, and approximately halved the total number of transitions to be fully investigated for the Nd III energy level analysis. However, this did not mean that a line classified as belonging to a species other than Nd III could not possibly be from Nd III as line blending is possible.

6.3 Nd III Line Classification and Energy Level Identification

6.3.1 Principal Methods to Establish New Energy Levels

Repeated Energy Separations of Pairs of Transitions

When no experimental energy levels of an atom are known, one can begin by looking for repeated wavenumber differences between pairs of observed lines [24]. For example, consider the 4 energy levels and the 4 transitions observed between them illustrated in Figure 6.1. It is seen that $\sigma_{1,3} - \sigma_{2,3} = \sigma_{1,4} - \sigma_{2,4} = E_2 - E_1$, where the two line pairs $(\sigma_{1,3}, \sigma_{2,3})$ and $(\sigma_{1,4}, \sigma_{2,4})$

are transitions from two separate upper levels to a common pair of lower levels E_1 and E_2 . Within some tolerance, set by the observed wavenumber uncertainties, the more line pairs with the same energy difference, the more likely a correct energy separation is found. Initially, when no energy levels are known for an atom, one would also look for transitions to the ground term levels, which typically involve the most populated levels with the strongest lines. Further clues could also be obtained from spectral line self-absorption features or largest energy gaps belonging only to the lowest-lying levels.

Intensity Patterns of Transitions

Detailed theoretical calculations of atomic structure and transition probabilities are the key guides in the term analysis process. Experimentally found tentative energy levels can be confirmed or otherwise identified with much confidence by comparing observed relative line intensities with corresponding theoretical transition probabilities and thermal conditions of the light source. With a few energy levels confidently found, one can begin to expand the energy level system one level at a time. To establish a new energy level this way, a set of observed lines must correspond to the energy level differences between the new level and existing known levels and have the expected relative intensity pattern, particularly for the transitions with the highest transition probabilities and branching fractions as these are generally most accurately theoretically predicted (see discussions of [Equation 2.26](#)). In the example shown in [Figure 6.2](#), three transitions are expected to be observed for E_{new} , the observed wavenumbers must satisfy

$$E_{\text{new}} - \Delta < E_1 + \sigma_1, E_2 + \sigma_2, E_3 - \sigma_3 < E_{\text{new}} + \Delta, \quad (6.1)$$

where Δ is comes from observed wavenumber uncertainties, and the relative intensity pattern of the three lines should agree with expectations from theory and/or observations of transitions within similar spectral regions, with similar transition probabilities, and with similar upper-level energies and configurations. In complex atomic spectra with tens of thousands of lines, a match such as the one in [Figure 6.2](#) could be ambiguous due to the finite size of Δ . While the confidence of a correct level identification could be largely improved with an increased number of lines classified for the new level, many energy levels may not have more than a few lines to known levels with high enough transition probabilities and/or populations to be observed in the experimental spectra. Additionally, the observable lines may also lie outside the spectral range

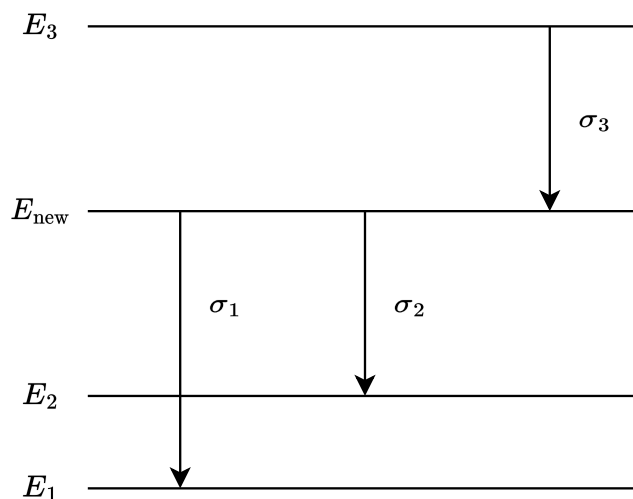


Figure 6.2: Grotrian diagram of 3 known energy levels to be connected by a new level and three newly classified transitions.

of the available data. Hence, high resolving powers (to reduce Δ) and wide spectral ranges (to measure all lines of interest) are crucial to the feasibility of term analyses.

Candidate lines and candidate energy levels

When classifying transitions of a new level using the criteria illustrated by [Figure 6.2](#) and [Equation 6.1](#), sets of candidate lines and their corresponding candidate energy levels were produced by the *LEVHAMD* program, in which all observed wavenumbers were added to and subtracted from a set of input known levels that were expected to have observed transitions to/from the new level to be found. This essentially produces all possible values of the new level energy based on the previously determined input levels and the observed line list. Energy level values that repeat within $\pm\Delta$ within some energy search range, chosen using the predicted energy and its probable error, would then become candidates for the new level. The input known levels were usually selected as those with the strongest transitions to/from the level being searched for. A minimum number of lines per level could be set to filter out candidate levels that do not have the desired number of observed transitions, up to the number of input levels.

An example output of *LEVHAMD* is shown in [Figure 6.3](#) for a simplified illustration of the analysis process, where four candidate levels were found within $\pm 20 \text{ cm}^{-1}$ of the predicted energy of a level of interest from four sets of candidate lines to the two input lower levels.

ENERGY	WAVENUM	INTENSITY	LEVEL	J	New level
12181.327 +	16240.753	3.8 8	4f4 5F4	4.0	28422.080
2387.544 +	26034.565	3.7 20	4f4 5I6	6.0	28422.109
					0.029
2387.544 +	26043.278	14.4 104	4f4 5I6	6.0	28430.822
12181.327 +	16249.536	1.37 5	4f4 5F4	4.0	28430.862
					0.040
2387.544 +	26051.362	1.18 8	4f4 5I6	6.0	28438.906
12181.327 +	16257.613	18.7 56	4f4 5F4	4.0	28438.940
					0.034
2387.544 +	26052.505	1.96 17	4f4 5I6	6.0	28440.049
12181.327 +	16258.731	2.3 12	4f4 5F4	4.0	28440.057
					0.008

Figure 6.3: Example output of *LEVHAMD* from a level search of $28440.047 \text{ cm}^{-1}$ (final value, see section 6.4) using two lower levels at 2387.544 cm^{-1} and $12181.327 \text{ cm}^{-1}$. The WAVENUM column contains wavenumbers from the PDL line list. The columns under INTENSITY are relative intensity (1/200 of the values in Table D.1) and SNR respectively. Repeated level energies within each of the four sets of candidate lines are in the final column and were filtered to deviate no more than 0.05 cm^{-1} and to lie within $\pm 20 \text{ cm}^{-1}$ of the correct level candidate (which would be the theoretically predicted energy in a real analysis with much larger range, see later discussions).

To eliminate the three coincidental matches, the relative intensities of the candidate lines are compared with theoretical branching fractions. In this case, the transitions from the new level to the 2387.544 cm^{-1} and 12181.327 cm^{-1} levels had predicted $g_u A$ values of $1.1 \times 10^6\text{ s}^{-1}$ and $1.8 \times 10^6\text{ s}^{-1}$ respectively. The line intensities for the middle candidates differed by more than an order of magnitude, they were therefore incorrect classifications. This left an ambiguity between the top and bottom candidate levels of [Figure 6.3](#) because neither the observed relative intensities nor the theoretical calculations were accurate enough to pick out the correct candidate, more information regarding the expected transitions was needed. As the two sets of candidate line intensities differ by a factor of 2, one may compare the line intensities with correctly classified lines in the same spectral region with similar transition probabilities and upper-level energies, if such data were available. In the case where no lines are blended, the deviation between repeated level energies from a set of candidate lines should be within measured wavenumber uncertainties (a few 10^{-3} cm^{-1}). This would raise the confidence in the bottom candidate level at 28440 cm^{-1} in [Figure 6.3](#) with deviation between repeated level energies at 0.008 cm^{-1} as opposed to 0.029 cm^{-1} for the candidate at 28422 cm^{-1} . Hence, the bottom candidate is the most likely identification.

The number of candidate levels and sets of candidate lines vary depending on the level energy search range, the repeated level energy tolerance Δ , the minimum number of transitions matched per candidate level used to filter candidates with too few lines, and the line densities of spectral regions expected to contain the transitions involving the new level. For example, the search range (discussed throughout the rest of this chapter) is usually of order $\pm 200\text{ cm}^{-1}$ around the level energies predicted by the parameterised Cowan code and Δ is usually 0.05 cm^{-1} , which is the largest wavenumber uncertainty in the Nd-Ar PDL FT spectral line list, and new levels are usually identified using two or three lines to two or three known levels. If the new level is to be identified using transitions in the relatively line-sparse UV, there are usually around 10 candidate levels. If the new level is to be identified using transitions lying only in the line-rich visible, there are usually around 100 candidates. Moreover, the correct level energy may not even be one of these candidate levels, this is particularly common when transitions of the new level are weak, where they could often be not observed, not fitted for the line list, or were blended with one or more other spectral lines.

Classification criteria and confidence

The energy search range in the simple example of [Figure 6.3](#) was only $\pm 20 \text{ cm}^{-1}$ and ten times less than the usual $\pm 200 \text{ cm}^{-1}$. This means that the number of ambiguous candidate levels is nearly always much greater, where corroboration with other experimental evidence is required to resolve the ambiguities. The candidate lines for a Nd III energy level were assessed using a list of criteria. Including all considerations discussed so far, the set of candidate lines should:

1. match the energy differences between known levels and the level of interest, within a tolerance of approximately the observed wavenumber uncertainties, i.e., Ritz wavenumbers after energy level optimisation should fall within observed wavenumber uncertainties (see [section 6.4](#) for the best estimates of level energies),
2. satisfy the rigorous E1 transition selection rules in the absence of external fields, i.e., $\Delta J = 0 \pm 1$ (but not $J = 0 \leftrightarrow 0$) and change of parity,
3. be within the expected wavenumber range, subject to the accuracy of theoretical calculations, which are generally around $\pm 200 \text{ cm}^{-1}$ during the analysis of this work,
4. have relative intensities in agreement with their predicted values, subject to uncertainties of experimental and theoretical values,
5. if possible, correspond to a tentative energy level that would subsequently enable the identification of further levels,
6. exhibit the expected isotope or hyperfine structure line profiles,
7. have the expected relative intensities in spectra acquired under different thermal conditions, e.g., stars, the cooler HCL, or hotter VS,
8. have the correct Zeeman patterns in stellar spectra or other suitable light sources,
9. and not be lines from other atomic species ([Table 6.1](#)).

Generally, meeting the first four criteria was necessary for a tentative level identification, and meeting the rest would improve confidence in the identification (if such data were available). In a few cases, only one relatively strong transition was expected to be observed for a new

energy level. Correct classifications of such transitions were possible by meeting many of the criteria from 3 to 9. Criterion 3 depended on the quality of theoretical calculations; energy levels from very poorly known configurations would require a greater wavenumber search range due to less accurate predictions, systematic shifts in level energies may be present, e.g., due to the inaccurate ab initio configuration averages and radial integrals, but this can be gauged after levels belonging to the same configuration and/or term are found (their energy shifts would be similar). Criterion 4 was more strict for lines with the highest transition probabilities, as these were generally found to be more accurately predicted theoretically. Caution was also required when considering transition probabilities involving poorly known configurations, as their Cowan code parameters were less well-constrained. Criterion 5 may not be immediately met after a tentative classification, but the confidence in this classification would be boosted greatly if it results in the classification of one or more energy levels. Criterion 6 was particularly useful for classifying the $4f^4 - 4f^35d$ transitions (see [subsection 6.3.2](#) for details). Criterion 7-9 were very important for the transitions between higher-lying $4f^4$ and $4f^35d$ levels since their isotope line profiles were not always available due to blends and low SNR (assistance provided by the HCL spectra is discussed in [subsection 6.3.3](#)).

Using the methodology described, the energy level system of Nd III was expanded level by level until the classification of any new levels became limited by the extent and accuracy of the experimental and theoretical data. For example, for candidate lines expected to be at low SNR (~ 10), the number of coincidental matches was too large because weak lines were much more common and more susceptible to blending, isotope profiles could not be observed reliably for weak lines, and weak lines have more uncertain wavenumber and intensity measurements. Furthermore, the weak lines may not have been fitted due to algorithmic and human limitations in the creation of the line list. Theoretical calculations can also become difficult for higher-lying levels because of increasing level densities, where slight changes in semi-empirical parameters can produce quite different eigenvector compositions and hence transition probabilities. In other words, the number of ambiguous matches increased exponentially with uncertainties in experimental measurements and theoretical calculations.

6.3.2 Line Classification Assistance from Nd III Isotope Structure

Transitions involving the same configurations of an atom will generally show similar isotope line profiles due to similar isotopic field shifts (more dominant in heavier elements such as Nd) of their corresponding energy levels, i.e., similar mean electron distance from the nucleus. This provided a very useful clue in line classification, and had also been used in the empirical spectrum analyses of Nd I and Nd II [74–76]. Observations of Nd III isotope structure had first been made by Maria Aldenius [83]. Examples observed in the Nd-Ar PDL spectra I recorded are shown in Figure 6.4. Almost all classified $4f^4 - 4f^35d$ transitions of Nd III show an unresolved ^{150}Nd right side wing in the FT spectra (e.g. see Figure 6.4), which turned out to be an essential clue to their classifications at sufficient SNRs. The Nd II line in Figure 6.6 observed in the HCL was slightly asymmetric, with possibly the ^{150}Nd wing on the left, this line profile was also commonly strong and belonged to Nd II lines, which helped with their identifications.

The transition $4f^4\ ^5I_6 - 4f^3(^4I^\circ)6s\ (\frac{9}{2}, \frac{1}{2})^\circ_5$ was the only classified Nd III line with resolved ^{142}Nd , ^{144}Nd , and ^{146}Nd isotope components in the HCL spectrum. The ^{148}Nd and ^{150}Nd components at higher wavenumbers are uncertain due to smaller relative abundances, low SNRs, and hyperfine structure of the ^{143}Nd and ^{145}Nd isotopes. The likelihood of the $4f^4\ ^5I_6 - 4f^3(^4I^\circ)6s\ (\frac{9}{2}, \frac{1}{2})^\circ_5$ line being a blend was very low, because: 1) the Ritz wavenumber of this line was within its COG wavenumber uncertainty, 2) the $4f^3(^4I^\circ)6s\ (\frac{9}{2}, \frac{1}{2})^\circ_5$ level has 8 classified transitions and is thus confidently established, 3) the relatively increased line width agreed with other transitions involving the $4f^3(^4I^\circ)6s$ sub-configuration, since 6s electrons penetrate the core and are expected to be affected by isotope shifts more, and 4) this pattern was consistent with those observed for Nd I (e.g. 19668.1 cm^{-1} of Figure 5.12), Nd II (e.g. Figure 2 of [155]), and those of Figure 5.9.

Identification of the species and configurations involved in a line is not guaranteed using its isotope structure line profile. Any line resembling the unresolved isotope structure line profiles could also just be a blend, and some Nd II lines also showed the same profile as those of $4f^4 - 4f^35d$ of Nd III. So having the expected isotope structure line profile unfortunately does not guarantee the correct classification. In weak lines, isotope shifts may not be observable, which is the case for observed transitions involving the $4f^36p$, $4f^37s$, and $4f^36d$ configurations, where the lines are weak and further in the UV with broader Doppler widths, whether their isotope shifts were observed is rather uncertain.

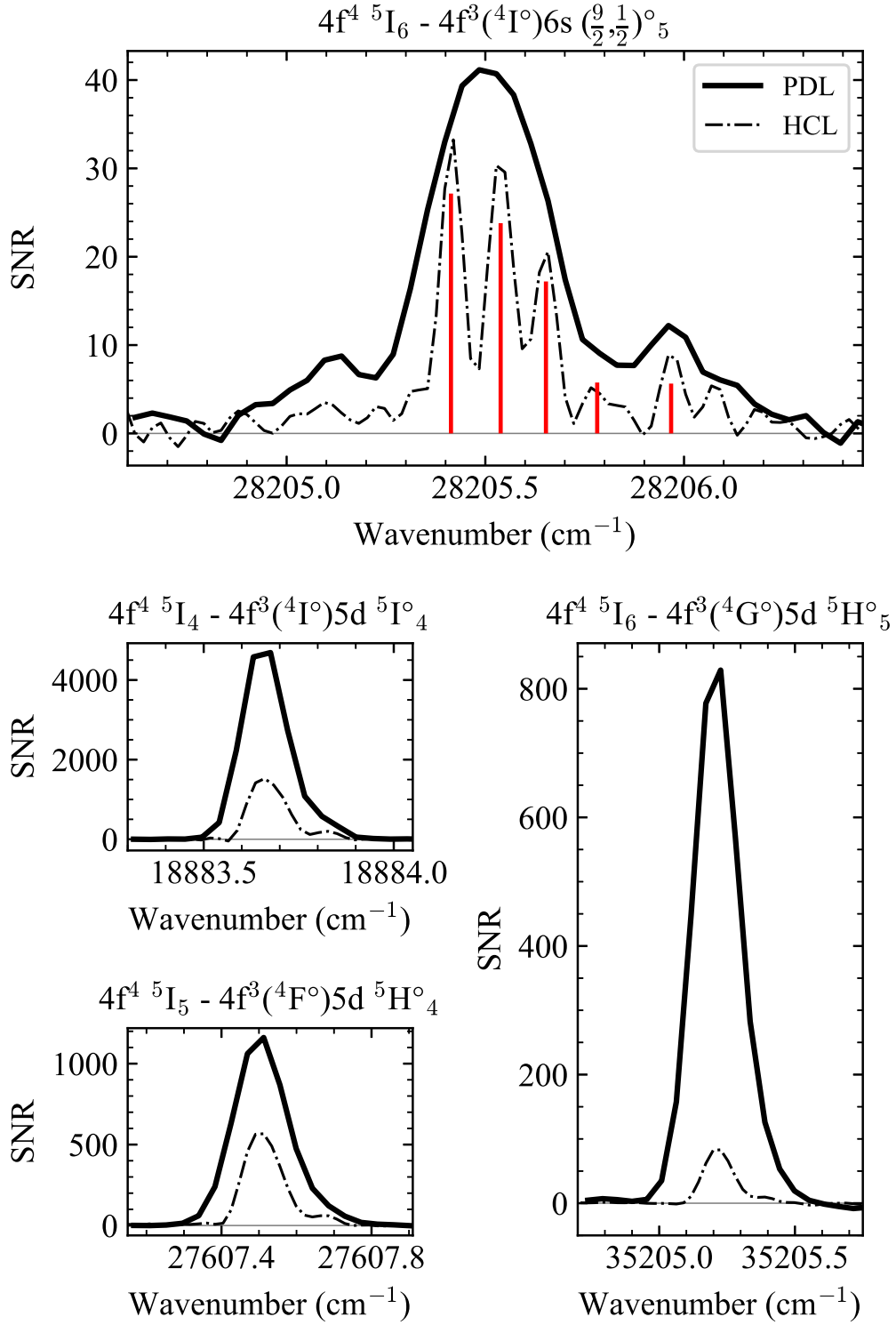


Figure 6.4: Isotope shifts in four Nd III lines observed with the Nd-Ar PDL (solid) and HCL (dash-dotted) light sources. For $4f^4 \ ^5I_6 - 4f^3(4I^o)6s \ (\frac{9}{2}, \frac{1}{2})^o_5$ at the top, isotope components of ^{142}Nd , ^{144}Nd , ^{146}Nd , ^{148}Nd , and ^{150}Nd are marked tentatively from left to right with red vertical lines in relative abundance ratios from [140], remaining features are likely to be hyperfine structures of ^{143}Nd and ^{145}Nd or blended weak lines. Plot from Ding et al. (2024) [96].

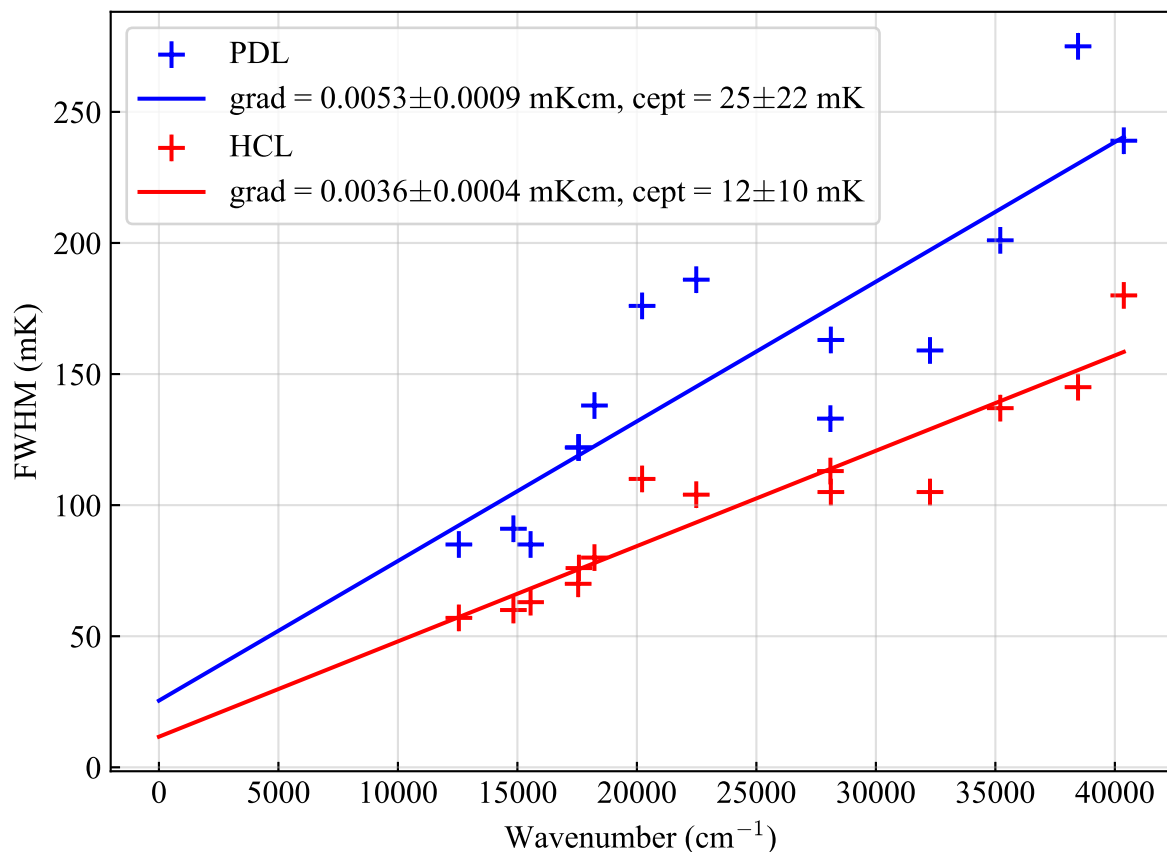


Figure 6.5: FWHM ($1 \text{ mK} = 10^{-3} \text{ cm}^{-1} = 30 \text{ MHz}$) plotted against wavenumber for the PDL (blue) and HCL (red) Nd-Ar spectra. The lines selected were symmetric, not Ar lines, and belong to both spectra. The species of origin was not considered.

6.3.3 Line Classification Assistance from Nd-Ar Hollow Cathode FT Spectra

The primary assistance in weak line and blend identification was provided by the HCL spectra, which contain lines of a Nd-Ar discharge with narrower line widths and lower effective temperature. This was illustrated in [Figure 5.9](#), [Figure 5.12](#), and [Figure 6.4](#). [Figure 6.5](#) plots the FWHM of symmetric lines of the PDL and HCL against wavenumber. The narrower typical FWHM was strong evidence for lower effective temperatures in the Nd-Ar HCL discharge, as Doppler broadening dominates line shape in these high-resolution spectra. Moreover, instrumental ringing was observed in the HCL spectra, again indicating narrower lamp line widths compared to the PDL.

Further evidence for lower effective temperatures in the HCL were the relative intensities of

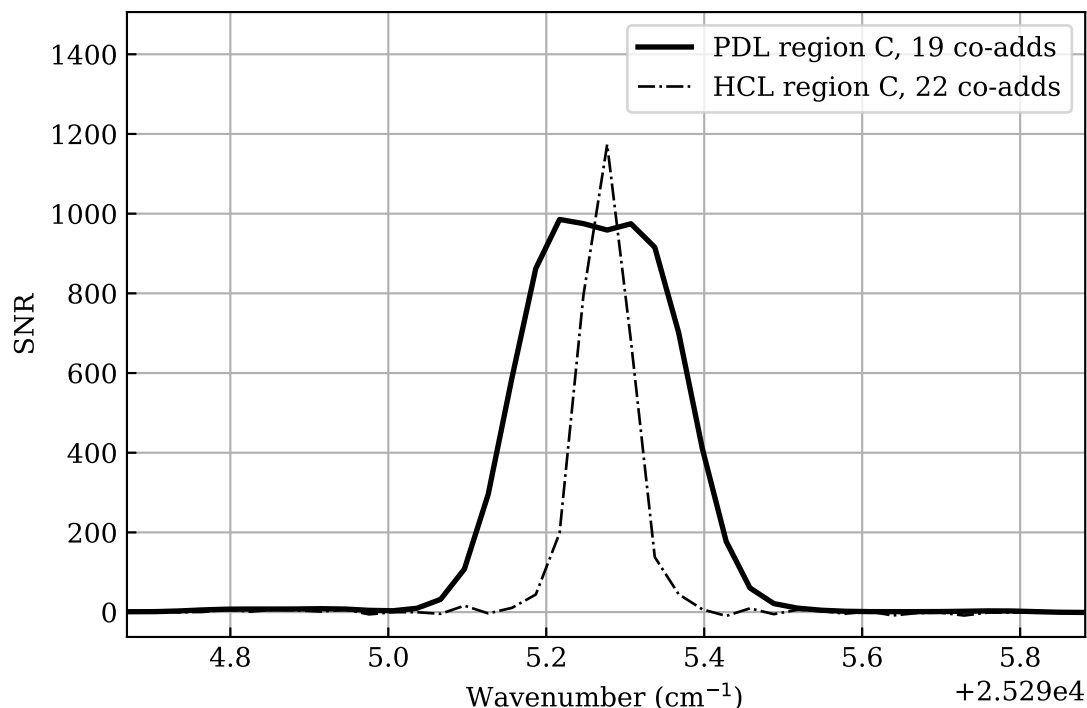


Figure 6.6: Transition of Nd II from the energy level $25295.28 \text{ cm}^{-1} (J = 7/2)$ to ground, observed in both the HCL and PDL spectra. Self-reversal is observed in the Nd-Ar PDL spectrum.

known Nd I transitions. Transitions of Nd I could also be identified because Nd I was the only Nd species with reduced relative intensities in the PDL, this can be seen from Figure 5.12. This was of course assumed not always true as lines belonging to other species may blend with a Nd I line in the PDL, which may suggest higher relative intensities in the PDL without further investigation.

Self-absorption was only observed for some known lines of Nd II in the PDL spectra. An example is shown in Figure 6.6, which is a classified transition to the ground with strong enough self-absorption to show self-reversal in the PDL. Self-absorbed lines generally show an upside down ‘W’ in the fit residual [116]. The line in Figure 5.12 at 19660.2 cm^{-1} shows this feature but is unclassified, indicating its possibility of being an unclassified Nd II transition¹.

¹After analysis of this line in stellar spectra (March 2024 [138, 156]), this line was concluded to most likely belong to Nd III with label $4f^4 \text{ } ^5\text{S}_2 - 4f^3(^4\text{F})5d \text{ } ^5\text{P}_2$, but both levels were unable to be established relative to the ground level due to weak lines connecting them. So self-absorption could occur for Nd III lines too, especially if their lower levels have very long lifetimes, in terms of low spontaneous de-excitation rate and low plasma collisional excitation rate.

Nd-Ne HCL FT spectra were not used due to poorer Nd III SNRs compared to the Nd-Ar HCL spectra. However, potential applications are indicated at the conclusion of the Nd III term analysis (see [section 7.5](#)).

6.4 Energy Level Optimisation and Ritz Wavenumber Uncertainties

When identifying an energy level, the most confident set of candidate lines was added to the existing list of classified lines, which were then used to determine the best estimates of energies and energy uncertainties of the new level and previously identified levels. This task was handled by the program *LOPT* [157], which optimises level energies based on the input of a list of observed energy separations (i.e. line wavenumbers) and their uncertainties. Any issues with the new set of candidate lines may come to light if the new best estimates of the Ritz wavenumbers (best estimate of energy level separations) of classified transitions disagree with observed wavenumbers. In *LOPT*'s design, Ritz wavenumbers deviating from their observed wavenumbers by more than $1.2\times$ their observed wavenumber uncertainties are flagged, this choice of threshold appears empirical (e.g. $1\times$ may induce too many false classifications, especially for weak lines), is only used to indicate likely problems with the lines, and does not affect the optimisation. In almost all cases, the addition of a set of lines for a new level that causes this problem is due to either incorrect/spurious line classifications or an issue with line wavenumbers, which can occur with weak or blended lines. The agreement of optimised energy levels with observed wavenumber uncertainties is a crucial criterion for correct classifications.

6.4.1 Optimum Energies and Energy Uncertainties

The *LOPT* program minimises the quantity F for N excited energy levels, where F is a weighted sum of the squared differences between the energy differences to be optimised (Ritz wavenumbers) and the observed energy differences between all pairs of the N levels (the observed line

wavenumbers). Using notations from the paper [157],

$$F = \sum_{i=0}^N \sum_{j=1}^N (E_j - E_i - s_{ij})^2 w_{ij}, \quad (6.2)$$

where s_{ij} is the observed wavenumber of the transition from the upper level E_j to the lower level E_i , the weights $w_{ij} = (\delta s_{ij})^{-2}$ are inverse squares of the absolute uncertainties of s_{ij} , which are zero if $i = j$. By setting the derivative of F with respect to either E_j or E_i to be zero, one can obtain a system of N linear equations for the N excited energies ($i > 0$) given by

$$S_i = \sum_{j=0}^N \left[\left(\delta_{ij} \sum_{k=0}^N w_{kj} \right) - w_{ij} \right] E_j = \sum_{j=0}^N W_{ij} E_j, \quad (6.3)$$

and also

$$S_i = \sum_{j=0}^N w_{ij} s_{ij}, \quad (6.4)$$

with δ_{ij} as the Kronecker delta and the ground level energy $E_0 = 0$. Hence, *LOPT* calculates optimum level energies E_j by computing the product between the inverse of the $\underline{\underline{W}}$ matrix and the $\underline{\underline{S}}$ vector, both of which are determined solely by the observed wavenumbers and their associated uncertainties.

The variance a_{ij}^2 of the Ritz wavenumber $E_j - E_i$ is [157]

$$\begin{aligned} a_{ij}^2 &= \text{Var}(E_j) + \text{Var}(E_i) - 2\text{Cov}(E_i, E_j) \\ &= (\underline{\underline{W}}^{-1})_{ii} + (\underline{\underline{W}}^{-1})_{jj} - 2(\underline{\underline{W}}^{-1})_{ij}. \end{aligned} \quad (6.5)$$

Uncertainty in level energy is estimated as the uncertainty of the transition wavenumber from the level to the ground, i.e., $i = 0$ in the above.

6.4.2 Effects of Systematic Shifts on Uncertainties

Uncertainties in absolute wavenumber calibration imply non-zero systematic shifts. These are a part of the total wavenumber uncertainties that are included only in the weights of the level optimisation, therefore uncertainties due to systematic shifts are not considered in a_{ij}^2 of Equation 6.5. In *LOPT* [157], the possible systematic wavenumber shift δ_K of a spectrum K is

estimated as the smallest input wavenumber uncertainty of the spectrum, so that the observed wavenumbers of the spectrum s_{ijK} could differ from the unshifted wavenumbers s_{ijK}^* by δ_K ;

$$s_{ijK} = s_{ijK}^* + \delta_K \quad (6.6)$$

The possible shift δE_{jK} in the optimised energies E_j of Equation 6.3 due to the possible wavenumber shift of spectrum K is estimated as

$$\delta E_{jK} = \sum_{i,m} \frac{\partial E_j}{\partial s_{imK}} \delta_K = \delta_K \sum_{i,m} W_{ij}^{-1} w_{imK}. \quad (6.7)$$

The possible shift of the Ritz wavenumber between two energy levels E_i and E_j is then $\delta E_{iK} - \delta E_{jK}$, and a more appropriate Ritz wavenumber uncertainty b_{ij} is estimated as

$$b_{ij}^2 = a_{ij}^2 + \sum_K (\delta E_{jK} - \delta E_{iK})^2, \quad (6.8)$$

using a_{ij}^2 of Equation 6.5. This b_{ij}^2 is the square of the Ritz wavenumber uncertainty in the lines output file of *LOPT* when using its feature to estimate uncertainties due to potential systematic shifts. The more appropriate estimate for optimised level energy E_j is estimated as b_{0j} , which is the uncertainty of the Ritz wavenumber between the level and the ground level, and is the *D2* column in the *LOPT* levels output file.

The index K included all six Nd-Ar PDL FT spectra of Table 4.6, and b_{ij} was used for all Ritz wavenumber and optimised level energy uncertainties of Nd III in this work. The possible shifts to Ritz wavenumbers $\delta E_{jK} - \delta E_{iK}$ and shifts to level energies δE_{jK} were generally negligible compared to a_{ij} . A few significant δE_{jK} shifts were around 0.002 cm^{-1} and very few were up to 0.005 cm^{-1} . These were always within the observed wavenumber uncertainties and usually attributed to lines and levels involving lines that lie far from the spectrum containing Ar II calibration lines, e.g., not in the spectra B, C, and D, and due to systematic uncertainty buildup. The highest estimated shift δE_{jK} is 0.005 cm^{-1} and is not unexpected as it is also the highest estimated systematic wavenumber uncertainty for spectrum F in the VUV (see Figure 5.15).

6.5 Term Analysis Methodology for Nd III

The approach I took was to identify Nd III energy levels one at a time by carefully classifying their transitions to known levels. First, previously experimentally established energy levels were validated or revised one at a time using the experimental observations and *LOPT* optimisations of energy levels. After revising previously known Nd III energy levels, the search for previously experimentally unknown levels began. The thought process when identifying one energy level and when classifying the transitions of the level is summarised in [Figure 6.7](#) and was iterated until the analysis could no longer proceed outside the red dashed box shown. Blended and weak lines with uncertain wavenumbers were weighted zero in the level energies optimisation as including them will reduce the accuracy of optimised energies. In addition to the steps mentioned in [Figure 6.7](#), once a few new energy levels are identified, they could be used in improving the semi-empirical calculations using Cowan's codes (reduce uncertainties of theoretical calculations used as guides), which then helped with eliminating ambiguities or identifying previously not predicted relative intensity patterns.

I would like to emphasise that the ability to resolve ambiguous candidate levels (in the red dashed box of [Figure 6.7](#)) was greatly hindered when spectral lines of interest were fitted incorrectly or not fitted at all, either due to being too weak or in a blend. Therefore, one would repeatedly check the spectrum by eye at expected transition wavenumbers for missing lines and require very frequent adjustments of the line list. Maximising the efficiency of this process was arguably the biggest motivation for creating the line fitting program ([subsection 5.3.6](#) and [Appendix B](#)). The Nd III term analysis was also greatly streamlined by customising the outputs and converting between the input and outputs of the four programs: *LEVHAMD*, *STRANS*, *LOPT*, and the line fitting program written during this work.

6.6 Confirmation and Revision of Known Nd III Levels

At the beginning of the analysis, the five levels of the ground term $4f^4\ ^5I$ were assumed to be correctly identified by Dr H. M. Crosswhite [20, 73]. These identifications have now been confirmed as the five levels enabled the identification of more than 250 interconnected energy levels belonging to the $4f^4$, $4f^35d$, $4f^36s$, $4f^36p$, $4f^37s$, $4f^36d$, and $4f^35f$ configurations. Prior to the

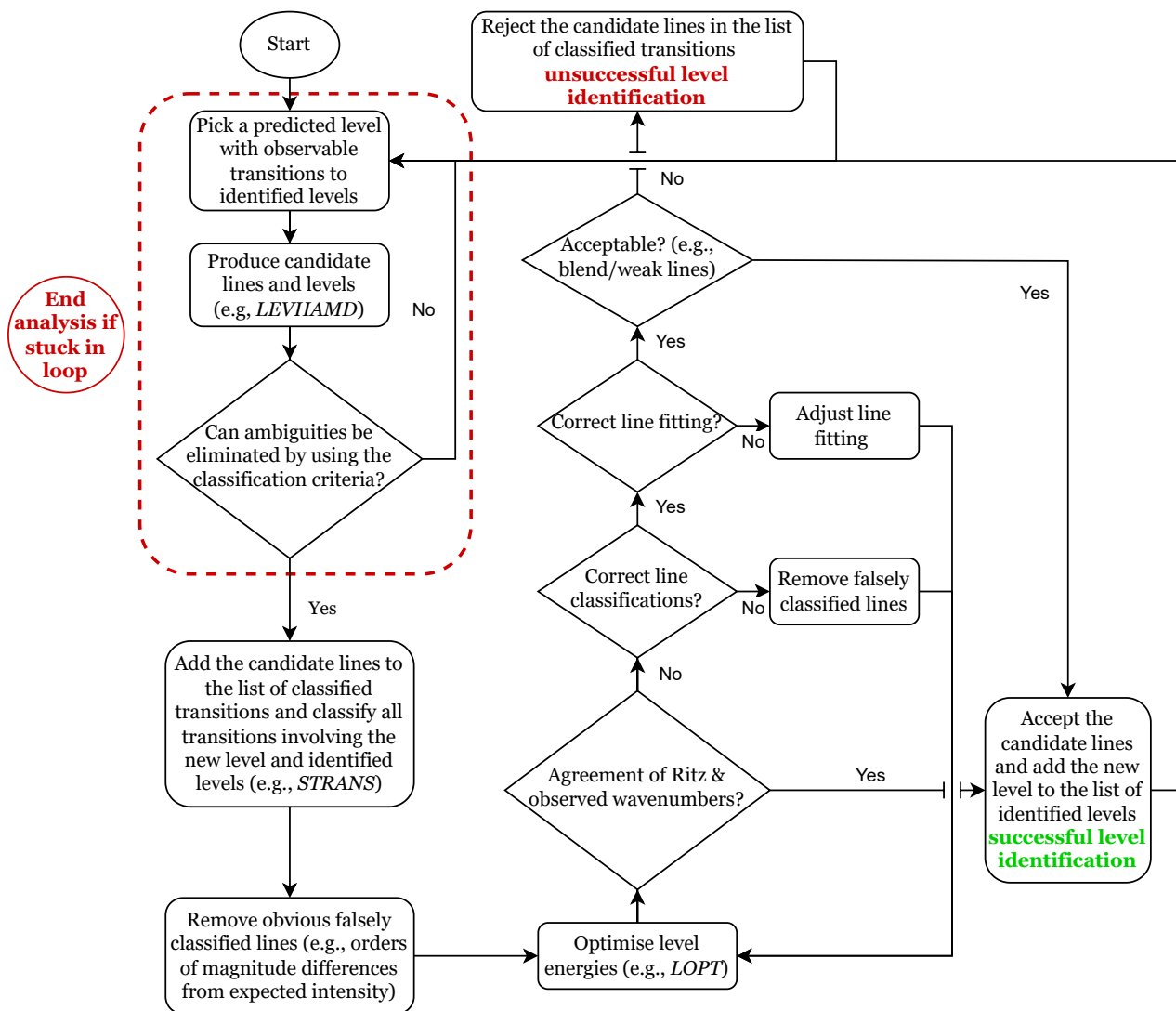


Figure 6.7: Flow chart summarising the empirical spectrum analysis of Nd III.

semi-empirical atomic structure calculations using Cowan’s codes, theoretical guidance in the search for energy levels of Nd III was from Nd III atomic structure and transition probability calculations of Gaigalas et al. (2019) [81], as well as level energies and eigenvector compositions of Zhang et al. (2002) [86] and Ryabchikova et al. (2006) [63]. These theoretical calculations allowed the analysis documented in this section, to check previously known energy levels, to be carried out completely. As discussed in subsection 1.4.1, only 40 energy levels of Nd III were experimentally known previously; five belong to the ground quintet term $4f^4 \ ^5I$, and 35 belong to the $4f^3 5d$ singly excited configuration. This section is aimed to be merely a summary and discussion of the confirmation of 39 of these levels and the revision of one level. Exact details of the changes in energy levels and transition classifications can be inferred between results of the present work [96] and previous work [20, 63, 73].

I would like to note that the information in this section and the next section are very dense. These two sections are a chronological record of how the results of the Nd III term analysis were obtained over ten months, and they are written for demonstrations of the discussed methodologies and organised for future references of Nd III analyses. The diagram of Figure 2.1 should be particularly helpful for the discussions involving level labels. Results of the Nd III term analysis are summarised in section 6.8 if one is interested in the overall picture.

6.6.1 H. M. Crosswhite’s Identifications - NIST ASD Energy Levels

Currently, the number of Nd III energy levels on the NIST ASD [20] is 29, all of which were likely identified by Dr H. M. Crosswhite [73, 84, 85]. These were revised without considering the more recent analysis of Ryabchikova et al. (2006) [63], because the analysis of Ryabchikova et al. (2006) [63] depended on these results produced by Dr H. M. Crosswhite.

$4f^3(^4I^\circ)5d \ ^5K^\circ$ levels

All five levels of the $4f^3(^4I^\circ)5d \ ^5K^\circ$ term identified by H. M. Crosswhite were confirmed. These levels were well represented by the *LS* coupling basis functions corresponding to their labels, which make up $\gtrsim 90\%$ of their compositions. The $4f^4 \ ^5I_{J-1} - 4f^3(^4I^\circ)5d \ ^5K^\circ_J$ lines were the strongest lines in the $16\,000\text{ cm}^{-1}$ region and well separated from intense lines of transitions from higher-lying terms of the $4f^3(^4I)5d$ sub-configuration to the ground term.

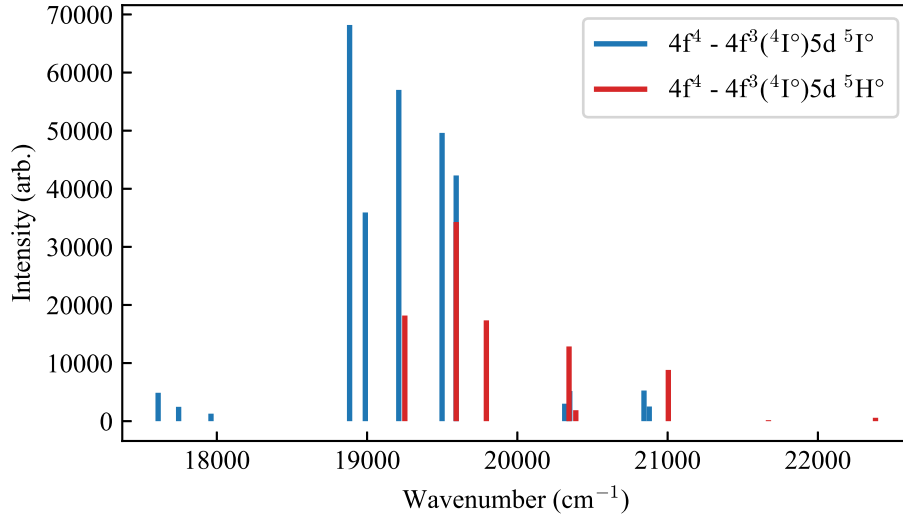


Figure 6.8: Classified transitions from $4f^3(^4I^\circ)5d\ ^5I^\circ$ and $4f^3(^4I^\circ)5d\ ^5H^\circ$ to the ground term in the Nd-Ar PDL FT spectral line list. Intensities are calibrated relative intensities from Table D.1.

$4f^3(^4I^\circ)5d\ ^5I^\circ$ and $4f^3(^4I^\circ)5d\ ^5H^\circ$ levels

The $^5I^\circ$ and $^5H^\circ$ terms of $4f^3(^4I^\circ)5d$ lie approximately 3500 cm^{-1} and 4500 cm^{-1} higher than the $4f^3(^4I^\circ)5d\ ^5K^\circ$ term respectively. However, their strongest transitions, $4f^4\ ^5I_J - 4f^3(^4I^\circ)5d\ ^5I^\circ_J$ and $4f^4\ ^5I_{J+1} - 4f^3(^4I^\circ)5d\ ^5H^\circ_J$, lie in the same spectral region around 19500 cm^{-1} , see Figure 6.8. Dr Crosswhite's $4f^3(^4I^\circ)5d\ ^5I^\circ$ (five) and $4f^3(^4I^\circ)5d\ ^5H^\circ$ (four) levels only agreed with the $4f^3(^4I^\circ)5d\ ^5I^\circ_{4,7}$ levels identified in the present work. However, most of the strong lines of Figure 6.8 were within her line list (see Table E.1), except for the main lines of $4f^3(^4I^\circ)5d\ ^5H^\circ_{5,6}$ classified in the Nd-Ar PDL spectrum. In the correct identification of the $4f^3(^4I^\circ)5d\ ^5I^\circ$ and $4f^3(^4I^\circ)5d\ ^5H^\circ$ levels, these strong lines were rearranged and reassigned to different levels of the $4f^3(^4I^\circ)5d\ ^5I^\circ$ and $4f^3(^4I^\circ)5d\ ^5H^\circ$ terms.

The errors in Dr Crosswhite's results were not surprising because the correct line classifications would require sufficiently accurate relative intensity measurements, which were not available because Dr Crosswhite's spectra were recorded on photographic plates that have a non-linear intensity response and low dynamic range compared to FT spectra recorded using PMTs (see [84, 85] and column 1 of Table E.1), and the lower resolutions of grating spectroscopy could have caused overestimates in intensities due to unresolved blends.

$4f^3(^4F^\circ)5d\ ^5H^\circ$ levels

Of the five levels of the $4f^3(^4F^\circ)5d\ ^5H^\circ$ term identified by H. M. Crosswhite, only the levels with $J = 4, 7$ were confirmed. Similar to the situation with $4f^3(^4I^\circ)5d\ ^5I^\circ$ and $4f^3(^4I^\circ)5d\ ^5H^\circ$, some of these strong lines were classified as involving levels with incorrectly assigned J values, likely owing to their inaccurate relative intensities on her photographic plates. For example, Dr Crosswhite had assigned the line at 27675.024 cm^{-1} as $4f^4\ ^5I_7 - 4f^3(^4F^\circ)5d\ ^5H^\circ_6$ rather than $4f^4\ ^5I_4 - 4f^3(^4F^\circ)5d\ ^5H^\circ_3$ (final classification), and her assignment of $4f^4\ ^5I_4 - 4f^3(^4F^\circ)5d\ ^5H^\circ_3$ was 27788.191 cm^{-1} , which is now classified as $4f^4\ ^5I_6 - 4f^3(^4F^\circ)5d\ ^5H^\circ_5$. Her classification for the main line $4f^4\ ^5I_7 - 4f^3(^4F^\circ)5d\ ^5H^\circ_6$ ($\Delta J = +1$) had a low intensity in her line list, which is almost two orders of magnitude lower than expected in the Nd-Ar PDL FT spectrum of the present work. A new candidate for the main line $4f^4\ ^5I_7 - 4f^3(^4F^\circ)5d\ ^5H^\circ_6$ ($\Delta J = +1$) was found at 27431.909 cm^{-1} , which was confirmed by the expected and observed weaker $\Delta J = 0$ transition to the ground term from $4f^3(^4F^\circ)5d\ ^5H^\circ_6$ at 28758.912 cm^{-1} .

It is also worth noting another factor that potentially contributed to these errors; in the 1970s, Dr Crosswhite and her colleagues would not have had the well-developed computational tools of today to perform sufficiently accurate atomic structure and transition probability calculations.

Remaining Five of the 29 Levels Found by Dr Crosswhite

In the present Nd III term analysis, the leading percentages of the eigenvector compositions of the $4f^3(^4F^\circ)5d\ ^5H^\circ_{5,6,7}$ levels were calculated to be only $\sim 50\%$. Another set of $J = 5, 6, 7$ energy levels also share the same (but lower percentages) leading components $4f^3(^4F^\circ)5d\ ^5H^\circ_{5,6,7}$. The $J = 5$ level of the lower-percentage set of levels was identified and then labelled using its second largest eigenvector component $4f^3(^4H^\circ)5d\ ^3I^\circ_5$, which was the confirmation of Dr Crosswhite's level belonging to the $4f^3(^4F^\circ)5d$ sub-configuration at 29397.423 cm^{-1} without an assigned term.

The term-less level Dr Crosswhite had identified as belonging to the $4f^3(^4I^\circ)5d$ sub-configuration at 24003.230 cm^{-1} has been very confidently confirmed with three transitions to the ground term and given the new label $4f^3(^4I^\circ)5d\ ^3I^\circ_7$.

The remaining identifications by Dr Crosswhite for $4f^3(^4I^\circ)5d\ ^3K^\circ_8$ and two other levels without

term assignments were not confirmed. Overall, 16 of the 29 energy levels identified by Dr Crosswhite and currently on the NIST database [20] were confirmed, and 13 were revised. These results are exactly the same as the only other and most recent Nd III term analysis by Ryabchikova et al. (2006) [63].

6.6.2 Confirmation of Energy Levels by Ryabchikova et al. (2006)

The most recent publication of experimental Nd III energy levels by Ryabchikova et al. (2006) [63] contained a list of 40 levels, five of which are the levels of the ground term (same identification as Dr Crosswhite's) and 35 of which were assigned the $4f^35d$ configuration. Eigenvector compositions had also been calculated [63] for energy levels up to $33\,000\text{ cm}^{-1}$. Prior to comparing my results with Ryabchikova et al. (2006) [63], I had identified 32 energy levels and most of these were assigned to the ground term, $4f^3(^4F^\circ)5d\ ^5H^\circ$ term, and $^5K^\circ$, $^5I^\circ$, $^5H^\circ$ (except for $J = 3$), and $^3I^\circ$ terms of the $4f^3(^4I^\circ)5d$ sub-configuration. All of these 32 levels were in excellent agreement with Ryabchikova et al. (2006) [63], with the exception that their energy values were around 0.01 cm^{-1} lower. This was due to their use of peak wavenumbers by Alde-nius (2001) [83] rather than the COG wavenumbers used in the present work to account for isotope shifts. The $4f^3(^4I^\circ)5d\ ^3K^\circ_{6,7,8}$, $4f^3(^4I^\circ)5d\ ^5G^\circ_{3,4,5}$, and $4f^3(^2H2^\circ)5d\ ^3I^\circ_5$ levels (my labels) identified by [63] were soon confirmed.

6.6.3 Revision of $4f^3(^4I^\circ)5d\ ^5H^\circ_3$ by Ryabchikova et al. (2006)

$4f^3(^4I^\circ)5d\ ^5H^\circ_3$ was the only tentative classification by Ryabchikova et al. (2006) [63], and its proposed transition to the ground was not observed in the Nd-Ar PDL spectrum. This level was eventually identified at 19593.094 cm^{-1} , using its transitions from $4f^3(^4I^\circ)6p\ ^5I_4$ and $4f^3(^4I^\circ)6p\ ^5H_3$ (see subsection 6.7.1 for their identifications). The very high SNR resonance line of this level, $4f^4\ ^5I_4 - 4f^3(^4I^\circ)5d\ ^5H^\circ_3$, was a blend at 19593 cm^{-1} with $4f^4\ ^5I_6 - 4f^3(^4I^\circ)5d\ ^5I^\circ_6$, which Dr Crosswhite had originally identified as $4f^4\ ^5I_8 - 4f^3(^4I^\circ)5d\ ^5I^\circ_8$. The blend is shown in Figure 6.9. This blended line profile was most likely unresolved in Dr Crosswhite's grating spectra, which led to her classification of just one transition for it. In the Nd-Ar PDL FT spectrum, this line could be interpreted as the two Nd III lines $4f^4\ ^5I_6 - 4f^3(^4I^\circ)5d\ ^5I^\circ_6$ (stronger left component) and $4f^4\ ^5I_4 - 4f^3(^4I^\circ)5d\ ^5H^\circ_3$ (weaker right component, with the ^{150}Nd isotope

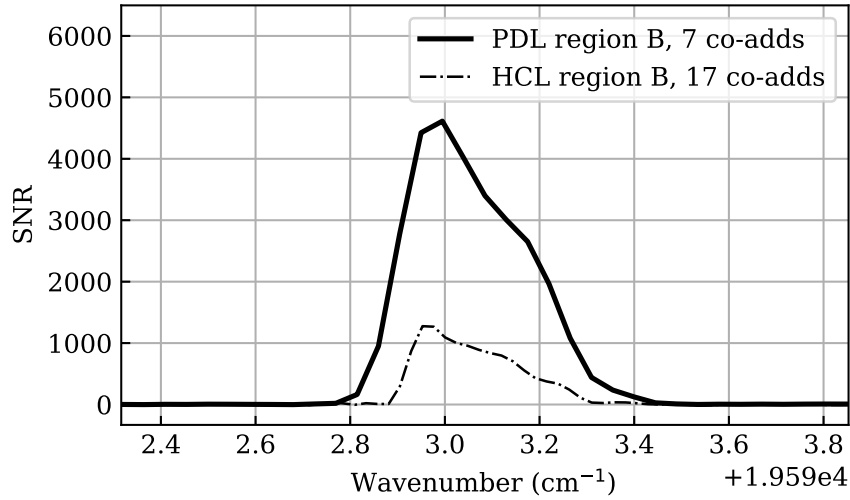


Figure 6.9: Blend of the $4f^4 \ ^5I_6 - 4f^3(^4I^\circ)5d \ ^5I^\circ_6$ and $4f^4 \ ^5I_4 - 4f^3(^4I^\circ)5d \ ^5H_3$ transitions at 19593 cm^{-1} , observed in both the HCL and PDL Nd-Ar spectra.

wing visible). However, the HCL line profile suggested the existence of more than two lines, and so in the final PDL line list, this blend was fitted as three lines (but weighted zero in level optimisation), where the right-most component was classified as a Nd II transition. The relative intensities of the two Nd III lines were then reasonable compared to their theoretically predicted values.

In the literature, the blended Nd II line belongs to the upper level at 25080.9 cm^{-1} with $J = 11/2$ and no configuration assignment, but its experimental lifetime has been measured by Den Hartog et al. (2003) [158]. Strangely, this blended Nd II line at 19593 cm^{-1} was not within published line list of transition probabilities, but it was used by Ryabchikova et al. (2006) [63] for stellar synthesis and correct classification of its blend with $4f^4 \ ^5I_6 - 4f^3(^4I^\circ)5d \ ^5I^\circ_6$, without realising that the strong $4f^4 \ ^5I_4 - 4f^3(^4I^\circ)5d \ ^5H_3$ transition was also a part of the blend. Whether there are more or fewer lines other than the two Nd III lines in this blend is still uncertain.

Overall, my analysis and revision of Dr Crosswhite’s energy levels and transitions completely agreed with those concluded by Ryabchikova et al. (2006) [63]. The one level tentatively identified by Ryabchikova et al. (2006) [63] was revised during the search for the previously unknown $4f^36p$ levels (see subsection 6.7.1).

6.7 Searching for Unknown Energy Levels of Nd III

After the confirmation of all previously published Nd III energy levels, the search for new levels began. Ryabchikova et al. (2006) [63] did not propose any more tentative energy levels other than the 40 levels they presented. There exists another line list of Dr Crosswhite (not the one in [Appendix E](#)), which has upper and lower level energies and J values for each line. This other line list of Dr Crosswhite also circulates within the astronomical community [63, 156], but it was not useful at all in the present Nd III term analysis, i.e., no agreement. Therefore, no tentative energy levels from previous works were available or confirmed for the search for unknown Nd III levels.

This section is the longest section of the thesis and contains specific discussions on how previously unknown Nd III energy levels were identified in chronological order. This section is aimed to be a demonstration of the methodologies discussed in the previous parts of the thesis and a reference for future Nd III term analyses. Results are summarised in [section 6.8](#) and please refer to [Figure 2.1](#) for discussions involving energy level labels.

Although no previously published eigenvector compositions of the $4f^3(^4I^\circ)6p$ and $4f^3(^4I^\circ)6s$ levels were available, transition probability and level energy data from Gaigalas et al. (2019) [81] were sufficient to guide my analysis to establish all 40 $4f^3(^4I^\circ)5d$ ([subsection 6.7.1](#)), 29 $4f^3(^4I^\circ)6p$ ([subsection 6.7.1](#)), and all 8 $4f^3(^4I^\circ)6s$ levels ([subsection 6.7.2](#)). A few higher-lying $4f^35d$ levels (above $35\,000\text{ cm}^{-1}$), particularly those of the $4f^3(^4G^\circ)5d\ ^5H^\circ$ and $^5I^\circ$ terms, were also identified without eigenvector composition data (see [subsection 6.7.3](#)), which were only available for levels under $33\,000\text{ cm}^{-1}$ [63, 86].

Limitations of previous theoretical calculations of Nd III atomic structure came to light after identifying levels of the $4f^3(^4G^\circ)5d$ sub-configuration; more accurate parameterised Cowan code atomic structure calculations ([subsection 6.7.4](#)) were then used as the approach for theoretical guidance of the Nd III term analysis. Furthermore, the continuation of the analysis was significantly aided by Nd spectra of stars and vacuum sliding sparks. The access to more accurate calculations and the different Nd spectra were acquired through collaboration with the lead authors of Ryabchikova et al. (2006) [63], Dr Ryabtsev and Dr Ryabchikova. All discussions between [subsection 6.7.4](#) and [subsection 6.7.18](#) are on the results of the collaboration.

6.7.1 Completing the $4f^3(^4I^\circ)5d$ and $4f^3(^4I^\circ)6p$ Sub-configurations

The three levels of the $4f^3(^4I^\circ)5d\ ^3H^\circ$ term were identified and assigned. The remaining unidentified levels of the $4f^3(^4I^\circ)5d$ sub-configuration were then those of the $^3,^5L^\circ$ and $^3G^\circ$ terms and the $^5G^\circ_{2,6}$ levels. Transitions from $^3,^5L^\circ$ to the $4f^4\ ^5I$ ground term levels were very weak, which follows from the LS coupling selection rules ($\Delta L = \pm 1$) due to the high purities of $^3,^5L^\circ$ and $4f^4\ ^5I$ in the LS coupling basis ($> 80\%$ for the triplet, $> 90\%$ for the quintet, and $> 96\%$ for the ground term). This is similar for the $^3,^5G^\circ$ terms, but their much lower purities ($\sim 50\%$) allowed stronger transitions to the $4f^4\ ^5I$ ground term levels. The extreme J values of the $^5G^\circ_2$ and $^5L^\circ_{10}$ levels have no allowed E1 transitions ($\Delta J = \pm 1, 0$) to the ground term levels ($J = 4, 5, 6, 7, 8$). So the search for the remaining $4f^3(^4I^\circ)5d$ levels required classification of their transitions from the $4f^3(^4I^\circ)6p$ levels, which were yet to be identified.

Classifications of the $4f^3(^4I^\circ)5d - 4f^3(^4I^\circ)6p$ transitions in the Nd-Ar PDL FT spectra were possible for two main reasons: 1) the lines fall within the line-sparse UV region ($> 30\,000\text{ cm}^{-1}$) and are associated with relatively few ambiguous possible candidate energy levels, and 2) the $4f^3(^4I^\circ)6p$ levels had many more observable transitions to lower levels compared to the $4f^3(^4I^\circ)5d$ levels, which reduced the number of candidate levels further. For the $4f^3(^4I^\circ)5d$ levels, there were, at most, three observable transitions ($\Delta J = 0, \pm 1$) to lower levels of the ground term $4f^4\ ^5I$, because other levels of the $4f^4$ configuration were unknown and the associated $4f^4 - 4f^3(^4I^\circ)5d$ transitions lie above the infrared wavelength limit of the Imperial College VUV FT spectrometer and are much weaker.

The levels $4f^3(^4I^\circ)6p\ ^5I_{5,6}$ were first identified using five transitions each. Their identifications were crucial in gauging the observed relative intensities of all $4f^3(^4I^\circ)5d - 4f^3(^4I^\circ)6p$ transitions, and gauging the energy offsets of the $4f^3(^4I^\circ)6p$ levels in theoretical calculations by Gaigalas et al. (2019) [81]. With the expected intensities and wavenumber offsets established, the $^5G^\circ_2$ and $^5L^\circ_{10}$ levels of $4f^3(^4I^\circ)5d$ were found using only a single line each. The $4f^3(^4I^\circ)5d\ ^5G^\circ_2 - 4f^3(^4I^\circ)6p\ ^5H_3$ transition at 42870.371 cm^{-1} was the sole candidate within $\pm 300\text{ cm}^{-1}$ of the expected wavenumber, and the very intense (relative to other $4f^35d - 4f^36p$ transitions) $4f^3(^4I^\circ)5d\ ^5L^\circ_{10} - 4f^3(^4I^\circ)6p\ ^5K_9$ at 47208.733 cm^{-1} was the sole candidate between $42\,000$ - $49\,000\text{ cm}^{-1}$.

Finding all levels of the $4f^3(^4I^\circ)6p$ sub-configuration helped with identifying the still unknown

levels of the $4f^3(^4I^\circ)5d$ sub-configuration. At this stage, only $4f^3(^4I^\circ)5d\ ^3G^\circ_5$ of the $4f^3(^4I^\circ)5d$ sub-configuration remained uncertain due to having only very weak but observable transitions to $4f^4\ ^5I$ and from $4f^3(^4I^\circ)6p\ ^3H_6$. The $4f^3(^4I^\circ)5d\ ^3G^\circ_5$ level was later revised during the search for $4f^4\ ^5F_4$ (subsection 6.7.15).

6.7.2 Completing the $4f^3(^4I^\circ)6s$ Sub-configuration

Once all $4f^3(^4I^\circ)6p$ levels were identified, searching for the eight levels of $4f^3(^4I^\circ)6s\ ^{3,5}I^\circ$ became very simple. Each of the $4f^3(^4I^\circ)6s$ levels were identified using at least five transitions from the $4f^3(^4I^\circ)6p$ levels, but this analysis had some complications.

Firstly, the energies of the $4f^3(^4I^\circ)6s$ levels were similar to many levels of the same parity $4f^35d$ configuration, and mixing between these two configurations was observed in the eigenvector compositions. Consequently, the predicted transition probabilities involving the $4f^3(^4I^\circ)6s$ levels agreed less well with observed relative intensities compared to transitions not involving $4f^36s$. Secondly, some $4f^3(^4I^\circ)6s - 4f^3(^4I^\circ)6p$ lines were expected to lie within spectrum D of Table 4.6 and were therefore affected by the photon noise from this intense and line-rich region, and thus would have low SNRs and more uncertain intensities. Thirdly, these intensities also needed to be compared with $4f^3(^4I^\circ)6s - 4f^3(^4I^\circ)6p$ lines from spectrum E, which is less reliable than comparing lines within the same spectrum, due to observation on different days and lamp conditions (e.g. different plasma conditions and hence level populations). Lastly, the $4f^3(^4I^\circ)6s - 4f^3(^4I^\circ)6p$ lines had larger widths because the 6s electron orbital penetrates closer to the nucleus, and so the levels are affected more by nuclear perturbation effects (see Figure 6.4).

When the $4f^3(^4I^\circ)6s$ levels were identified, optimisation of their level energies required adjustments to the fitting of the spectral lines of the classified $4f^3(^4I^\circ)6s - 4f^3(^4I^\circ)6p$ transitions to reach agreements between observed wavenumber uncertainty and Ritz wavenumbers. Particularly, the wider and weaker lines required manual COG fits, and isotope or hyperfine component transitions could be lost in the noise. The less accurate and difficult-to-fit wavenumbers did not fully prevent their classifications because: 1) a large number of lines were observed involving the $4f^3(^4I^\circ)6s$ levels due to the knowledge of all $4f^3(^4I^\circ)6p$ levels, which removed ambiguous candidate levels; 2) the collective agreement in larger observed line widths of the $4f^3(^4I^\circ)6s - 4f^3(^4I^\circ)6p$ lines due to more significant nuclear effects; and 3) the classifications of additionally

observed $4f^4\ ^5I - 4f^3(^4I^\circ)6s$ transitions.

The $4f^3(^4I^\circ)6s$ levels were eventually labelled using jj coupling of the $6s$ electron with $4f^3(^4I^\circ)$. This was because of the much higher purities of these levels under this coupling scheme; the $6s$ orbital has appreciable probability density near the nucleus, but the bulk of the probability density function is very far from that of the $4f$ orbital, therefore the coulomb interaction between the $4f^3$ and the $6s$ electrons is much smaller compared to the coulomb interaction between the $4f^3$ and the $5d$ electrons.

6.7.3 Locating the $4f^3(^4G^\circ)5d$ Sub-configuration

All of the strongest lines in spectrum E are around $35\,000\text{ cm}^{-1}$ and show the Nd III $4f^4 - 4f^35d$ isotope structure line profile (Figure 6.4). Their relative line intensities correspond to those of $4f^4\ ^5I - 4f^3(^4G^\circ)5d\ ^5H^\circ$ predicted by Gaigalas et al. (2019) [81], but their wavenumbers were about 2500 cm^{-1} lower than their calculated values from Gaigalas et al. (2019) [81]. Nevertheless, their very high intensities in this spectral region essentially reduced the number of ambiguous candidate energy levels to zero.

The $4f^3(^4G^\circ)5d\ ^5H_{4,5,6,7}^\circ$ levels were identified. However, There were two candidate energy levels for $4f^3(^4G^\circ)5d\ ^5H_3^\circ$ using at 34856.862 and 35576.326 cm^{-1} which could not be resolved as only the transition to the ground level $4f^4\ ^5I_4$ was expected to be observed due to the ΔJ selection rule and no other $4f^4$ levels with allowed J values were known. The level at 34856.862 cm^{-1} was eventually labelled $4f^3(^4G^\circ)5d\ ^5G_3^\circ$ and the level at 35576.326 cm^{-1} was eventually labelled $4f^3(^4G^\circ)5d\ ^5H_3^\circ$.

The $4f^4\ ^5I - 4f^3(^4G^\circ)5d\ ^5I^\circ$ transitions were much weaker, but the strongest lines were sufficient in SNR to show the expected isotope line profiles (Figure 6.4), which enabled the identification of $4f^3(^4G^\circ)5d\ ^5I_{4,5,7,8}^\circ$. Two candidates for the two levels leading with $4f^3(^4G^\circ)5d\ ^5I_6^\circ$ [81] at 34994.015 cm^{-1} and 35154.434 cm^{-1} were also identified and will be discussed in subsection 6.7.6.

The $4f^3(^4G^\circ)5d\ ^5I_7^\circ$ level was found with nine transitions, with lines from the levels of the $4f^3(^4I^\circ)6p$ sub-configuration. These lines were first labelled as incorrect classifications due to their unexpectedly high observed relative intensities compared with theoretical calculations of

Gaigalas et al. (2019) [81]. However, they were later found to be correct due to an almost 50/50 mix of the $4f^3(^4G^\circ)5d\ ^5I^\circ_7$ level with the $4f^3(^4I^\circ)6s\ ^3I^\circ_7$ level from another configuration. This is discussed in [subsection 6.7.5](#) and was identified using new semi-empirical Cowan code Nd III atomic structure calculations, discussed in the next subsection.

6.7.4 New Cowan Code Nd III Atomic Structure Calculations

Since the theoretical calculations of Gaigalas et al. (2019) [81] have begun limiting the analysis (discussed in the previous subsection), improvements to theoretical guidance were needed. This was achieved through collaboration with Dr Ryabtsev, where he made new calculations iteratively as new experimental energy levels were identified (see [subsection 2.2.8](#) and [Appendix A](#) for details of the final iteration). At this point, the collaboration with Dr Ryabtsev and Dr Ryabchikova formally began, where analysis using stellar and VS Nd grating spectra also became possible.

Using the newly calculated eigenvector compositions, several previously classified $4f^35d$ levels were relabelled, and those without labels were assigned using *LS*-coupling eigenfunctions. There were shifts of order 2000 cm^{-1} in the newly calculated level energies (see [Table C.1](#)) compared to predictions by Gaigalas et al. (2019) [81] of unknown $4f^35d$ levels lying above $30\,000\text{ cm}^{-1}$. Candidate energy levels predicted to unlikely have observable lines by Gaigalas et al. (2019) [81] became good targets for level searching. For example, the transition probabilities of the $4f^3(^2H_2)5d\ ^3K_6$ transitions down to $4f^4$ were one magnitude higher in the newly parameterised Cowan code calculations compared to predictions of Gaigalas et al. (2019) [81], and the upper level was found with the line intensities expected from the new Cowan code calculations. This was likely due to significantly differing eigenvector compositions between the atomic structure calculations (see [subsection 2.3.2](#)).

Each time new sets of levels were found, the Cowan code calculation was repeated and further parameterised using the new levels. With each iteration, already identified $4f^35d$ levels deviating by more than $\sim 150\text{ cm}^{-1}$ from their predicted positions were highlighted as questionable. In most cases, this corresponded to incorrect classifications. This implied that the search range and predicted energy uncertainties were around $\pm 200\text{ cm}^{-1}$ for the yet-to-be-identified $4f^35d$ levels.

Table 6.2: Theoretical $g_u A$ values (s^{-1}) and Nd-Ar PDL FT spectra SNR and relative intensities of three transitions from $4f^3(^4I^\circ)6p$ to $4f^3(^4G^\circ)5d\ ^5I^\circ_7$

Upper Level	SNR	Relative Intensity	Cowan Code	Cowan Code (no 6s fit)	Gaigalas et al. (2019)
$4f^3(^4I^\circ)6p\ ^3H_6$	13	160	2.1×10^9	2.9×10^8	5.3×10^6
$4f^3(^4I^\circ)6p\ ^3I_7$	8	64	1.8×10^9	1.7×10^8	5.1×10^6
$4f^3(^4I^\circ)6p\ ^3K_8$	8	90	1.6×10^9	6.0×10^7	2.3×10^5
Predicted $4f^3(^4I^\circ)6s\ (\frac{15}{2}, \frac{1}{2})^\circ_7$ Energy			37094 cm^{-1}	37404 cm^{-1}	37922 cm^{-1}
Predicted $4f^3(^4G^\circ)5d\ ^5I^\circ_7$ Energy			36847 cm^{-1}	36877 cm^{-1}	39901 cm^{-1}
Energy Difference			247 cm^{-1}	527 cm^{-1}	-1979 cm^{-1}

Improved accuracy of the theoretical guidance provided by new Cowan code calculations and experimental guidance provided by stellar and VS Nd spectra will be demonstrated in the remaining subsections.

6.7.5 Configuration Mixing between $4f^35d$ and $4f^36s$ in $4f^3(^4G^\circ)5d\ ^5I^\circ_7$

The higher accuracy of the new Cowan code calculations was demonstrated from the identification of the $4f^3(^4G^\circ)5d\ ^5I^\circ_7$ level at $36890.348\ \text{cm}^{-1}$ (previously discussed at the end of subsection 6.7.3). This level was concluded to be heavily mixed with $4f^3(^4I^\circ)6s\ (\frac{15}{2}, \frac{1}{2})^\circ_7$. Three $4f^3(^4G^\circ)5d\ ^5I^\circ_7 - 4f^3(^4I^\circ)6p$ lines with the highest calculated transition probabilities are listed in Table 6.2, the $g_u A$ and level energy values from new parameterised Cowan code calculations including the new $4f^3(^4I^\circ)6s$ levels, Cowan code calculations without parameterisation of the $4f^3(^4I^\circ)6s$ levels [63], and calculations of Gaigalas et al. (2019) [81] are in the final three columns. For context, the three upper $4f^3(^4I^\circ)6p$ levels are very similar in energies and a transition to $4f^3(^4I^\circ)5d$ with $gA = 2 \times 10^9\ \text{s}^{-1}$ was expected to have an observed relative intensity of around 120, which only agrees with the Cowan code calculations after fitting the semi-empirical parameters with the identified $4f^3(^4I^\circ)6s$ (and $4f^3(^4I^\circ)5d$) levels.

Without using $4f^3(^4I^\circ)6s$ for parameterisation, $36890.348\ \text{cm}^{-1}$ ($J = 7$) was calculated to be composed of 70% of $4f^3(^4I^\circ)6s\ ^3I^\circ_7$ and 9% $4f^3(^4G^\circ)5d\ ^5I^\circ_7$ [63]. The final eigenvector composition of $36890.348\ \text{cm}^{-1}$ was 44% $4f^3(^4G^\circ)5d\ ^5I^\circ_7$ and 43% $4f^3(^4I^\circ)6s\ ^3I^\circ_7$, this composition is similar when the two levels are considered in the basis using jj -coupling of the excited electron

with the LS terms of the $4f^3$ electrons. Similarly, $4f^3(^4I^\circ)6s\ (\frac{15}{2}, \frac{1}{2})^\circ_7$ (37089.599 cm^{-1} , $J = 7$) was predicted to mix more with the $4f^3(^4G^\circ)5d\ J = 7$ level at 36890.348 cm^{-1} after parameterising the Cowan code with the $4f^3(^4I^\circ)6s$ levels, relative intensities of its observed transitions to $4f^4$ were also in better agreement with the orders-of-magnitude higher predicted transition probabilities compared to previous calculations without any $4f^3(^4I^\circ)6s$ parameterisation. Any observed $4f^4 - 4f^36s$ transitions (e.g. $4f^4\ ^5I_6 - 4f^3(^4I^\circ)6s\ (\frac{9}{2}, \frac{1}{2})^\circ_5$ of Figure 6.4) were also very likely results of mixing between the $4f^4$ and $4f^35d$ configurations.

6.7.6 Zeeman Splitting and J Values of 34994 cm^{-1} and 35154 cm^{-1}

The two levels observed at 34994 cm^{-1} and 35154 cm^{-1} were highly mixed in the final calculations, with leading eigenvector percentages of less than 25%. Their labels could not be assigned using the labels given by Gaigalas et al. (2019) [81] (no eigenvector composition data). These two levels caused much confusion from incorrect tentative classifications. In the screenshot of Figure 6.12, 34994.015 cm^{-1} was labelled $4f^3(^4F^\circ)5d\ ^3H^\circ_6$. At first, 34994.015 cm^{-1} was labelled $4f^3(^4G^\circ)5d\ ^5I^\circ_6$ and 35154.437 cm^{-1} had the label $4f^3(^4F^\circ)5d\ ^3H^\circ_6$, the two labels were swapped at the time of Figure 6.12. A better candidate for $4f^3(^4G^\circ)5d\ ^5I^\circ_6$ was later found using the new Cowan code calculations at 35549.5647 cm^{-1} , which left 34994.015 cm^{-1} and 35154.437 cm^{-1} for term assignment and reconsideration.

The lines $4f^4\ ^5I_{5,6} - 34994.015\ \text{cm}^{-1}$ and $4f^4\ ^5I_{5,6} - 35154.437\ \text{cm}^{-1}$ were the only observable lines to other known levels during the initial identifications of the two levels, one with $J = 5$ and one with $J = 6$. By coincidence, these four lines had the same (within uncertainties) predicted and observed relative intensities. Since the difference between the two observed energies was also on the order of the energy uncertainties predicted by the Cowan code ($\pm 200\ \text{cm}^{-1}$) and the two levels were predicted highly mixed (not suitable to apply LS -coupling selection rules), there was no reliable method of distinguishing between the two except by possibly considering the intensity of the observed $4f^4\ ^5G_5 - 34994.015\ \text{cm}^{-1}$ line, but the $4f^4\ ^5G_5$ level itself was uncertain at the time. Unfortunately, the two J values were assigned the wrong way around.

This mistake remained hidden for two months until Dr Ryabchikova performed the stellar spectral synthesis of HD 144897. She used an effective magnetic field strength of 8.8 kG and investigated the $4f^4\ ^3K_{2,6} - 34994.015\ \text{cm}^{-1}$ transition, see Figure 6.10. The existence of Zeeman

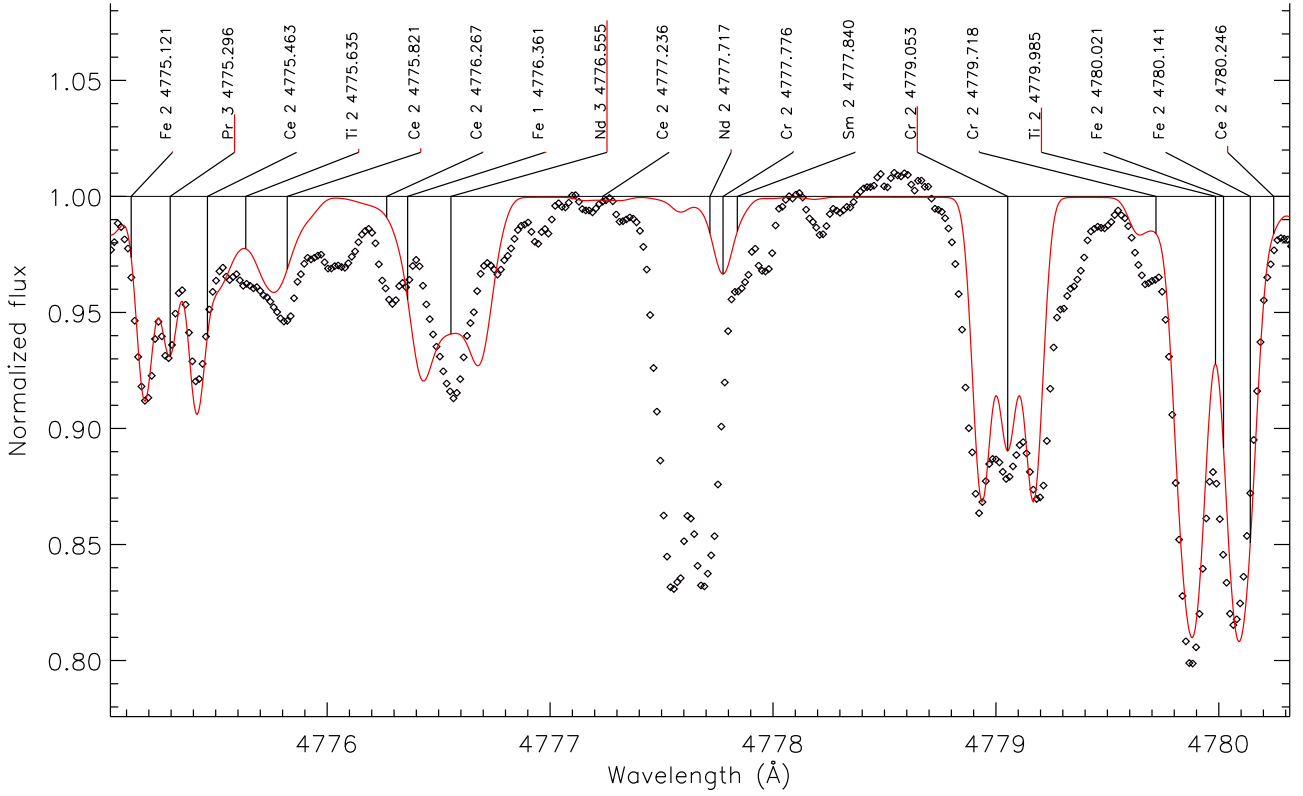


Figure 6.10: Spectral synthesis of $4f^4 \ ^3K_{26} - 34994.015 \text{ cm}^{-1}$ (incorrect) at 4776.56 Å of HD 144897 with an effective magnetic field strength of 8.8 kG [156]. The diamonds are the observed absorption spectrum and the red curve is the synthetic absorption spectrum.

splitting of atomic energy levels is readily observed in the three lines belonging to Pr III, Cr II, and Ti II (nearly). However, for Nd III at 4776.555 Å , the predicted Zeeman pattern did not match, which conclusively showed the incorrect level label and J value assignment of the level at $34994.015 \text{ cm}^{-1}$.

When $4f^4 \ ^3K_{26}$ was found (subsection 6.7.12), $34994.015 \text{ cm}^{-1}$ was incorrectly identified as $4f^3(4F^\circ)5d \ ^3H^\circ_6$. One may expect the incorrect $4f^3(4F^\circ)5d \ ^3H^\circ_6$ level to have no observable transition to the $4f^4 \ ^3K_{26}$ level, but by another coincidence, a line exists in the Nd-Ar PDL FT spectrum which agrees with the Ritz wavenumber and relative intensity of $4f^4 \ ^3K_{26} - 4f^3(4F^\circ)5d \ ^3H^\circ_6$, even when the upper-level energy was incorrect at $34994.015 \text{ cm}^{-1}$. This can also be seen in the 4776.555 Å line also observed in the stellar spectrum in Figure 6.10 if the Zeeman pattern matched. The same coincidence occurred for the classification of $4f^4 \ ^3K_{27} - 34994.015 \text{ cm}^{-1}$ in a plausible blend. These two imposter lines did ‘help’ with the identifications of their lower levels $4f^4 \ ^3K_{6,7}$ by increasing the number of lines classified per level to further remove ambiguities. In the end, only the incorrect Zeeman pattern in the stellar spectrum revealed the wrong level assignments, and $34994.015 \text{ cm}^{-1}$ was given the final label

33839.217	-0.043	960	634	4f36s~4I3I/	5.0 *	-4f36p_4I5H/	4.0 *	32605.900 -	66445.160
33846.092	0.179	971	573	4f36s~4I3I/	5.0 *	-4f36p_4I3K/	6.0 *	32605.900 -	66451.813
33666.909	0.012	970	563	4f36s~4I3I/	5.0 *	-4f36p_4I5H/	5.0 *	32605.900 -	66272.797
44630.377	0.169	302	128	4f36s~4I3I/	5.0 *	-4f36p_2H1I2	6.0 *	32605.900 -	77236.108
31744.895	-0.012	813	90	4f36s~4I3I/	5.0 *	-4f36p_4I3I/	5.0 *	32605.900 -	64350.807
40642.287	0.287	287	90	4f36s~4I3I/	5.0 *	-4f36p_2H3I2	5.0 *	32605.900 -	73247.900
32417.710	-0.026	793	64	4f36s~4I3I/	5.0 *	-4f36p_4I3K/	6.0 *	32605.900 -	65023.636
41653.154	0.050	256	56	4f36s~4I3I/	5.0 *	-4f36p_4F5G/	4.0 *	32605.900 -	74259.004
38220.062	-0.042	164	35	4f36s~4I3I/	5.0 *	-4f36p_4I3H/	6.0 *	32605.900 -	70826.004
31638.008	-0.004	348	28	4f36s~4I3I/	5.0 *	-4f36p_4I5I/	4.0 *	32605.900 -	64243.912
35741.633	-0.055	287	27	4f36s~4I3I/	5.0 *	-4f36p_4I3I/	6.0 *	32605.900 -	68347.588
43820.954	0.204	234	489	4f35d~2H1I2	6.0 *	-4f36p_2H3I2	6.0 *	32823.700 -	76644.450
33673.560	0.037	542	61	4f35d~2H1I2	6.0 *	-4f36p_4I5I/	7.0 *	32823.700 -	66497.223
31798.259	-0.050	580	32	4f35d~2H1I2	6.0 *	-4f36p_4I5K/	7.0 *	32823.700 -	64622.009
31725.911	-0.011	488	29	4f35d~2H1I2	6.0 *	-4f36p_4I5I/	6.0 *	32823.700 -	64549.622
33449.035	-0.062	245	27	4f35d~2H1I2	6.0 *	-4f36p_4I5H/	5.0 *	32823.700 -	66272.797
35523.879	-0.009	558	26	4f35d~2H1I2	6.0 *	-4f36p_4I3I/	6.0 *	32823.700 -	68347.588
35789.467	-0.046	586	23	4f35d~2H1I2	6.0 *	-4f36p_4I3H/	5.0 *	32823.700 -	68613.213
33628.019	-0.094	559	17	4f35d~2H1I2	6.0 *	-4f36p_4I3K/	6.0 *	32823.700 -	66451.813
35683.622	-0.063	418	11	4f35d~2H1I2	6.0 *	-4f36p_4I3K/	7.0 *	32823.700 -	68507.385

Figure 6.11: Classified transitions of $4f^3(^2H2^\circ)5d\ ^1H^\circ_5$ and $4f^3(^2H2^\circ)5d\ ^1I^\circ_6$ in the Nd vacuum spark grating spectra line list [138]. Column 1 is the observed wavenumber, column 2 is the difference from Ritz wavenumber, column 3 is the observed intensity (greater than the values in Table D.2 by a factor of 10), column 4 is the g_uA value from Cowan code calculations at the time in 10^6 s^{-1} , and the remaining columns give level information of the line.

$4f^3(^2H2^\circ)5d\ ^3H^\circ_5$ and 35154 cm^{-1} was given the final label $4f^3(^4F^\circ)5d\ ^3H^\circ_6$.

6.7.7 The Singlets $^1H^\circ_5$ and $^1I^\circ_6$ of $4f^3(^2H2^\circ)5d$

These two levels were highly mixed, in the final Cowan code calculations, $4f^3(^2H2^\circ)5d\ ^1H^\circ_5$ was the leading component of 32605.894 cm^{-1} at 15% and $4f^3(^2H2^\circ)5d\ ^1I^\circ_6$ was the leading component of 32823.701 cm^{-1} at 26%. The mixing allowed many transitions to originate from the $4f^3(^4I^\circ)6p$ sub-configuration. These were initially observed at high intensities in the Nd VS grating spectra and later confirmed to be just above the noise level in the Nd-Ar PDL spectra, which enabled classifications of the transitions from these two levels to terms of the $4f^4$ configuration. Identifications of the $4f^3(^2H2^\circ)5d\ ^1H^\circ_5$ and $4f^3(^2H2^\circ)5d\ ^1I^\circ_6$ levels using the Nd-Ar PDL spectra alone would be quite difficult due to low intensities or unobserved lines, for example, 8 out of the 10 lines eventually classified for $4f^3(^2H2^\circ)5d\ ^1H^\circ_5$ were blended and under 10 SNR in the Nd-Ar PDL FT spectra. The relatively large number of transitions from the $4f^36p$ configuration seen in the Nd VS spectra provided plenty of evidence to resolve ambiguities and are shown in the screenshots of Figure 6.11.

6.7.8 Higher-lying $4f^36p$ Energy Levels

Similar to how $4f^3(^2H^{\circ})5d\ ^1H^{\circ}_5$ and $4f^3(^2H^{\circ})5d\ ^1I^{\circ}_6$ were found, the $4f^3(^4F^{\circ})6p\ ^5G_{2,3,4,5}$, $4f^3(^2H^{\circ})6p\ ^3I_{5,6}$, and $4f^3(^2H^{\circ})6p\ ^1I_6$ energy levels were identified using the Nd vacuum spark grating line list. Some classified transitions involving these higher-lying $4f^36p$ levels were also listed in [Figure 6.11](#). Not all first attempts at finding these levels were successful, especially for levels with less than around 4 candidate lines from the grating line list. Only levels with the strongest transitions (at least the main line) observed in the Nd-Ar PDL spectrum were concluded as correct identifications.

6.7.9 Challenges in Finding Unknown $4f^4$ Energy Levels

At this stage of the Nd III term analysis, the experimentally known levels of the ground configuration $4f^4$ were still only the five of the ground term $4f^4\ ^5I$. This had become quite limiting in the search for the remaining higher-lying $4f^35d$ levels because the transition probabilities of lines from these higher-lying $4f^35d$ levels to the ground term were low.

Transitions between the higher-lying $4f^35d$ levels and higher-lying $4f^4$ levels have relatively higher transition probabilities. However, higher-lying $4f^35d$ levels had much lower populations, which resulted in weak or unobservable lines in the Nd-Ar PDL FT spectra. This issue is worsened by the fact that the majority of the remaining unclassified $4f^4 - 4f^35d$ transitions were also expected to lie in the line-rich visible spectral region with high photon noise. For these reasons, accurate theoretical calculations became invaluable; the number of ambiguous candidate energy levels could be reduced by using narrower wavenumber and relative intensity search ranges. Moreover, the availability of VS and stellar spectra of Nd III became necessary in the reduction of ambiguous matches of the weaker $4f^4 - 4f^35d$ transitions towards the end (see [subsection 6.7.15](#)).

One of the biggest challenges in advancing the analysis was the lack of energy levels identified in the $4f^4$ configuration. This meant that the energy parameters of the Cowan code for this configuration were much less well-constrained, and potential energy offsets were unknown. Therefore the predicted level energies for $4f^4$ were much more uncertain compared to those for $4f^35d$. This was eventually overcome through classifications of many lines (> 3) for the first

new levels of $4f^4$, and confirmations in stellar spectral analyses made by Dr Ryabchikova.

6.7.10 Finding the $4f^4 \ ^5G_5$ Energy Level

The first new level of the $4f^4$ configuration was the $4f^4 \ ^5G_5$ energy level. The $4f^3(^4G^\circ)5d \ ^5G^\circ_{4,5,6}$ levels were expected to have observed transitions to $4f^4 \ ^5G_5$ in the Nd-Ar PDL FT spectra. These three levels were found using the new Cowan code calculations with their transitions to the $4f^4 \ ^5I$ levels. Transition probabilities for the $4f^4 \ ^5I - 4f^3(^4G^\circ)5d \ ^5G^\circ_{4,5}$ transitions were predicted around an order of magnitude lower by Gaigalas et al. (2019) [81], which had previously prevented their confident identifications. The $4f^4 \ ^5G_5 - 4f^3(^4G^\circ)5d \ ^5G^\circ_5$ transition was the best option for identifying the $4f^4 \ ^5G_5$ level. This line was expected to have sufficient SNR to have an observable isotope profile (e.g. Figure 6.4), whereas the three other observable transitions from the known levels $4f^3(^4G^\circ)5d \ ^5G^\circ_4$, $4f^3(^4G^\circ)5d \ ^5G^\circ_6$, and $4f^3(^4G^\circ)5d \ ^5H^\circ_5$ were expected around the noise level. This was a problem because any line around the noise level in the line-rich visible region had a very high chance of being either blended or not fitted.

In the calculations by Ryabchikova et al. (2006) [63], $4f^4 \ ^5G_5$ was predicted to lie at 17307 cm^{-1} . Since there existed another predicted level with the same leading term $4f^4 \ ^5G_5$ at 15801 cm^{-1} , the search for $4f^4 \ ^5G_5$ was performed within the $15\,000\text{--}20\,000 \text{ cm}^{-1}$ range, where any set of candidate lines containing more than two lines and a strong $4f^4 \ ^5G_5 - 4f^3(^4G^\circ)5d \ ^5G^\circ_5$ candidate line at the expected intensity with the correct isotope profile was considered. Any missing wavenumbers or unexpectedly high intensities were manually checked in the observed Nd-Ar PDL and HCL FT spectra for unfitted or blended lines respectively.

A candidate for $4f^4 \ ^5G_5$ was tentatively found at $18313.004 \text{ cm}^{-1}$, with $4f^4 \ ^5G_5 - 4f^3(^4G^\circ)5d \ ^5G^\circ_5$ at the expected intensity and showing the expected isotope line profile, $4f^4 \ ^5G_5 - 4f^3(^4G^\circ)5d \ ^5G^\circ_6$ at 5 SNR, and $4f^4 \ ^5G_5 - 4f^3(^4G^\circ)5d \ ^5H^\circ_5$ blended at SNR 10. This new level revealed that $4f^4 \ ^5G_5 - 4f^3(^4G^\circ)5d \ ^5G^\circ_4$ was in a weak, wide, and blended line profile that had been fitted as one line in the line list, where the initially fitted wavenumber was far from the expected Ritz wavenumber, further highlighting the difficulty and importance in obtaining accurate line lists.

This identification of $4f^4 \ ^5G_5$ became more and more certain over a period of three months during which the following events developed: 1) the Slater integral values of the calculations were adjusted by considering those of neighbouring ions which resulted in a prediction of 18116 cm^{-1} ,

2	21298.3998	4f4 5G5*	4G5d 5G6	18312.988	39611.3883	4693.863 bl. Cr2	4693.91 bl. Ce2 93.88
3	19664.6547	4f4 5G5*	4G5d 5G5	18312.988	37977.6432	5083.690 blend room is available	5083.86
3	19279.7705	4f4 5G5*	4G5d 5H5	18312.988	37592.759	Si2 blend	5185.36 Tm3 blend
3	18204.3612	4f4 5G5*	4G5d 5G4	18312.988	36517.3497	5491.657 weak line	5491.68
3	16681.0256	4f4 5G5*	4F5d 3H6	18312.988	34994.0141	5993.2	5993.19
3	47810.8500	4f4 5G5*	4G5d 5H5	18312.988	37592.759		

Figure 6.12: Classifications of five transitions to $4f^4 \ ^5G_5$ with comments for the stars HD 170973 and HD 217522 in the final two columns, respectively [156]. The first column is the transition wavenumber and columns 2-5 are the levels information.

which was remarkably close to the observed value, 2) the classifications of the five transitions to $4f^4 \ ^5G_5$ were confirmed by Dr Ryabchikova in two separate stars HD 170973 and HD 217522 with effective temperatures of 11 000 K and 6750 K, respectively, details are in Figure 6.12, and 3) stellar spectral synthesis of HD 170973 for Nd III abundance was performed later by Dr Ryabchikova, and these lines remain confirmed.

6.7.11 Finding the $4f^4 \ ^3K2_7$ Energy Level

In the search for the $4f^4 \ ^3K2$ term, a separate line list of 441 lines was created for the input of *LEVHAM*. This list includes PDL wavenumbers of lines observed in both the Nd-Ar PDL line list and Dr Crosswhite's unclassified Nd III line lists (see Appendix E), plus lines that were only observed in Dr Crosswhite's line list (using her wavenumbers), and a small list of 37 lines from the Nd-Ar PDL spectra that were noted to have the characteristic $4f^4 - 4f^3 5d$ isotope line profile (Figure 6.4). Therefore, only the lines Dr Crosswhite and I had classified to be likely of Nd III and the lines Dr Crosswhite had observed but were too weak in the Nd-Ar PDL spectra were included in the level search for the $4f^4 \ ^3K2$ term. The search for $4f^4 \ ^3K2_8$ was first attempted using this line list but without success. For $4f^4 \ ^3K2_7$ (and $4f^4 \ ^5F_5$, see subsection 6.7.13), this was however very effective. Unfortunately, this line list did not prove useful for the search of any other levels.

$4f^4 \ ^3K2_7$ was predicted to be at 15557 cm^{-1} . This was uncertain as the $4f^4$ parameters of the Cowan code were still poorly constrained at the time, using only the ground term and, at the time, tentative $4f^4 \ ^5G_5$. Since the new input for *LEVHAM* only had 441 lines, the number of ambiguous candidate levels was expected to be very low, therefore the search range was set between $7000\text{-}25\,000 \text{ cm}^{-1}$. Any potential level energy matched with more than two lines to five input known levels within a tolerance of 0.15 cm^{-1} was examined. One of the five known levels was the incorrect $4f^3(^4F^\circ)5d \ ^3H^\circ_6$ (see subsection 6.7.6). The output of *LEVHAM* is

ENERGY	WAVENUM	INTENSITY		LEVEL	J	New level
34994.014 -	26345.467	6.1	60	4F5d 3H6	6.0	8648.547
39058.272 -	30409.681	0.00	0	4G5d 5H6	6.0	8648.591
						0.044
39058.272 -	29944.433	0.00	0	4G5d 5H6	6.0	9113.840
36890.348 -	27776.374	1.21	14	4G5d 5I7	7.0	9113.974
						0.134
36890.348 -	27679.750	1.08	12	4G5d 5I7	7.0	9210.598
39058.272 -	29847.615	0.00	0	4G5d 5H6	6.0	9210.658
						0.060
39058.272 -	29455.411	7.9	64	4G5d 5H6	6.0	9602.862
31781.802 -	22178.875	2.7	13	b2H5d 3K7	7.0	9602.927
						0.065
39058.272 -	27920.178	0.00	0	4G5d 5H6	6.0	11138.095
34994.014 -	23855.908	0.00	0	4F5d 3H6	6.0	11138.105
						0.010
36890.348 -	21736.570	0.00	0	4G5d 5I7	7.0	15153.778
39058.272 -	23904.473	3.1	15	4G5d 5H6	6.0	15153.799
31781.802 -	16627.998	4.9	20	b2H5d 3K7	7.0	15153.804
32832.446 -	17678.638	7.8	35	4F5d 5H7	7.0	15153.809
						0.031
31781.802 -	15716.194	4.2	11	b2H5d 3K7	7.0	16065.608
36890.348 -	20824.631	0.00	0	4G5d 5I7	7.0	16065.717
						0.109

Figure 6.13: *LEVHAM* output in the search for $4f^4\ ^3K2_7$. The columns are: input connecting level energy, observed wavenumber, intensity and SNR of the observed line, level and J value of the input connecting level, the candidate level energy of the new level, and the maximum deviation of the new level energy derived from different line and level combinations. The meaning of various columns is also in the discussions of Figure 6.3. Lines with zero intensity and SNR were observed only in Dr Crosswhite's unclassified Nd III line list (Appendix E).

shown in [Figure 6.13](#) in its entirety, showing spurious level candidates as well as a clear new level. Evidently, there is no doubt $4f^4 \ ^3K_{27}$ is at 15153.8 cm^{-1} , where four lines from the combined line list matched the Ritz wavenumber differences between 15153.8 cm^{-1} and four different known levels within 0.03 cm^{-1} with the expected relative line intensity pattern. The line at $21736.570 \text{ cm}^{-1}$ from Dr Crosswhite's line list was not observed in the Nd-Ar PDL spectra, $23904.473 \text{ cm}^{-1}$ was observed in both Nd-Ar PDL and Crosswhite's line list, and $16627.998 \text{ cm}^{-1}$ and $17678.638 \text{ cm}^{-1}$ were absent in Crosswhite's list of unclassified Nd III lines but seen in the Nd-Ar PDL spectrum.

6.7.12 Finding the $4f^4 \ ^3K_{26}$ Energy Level

The identification of $4f^3(^2H^{\circ})6p \ ^3I_6$ (discussed back in [subsection 6.7.8](#)) revealed the incorrect identification of $4f^3(^2H^{\circ})5d \ ^3K_{26}^{\circ}$, as the transition between these two levels was predicted to be very strong but the line was missing in both the Nd-Ar PDL and Nd vacuum spark spectra. The correct identification for $4f^3(^2H^{\circ})5d \ ^3K_{26}^{\circ}$ was the missing key to identifying $4f^4 \ ^3K_{26}$, because the $4f^4 \ ^3K_{26} - 4f^3(^2H^{\circ})5d \ ^3K_{26}^{\circ}$ transition was expected at intermediate relative intensities with observable $4f^4 - 4f^35d$ isotope profile. The number of ambiguous candidate levels was significantly reduced with the requirement of this line to be in the set of candidate lines.

Since $4f^4 \ ^3K_{27}$ was found around 400 cm^{-1} lower than its predicted value at the time, $4f^4 \ ^3K_{26}$ (predicted 14450 cm^{-1}) was also expected to have a similar offset and to lie at around 14000 cm^{-1} . Using the Nd-Ar PDL line list, a tolerance of 0.05 cm^{-1} , and the search range $13800\text{-}14300 \text{ cm}^{-1}$, any *LEVHAM* matches of three or more lines to eight known levels were examined. From these parameters, there existed only one match with more than three candidate lines to known levels at 14064.3 cm^{-1} , which were reasonably consistent with relative intensities and line profiles in the Nd-Ar HCL FT spectra. The confidence in this identification later greatly rose with agreement shown in lines of stellar spectra and from consistency with transitions later classified involving the $4f^4 \ ^3K_{26}$ level.

6.7.13 Finding the $4f^4 \ ^5F_5$ Energy Level

The combined line list of 441 lines likely belonging to Nd III used to identify $4f^4 \ ^3K_{27}$ in [subsection 6.7.11](#) also enabled the identification of $4f^4 \ ^5F_5$ at 13210.28 cm^{-1} using only two lines that were both present in the Nd-Ar PDL and Dr Crosswhite's line lists. These lines were the moderately intense transition $4f^4 \ ^5F_5 - 4f^3(^4I^\circ)5d \ ^5G^\circ_6$ with observable $4f^4 - 4f^35d$ isotope line profile and the weaker $4f^4 \ ^5F_5 - 4f^3(^4G^\circ)5d \ ^5I^\circ_5$ transition. The *LEVHAM* search range was between $5000\text{--}25\,000 \text{ cm}^{-1}$ with a tolerance of 0.2 cm^{-1} for any candidate level of two observed lines to four known levels. Only three candidate levels were indicated by *LEVHAM* using the combined line list of 441 lines, the correct candidate level was as obvious as when $4f^4 \ ^3K_{27}$ was identified in [Figure 6.13](#).

The $4f^4 \ ^5F_5 - 4f^3(^4G^\circ)5d \ ^5G^\circ_5$ transition was found to be an unfitted line due to low SNR in the Nd-Ar PDL spectrum. Transitions from $4f^3(^2H2^\circ)5d \ ^1I^\circ_6$, $4f^3(^4H2^\circ)5d \ ^1H^\circ_5$, $4f^3(^4F^\circ)5d \ ^5H^\circ_6$, and $4f^3(^2G1^\circ)5d \ ^3H^\circ_6$ were then classified at the expected intensities, further confirming the identification of $4f^4 \ ^5F_5$.

6.7.14 Finding the $4f^4 \ ^3K_{28}$ Energy Level

The final, and successful, attempt at locating $4f^4 \ ^3K_{28}$ was made using the combined line list of [subsection 6.7.11](#). This time, all known energy levels with $J = 7, 8, 9$ from the odd-parity configurations were input as the known levels of *LEVHAM*, which totaled 25 levels. This was to search for transitions that may be predicted as too weak to be observed but were in fact observed experimentally. The number of ambiguous candidate levels from this many input levels was manageable since the combined line list contained only 441 lines. As $4f^4 \ ^3K_{27}$ had been found with a negative offset of around 400 cm^{-1} , the suitable search range for $4f^4 \ ^3K_{28}$ was around $\pm 200 \text{ cm}^{-1}$ of its predicted value minus 400 cm^{-1} . Transitions from seven known levels to $4f^4 \ ^3K_{28}$ at 16459.1 cm^{-1} were successfully found. Then, the confident identification of $4f^3(^2H2^\circ)5d \ ^3K_{28}^\circ$ was made with the strong $4f^4 \ ^3K_{28} - 4f^3(^2H2^\circ)5d \ ^3K_{28}^\circ$ transition showing clear $4f^4 - 4f^35d$ isotope profile.

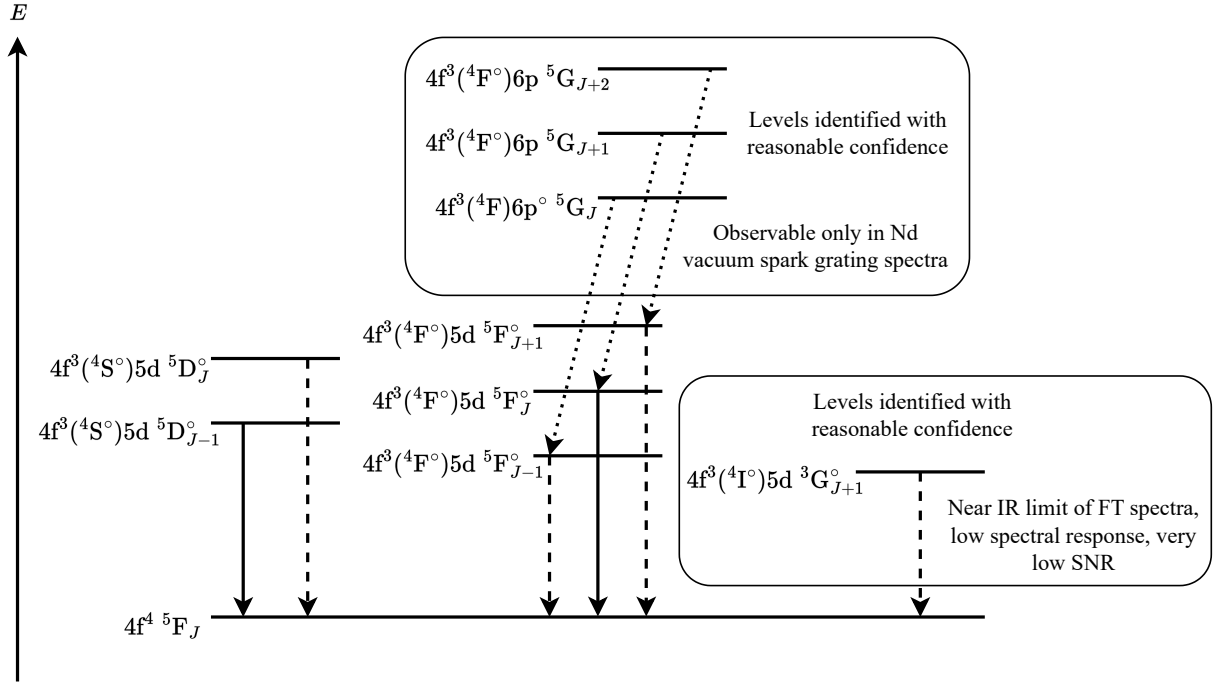


Figure 6.14: Summary of the main levels and transitions involved in identifying the $4f^4 \ ^5F_J$ levels for $J = 2, 3, 4$. Solid arrows indicate transitions with moderate to high SNR in the Nd-Ar PDL FT spectra with observable isotope shift line profiles, dashed arrows indicate low SNR transitions in the Nd-Ar PDL FT spectra which were prone to blends and were commonly not fitted, and dotted arrows indicate transitions observed only in the Nd vacuum spark grating spectra.

6.7.15 Finding the $4f^4 \ ^5F_{2,3,4}$, $4f^3(4F^o)5d \ ^5F^o$, and $4f^3(4S^o)5d \ ^5D^o$ Energy Levels

For the search and analysis of these levels, the approach had to be no longer establishing one level at a time by classifying lines between the new level and known levels (e.g. Figure 6.2) but by classifying lines from multiple levels at the same time to connect multiple levels to the known network of levels. The exact situation is illustrated in Figure 6.14, where all levels were previously unknown except for the $4f^3(4F)6p \ ^5G$ and $4f^3(4I)5d \ ^3G$ levels, which were identified with reasonable confidence, but were then either verified or corrected in the analysis of the $4f^4 \ ^5F_{2,3,4}$ levels.

The $4f^4 \ ^5F_J - 4f^3(4S^o)5d \ ^5D^o_{J-1}$ and $4f^4 \ ^5F_J - 4f^3(4F^o)5d \ ^5F^o_J$ transitions (solid arrows in Figure 6.14), were expected to be the remaining highest intensity unclassified lines of Nd III in the Nd-Ar PDL FT spectra. Particularly, the $4f^4 \ ^5F_J - 4f^3(4S^o)5d \ ^5D^o_{J-1}$ transitions for $J > 1$ were intense enough to be classifiable without any knowledge of the experimental level

Table 6.3: Predicted and Observed $4f^4 \ ^5F_J - 4f^3 5d(^4S^\circ) \ ^5D^\circ_{J-1}$ Transitions

Transition	gA (10^7 s^{-1})	SNR	I_{calc} (arb.)	I_{obs} (arb.)	σ_{calc} (cm^{-1})	σ_{obs} (cm^{-1})	$\Delta\sigma$ (cm^{-1})
$4f^4 \ ^5F_5 - 4f^3 5d(^4S^\circ) \ ^5D^\circ_4$	5.80	212	3200	5000	21211	21209.5986	1
$4f^4 \ ^5F_4 - 4f^3 5d(^4S^\circ) \ ^5D^\circ_3$	6.06	221	4400	5500	21230	21219.4957	10
$4f^4 \ ^5F_3 - 4f^3 5d(^4S^\circ) \ ^5D^\circ_2$	3.74	75	3000	2700	21479	21480.7637	2
$4f^4 \ ^5F_2 - 4f^3 5d(^4S^\circ) \ ^5D^\circ_1$	1.97	49	1700	1800	21650	21600.3924	50

energies. This was possible from agreements with other $4f^4 - 4f^3 5d$ isotope line profiles, with Crosswhite’s unclassified line list, and with the Cowan code calculations, see [Table 6.3](#) where relative intensities of the fourth column I_{calc} were from an analysis further described in [section 7.4](#) with Boltzmann temperature 7300 K. However, the $4f^4 \ ^5F_J - 4f^3(^4S^\circ) 5d \ ^5D^\circ_J$ transitions were expected to appear around the noise level in the Nd-Ar PDL spectrum, and the $4f^4 \ ^5F_J - 4f^3(^4F^\circ) 5d \ ^5F^\circ_J$ transitions were not classifiable without knowing the experimental energy of least one level involved in these transitions. Therefore, while there were good candidates for the strong lines, they could not initially be connected to the network of identified levels.

The starting point was to find $4f^4 \ ^5F_4$. Since $4f^4 \ ^5F_5$ was identified, $4f^3 5d(^4S^\circ) \ ^5D^\circ_4$ was established with its strong transition to $4f^4 \ ^5F_5$ (top row of [Table 6.3](#)). $4f^3(^4F^\circ) 5d \ ^5F^\circ_5$ was then identified using its UV transitions to the ground term, to $4f^4 \ ^5F_5$, and from $4f^3(^4F^\circ) 6p \ ^5G_6$. Therefore, $4f^4 \ ^5F_4$ was searched for using only low SNR transitions from $4f^3(^4S^\circ) 5d \ ^5D^\circ_4$, $4f^3(^4F^\circ) 5d \ ^5F^\circ_5$, $4f^3(^4I^\circ) 5d \ ^3G^\circ_5$, and a few other levels not shown in [Figure 6.14](#). This resulted in ambiguous candidate levels for $4f^4 \ ^5F_4$ as the low SNR lines were highly susceptible to blending and were commonly not fitted. However, transitions of the correct candidate energy for $4f^4 \ ^5F_4$ agreed with stellar spectra and thus enabled identification of other levels of the terms in [Figure 6.14](#) for $J = 4$. With $4f^4 \ ^5F_4$ established, similar analysis procedures were iterated for $4f^4 \ ^5F_3$ and then for $4f^4 \ ^5F_2$, while making sure all classified transitions agreed between Nd-Ar PDL FT spectra and stellar spectra.

In the end, several candidate energies for each of the $4f^4 \ ^5F_{2,3,4}$ levels were checked in stellar spectra. An example of false classification from disagreement with stellar spectra is shown in [Figure 6.15](#). In the centre section of this plot, two Nd III lines falsely classified in the Nd-Ar PDL FT spectra were not observed in HD170973. The $4f^4 \ ^5F_2 - 4f^3(^4S^\circ) 5d \ ^5D^\circ_2$ transition

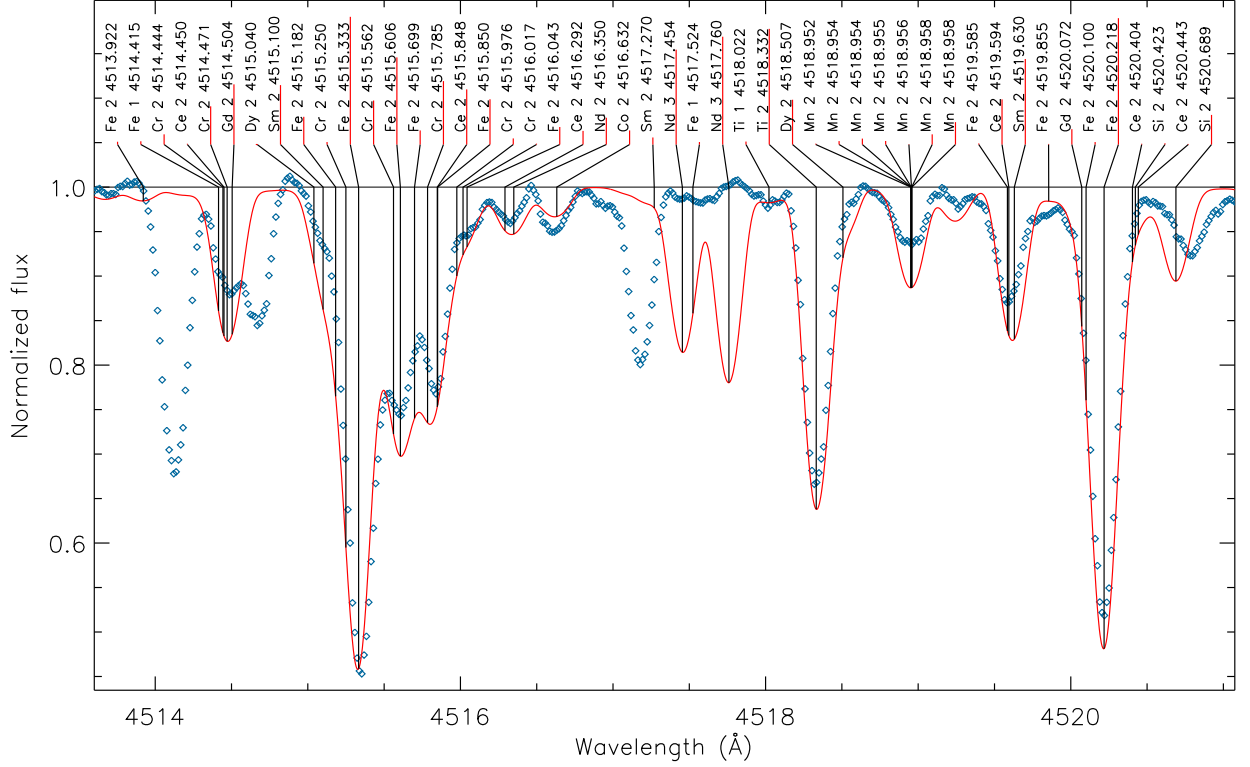


Figure 6.15: Stellar spectrum showing false classifications for $4f^4 \ ^5G_4 - 4f^3(^4G^\circ)5d \ ^5F^\circ_3$ at $4517.5 \text{ \AA}$ and $4f^4 \ ^5F_2 - 4f^3(^4S^\circ)5d \ ^5D^\circ_2$ at $4517.8 \text{ \AA}$ [156]. The observed spectrum of HD170973 is traced by the blue diamonds, the synthesised spectrum is the red curve.

at $4517.8 \text{ \AA}$ concerns the weak transition shown on the left-hand side of Figure 6.14, which was difficult to find and classify due to low SNR and line blending. Remarkably, the nearby unidentified line at $4517.2 \text{ \AA}$ in the spectrum of HD170973 in Figure 6.15 turned out to be the most convincing and final classification for $4f^4 \ ^5F_2 - 4f^3(^4S^\circ)5d \ ^5D^\circ_2$, it was $0.6 \text{ \AA}$ away from the initially false classification. Unfortunately, no suitable candidate for $4f^4 \ ^5G_4 - 4f^3(^4G^\circ)5d \ ^5F^\circ_3$ could be found and the $4f^3(^4G^\circ)5d \ ^5F^\circ_3$ level still remains experimentally unknown as too few of its lines were expected at suitable SNRs in the Nd-Ar PDL FT spectra.

Identifying the $4f^4 \ ^5F_{2,3,4}$ levels was arguably the most challenging analysis of this project, requiring three months of three physicists and spectra of three very different plasmas containing Nd III measured at three separate cutting-edge high-resolution spectroscopy facilities.

6.7.16 Finding the $4f^4\ ^5G_{3,4}$ and $4f^4\ ^3H_4$ Energy Levels

Multiple attempts to find these levels were initially unsuccessful, but the breakthrough was the identification of the $4f^3(^4F^\circ)5d\ ^5F^\circ$ levels from the challenging identification of the $4f^4\ ^5F_{2,3,4}$ levels just described. Transitions from the previously identified levels to the $4f^4\ ^5G_{3,4}$ and $4f^4\ ^3H_4$ levels were low in SNR and prone to blends, but with the addition of the $4f^3(^4F^\circ)5d\ ^5F^\circ$ levels, the number of lines classifiable for each of these levels increased to a degree where the number of ambiguous candidate levels was resolvable, although careful analysis of blends and agreement with stellar spectra were still required.

6.7.17 Levels of the $4f^3(^4I^\circ)7s$ and $4f^3(^4I^\circ)6d$ Sub-configurations

No energy levels from $4f^37s$ and $4f^36d$ configurations were experimentally identified at this stage of the analysis. I had made prior attempts using calculations from Gaigalas et al. (2019) [81] without success, but a large group of low SNR, unclassified lines around $40\,000\text{ cm}^{-1}$ was of unknown origin. This mystery was resolved when Dr Ryabtsev provided updated Cowan code calculations including these configurations and a list of many dozens of levels he had identified as belonging to these configurations using the Nd VS grating spectra. The average energies for the $4f^37s$ and $4f^36d$ levels calculated by Gaigalas et al. (2019) [81] were found to be about 6500 cm^{-1} higher than observed, and therefore any original search for these levels was in an irrelevant spectral region, far from the group of unclassified lines around $40\,000\text{ cm}^{-1}$. The importance of accurate semi-empirical atomic structure calculations in term analyses was highlighted again.

I found that many $4f^37s$ and $4f^36d$ levels identified by Dr Ryabtsev were consistent with the Nd-Ar PDL FT spectra, with a few false classifications but confident candidate levels were later identified. Following this comparison, expected relative intensities were established for the $4f^36p - 4f^37s$ and $4f^36p - 4f^36d$ transitions observed in the Nd-Ar PDL FT spectra, and analysis using these spectra for the two configurations was thus enabled. However, the transition probabilities of the $4f^4 - 4f^37s$ and $4f^4 - 4f^36d$ transitions and low upper level populations meant that these lines were very weak in the Nd-Ar PDL FT spectra. Nevertheless, the Nd-Ar PDL FT spectra have the advantage of high resolution and fewer lines observed in the UV region, compared to the lower-resolution and line-rich Nd vacuum spark grating spectra in the same region, which

are prone to blends. Therefore, observing the spectra of Nd III at two very different thermal conditions (PDL and VS) greatly helped in resolving ambiguous identifications, the advantages of both spectroscopic methods complemented each other. Moreover, no $4f^36p - 4f^37s$ and $4f^36p - 4f^36d$ transitions were observed in the Nd-Ar HCL spectra, which was also a useful hint for the classifications of these lines.

Only the $4f^3(^4I^\circ)6p$ sub-configuration was well established, so all identified $4f^37s$ and $4f^36d$ levels belong only to the $4f^3(^4I^\circ)$ parent term. All 8 levels of the $4f^3(^4I^\circ)7s$ and 38 of the 40 levels of the $4f^3(^4I^\circ)6d$ configuration were identified. Similar to the $4f^3(^4I^\circ)6s$ levels, the $4f^3(^4I^\circ)7s$ levels were well represented by eigenfunctions from jj -coupling between the $4f^3(^4I^\circ)$ core and the excited 7s electron; the eigenvector composition of each of the $4f^3(^4I^\circ)7s$ is comprised of more than 95% purely its corresponding jj -coupled eigenfunction and the impressively calculated level energies deviated by no more than 10 cm^{-1} from the observed energy values.

6.7.18 Levels of the $4f^35f$ Configuration

Although the $4f^37s - 4f^35f$ and $4f^36d - 4f^35f$ transitions have high transition probabilities and may be produced at reasonable intensities in the PDL, they were beyond the experimental spectral range in the IR of the Imperial College VUV FT spectrometer, and could be masked by the photon noise of the line-rich IR region.

In total, 70 levels of the $4f^35f$ configuration were identified only using 172 $4f^35d - 4f^35f$ transitions observed in the Nd VS grating spectra (see [section 4.7](#)). All 56 levels of the $4f^3(^4I^\circ)5f$ sub-configuration were identified. These levels were optimised by fixing the connecting $4f^35d$ level energies at values optimised using only FT wavenumbers ([Table D.1](#)). This was to prevent the $4f^35d$ level energies in the optimisation from being affected by the grating spectra wavenumbers, which are prone to blends and have an order of magnitude higher uncertainty due to the much lower resolving powers of grating spectrometers compared to FT spectrometers. Any doubly identified $4f^35d - 4f^35f$ transitions were weighted according to the ratio between their g_uA values calculated using the Cowan code.

6.8 Term Analysis Results

Results of the analysis of the previous two sections are presented in this section, which includes full tables of Ding et al. (2024) [96] and additional results for the $4f^37s$, $4f^36d$, and $4f^35f$ configurations. Newly identified energy levels of the $4f^36s$ and $4f^37s$ configurations enabled a revision of the Nd III ionisation energy at twice the previous accuracy [109, 159] at $178070 \pm 330 \text{ cm}^{-1}$, this calculation was performed by Dr Ryabstev and will be described in detail in a future publication [160]. The classifications of the $4f^35d - 4f^35f$ transitions and identifications of the $4f^35f$ levels were purely Dr Ryabtsev's work (see subsection 6.7.18), these are included in the thesis for completeness and for presenting the collaboration. Most $4f^36d$ and $4f^37s$ levels were also first identified by Dr Ryabtsev (see subsection 6.7.17), they were later verified and more were identified by me using the Nd-Ar PDL FT spectra. Please refer to the published Nd III line and level lists for final results that are also machine-readable [96, 160]. Most results in tables of Appendix C and Appendix D are final and these tables can be viewed as records that led to the final results.

6.8.1 List of Identified Energy Levels

In total, 258 energy levels were experimentally identified, 219 of which were identified for the first time, and 39 previously reported levels were confirmed. The list of Nd III energy levels is in Appendix C. Most energy level identifications were documented in detail in the section 6.6 and section 6.7. For the levels undocumented, their identifications and line classifications were straightforward, meeting many classification criteria (section 6.3), e.g., agreement with the parameterised Cowan code calculations, stellar and vacuum spark spectra, and zero ambiguous matches. Figure 6.16 shows a comparison of the extent and positions of the 258 identified energy levels with those currently in the NIST ASD [20] and those predicted using the Cowan code. Evidently, there are many predicted Nd III energy levels that have yet to be identified and confirmed.

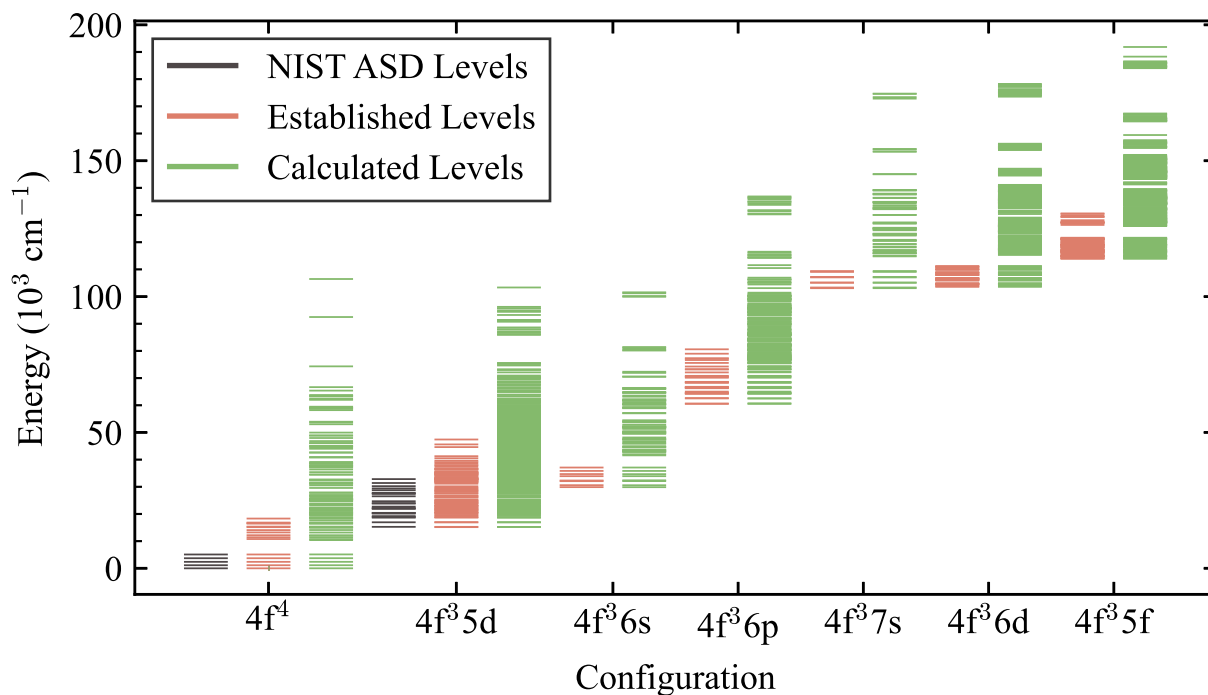


Figure 6.16: Plot showing Nd III energy levels on the NIST ASD [20] (black), levels identified from this work (coral), and levels predicted by the Cowan code calculations performed in the present work (green, below 192000cm^{-1}).

6.8.2 Transitions Classified from Laboratory Sources

The Nd III level energies of Table C.1 were optimised using 577 transitions classified and measured from the Nd-Ar PDL FT spectra and 172 $4f^3 5d - 4f^3 5f$ transitions measured from the Nd VS grating spectra in the far UV, these lines are illustrated in Figure 6.17. The $4f^3 5d$ level energies were fixed in the optimisation of the $4f^3 5f$ level energies. In the spectral range overlap between the Nd-Ar PDL FT spectra and the Nd VS spectra, all lines observed in the Nd-Ar PDL FT spectra were observed in the Nd VS spectra. Additionally, 208 transitions that were too weak to be observed in the Nd-Ar PDL FT spectra were observed in the Nd VS spectra, because the Nd VS source had a higher effective temperature (see Figure 7.5 and Figure 7.7). In total, 957 transitions of Nd III were classified. Ritz wavenumbers can also be calculated for unobserved weaker transitions or transitions lying outside the experimental spectral regions using known level energies. The lists of observed transitions from both the Nd-Ar PDL FT spectra and Nd VS grating spectra are listed in Appendix D, wavenumber uncertainties of these spectra are down to a few parts in 10^8 and 10^7 , respectively.

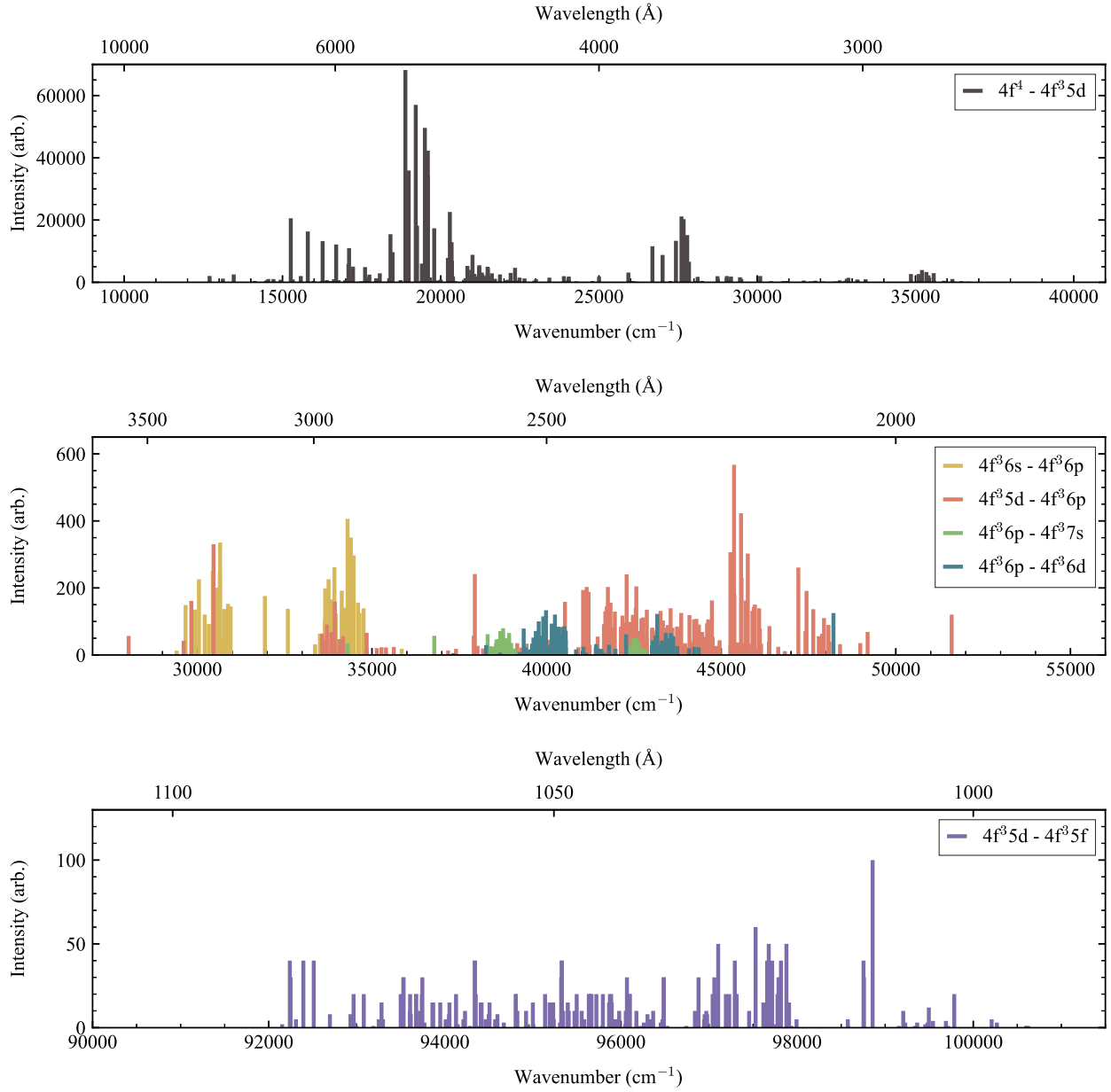


Figure 6.17: 577 transitions observed in the Nd-Ar PDL FT spectra (top and middle) and 172 transitions observed in the Nd VS spectra (bottom) used to optimise Nd III level energies with LOPT [157]. The three observed $4f^4 - 4f^3 6s$ transitions are not shown (introduces awkward intensity scale). The intensity scales are the same as those of Table D.1 and Table D.2.

6.9 Summary of the Term Analysis of Nd III

Observed transitions of Nd III were identified from the Nd-Ar PDL FT spectra. The configuration, term, J value, and energy of upper and lower energy levels were assigned for each identified Nd III transition, through consideration of semi-empirical calculations of energy separations and relative intensities, isotope shifts of Nd III energy levels, relative intensities observed in light sources of different plasma conditions (PDL, HCL, VS, and stars), and agreement with energies of the identified levels. The methodologies and considerations used to revise and identify energy levels are documented. Measured wavenumbers and classifications of Nd III transitions were input into *LOPT* [157] for best estimates of level energies. Agreement was found between 39 of 40 previously experimentally established energy levels, the remaining level was revised using the much more extensive experimental data of the present work. In total, 258 energy levels were identified, of which 219 are new and were identified for the first time, using 957 observed transitions involving the $4f^3(4f + 5d + 6s + 6p + 7s + 6d + 5f)$ configurations.

Chapter 7

Outlook from the Analysis of Nd III Atomic Structure

7.1 Introduction

The present work has substantially increased the number of transitions of Nd III available to stellar astrophysics and the immediate impact of the present work on stellar spectroscopy is presented in [section 7.2](#). The experimental knowledge of Nd III atomic structure remains incomplete, but investigations extending the analysis of the present work are ongoing, see [section 7.3](#). The later sections of this chapter summarises possible future analyses on Nd III or other atoms using similar methodologies; [section 7.4](#) discusses capabilities of the Nd-Ar PDL light source in hindsight, [section 7.5](#) lists some potential strategies to extend the present analysis, and lastly, [section 7.6](#) contain general remarks on the methodologies successfully employed in the present work.

7.2 Applications to Astrophysical Spectra

The number of classified transitions of Nd III has increased from 70 [\[63\]](#) by an order of magnitude to 964. These wavelengths are now measured accurately up to a few parts in 10^8 between the VUV and near IR range (185-870 nm). These will enable more reliable modelling of stellar

absorption lines involving Nd III when combined with the semi-empirically calculated transition probabilities and Landé g -factors from the present work or future experimental or theoretical work. Some applications in stellar spectral syntheses have been presented in [Figure 6.12](#), [Figure 6.10](#), and [Figure 6.15](#). These astrophysical application results, and those presented in this section were produced by Dr Ryabchikova, who greatly aided the analysis of Nd III in the visible region, where agreement between laboratory and stellar spectra was crucial in the classification of Nd III spectral lines in that region.

Examples of improved stellar spectra synthesis using newly classified Nd III transitions are shown in [Figure 7.1](#), [Figure 7.2](#), and [Figure 7.3](#), where Nd III spectral lines with previously unknown identities can now be analysed to yield stellar atmospheric properties, such as temperature, abundance, magnetic field strength, and atmospheric pulsational amplitudes. Stellar spectra of the three figures were measured by the UVES at the VLT (see [subsection 1.1.2](#) and [section 4.7](#)). In [Figure 7.1](#), the applicability of results from the present work to stars of varying temperatures and magnetic fields are demonstrated. In [Figure 7.2](#), newly classified Nd III transitions all show pulsation signals, which were deduced from residuals (red) of the fits to the time-averaged spectrum (black). As discussed in [subsection 1.2.3](#), Nd III lines tend to show clear signs of pulsation in roAp-type stars, i.e., double peak residuals due to Doppler shifts from the rapid expansion and contraction of the stellar atmosphere, compared to lines from non-REE species. The newly classified Nd III lines will be useful in similar future investigations of roAp stars. In [Figure 7.3](#), a Nd III transition unobserved in the laboratory spectra was successfully synthesised. The successful spectral synthesis of Nd III transitions unobserved in the laboratory due to limited laboratory spectral range further confirmed the validity and accuracy of the new experimental level energies and theoretical transition probabilities. [Figure 7.3](#) also demonstrates that the number of available transitions for stellar spectral modelling can be larger than the number of transitions newly classified directly in the laboratory.

The increased number of transitions available for measurements of stellar properties will give more accurate conclusions compared to using fewer transitions. This is especially true when blends are involved, which can be very common in stellar spectra. One would need information on all atomic transitions in a blend to correctly model the blend or look elsewhere in the stellar spectrum for unblended lines, the success of either approach greatly depends on the number of experimentally known transitions. Experimentally identifying level and transition energies is

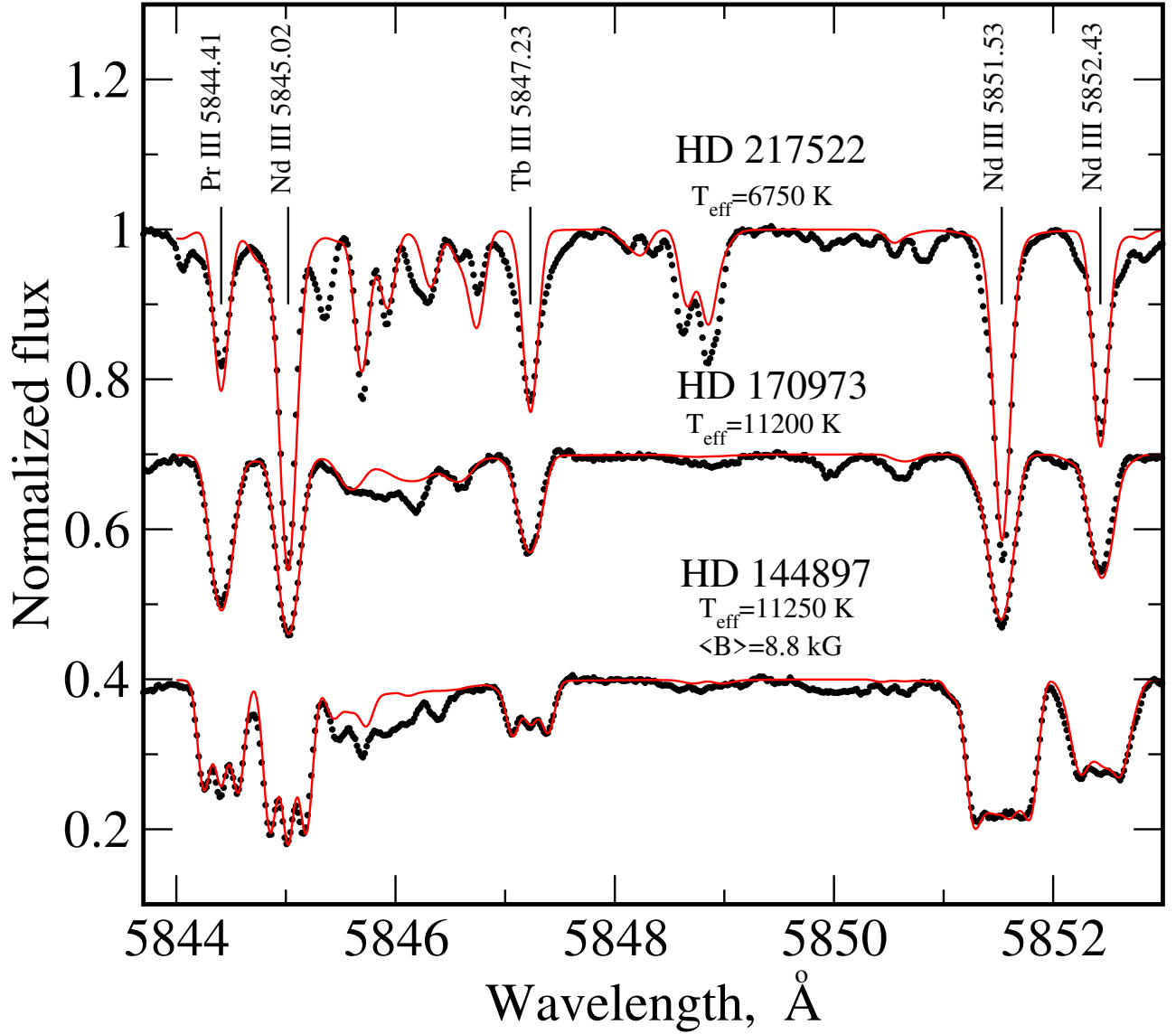
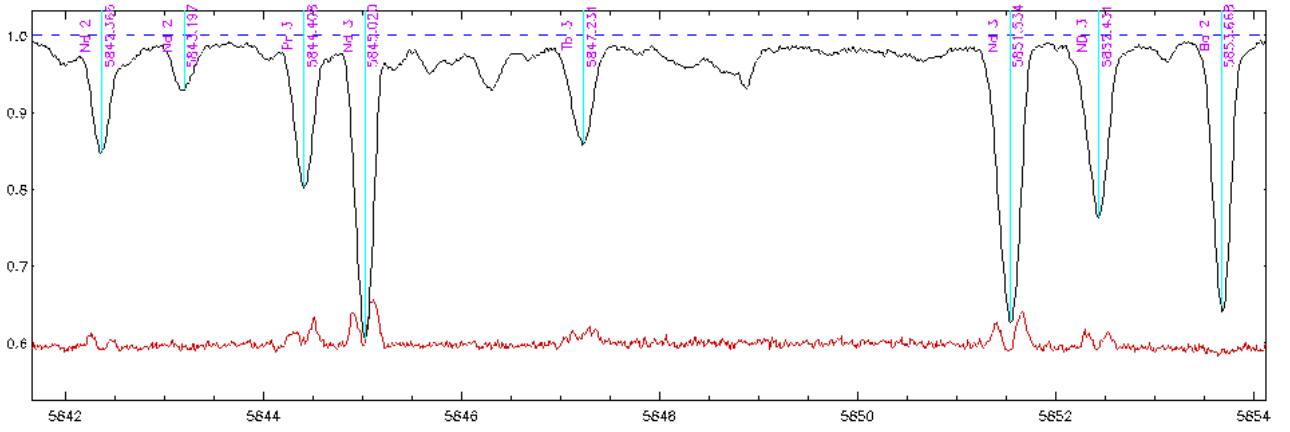
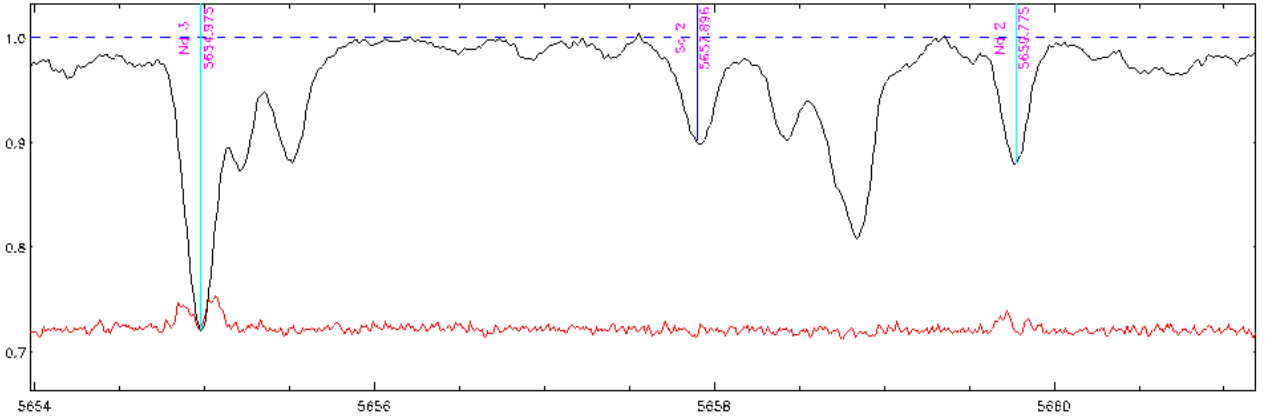


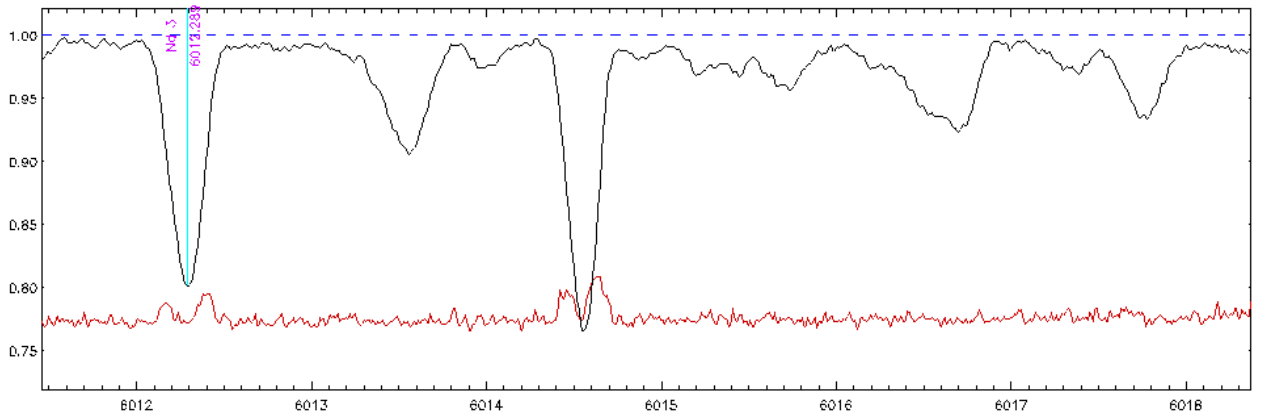
Figure 7.1: Synthesis (red line) of three stellar spectra (black dotted line) in the region with the transitions $4f^4 \ ^5I_8 - 4f^3(^4I)5d \ ^5K_9$ at 5845.0 Å, $4f^4 \ ^5I_7 - 4f^3(^4I)5d \ ^3I_6$ at 5851.5 Å, and $4f^4 \ ^3K_{26} - 4f^3(^4F)5d \ ^5H_6$ at 5852.4 Å using theoretical Nd III transition probabilities and Landè g-factors calculated in the present work [138, 156].



(a) The same three Nd III transitions as the ones shown in Figure 7.1.



(b) $4f^4 \ ^3K_{27} - 4f^3(^4F)5d \ ^5H_7$ at 5655.0 Å, previously unclassified.



(c) $4f^4 \ ^3K_{27} - 4f^3(^2H_2)5d \ ^3K_7$ at 6012.3 Å, previously unclassified

Figure 7.2: Pulsational characteristics observed in previously and newly classified Nd III lines in the pulsating Ap star HD 24712. These are screenshots provided by Dr Ryabchikova [156], the y -axis shows normalised flux and the x -axis shows wavelength in Å. The black curve is the time-averaged spectrum and the red curve shows residuals from the time-series spectra [156].

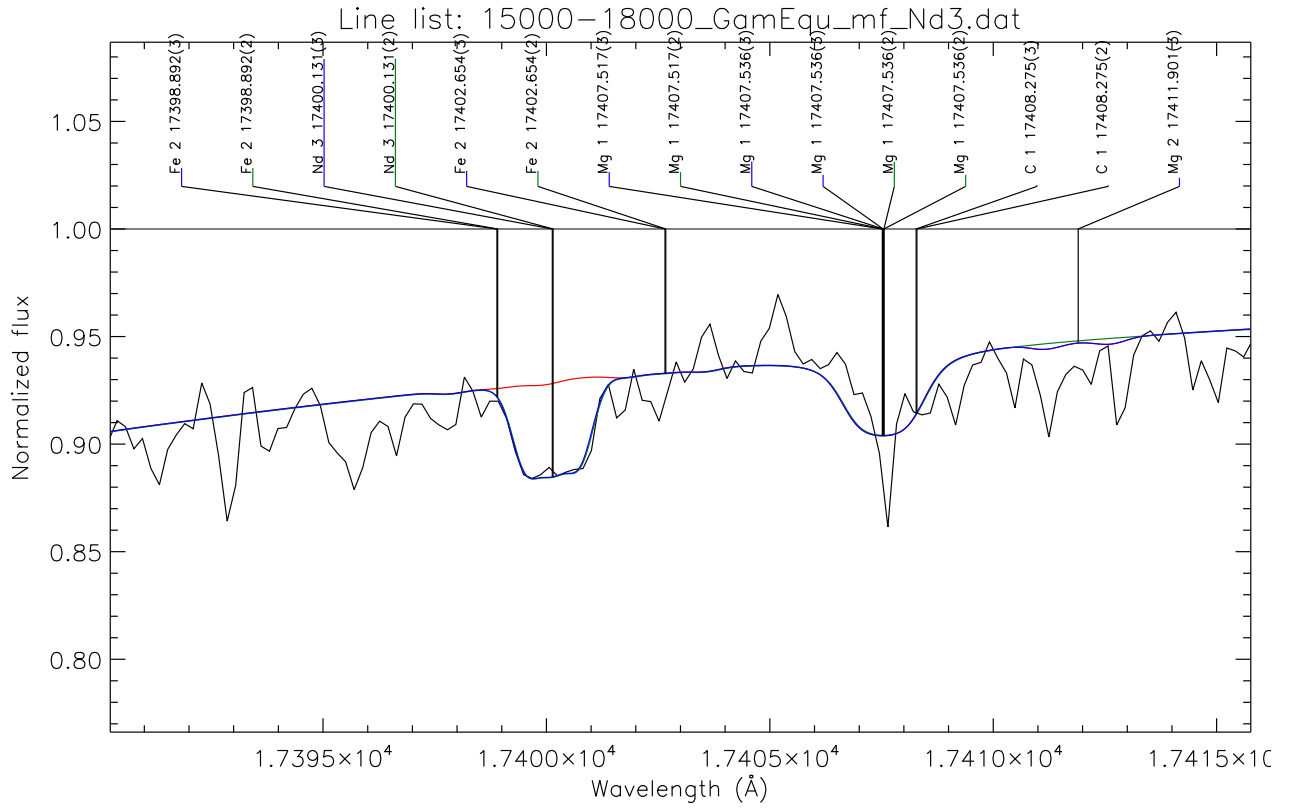


Figure 7.3: Previously unidentified line $4f^4 \ ^5G_5 - 4f^3(^4I) \ ^5H_6$ at $17400.13 \text{ \AA}$ of γ Equulei with agreement in line strength and width from calculated transition probability and Landè g-factors. Black is the observed spectrum, and red and blue are synthesised spectra with and without the Nd III transition, respectively [156].

also the prerequisite to experimentally or theoretically determining accurate transition probabilities and Landé g -factors used for the analysis of stellar spectra, the importance of term analysis in obtaining useful atomic data is therefore emphasised.

To illustrate the importance of accurate knowledge of energy levels and hence term analysis for transition probability calculations, Nd abundance in the star HD 170973 was determined using the new semi-empirical transition probability and Landè g -factor calculations [138, 156] (publication under consideration). Results were compared to Nd abundance values obtained using Nd II lines with experimental transition probabilities [158] and transition probabilities calculated by Gaigalas et al. (2019) [81] and shown in Figure 7.4. Agreement was found between the stellar Nd abundances obtained from experimental Nd II transition probabilities and those obtained from the semi-empirical Nd III transition probabilities of this work, but a significant discrepancy (~ 0.6 dex) is observed for the Nd abundance obtained using calculated transition probabilities from Gaigalas et al. (2019) [81].

The slight underestimate of stellar Nd abundance using Nd III transition probabilities from the present work in Figure 7.4 could be due to the underestimation of level lifetimes, which was observed in previously published semi-empirical calculations using similar methods [63, 86]. Consideration of the $5p^6$ core may be required for more accurate calculations of Nd III lifetimes. In the analysis of Nd IV [77, 78], inclusion of configuration interaction of the core-excited $5p^5 4f^3 5d$ configuration with the $5p^6 4f^2 5d$ configuration increased the $5p^6 4f^2 5d$ level lifetimes by up to a factor of two, this increase was illustrated in Figure 2 of Arab et al. (2019) [78]. Similar effects from considering the $5p$ core-excitation were also observed for Nd V [79, 80]. For improvements in transition probability calculations, one could include $5p^5 4f^3 5d$ directly in the configuration interaction space and look for experimental evidence of those energy levels, use a polarised electrostatic potential to approximate the existence of the $5p$ core-electron excitation, or scale the radial electric dipole integrals in evaluation of line strengths [111].

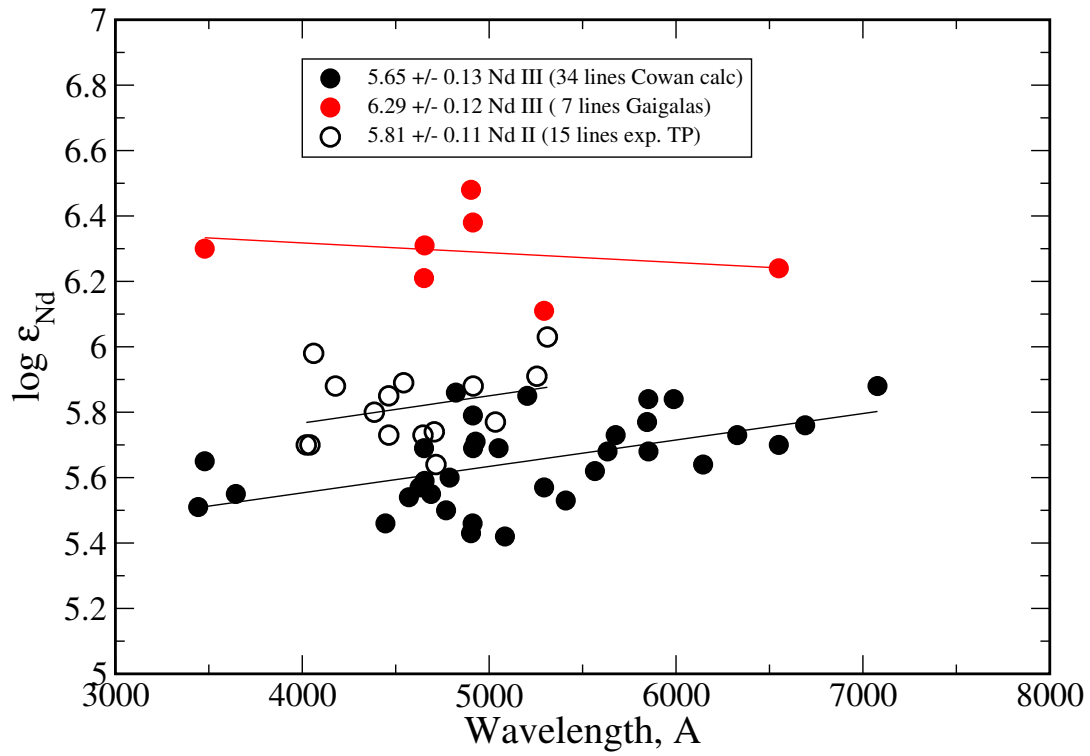


Figure 7.4: Nd abundance estimated for the star HD 170973, using theoretical Nd III transition probabilities from [81] (red circles), experimental Nd II transition probabilities from [158] (white circles), and semi-empirical Nd III transition probabilities calculated in this work (black circles) [138, 156].

7.3 Ongoing Work

Extended laboratory measurements of lifetimes and branching ratios of the new Nd III energy levels are now possible. For example, knowing the new level energies implies knowing which laser wavelengths can be used to excite Nd III atoms to corresponding levels for fluorescence lifetime investigations (e.g. [86]). Furthermore, FT spectroscopy measurements can be chosen to reliably measure branching fractions as the exact wavenumbers of the transitions are now known. Experimental transition probabilities would produce even more reliable transition probabilities compared to those calculated in this work and would provide more reliable stellar absorption line fitting and abundance determinations. A set of Nd-Ar HCL spectra was recorded using the Imperial College VUV FT spectrometer for branching fraction measurements in collaboration with Dr M. T. Belmonte of the University of Valladolid. Further measurements and analysis are ongoing within her research group to determine absolute transition probabilities of Nd III using the lifetime measurements of five energy levels by Zhang et al. (2002) [86] and theoretical lifetimes of Nd III. The Nd-Ar HCL spectra were recorded using the same Nd cathode used to record the Nd-Ar and Nd-Ne HCL spectra of the present work, and the cathode was finally depleted after the branching fraction measurements (Figure 4.9).

The lifetimes calculated in the present work using the parameterised Cowan code, are on average 70% of the five lifetimes measured by Zhang et al. (2002) [86], and three times larger compared to those calculated by Gaigalas et al. (2019) [81]. To investigate potential offsets in the calculated absolute transition probabilities, configurations involving the excitation of a 5p electron from the $5p^6$ core are being considered in the configuration interaction space by Dr Ryabtsev. From previous studies of Nd IV [77, 78] and Nd V [79, 80], including the interaction between the $5p^5 4f^n 5d$ and $5p^6 4f^{n-1} 5d$ configurations significantly reduces transition probabilities of the $5p^6 4f^n - 5p^6 4f^{n-1} 5d$ transitions. The lowest levels of the 5p-excited configurations are estimated to lie around $140\,000\text{ cm}^{-1}$. Due to the small overlap in energy between the 5p-excited configurations and the levels identified in the present work (highest level at $130\,000\text{ cm}^{-1}$), changes to the eigenvector composition and branching fractions of the identified levels were very small. These changes were not significant enough to invalidate level identifications of Table C.1. In fact, small improvements to calculated branching fractions were observed for some levels of the $4f^3 5d$ and $4f^3 6p$ configurations, where calculations including 5p-excited configurations produced transition probabilities agreeing better with their observed relative intensities. VS spectrum

number 1 of Table 4.7 is expected to contain $5p^64f^4 - 5p^54f^45d$ transitions around 450 Å, this and the overall offset in level lifetimes is being investigated by Dr Ryabtsev [138, 160].

7.4 Nd Discharge Lamp Thermal Conditions

It is useful to consider the plasma conditions of a light source in the spectroscopic measurements of its atoms and ions, e.g., level populations of a transition will determine the photon (or intensity) flux of its transitions. This was not possible for Nd III at the experimental stage of this project because its energy levels are largely unknown. However, the success of the Nd III term analysis enabled reasonable estimations of temperatures and relative level populations of Nd III ions in the Nd-Ar PDL, which helped with expectations of SNRs of unclassified Nd III transitions. These insights will also aid future experiments using similar instrumentation.

Nd-Ar PDL Temperature

Transitions between the higher-lying $4f^4$ and $4f^35d$ levels lie within the line-rich IR-visible spectral regions and were relatively weak in intensity due to relatively low upper level populations. In tackling difficulties encountered back when searching for $4f^4$ levels (subsection 6.7.9), estimates were made for level populations and hence relative line intensities of the Nd-Ar PDL spectra using the Cowan code transition probabilities and the Boltzmann distribution, which were direct applications of Equation 2.20 and Equation 2.33 respectively.

The Nd-Ar PDL discharge was estimated to have an effective temperature of roughly 7300 K. This temperature matched best with the observed relative intensities of the strongest $4f^4\ ^5I - 4f^3(^4I)5d\ ^5I$ and $4f^4\ ^5I - 4f^3(^4I)5d\ ^5K$ transitions, see the top two plots of Figure 7.5. The predicted relative intensities of these lines using temperatures more than 500 K away from 7300 K did not agree with their observed relative intensity patterns. Temperature estimates obtained using PDL line widths, i.e., using Figure 6.5 and Equation 2.37, were around 8000 K, which is in agreement given the 16% uncertainty in the gradient in Figure 6.5.

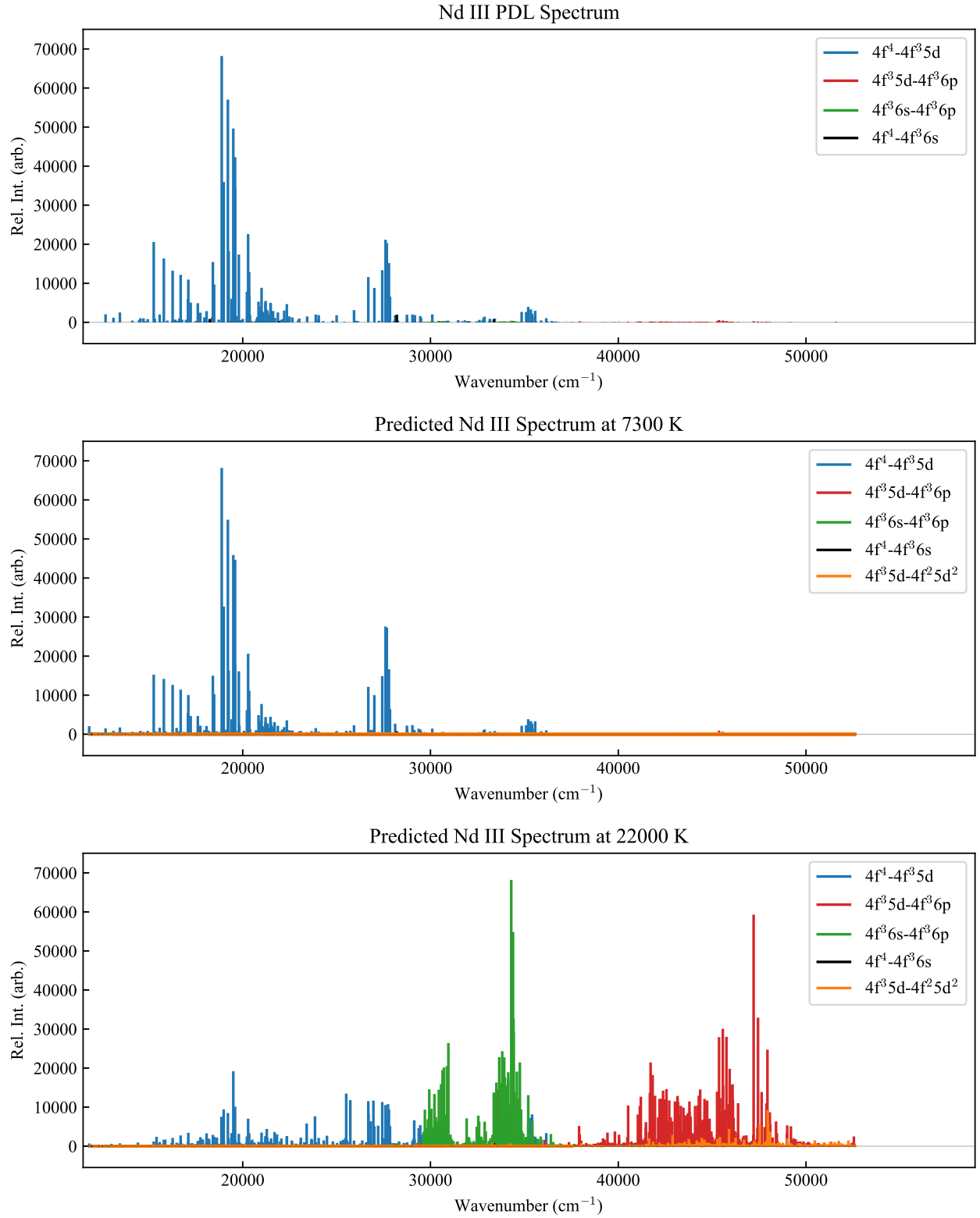


Figure 7.5: Predicted Nd III spectrum using a temperature estimate of 7300 K (middle) and 22000 K (bottom) and weighted transition probabilities from the Cowan code calculations, with highest intensity scaled to the maximum relative intensity of the observed Nd-Ar PDL spectrum (top). The height of each line represents relative photon flux of Table D.1. Theoretical wavenumbers are used for lines involving missing levels. The three y-axes are not on the same scale.

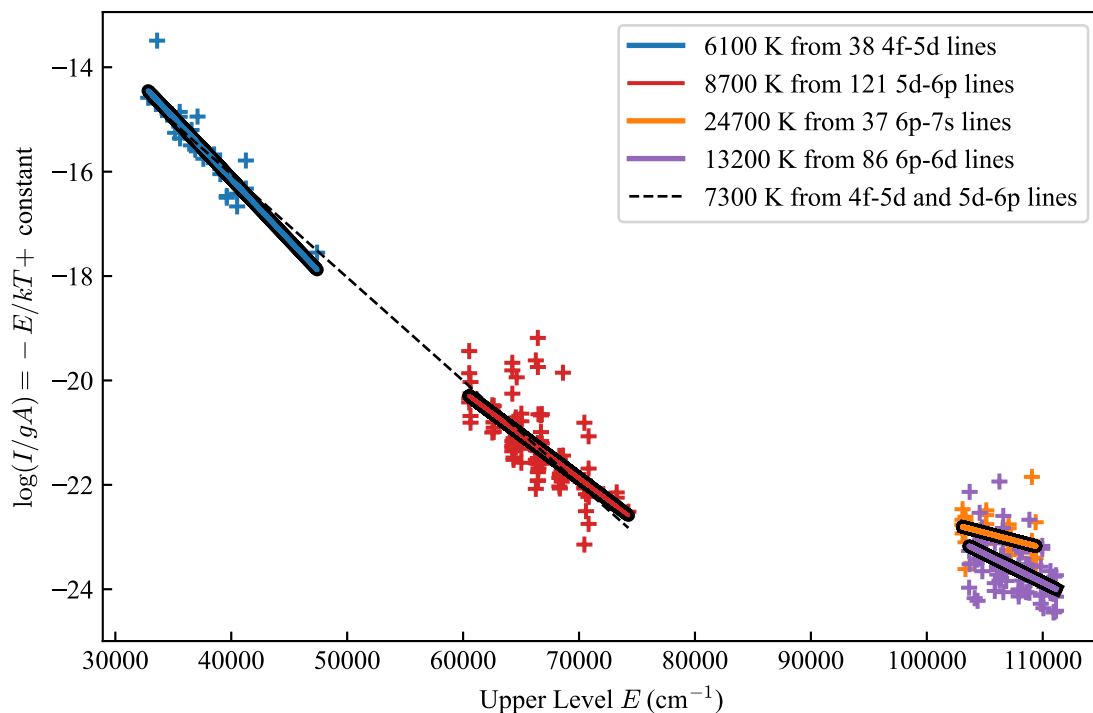


Figure 7.6: Boltzmann plot of Nd III transitions in spectrum E of the Nd-Ar PDL using transition probabilities calculated using the Cowan code during the analysis of Nd III atomic structure. Each cross is an observed transition (all SNRs above 3). Linear fits were made to each group of transitions and temperatures were estimated, the dashed line is a fit to transitions from both the $4f^4 - 4f^35d$ and $4f^35d - 4f^36p$ arrays.

Boltzmann Plot of Nd-Ar PDL FT Spectrum E

Four separate transition groups, $4f^4 - 4f^35d$, $4f^35d - 4f^36p$, $4f^36p - 4f^37s$, and $4f^36p - 4f^35d$ are observed in one Nd-Ar PDL FT spectrum (spectrum E of Table 4.6), with upper-level energies spanning 35 000 to 110 000 cm^{-1} . This offered a good opportunity to investigate whether the level populations, $N_j(t)$ of Equation 2.20, resemble the Boltzmann distribution of Equation 2.33, because the relative intensities of these lines are measured simultaneously, during one experiment.

A Boltzmann plot is made by plotting the log of the ratio between observed relative intensities and their calculated weighted transition probabilities against upper-level energies. Boltzmann plots can be used to estimate absolute transition probabilities using experimentally measured branching fractions. This is applicable when, over some energy range, the level populations follow the Boltzmann distribution and a sufficient number of accurate transition probabilities are available, see cases for Ce I [161] and Kr III [162]. The Boltzmann plot is shown in

Figure 7.6 for the Nd III lines in spectrum E. The reasonable conclusion that can be drawn from this analysis is that the level populations of Nd III in the Nd-Ar PDL plasma somewhat follow the Boltzmann distribution, with particular departure from the distribution for levels above $100\,000\text{ cm}^{-1}$. This is clearly seen from the fact that the dashed line would not fit data points above $100\,000\text{ cm}^{-1}$. Lines originating from higher-lying levels are weaker due to lower population, resulting in lower SNR and more uncertain measured intensities. Moreover, fewer levels are identified in the higher-lying, higher level density configurations, which means that accurate transition probability calculations are also more difficult. This explains the increasing spread of data points around the fits in Figure 7.6 as upper-level energy increases, and that any conclusions made for the populations of higher-lying levels are also less accurate. Furthermore, the levels above $100\,000\text{ cm}^{-1}$ are likely to be influenced more by the 5p-excited configurations that are not included in the current calculations. Nevertheless, the Boltzmann distribution was shown to be suitable as a first-order estimation of relative level populations in the Nd-Ar PDL, which could be useful when considering the choice of future experimental parameters.

Vacuum Spark Temperature

Dr Ryabtsev performed a Boltzmann plot on the Nd vacuum spark grating line list under the assumption of Boltzmann distribution of energy level populations, which resulted in a rough temperature estimate of $22\,000\text{ K}$. The plot is shown in Figure 7.7 and the predicted Nd III spectrum for this temperature is shown at the bottom of Figure 7.5. As seen from the spread of points around the straight line, the uncertainty of this temperature is very high, because the relative intensity measurements were made using the amount of photographic plate darkening for each line, which is very uncertain and has very low dynamic range. Furthermore, calculated transition probabilities are more uncertain for the weaker lines observed in the VS spectra.

Implications

Evidently, higher-lying levels of Nd III were much better populated in the Nd vacuum spark discharge source. This is unsurprising as the VS source is commonly used in grating spectroscopy to excite higher ionisation states. The temperature analyses of Figure 7.5 and Figure 7.7 were carried out after the observation of $4f^35d - 4f^36p$ lines in the Nd VS grating spectra that were

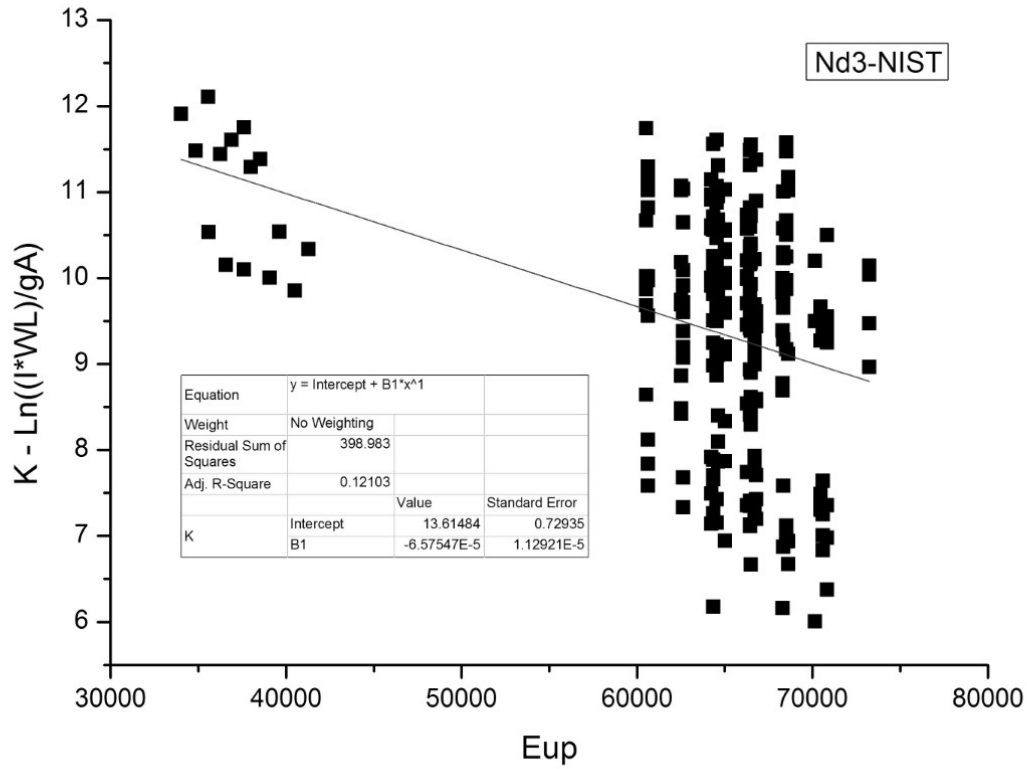


Figure 7.7: Nd vacuum spark temperature estimation using measured Nd III transition intensities and weighted transition probabilities calculated using the Cowan code [138]. The y-axis is the natural log of energy level population determined using Equation 2.20, the x-axis is the upper level energy in Equation 2.33 in units of cm^{-1} , and the gradient is $(k_B T)^{-1}$ in units of cm .

too weak to be observed in the PDL.

From Figure 7.5, the observed relative intensities of the remaining Nd III transitions involving unknown levels could be estimated by comparing them with the already classified Nd III transitions, and the expected relative intensities of the unclassified transitions can be mapped to their expected SNRs (dependent on the spectral regions) so that one could gauge whether a transition was likely to be observable in the Nd-Ar PDL FT spectra. Hence, energy levels with multiple such observable transitions to or from known levels could in principle be experimentally identified. For example, the analysis of Figure 7.5 was carried out before the identification of $4f^4$ levels that are not from the ground term, which indicated that most of the $4f^4 - 4f^3 5d$ transitions involving higher-lying $4f^4$ levels were around the noise level.

Overall, the temperature and relative intensity analysis were helpful for further familiarisation

with the observed Nd-Ar PDL and Nd vacuum spark spectra. Around 10^4 lines of the 21584 lines observed in the Nd-Ar PDL are classified as belonging to Nd I-II, Nd IV, Ar I-III, and Fe I-II (Table 6.1), and only 577 lines are classified as belonging to Nd III. From looking at the upper two plots of Figure 7.5, most of the high-intensity and high-SNR Nd III lines in the Nd-Ar PDL spectra have now been classified. This means the majority of remaining 10^4 unclassified transitions are not likely to be from Nd III, but are expected to be from Nd I-II. Furthermore, the charge transfer reaction [147] is expected between Ar^+ and Nd to enhance populations of some Nd II energy levels. Therefore, PDL is expected to be an ideal light source to investigate Nd II since Nd I line intensities are dramatically smaller in the PDL compared to the HCL. I would like to note that the strongest line in the Nd-Ar PDL spectrum with SNR 8400 remains unidentified.

The atomic structures of Nd I-III are concluded to still remain experimentally incomplete, given that thousands of unclassified lines could belong to Nd I-II and only levels of the first parent term of the 4f-excited configurations of Nd III are well established, and levels from other parent terms of Nd III remain poorly known.

7.5 Possible Experimental Strategies for Future Nd III Term Analyses

Nd III transitions with unknown energy levels will remain unavailable for high-resolution stellar spectroscopy until the present work is extended because the accuracy of calculated transition wavelengths is insufficient - wavelengths measured and classified through high-resolution spectroscopy are required. The accuracy requirement is less stringent for investigations of spectra of kilonovae, as the lines are broadened by the expansion of the kilonovae ejecta such that wavenumber accuracies of the theoretical calculations for observed levels become much less significant. However, transition probabilities are then the key atomic data that determine the large scale spectral features of kilonovae. Nevertheless, gaining further experimental validation such as observing predicted levels of different configurations will benchmark theoretical and constrain semi-empirical atomic structure calculations of Nd III, which will help to reduce uncertainties in kilonovae opacity calculations. Therefore, future term analysis of Nd III will still improve the availability of atomic data for astrophysical applications, as is the case for most

atoms and ions.

The knowledge of Nd III atomic structure is now much more accurate with 258 levels identified from seven different configurations. This will aid future experiments specifically designed to identify particular still-unknown levels and configurations. For example, in FT spectroscopy, instead of searching for lamp conditions that maximise SNRs of the resonance transitions (as was done in the present work), one could look for lamp conditions with the highest SNRs for transitions between higher-lying levels, one could reduce the spectral range of the FT spectrometer to reduce photon noise (improving SNR) to target predicted transition wavenumbers of unclassified lines that are now more accurate due to better parameterisation of semi-empirical calculations. In grating spectroscopy, vacuum spark sources are expected to be able to populate the unknown higher-lying Nd III levels much better. One could alter spark currents for a wide range of effective plasma temperatures to aid line classification or increase exposure times to reveal weak lines of unknown energy levels.

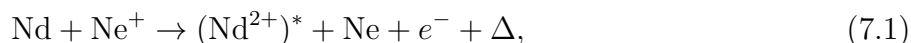
7.5.1 Experimentally Unknown Configurations of Interest

No levels were identified for the lowest doubly excited configurations of Nd III, $4f^25d^2$ and $4f^25d6p$. The strongest $4f^35d - 4f^25d^2$ transitions are to the still unknown $4f^35d$ levels. Therefore, identification of levels from the doubly excited configurations may require an extension of the experimental knowledge of the $4f^35d$ levels. Experimentally identifying levels from the doubly excited configurations should also improve semi-empirical calculations. The energy ranges of the $4f^25d^2$ and $4f^25d6p$ configurations are expected to overlap many other configurations. Therefore, configuration interaction will likely shift in the predicted energies of the doubly excited configurations, affecting theoretical transition probabilities by changing the predicted eigenvector compositions.

As discussed in [section 7.2](#) and [section 7.3](#), the possibility of core-excited configuration $5p^54f^45d$ of Nd III should be investigated, as its interaction with the $4f^35d$ configuration could explain underestimated theoretical lifetimes of the $4f^35d$ levels in the Cowan code calculations in this work and previous studies [63, 86]. The $5p^64f^4 - 5p^54f^45d$ transitions are expected to lie below 100 nm, which would not be observable by the Imperial College VUV FT spectrometer and would likely require grating spectroscopy of Nd III.

7.5.2 Resonance Plasma Collisional Cross-sections

Levels of the $4f^35d$ configuration may be better populated. Specifically, the Duffendack-Penning reaction [163] could be useful for enhancing populations of Nd III energy levels lying in the $4f^35d$ configuration. This enhancement can be seen when comparing the Nd-Ar and Nd-Ne HCL FT spectra, where intermediate-lying $4f^35d$ levels showed higher level populations in the Nd-Ne HCL as the transitions down from these levels were relatively more prominent. In this context, the Duffendack-Penning reaction refers to the resonance cross-section (high probability) for the collisional reaction



where Δ indicates an energy range for this resonance reaction and the atoms are in the ground state except for $(\text{Nd}^{2+})^*$, which is Nd III in an excited state. In this reaction, the ionisation energy of Ne is greater than the ionisation energy of Nd I and Nd II combined by about $42\,000\text{ cm}^{-1}$, which enhances population in the $(\text{Nd}^{2+})^*$ levels that are about $42\,000\text{ cm}^{-1}$ above the ground state of Nd III within an energy range Δ of order 1 eV or around $10\,000\text{ cm}^{-1}$. An example observation of this population enhancement is shown in Figure 7.8, where the line from the level 35576 cm^{-1} to the ground level more than doubled in SNR in the Nd-Ne spectrum. A less dramatic enhancement was observed for the lower-lying $4f^3(4F^\circ)5d\ 5H^\circ$ levels with energies around $30\,000\text{ cm}^{-1}$, this was expected as their energies deviate more than Δ from around $42\,000\text{ cm}^{-1}$. Transitions from the low-lying $4f^3(4I^\circ)5d$ levels were in fact significantly higher in SNR in the Nd-Ar HCL spectrum, opposite to the situation shown in Figure 7.8. Although the SNR of all Nd III lines in the Nd-Ar PDL was still greater in general, running the Nd PDL using Ne as the carrier gas could be considered in the next step of the analysis of the $4f^35d$ configuration.

7.6 Remarks on Key Strategies in the Analysis of Complex Atomic Structure

I expect the strategies mentioned in this final section to be applicable to future term analyses of the extremely complex spectra of the REE atoms and ions.

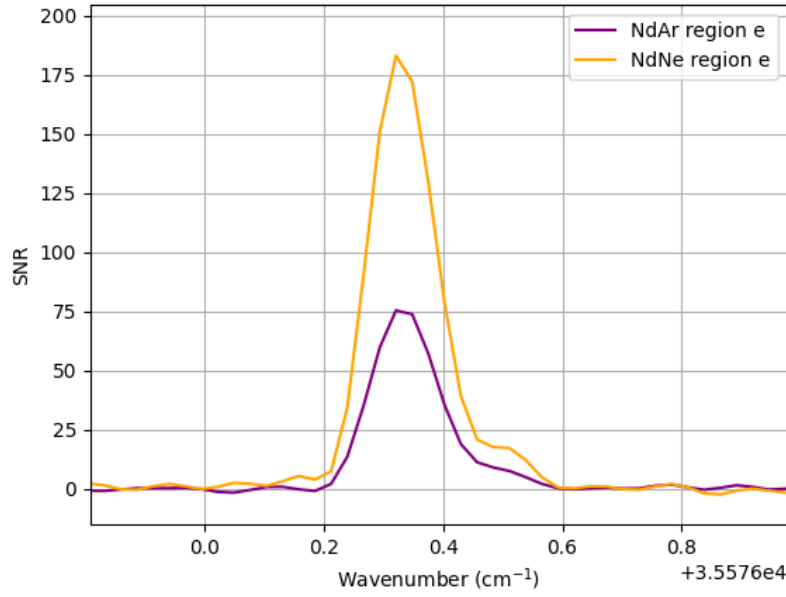


Figure 7.8: Observation of the previously unclassified Nd III transition from $4f^3(^4G^\circ) \ ^5H^\circ_3$ ($E = 35576.327 \text{ cm}^{-1}$) to the ground energy level in the Nd HCL running with Ar (purple, 28 interferogram co-adds) and Ne (orange, 23 interferogram co-adds) carrier gases. The two spectra were measured with the same resolution, spectral range, and aperture using the same detector without optical filters.

7.6.1 Variety of Light Source Thermal Conditions

In hindsight, most spurious ambiguous candidate energy levels in the level searching process likely originated from transitions of Nd I and Nd II. The analysis of the PDL spectra would have been much more difficult without the HCL spectra with their higher-resolution, narrower Doppler widths, different Nd ion fractions, and different relative intensities to aid line classification. Going forwards, any detailed analysis of Nd or complex lanthanide atomic spectra should aim to obtain spectra at significantly different effective temperatures and plasma conditions, as the separation of lines of the atom of interest from other lines of the atom and lines of other species is crucial in their classification. For example, the spectra of PDL, HCL, vacuum sparks, and stars of varying surface magnetic fields were available for this project. To the best of my knowledge, this combination of data sources is amongst the most extensive in a term analysis of this kind.

7.6.2 Wide Spectral Range and High Spectral Resolution

The more transitions observed for a level, the easier and more confident its identification becomes. Access to a wide spectral range (generally from IR to VUV) remains a key requirement for large-scale atomic structure investigations. Moreover, the ability to resolve individual transitions of a complex spectrum is essential, as the number of ambiguous classifications and spurious candidate energy levels rises exponentially with experimental uncertainties. The relative intensities of the transitions must also be measured to accuracies comparable with the accuracies of theoretical transition probabilities to make meaningful classifications from matching relative intensity patterns. High-resolution FT and grating spectroscopy¹ were able to accommodate these requirements.

7.6.3 Accurate and Complete Line Lists

The method of identifying energy levels and classifying transitions greatly depends on the accuracy and completeness of the line list. During the creation of the line list, many weak lines were considered to be noise, and many blends were unknown and not fitted due to the lack of available atomic data and the sheer amount of labour required to carefully fit these lines due to their ubiquity. While experience and familiarity with the spectra would help with the line list creation, fitting all observed lines correctly is unrealistic, e.g., isotope structure could be mistaken as blends, line blending with isotope structure requires non-trivial fitting, and the dilemma of whether a weak line is noise. For this reason, the line list is almost certainly subject to change during the analysis, and an efficient way of altering the line list during the energy level analysis, such as the computer program created in this work ([subsection 5.3.6](#) and [Appendix B](#)), should be an essential consideration in the analysis of complex atomic spectra.

¹Photographic plate intensity measurements are very uncertain, but they were still useful in the Nd III term analysis (see [section 4.7](#)). Grating spectroscopy with charge-coupled devices or image plates [[133](#), [164](#)] as detectors can achieve good intensity accuracy.

7.6.4 Accurate Atomic Structure and Transition Probability Calculations

Limitations of ab initio atomic structure and transition probability calculations for the analysis of Nd III atomic structure were demonstrated by the results of the present work. While these calculations [81] for Nd III provided a good starting point for the analysis of lower-lying levels at lower level densities, they were not able to achieve the accuracy required for the analysis of higher-lying levels (e.g. see subsection 6.7.5, subsection 6.7.6, and subsection 6.7.17). Even for semi-empirical calculations [63, 86], an insufficient number of observed levels will not be able to constrain the Cowan code energy parameters to provide enough accuracy, especially for identifying levels of poorly known configurations and levels with limited number of lines confidently observed above the noise level. Therefore, the current best approach in the analysis of Nd and complex lanthanide atomic structures should ideally include accurate (most likely semi-empirical) calculations made iteratively with new experimentally found energy levels to minimise line classification ambiguities. These calculations also often reveal potential errors in the analysis of experimental data provided there is familiarity with the accuracies achievable in the calculations for the specific analysis and atom. For example, if a Nd III energy level was experimentally identified to be $\sim 150 \text{ cm}^{-1}$ away from the value calculated by Dr Ryabtsev using the Cowan code, doubts were raised if calculations for many other known levels of the same (sub)configuration are accurate within $\sim 50 \text{ cm}^{-1}$.

Chapter 8

Hyperfine Structure Analysis of Co II Energy Levels

8.1 Introduction

Cobalt has only one naturally occurring isotope (^{59}Co) with nuclear spin quantum number $I = 7/2$, which means atomic energy levels of Co II exhibit HFS. The ground configuration of Co II is $[\text{Ar}]3d^8$, but the second lowest-lying configuration $[\text{Ar}]3d^74s$ has larger electron densities near the nucleus so that strong transitions of Co II (e.g. $3d^74s - 3d^74p$) are expected to be significantly affected by HFS. As discussed in [subsection 1.2.3](#), the HFS of atomic energy levels can be observed in absorption lines of high-resolution stellar spectra, and its consideration is significant in modern stellar atmospheric abundance analyses using both local and non-local thermodynamic equilibrium models. The HFS splitting of the energy levels of a transition causes broadening and distortion of its line profile from the expected fine structure transition. This splitting is determined by the HFS magnetic interaction (A) and electric quadrupole interaction (B) constants of the two fine structure energy levels ([Equation 2.29](#)). The A constants are of most interest as these contribute most to the HFS energy level splitting.

To determine HFS constants data for Co II energy levels, previously measured experimental FT spectra of a Co HCL with either Ar or Ne carrier gas were used (see [section 8.2](#)). Parameters governing HFS line profiles were fitted using the observed Co II spectral lines of these spectra. The challenges were fitting a large number of parameters (~ 10) for spectral lines typically with

around 15 data points across the overall line profile and that many strong lines of Co II lie in the UV with large Doppler widths (Equation 2.37), which means that hyperfine transitions are not well resolved in general. To address this, a custom computer program was created to efficiently produce initial parameter values and fit them (see section 8.3). Parameter constraints were carefully investigated for each fit, which is discussed in section 8.4 and section 8.5. Details of the overall approach of the analysis are discussed in section 8.6. Lastly, results and comparisons with more recent literature on HFS of Co II are presented in section 8.7 and section 8.8, respectively.

8.2 Fourier Transform Spectra of Cobalt

High-resolution Fabry-Pérot and laser spectroscopy techniques allow more accurate measurements of HFS of atomic energy levels compared to FT spectroscopy, but their spectral range is limited, leading to low efficiency in obtaining HFS constants for large numbers of energy levels. The wide spectral range of FT spectroscopy (IR to VUV) can measure transitions between many different energy levels. Although the resolution of FT spectroscopy is lower, the wide spectral range available to FT spectroscopy enables observations of transitions connecting an energy level to multiple different levels. This provides independent measurements of the A and B HFS constants, which allow reliable and accurate results for stellar astrophysical applications to be obtained (e.g. for Co II [64,97]). FT spectroscopy is capable of higher resolving powers compared to spectrometers used in stellar spectroscopy, which means any HFS observed in stellar spectra can be better investigated in laboratory FT spectra and measured with sufficient accuracy. Therefore, FT spectroscopy is one of the primary tools in extensive HFS analyses of atomic energy levels.

The Co FT spectra used in the present HFS analysis were recorded within the region 3000–63 000 cm^{−1} (33333–1587 Å) for the extensive atomic structure analyses of Co I [165] and Co II [100–102], and were also used for the HFS analysis of Co I [166]. Spectra of the visible-UV region were recorded using the f/25 VUV FT spectrometer at Imperial College and spectra of the IR region were recorded using the 1 m f/55 FT spectrometer at the National Solar Observatory at Kitt Peak in Arizona. Spectral resolutions of the spectra were chosen such that the instrumental profiles of the FT spectrometers were much smaller than the Doppler widths

of the spectral lines, thereby observing line profiles close to the true line profiles emitted from the HCL. The resolutions were 0.05 cm^{-1} , 0.036 cm^{-1} , and 0.0139 cm^{-1} in the UV, visible, and IR, respectively. The HCL was run using a pure Co cathode at pressures of 1 mbar and 2–3 mbar of Ar and Ne carrier gases, respectively. More experimental details can be found in Pickering et al. (1998) [100].

8.3 Custom Analysis Program - *hfs_fit*

Model fine structure line profiles were produced using hyperfine component transitions calculated using Equation 2.29, Equation 2.30, and Voigt profiles (subsection 2.5.3). The model profiles were fitted to observed line profiles to obtain parameters such as the A and B constants of the upper and lower levels, Gaussian and Lorentzian widths of the Voigt profiles, and COG wavenumber of the fine structure line.

A method to efficiently and accurately produce initial guesses of fit parameters (e.g. HFS constants) was required for line profile fitting. This was because the existing Co II HFS data in the literature were very limited, where HFS A constants were known for only 28 out of almost 500 known energy levels of Co II (see subsection 1.4.2). It was common for both upper and lower levels of a transition of Co II to have unknown A constants. This placed very few constraints on the fit parameters (see section 8.5 for details). Moreover, strong transitions of Co II lie deeper in the UV compared to those of Co I, where hyperfine component transitions are more commonly unresolved due to larger Doppler widths (Equation 2.37). Therefore, methods from the HFS analysis of Co I [166] were expected to be less effective for Co II HFS analysis, which needed to be addressed and this prompted me to create the *hfs_fit* computer program [167].

8.3.1 Initial Parameter Determination

Initial guesses for fit parameters are determined visually through manual variation of sliders to adjust parameters in the fit. The process is illustrated in Figure 8.1 and Figure 8.2, where the only difference between the two sets of parameters is the A constant of the lower level. Using this program, the problem of obtaining initial parameters for optimisation was reduced to an efficient trial-and-error search with instant visual feedback from varying any parameter

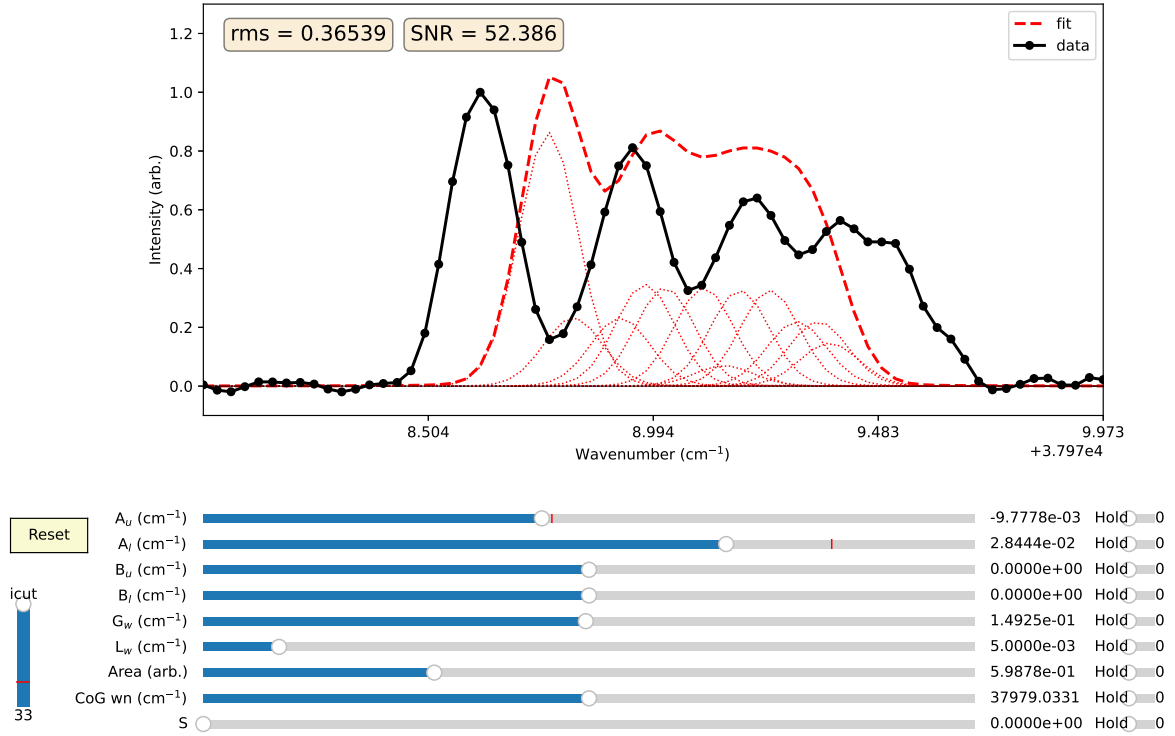


Figure 8.1: *hfs_fit* user interface showing a plot of model line profile (red dashed line) from a poor set of parameter values for the observed (black line with dots) 4s – 4p transition of Co II at 37979.042 cm⁻¹. The thinner red dotted lines are Voigt profiles of the component HFS transitions that are added together to produce the model line profile. The meaning of *rms* and *icut* will be explained in subsection 8.3.2 and subsection 8.3.3, respectively.

of the fit. Furthermore, the program allowed convenient estimations of uncertainties based on examining worst fits.

The parameters of Figure 8.1 and Figure 8.2 with horizontal sliders are, from top to bottom: A_u constant of the upper level, A_l constant of the lower level, B_u constant of the upper level, B_l constant of the lower level, Gaussian (Doppler) width G_w of the component transitions, Lorentzian (resonance, pressure, and natural) width L_w of the component transitions, the area under the amplitude-normalised curve, the COG wavenumber, and the self-absorption parameter (see section 8.4 for more details). The possible values of each parameter are crucial to their mean value and uncertainty estimation. The rest of this chapter is dedicated to discussing the optimisation of parameter values and considerations for parameter constraint in the Co II HFS analysis, as well as presenting the analysis results and their uncertainties.

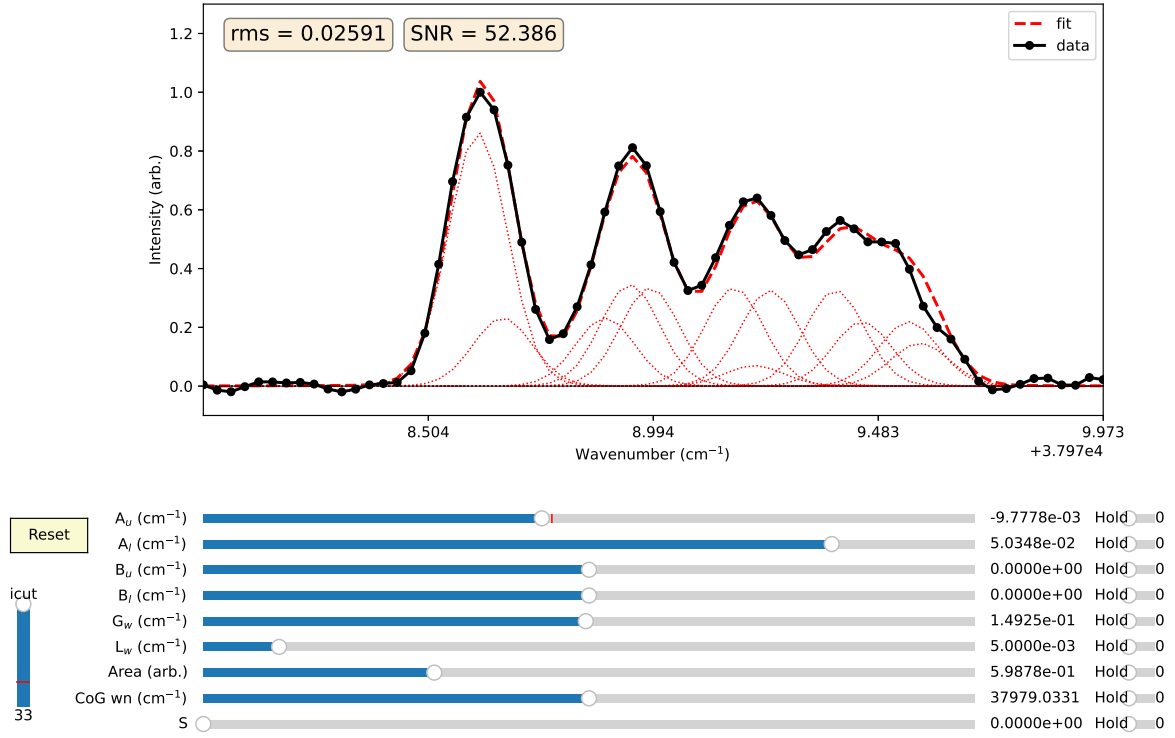


Figure 8.2: *hfs_fit* user interface showing a plot of model line profile (red dashed line) from a good set of parameter values for the observed (black line with dots) 4s – 4p transition of Co II at 37979.042 cm⁻¹. The thinner red dotted lines are Voigt profiles of the component HFS transitions that are added together to produce the model line profile. The meaning of *rms* and *icut* will be explained in [subsection 8.3.2](#) and [subsection 8.3.3](#), respectively.

8.3.2 Least-squares Fit by Simulated Annealing

After obtaining a set of satisfactory initial parameters, such as those of [Figure 8.2](#), the parameters are optimised using the simulated annealing algorithm. The optimisation method was inspired by the program used for the Co I HFS analysis [166, 168] written by Dr J. Brault and the program *XGREMLIN* [122], both of which employ the simulated annealing method for many-parameter optimisation [169, 170]. The algorithm is a Monte Carlo method requiring an initial guess for each parameter. In an iteration, each parameter is randomly sampled from a specified distribution that is usually centered around the current parameter value. If the new set of parameters decreases the loss (e.g. sum of squared differences between model and observation becomes smaller and more optimal), they are accepted. If the new set of parameters increase the loss, they are accepted under a probability that exponentially decreases with the increase in loss and decreases with increasing number of iterations.

Aside from the simplicity and ease of implementation of the simulated annealing algorithm, there were two more reasons for using the algorithm. First and most importantly, it can escape local minima and find the global minimum when less optimal parameters in an iteration are accepted by chance. Aiming to find the global minimum is an important consideration for a many-parameter optimisation problem such as HFS line profile fitting. Secondly, it was commonly used in HFS analyses [122, 166, 168] and therefore was considered suitable for the task.

In *hfs_fit* [167], the quantity minimised is the standard deviation of the residuals of the fit (*rms* in Figure 8.1 and Figure 8.2):

$$r^j = \sqrt{\frac{1}{N - k} \sum_i^N (I_i^{\text{fit}} - I_i^{\text{obs}})^2}, \quad (8.1)$$

where j is the iteration number, N is the number of observed data points across the fitted line profile, k is the number of fitted parameters, I_i^{fit} is the model line profile, and I_i^{obs} is the observed line profile. When a new set of parameters is generated in the next iteration $j + 1$ such that $r^{j+1} > r^j$, the acceptance probability of the new (but less optimal) set of parameters is

$$p = e^{-(r^{j+1} - r^j)/T}, \quad (8.2)$$

where T is the temperature parameter. From observing the efficiency and accuracy of the optimisation algorithm, the initial value of T was chosen as a fifth of r^0 and was multiplied by 0.98 after each iteration. Similarly, the final iteration was chosen such that $T < 10^{-10}$ (no probability of accepting parameters with higher loss), and the number of iterations was generally around 10^3 .

For the random sampling of parameter values during an iteration, a Gaussian distribution was assigned to each parameter, centered around the parameter with a width (standard deviation). These widths are also determined from experience with using the optimisation algorithm, their default values are 0.001 cm^{-1} (30 MHz) for A_u , A_l , B_u , B_l , L_w , and the COG wavenumber, 0.01 cm^{-1} for G_w , 0.05 for the area under the line profile (all line profiles were normalised with peak values at unity), and 0.1 for the self-absorption parameter (section 8.4). If necessary, parameters could be held fixed during an optimisation, which can be specified by changing the *hold* slider values of Figure 8.1 and Figure 8.2. Fixing parameter values is often necessary when

the parameters could be optimised to values disagreeing with their known uncertainties, e.g., when the A constant of the lower level is known accurately and the A constant of the upper level is unknown.

8.3.3 Treating Instrumental Ringing

In most cases, line widths were limited by Doppler broadening alone. However, in a handful of cases, the fitting process needed to consider instrumental ringing. When the instrumental line width becomes comparable to the true line width, ringing artefacts are observable around spectral lines (see [subsection 3.3.3](#)). This was common in the IR Co HCL FT spectra used for the Co II HFS analysis. Instrumental ringing is mostly due to the finite mirror displacement (finite optical path difference) of the FT spectrometers, which apodises the ideal interferogram with a box function, and convolves the spectrum with a sinc function (e.g. [Figure 3.6](#) and [Figure 3.7](#)). If unconsidered, distortions to the true line profiles from this convolution will cause inaccuracies in the determined HFS constants.

Instrumental ringing was addressed by mimicking the apodisation of the interferogram, where the model spectral line was Fourier transformed, multiplied by a box function in the interferogram domain, and then reverse transformed back into the spectrum domain to match the observed instrumental ringing [[119](#)]. The integer parameter *icut* of *hfs_fit* (see [Figure 8.1](#) and [Figure 8.2](#)) specified the transformed data point index as the width of the box function. A fit to the instrumental ringing of an IR line with significant HFS is shown in [Figure 8.3](#), where regions without hyperfine transitions (vertical red lines) have spectral features significantly above the noise level and are well fitted by the model line profile.

By the convolution theorem, the above discussed method is the same as convolving the spectrum with a sinc function, which is also viable [[172](#)]. A more accurate instrumental profile [[173,174](#)] could also be used. The difference between these methods and the model profile transform apodisation method is not expected to be significant compared to the uncertainties of the HFS constants obtained for the Co II energy levels. However, not addressing the instrumental artefacts was observed to produce differences in Co II HFS constants that were comparable to their uncertainties.

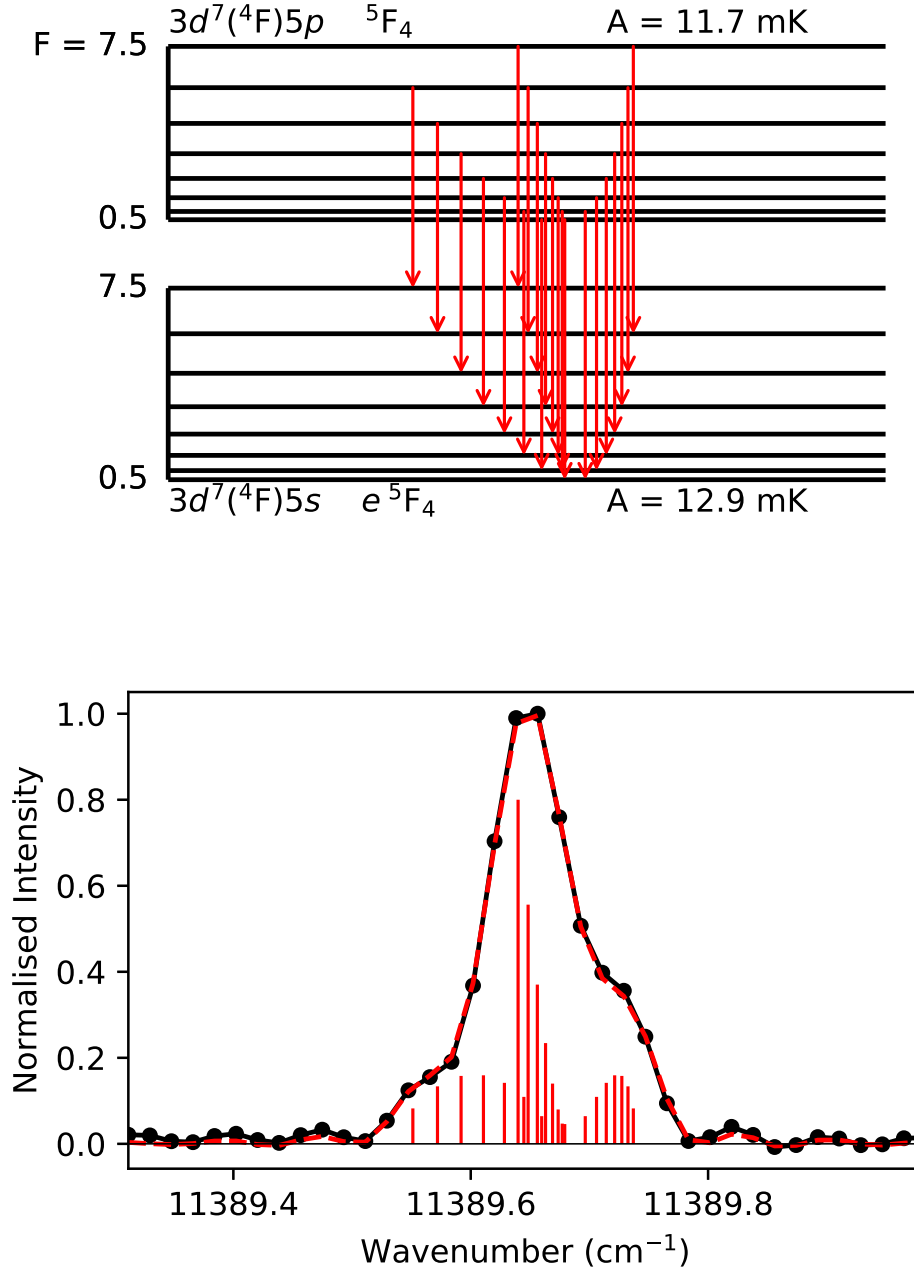


Figure 8.3: A $5s - 6p$ transition of Co II at $11389.710 \text{ cm}^{-1}$ in the IR with SNR of 160. The top plot shows a transition diagram illustrating the location and origin of the hyperfine component transitions, their relative intensities are shown as red vertical lines in the bottom plot. The bottom plot shows the observed (black line with dots) and fitted (red dashed line) line profiles. Units for A constants are in milli-Kayser which is equivalent to 0.001 cm^{-1} or 30 MHz. Figure from Ding & Pickering (2020) [171].

8.4 Considerations for Self-Absorption

Another difficulty in the HFS analysis is the existence of the self-absorption of spectral lines in the Co HCL FT spectra. As discussed in [subsection 2.5.4](#), self-absorption distorts and broadens spectral lines and prevents accurate determination of HFS constants of the associated energy levels. The method used to address effects of self-absorption for the HFS analysis of Co I [166, 168] is to introduce a self-absorption parameter S (bottom slider of [Figure 8.1](#) and [Figure 8.2](#)), where the initial line profile $I_0(\sigma)$ after self-absorption $I_{SA}(\sigma)$ is

$$I_{SA}(\sigma) = I_0(\sigma)e^{-SI_0(\sigma)}. \quad (8.3)$$

This has the same functional form as [Equation 2.38](#), where S is positive and increases with increasing amount of self-absorption. However, as discussed in [subsection 2.5.4](#), [Equation 2.38](#) arises from considering a constant spectral energy density across the line profile, which is itself an approximation as the spectral energy density primarily comes from the emission line profile of the fine structure transition, which is even less true for lines broadened by HFS [116]. Nevertheless, [Equation 8.3](#) was implemented into *hfs_fit* [167], expecting potential improvements when fitting lines affected slightly by self-absorption.

Generally, the parameter S was negligible for lines without self-absorption and was no greater than ~ 0.2 when a line profile showed signs of self-absorption. In the latter case, an S value of 0.2 reduced the fit residuals compared to S fixed at zero, but not to the extent expected from good fits of line profiles without any self-absorption. Therefore, the model in [Equation 8.3](#) was concluded to be an inaccurate description for lines significantly affected by self-absorption within the Co HCL. However, the S value was a useful indicator for problems with the line profile, such as self-absorption and blending with other transitions, generally accompanied by anomalous widths and/or a different profile in a different spectrum with different HCL conditions. Where possible, lines affected by self-absorption (and blends) were not used to determine the HFS constants of the corresponding levels. If a level contained only lines affected by self-absorption, (e.g. the ground term triplet $3d^8\ ^3F$), relatively large uncertainties were estimated for the HFS constants based on worst fits using the sliders of the *hfs_fit* program [167].

It is worth noting that fitting line profiles affected by self-absorption was attempted using a separate S value for each hyperfine component transition, to accommodate factors such as

spectral energy density wavenumber dependence across the line profile and hyperfine level populations due to different statistical weights. This method produced Doppler widths and A values that agreed with their values determined from other lines unaffected by self-absorption. However, the number of fit parameters was generally tripled due to the large number of hyperfine transitions, exceeding the number of data points across the line profile and likely overfitted the data. Therefore, a separate S value for each hyperfine component transition could not be concluded as a more accurate description of the observed self-absorption. Beyond the scope of the present work, reduction in the number of parameters may be possible by investigating fully resolved but self-absorbed hyperfine transitions observed in experimental spectra and by considering relative hyperfine transition intensities, relative hyperfine level populations, and spectral energy densities corresponding to the full fine structure emission line profile.

8.5 Parameter Constraints

To effectively determine optimal parameter values and the widths of their random sampling distributions, the sensitivity of the model line profile (in relation to the observed profile) from varying each parameter was investigated.

8.5.1 Well-constrained Parameters

For a spectral line profile, the COG wavenumber and the area under the line were calculable quantities, so acquiring their initial values was trivial. A slight adjustment of these two parameters was required if the line was noisy or slightly blended with other lines. The area under the line profile was slightly affected by the self-absorption parameter S^1 , which is also commonly negligibly small as only a small number of lines were affected by self-absorption. The Lorentzian width component is mainly due to the pressure broadening of the spectral lines, which is constant throughout a spectrum. However, unexpectedly large L_w in a fit was nearly always a sign of self-absorption. The apodisation parameter $icut$ was always at the highest value for fully resolved lines and was simple to determine for lines with ringing, as only one

¹Equation 8.3 was applied after normalisation of the peak line intensity.

particular integer value fitted the ringing the best. Lastly, the electric quadrupole interaction constants of Co II, B_u and B_l , were concluded to be too small to be measurable due to insufficient resolution of the Co HCL FT spectra, similar to most HFS analyses by FT spectroscopy (e.g. [97, 166, 173–175]). These two parameters were never fixed but were also never optimised to values significant compared to their uncertainties. Furthermore, the line profile was mostly only sensitive to the difference between B_u and B_l rather than their particular values. The B constant was estimated for only one energy level, 5 ± 4 mK ($1 \text{ mK} = 0.001 \text{ cm}^{-1} = 30 \text{ MHz}$) for $3d^7(^4P)4s \text{ a}^5P_2$.

8.5.2 Poorly Constrained and Most Significant Parameters

The model line profile was most sensitive to the Gaussian (Doppler) width, G_w , and the magnetic hyperfine interaction constants of the upper and lower energy levels, A_u and A_l , respectively. Accurately determining these three parameters comprised the majority of the HFS analysis. The dominating width of the Voigt profiles was G_w , around an order of magnitude larger than the Lorentzian component L_w , so G_w was expected to significantly affect the line profiles². The high sensitivity of the line profile to the A constants was also expected since they generally dominate the hyperfine energy level splitting (compared to the B constants) and are the most important in modelling stellar absorption lines.

The three parameters A_u , A_l , and G_w are generally well-constrained for line profiles showing pronounced HFS where hyperfine component transitions are fully or partially resolved (e.g. Figure 8.2). In these cases, the three parameters can be determined at 5 to 10% accuracy without any prior information on the parameters. However, around half of the ~ 700 line profiles analysed in the present work have fully unresolved HFS component transitions, where the three parameters were poorly constrained and extra considerations were required for their correct determination.

²Typical G_w values are 25 mK around 5000 cm^{-1} , 50 mK around $10\,000 \text{ cm}^{-1}$, 80 mK around $20\,000 \text{ cm}^{-1}$, and up to 200 mK around $50\,000 \text{ cm}^{-1}$ for the Co HCL FT spectra.

Unresolved HFS Component Transitions

The lack of constraint and difficulty in the determination of the three parameters from line profiles with unresolved HFS is illustrated by [Figure 8.4](#) and [Figure 8.5](#). The line profile cannot be fitted by a single Voigt profile and is composed of multiple unresolved Voigt profiles from the individual hyperfine component transitions. However, the range of possible A constants that can fit the profile was over 20 mK, this range was deduced from the simulated annealing optimisations using different initial guesses and random seeds, as well as estimations by worst fits. From analysing this line alone, the A constants cannot be determined with satisfactory accuracy. For example, for a transition of a level with highly uncertain A constant to another level with accurately known A constant, variation of the uncertain A constant within ± 20 mK would produce significantly different total line widths, such as the 20 mK difference in one A constant of the model line profiles of [Figure 8.1](#) and [Figure 8.2](#), and the 10 mK difference in the HFS analysis of the stellar absorption line of [Figure 1.8](#).

Fine structure line profiles similar to that of [Figure 8.4](#) and [Figure 8.5](#) were common but never analysed without existing information on the expected value and uncertainty of at least G_w and one of either A_u or A_l . Constraints on the three parameters are much tighter for line profiles with resolved or partially resolved HFS component transitions. Such profiles were the first selected to be analysed and these would then go on to provide key information for profiles with poorly constrained G_w , A_u , and A_l . For instance, G_w can be gauged from the Doppler broadening relation with wavenumber ([Equation 2.37](#)) from well-fitted profiles, and one of the A constants could be obtained from line profiles with resolved HFS component transitions.

Considering Electron Configurations of Energy Levels

Consideration of the configurations of the energy levels can also allow checks on the new A constants. In [Figure 8.4](#) and [Figure 8.5](#) where there are ambiguous results for A values, the lower level contains an electron in the 4p orbital ($l = 1$) and the upper level contains an electron in the 4d orbital ($l = 2$). The electron density near the nucleus is generally larger for the 4p orbital, and therefore the size of HFS splitting is expected to be larger for the lower level, suggesting the A constants of [Figure 8.5](#) to be less likely, which was indeed the case.

It is worth noting that when the J values of two energy levels of a transition are equal, the A

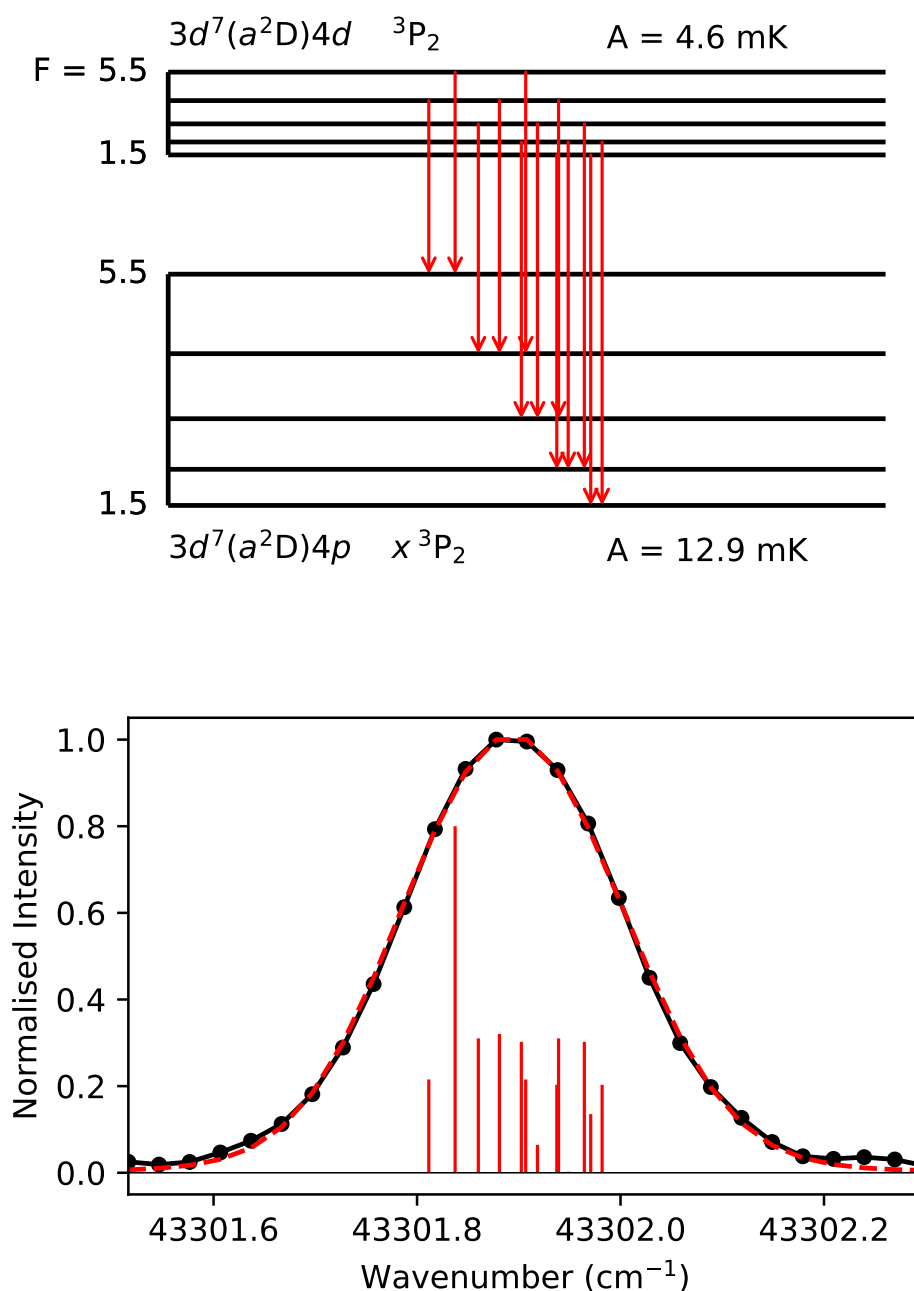


Figure 8.4: A 4p – 4d transition of Co II at $43301.944 \text{ cm}^{-1}$ in the UV with SNR of 80. The top plot shows a transition diagram illustrating the location and origin of the hyperfine component transitions, their relative intensities are shown as red vertical lines in the bottom plot. The bottom plot shows the observed (black line with dots) and fitted (red dashed line) line profiles. Units for A constants are in milli-Kayser which is equivalent to 0.001 cm^{-1} or 30 MHz. Figure from Ding & Pickering (2020) [171]. Please note that these two A constants were not obtainable using this line profile alone.

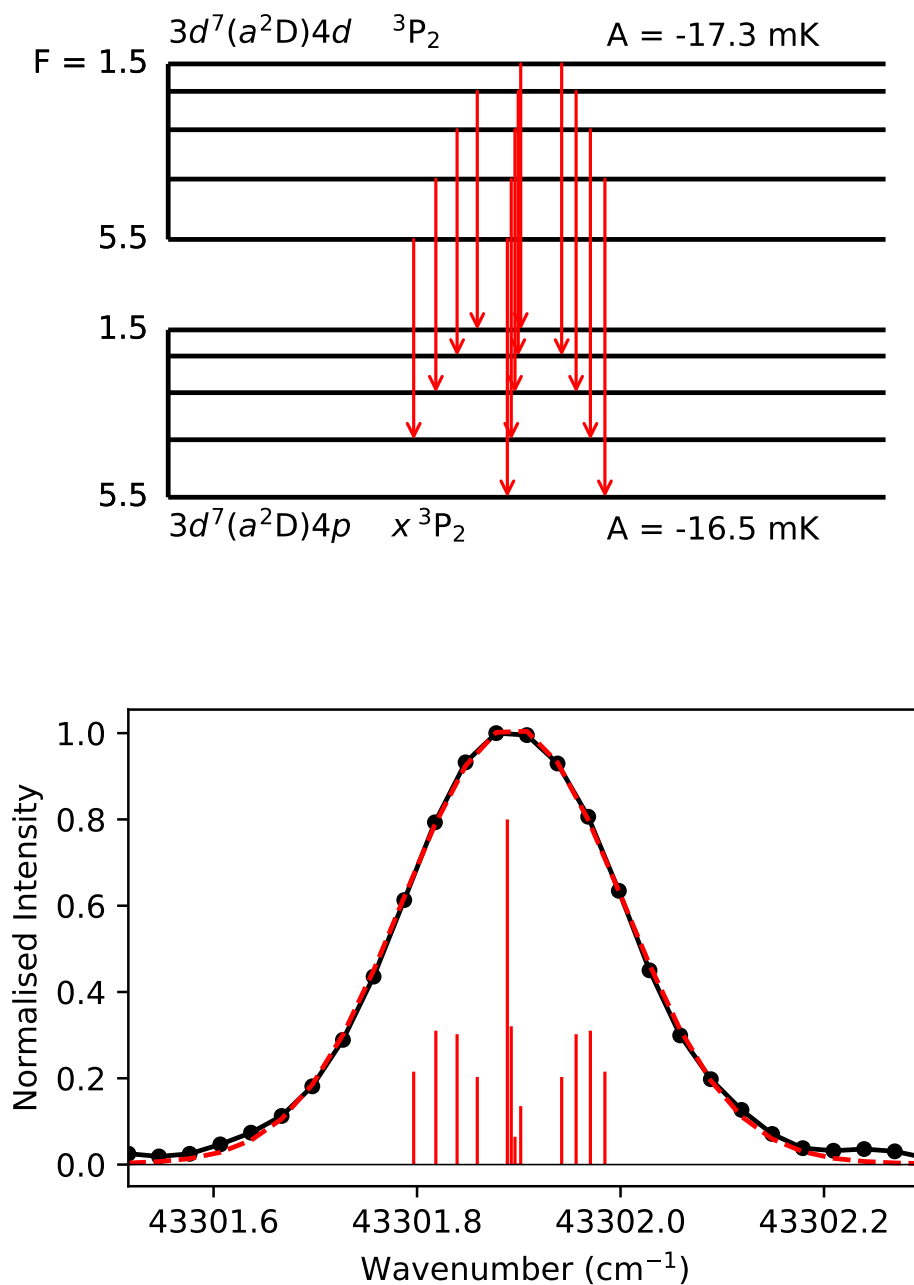


Figure 8.5: Same plot as Figure 8.4, except with very different A constants and similar Gaussian width G_w . This set of A constants does not agree with their values determined using other transitions involving either of the two energy levels. Figure from Ding & Pickering (2020) [171].

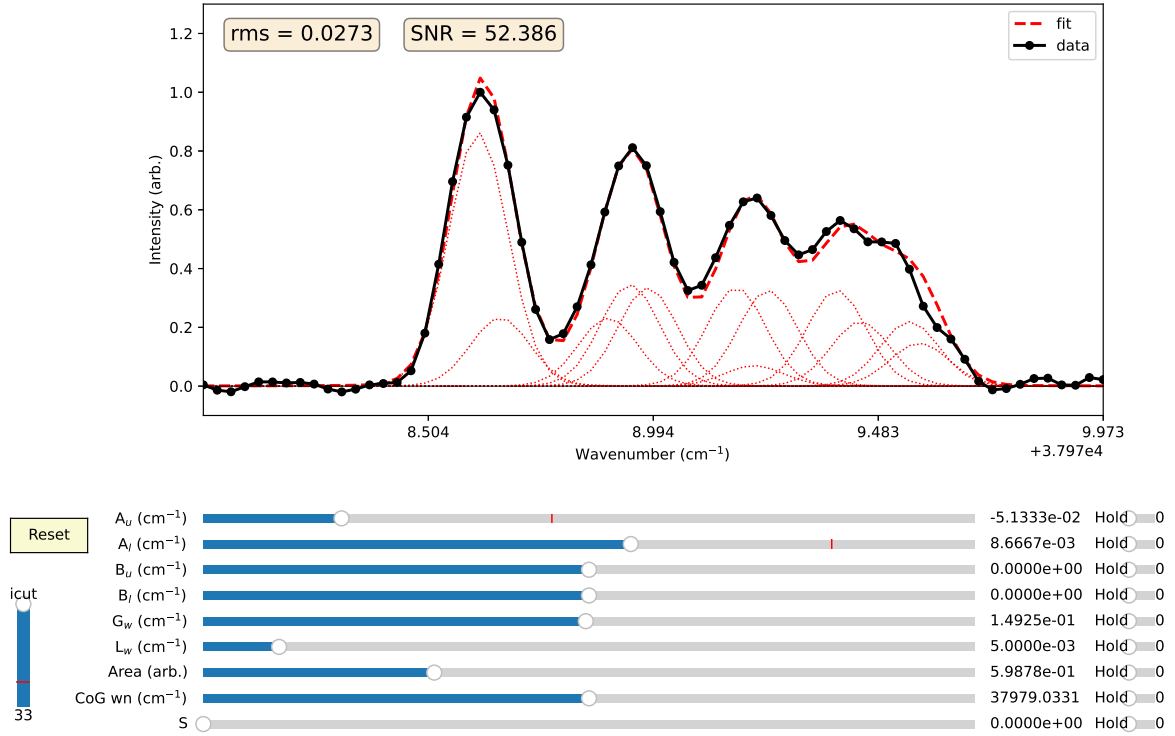


Figure 8.6: Same plot as Figure 8.2, but with $A_u = -A_l$. The transition is between two $J = 2$ energy levels.

constants of the two levels can swap values and signs ($A_u = -A_l$) and still fit the line profile. This is due to the symmetry of the 6- j symbol of Equation 2.29, where the value of the symbol is unchanged from swapping two values of the bottom row (J' and F') with corresponding values (J and F) with the top row. An example is shown in Figure 8.6, where $A_u = -51$ mK and $A_l = 9$ mK, but can also be³ $A_u = -10$ mK and $A_l = 50$ mK according to Figure 8.2. Again, the correct pair of A constants can be gauged by considering configurations of the energy levels. The transition is from a 4p level to a 4s level, and the 4s orbital electron densities are greater near the nucleus, therefore the lower level is expected to have greater HFS splitting and so the A constants from Figure 8.2 are more likely to be correct.

³The difference of 1 mK is within uncertainties and implemented here to avoid an exact replica of the plot in Figure 8.2 in the interest of demonstration.

Agreement of A Constants between Different Transitions and Lamp Conditions

One of the most important requirements in the reliable determination of the A constant of an energy level is achieving consistency between its optimised value across line profiles observed for transitions to/from different energy levels and between transitions of the energy level observed in different lamp conditions (e.g. Ar or Ne carrier gas). Not only does this consistency reduce the constraint on lines with unresolved HFS, but also problems such as self-absorption or line blending are also indicated. This is discussed in the previous Co II HFS analysis [97] and potential problems when this consistency cannot be achieved (generally due to limited extent and SNR of spectral data) will be illustrated in [section 8.8](#). All A constants determined in the present work were analysed using at least two transitions to different levels, and in most cases in both the Co-Ar and Co-Ne spectra.

8.5.3 Parameter Mean and Uncertainty Estimation

Variability from Random Seeds

The simulated annealing algorithm used random sampling and optimised parameters over $\sim 10^3$ iterations. The final parameter values were therefore dependent on the samples made and the random seed. For each optimisation, after setting initial parameter values, 20 separate optimisations were made using different seeds. The resulting distributions of each parameter were used to estimate their mean values and standard uncertainties. This method can indicate parameter constraints of A_u , A_l , and G_w since the 20 optimised values likely lie on a flat global minimum where any location within the minimum (generally along the A_u , A_l , and G_w axes and the axes of the negligible B_u and B_l parameters) has the same fit residuals. For the important A constants, their standard uncertainty from 20 optimisations was usually 1 mK for line profiles with asymmetry and partially resolved HFS components (e.g. [Figure 8.3](#)), and up to 10 mK for symmetric line profiles with unresolved HFS components (e.g. [Figure 8.4](#)).

A Constants

The mean and uncertainty of an A constant were mainly determined using the weighted average and weighted standard deviation of values obtained from fitting as many transitions of the

energy level observed from as many spectra as possible. The unnormalised weights w were determined using SNRs and the amount of complexity across the line profile, specifically

$$w = \text{SNR} \times \left(\sum_i \left| \frac{I_{i+1} - I_i}{\Delta\sigma} \right| \right)^3, \quad (8.4)$$

where I_i is normalised intensity of the model line profile and i is the index in the wavenumber axis. The wavenumber range of each line profile was also normalised to be from 0 to 1 (i.e. from $[\sigma_{\min}, \sigma_{\max}]$ to $[\sigma_{\min} - \sigma_{\min}, (\sigma_{\max} - \sigma_{\min})/(\sigma_{\max} - \sigma_{\min})]$), $\Delta\sigma$ is the resolution after this normalisation (i.e. $\Delta\sigma/(\sigma_{\max} - \sigma_{\min})$), and so profiles with fewer data points were also weighted less. The amount of complexity is measured by the summation of the absolute value of the derivative-like quantity, which is larger for profiles similar to that of [Figure 8.2](#) compared to profiles similar to that of [Figure 8.4](#). This summation is cubed to be weighted more than the SNR since the constraint on A constants depended much more on whether hyperfine component transitions were resolved. The SNR also does not affect the line profile except at very low values (less than around 10), in which case the line profiles would be too unreliable for HFS analysis.

The weighted mean and standard deviation method required a sufficient number of samples. A significant fraction of levels did not have more than five lines suitable for fitting, in which case the variability of optimal A values from the fits was the indicator for uncertainty instead and the weighted estimation was not used. In this case, the estimations of the A constant and its uncertainty were made using worst fits, where fits were made at mean values and extremes of possible values of the other A constant and G_w based on their uncertainties.

Gaussian (Doppler) Width G_w

The expected G_w and its standard uncertainty was obtained from the distribution of the already fitted lines. [Figure 8.7](#) shows the relationship of the fitted G_w against wavenumber for one UV Co HCL FT spectrum, where the standard uncertainty σ was determined using the root-mean-squared residuals between the observed values and the linear fit. There are five points beyond the 3σ region, these were a part of the linear fit and are examples of indications of self-absorbed lines that were generally avoided in the determination of the final A constant values.

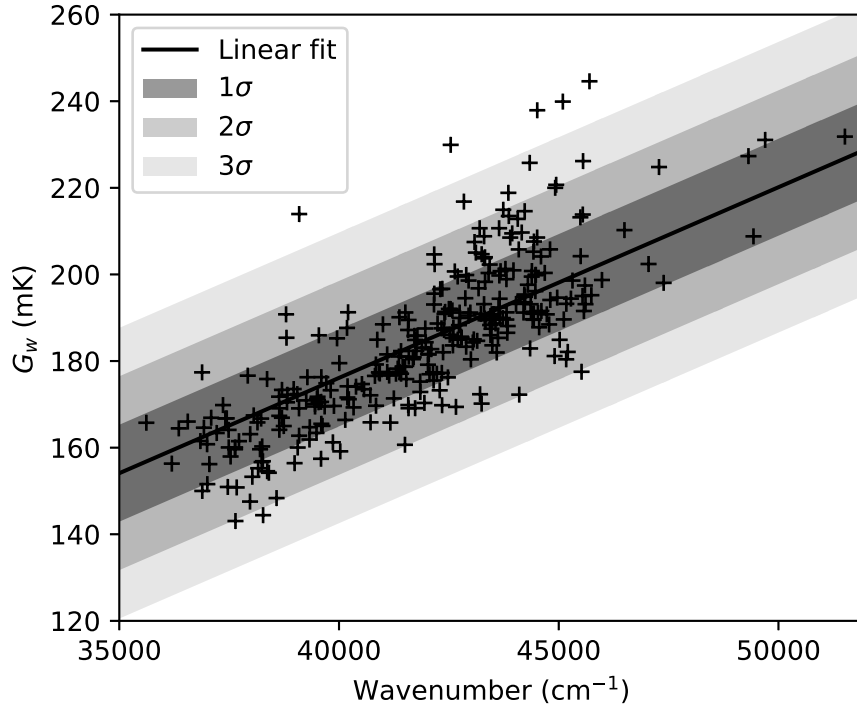


Figure 8.7: Doppler width relation with wavenumber within a UV Co HCL FT spectrum, the standard deviations of the fit residuals are shown using the shaded regions. Figure from [171].

8.6 Strategy of Analysis

As discussed in [subsection 8.5.2](#), the knowledge of one A constant of a transition simplifies the HFS analysis of the transition greatly and reduces the range of possible optimal values for the other A constant and G_w . Whenever an A constant and its uncertainty were determined, it would then become a reference A constant for the HFS analysis of other transitions involving its energy level. This process was iterated until further analysis became limited by the spectral range (i.e. no further lines to analyse within the observed spectra) or the SNR of the spectral lines being too poor for reliable analysis. Due to the iterative nature of this method, the initial set of reference A values needed to be as accurate as possible. There could be systematic errors for the A constants determined later in the analysis if the initial reference A constants were incorrect. For the Co II HFS analysis, no accurate A and B constants were available from Fabry-Pérot or laser spectroscopy measurements, and the only available measurements were the 28 A constants from FT spectroscopy [64, 97], which were expected to have similar accuracy compared to the present analysis. Therefore, the use of these 28 known A constants as references was not expected to give more accurate results, and to avoid any potential systematic errors in

the known A constants, the Co II HFS analysis began with no reference A or B constants of Co II energy levels.

The first step was to analyse all observed transitions showing pronounced HFS, where individual hyperfine component transitions were fully or partially resolved and accurate A constants could be determined without any prior information on A_u , A_l , and G_w . These lines could be identified in the line list [100–102, 165] from their anomalously large total line widths and from the fact that their lower levels belong to the $3d^74s$ configuration which generally has the largest HFS splitting. Examples include the line of Figure 8.2 and Figure 8.8. In Figure 8.8, the strongest hyperfine component transition is resolved, which provided an accurate measurement of G_w . As discussed in subsection 8.5.2, the A_u , A_l , and G_w parameters were well-constrained on these line profiles, and the goal for fitting as many of them as possible at the start of the Co II HFS analysis was to obtain an initial set of reference A constants and expectations for G_w based on its dependence on wavenumber (e.g. Figure 8.7).

In the UV region, within $36\,000\text{--}42\,000\text{ cm}^{-1}$, A_u , A_l , and G_w values of 18 lines were determined from two spectra (with Ar and Ne carrier gases respectively) to $\sim 5\%$ accuracy. Consistency, within uncertainties, with other transitions of the levels associated with these 18 transitions was also checked and achieved. With the initial set of reference A constants and expectations for G_w established, the analysis progressed and more A constants were determined, which were then used eventually as references for the analysis of line profiles with unresolved hyperfine components. Generally, one particular level's A constant was analysed at a time, which involves fitting all observed transitions of the associated energy level and estimating the mean A value and its uncertainty before moving on to determining another A constant of a different level. The analysis concluded when no observed transitions of the remaining Co II energy levels with unknown A constants were suitable for HFS analysis, e.g., no reference A constants, unresolved hyperfine component transitions, and/or line SNRs $\lesssim 10$.

8.7 Summary of Results

In total, magnetic dipole interaction A constants were determined for 292 energy levels of Co II, 264 of which were previously unknown, and these are listed in Appendix F. The electric quadrupole interaction B constant was estimated for one level, $3d^7(^4P)4s\ a^5P_2$, at $5 \pm 4\text{ mK}$

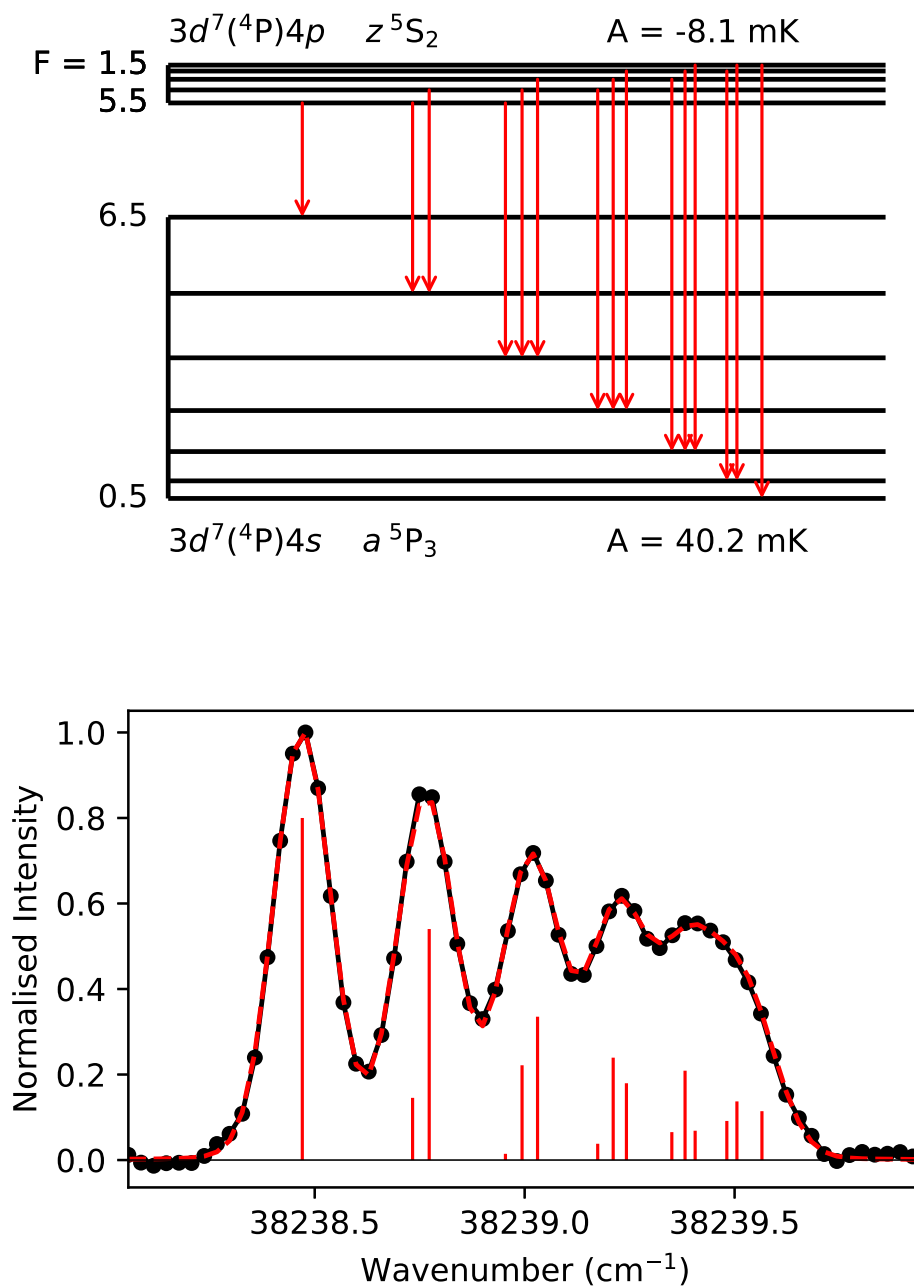


Figure 8.8: A $4s - 4p$ transition of Co II at $38238.969 \text{ cm}^{-1}$ in the UV with SNR of 70, observed with a resolved hyperfine component transition. The top plot shows a transition diagram illustrating the location and origin of the hyperfine component transitions, their relative intensities are shown as red vertical lines in the bottom plot. The bottom plot shows the observed (black line with dots) and fitted (red dashed line) line profiles. Units for A constants are in milli-Kayser which is equivalent to 0.001 cm^{-1} or 30 MHz. Figure from Ding & Pickering (2020) [171].

(1 mK = 0.001 cm⁻¹ = 30 MHz) using 14 fitted line profiles. The A constants were between -32.5 mK and 59.5 mK. Uncertainties of 90% of the A constants were between ± 0.4 mK and ± 3.0 mK and the remaining 10% were estimated at uncertainties up to ± 7 mK. These results were obtained from fitting over 700 observed spectral lines of the Co HCL FT spectra (section 8.2). All 28 previously known A constants [64,97] agree with their values determined in the present work within their combined uncertainties. As expected, the size of the A constants was the largest for configurations with a lone s ($l = 0$) electron, having the highest probability density near the nucleus. The size of the A constants decreased overall with increasing principal and angular momentum quantum number. The A constant of only one level of the 3d⁷5d configuration was determined and no A constants were determined for any levels of the 3d⁷5g configuration.

8.8 Comparisons with More Recent Literature

8.8.1 Laser Spectroscopy by Koszorús et al. (2023)

The HFS of ten Co II energy levels were investigated using laser spectroscopy by Koszorús et al. (2023) [176]. Their results agree with those in the present work, but their accuracies were two orders of magnitude higher due to the reduction of Doppler widths to sizes comparable to the natural line widths. As discussed, despite the high accuracy of laser spectroscopic techniques, the accuracy required for stellar spectral synthesis is already met through FT spectroscopy [64,97]. The wide spectral range of FT spectroscopy allows efficient determination of HFS constants for a large number of Co II levels, which is not achievable by the small spectral range of laser spectroscopic methods. Nevertheless, the accurate measurements by [176] will be excellent reference HFS constants for future similar work on Co II HFS.

8.8.2 Independent Analysis of Archival FT Spectra by Fu et al. (2021)

A few months after the publication of my results of the Co II HFS analysis [171], Fu et al. (2021) [177] published an analysis in JQSRT on the determination of 61 magnetic dipole interaction

Table 8.1: Table of 17 Co II Energy Levels with A Constants Inconsistent with Fu et al. (2021)

Config.	Term	J	Energy ^a (cm ⁻¹)	N	A^a (mK)	ΔA^a (mK)	A^b (mK)	ΔA^b (mK)	Diff. (mK)
3d ⁸	a ³ P	1	13404.321	2	-3.0	5.0	-11.9	1.6	8.9
3d ⁷ (² G)4s	a ³ G	5	21624.528	13	40.8	0.7	4.4	0.9	36.4
3d ⁷ (² G)4s	a ³ G	4	22009.344	17	22.7	0.4	30.8	5.9	-8.1
3d ⁷ (² P)4s	c ³ P	2	24886.400	14	51.8	1.0	11.2	3.5	40.6
3d ⁷ (² P)4s	a ¹ P	1	27585.138	4	26.4	0.9	15.0	8.7	11.4
3d ⁷ (² H)4s	a ³ H	4	27902.161	4	9.5	1.9	-10.3	1.1	19.8
3d ⁷ (² H)4s	a ¹ H	5	30567.173	10	29.9	1.3	-7.6	0.9	37.5
3d ⁷ (⁴ F)4p	z ³ D	1	52684.634	6	46.7	1.2	40.0	1.1	6.7
3d ⁷ (⁴ P)4p	y ⁵ D	3	61240.746	4	8.4	1.6	5.6	0.9	2.8
3d ⁷ (² G)4p	z ³ H	5	63306.686	7	22.1	0.7	24.5	0.9	-2.4
3d ⁷ (⁴ P)4p	y ³ D	3	63586.987	8	5.6	1.0	-23.4	3.5	29.0
3d ⁷ (² G)4p	z ³ H	6	63597.396	1	16.0	2.0	-14.4	0.9	30.4
3d ⁷ (² G)4p	z ¹ G	4	64401.359	8	22.2	1.1	-23.6	0.9	45.8
3d ⁷ (² P)4p	z ³ P	1	65028.512	5	5.1	0.7	-39.8	3.5	44.9
3d ⁷ (² P)4p	x ³ D	3	67524.021	3	10.5	1.5	-19.4	3.5	29.9
3d ⁷ (a ² D)4p	w ³ D	1	69317.077	1	22.2	0.7	-8.3	10.0	30.5
3d ⁷ (² H)4p	z ¹ I	6	69617.495	1	24.0	2.0	-6.7	3.4	30.7

^a Ding & Pickering (2020) [171]

^b Fu et al. (2021) [177]

N is the number of line profiles used in the present work to determine the mean value and uncertainties of the A constants, excluding blends, self-absorbed, or low SNR lines used to check consistency. 1 mK = 0.001 cm⁻¹ = 30 MHz. The differences in A values of the two papers are given in the final column. Table from Ding & Pickering (2022) [178].

HFS (A) constants of Co II using archival FT spectra from the National Solar Observatory. Surprisingly, the authors and reviewers of Fu et al. (2021) [177] appeared to be unaware of the existence of the published results of the present work. Upon comparing the results of the present work with those from Fu et al. (2021) [177], 17 A constants were found to be in disagreement. Summarised in Table 8.1, all discrepancies between each of the 17 A constants were greater than the joint uncertainties from both measurements and most were greater by more than an order of magnitude of the uncertainties.

The discrepancies of Table 8.1 were investigated in detail in Ding & Pickering (2022) [178], and are clear examples of insufficient consideration of parameter constraints, particularly those of A_u and A_l . Most of the discrepancies, also the largest, arose from Fu et al. (2021) [177] not

achieving consistent A constant values between different transitions of different energy levels. Particularly, errors in the A constants of $3d^7(^2G)4s\ a^3G_5$ and $3d^7(^2P)4s\ c^3P_2$ caused a cascade of errors in the flawed determination of the A constants for ten other Co II energy levels. This was deduced from following the list of transitions used by Fu et al. (2021) [177] to determine the disagreeing A constants, where the errors started with using the incorrect A constants of $3d^7(^2G)4s\ a^3G_5$ and $3d^7(^2P)4s\ c^3P_2$ as reference A constants. The exact number of transitions analysed by Fu et al. (2021) [177] for each of their A constants is unknown, but appeared generally fewer compared to the present work.

The remaining five other smaller discrepancies were considered possible due to different FT spectra and lamp conditions, e.g., differences in resolution, Doppler widths, and amount of self-absorption. One A constant determined by Fu et al. (2021) [177] was not determined in the present work, due to the lack of transitions observed at satisfactory SNRs. This was for the $3d^64s^2\ a^5D_4$ level, with 12.0 ± 1.8 mK [177] which agrees with the weak spectral lines of this level observed in our set of Co HCL FT spectra, after considering the expected G_w and reference A constants.

8.8.3 Semi-empirical Calculations of Co II HFS

Similar to the semi-empirical calculations of the atomic structure of Nd III (subsection 2.2.8 and Appendix A), HFS constants of the energy levels of an atom can be calculated using theoretical parameters fitted using known HFS constants. Semi-empirical calculations of Co II HFS were published [179–181] in 2023 using the available experimental A constants of Co II from the present (292) and other work [97, 177] (28 and 61, respectively). Comparison between the semi-empirical calculations showed excellent agreement with results of the present Co II HFS analysis.

In the initial stages of the new semi-empirical calculations [179–181], the 17 disagreeing A constants of Table 8.1 were excluded from the semi-empirical parameter fitting. The calculations on average deviated from available experimental A constants by ~ 1.5 mK. The calculations did not agree with 15 of the 17 problematic A constants of Table 8.1 determined by Fu et al. (2021) [177], which further supported the conclusion that the discrepancies were caused by the flawed analysis of weak and experimentally unclassified lines by Fu et al. (2021) [177], as was

pointed out [178].

The two A constants calculated to agree better with results from Fu et al. (2021) [177] and slightly disagree with results from the present work were not part of the cascade of errors made by Fu et al. (2021) [177] due to incorrect reference A constants for $3d^7(^2G)4s\ a^3G_5$ and $3d^7(^2P)4s\ c^3P_2$ [178]. Both A constants were determined with a high uncertainty of ± 5 mK in the present work due to non-ideal line profiles for HFS fitting, small discrepancies were therefore not unexpected.

The first disagreement was in the low-lying ground configuration level, $3d^8\ a^3P_1$, with an A constant of -2 ± 5 mK determined in the present work, 12 ± 2 mK in Fu et al. (2021) [177], and 11.0 ± 1.5 mK in calculations [179, 181]. Only two line profiles were suitable for HFS fitting of the A constant of this level, which were the $3d^8\ a^3P_1 - 3d^7(^4P)4p\ z^3D_{2,1}$ transitions. Both of these lines showed obvious signs of self-absorption in the Co-Ar HCL FT spectrum and slight signs of self-absorption in the Co-Ne HCL FT spectrum. The two lines observed in the Co-Ne HCL FT spectrum were used to determine the A constant of $3d^8\ a^3P_1$ through the method of worst fitting while keeping the reference A value fixed at expected values for the $3d^7(^4P)4p\ z^3D_{2,1}$ levels. The spectral lines of the archival Co FT spectra used by Fu et al. (2021) [177] may have been recorded at lower currents and so were free from self-absorption.

The second disagreeing A constant belongs to the $3d^7(^4P)4p\ y^5D_3$ level, determined as 8.4 ± 1.6 mK in the present work, 5.6 ± 0.9 mK in Fu et al. (2021) [177], and 6.4 ± 1.5 mK in calculations [180, 181]. All results agree within joint uncertainties, but the value from the present work agrees less well with the other two. The value 8.4 ± 1.6 mK was determined using four line profiles - the $3d^74s\ a^5P_{2,3} - 3d^7(^4P)4p\ y^5D_3$ transitions observed in both the Co-Ar and Co-Ne HCL FT spectra. These two transitions in the Co-Ne spectrum were around 120 SNR, half of the SNR of those observed in the Co-Ar spectrum, but fit residuals in the Co-Ne spectrum were poorer, possibly due to unknown blending or slight self-absorption. Furthermore, the A constant of $3d^7(^4P)4p\ y^5D_3$ was determined very consistently at 7.6 and 7.4 mK respectively using the two lines from the Co-Ar spectrum, as opposed to 10.9 mK and 8.7 mK determined from the Co-Ne spectrum. Therefore, a better estimate for the A constant of $3d^7(^4P)4p\ y^5D_3$ could be 7.5 ± 1.6 mK, in better agreement with the more recent literature values [177, 180, 181].

Additionally, eight A constants of the new semi-empirical calculations [179–181] that were not reported by Fu et al. (2021) [177] also disagree with their values determined in the present

Table 8.2: Table of 8 Co II Energy Levels with A Constants Inconsistent with Recent Semi-empirical Calculations

Config.	Term	J	Energy ^a (cm ⁻¹)	N	A_{obs}^a (mK)	ΔA_{obs}^a (mK)	A_{calc}^b (mK)	ΔA_{calc}^b (mK)	Diff. (mK)
3d ⁸	a ³ F	2	1597.197	1	33	5	42	1.5	9
3d ⁸	a ³ P	2	13260.688	3	17	2	13	1.5	4
3d ⁷ (⁴ P)5s	⁵ P	1	99552.560	1	17	6	-12	1.5	29
3d ⁷ (a ² D)5s	³ D	1	108500.862	2	-7	3	32	1.5	39
3d ⁷ (⁴ F)4f	4.5[6.5]	6	110008.482	5	19	2	8	1.5	11
3d ⁷ (⁴ F)4f	3.5[0.5]	1	111014.319	1	19	2	10	1.5	9
3d ⁷ (⁴ F)4f	2.5[1.5]	1	111562.737	3	8	2	3	1.5	5
3d ⁷ (a ² D)4d	¹ P	1	113857.84	2	18	2	11	1.5	7

^a Ding & Pickering (2020) [171]

^b Klempka et al. (2023) [179, 180] and Elantkowska et al. (2023) [181]

N is the number of line profiles used in the present work to determine the mean value and uncertainties of the A constants, excluding blends, self-absorbed, or low SNR lines used to check consistency. 1 mK = 0.001 cm⁻¹ = 30 MHz.

work. These are summarised in Table 8.2 and the discrepancies were investigated. The largest and most concerning discrepancies belong to the A constants of the two 3d⁷5s levels, both fitted from only one line profile with unresolved HFS and with consistency checked using other weaker transitions (SNR ~ 10). The limited number of lines is because transitions of these two 3d⁷5s levels were not observed in the Co-Ar HCL FT spectrum, and observed only in the Co-Ne HCL FT spectrum likely due to enhanced population of the 3d⁷5s levels from the charge transfer reaction between Ne⁺ and Co [100, 147]. From holding reference A constants and G_w at expected values for the line profiles of these two levels, both A_{obs} and A_{calc} of Table 8.2 can fit the line profiles with unresolved HFS. Therefore, the lack of sufficient experimental data likely caused the inability to constrain these two A constants and explain their large discrepancies from semi-empirical calculations. Indeed, these two A constants are example results from the most challenging and uncertain HFS analyses of my work, dozens of other A constants were also determined using similarly limiting experimental data, but their results agreed very well within joint uncertainties with the semi-empirical calculations. The A constants of 3d⁷(⁴P)5s ⁵P₁ and 3d⁷(a²D)5s ³D₁ in the new calculations [179, 181] are concluded to likely be the more accurate values, especially for 3d⁷(a²D)5s ³D₁, where the re-analysis of a 70 SNR blend agreed much better with $A = 32$ mK. This is illustrated in Figure 8.9, where the COG wavenumber is the Ritz wavenumber between the two Co II energy levels. If A_u is set at the value -7 mK determined in the present work, the red dashed profile would be much wider, exceeding what

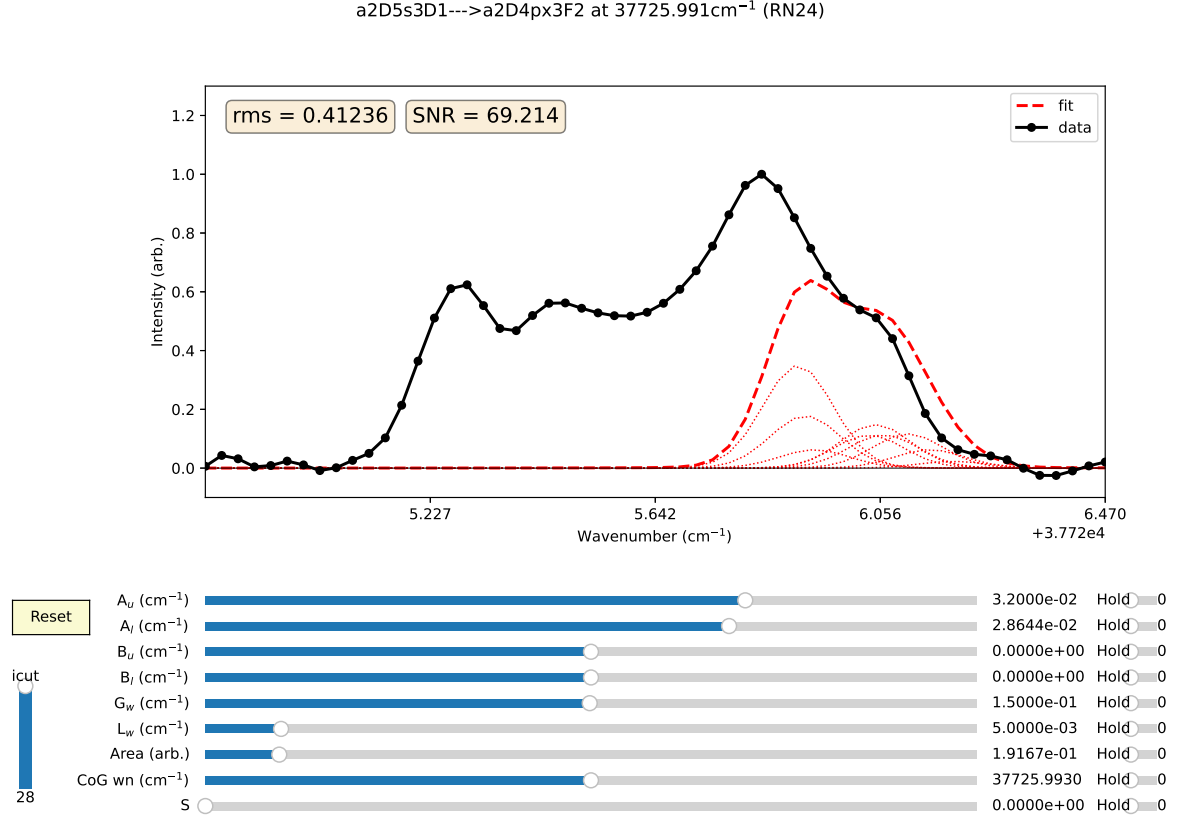


Figure 8.9: *hfs_fit* user interface with the A_u constant of $3d^7(a^2D)5s\ ^3D_1$ (upper level) set at the value 32 mK semi-empirically calculated by Elantkowska et al. (2023) [181] and the A_l constant set at the value experimentally determined in the present Co II HFS analysis. This Co II line is blended with a transition of Co I [165].

is observed in this blend on the right hand side.

Similarly limited experimental data also plagued the analysis of the A constants of the $3d^8\ a^3F_2$ and a^3P_2 levels and the $3d^7(a^2D)4d\ ^1P_1$ level of Table 8.2, where all available line profiles were with unresolved HFS. Transitions involving the two $3d^8$ levels were affected by self-absorption to a small extent, and those with the smallest G_w and L_w width parameters were used in worst-fit estimation of the A constants. Nevertheless, the discrepancies are only slightly greater than the joint uncertainties, which could indicate underestimates in the uncertainties of the observed A constants.

On the other hand, A_{obs} of the three $3d^7(^4F)4f$ levels of Table 8.2 were determined using high SNR line profiles showing partially resolved hyperfine component transitions in the IR (similar to that of Figure 8.8). Model line profiles using A_{calc} [179–181] produced line profiles that are too narrow compared to the observed high SNR lines. In particular, when A_{calc} [179–181] were used for both upper and lower levels to model the five transitions used to determine the

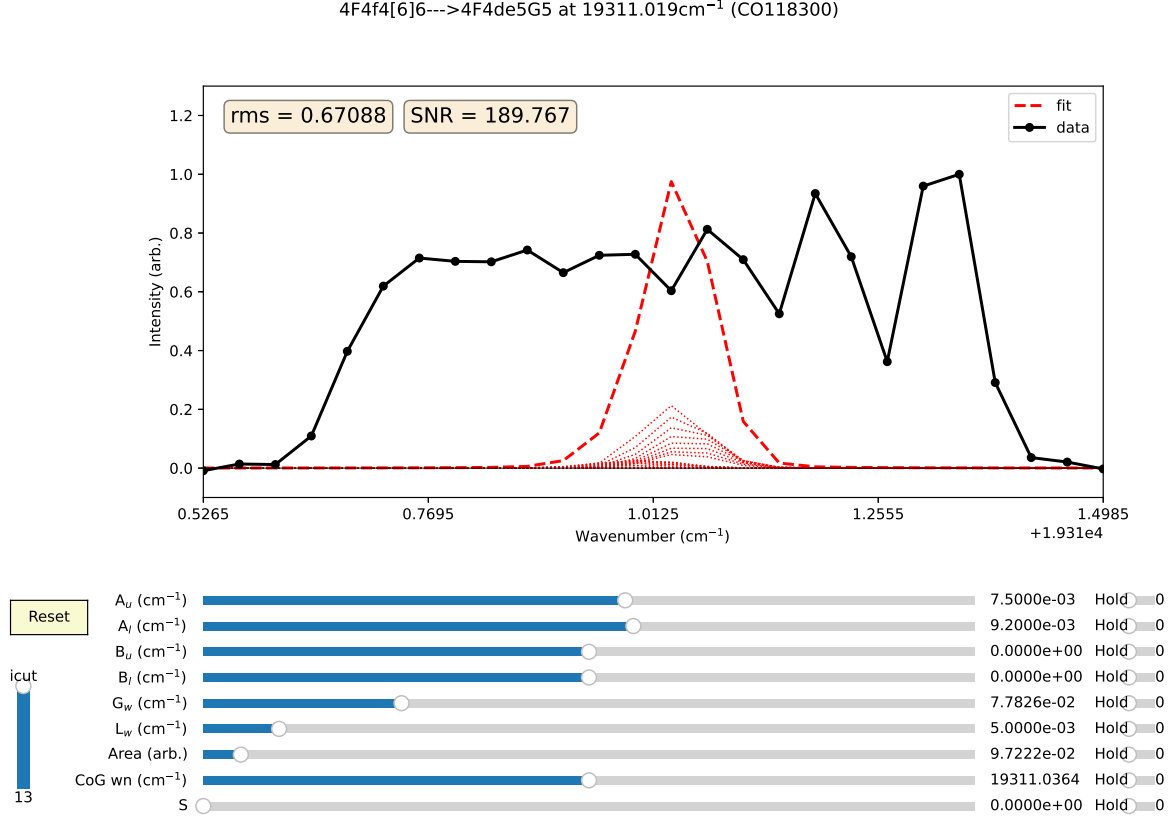


Figure 8.10: *hfs_fit* user interface with $A_u = 7.5$ mK for upper level $3d^7(^4F)4f\ 3.5[6.5]_6$ and $A_l = 9.2$ mK for lower level $3d^7(^4F)4d\ ^5G_5$. Both A constants are values semi-empirically calculated by Elantkowska et al. (2023) [181].

A constant of $3d^7(^4F)4f\ 4.5[6.5]_6$, all five line profiles were symmetric with no resolved HFS components and dramatically narrower than the observed profiles. An example is shown in Figure 8.10, where the observed profile is completely different from the model profile computed using upper and lower A calculated by Elantkowska et al. (2023) [181]. The semi-empirically calculated A constant of the lower level $3d^7(^4F)4d\ ^5G_5$ (9.2 ± 1.5 mK) agrees with its value determined experimentally in the present work (6 ± 3 mK) [171]. If 7.5 mK (the calculated value [181]) is used as A_u for the upper level, the A_l constant of the lower level must be -7 mK for the correct line width. This produces a visibly poorer fit of the smaller hyperfine components and -7 mK agrees with neither 6 ± 3 mK nor 9.2 ± 1.5 mK.

Since A_{calc} of other $3d^74f$ levels agree very well with the experimental values determined in the present work, the discrepancies between the three observed and calculated A constants of the $3d^74f$ levels of Table 8.2 could be due to outliers in the calculations and could indicate a larger uncertainty for A_{calc} of the $3d^74f$ configuration (larger than ± 1.5 mK), which would then agree with the experimental values as the discrepancies would be similar to the joint uncertainties.

Despite the inconsistencies discussed between ten A constants determined in the present work and those from the new semi-empirical calculations [179–181], the other 282 A constants are in very good agreement. Eight of the ten discrepancies were concluded to be only slightly significant and were due to limited experimental data and underestimation of experimental and theoretical uncertainties. It is worth noting that another set of semi-empirical calculations by Dr Peter Uylings and Dr Ton Raassen (private communications) included levels of the $3d^8$ and $3d^74f$ configurations, their results for the five $3d^8$ and $3d^74f$ levels of Table 8.2 agreed better with the experimental values determined in the present work.

In summary, only the two A constants of $3d^7(^4P)5s\ ^5P_1$ and $3d^7(a^2D)5s\ ^3D_1$ determined in the present work are potentially incorrect (wrong signs) when compared to recent semi-empirical calculations by [179–181]. Overall, the methodologies presented and performed in this chapter have been shown to be reliable for the determination of HFS A constants for the application of astrophysics, given that only two out of the 292 A constants determined suffered major discrepancies from semi-empirical calculations. These two A constants likely require further investigation.

8.9 Summary of the Analysis of Co II HFS

Magnetic dipole interaction HFS A constants of 292 energy levels were determined using least-squares fitting of observed Co II line profiles in Co HCL FT spectra ranging from the IR to the UV, and the electric quadrupole interaction B constant was estimated for one level. In tackling the challenges arising from no prior highly accurate HFS constants of Co II and many unresolved hyperfine transitions in the observed FT spectra, a computer program was created to efficiently pinpoint initial HFS line profile parameters for optimisation through user-interactive parameter variation with immediate visual feedback. The constraints of various parameters of the subsequent line profile fitting were carefully considered using properties of the FT spectra, the structure of the line profiles, the range of optimal values, the Doppler width relation, and agreement with A constant values determined using transitions involving other levels and within Co HCL FT spectra of varying lamp conditions.

Results agree with all 28 previously known A constants determined by FT spectroscopy [64, 97]. Comparisons made between the results of the present work and those from the more

recent literature [177, 179–181] showed good agreement. A small number of discrepancies were investigated and resolved, and semi-empirical calculations are in agreement for an overwhelming majority of the A constants determined in the present work, where only 2 of the 292 A constants determined in the present work could be erroneous due to limitations of the experimental spectra used.

Chapter 9

Conclusions

I recorded Nd spectra covering the full spectral range of the Imperial College VUV FT spectrometer and analysed them to experimentally identify energy levels and transitions of Nd III. Supplemented by grating spectroscopy and semi-empirical calculations, a significant extension to the experimental knowledge of the Nd III energy level system was achieved. I also discussed the outlook and possible future work on the atomic data of Nd III. In the penultimate chapter, I described the analysis of the HFS of Co II energy levels. This conclusion chapter contains a summary of all results obtained in the work of my thesis, which are significant advancements in the available atomic reference data of the spectrum and energy levels of Nd III and HFS of energy levels in Co II.

9.1 Energy Levels and Transitions of Nd III

In the present work, 258 energy levels of the $4f^4$, $4f^35d$, $4f^36s$, $4f^36p$, $4f^37s$, $4f^36d$, and $4f^35f$ configurations of Nd III were experimentally identified using 957 transitions of Nd III observed and classified from the laboratory spectra of Nd. Of the previously experimentally established 40 energy levels [63], 39 were confirmed and one was revised. A total of 219 energy levels were previously unknown and identified for the first time. I determined level energies for all levels except for the $4f^35f$ configuration, using FT spectra of the Nd-Ar PDL that I recorded using the Imperial College VUV high-resolution FT spectrometer within the region $11\,500\text{--}54\,000\text{ cm}^{-1}$ (870-185 nm) at resolving powers up to 10^6 . Transition and level energies are accurate to a

few parts in 10^8 and far exceeding the accuracy requirements for modern stellar absorption line analyses. For the classification of transitions of Nd III, I considered theoretically calculated level energies, level energy separations, and transition probabilities, as well as the comparison between the Nd-Ar PDL spectra and the Nd-Ar HCL spectra of lower effective temperatures. These results are the most extensive and accurate (to a few 10^{-3} cm^{-1}) Nd III energy level and transition wavenumber data to date.

The latter half of the term analysis of Nd III was enabled by carrying out new semi-empirical calculations of Nd III atomic structure and transition probabilities using the Cowan code, and observing Nd spectra at a variety of plasma conditions: in the HCL, vacuum sliding sparks, and stars of differing magnetic fields. The new semi-empirical calculations, stellar spectra, and spectra of vacuum sliding sparks were made available through international collaboration with the lead authors of the previous Nd III term analysis [63], Dr Alexander Ryabtsev and Dr Tatiana Ryabchikova. Note that the energy levels and transitions of the $4f^35f$ configuration were analysed by Dr Ryabtsev, and these results were only briefly included in this thesis for completeness.

Results for energy levels and transitions involving the $4f^4$, $4f^35d$, $4f^36s$, and $4f^36p$ configurations and the overall methodology have been published [96], and remaining results are being prepared for publication [160]. The present work will not only benchmark and improve future semi-empirical atomic structure calculations of Nd III, but also enable wider and more reliable astrophysical applications of Nd III, such as elemental abundance analyses of kilonovae and chemically peculiar stars, and studies of pulsational wave propagation in these stars.

9.2 Hyperfine Structure Interaction Constants of Co II

Energy Levels

By analysis of archival spectra, used originally for the most recent term analyses of Co I [166] and Co II [100–102], the most significant HFS interaction constant, the magnetic dipole interaction A constant was determined for 298 energy levels of Co II. My results agree with all 28 previously determined A constants and I determined 264 A constants for the first time. The less significant electric quadrupole B constant was determined only for one energy level, as the resolutions of

the Co FT spectra were insufficient. I showed that even if no accurate HFS constants for the Co II atom were known previously, and when the majority of line profiles have no resolved HFS component transitions, reliable determination of the A constants is achievable by using a few dozen line profiles with resolved HFS as references. Energy levels of the $3d^75g$ configurations did not show significant HFS, therefore. Similarly, the A constant of only one level of the $3d^75d$ configuration was determined. The vast majority of experimentally known Co II energy levels with significant HFS now have measured A constants, enabling much more reliable Co II stellar absorption line analyses.

Results for the HFS constants of Co II were published in 2020 [171]. Since then, several further measurements and theoretical calculations have been made for Co II HFS. An overwhelming agreement was found between the results of the present work and the results of the more recent Co II HFS investigations. Disagreements with experimental measurements that used poorer quality spectra [177] were resolved [178]. Newly published semi-empirical calculations of Co II HFS [179–181] agreed with 290 of the 292 A constants determined in my work.

9.3 Impacts and Future Work

The methodologies employed in my thesis are expected to be effective in similar analyses for other atoms and ions. FT spectroscopy has been shown to be the most suitable experimental method currently available for the analysis of extremely complex REE spectra and for obtaining a large number of HFS constants for an atom or ion. In addressing the lack of atomic data for kilonovae investigations, FT spectroscopy of other REEs in the future is not unexpected.

Results of the Co II HFS analysis has already been applied by astronomers to achieve better Co abundance values [182]. However, the two A constants disagreeing with new semi-empirical calculations were determined using line profiles limited by noise and resolution of the FT spectra used in the present work, they should require further investigation. FT spectroscopy targeting the transitions of the two levels would be a reasonable approach, e.g., narrower spectral ranges to boost SNR and lower currents to avoid self-absorption.

Experimentally identified energy levels of Nd III have led to more effective stellar Nd III spectral line analyses and the beginning of measurements of Nd III transition probabilities (Chapter 7).

Improvements to the results of the Nd III term analysis should be possible. Identifying levels of the doubly-excited configurations $4f^25d^2$ and $4f^25d6p$ is expected to improve parameterisation of the Cowan code significantly. Finding these configurations may also require further investigations of the $4f^35d$ configuration, where running Ne in the PDL looks promising.

Much of the atomic structure of Nd I-II remains experimentally unknown, where $\sim 10^4$ lines remain unclassified in the Nd-Ar PDL spectra. In retrospect, the Nd-Ar PDL populated Nd II levels the best, while the Nd HCL populated Nd I levels the best. Since the majority of Nd III transitions in the spectra I recorded are expected to have been classified (only 577 out of $\sim 20\,000$), and that transitions of Nd IV were essentially negligible, a term analysis of Nd I-II is very realistic with extra measurements of Nd-Ar and Nd-Ne FT spectra in the IR, because the lines between the two different ionisation stages are separable between the PDL and HCL.

Afterword – The experimental determination of atomic structure and transitions is an incredibly difficult task. It requires very sophisticated laboratory instrumentation, physical theories, and analysis software, I am in awe. I would like to believe that my results are a step towards answering our philosophical questions about the universe, although the progress made by my thesis may seem negligible, as if it was no more than one Nd atom compared to all of the Nd metal I have obliterated (about 10^{28} Nd atoms).

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Appendix A

Nd III Cowan Code Parameters

Semi-empirical calculations of Nd III atomic structure were carried out by Dr Ryabtsev using the Cowan code and all experimentally identified energy levels [96]. [Table A.1](#) [96] lists the semi-empirical parameters: the first column is the parity of the configuration; the second column is the configuration; the third column is the other configuration for configuration interaction parameters; the fourth column is the name of the parameter (explained in [Chapter 2](#)); the fifth column is the least-squares fit (LSF) value of the parameter determined using experimental level energies; the sixth column is the standard deviation of the fit; the seventh column is the flag indicating whether a parameter was fixed; the eighth column is the group of the parameter, where parameters of the same group were fixed at the same ratios (final column); the ninth column is the ab initio value of the parameters; and the final column is the ratio between LSF and HFR values, where the difference is used for E_{av} in units of cm^{-1} .

Table A.1: Nd III Cowan Code Parameters

Parity	Config.	Interacting Config.	Param.	LSF (cm ⁻¹)	Unc. (cm ⁻¹)	Fixed?	Group	HFR (cm ⁻¹)	Ratio
e	4f ⁴		E_{av}	32348	22			35503	-3155
e	4f ⁴		$F^2(4f,4f)$	71335	105			92636	0.770
e	4f ⁴		$F^4(4f,4f)$	40755	201			57680	0.707
e	4f ⁴		$F^6(4f,4f)$	35267		fixed		41372	0.852
e	4f ⁴		$\alpha(4f)$	8		fixed		0	0
e	4f ⁴		$\beta(4f)$	-310		fixed		0	0
e	4f ⁴		$\gamma(4f)$	1110		fixed		0	0
e	4f ⁴		$\zeta(4f)$	782	4			849	0.921
e	4f ³ 6p		E_{av}	88343	29			79811	8544
e	4f ³ 6p		$F^2(4f,4f)$	78655	146			102329	0.769
e	4f ³ 6p		$F^4(4f,4f)$	49923	164			64196	0.778
e	4f ³ 6p		$F^6(4f,4f)$	39344		fixed		46180	0.852
e	4f ³ 6p		$\alpha(4f)$	22		fixed		0	0
e	4f ³ 6p		$\beta(4f)$	-600		fixed		0	0
e	4f ³ 6p		$\gamma(4f)$	1450		fixed		0	0
e	4f ³ 6p		$\zeta(4f)$	888	2			954	0.930
e	4f ³ 6p		$\zeta(6p)$	2467	10			1989	1.240
e	4f ³ 6p		$F^1(4f,6p)$	739	45			0	0
e	4f ³ 6p		$F^2(4f,6p)$	6396	359			7861	0.814
e	4f ³ 6p		$G^2(4f,6p)$	2082	55			1981	1.051
e	4f ³ 6p		$G^3(4f,6p)$	0		fixed		0	0
e	4f ³ 6p		$G^4(4f,6p)$	1490	93			1791	0.832
e	4f ² 5d ²		E_{av}	96505		fixed		80505	16000
e	4f ² 5d ²		$F^2(4f,4f)$	83976		fixed		109034	0.77
e	4f ² 5d ²		$F^4(4f,4f)$	53651		fixed		68734	0.781
e	4f ² 5d ²		$F^6(4f,4f)$	42232		fixed		49543	0.852
e	4f ² 5d ²		$\alpha(4f)$	22		fixed		0	0
e	4f ² 5d ²		$\beta(4f)$	-600		fixed		0	0
e	4f ² 5d ²		$\gamma(4f)$	1450		fixed		0	0
e	4f ² 5d ²		$F^2(5d,5d)$	31880		fixed		44712	0.713
e	4f ² 5d ²		$F^4(5d,5d)$	19912		fixed		29676	0.671
e	4f ² 5d ²		$\alpha(5d)$	0		fixed		0	0
e	4f ² 5d ²		$\beta(5d)$	0		fixed		0	0
e	4f ² 5d ²		$T(5d)$	0		fixed		0	0
e	4f ² 5d ²		$\zeta(4f)$	972		fixed		1043	0.932
e	4f ² 5d ²		$\zeta(5d)$	928		fixed		982	0.945
e	4f ² 5d ²		$F^1(4f,5d)$	0		fixed		0	0
e	4f ² 5d ²		$F^2(4f,5d)$	20552		fixed		27943	0.735
e	4f ² 5d ²		$F^3(4f,5d)$	0		fixed		0	0
e	4f ² 5d ²		$F^4(4f,5d)$	14698		fixed		13649	1.077
e	4f ² 5d ²		$G^1(4f,5d)$	8707		fixed		12140	0.717
e	4f ² 5d ²		$G^2(4f,5d)$	0		fixed		0	0
e	4f ² 5d ²		$G^3(4f,5d)$	9206		fixed		10146	0.907

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Table C.1: Nd III Cowan Code Parameters (continued)

Parity	Config.	Interacting Config.	Param.	LSF (cm ⁻¹)	LSF Unc. (cm ⁻¹)	Fixed?	Group	HFR	Ratio
e	4f ² 5d ²		$G^4(4f,5d)$	0		fixed		0	0
e	4f ² 5d ²		$G^5(4f,5d)$	5248		fixed		7821	0.671
e	4f ³ 5f		E_{av}	139781	20			130790	8991
e	4f ³ 5f		$F^2(4f,4f)$	78489	120			102542	0.765
e	4f ³ 5f		$F^4(4f,4f)$	50724	149			64340	0.788
e	4f ³ 5f		$F^6(4f,4f)$	39436		fixed		46287	0.852
e	4f ³ 5f		$\alpha(4f)$	22		fixed		0	0
e	4f ³ 5f		$\beta(4f)$	-600		fixed		0	0
e	4f ³ 5f		$\gamma(4f)$	1450		fixed		0	0
e	4f ³ 5f		$\zeta(4f)$	884	2			956	0.924
e	4f ³ 5f		$\zeta(5f)$	21		fixed		21	1
e	4f ³ 5f		$F^1(4f,5f)$	0		fixed		0	0
e	4f ³ 5f		$F^2(4f,5f)$	2828	115			4027	0.702
e	4f ³ 5f		$F^3(4f,5f)$	0		fixed		0	0
e	4f ³ 5f		$F^4(4f,5f)$	1174	244			1575	0.747
e	4f ³ 5f		$F^5(4f,5f)$	0		fixed		0	0
e	4f ³ 5f		$F^6(4f,5f)$	880	127			1010	0.875
e	4f ³ 5f		$G^0(4f,5f)$	756	14			2811	0.269
e	4f ³ 5f		$G^1(4f,5f)$	0		fixed		0	0
e	4f ³ 5f		$G^2(4f,5f)$	1293	104			1846	0.701
e	4f ³ 5f		$G^3(4f,5f)$	0				0	0
e	4f ³ 5f		$G^4(4f,5f)$	650	208			1238	0.525
e	4f ³ 5f		$G^5(4f,5f)$	0				0	0
e	4f ³ 5f		$G^6(4f,5f)$	937	93			911	1.028
e	4f ⁴	4f ³ 6p	$RD^2(4f,4f,4f,6p)$	-3309		fixed		-4727	0.7
e	4f ⁴	4f ³ 6p	$RD^4(4f,4f,4f,6p)$	-2193		fixed		-3133	0.7
e	4f ⁴	4f ² 5d ²	$RD^1(4f,4f,5d,5d)$	12604		fixed		18006	0.7
e	4f ⁴	4f ² 5d ²	$RD^3(4f,4f,5d,5d)$	9601		fixed		13715	0.7
e	4f ⁴	4f ² 5d ²	$RD^5(4f,4f,5d,5d)$	7186		fixed		10265	0.7
e	4f ⁴	4f ³ 5f	$RD^0(4f,4f,4f,5f)$	881		fixed		1259	0.7
e	4f ⁴	4f ³ 5f	$RD^2(4f,4f,4f,5f)$	8202		fixed		11716	0.7
e	4f ⁴	4f ³ 5f	$RD^4(4f,4f,4f,5f)$	5368		fixed		7669	0.7
e	4f ⁴	4f ³ 5f	$RD^6(4f,4f,4f,5f)$	3914		fixed		5591	0.7
e	4f ³ 6p	4f ² 5d ²	$RD^1(4f,6p,5d,5d)$	2695		fixed		3849	0.7
e	4f ³ 6p	4f ² 5d ²	$RD^3(4f,6p,5d,5d)$	574		fixed		819	0.7
e	4f ³ 6p	4f ³ 5f	$RD^2(4f,6p,4f,5f)$	-2121		fixed		-3030	0.7
e	4f ³ 6p	4f ³ 5f	$RD^4(4f,6p,4f,5f)$	-506		fixed		-723	0.7
e	4f ³ 6p	4f ³ 5f	$RE^2(4f,6p,4f,5f)$	-319		fixed		-456	0.7
e	4f ³ 6p	4f ³ 5f	$RE^4(4f,6p,4f,5f)$	-210		fixed		-300	0.7
e	4f ² 5d ²	4f ³ 5f	$RD^1(5d,5d,4f,5f)$	-3112		fixed		-4445	0.7
e	4f ² 5d ²	4f ³ 5f	$RD^3(5d,5d,4f,5f)$	-1172		fixed		-1674	0.7
e	4f ² 5d ²	4f ³ 5f	$RD^5(5d,5d,4f,5f)$	-584		fixed		-834	0.7
o	4f ³ 5d		E_{av}	44999	43			36770	8229
o	4f ³ 5d		$F^2(4f,4f)$	78070	397		1	101378	0.770

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Table C.1: Nd III Cowan Code Parameters (continued)

Parity	Config.	Interacting Config.	Param.	LSF (cm ⁻¹)	LSF Unc. (cm ⁻¹)	Fixed?	Group	HFR	Ratio
o	4f ³ 5d		$F^4(4f,4f)$	49616	383		2	63552	0.781
o	4f ³ 5d		$F^6(4f,4f)$	38949	554		3	45705	0.852
o	4f ³ 5d		$\alpha(4f)$	22		fixed		0	0
o	4f ³ 5d		$\beta(4f)$	-600		fixed		0	0
o	4f ³ 5d		$\gamma(4f)$	1450		fixed		0	0
o	4f ³ 5d		$\zeta(4f)$	882	2		4	947	0.932
o	4f ³ 5d		$\zeta(5d)$	785	7			831	0.945
o	4f ³ 5d		$F^1(4f,5d)$	953	81			0	0
o	4f ³ 5d		$F^2(4f,5d)$	19310	119			26408	0.731
o	4f ³ 5d		$F^3(4f,5d)$	0		fixed		0	0
o	4f ³ 5d		$F^4(4f,5d)$	13958	275			13022	1.072
o	4f ³ 5d		$G^1(4f,5d)$	9138	39			12824	0.713
o	4f ³ 5d		$G^2(4f,5d)$	1689	198			0	0
o	4f ³ 5d		$G^3(4f,5d)$	9205	142			10202	0.902
o	4f ³ 5d		$G^4(4f,5d)$	0		fixed		0	0
o	4f ³ 5d		$G^5(4f,5d)$	5148	126			7735	0.666
o	4f ³ 6s		E_{av}	55647	49			47956	7691
o	4f ³ 6s		$F^2(4f,4f)$	78723	400		1	102226	0.770
o	4f ³ 6s		$F^4(4f,4f)$	50064	387		2	64126	0.781
o	4f ³ 6s		$F^6(4f,4f)$	39310	559		3	46129	0.852
o	4f ³ 6s		$\alpha(4f)$	22		fixed		0	0
o	4f ³ 6s		$\beta(4f)$	-600		fixed		0	0
o	4f ³ 6s		$\gamma(4f)$	1450		fixed		0	0
o	4f ³ 6s		$\zeta(4f)$	886	2		4	953	0.932
o	4f ³ 6s		$G^3(4f,6s)$	2393	72			2870	0.834
o	4f ³ 7s		E_{av}	128335	48			119629	8706
o	4f ³ 7s		$F^2(4f,4f)$	78941	401		1	102509	0.770
o	4f ³ 7s		$F^4(4f,4f)$	50214	388		2	64317	0.781
o	4f ³ 7s		$F^6(4f,4f)$	39431	561		3	46270	0.852
o	4f ³ 7s		$\alpha(4f)$	22		fixed		0	0
o	4f ³ 7s		$\beta(4f)$	-600		fixed		0	0
o	4f ³ 7s		$\gamma(4f)$	1450		fixed		0	0
o	4f ³ 7s		$\zeta(4f)$	888	2		4	956	0.932
o	4f ³ 7s		$G^3(4f,7s)$	714	76			917	0.779
o	4f ³ 6d		E_{av}	129569	47			120621	8948
o	4f ³ 6d		$F^2(4f,4f)$	78876	401		1	102424	0.770
o	4f ³ 6d		$F^4(4f,4f)$	50169	388		2	64259	0.781
o	4f ³ 6d		$F^6(4f,4f)$	39394	560		3	46227	0.852
o	4f ³ 6d		$\alpha(4f)$	22		fixed		0	0
o	4f ³ 6d		$\beta(4f)$	-600		fixed		0	0
o	4f ³ 6d		$\gamma(4f)$	1450		fixed		0	0
o	4f ³ 6d		$\zeta(4f)$	890	2		4	955	0.932
o	4f ³ 6d		$\zeta(6d)$	199	8			174	1.143
o	4f ³ 6d		$F^1(4f,6d)$	0		fixed		0	0

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Table C.1: Nd III Cowan Code Parameters (continued)

Parity	Config.	Interacting Config.	Param.	LSF (cm ⁻¹)	LSF Unc. (cm ⁻¹)	Fixed?	Group	HFR	Ratio
o	4f ³ 6d		$F^2(4f,6d)$	4206	199			5283	0.796
o	4f ³ 6d		$F^3(4f,6d)$	0		fixed		0	0
o	4f ³ 6d		$F^4(4f,6d)$	2299	355			2328	0.988
o	4f ³ 6d		$G^1(4f,6d)$	1356	70			1938	0.700
o	4f ³ 6d		$G^2(4f,6d)$	0		fixed		0	0
o	4f ³ 6d		$G^3(4f,6d)$	1743	246			1723	1.011
o	4f ³ 6d		$G^4(4f,6d)$	0		fixed		0	0
o	4f ³ 6d		$G^5(4f,6d)$	1248	176			1355	0.920
o	4f ² 5d6p		E_{av}	147563		fixed		131563	16000
o	4f ² 5d6p		$F^2(4f,4f)$	84517		fixed		109736	0.770
o	4f ² 5d6p		$F^4(4f,4f)$	54025		fixed		69213	0.781
o	4f ² 5d6p		$F^6(4f,4f)$	42535		fixed		49898	0.852
o	4f ² 5d6p		$\alpha(4f)$	22		fixed		0	0
o	4f ² 5d6p		$\beta(4f)$	-600		fixed		0	0
o	4f ² 5d6p		$\gamma(4f)$	1450		fixed		0	0
o	4f ² 5d6p		$\zeta(4f)$	978		fixed		1049	0.932
o	4f ² 5d6p		$\zeta(5d)$	1033		fixed		1094	0.945
o	4f ² 5d6p		$\zeta(6p)$	2683		fixed		2146	1.25
o	4f ² 5d6p		$F^1(4f,5d)$	0		fixed		0	0
o	4f ² 5d6p		$F^2(4f,5d)$	22410		fixed		29880	0.75
o	4f ² 5d6p		$F^3(4f,5d)$	0		fixed		0	0
o	4f ² 5d6p		$F^4(4f,5d)$	11061		fixed		14748	0.75
o	4f ² 5d6p		$F^1(4f,6p)$	0		fixed		0	0
o	4f ² 5d6p		$F^2(4f,6p)$	5860		fixed		7813	0.75
o	4f ² 5d6p		$F^1(5d,6p)$	0		fixed		0	0
o	4f ² 5d6p		$F^2(5d,6p)$	15285		fixed		20380	0.75
o	4f ² 5d6p		$G^1(4f,5d)$	9690		fixed		12920	0.75
o	4f ² 5d6p		$G^2(4f,5d)$	0		fixed		0	0
o	4f ² 5d6p		$G^3(4f,5d)$	8201		fixed		10934	0.75
o	4f ² 5d6p		$G^4(4f,5d)$	0		fixed		0	0
o	4f ² 5d6p		$G^5(4f,5d)$	6349		fixed		8465	0.75
o	4f ² 5d6p		$G^2(4f,6p)$	1443		fixed		1925	0.75
o	4f ² 5d6p		$G^3(4f,6p)$	0		fixed		0	0
o	4f ² 5d6p		$G^4(4f,6p)$	1312		fixed		1750	0.75
o	4f ² 5d6p		$G^1(5d,6p)$	7023		fixed		9364	0.75
o	4f ² 5d6p		$G^2(5d,6p)$	0		fixed		0	0
o	4f ² 5d6p		$G^3(5d,6p)$	5782		fixed		7709	0.75
o	4f ³ 5d	4f ³ 6s	$RD^2(4f,5d,4f,6s)$	-455		fixed		-650	0.7
o	4f ³ 5d	4f ³ 6s	$RE^3(4f,5d,4f,6s)$	1403		fixed		2004	0.7
o	4f ³ 5d	4f ³ 7s	$RD^2(4f,5d,4f,7s)$	-52		fixed		-74	0.7
o	4f ³ 5d	4f ³ 7s	$RE^3(4f,5d,4f,7s)$	730		fixed		1043	0.7
o	4f ³ 5d	4f ³ 6d	$RD^0(4f,5d,4f,6d)$	0		fixed		0	0
o	4f ³ 5d	4f ³ 6d	$RD^2(4f,5d,4f,6d)$	6412		fixed		9159	0.7
o	4f ³ 5d	4f ³ 6d	$RD^4(4f,5d,4f,6d)$	3556		fixed		5080	0.7

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Table C.1: Nd III Cowan Code Parameters (continued)

Parity	Config.	Interacting Config.	Param.	LSF (cm ⁻¹)	LSF Unc. (cm ⁻¹)	Fixed?	Group	HFR	Ratio
o	4f ³ 5d	4f ³ 6d	$RE^1(4f,5d,4f,6d)$	3386		fixed		4837	0.7
o	4f ³ 5d	4f ³ 6d	$RE^3(4f,5d,4f,6d)$	2864		fixed		4092	0.7
o	4f ³ 5d	4f ³ 6d	$RE^5(4f,5d,4f,6d)$	2216		fixed		3165	0.7
o	4f ³ 5d	4f ² 5d6p	$RD^2(4f,4f,4f,6p)$	-3097		fixed		-4425	0.7
o	4f ³ 5d	4f ² 5d6p	$RD^4(4f,4f,4f,6p)$	-1972		fixed		-2817	0.7
o	4f ³ 5d	4f ² 5d6p	$RD^1(4f,5d,5d,6p)$	4080		fixed		5829	0.7
o	4f ³ 5d	4f ² 5d6p	$RD^3(4f,5d,5d,6p)$	1287		fixed		1838	0.7
o	4f ³ 5d	4f ² 5d6p	$RE^2(4f,5d,5d,6p)$	-1287		fixed		-1838	0.7
o	4f ³ 5d	4f ² 5d6p	$RE^4(4f,5d,5d,6p)$	-556		fixed		-794	0.7
o	4f ³ 6s	4f ³ 7s	$RD^0(4f,6s,4f,7s)$	0		fixed		0	0
o	4f ³ 6s	4f ³ 7s	$RE^3(4f,6s,4f,7s)$	1128		fixed		1611	0.7
o	4f ³ 6s	4f ³ 6d	$RD^2(4f,6s,4f,6d)$	2073		fixed		2961	0.7
o	4f ³ 6s	4f ³ 6d	$RE^3(4f,6s,4f,6d)$	805		fixed		1149	0.7
o	4f ³ 6s	4f ² 5d6p	$RD^1(4f,6s,5d,6p)$	-8507		fixed		-12152	0.7
o	4f ³ 6s	4f ² 5d6p	$RE^2(4f,6s,5d,6p)$	-1212		fixed		-1732	0.7
o	4f ³ 7s	4f ³ 6d	$RD^2(4f,7s,4f,6d)$	113		fixed		161	0.7
o	4f ³ 7s	4f ³ 6d	$RE^3(4f,7s,4f,6d)$	418		fixed		597	0.7
o	4f ³ 7s	4f ² 5d6p	$RD^1(4f,7s,5d,6p)$	-1384		fixed		-1976	0.7
o	4f ³ 7s	4f ² 5d6p	$RE^2(4f,7s,5d,6p)$	-450		fixed		-643	0.7
o	4f ³ 6d	4f ² 5d6p	$RD^1(4f,6d,5d,6p)$	-3448		fixed		-4925	0.7
o	4f ³ 6d	4f ² 5d6p	$RD^3(4f,6d,5d,6p)$	-1050		fixed		-1499	0.7
o	4f ³ 6d	4f ² 5d6p	$RE^2(4f,6d,5d,6p)$	-975		fixed		-1393	0.7
o	4f ³ 6d	4f ² 5d6p	$RE^4(4f,6d,5d,6p)$	-650		fixed		-929	0.7

Appendix B

Custom Spectral Line Fitting Program Functionalities

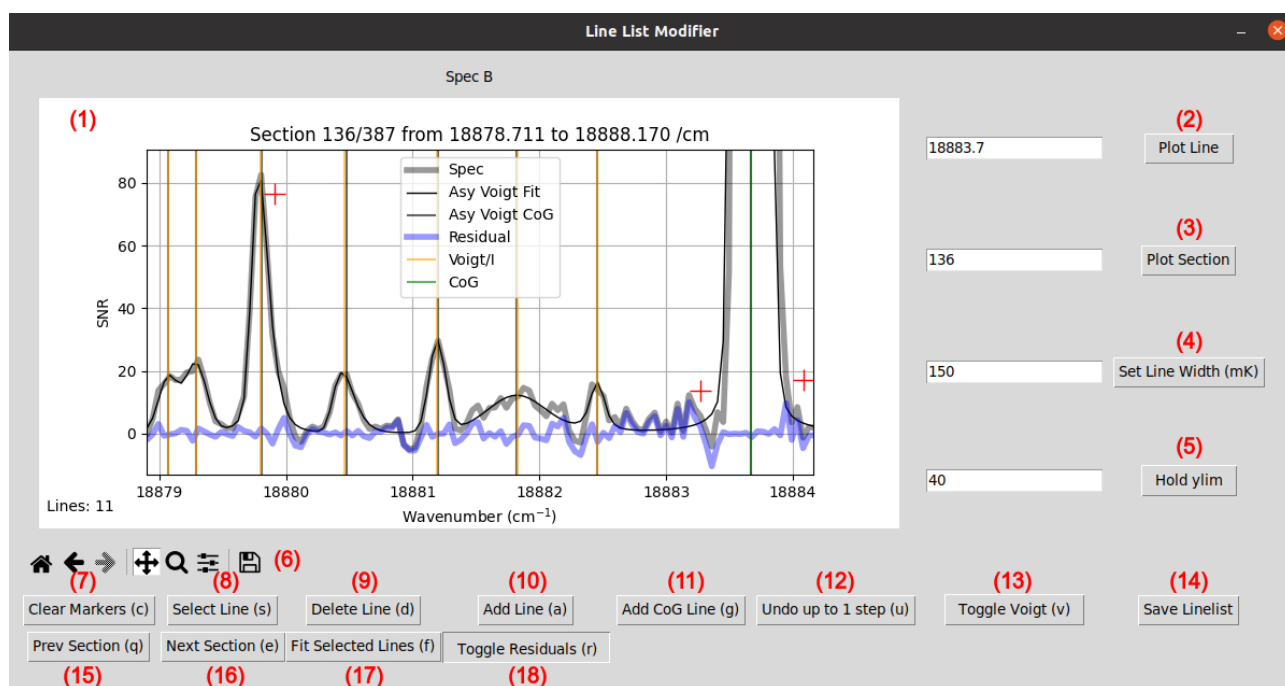


Figure B.1: Graphical user interface of the line fitting program used to alter the line list during the analysis of Nd III atomic structure.

A spectrum fitting program was created in Python to optimise the workflow of an evolving line list of the Nd-Ar PDL FT spectra (subsection 5.3.6). The graphical user interface is shown again in Figure B.1, the functionalities are explained as follows:

- (1) The default *matplotlib* plotting interface, showing the spectrum in grey, fitted spectrum

using the asymmetric Voigt profiles in black, and the residuals in blue. The vertical yellow lines are wavenumbers fitted using Voigt profiles using *XGREMLIN* [122], the vertical black lines (very close to the yellow lines) are wavenumbers fitted using the asymmetric Voigt profiles, and the vertical green lines are wavenumbers fitted using the COG method, which are treated as Voigt profiles in the fitted spectrum and residuals arrays.

- (2) Upon entering a float value and clicking the button, the line (currently in the line list) with the closest wavenumber to that value will be plotted in (1). This will change the spectrum accordingly if the entered value lies outside the currently plotted spectrum.
- (3) Upon entering an integer value and clicking the button, the corresponding section (see title of (1)) of the current spectrum will be plotted. The spectra were automatically divided into sections with around 10 to 20 lines per section, as fitting more than these numbers of lines at a time proved challenging for the *scipy.optimize.curve_fit* function, e.g., unfeasible convergence rates due to too many parameters.
- (4) The FWHM of the new line to be added to and fitted for the line list, in units of mK which is 10^{-3} cm^{-1} .
- (5) Toggle whether to plot at a maximum SNR (y-axis) when switching between sections or lines. This is useful when investigating the weak and blended lines.
- (6) Default *matplotlib* buttons for (1). The currently selected cross button is essentially the only button used, which allows convenient dragging (left click hold) and squeezing/stretching (right click hold) of the view.
- (7)-(18) Any letters in parentheses are keyboard shortcuts.
- (7) Markers are red crosses, which are created with a mouse click within (1), there are currently three markers. This button removes all markers.
- (8) All lines in the line list closest to each of the markers will be selected. Selected lines will have red vertical lines, and multiple selections of one line will be automatically prevented.
- (9) All selected lines will be removed from the line list, and the fit and residual curves of (1) are updated.

- (10) Lines will be added to all marker positions using the markers' wavenumbers (x values), SNRs (y values), and the width in (4), and the fit and residual curves of (1) are updated. These will show in the line list as not fitted but will provide initial values for the fit.
- (11) Add a COG fitted line to the line list using two markers, e.g., the two markers around 18883.7 cm^{-1} in [Figure B.1](#). The fit and residual curves of (1) are updated. The COG fitting was done using cubic spline interpolation to allow more reasonable wavenumber limits, e.g., the optimal wavenumber limits in a slightly blended line may lie in between the data points allowed by spectral resolution.
- (12) Reverse the latest change of the line list. Plots in (1) are updated accordingly.
- (13) Toggling whether to fix a of [Equation 5.2](#) at zero in the fit. This is particularly useful when fitting weaker lines and blends, e.g., an asymmetric line profile could be a blend rather than due to isotope shifts.
- (14) Save all changes to the line list. The line list itself is stored as a .csv file (5.6 MB for about 20 000 lines) and handled by *pandas*.
- (15) Plot the previous section, which allows the modification of the line list in that spectral region.
- (16) Plot the next section, which allows the modification of the line list in that spectral region.
- (17) All selected lines are fitted. Not selected lines will not be fitted. This functionality is quite useful in fitting blends as often the weaker lines of blends require more human intervention.
- (18) Toggle the residual curve of (1), as the plot can get crowded.

Appendix C

Nd III Energy Levels Experimentally Identified

Please refer to the published Nd III line and level lists for final results that are also machine-readable [96, 160]. Most energy levels in this appendix are final, and the table can be viewed as a record that led to the final results.

All 258 identified energy levels of Nd III are presented in Table C.1, 219 of these levels were identified for the first time, and 39 previously identified levels were confirmed. The first 3 columns of the table are the configuration, term, and J value assignments for the level, parent terms of the $4f^3$ core electrons are in parentheses, any number following a term symbol is used to distinguish recurrent terms of equivalent electrons, and a $^\circ$ following a term symbol indicates a term of odd parity. The fourth column is the optimised energy and its associated uncertainty in parentheses in units represented by the final decimal place of the energy value, the fifth column lists the number of lines used to optimise energy for each level in the Nd-Ar PDL FT spectra, the number in parentheses is the number of blended or weak lines weighted zero in the level energy optimisation. The sixth and seventh columns are the differences between observed and calculated values of the present work using the parameterized Cowan code and of Gaigalas et al. (2019) [81] respectively (some $4f^35f$ levels are missing values in this column because they could not be compared [138], likely due to the missing eigenvector composition data of Gaigalas et al. (2019) [81]). The remaining columns list the Landé g -factors and three leading eigenvector percentages calculated using the Cowan code in this work.

Table C.1: Observed Nd III Energy Levels

Assignment			Energy	N	ΔE_1	ΔE_2	g_J	Eigenvector Composition		
Conf.	Term	J	(cm^{-1})			(cm^{-1})		(%)		
$4f^4$	5I	4	0.000(0)	22(5)	-8	0	0.604	97 $4f^4$ 5I	1 $4f^4$ 3H4	1 $4f^4$ 3H3
		5	1137.794(2)	31(7)	-3	65	0.901	98 $4f^4$ 5I	1 $4f^4$ 3H4	
		6	2387.544(2)	34(7)	-4	124	1.071	99 $4f^4$ 5I		
		7	3714.548(2)	29(6)	-12	172	1.177	98 $4f^4$ 5I	1 $4f^4$ 3K2	
		8	5093.257(3)	17(4)	-23	209	1.247	96 $4f^4$ 5I	2 $4f^4$ 3K2	1 $4f^4$ 3K1
$4f^4$	5F	2	10773.962(12)	4(3)	26	-1325	1.007	93 $4f^4$ 5F	3 $4f^4$ 3D1	1 $4f^4$ 3D2
		3	11424.605(7)	9(1)	23	-1300	1.244	95 $4f^4$ 5F	1 $4f^4$ 3D1	1 $4f^4$ 3F3
		4	12181.327(5)	13(2)	32	-1279	1.330	92 $4f^4$ 5F	3 $4f^4$ 3G2	1 $4f^4$ 3F3
		5	13210.278(6)	10(4)	41	-1234	1.387	93 $4f^4$ 5F	3 $4f^4$ 3G2	1 $4f^4$ 3G1
$4f^4$	3K2	6	14064.277(4)	8(3)	-26	-1002	0.860	78 $4f^4$ 3K2	20 $4f^4$ 3K1	
		7	15153.807(5)	11(3)	2	-1027	1.005	69 $4f^4$ 3K2	18 $4f^4$ 3K1	11 $4f^4$ 3L
		8	16459.136(6)	8(5)	66	-1007	1.105	63 $4f^4$ 3K2	14 $4f^4$ 3K1	11 $4f^4$ 3L
$4f^4$	5G	3	15349.601(4)	5(3)	-1	-2018	0.885	73 $4f^4$ 5G	14 $4f^4$ 3G2	7 $4f^4$ 3G3
		4	16831.344(9)	5(3)	-75	-1944	1.051	69 $4f^4$ 5G	13 $4f^4$ 3H4	10 $4f^4$ 3H3
		5	18313.004(4)	7(3)	-26	-1825	1.167	57 $4f^4$ 5G	18 $4f^4$ 3H4	17 $4f^4$ 3H3
$4f^4$	3H4	5	16622.337(5)	7(1)	-11	-1316	1.157	36 $4f^4$ 5G	21 $4f^4$ 3H4	13 $4f^4$ 3H3
$4f^3(4I^\circ)5d$	$^5L^\circ$	6	15158.154(7)	2(0)	-52	-100	0.724	93 $(4I^\circ)5d$ $^5L^\circ$	3 $(^2H2^\circ)5d$ $^3K^\circ$	3 $(4I^\circ)5d$ $^3K^\circ$
		7	16952.835(8)	2(0)	-29	-32	0.914	97 $(4I^\circ)5d$ $^5L^\circ$	2 $(^2H2^\circ)5d$ $^3K^\circ$	1 $(4I^\circ)5d$ $^3K^\circ$
		8	18861.064(7)	4(1)	-12	26	1.043	99 $(4I^\circ)5d$ $^5L^\circ$	1 $(^2H2^\circ)5d$ $^3K^\circ$	
		9	20859.732(8)	2(0)	1	74	1.133	99 $(4I^\circ)5d$ $^5L^\circ$		
		10	22932.276(9)	1(0)	11	61	1.200	99 $(4I^\circ)5d$ $^5L^\circ$	1 $(^2K^\circ)5d$ $^3M^\circ$	
$4f^3(4I^\circ)5d$	$^5K^\circ$	5	15262.437(3)	5(0)	17	134	0.688	87 $(4I^\circ)5d$ $^5K^\circ$	8 $(4I^\circ)5d$ $^3I^\circ$	3 $(^2H2^\circ)5d$ $^3I^\circ$
		6	16938.068(7)	5(1)	36	217	0.912	94 $(4I^\circ)5d$ $^5K^\circ$	4 $(4I^\circ)5d$ $^3I^\circ$	2 $(^2H2^\circ)5d$ $^3I^\circ$
		7	18656.272(3)	7(0)	46	273	1.054	97 $(4I^\circ)5d$ $^5K^\circ$	1 $(4I^\circ)5d$ $^3I^\circ$	1 $(^2H2^\circ)5d$ $^3I^\circ$
		8	20410.897(3)	7(0)	49	306	1.150	97 $(4I^\circ)5d$ $^5K^\circ$	1 $(4I^\circ)5d$ $^3L^\circ$	1 $(^2K^\circ)5d$ $^3L^\circ$
		9	22197.115(3)	5(1)	44	315	1.218	96 $(4I^\circ)5d$ $^5K^\circ$	3 $(4I^\circ)5d$ $^3L^\circ$	2 $(^2K^\circ)5d$ $^3L^\circ$
$4f^3(4I^\circ)5d$	$^5I^\circ$	4	18883.669(2)	5(0)	76	170	0.634	83 $(4I^\circ)5d$ $^5I^\circ$	13 $(4I^\circ)5d$ $^3H^\circ$	1 $(4G^\circ)5d$ $^3H^\circ$
		5	20348.742(2)	7(0)	50	140	0.920	74 $(4I^\circ)5d$ $^5I^\circ$	12 $(4I^\circ)5d$ $^3H^\circ$	5 $(4I^\circ)5d$ $^3I^\circ$
		6	21980.522(3)	5(1)	24	136	1.081	68 $(4I^\circ)5d$ $^5I^\circ$	11 $(4I^\circ)5d$ $^3I^\circ$	8 $(4I^\circ)5d$ $^3H^\circ$
		7	22702.777(3)	12(0)	36	204	1.150	58 $(4I^\circ)5d$ $^5I^\circ$	21 $(4I^\circ)5d$ $^3I^\circ$	12 $(4I^\circ)5d$ $^3K^\circ$
$4f^3(4I^\circ)5d$	$^5H^\circ$	8	24592.259(3)	7(0)	16	291	1.231	85 $(4I^\circ)5d$ $^5I^\circ$	12 $(4I^\circ)5d$ $^3K^\circ$	2 $(^2K^\circ)5d$ $^3K^\circ$
		3	19593.094(4)	3(1)	-15	-160	0.591	62 $(4I^\circ)5d$ $^5H^\circ$	22 $(4I^\circ)5d$ $^3G^\circ$	5 $(4F^\circ)5d$ $^5H^\circ$
		4	20388.995(2)	6(0)	-67	-76	0.836	43 $(4I^\circ)5d$ $^5H^\circ$	32 $(4I^\circ)5d$ $^3H^\circ$	9 $(4I^\circ)5d$ $^5I^\circ$
		5	22181.299(11)	4(1)	-43	62	1.035	56 $(4I^\circ)5d$ $^5H^\circ$	16 $(4I^\circ)5d$ $^3I^\circ$	11 $(4I^\circ)5d$ $^3H^\circ$
		6	24058.518(3)	5(0)	-48	66	1.128	50 $(4I^\circ)5d$ $^5H^\circ$	26 $(4I^\circ)5d$ $^3I^\circ$	5 $(4I^\circ)5d$ $^3K^\circ$
$4f^3(4I^\circ)5d$	$^3I^\circ$	7	26097.906(4)	7(2)	-56	76	1.193	46 $(4I^\circ)5d$ $^5H^\circ$	28 $(4I^\circ)5d$ $^3I^\circ$	13 $(4I^\circ)5d$ $^3K^\circ$
		5	19616.622(2)	5(0)	-17	-5	0.865	54 $(4I^\circ)5d$ $^3I^\circ$	17 $(4I^\circ)5d$ $^5I^\circ$	9 $(4I^\circ)5d$ $^5K^\circ$
		6	20799.349(3)	8(3)	0	22	1.026	40 $(4I^\circ)5d$ $^3I^\circ$	26 $(4I^\circ)5d$ $^5I^\circ$	11 $(4I^\circ)5d$ $^3K^\circ$
$4f^3(4I^\circ)5d$	$^5G^\circ$	7	24003.225(3)	8(1)	10	61	1.171	37 $(4I^\circ)5d$ $^3I^\circ$	33 $(4I^\circ)5d$ $^5I^\circ$	16 $(4I^\circ)5d$ $^5H^\circ$
		2	21477.328(8)	1(0)	7	-9	0.344	93 $(4I^\circ)5d$ $^5G^\circ$	3 $(^2H2^\circ)5d$ $^3F^\circ$	3 $(4G^\circ)5d$ $^5G^\circ$
		3	21479.404(2)	4(0)	1	-112	0.800	54 $(4I^\circ)5d$ $^5G^\circ$	20 $(4I^\circ)5d$ $^5H^\circ$	19 $(4I^\circ)5d$ $^3G^\circ$
		4	23010.450(9)	5(2)	-2	-55	1.030	55 $(4I^\circ)5d$ $^5G^\circ$	17 $(4I^\circ)5d$ $^3H^\circ$	12 $(4I^\circ)5d$ $^5H^\circ$
		5	24878.412(10)	5(1)	-14	-61	1.148	47 $(4I^\circ)5d$ $^5G^\circ$	29 $(4I^\circ)5d$ $^3H^\circ$	7 $(4I^\circ)5d$ $^5H^\circ$
		6	26670.461(7)	6(1)	-29	-150	1.243	48 $(4I^\circ)5d$ $^5G^\circ$	26 $(4I^\circ)5d$ $^3H^\circ$	6 $(4G^\circ)5d$ $^3H^\circ$

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Table C.1: Observed Nd III Energy Levels (continued)

Assignment			Energy (cm ⁻¹)	<i>N</i>	$\Delta E_1 \ \Delta E_2$		<i>g</i>	Eigenvector Composition		
Conf.	Term	<i>J</i>			(cm ⁻¹)			(%)		
4f ³ (⁴ I°)5d	³ H°	4	21491.882(3)	6(1)	11	-201	0.952	31 (⁴ I°)5d ⁵ H°	20 (⁴ I°)5d ³ G°	19 (⁴ I°)5d ⁵ G°
		5	23347.721(3)	5(0)	14	-126	1.149	37 (⁴ I°)5d ⁵ G°	20 (⁴ I°)5d ⁵ H°	18 (⁴ I°)5d ³ H°
		6	25034.832(6)	6(3)	-30	-127	1.244	43 (⁴ I°)5d ⁵ G°	23 (⁴ I°)5d ³ H°	16 (⁴ I°)5d ⁵ H°
4f ³ (⁴ I°)5d	³ K°	6	23120.073(4)	7(1)	-37	-52	0.931	57 (⁴ I°)5d ³ K°	12 (⁴ I°)5d ⁵ H°	8 (² H2°)5d ³ K°
		7	25319.579(6)	5(2)	-21	21	1.096	51 (⁴ I°)5d ³ K°	25 (⁴ I°)5d ⁵ H°	8 (² H2°)5d ³ K°
		8	27441.911(4)	5(0)	14	-23	1.138	69 (⁴ I°)5d ³ K°	12 (⁴ I°)5d ⁵ I°	11 (² H2°)5d ³ K°
4f ³ (⁴ I°)5d	³ G°	3	23891.226(4)	3(0)	11	-300	0.796	48 (⁴ I°)5d ³ G°	36 (⁴ I°)5d ⁵ G°	8 (⁴ I°)5d ⁵ H°
		4	26140.225(8)	4(2)	10	-382	1.060	66 (⁴ I°)5d ³ G°	20 (⁴ I°)5d ⁵ G°	5 (⁴ I°)5d ⁵ H°
		5	28440.047(5)	3(0)	-4	-489	1.194	77 (⁴ I°)5d ³ G°	8 (⁴ I°)5d ⁵ G°	3 (⁴ F°)5d ³ G°
4f ³ (⁴ I°)5d	³ L°	7	24497.165(5)	4(1)	-29	-454	0.891	82 (⁴ I°)5d ³ L°	7 (² K°)5d ³ L°	3 (⁴ I°)5d ³ K°
		8	26676.685(8)	5(2)	1	-443	1.019	85 (⁴ I°)5d ³ L°	7 (² K°)5d ³ L°	2 (⁴ I°)5d ⁵ K°
		9	28877.321(7)	3(0)	21	-454	1.113	84 (⁴ I°)5d ³ L°	8 (² K°)5d ³ L°	4 (⁴ I°)5d ⁵ K°
4f ³ (⁴ F°)5d	⁵ H°	3	27675.024(2)	1(0)	-55	-1819	0.589	77 (⁴ F°)5d ⁵ H°	6 (⁴ I°)5d ⁵ H°	4 (² D1°)5d ³ G°
		4	28745.307(3)	2(1)	-54	-1761	0.907	86 (⁴ F°)5d ⁵ H°	6 (⁴ I°)5d ⁵ H°	2 (² D1°)5d ³ G°
		5	30175.737(3)	7(0)	-52	-1676	1.040	52 (⁴ F°)5d ⁵ H°	10 (² H2°)5d ³ I°	5 (⁴ I°)6s ⁵ I°
		6	31146.457(3)	4(1)	-50	-1494	1.111	56 (⁴ F°)5d ⁵ H°	18 (² H2°)5d ³ K°	5 (⁴ I°)5d ⁵ H°
		7	32832.447(3)	5(2)	-17	-1401	1.142	41 (⁴ F°)5d ⁵ H°	33 (² H2°)5d ³ K°	7 (² K°)5d ³ K°
4f ³ (⁴ F°)5d	⁵ D°	3	28118.535(2)	2(0)	60	-1800	1.297	26 (⁴ F°)5d ⁵ D°	24 (⁴ S°)5d ⁵ D°	9 (⁴ F°)5d ⁵ H°
4f ³ (⁴ F°)5d	⁵ F°	2	31888.511(7)	3(1)	-41	-2129	1.057	75 (⁴ F°)5d ⁵ F°	6 (⁴ F°)5d ³ P°	5 (⁴ S°)5d ³ D°
		3	32489.101(7)	5(4)	-12	-2131	1.227	69 (⁴ F°)5d ⁵ F°	7 (⁴ S°)5d ³ D°	3 (⁴ F°)5d ⁵ D°
		4	33603.488(6)	6(0)	60	-2264	1.121	48 (⁴ F°)5d ⁵ F°	18 (² H2°)5d ³ H°	6 (² G1°)5d ³ H°
		5	34511.186(7)	4(1)	-35	-2116	1.237	54 (⁴ F°)5d ⁵ F°	13 (² H2°)5d ¹ H°	7 (⁴ G°)5d ⁵ I°
		6	35154.437(5)	4(0)	56	-1536	1.116	21 (⁴ G°)5d ⁵ I°	20 (⁴ F°)5d ³ H°	9 (² H2°)5d ³ H°
4f ³ (⁴ F°)5d	⁵ G°	6	33210.660(12)	5(3)	-36	-1579	1.129	34 (² H2°)5d ³ I°	34 (⁴ F°)5d ⁵ G°	7 (² H1°)5d ³ I°
4f ³ (² H2°)5d	³ I°	5	29397.423(3)	6(1)	-113	-1501	0.995	32 (⁴ F°)5d ⁵ H°	16 (² H2°)5d ³ I°	7 (² G1°)5d ³ I°
		7	35188.278(12)	4(2)	-9	-969	1.136	54 (² H2°)5d ³ I°	13 (² H1°)5d ³ I°	4 (² G1°)5d ³ I°
4f ³ (² H2°)5d	³ K°	6	29643.186(3)	5(1)	8	-1212	0.994	22 (² H2°)5d ³ K°	15 (⁴ I°)5d ³ K°	8 (² H2°)5d ¹ I°
		7	31781.802(6)	5(1)	9	-1352	1.154	37 (⁴ F°)5d ⁵ H°	23 (² H2°)5d ³ K°	9 (² G1°)5d ³ I°
		8	34534.549(7)	3(0)	-0	-1188	1.129	58 (² H2°)5d ³ K°	12 (² K°)5d ³ K°	9 (⁴ I°)5d ³ K°
4f ³ (² H2°)5d	¹ H°	5	32605.894(7)	10(6)	37	-1372	1.071	14 (² H2°)5d ¹ H°	11 (⁴ F°)5d ⁵ F°	9 (² H2°)5d ³ H°
4f ³ (² H2°)5d	¹ I°	6	32823.701(6)	3(0)	32	-1331	1.079	26 (² H2°)5d ¹ I°	19 (⁴ F°)5d ⁵ G°	13 (² H2°)5d ³ I°
4f ³ (² H2°)5d	³ G°	4	33135.917(5)	6(1)	-38	-2324	1.043	27 (⁴ F°)5d ⁵ F°	14 (² H2°)5d ³ G°	13 (⁴ G°)5d ⁵ I°
4f ³ (² H2°)5d	³ H°	5	34994.015(6)	5(1)	-22	-1995	1.100	23 (² H2°)5d ³ H°	11 (⁴ F°)5d ³ H°	10 (² H2°)5d ³ G°
4f ³ (² H2°)5d	¹ G°	4	36517.350(4)	6(3)	-36	-2641	1.054	32 (⁴ G°)5d ⁵ G°	26 (⁴ G°)5d ⁵ H°	9 (² H2°)5d ¹ G°
4f ³ (² G1°)5d	³ H°	6	31559.217(3)	6(3)	48	-1402	1.120	20 (⁴ F°)5d ⁵ G°	18 (⁴ F°)5d ⁵ H°	16 (² H2°)5d ³ K°
4f ³ (² G1°)5d	³ G°	3	34856.862(4)	3(2)	-20	-2332	0.780	29 (⁴ G°)5d ⁵ H°	16 (² G1°)5d ³ G°	15 (⁴ G°)5d ⁵ G°
4f ³ (⁴ S°)5d	⁵ D°	1	32374.355(13)	1(0)	-15	-1850	1.036	37 (⁴ S°)5d ⁵ D°	12 (⁴ F°)5d ⁵ D°	11 (⁴ S°)5d ³ D°
		2	32905.369(7)	2(1)	24	-1671	1.322	37 (⁴ S°)5d ⁵ D°	29 (⁴ F°)5d ⁵ D°	11 (² H2°)5d ³ F°
		3	33400.822(5)	2(0)	23	-1705	1.374	33 (⁴ S°)5d ⁵ D°	29 (⁴ F°)5d ⁵ D°	7 (⁴ G°)5d ⁵ D°
		4	34419.877(6)	2(0)	65	-1826	1.352	29 (² H2°)5d ³ F°	27 (⁴ S°)5d ⁵ D°	15 (⁴ F°)5d ⁵ D°
4f ³ (⁴ G°)5d	⁵ I°	4	32829.311(5)	2(0)	1	-2053	0.786	61 (⁴ G°)5d ⁵ I°	6 (⁴ F°)5d ³ F°	5 (⁴ G°)5d ³ F°
		5	34017.306(4)	4(1)	36	-2323	0.944	76 (⁴ G°)5d ⁵ I°	8 (⁴ F°)5d ⁵ F°	5 (² H2°)5d ³ I°
		6	35549.565(4)	3(0)	16	-2719	1.100	57 (⁴ G°)5d ⁵ I°	12 (⁴ F°)5d ³ H°	5 (⁴ F°)5d ⁵ G°
		7	36890.347(8)	8(3)	42	-3010	1.146	44 (⁴ G°)5d ⁵ I°	43 (⁴ I°)6s ³ I°	4 (² K°)5d ³ K°

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Table C.1: Observed Nd III Energy Levels (continued)

Assignment			Energy	N	ΔE_1	ΔE_2	g	Eigenvector Composition		
Conf.	Term	J	(cm ⁻¹)			(cm ⁻¹)		(%)		
4f ³ (⁴ G°)5d	⁵ H°	8	38517.773(5)	3(1)	14	-2845	1.193	65 (⁴ G°)5d ⁵ I°	21 (² K°)5d ³ K°	5 (² K°)5d ³ L°
		3	35576.326(4)	2(0)	53	-2129	0.692	48 (⁴ G°)5d ⁵ H°	25 (⁴ G°)5d ⁵ G°	9 (⁴ F°)5d ³ G°
		4	36235.179(4)	3(1)	-29	-1689	1.005	33 (⁴ G°)5d ⁵ H°	8 (² H2°)5d ³ F°	7 (² H2°)5d ³ G°
		5	37592.759(3)	5(1)	-28	-3092	1.109	67 (⁴ G°)5d ⁵ H°	14 (⁴ G°)5d ⁵ G°	4 (⁴ F°)5d ³ H°
		6	39058.274(4)	4(0)	68	-2695	1.189	62 (⁴ G°)5d ⁵ H°	11 (⁴ G°)5d ⁵ G°	4 (² H2°)5d ³ I°
4f ³ (⁴ G°)5d	⁵ G°	7	40505.082(5)	3(1)	134	-2793	1.210	55 (⁴ G°)5d ⁵ H°	11 (⁴ G°)5d ³ I°	11 (² K°)5d ³ I°
		4	36572.870(4)	3(1)	-15	-3016	1.069	35 (⁴ G°)5d ⁵ G°	23 (⁴ G°)5d ⁵ H°	6 (² G1°)5d ³ G°
		5	37977.641(4)	6(1)	-37	-2649	1.208	50 (⁴ G°)5d ⁵ G°	8 (⁴ G°)5d ⁵ H°	4 (² H2°)5d ³ H°
4f ³ (⁴ G°)5d	³ I°	6	39611.389(5)	3(0)	-45	-2897	1.223	45 (⁴ G°)5d ⁵ G°	18 (⁴ G°)5d ⁵ H°	5 (² K°)5d ¹ I°
		6	44609.232(5)	2(0)	21	-3380	1.018	34 (⁴ G°)5d ³ I°	16 (² K°)5d ³ I°	7 (² H1°)5d ³ I°
4f ³ (² K°)5d	³ I°	7	45592.778(7)	1(0)	-28	-3468	1.117	41 (⁴ G°)5d ³ I°	18 (² K°)5d ³ I°	7 (² I°)5d ³ K°
		7	41260.027(4)	3(0)	17	-2715	1.173	49 (² K°)5d ³ I°	26 (⁴ G°)5d ⁵ H°	8 (⁴ G°)5d ³ I°
4f ³ (⁴ D°)5d	⁵ F°	4	47404.355(8)	3(0)	-35	-5744	1.217	47 (⁴ D°)5d ⁵ F°	18 (⁴ D°)5d ⁵ G°	8 (² D1°)5d ¹ G°
4f ³ (⁴ I°)6s	(⁹ / ₂ , ¹ / ₂)°	4	29873.222(6)	5(1)	15	-1108	0.607	96 (⁴ I°)6s (⁹ / ₂ , ¹ / ₂)°	2 (² H°)6s (⁹ / ₂ , ¹ / ₂)°	1 (⁴ G°)5d (⁵ / ₂ , ³ / ₂)°
		5	30593.085(5)	7(0)	25	-999	0.903	74 (⁴ I°)6s (⁹ / ₂ , ¹ / ₂)°	12 (⁴ I°)6s (¹¹ / ₂ , ¹ / ₂)°	3 (⁴ F°)5d (⁵ / ₂ , ⁵ / ₂)°
4f ³ (⁴ I°)6s	(¹¹ / ₂ , ¹ / ₂)°	6	32075.658(8)	6(0)	-23	-1056	1.063	90 (⁴ I°)6s (¹¹ / ₂ , ¹ / ₂)°	6 (⁴ I°)6s (¹³ / ₂ , ¹ / ₂)°	1 (² H°)5d (¹¹ / ₂ , ³ / ₂)°
		5	32309.729(9)	7(4)	-64	-930	0.873	81 (⁴ I°)6s (¹¹ / ₂ , ¹ / ₂)°	11 (⁴ I°)6s (⁹ / ₂ , ¹ / ₂)°	1 (² H°)5d (⁹ / ₂ , ⁵ / ₂)°
4f ³ (⁴ I°)6s	(¹³ / ₂ , ¹ / ₂)°	7	33906.143(8)	6(1)	-2	-1028	1.174	95 (⁴ I°)6s (¹³ / ₂ , ¹ / ₂)°	3 (⁴ I°)6s (¹⁵ / ₂ , ¹ / ₂)°	
		6	34687.230(7)	4(0)	28	-993	1.035	85 (⁴ I°)6s (¹³ / ₂ , ¹ / ₂)°	7 (⁴ I°)6s (¹¹ / ₂ , ¹ / ₂)°	3 (⁴ G°)5d (⁹ / ₂ , ³ / ₂)°
4f ³ (⁴ I°)6s	(¹⁵ / ₂ , ¹ / ₂)°	8	35839.828(11)	5(2)	7	-1028	1.248	98 (⁴ I°)6s (¹⁵ / ₂ , ¹ / ₂)°	1 (² K°)6s (¹⁵ / ₂ , ¹ / ₂)°	
		7	37089.599(6)	8(3)	-3	-832	1.148	50 (⁴ I°)6s (¹⁵ / ₂ , ¹ / ₂)°	27 (⁴ G°)5d (⁹ / ₂ , ⁵ / ₂)°	8 (⁴ G°)5d (¹¹ / ₂ , ³ / ₂)°
4f ³ (⁴ I°)6p	⁵ K	5	60526.067(5)	14(0)	14	321	0.719	71 (⁴ I°)6p ⁵ K	22 (⁴ I°)6p ³ I	3 (⁴ I°)6p ⁵ I
		6	62520.646(5)	15(0)	21	358	0.941	67 (⁴ I°)6p ⁵ K	17 (⁴ I°)6p ³ I	9 (⁴ I°)6p ⁵ I
		7	64622.006(5)	15(2)	12	373	1.083	57 (⁴ I°)6p ⁵ K	20 (⁴ I°)6p ⁵ I	12 (⁴ I°)6p ³ K
		8	68302.664(7)	11(0)	18	524	1.168	62 (⁴ I°)6p ⁵ K	21 (⁴ I°)6p ⁵ I	17 (⁴ I°)6p ³ K
		9	70141.009(8)	6(0)	9	483	1.221	99 (⁴ I°)6p ⁵ K	1 (² K°)6p ³ L	
4f ³ (⁴ I°)6p	⁵ I	4	60638.963(4)	15(2)	-95	207	0.711	50 (⁴ I°)6p ⁵ I	36 (⁴ I°)6p ³ H	9 (⁴ I°)6p ⁵ H
		5	62640.266(4)	14(1)	89	411	0.977	48 (⁴ I°)6p ⁵ I	26 (⁴ I°)6p ³ H	20 (⁴ I°)6p ⁵ H
		6	64549.620(4)	11(0)	26	383	1.119	47 (⁴ I°)6p ⁵ I	31 (⁴ I°)6p ⁵ H	13 (⁴ I°)6p ³ H
		7	66497.225(6)	18(3)	15	509	1.122	41 (⁴ I°)6p ⁵ I	28 (⁴ I°)6p ⁵ K	19 (⁴ I°)6p ³ K
		8	66792.024(6)	17(3)	-8	368	1.182	37 (⁴ I°)6p ⁵ K	37 (⁴ I°)6p ⁵ I	24 (⁴ I°)6p ³ K
4f ³ (⁴ I°)6p	⁵ H	4	64243.914(5)	17(1)	10	494	0.752	42 (⁴ I°)6p ⁵ I	32 (⁴ I°)6p ⁵ H	23 (⁴ I°)6p ³ H
		3	64347.699(7)	9(0)	-26	443	0.507	96 (⁴ I°)6p ⁵ H	3 (² H2°)6p ³ G	1 (⁴ G°)6p ⁵ H
		6	65023.633(5)	17(1)	-7	542	0.950	40 (⁴ I°)6p ³ K	24 (⁴ I°)6p ⁵ K	16 (⁴ I°)6p ³ I
		5	66272.802(7)	12(0)	11	562	0.954	37 (⁴ I°)6p ⁵ H	34 (⁴ I°)6p ³ I	18 (⁴ I°)6p ⁵ I
		7	66717.513(6)	18(2)	-9	379	1.191	49 (⁴ I°)6p ⁵ H	27 (⁴ I°)6p ³ I	12 (⁴ I°)6p ⁵ K
4f ³ (⁴ I°)6p	³ I	5	64350.812(5)	18(0)	16	525	0.850	36 (⁴ I°)6p ³ I	25 (⁴ I°)6p ⁵ I	22 (⁴ I°)6p ⁵ K
		6	68347.584(6)	14(2)	2	557	1.091	49 (⁴ I°)6p ³ I	36 (⁴ I°)6p ⁵ H	8 (⁴ I°)6p ⁵ I
		7	70460.602(7)	14(3)	-14	548	1.186	59 (⁴ I°)6p ³ I	32 (⁴ I°)6p ⁵ H	3 (⁴ I°)6p ⁵ I
4f ³ (⁴ I°)6p	³ H	4	66445.159(7)	13(1)	3	519	0.851	56 (⁴ I°)6p ⁵ H	37 (⁴ I°)6p ³ H	4 (⁴ I°)6p ⁵ I
		5	68613.221(8)	11(0)	9	553	1.046	61 (⁴ I°)6p ³ H	32 (⁴ I°)6p ⁵ H	3 (⁴ I°)6p ⁵ I
		6	70826.009(8)	13(1)	-1	573	1.167	79 (⁴ I°)6p ³ H	14 (⁴ I°)6p ⁵ H	2 (⁴ I°)6p ³ I
4f ³ (⁴ I°)6p	³ K	6	66451.812(6)	14(1)	-4	575	0.973	47 (⁴ I°)6p ³ K	28 (⁴ I°)6p ⁵ I	9 (⁴ I°)6p ⁵ H
		7	68507.387(6)	13(0)	-11	592	1.094	55 (⁴ I°)6p ³ K	34 (⁴ I°)6p ⁵ I	7 (⁴ I°)6p ⁵ H
		8	70599.570(7)	16(0)	-23	591	1.176	57 (⁴ I°)6p ³ K	41 (⁴ I°)6p ⁵ I	1 (² K°)6p ¹ L

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Table C.1: Observed Nd III Energy Levels (continued)

Assignment			Energy (cm ⁻¹)	N	ΔE_1 (cm ⁻¹)	ΔE_2 (cm ⁻¹)	g	Eigenvector Composition		
Conf.	Term	J						(%)		
4f ³ (⁴ F°)6p	⁵ G	2	72088.930(17)	1(0)	-22	-1959	0.427	77 (⁴ F°)6p ⁵ G	14 (⁴ F°)6p ³ F	4 (² D1°)6p ³ F
		3	73201.950(28)	1(0)	-11	-1919	0.947	73 (⁴ F°)6p ⁵ G	12 (⁴ F°)6p ³ F	6 (⁴ F°)6p ³ G
		4	74258.973(22)	2(0)	-8	-1861	1.112	47 (⁴ F°)6p ⁵ G	15 (⁴ F°)6p ³ G	8 4f ⁴ ¹ G3
		5	75579.962(31)	1(0)	-41	-1661	1.175	30 (⁴ F°)6p ⁵ G	26 (⁴ F°)6p ³ G	16 (⁴ F°)6p ⁵ F
		6	78974.826(24)	1(0)	-17	-1467	1.217	61 (⁴ F°)6p ⁵ G	16 (² H2°)6p ¹ I	9 (² H2°)6p ³ I
4f ³ (² H2°)6p	³ I	5	73247.950(16)	2(0)	34	-1068	0.961	39 (² H2°)6p ³ I	10 (² H2°)6p ¹ H	6 (² H1°)6p ³ I
		6	76644.575(28)	1(0)	-59	-1037	1.053	54 (² H2°)6p ³ I	9 (² H1°)6p ³ I	8 (² H2°)6p ³ H
4f ³ (² H2°)6p	¹ I	6	77236.125(23)	3(1)	86	-938	1.129	34 (² H2°)6p ¹ I	19 (⁴ F°)6p ⁵ G	16 (² H2°)6p ³ H
4f ³ (⁴ I°)7s	(⁹ / ₂ , ¹ / ₂)°	4	103085.765(10)	5(0)	-6	-6606	0.605	97 (⁴ I°)7s (⁹ / ₂ , ¹ / ₂)°	3 (² H°)7s (⁹ / ₂ , ¹ / ₂)°	
		5	103335.469(8)	5(0)	-4	-6655	0.866	96 (⁴ I°)7s (⁹ / ₂ , ¹ / ₂)°	3 (² H°)7s (⁹ / ₂ , ¹ / ₂)°	1 (⁴ I°)7s (¹¹ / ₂ , ¹ / ₂)°
4f ³ (⁴ I°)7s	(¹¹ / ₂ , ¹ / ₂)°	5	105124.885(11)	5(1)	7	-6621	0.873	98 (⁴ I°)7s (¹¹ / ₂ , ¹ / ₂)°	1 (⁴ I°)7s (⁹ / ₂ , ¹ / ₂)°	1 (² H°)7s (¹¹ / ₂ , ¹ / ₂)°
		6	105131.521(11)	8(2)	10	-6610	1.057	98 (⁴ I°)7s (¹¹ / ₂ , ¹ / ₂)°	1 (² H°)7s (¹¹ / ₂ , ¹ / ₂)°	1 (⁴ I°)7s (¹³ / ₂ , ¹ / ₂)°
4f ³ (⁴ I°)7s	(¹³ / ₂ , ¹ / ₂)°	7	107058.347(9)	5(0)	6	-6601	1.173	99 (⁴ I°)7s (¹³ / ₂ , ¹ / ₂)°		
		6	107232.851(13)	4(1)	5	-6646	1.039	99 (⁴ I°)7s (¹³ / ₂ , ¹ / ₂)°	1 (⁴ I°)7s (¹¹ / ₂ , ¹ / ₂)°	
4f ³ (⁴ I°)7s	(¹⁵ / ₂ , ¹ / ₂)°	8	109068.145(12)	6(0)	-8	-6619	1.249	99 (⁴ I°)7s (¹⁵ / ₂ , ¹ / ₂)°	1 (² K°)7s (¹⁵ / ₂ , ¹ / ₂)°	
		7	109390.838(12)	5(0)	-9	-6691	1.147	98 (⁴ I°)7s (¹⁵ / ₂ , ¹ / ₂)°	1 (² K°)7s (¹⁵ / ₂ , ¹ / ₂)°	
4f ³ (⁴ I°)6d	⁵ K°	5	103652.472(9)	3(1)	0	-6059	0.695	84 (⁴ I°)6d ⁵ K°	11 (⁴ I°)6d ³ I°	2 (² H2°)6d ³ I°
		6	104612.324(10)	4(0)	14	-6032	0.909	61 (⁴ I°)6d ⁵ K°	27 (⁴ I°)6d ³ K°	7 (⁴ I°)6d ⁵ I°
		7	106077.365(15)	4(0)	10	-6040	1.007	40 (⁴ I°)6d ⁵ K°	21 (⁴ I°)6d ³ K°	18 (⁴ I°)6d ⁵ L°
		8	107926.405(11)	6(0)	-1	-6045	1.134	66 (⁴ I°)6d ⁵ K°	13 (⁴ I°)6d ⁵ L°	10 (⁴ I°)6d ³ K°
		9	109832.461(10)	3(0)	-22	-6075	1.209	86 (⁴ I°)6d ⁵ K°	8 (⁴ I°)6d ⁵ L°	4 (⁴ I°)6d ³ L°
4f ³ (⁴ I°)6d	⁵ L°	6	103695.078(8)	3(0)	-1	-6104	0.728	91 (⁴ I°)6d ⁵ L°	4 (⁴ I°)6d ³ K°	3 (² H2°)6d ³ K°
		7	104797.903(7)	3(1)	12	-6075	0.916	70 (⁴ I°)6d ⁵ L°	20 (⁴ I°)6d ³ L°	7 (⁴ I°)6d ⁵ K°
		8	106410.353(9)	3(0)	15	-6063	1.048	78 (⁴ I°)6d ⁵ L°	13 (⁴ I°)6d ³ L°	8 (⁴ I°)6d ⁵ K°
		9	108209.894(9)	2(0)	6	-6075	1.137	88 (⁴ I°)6d ⁵ L°	6 (⁴ I°)6d ³ L°	6 (⁴ I°)6d ⁵ K°
		10	110125.394(9)	1(0)	-15	-6134	1.199	99 (⁴ I°)6d ⁵ L°	1 (² K°)6d ³ M°	
4f ³ (⁴ I°)6d	⁵ I°	4	104130.404(13)	4(1)	12	-6047	0.632	85 (⁴ I°)6d ⁵ I°	11 (⁴ I°)6d ³ H°	2 (² H2°)6d ³ H°
		5	106052.139(18)	3(1)	10	-6046	0.925	47 (⁴ I°)6d ⁵ I°	22 (⁴ I°)6d ³ H°	15 (⁴ I°)6d ³ I°
		7	107906.087(31)	4(3)	-2	-6043	1.127	43 (⁴ I°)6d ⁵ I°	19 (⁴ I°)6d ³ I°	18 (⁴ I°)6d ⁵ K°
		6	108026.950(14)	4(1)	-3	-6065	1.116	30 (⁴ I°)6d ⁵ I°	28 (⁴ I°)6d ⁵ H°	16 (⁴ I°)6d ³ H°
		8	109959.872(22)	5(3)	-20	-6068	1.222	76 (⁴ I°)6d ⁵ I°	10 (⁴ I°)6d ³ K°	10 (⁴ I°)6d ⁵ K°
4f ³ (⁴ I°)6d	⁵ H°	3	104379.920(110)	2(2)	7	-6106	0.573	72 (⁴ I°)6d ⁵ H°	24 (⁴ I°)6d ³ G°	2 (² H2°)6d ³ G°
		4	106265.687(12)	3(1)	5	-6108	0.995	33 (⁴ I°)6d ⁵ H°	32 (⁴ I°)6d ³ G°	24 (⁴ I°)6d ⁵ G°
		5	106560.907(10)	3(0)	4	-6055	1.025	54 (⁴ I°)6d ⁵ H°	26 (⁴ I°)6d ³ I°	8 (⁴ I°)6d ³ H°
		6	108568.311(12)	3(0)	-5	-6055	1.108	43 (⁴ I°)6d ⁵ H°	43 (⁴ I°)6d ³ I°	4 (⁴ I°)6d ³ K°
		7	110057.560(17)	2(0)	-23	-6097	1.231	60 (⁴ I°)6d ⁵ H°	19 (⁴ I°)6d ³ I°	16 (⁴ I°)6d ⁵ I°
4f ³ (⁴ I°)6d	³ I°	5	104560.563(11)	3(0)	1	-6050	0.885	42 (⁴ I°)6d ⁵ I°	40 (⁴ I°)6d ³ I°	7 (⁴ I°)6d ⁵ H°
		6	105866.787(12)	4(0)	7	-6043	0.967	31 (⁴ I°)6d ³ I°	26 (⁴ I°)6d ⁵ K°	19 (⁴ I°)6d ³ K°
		7	110669.386(15)	3(0)	-26	-6081	1.179	59 (⁴ I°)6d ³ I°	31 (⁴ I°)6d ⁵ H°	5 (⁴ I°)6d ³ K°
4f ³ (⁴ I°)6d	³ H°	4	104753.498(16)	2(0)	-1	-6083	0.875	46 (⁴ I°)6d ⁵ H°	39 (⁴ I°)6d ³ H°	7 (⁴ I°)6d ⁵ G°
		5	108852.966(10)	3(1)	-6	-6070	1.085	56 (⁴ I°)6d ³ H°	25 (⁴ I°)6d ⁵ G°	9 (⁴ I°)6d ⁵ H°
		6	111010.298(12)	2(0)	-24	-6097	1.183	73 (⁴ I°)6d ³ H°	14 (⁴ I°)6d ⁵ G°	5 (⁴ I°)6d ⁵ H°
4f ³ (⁴ I°)6d	⁵ G°	3	104793.195(13)	2(0)	-13	-6132	0.795	48 (⁴ I°)6d ⁵ G°	32 (⁴ I°)6d ³ G°	17 (⁴ I°)6d ⁵ H°
		2	104804.440(18)	1(0)	22	-6091	0.342	96 (⁴ I°)6d ⁵ G°	3 (² H2°)6d ³ F°	
		4	106757.677(11)	2(0)	-2	-6080	0.953	40 (⁴ I°)6d ⁵ G°	38 (⁴ I°)6d ³ H°	13 (⁴ I°)6d ⁵ H°

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Table C.1: Observed Nd III Energy Levels (continued)

Assignment			Energy (cm ⁻¹)	N	ΔE_1 (cm ⁻¹)	ΔE_2 (cm ⁻¹)	g	Eigenvector Composition		
Conf.	Term	J						(%)		
4f ³ (⁴ I°)6d	³ L°	7	106600.460(8)	3(0)	21	-6038	0.939	60 (⁴ I°)6d ³ L°	29 (⁴ I°)6d ⁵ K°	7 (⁴ I°)6d ⁵ L°
		8	108857.156(11)	2(0)	16	-6043	1.036	78 (⁴ I°)6d ³ L°	13 (⁴ I°)6d ⁵ K°	6 (⁴ I°)6d ⁵ L°
		9	111146.752(10)	2(0)	-1	-6072	1.118	89 (⁴ I°)6d ³ L°	7 (⁴ I°)6d ⁵ K°	3 (⁴ I°)6d ⁵ L°
4f ³ (⁴ I°)6d	³ K°	6	106603.805(13)	2(0)	23	-6011	0.978	43 (⁴ I°)6d ⁵ I°	41 (⁴ I°)6d ³ K°	6 (⁴ I°)6d ⁵ H°
		7	108729.681(12)	3(0)	20	-6011	1.068	59 (⁴ I°)6d ³ K°	30 (⁴ I°)6d ⁵ I°	3 (⁴ I°)6d ³ L°
		8	110926.461(13)	2(0)	2	-6040	1.140	76 (⁴ I°)6d ³ K°	16 (⁴ I°)6d ⁵ I°	3 (⁴ I°)6d ³ L°
4f ³ (⁴ I°)6d	³ G°	3	106853.659(11)	1(0)	27	-6077	0.813	49 (⁴ I°)6d ⁵ G°	41 (⁴ I°)6d ³ G°	8 (⁴ I°)6d ⁵ H°
		4	108951.734(15)	1(0)	-14	-6118	1.056	62 (⁴ I°)6d ³ G°	27 (⁴ I°)6d ⁵ G°	6 (⁴ I°)6d ⁵ H°
		5	111138.018(18)	1(0)	-31	-6149	1.196	79 (⁴ I°)6d ³ G°	12 (⁴ I°)6d ⁵ G°	4 (⁴ I°)6d ³ H°
4f ³ (⁴ I°)5f	⁵ M	7	114015.1(5)	2(1)	-2	-6866	0.767	89 (⁴ I°)5f ⁵ M	7 (⁴ I°)5f ⁵ L	3 (² H2°)5f ³ L
		8	114831.2(3)	3(0)	-7	-6875	0.928	62 (⁴ I°)5f ⁵ M	23 (⁴ I°)5f ³ M	10 (⁴ I°)5f ⁵ L
		9	116389.9(4)	2(0)	6	-6842	1.044	73 (⁴ I°)5f ⁵ M	14 (⁴ I°)5f ³ M	11 (⁴ I°)5f ⁵ L
		10	118152.2(4)	2(0)	8	-6879	1.123	85 (⁴ I°)5f ⁵ M	8 (⁴ I°)5f ⁵ L	7 (⁴ I°)5f ³ M
		11	120036.1(6)	1(0)	-1	-7401	1.181	99 (⁴ I°)5f ⁵ M	1 (² K°)5f ³ N	
4f ³ (⁴ I°)5f	⁵ L	6	114016.4(6)	1(0)	-20	-6812	0.748	81 (⁴ I°)5f ⁵ L	13 (⁴ I°)5f ⁵ K	2 (² H2°)5f ³ K
		7	114747.2(4)	3(0)	-8	-6826	0.927	48 (⁴ I°)5f ⁵ L	27 (⁴ I°)5f ³ L	16 (⁴ I°)5f ⁵ K
		8	116315.8(3)	4(0)	6	-6808	1.040	47 (⁴ I°)5f ⁵ L	18 (⁴ I°)5f ⁵ K	17 (⁴ I°)5f ³ L
		9	118088.7(3)	3(0)	4	-6805	1.131	62 (⁴ I°)5f ⁵ L	15 (⁴ I°)5f ⁵ K	14 (⁴ I°)5f ⁵ M
		10	120013.8(4)	3(0)	-5	-6862	1.191	89 (⁴ I°)5f ⁵ L	10 (⁴ I°)5f ⁵ M	1 (² K°)5f ³ M
4f ³ (⁴ I°)5f	⁵ K	5	114021.3(4)	2(0)	-18	-6808	0.701	81 (⁴ I°)5f ⁵ K	13 (⁴ I°)5f ³ I	2 (² H2°)5f ³ I
		6	114846.8(3)	4(0)	-1	-6815	0.904	47 (⁴ I°)5f ⁵ K	33 (⁴ I°)5f ³ K	6 (⁴ I°)5f ⁵ I
		7	116433.7(3)	4(0)	16	-6818	0.993	32 (⁴ I°)5f ⁵ L	28 (⁴ I°)5f ⁵ K	24 (⁴ I°)5f ³ K
		8	118199.5(3)	4(0)	18	-6746	1.125	61 (⁴ I°)5f ⁵ K	24 (⁴ I°)5f ⁵ L	9 (⁴ I°)5f ³ K
		9	119913.5(4)	3(0)	5		1.203	80 (⁴ I°)5f ⁵ K	18 (⁴ I°)5f ⁵ L	1 (² K°)5f ³ L
4f ³ (⁴ I°)5f	⁵ H	3	114190.1(4)	2(0)	5	-6801	0.551	82 (⁴ I°)5f ⁵ H	11 (⁴ I°)5f ³ G	3 (⁴ I°)5f ⁵ G
		4	114728.7(4)	3(1)	-12	-6793	0.888	72 (⁴ I°)5f ⁵ H	9 (⁴ I°)5f ⁵ I	8 (⁴ I°)5f ⁵ G
		5	116308.2(3)	3(0)	-9		1.002	54 (⁴ I°)5f ⁵ H	31 (⁴ I°)5f ³ I	6 (⁴ I°)5f ⁵ G
		6	118409.1(5)	2(1)	16		1.076	43 (⁴ I°)5f ³ I	36 (⁴ I°)5f ⁵ H	13 (⁴ I°)5f ³ K
		7	120438.8(3)	3(1)	-15		1.184	36 (⁴ I°)5f ⁵ H	30 (⁴ I°)5f ³ I	12 (⁴ I°)5f ⁵ I
4f ³ (⁴ I°)5f	³ I	5	114806.2(4)	2(0)	-24		0.915	45 (⁴ I°)5f ³ I	21 (⁴ I°)5f ⁵ H	14 (⁴ I°)5f ⁵ I
		6	116143.3(3)	4(0)	-10		0.971	37 (⁴ I°)5f ³ I	26 (⁴ I°)5f ⁵ K	12 (⁴ I°)5f ³ K
		7	118346.0(3)	4(0)	-10		1.112	32 (⁴ I°)5f ³ I	17 (⁴ I°)5f ⁵ H	17 (⁴ I°)5f ³ K
4f ³ (⁴ I°)5f	⁵ F	1	114975.9(5)	1(0)	-6	-6906	0.013	96 (⁴ I°)5f ⁵ F	3 (² H2°)5f ³ D	
		2	115151.6(8)	2(2)	6	-6824	0.850	58 (⁴ I°)5f ⁵ F	25 (⁴ I°)5f ³ F	8 (⁴ I°)5f ⁵ G
		3	116869.3(4)	2(0)	12	-5260	1.019	52 (⁴ I°)5f ⁵ F	32 (⁴ I°)5f ³ G	6 (⁴ I°)5f ⁵ H
		4	118930.7(4)	2(0)	9		1.229	60 (⁴ I°)5f ⁵ F	21 (⁴ I°)5f ³ G	6 (⁴ I°)5f ⁵ G
		5	120899.4(4)	2(0)	3		1.367	75 (⁴ I°)5f ⁵ F	20 (⁴ I°)5f ⁵ G	1 (² K°)5f ³ G
4f ³ (⁴ I°)5f	³ G	3	115194.8(5)	2(1)	23	-6715	0.900	41 (⁴ I°)5f ³ G	22 (⁴ I°)5f ⁵ G	13 (⁴ I°)5f ⁵ F
		4	116819.1(4)	3(1)	15		0.891	38 (⁴ I°)5f ⁵ I	28 (⁴ I°)5f ³ G	14 (⁴ I°)5f ⁵ H
		5	121134.9(4)	3(2)	-4		1.176	64 (⁴ I°)5f ³ G	14 (⁴ I°)5f ³ H	10 (⁴ I°)5f ⁵ G
4f ³ (⁴ I°)5f	⁵ G	2	115647.5(6)	1(0)	71		0.605	40 (⁴ I°)5f ⁵ G	23 (⁴ I°)5f ³ F	7 (² G2°)6p ³ F
		3	117156.6(4)	2(0)	-28		0.979	53 (⁴ I°)5f ⁵ G	29 (⁴ I°)5f ³ F	9 (⁴ I°)5f ⁵ F
		5	118820.0(4)	2(0)	11		1.143	26 (⁴ I°)5f ³ G	21 (⁴ I°)5f ⁵ G	18 (⁴ I°)5f ⁵ H
		4	119068.2(4)	2(0)	-7		1.081	38 (⁴ I°)5f ⁵ G	25 (⁴ I°)5f ³ G	13 (⁴ I°)5f ³ F
		6	121102.4(3)	4(1)	-32		1.278	65 (⁴ I°)5f ⁵ G	14 (⁴ I°)5f ³ H	13 (⁴ I°)5f ⁵ H

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Table C.1: Observed Nd III Energy Levels (continued)

Assignment			Energy	N	ΔE_1 ΔE_2	g	Eigenvector Composition		
Conf.	Term	J	(cm^{-1})		(cm^{-1})		(%)		
$4f^3(4I^\circ)5f$	5I	4	115852.3(3)	4(0)	-26	0.801	38 ($4I^\circ$)5f 5I	35 ($4I^\circ$)5f 3H	17 ($4I^\circ$)5f 3G
		5	117539.8(3)	4(0)	-8	0.970	58 ($4I^\circ$)5f 5I	24 ($4I^\circ$)5f 3H	6 ($4I^\circ$)5f 5G
		6	119280.8(3)	4(1)	4	1.085	66 ($4I^\circ$)5f 5I	12 ($4I^\circ$)5f 3H	6 ($4I^\circ$)5f 5K
		7	120883.6(6)	1(0)	-39	1.158	53 ($4I^\circ$)5f 5I	29 ($4I^\circ$)5f 3I	5 ($4I^\circ$)5f 5K
		8	121652.0(3)	5(0)	10	1.237	88 ($4I^\circ$)5f 5I	6 ($4I^\circ$)5f 3K	2 ($4I^\circ$)5f 5K
$4f^3(4I^\circ)5f$	3L	7	116649.9(3)	5(1)	16 -6852	0.939	56 ($4I^\circ$)5f 3L	32 ($4I^\circ$)5f 5K	4 ($4I^\circ$)5f 5L
		8	118924.9(3)	4(0)	24	1.025	71 ($4I^\circ$)5f 3L	8 ($4I^\circ$)5f 5K	7 ($4I^\circ$)5f 5L
		9	121186.4(4)	2(0)	11	1.110	86 ($4I^\circ$)5f 3L	4 ($4I^\circ$)5f 5L	4 ($4I^\circ$)5f 3M
$4f^3(4I^\circ)5f$	3M	8	116737.1(4)	2(0)	-3 -6941	0.914	69 ($4I^\circ$)5f 3M	17 ($4I^\circ$)5f 5M	8 ($4I^\circ$)5f 5L
		9	119070.0(4)	2(0)	-2 -6962	1.022	81 ($4I^\circ$)5f 3M	11 ($4I^\circ$)5f 5M	4 ($4I^\circ$)5f 5L
		10	121388.6(5)	1(0)	-14	1.102	91 ($4I^\circ$)5f 3M	5 ($4I^\circ$)5f 5M	2 ($4I^\circ$)5f 5L
$4f^3(4I^\circ)5f$	3K	6	116987.9(3)	4(1)	22	1.038	36 ($4I^\circ$)5f 3K	35 ($4I^\circ$)5f 5H	17 ($4I^\circ$)5f 5I
		7	119057.9(3)	5(2)	22	1.134	40 ($4I^\circ$)5f 3K	35 ($4I^\circ$)5f 5H	17 ($4I^\circ$)5f 5I
		8	121043.8(3)	4(0)	24	1.122	76 ($4I^\circ$)5f 3K	8 ($4I^\circ$)5f 5K	6 ($4I^\circ$)5f 3L
$4f^3(4I^\circ)5f$	3F	2	117172.4(5)	1(0)	-2	0.711	40 ($4I^\circ$)5f 3F	33 ($4I^\circ$)5f 5F	22 ($4I^\circ$)5f 5G
		3	119219.7(5)	1(0)	-16	1.072	59 ($4I^\circ$)5f 3F	21 ($4I^\circ$)5f 5F	11 ($4I^\circ$)5f 5G
		4	121403.6(5)	1(0)	3	1.237	75 ($4I^\circ$)5f 3F	10 ($4I^\circ$)5f 5F	7 ($4I^\circ$)5f 3G
$4f^3(4I^\circ)5f$	3H	4	117418.5(4)	2(0)	-5	0.980	40 ($4I^\circ$)5f 3H	29 ($4I^\circ$)5f 5G	16 ($4I^\circ$)5f 5F
		5	119385.9(5)	2(1)	-10	1.131	45 ($4I^\circ$)5f 3H	32 ($4I^\circ$)5f 5G	10 ($4I^\circ$)5f 5F
		6	121493.7(4)	2(0)	-28	1.194	65 ($4I^\circ$)5f 3H	23 ($4I^\circ$)5f 5G	5 ($4I^\circ$)5f 3I
$4f^3(4F^\circ)5f$	5I	5	126361.9(6)	1(0)	42	0.943	47 ($4F^\circ$)5f 5I	22 ($4F^\circ$)5f 3I	18 ($4F^\circ$)5f 5H
		6	127153.8(3)	3(0)	-32	1.064	51 ($4F^\circ$)5f 5I	9 ($^2H2^\circ$)5f 3K	7 ($4F^\circ$)5f 5H
		7	128096.7(6)	1(0)	0	1.160	70 ($4F^\circ$)5f 5I	9 ($4F^\circ$)5f 5H	7 ($4F^\circ$)5f 3I
		8	129317.8(6)	1(1)	-7	1.185	70 ($4F^\circ$)5f 5I	17 ($^2H2^\circ$)5f 3L	4 ($^2H2^\circ$)5f 1L
$4f^3(4F^\circ)5f$	5H	5	127320.9(6)	1(0)	-3	1.064	33 ($4F^\circ$)5f 5I	20 ($4F^\circ$)5f 5H	13 ($4F^\circ$)5f 5G
		7	129309.5(4)	3(2)	1	1.201	60 ($4F^\circ$)5f 5H	12 ($^2H2^\circ$)5f 3K	12 ($4F^\circ$)5f 5I
$4f^3(4F^\circ)5f$	3I	7	129725.5(4)	2(0)	3	1.086	59 ($4F^\circ$)5f 3I	14 ($^2H2^\circ$)5f 3L	6 ($^2H2^\circ$)5f 3K
$4f^3(^2H2^\circ)5f$	3L	7	126956.7(6)	1(0)	-25	0.977	38 ($^2H2^\circ$)5f 3L	10 ($^2H2^\circ$)5f 1K	6 ($4F^\circ$)5f 3I
		8	127432.6(5)	1(0)	1	1.077	34 ($^2H2^\circ$)5f 3L	17 ($4F^\circ$)5f 5I	15 ($^2H2^\circ$)5f 1L
		9	130408.4(6)	1(0)	26	1.117	79 ($^2H2^\circ$)5f 3L	13 ($^2H1^\circ$)5f 3L	6 ($4G^\circ$)5f 5K
$4f^3(^2H2^\circ)5f$	3K	6	127120.7(4)	3(0)	-21	1.002	31 ($^2H2^\circ$)5f 3K	22 ($4F^\circ$)5f 5H	10 ($4F^\circ$)5f 3I
		7	127447.8(4)	2(0)	-1	1.056	23 ($^2H2^\circ$)5f 3K	18 ($^2H2^\circ$)5f 3L	17 ($4F^\circ$)5f 5H
		8	130594.8(4)	2(0)	23	1.119	71 ($^2H2^\circ$)5f 3K	14 ($^2H1^\circ$)5f 3K	6 ($^2H2^\circ$)5f 3L
(115488)5f		2	115488.1(4)	2(0)	57	0.673	25 ($4I^\circ$)5f 5G	14 $4f^2(^3P)5d^2$ 3F	10 $4f^2(^3F)5d^2$ 3F

Appendix D

Nd III Transitions Classified from Laboratory Plasmas

Please refer to the published Nd III line and level lists for final results that are also machine-readable [96,160], where cancellation factors can also be found [160]. Most lines in this appendix are final, and the tables can be viewed as a record that led to the final results.

All 957 transitions of Nd III classified from the PDL and VS light sources are presented in this appendix in two tables, respectively. The relative intensity values in both tables were adjusted so that they are roughly comparable with each other, except for the $4f^35d - 4f^35f$ transitions which were not observable by FT spectroscopy.

Transitions classified in the Nd-Ar PDL FT spectra are listed in [Table D.1](#). The first column is the signal-to-noise ratio. The second column is the calibrated relative intensity corresponding to relative photon counts. The third and fourth columns are the weighted transition probability and log of the weighted (absorption) oscillator strength calculated using the Cowan code, where g_u and g_l refer to statistical weights of the upper and lower energy levels respectively. The fifth column is the full width at half maximum of the fitted line. The sixth and seventh columns are observed wavenumber and Ritz wavenumber from level optimisation. The eighth column is the wavenumber difference between observed and Ritz values. The ninth column is the Ritz air wavelength converted using the three-term dispersion formula from Peck & Reeder (1972) [183]. The tenth to fifteenth columns contain information on the energy levels associated with the transition. The final column contains comments of the observed transition, where

‘B/W’ indicates a blended or weak line with unreliable wavenumber and intensity, which was omitted from level optimisation. Uncertainties are in parentheses in units of the final decimal place.

Transitions observed and classified in the Nd VS grating spectra are listed in [Table D.2](#). The first column is the approximate relative intensity corresponding to relative energy flux, a ‘db’ following an intensity value indicates a doubly identified line (unresolved blend). The second and third columns are weighted transition probability and log of the weighted (absorption) oscillator strength calculated using the Cowan code, where g_u and g_l refer to statistical weights of the upper and lower energy levels respectively. The fourth column is the calibrated wavelength of the observed line with minimum uncertainty at ± 0.006 Å estimated for unblended and symmetric lines of moderate intensity. The fifth column is the Ritz wavelength resulting from the level optimisation, uncertainty is in parentheses in units of the final decimal place. The sixth column is the air Ritz wavelength (empty for the transitions involving 5f levels around 100 nm) converted using the three-term dispersion formula from Peck & Reeder (1972) [\[183\]](#). The seventh to tenth columns contain information on energy levels associated with the transition. The Nd VS grating spectra Ritz wavelengths of transitions *not* belonging to the $4f^35d - 4f^35f$ transition array were obtained from their input into the *LOPT* program with an ‘M’ (masked) flag, which assigned them with zero weights and therefore were neglected in the level energy optimisation. This was because these lines were an order of magnitude higher in uncertainty and would not have significantly contributed to the optimised level energies, moreover, the lower-resolution and more line-rich grating spectra in the UV were much more prone to blends, and less reliable wavelengths were also expected. Therefore, there was no guarantee that the Ritz wavenumber and level energy uncertainties would improve from including these lines in the level optimisation, and there was a chance of deterioration of the accuracy of results obtained purely by FT spectroscopy since the original grating spectra were not available to check for blends.

Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm ⁻¹)	σ (cm ⁻¹)	σ_{Ritz} (cm ⁻¹)	$\sigma - \sigma_{\text{Ritz}}$ (cm ⁻¹)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm ⁻¹)	E_u (cm ⁻¹)	Note
4	2000	3.8×10^6	-1.45	0.187	12697.081(22)	12697.085(11)	-0.004	7873.6573(68)	4f ⁴	5F ₄	4f ³ (⁴ I°)5d	5G° ₅	12181.327	24878.412	
6	1200	1.8×10^6	-1.80	0.110	13117.264(12)	13117.264(12)	0.000	7621.4430(70)	4f ⁴	5F ₂	4f ³ (⁴ I°)5d	3G° ₃	10773.962	23891.226	
11	2500	6.3×10^6	-1.28	0.130	13460.188(15)	13460.183(8)	0.005	7427.2738(46)	4f ⁴	5F ₅	4f ³ (⁴ I°)5d	5G° ₆	13210.278	26670.461	
4	430	2.3×10^5	-2.76	0.134	14124.631(17)	14124.643(3)	-0.012	7077.8735(15)	4f ⁴	5I ₅	4f ³ (⁴ I°)5d	5K° ₅	1137.794	15262.437	
6	590	3.2×10^6	-1.64	0.151	14489.386(13)	14489.379(5)	0.007	6899.7035(22)	4f ⁴	3K2 ₇	4f ³ (² H2°)5d	3K° ₆	15153.807	29643.186	
12	1000	4.5×10^5	-2.50	0.136	14550.517(13)	14550.524(7)	-0.007	6870.7090(34)	4f ⁴	5I ₆	4f ³ (⁴ I°)5d	5K° ₆	2387.544	16938.068	
13	1000	1.9×10^6	-1.88	0.145	14715.629(12)	14715.620(9)	0.009	6793.6253(40)	4f ⁴	5F ₃	4f ³ (⁴ I°)5d	3G° ₄	11424.605	26140.225	
5	220	2.3×10^6	-1.80	0.089	14822.931(26)	14822.913(6)	0.018	6744.4506(26)	4f ⁴	5G ₅	4f ³ (² H2°)5d	3G° ₄	18313.004	33135.917	B/W
12	820	6.3×10^5	-2.37	0.141	14941.721(13)	14941.724(3)	-0.003	6690.8208(13)	4f ⁴	5I ₇	4f ³ (⁴ I°)5d	5K° ₇	3714.548	18656.272	
312	21000	5.8×10^6	-1.43	0.178	15262.437(2)	15262.437(2)	0.000	6550.2241(9)	4f ⁴	5I ₄	4f ³ (⁴ I°)5d	5K° ₅	0.000	15262.437	
12	800	5.9×10^5	-2.42	0.128	15317.632(13)	15317.640(4)	-0.008	6526.6177(15)	4f ⁴	5I ₈	4f ³ (⁴ I°)5d	5K° ₈	5093.257	20410.897	
15	910	7.1×10^6	-1.34	0.123	15322.669(10)	15322.666(7)	0.003	6524.4769(28)	4f ⁴	3K2 ₈	4f ³ (² H2°)5d	3K° ₇	16459.136	31781.802	
39	2000	1.1×10^7	-1.17	0.150	15578.912(4)	15578.909(4)	0.003	6417.1610(14)	4f ⁴	3K2 ₆	4f ³ (² H2°)5d	3K° ₆	14064.277	29643.186	
5	110	1.5×10^6	-2.04	0.064	15657.794(10)	15657.757(11)	0.037	6384.8457(45)	4f ⁴	5G ₄	4f ³ (⁴ F°)5d	5F° ₃	16831.344	32489.101	B/W
378	16000	7.5×10^6	-1.35	0.135	15800.273(2)	15800.274(7)	-0.001	6327.2546(29)	4f ⁴	5I ₅	4f ³ (⁴ I°)5d	5K° ₆	1137.794	16938.068	B/W
9	450	5.8×10^6	-1.47	0.162	15983.560(9)	15983.557(7)	0.003	6254.6995(26)	4f ⁴	3H4 ₅	4f ³ (² H2°)5d	1H° ₅	16622.337	32605.894	
12	460	1.8×10^6	-1.99	0.099	16258.731(14)	16258.720(6)	0.011	6148.8440(24)	4f ⁴	5F ₄	4f ³ (⁴ I°)5d	3G° ₅	12181.327	28440.047	
341	13000	9.4×10^6	-1.27	0.146	16268.729(2)	16268.7280(19)	0.001	6145.0614(7)	4f ⁴	5I ₆	4f ³ (⁴ I°)5d	5K° ₇	2387.544	18656.272	
10	330	2.6×10^6	-1.84	0.134	16373.319(8)	16373.311(6)	0.008	6105.8100(21)	4f ⁴	3K2 ₈	4f ³ (⁴ F°)5d	5H° ₇	16459.136	32832.447	B/W
12	680	4.0×10^6	-1.65	0.165	16405.400(14)	16405.410(5)	-0.010	6093.8632(17)	4f ⁴	3K2 ₇	4f ³ (² G1°)5d	3H° ₆	15153.807	31559.217	
8	370	2.5×10^6	-1.86	0.177	16538.917(12)	16538.910(7)	0.007	6044.6739(27)	4f ⁴	5G ₃	4f ³ (⁴ F°)5d	5F° ₂	15349.601	31888.511	
20	990	7.3×10^6	-1.40	0.158	16627.998(9)	16627.995(6)	0.003	6012.2891(21)	4f ⁴	3K2 ₇	4f ³ (² H2°)5d	3K° ₇	15153.807	31781.802	
8	320	4.7×10^6	-1.60	0.155	16681.022(10)	16681.011(5)	0.011	5993.1805(19)	4f ⁴	5G ₅	4f ³ (² H2°)5d	3H° ₅	18313.004	34994.015	
4	120	3.3×10^5	-2.75	0.120	16693.937(19)	16693.930(7)	0.007	5988.5425(24)	4f ⁴	5F ₃	4f ³ (⁴ F°)5d	5D° ₃	11424.605	28118.535	
327	12000	1.2×10^7	-1.19	0.150	16696.350(2)	16696.3490(19)	0.001	5987.6749(7)	4f ⁴	5I ₇	4f ³ (⁴ I°)5d	5K° ₈	3714.548	20410.897	
13	670	5.2×10^6	-1.56	0.187	16772.159(14)	16772.144(9)	0.015	5960.6157(33)	4f ⁴	5G ₄	4f ³ (⁴ F°)5d	5F° ₄	16831.344	33603.488	
16	650	5.7×10^6	-1.53	0.180	16981.159(12)	16981.151(6)	0.008	5887.2507(22)	4f ⁴	3H4 ₅	4f ³ (⁴ F°)5d	5F° ₄	16622.337	33603.488	
23	1200	7.8×10^6	-1.40	0.194	17082.189(8)	17082.180(4)	0.009	5852.4315(12)	4f ⁴	3K2 ₆	4f ³ (⁴ F°)5d	5H° ₆	14064.277	31146.457	

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm ⁻¹)	σ (cm ⁻¹)	σ_{Ritz} (cm ⁻¹)	$\sigma - \sigma_{\text{Ritz}}$ (cm ⁻¹)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm ⁻¹)	E_u (cm ⁻¹)	Note
139	6000	6.2×10^6	-1.50	0.209	17084.810(2)	17084.801(3)	0.009	5851.5337(10)	4f ⁴	5I ₇	4f ³ (⁴ I°)5d	3I° ₆	3714.548	20799.349	B/W
310	11000	1.5×10^7	-1.11	0.150	17103.858(2)	17103.8580(19)	0.000	5845.0139(6)	4f ⁴	5I ₈	4f ³ (⁴ I°)5d	5K° ₉	5093.257	22197.115	
6	150	2.3×10^6	-1.93	0.103	17139.522(11)	17139.500(7)	0.022	5832.8589(25)	4f ⁴	5G ₃	4f ³ (⁴ F°)5d	5F° ₃	15349.601	32489.101	B/W
114	5000	4.2×10^6	-1.67	0.185	17229.078(2)	17229.078(2)	0.000	5802.5322(7)	4f ⁴	5I ₆	4f ³ (⁴ I°)5d	3I° ₅	2387.544	19616.622	
7	340	2.9×10^6	-1.85	0.211	17494.914(14)	17494.940(4)	-0.026	5714.3531(13)	4f ⁴	3K ₂₆	4f ³ (² G1°)5d	3H° ₆	14064.277	31559.217	B/W
119	4900	7.7×10^6	-1.43	0.174	17609.518(2)	17609.520(2)	-0.002	5677.1711(6)	4f ⁴	5I ₈	4f ³ (⁴ I°)5d	5I° ₇	5093.257	22702.777	
35	1600	1.6×10^7	-1.11	0.166	17678.638(5)	17678.640(4)	-0.002	5654.9743(12)	4f ⁴	3K ₂₇	4f ³ (⁴ F°)5d	5H° ₇	15153.807	32832.447	
70	2500	1.7×10^6	-2.09	0.182	17745.875(3)	17745.875(2)	0.000	5633.5487(7)	4f ⁴	5I ₅	4f ³ (⁴ I°)5d	5I° ₄	1137.794	18883.669	
9	310	1.1×10^5	-3.29	0.164	17936.225(20)	17936.179(6)	0.046	5573.7758(19)	4f ⁴	5F ₅	4f ³ (⁴ F°)5d	5H° ₆	13210.278	31146.457	B/W
51	1300	1.1×10^6	-2.29	0.167	17961.198(4)	17961.198(2)	0.000	5566.0117(7)	4f ⁴	5I ₆	4f ³ (⁴ I°)5d	5I° ₅	2387.544	20348.742	
21	480	4.9×10^6	-1.65	0.154	18056.836(4)	18056.853(13)	-0.017	5536.5258(40)	4f ⁴	3K ₂₇	4f ³ (⁴ F°)5d	5G° ₆	15153.807	33210.660	B/W
124	2900	3.6×10^7	-0.78	0.158	18075.412(2)	18075.4130(19)	-0.001	5530.8408(6)	4f ⁴	3K ₂₈	4f ³ (² H2°)5d	3K° ₈	16459.136	34534.549	
7	190	2.2×10^6	-2.00	0.217	18204.307(16)	18204.346(4)	-0.039	5491.6680(13)	4f ⁴	5G ₅	4f ³ (² H2°)5d	1G° ₄	18313.004	36517.350	B/W
23	850	2.5×10^4	-3.95	0.185	18245.456(9)	18245.452(10)	0.004	5479.2954(29)	4f ⁴	3K ₂₆	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₅		14064.277	32309.729	B/W
9	280	4.0×10^5	-2.75	0.250	18348.955(12)	18348.939(6)	0.016	5448.3922(19)	4f ⁴	5F ₅	4f ³ (² G1°)5d	3H° ₆	13210.278	31559.217	B/W
48	1300	1.1×10^7	-1.31	0.173	18371.676(4)	18371.678(4)	-0.002	5441.6485(11)	4f ⁴	3H ₄₅	4f ³ (² H2°)5d	3H° ₅	16622.337	34994.015	
810	15000	1.7×10^7	-1.12	0.154	18411.805(2)	18411.8050(19)	0.000	5429.7888(6)	4f ⁴	5I ₆	4f ³ (⁴ I°)5d	3I° ₆	2387.544	20799.349	
533	9700	9.2×10^6	-1.39	0.150	18478.827(2)	18478.8280(18)	-0.001	5410.0946(5)	4f ⁴	5I ₅	4f ³ (⁴ I°)5d	3I° ₅	1137.794	19616.622	
30	670	8.2×10^6	-1.46	0.166	18729.140(6)	18729.142(13)	-0.002	5337.7882(37)	4f ⁴	3K ₂₈	4f ³ (² H2°)5d	3I° ₇	16459.136	35188.278	B/W
4677	68000	5.3×10^7	-0.65	0.150	18883.669(2)	18883.6690(18)	0.000	5294.1080(5)	4f ⁴	5I ₄	4f ³ (⁴ I°)5d	5I° ₄	0.000	18883.669	
102	2100	3.0×10^6	-1.90	0.188	18909.970(2)	18909.968(2)	0.002	5286.7451(6)	4f ⁴	5I ₈	4f ³ (⁴ I°)5d	3I° ₇	5093.257	24003.225	B/W
2366	36000	5.4×10^7	-0.65	0.167	18988.231(2)	18988.2290(17)	0.002	5264.9553(5)	4f ⁴	5I ₇	4f ³ (⁴ I°)5d	5I° ₇	3714.548	22702.777	
4868	57000	5.7×10^7	-0.64	0.272	19210.946(2)	19210.948(2)	-0.002	5203.9162(5)	4f ⁴	5I ₅	4f ³ (⁴ I°)5d	5I° ₅	1137.794	20348.742	
1443	18000	1.7×10^7	-1.16	0.161	19251.201(2)	19251.2010(19)	0.000	5193.0350(5)	4f ⁴	5I ₅	4f ³ (⁴ I°)5d	5H° ₄	1137.794	20388.995	
10	120	2.9×10^6	-1.93	0.162	19279.790(9)	19279.755(4)	0.035	5185.3438(10)	4f ⁴	5G ₅	4f ³ (⁴ G°)5d	5H° ₅	18313.004	37592.759	B/W
14	230	2.1×10^6	-2.08	0.159	19380.736(14)	19380.742(6)	-0.006	5158.3243(17)	4f ⁴	3K ₂₇	4f ³ (² H2°)5d	3K° ₈	15153.807	34534.549	
30	430	6.4×10^6	-1.59	0.159	19395.621(6)	19395.616(8)	0.005	5154.3684(21)	4f ⁴	5F ₅	4f ³ (² H2°)5d	1H° ₅	13210.278	32605.894	B/W
319	6000	6.9×10^6	-1.56	0.249	19405.510(2)	19405.525(3)	-0.015	5151.7364(9)	4f ⁴	5I ₇	4f ³ (⁴ I°)5d	3K° ₆	3714.548	23120.073	B/W
4150	50000	1.1×10^8	-0.36	0.169	19499.003(2)	19499.0020(19)	0.001	5127.0390(5)	4f ⁴	5I ₈	4f ³ (⁴ I°)5d	5I° ₈	5093.257	24592.259	

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm ⁻¹)	σ (cm ⁻¹)	σ_{Ritz} (cm ⁻¹)	$\sigma - \sigma_{\text{Ritz}}$ (cm ⁻¹)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm ⁻¹)	E_u (cm ⁻¹)	Note
19	290	3.4×10^6	-1.87	0.181	19507.273(5)	19507.261(5)	0.012	5124.8683(12)	4f ⁴	5G ₃	4f ³ (² G ^o)5d	3G ^o ₃	15349.601	34856.862	B/W
3854	42000	6.4×10^7	-0.60	0.162	19592.984(2)	19592.978(3)	0.006	5102.4473(7)	4f ⁴	5I ₆	4f ³ (⁴ I ^o)5d	5I ^o ₆	2387.544	21980.522	B/W
2418	34000	1.6×10^7	-1.20	0.209	19593.104(2)	19593.094(4)	0.010	5102.4171(11)	4f ⁴	5I ₄	4f ³ (⁴ I ^o)5d	5H ^o ₃	0.000	19593.094	B/W
20	240	7.8×10^5	-2.52	0.178	19613.418(9)	19613.423(7)	-0.005	5097.1285(17)	4f ⁴	5F ₅	4f ³ (² H ^o)5d	1I ^o ₆	13210.278	32823.701	
77	1600	9.3×10^5	-2.44	0.222	19661.576(3)	19661.555(3)	0.021	5084.6504(7)	4f ⁴	5I ₅	4f ³ (⁴ I ^o)5d	3I ^o ₆	1137.794	20799.349	B/W
75	680	2.0×10^7	-1.11	0.136	19664.636(1)	19664.6370(13)	-0.001	5083.8535(3)	4f ⁴	5G ₅	4f ³ (⁴ G ^o)5d	5G ^o ₅	18313.004	37977.641	
37	430	7.9×10^6	-1.51	0.147	19686.035(5)	19686.006(9)	0.029	5078.3350(24)	4f ⁴	5G ₄	4f ³ (² H ^o)5d	1G ^o ₄	16831.344	36517.350	B/W
38	360	1.1×10^7	-1.37	0.122	19741.524(4)	19741.526(9)	-0.002	5064.0527(24)	4f ⁴	5G ₄	4f ³ (⁴ G ^o)5d	5G ^o ₄	16831.344	36572.870	B/W
1653	17000	2.4×10^7	-1.04	0.157	19793.752(2)	19793.755(11)	-0.003	5050.6902(28)	4f ⁴	5I ₆	4f ³ (⁴ I ^o)5d	5H ^o ₅	2387.544	22181.299	B/W
9	200	3.8×10^5	-2.84	0.316	19895.012(14)	19895.013(6)	-0.001	5024.9838(14)	4f ⁴	3H ₄₅	4f ³ (² H ^o)5d	1G ^o ₄	16622.337	36517.350	
34	540	4.4×10^6	-1.78	0.224	19895.787(3)	19895.786(3)	0.001	5024.7886(8)	4f ⁴	5F ₄	4f ³ (⁴ F ^o)5d	3H ^o ₄	12181.327	32077.113	
28	520	2.9×10^6	-1.96	0.246	19925.633(8)	19925.639(6)	-0.006	5017.2603(14)	4f ⁴	5F ₅	4f ³ (² H ^o)5d	3G ^o ₄	13210.278	33135.917	
36	370	5.7×10^6	-1.67	0.141	19953.028(2)	19953.029(2)	-0.001	5010.3729(6)	4f ⁴	3K ₂₆	4f ³ (⁴ G ^o)5d	5I ^o ₅	14064.277	34017.306	
79	870	9.1×10^6	-1.47	0.159	20000.630(2)	20000.630(2)	0.000	4998.4481(6)	4f ⁴	3K ₂₇	4f ³ (⁴ F ^o)5d	3H ^o ₆	15153.807	35154.437	
555	7800	1.7×10^7	-1.21	0.202	20226.325(1)	20226.322(5)	0.003	4942.6731(13)	4f ⁴	5I ₈	4f ³ (⁴ I ^o)5d	3K ^o ₇	5093.257	25319.579	B/W
88	1000	1.3×10^7	-1.32	0.149	20226.725(1)	20226.7250(12)	0.000	4942.5746(3)	4f ⁴	5G ₃	4f ³ (⁴ G ^o)5d	5H ^o ₃	15349.601	35576.326	
1949	23000	4.4×10^7	-0.80	0.168	20288.679(2)	20288.6770(18)	0.002	4927.4821(4)	4f ⁴	5I ₇	4f ³ (⁴ I ^o)5d	3I ^o ₇	3714.548	24003.225	
20	180	1.4×10^6	-2.29	0.139	20307.804(4)	20307.774(7)	0.030	4922.8483(17)	4f ⁴	5F ₄	4f ³ (⁴ F ^o)5d	5F ^o ₃	12181.327	32489.101	B/W
217	3000	4.2×10^6	-1.82	0.164	20315.233(2)	20315.2330(17)	0.000	4921.0408(4)	4f ⁴	5I ₆	4f ³ (⁴ I ^o)5d	5I ^o ₇	2387.544	22702.777	
1079	13000	2.4×10^7	-1.06	0.171	20343.971(2)	20343.970(2)	0.001	4914.0895(5)	4f ⁴	5I ₇	4f ³ (⁴ I ^o)5d	5H ^o ₆	3714.548	24058.518	
376	5200	5.0×10^6	-1.74	0.199	20348.743(2)	20348.742(2)	0.001	4912.9371(5)	4f ⁴	5I ₄	4f ³ (⁴ I ^o)5d	5I ^o ₅	0.000	20348.742	
647	7000	8.0×10^6	-1.54	0.154	20354.089(2)	20354.0880(19)	0.001	4911.6467(5)	4f ⁴	5I ₅	4f ³ (⁴ I ^o)5d	3H ^o ₄	1137.794	21491.882	
165	1900	1.4×10^6	-2.30	0.160	20388.994(2)	20388.9950(19)	-0.001	4903.2376(5)	4f ⁴	5I ₄	4f ³ (⁴ I ^o)5d	5H ^o ₄	0.000	20388.995	
10	110	1.6×10^6	-2.24	0.138	20424.559(8)	20424.567(6)	-0.008	4894.6978(15)	4f ⁴	5F ₄	4f ³ (² H ^o)5d	1H ^o ₅	12181.327	32605.894	
27	340	2.9×10^6	-1.98	0.158	20463.905(3)	20463.906(3)	-0.001	4885.2883(8)	4f ⁴	5F ₃	4f ³ (⁴ F ^o)5d	5F ^o ₂	11424.605	31888.511	
12	140	1.6×10^6	-2.25	0.157	20630.414(7)	20630.463(7)	-0.049	4845.8471(17)	4f ⁴	3K ₂₈	4f ³ (⁴ I ^o)6s (¹⁵ / ₂ , ¹ / ₂) ^o ₇	(¹⁵ / ₂ , ¹ / ₂) ^o ₇	16459.136	37089.599	B/W
65	790	7.1×10^5	-2.61	0.150	20732.528(3)	20732.529(3)	-0.001	4821.9907(7)	4f ⁴	5I ₆	4f ³ (⁴ I ^o)5d	3K ^o ₆	2387.544	23120.073	
76	1300	2.2×10^6	-2.12	0.224	20782.616(2)	20782.617(5)	-0.001	4810.3691(11)	4f ⁴	5I ₇	4f ³ (⁴ I ^o)5d	3I ^o ₇	3714.548	24497.165	B/W
20	290	5.1×10^6	-1.75	0.151	20807.075(4)	20807.028(7)	0.047	4804.7255(15)	4f ⁴	5F ₅	4f ³ (⁴ G ^o)5d	5I ^o ₅	13210.278	34017.306	B/W

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm^{-1})	σ (cm^{-1})	σ_{Ritz} (cm^{-1})	$\sigma - \sigma_{\text{Ritz}}$ (cm^{-1})	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm^{-1})	E_u (cm^{-1})	Note
326	5300	7.0×10^6	-1.62	0.187	20842.729(2)	20842.728(2)	0.001	4796.4957(5)	4f ⁴	⁵ I ₅	4f ³ (⁴ I°)5d	⁵ I° ₆	1137.794	21980.522	
167	2500	5.6×10^6	-1.72	0.213	20877.711(2)	20877.711(2)	0.000	4788.4585(5)	4f ⁴	⁵ I ₇	4f ³ (⁴ I°)5d	⁵ I° ₈	3714.548	24592.259	
4	28	3.7×10^5	-2.90	0.084	20929.739(17)	20929.738(6)	0.001	4776.5552(13)	4f ⁴	³ K ₂₆	4f ³ (² H ^o)5d	³ H° ₅	14064.277	34994.015	B/W
64	1200	8.1×10^6	-1.56	0.188	20954.592(3)	20954.590(3)	0.002	4770.8902(7)	4f ⁴	⁵ F ₄	4f ³ (² H ^o)5d	³ G° ₄	12181.327	33135.917	
264	4000	6.5×10^6	-1.65	0.164	20960.177(2)	20960.1770(19)	0.000	4769.6184(4)	4f ⁴	⁵ I ₆	4f ³ (⁴ I°)5d	³ H° ₅	2387.544	23347.721	
20	400	8.6×10^6	-1.53	0.185	20970.419(10)	20970.422(5)	-0.003	4767.2882(12)	4f ⁴	³ H ₄₅	4f ³ (⁴ G°)5d	⁵ H° ₅	16622.337	37592.759	
492	8800	2.5×10^7	-1.07	0.186	21004.649(2)	21004.649(2)	0.000	4759.5198(5)	4f ⁴	⁵ I ₈	4f ³ (⁴ I°)5d	⁵ H° ₇	5093.257	26097.906	
139	2700	2.3×10^7	-1.11	0.165	21064.495(2)	21064.4960(19)	-0.001	4745.9972(4)	4f ⁴	⁵ F ₃	4f ³ (⁴ F°)5d	⁵ F° ₃	11424.605	32489.101	
12	400	4.8×10^6	-1.79	0.230	21090.151(18)	21090.160(5)	-0.009	4740.2219(12)	4f ⁴	³ K ₂₆	4f ³ (⁴ F°)5d	³ H° ₆	14064.277	35154.437	
91	1900	1.5×10^7	-1.30	0.163	21114.573(2)	21114.549(14)	0.024	4734.7465(31)	4f ⁴	⁵ F ₂	4f ³ (⁴ F°)5d	⁵ F° ₂	10773.962	31888.511	B/W
18	380	6.2×10^6	-1.68	0.168	21146.289(10)	21146.297(9)	-0.008	4727.6378(19)	4f ⁴	⁵ G ₄	4f ³ (⁴ G°)5d	⁵ G° ₅	16831.344	37977.641	
13	580	5.7×10^6	-1.72	0.271	21167.729(9)	21167.749(5)	-0.020	4722.8466(10)	4f ⁴	⁵ G ₃	4f ³ (² H ^o)5d	¹ G° ₄	15349.601	36517.350	B/W
212	5000	5.3×10^7	-0.75	0.162	21209.599(2)	21209.5990(19)	0.000	4713.5276(4)	4f ⁴	⁵ F ₅	4f ³ (⁴ S°)5d	⁵ D° ₄	13210.278	34419.877	
221	5500	6.0×10^7	-0.70	0.169	21219.496(2)	21219.4950(19)	0.001	4711.3293(4)	4f ⁴	⁵ F ₄	4f ³ (⁴ S°)5d	⁵ D° ₃	12181.327	33400.822	
5	150	5.7×10^6	-1.72	0.143	21298.391(16)	21298.385(5)	0.006	4693.8781(10)	4f ⁴	⁵ G ₅	4f ³ (⁴ G°)5d	⁵ G° ₆	18313.004	39611.389	
66	3100	3.9×10^7	-0.89	0.158	21300.908(3)	21300.908(3)	0.000	4693.3221(6)	4f ⁴	⁵ F ₅	4f ³ (⁴ F°)5d	⁵ F° ₅	13210.278	34511.186	
77	2400	7.2×10^6	-1.62	0.140	21320.273(2)	21320.284(6)	-0.011	4689.0567(13)	4f ⁴	⁵ I ₇	4f ³ (⁴ I°)5d	³ H° ₆	3714.548	25034.832	B/W
2	60	1.9×10^6	-2.20	0.133	21355.301(41)	21355.304(5)	-0.003	4681.3672(12)	4f ⁴	³ H ₄₅	4f ³ (⁴ G°)5d	⁵ G° ₅	16622.337	37977.641	B/W
38	2000	2.3×10^7	-1.12	0.177	21422.159(5)	21422.161(4)	-0.002	4666.7567(10)	4f ⁴	⁵ F ₄	4f ³ (⁴ F°)5d	⁵ F° ₄	12181.327	33603.488	
154	5000	5.8×10^6	-1.72	0.137	21479.404(2)	21479.4040(17)	0.000	4654.3196(4)	4f ⁴	⁵ I ₄	4f ³ (⁴ I°)5d	⁵ G° ₃	0.000	21479.404	
75	2700	3.7×10^7	-0.92	0.154	21480.764(1)	21480.7640(12)	0.000	4654.0249(3)	4f ⁴	⁵ F ₃	4f ³ (⁴ S°)5d	⁵ D° ₂	11424.605	32905.369	
93	4600	4.2×10^6	-1.87	0.194	21491.877(2)	21491.882(3)	-0.005	4651.6173(5)	4f ⁴	⁵ I ₄	4f ³ (⁴ I°)5d	³ H° ₄	0.000	21491.882	B/W
4	170	7.4×10^5	-2.62	0.195	21583.403(25)	21583.428(8)	-0.025	4631.8871(17)	4f ⁴	⁵ I ₈	4f ³ (⁴ I°)5d	³ L° ₈	5093.257	26676.685	
49	1800	1.9×10^7	-1.21	0.149	21600.392(4)	21600.393(4)	-0.001	4628.2492(8)	4f ⁴	⁵ F ₂	4f ³ (⁴ S°)5d	⁵ D° ₁	10773.962	32374.355	
33	1700	2.0×10^6	-2.19	0.178	21605.029(6)	21605.031(5)	-0.002	4627.2556(11)	4f ⁴	⁵ I ₇	4f ³ (⁴ I°)5d	³ K° ₇	3714.548	25319.579	
73	2900	4.2×10^6	-1.87	0.163	21615.679(3)	21615.6810(19)	-0.002	4624.9757(4)	4f ⁴	⁵ I ₆	4f ³ (⁴ I°)5d	³ I° ₇	2387.544	24003.225	
5	170	3.4×10^5	-2.96	0.175	21670.978(21)	21670.974(3)	0.004	4613.1750(6)	4f ⁴	⁵ I ₆	4f ³ (⁴ I°)5d	⁵ H° ₆	2387.544	24058.518	
7	220	1.8×10^6	-2.24	0.134	21711.313(11)	21711.312(7)	0.001	4604.6040(14)	4f ⁴	⁵ F ₃	4f ³ (² H ^o)5d	³ G° ₄	11424.605	33135.917	
28	1100	8.7×10^6	-1.56	0.163	21715.160(3)	21715.139(14)	0.021	4603.7925(30)	4f ⁴	⁵ F ₂	4f ³ (⁴ F°)5d	⁵ F° ₃	10773.962	32489.101	B/W

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm ⁻¹)	σ (cm ⁻¹)	σ_{Ritz} (cm ⁻¹)	$\sigma - \sigma_{\text{Ritz}}$ (cm ⁻¹)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm ⁻¹)	E_u (cm ⁻¹)	Note
3	40	6.0×10^6	-1.72	0.064	21736.505(19)	21736.540(9)	-0.035	4599.2597(18)	4f ⁴	³ K ₂₇	4f ³ (⁴ G°)5d	⁵ I° ₇	15153.807	36890.347	B/W
75	2500	3.8×10^6	-1.92	0.135	21872.654(2)	21872.656(9)	-0.002	4570.6375(19)	4f ⁴	⁵ I ₅	4f ³ (⁴ I°)5d	⁵ G° ₄	1137.794	23010.450	B/W
7	290	4.3×10^6	-1.87	0.192	21935.813(14)	21935.792(6)	0.021	4557.4820(13)	4f ⁴	³ K ₂₇	4f ³ (⁴ I°)6s (¹⁵ / ₂) ^o ₇	¹⁵ / ₂ ^o ₇	15153.807	37089.599	B/W
3	120	8.4×10^6	-1.58	0.184	21976.209(31)	21976.217(7)	-0.008	4549.0984(14)	4f ⁴	⁵ F ₃	4f ³ (⁴ S°)5d	⁵ D° ₃	11424.605	33400.822	
23	640	2.8×10^7	-1.06	0.126	22058.637(4)	22058.637(6)	0.000	4532.1009(13)	4f ⁴	³ K ₂₈	4f ³ (⁴ G°)5d	⁵ I° ₈	16459.136	38517.773	B/W
25	800	1.3×10^7	-1.40	0.146	22131.429(3)	22131.407(14)	0.022	4517.1987(29)	4f ⁴	⁵ F ₂	4f ³ (⁴ S°)5d	⁵ D° ₂	10773.962	32905.369	B/W
13	490	6.8×10^6	-1.68	0.148	22178.877(13)	22178.883(7)	-0.006	4507.5290(14)	4f ⁴	⁵ F ₃	4f ³ (⁴ F°)5d	⁵ F° ₄	11424.605	33603.488	
53	3000	3.4×10^6	-1.99	0.224	22209.925(4)	22209.927(2)	-0.002	4501.2285(5)	4f ⁴	⁵ I ₅	4f ³ (⁴ I°)5d	³ H° ₅	1137.794	23347.721	
5	380	6.7×10^6	-1.69	0.191	22238.565(37)	22238.550(6)	0.015	4495.4349(12)	4f ⁴	⁵ F ₄	4f ³ (⁴ S°)5d	⁵ D° ₄	12181.327	34419.877	
7	220	4.4×10^6	-1.88	0.124	22329.852(11)	22329.859(6)	-0.007	4477.0524(12)	4f ⁴	⁵ F ₄	4f ³ (⁴ F°)5d	⁵ F° ₅	12181.327	34511.186	
111	4600	1.5×10^7	-1.35	0.186	22348.654(2)	22348.654(2)	0.000	4473.2871(4)	4f ⁴	⁵ I ₈	4f ³ (⁴ I°)5d	³ K° ₈	5093.257	27441.911	
15	590	1.5×10^6	-2.35	0.148	22383.358(6)	22383.358(3)	0.000	4466.3515(6)	4f ⁴	⁵ I ₇	4f ³ (⁴ I°)5d	⁵ H° ₇	3714.548	26097.906	
46	1500	2.6×10^6	-2.11	0.139	22490.858(2)	22490.868(10)	-0.010	4445.0012(20)	4f ⁴	⁵ I ₆	4f ³ (⁴ I°)5d	⁵ G° ₅	2387.544	24878.412	B/W
26	1200	2.5×10^6	-2.14	0.174	22647.292(7)	22647.288(6)	0.004	4414.3000(11)	4f ⁴	⁵ I ₆	4f ³ (⁴ I°)5d	³ H° ₆	2387.544	25034.832	
16	520	1.8×10^6	-2.29	0.134	22955.912(5)	22955.913(7)	-0.001	4354.9520(14)	4f ⁴	⁵ I ₇	4f ³ (⁴ I°)5d	⁵ G° ₆	3714.548	26670.461	B/W
21	960	1.3×10^6	-2.43	0.192	23010.412(5)	23010.450(9)	-0.038	4344.6302(17)	4f ⁴	⁵ I ₄	4f ³ (⁴ I°)5d	⁵ G° ₄	0.000	23010.450	B/W
42	1500	1.5×10^6	-2.39	0.141	23432.293(4)	23432.257(7)	0.036	4266.4206(13)	4f ⁴	⁵ F ₃	4f ³ (² G ^o)5d	³ G° ₃	11424.605	34856.862	B/W
48	2000	3.3×10^6	-2.06	0.139	23891.226(4)	23891.226(4)	0.000	4184.4578(6)	4f ⁴	⁵ I ₄	4f ³ (⁴ I°)5d	³ G° ₃	0.000	23891.226	
7	380	1.7×10^5	-3.35	0.202	23897.021(13)	23897.038(6)	-0.017	4183.4400(10)	4f ⁴	⁵ I ₅	4f ³ (⁴ I°)5d	³ H° ₆	1137.794	25034.832	B/W
15	610	1.9×10^7	-1.30	0.147	23904.473(12)	23904.467(5)	0.006	4182.1399(8)	4f ⁴	³ K ₂₇	4f ³ (⁴ G°)5d	⁵ H° ₆	15153.807	39058.274	
35	1800	3.9×10^7	-1.00	0.171	24045.932(3)	24045.946(6)	-0.014	4157.5330(10)	4f ⁴	³ K ₂₈	4f ³ (⁴ G°)5d	⁵ H° ₇	16459.136	40505.082	B/W
13	750	2.1×10^6	-2.26	0.209	24053.841(8)	24053.852(5)	-0.011	4156.1664(9)	4f ⁴	⁵ F ₄	4f ³ (⁴ G°)5d	⁵ H° ₄	12181.327	36235.179	B/W
8	280	6.3×10^5	-2.80	0.120	24282.913(11)	24282.917(7)	-0.004	4116.9598(12)	4f ⁴	⁵ I ₆	4f ³ (⁴ I°)5d	⁵ G° ₆	2387.544	26670.461	
4	170	4.1×10^6	-2.00	0.161	24767.382(22)	24767.363(7)	0.019	4036.4311(11)	4f ⁴	⁵ F ₅	4f ³ (⁴ G°)5d	⁵ G° ₅	13210.278	37977.641	
12	390	2.4×10^7	-1.23	0.111	24800.886(6)	24800.891(5)	-0.005	4030.9741(9)	4f ⁴	³ K ₂₈	4f ³ (² K°)5d	³ I° ₇	16459.136	41260.027	
31	1800	2.7×10^6	-2.19	0.162	25002.418(3)	25002.431(8)	-0.013	3998.4805(13)	4f ⁴	⁵ I ₅	4f ³ (⁴ I°)5d	³ G° ₄	1137.794	26140.225	B/W
5	130	4.3×10^5	-3.00	0.095	25411.439(13)	25411.432(5)	0.007	3934.1229(7)	4f ⁴	⁵ F ₄	4f ³ (⁴ G°)5d	⁵ H° ₅	12181.327	37592.759	
85	3100	1.5×10^7	-1.48	0.235	25928.637(3)	25928.638(3)	-0.001	3855.6461(4)	4f ⁴	⁵ I ₇	4f ³ (² H ² °)5d	³ K° ₆	3714.548	29643.186	
17	390	1.2×10^6	-2.58	0.162	26052.505(6)	26052.503(5)	0.002	3837.3142(8)	4f ⁴	⁵ I ₆	4f ³ (⁴ I°)5d	³ G° ₅	2387.544	28440.047	

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm ⁻¹)	σ (cm ⁻¹)	σ_{Ritz} (cm ⁻¹)	$\sigma - \sigma_{\text{Ritz}}$ (cm ⁻¹)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm ⁻¹)	E_u (cm ⁻¹)	Note
9	260	2.1×10^5	-3.34	0.233	26140.232(13)	26140.225(8)	0.007	3824.436(12)	4f ⁴	⁵ I ₄	4f ³ (⁴ I°)5d	³ G° ₄	0.000	26140.225	B/W
527	12000	1.2×10^8	-0.60	0.197	26688.546(1)	26688.545(6)	0.001	3745.861(8)	4f ⁴	⁵ I ₈	4f ³ (² H2°)5d	³ K° ₇	5093.257	31781.802	B/W
416	8800	6.2×10^7	-0.89	0.199	27009.879(2)	27009.879(2)	0.000	3701.2958(3)	4f ⁴	⁵ I ₆	4f ³ (² H2°)5d	³ I° ₅	2387.544	29397.423	
12	390	1.2×10^5	-3.62	0.222	27255.649(9)	27255.642(3)	0.007	3667.9205(4)	4f ⁴	⁵ I ₆	4f ³ (² H2°)5d	³ K° ₆	2387.544	29643.186	B/W
648	13000	1.3×10^8	-0.59	0.197	27431.909(2)	27431.909(2)	0.000	3644.3512(3)	4f ⁴	⁵ I ₇	4f ³ (⁴ F°)5d	⁵ H° ₆	3714.548	31146.457	
1161	21000	1.5×10^8	-0.53	0.174	27607.514(2)	27607.513(2)	0.001	3621.1699(3)	4f ⁴	⁵ I ₅	4f ³ (⁴ F°)5d	⁵ H° ₄	1137.794	28745.307	
1169	20000	1.2×10^8	-0.63	0.165	27675.024(2)	27675.024(2)	0.000	3612.3361(3)	4f ⁴	⁵ I ₄	4f ³ (⁴ F°)5d	⁵ H° ₃	0.000	27675.024	
420	9100	1.2×10^8	-0.63	0.202	27739.190(1)	27739.1900(13)	0.000	3603.9798(2)	4f ⁴	⁵ I ₈	4f ³ (⁴ F°)5d	⁵ H° ₇	5093.257	32832.447	
679	15000	1.2×10^8	-0.63	0.213	27788.191(2)	27788.193(2)	-0.002	3597.6242(3)	4f ⁴	⁵ I ₆	4f ³ (⁴ F°)5d	⁵ H° ₅	2387.544	30175.737	
314	6600	6.1×10^7	-0.93	0.187	27844.670(2)	27844.669(2)	0.001	3590.3271(3)	4f ⁴	⁵ I ₇	4f ³ (² G1°)5d	³ H° ₆	3714.548	31559.217	
5	56	7.9×10^6	-1.82	0.103	28033.075(15)	28033.069(7)	0.006	3566.1972(9)	4f ³ (² H2°)5d	¹ H° ₅	4f ³ (⁴ I°)6p	⁵ I ₄	32605.894	60638.963	B/W
15	390	2.8×10^6	-2.27	0.188	28067.249(7)	28067.254(5)	-0.005	3561.8536(7)	4f ⁴	⁵ I ₇	4f ³ (² H2°)5d	³ K° ₇	3714.548	31781.802	
72	1700	1.3×10^7	-1.61	0.207	28118.535(2)	28118.5350(17)	0.000	3555.3575(2)	4f ⁴	⁵ I ₄	4f ³ (⁴ F°)5d	⁵ D° ₃	0.000	28118.535	
41	1900	6.0×10^6	-1.95	0.452	28205.543(8)	28205.541(5)	0.002	3544.3899(6)	4f ⁴	⁵ I ₆	4f ³ (⁴ I°)6s	$(\frac{9}{2}, \frac{1}{2})^\circ_5$	2387.544	30593.085	
20	440	2.7×10^6	-2.30	0.170	28259.610(9)	28259.629(3)	-0.019	3537.6059(4)	4f ⁴	⁵ I ₅	4f ³ (² H2°)5d	³ I° ₅	1137.794	29397.423	B/W
80	2000	1.2×10^7	-1.66	0.210	28745.320(3)	28745.307(3)	0.013	3477.8331(4)	4f ⁴	⁵ I ₄	4f ³ (⁴ F°)5d	⁵ H° ₄	0.000	28745.307	B/W
52	1000	1.1×10^7	-1.70	0.174	28758.912(2)	28758.913(2)	-0.001	3476.1877(3)	4f ⁴	⁵ I ₆	4f ³ (⁴ F°)5d	⁵ H° ₆	2387.544	31146.457	
80	2000	1.7×10^7	-1.52	0.222	29037.945(3)	29037.943(2)	0.002	3442.7834(3)	4f ⁴	⁵ I ₅	4f ³ (⁴ F°)5d	⁵ H° ₅	1137.794	30175.737	
23	480	8.8×10^7	-0.81	0.172	29091.350(8)	29091.351(8)	-0.001	3436.4627(9)	4f ⁴	⁵ G ₅	4f ³ (⁴ D°)5d	⁵ F° ₄	18313.004	47404.355	
33	780	9.6×10^6	-1.77	0.210	29109.158(7)	29109.153(6)	0.005	3434.3611(6)	4f ⁴	⁵ I ₇	4f ³ (² H2°)5d	¹ I° ₆	3714.548	32823.701	
34	720	1.1×10^7	-1.71	0.181	29117.901(6)	29117.899(2)	0.002	3433.3295(3)	4f ⁴	⁵ I ₇	4f ³ (⁴ F°)5d	⁵ H° ₇	3714.548	32832.447	
59	1400	1.7×10^8	-0.52	0.178	29133.642(3)	29133.642(4)	0.000	3431.4741(4)	4f ⁴	³ K ₂₈	4f ³ (⁴ G°)5d	³ I° ₇	16459.136	45592.778	
74	1800	5.7×10^6	-2.00	0.215	29171.708(2)	29171.673(3)	0.035	3427.0004(3)	4f ⁴	⁵ I ₆	4f ³ (² G1°)5d	³ H° ₆	2387.544	31559.217	B/W
3	14	9.5×10^7	-0.78	0.038	29407.603(15)	29407.626(7)	-0.023	3399.5029(8)	4f ³ (⁴ I°)6s	$(\frac{15}{2}, \frac{1}{2})^\circ_7$	4f ³ (⁴ I°)6p	⁵ I ₇	37089.599	66497.225	B/W
6	130	2.4×10^6	-2.38	0.187	29441.283(18)	29441.292(6)	-0.009	3395.6155(7)	4f ⁴	⁵ I ₈	4f ³ (² H2°)5d	³ K° ₈	5093.257	34534.549	
64	1600	1.5×10^8	-0.59	0.185	29455.425(2)	29455.4250(18)	0.000	3393.9862(2)	4f ⁴	³ K ₂₇	4f ³ (⁴ G°)5d	³ I° ₆	15153.807	44609.232	
53	1100	9.2×10^6	-1.80	0.180	29496.117(4)	29496.112(12)	0.005	3389.3044(14)	4f ⁴	⁵ I ₇	4f ³ (⁴ F°)5d	⁵ G° ₆	3714.548	33210.660	B/W
3	42	8.9×10^7	-0.82	0.123	29606.889(29)	29606.878(9)	0.011	3376.6238(10)	4f ³ (⁴ G°)5d	⁵ I° ₇	4f ³ (⁴ I°)6p	⁵ I ₇	36890.347	66497.225	
9	150	6.4×10^6	-1.96	0.144	29663.582(10)	29663.582(7)	0.000	3370.1689(8)	4f ³ (⁴ I°)6s	$(\frac{13}{2}, \frac{1}{2})^\circ_6$	4f ³ (⁴ I°)6p	³ I ₅	34687.230	64350.812	

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm ⁻¹)	σ (cm ⁻¹)	σ_{Ritz} (cm ⁻¹)	$\sigma - \sigma_{\text{Ritz}}$ (cm ⁻¹)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm ⁻¹)	E_u (cm ⁻¹)	Note
6	160	4.0×10^8	-0.17	0.227	29827.159(19)	29827.166(9)	-0.007	3351.6850(10)	4f ³ (⁴ G°)5d	5 ¹ ° ₇	4f ³ (⁴ I°)6p	5H ₇	36890.347	66717.513	B/W
6	140	8.1×10^8	0.13	0.184	29932.979(36)	29932.982(7)	-0.003	3339.8361(7)	4f ³ (⁴ I°)6s	($\frac{9}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p	5K ₅	30593.085	60526.067	
4	230	1.1×10^9	0.26	0.408	30045.886(34)	30045.878(6)	0.008	3327.2864(7)	4f ³ (⁴ I°)6s	($\frac{9}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p	5I ₄	30593.085	60638.963	
64	2000	2.8×10^7	-1.33	0.220	30095.005(2)	30095.021(11)	-0.016	3321.8530(12)	4f ⁴	5I ₈	4f ³ (² H2°)5d	3 ¹ ° ₇	5093.257	35188.278	B/W
5	120	1.2×10^9	0.29	0.193	30210.918(21)	30210.917(9)	0.001	3309.1092(10)	4f ³ (⁴ I°)6s	($\frac{11}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p	5K ₆	32309.729	62520.646	
5	82	1.1×10^6	-2.74	0.133	30218.395(18)	30218.350(7)	0.045	3308.2952(7)	4f ⁴	5I ₆	4f ³ (² H2°)5d	1H° ₅	2387.544	32605.894	B/W
2	92	6.7×10^8	0.04	0.310	30330.520(56)	30330.537(9)	-0.017	3296.0580(10)	4f ³ (⁴ I°)6s	($\frac{11}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p	5I ₅	32309.729	62640.266	B/W
13	360	3.6×10^6	-2.23	0.180	30436.147(16)	30436.157(6)	-0.010	3284.6196(6)	4f ⁴	5I ₆	4f ³ (² H2°)5d	1 ¹ ° ₆	2387.544	32823.701	
7	250	1.3×10^9	0.32	0.263	30445.008(16)	30444.988(8)	0.020	3283.6668(9)	4f ³ (⁴ I°)6s	($\frac{11}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p	5K ₆	32075.658	62520.646	
8	330	1.2×10^8	-0.71	0.306	30463.224(16)	30463.226(4)	-0.002	3281.7009(4)	4f ³ (⁴ I°)5d	5H° ₅	4f ³ (⁴ I°)6p	5I ₄	30175.737	60638.963	
4	94	7.3×10^6	-1.93	0.177	30544.961(25)	30544.955(5)	0.006	3272.9197(6)	4f ⁴	3K2 ₆	4f ³ (⁴ G°)5d	3 ¹ ° ₆	14064.277	44609.232	
6	200	1.7×10^9	0.44	0.260	30564.608(20)	30564.608(8)	0.000	3270.8152(9)	4f ³ (⁴ I°)6s	($\frac{11}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p	5I ₅	32075.658	62640.266	
6	250	2.0×10^9	0.50	0.294	30643.494(20)	30643.477(8)	0.017	3262.3966(9)	4f ³ (⁴ I°)6s	($\frac{13}{2}, \frac{1}{2}$)° ₇	4f ³ (⁴ I°)6p	5I ₆	33906.143	64549.620	
10	340	1.8×10^9	0.46	0.258	30652.843(12)	30652.845(7)	-0.002	3261.3995(7)	4f ³ (⁴ I°)6s	($\frac{9}{2}, \frac{1}{2}$)° ₄	4f ³ (⁴ I°)6p	5K ₅	29873.222	60526.067	
3	50	1.8×10^9	0.46	0.108	30715.840(22)	30715.863(9)	-0.023	3254.7081(9)	4f ³ (⁴ I°)6s	($\frac{13}{2}, \frac{1}{2}$)° ₇	4f ³ (⁴ I°)6p	5K ₇	33906.143	64622.006	B/W
5	140	9.2×10^8	0.16	0.201	30765.780(21)	30765.741(7)	0.039	3249.4313(7)	4f ³ (⁴ I°)6s	($\frac{9}{2}, \frac{1}{2}$)° ₄	4f ³ (⁴ I°)6p	5I ₄	29873.222	60638.963	B/W
5	130	2.5×10^7	-1.40	0.212	30782.037(24)	30782.018(9)	0.019	3247.7130(9)	4f ⁴	3H4 ₅	4f ³ (⁴ D°)5d	5F° ₄	16622.337	47404.355	
13	380	3.4×10^6	-2.27	0.212	30823.113(17)	30823.116(12)	-0.003	3243.3825(13)	4f ⁴	5I ₆	4f ³ (⁴ F°)5d	5G° ₆	2387.544	33210.660	
5	150	2.1×10^9	0.52	0.221	30877.699(22)	30877.685(12)	0.014	3237.6504(13)	4f ³ (⁴ I°)6s	($\frac{15}{2}, \frac{1}{2}$)° ₈	4f ³ (⁴ I°)6p	5H ₇	35839.828	66717.513	B/W
15	420	3.9×10^6	-2.21	0.177	30939.324(14)	30939.319(5)	0.005	3231.2005(5)	4f ⁴	5I ₅	4f ³ (⁴ F°)5d	3H° ₄	1137.794	32077.113	
4	140	2.4×10^9	0.57	0.296	30952.215(36)	30952.196(12)	0.019	3229.8561(13)	4f ³ (⁴ I°)6s	($\frac{15}{2}, \frac{1}{2}$)° ₈	4f ³ (⁴ I°)6p	5I ₈	35839.828	66792.024	B/W
8	120	4.1×10^6	-2.21	0.102	31468.133(9)	31468.100(6)	0.033	3176.9023(6)	4f ⁴	5I ₅	4f ³ (² H2°)5d	1H° ₅	1137.794	32605.894	B/W
15	540	6.7×10^6	-1.99	0.225	31473.724(15)	31473.730(11)	-0.006	3176.3340(11)	4f ⁴	5I ₇	4f ³ (² H2°)5d	3 ¹ ° ₇	3714.548	35188.278	
10	290	4.5×10^6	-2.17	0.194	31691.533(21)	31691.517(5)	0.016	3154.5052(5)	4f ⁴	5I ₅	4f ³ (⁴ G°)5d	5 ¹ ° ₄	1137.794	32829.311	
14	490	7.1×10^6	-1.98	0.211	31835.030(15)	31835.017(4)	0.013	3140.2853(3)	4f ⁴	5I ₇	4f ³ (⁴ G°)5d	5 ¹ ° ₆	3714.548	35549.565	
6	180	8.3×10^7	-0.91	0.191	31934.210(17)	31934.185(10)	0.025	3130.5332(10)	4f ³ (⁴ I°)6s	($\frac{11}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p	5H ₄	32309.729	64243.914	B/W
6	210	2.7×10^6	-2.40	0.216	31996.332(18)	31996.342(5)	-0.010	3124.4515(5)	4f ⁴	5I ₈	4f ³ (⁴ I°)6s	($\frac{15}{2}, \frac{1}{2}$)° ₇	5093.257	37089.599	
4	150	1.6×10^6	-2.63	0.228	31998.106(27)	31998.123(5)	-0.017	3124.2776(5)	4f ⁴	5I ₅	4f ³ (² H2°)5d	3G° ₄	1137.794	33135.917	
8	270	3.1×10^6	-2.35	0.205	32077.104(13)	32077.113(5)	-0.009	3116.5837(5)	4f ⁴	5I ₄	4f ³ (⁴ F°)5d	3H° ₄	0.000	32077.113	

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm ⁻¹)	σ (cm ⁻¹)	σ_{Ritz} (cm ⁻¹)	$\sigma - \sigma_{\text{Ritz}}$ (cm ⁻¹)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm ⁻¹)	E_u (cm ⁻¹)	Note
5	64	3.6×10^6	-2.28	0.078	32123.671(13)	32123.642(6)	0.029	3112.0694(6)	4f ⁴	⁵ I ₆	4f ³ (⁴ F°)5d	⁵ F° ₅	2387.544	34511.186	B/W
7	260	3.0×10^6	-2.37	0.222	32465.687(16)	32465.694(6)	-0.007	3079.2800(5)	4f ⁴	⁵ I ₅	4f ³ (⁴ F°)5d	⁵ F° ₄	1137.794	33603.488	
4	140	6.4×10^8	-0.04	0.274	32591.085(34)	32591.082(9)	0.003	3067.4325(8)	4f ³ (⁴ I°)6s	(¹³ ₂ , ¹ ₂)° ₇	4f ³ (⁴ I°)6p	⁵ I ₇	33906.143	66497.225	
25	620	1.0×10^7	-1.85	0.179	32606.470(9)	32606.471(5)	-0.001	3065.9848(5)	4f ⁴	⁵ I ₆	4f ³ (² H2°)5d	³ H° ₅	2387.544	34994.015	
23	450	9.5×10^6	-1.88	0.187	32766.894(10)	32766.893(5)	0.001	3050.9736(4)	4f ⁴	⁵ I ₆	4f ³ (⁴ F°)5d	³ H° ₆	2387.544	35154.437	
63	1100	1.2×10^7	-1.78	0.178	32829.311(4)	32829.311(4)	0.000	3045.1725(4)	4f ⁴	⁵ I ₄	4f ³ (⁴ G°)5d	⁵ I° ₄	0.000	32829.311	
81	1400	1.9×10^7	-1.58	0.185	32879.516(3)	32879.512(3)	0.004	3040.5229(3)	4f ⁴	⁵ I ₅	4f ³ (⁴ G°)5d	⁵ I° ₅	1137.794	34017.306	
16	280	3.0×10^6	-2.39	0.232	33135.909(16)	33135.917(5)	-0.008	3016.9945(4)	4f ⁴	⁵ I ₄	4f ³ (² H2°)5d	³ G° ₄	0.000	33135.917	
63	900	1.4×10^7	-1.72	0.193	33162.020(3)	33162.021(3)	-0.001	3014.6195(2)	4f ⁴	⁵ I ₆	4f ³ (⁴ G°)5d	⁵ I° ₆	2387.544	35549.565	
30	660	1.8×10^7	-1.61	0.323	33175.804(10)	33175.799(8)	0.005	3013.3675(7)	4f ⁴	⁵ I ₇	4f ³ (⁴ G°)5d	⁵ I° ₇	3714.548	36890.347	
6	32	1.8×10^9	0.38	0.095	33370.994(15)	33371.003(7)	-0.009	2995.7400(6)	4f ³ (⁴ I°)6s	(¹⁵ ₂ , ¹ ₂)° ₇	4f ³ (⁴ I°)6p	³ I ₇	37089.599	70460.602	
4	52	7.6×10^5	-2.99	0.202	33373.365(27)	33373.392(6)	-0.027	2995.5255(6)	4f ⁴	⁵ I ₅	4f ³ (⁴ F°)5d	⁵ F° ₅	1137.794	34511.186	
50	780	1.2×10^7	-1.79	0.240	33375.051(5)	33375.051(5)	0.000	2995.3766(5)	4f ⁴	⁵ I ₇	4f ³ (⁴ I°)6s	(¹⁵ ₂ , ¹ ₂)° ₇	3714.548	37089.599	
84	970	3.1×10^7	-1.38	0.197	33424.516(3)	33424.516(3)	0.000	2990.9436(3)	4f ⁴	⁵ I ₈	4f ³ (⁴ G°)5d	⁵ I° ₈	5093.257	38517.773	
4	64	1.9×10^9	0.40	0.277	33509.956(33)	33509.971(8)	-0.015	2983.3159(7)	4f ³ (⁴ I°)6s	(¹⁵ ₂ , ¹ ₂)° ₇	4f ³ (⁴ I°)6p	³ K ₈	37089.599	70599.570	
8	64	1.9×10^9	0.40	0.161	33570.216(14)	33570.255(9)	-0.039	2977.9584(8)	4f ³ (⁴ G°)5d	⁵ I° ₇	4f ³ (⁴ I°)6p	³ I ₇	36890.347	70460.602	B/W
3	36	1.3×10^5	-3.76	0.261	33603.468(50)	33603.488(6)	-0.020	2975.0131(5)	4f ⁴	⁵ I ₄	4f ³ (⁴ F°)5d	⁵ F° ₄	0.000	33603.488	
8	110	1.0×10^9	0.12	0.256	33650.833(16)	33650.829(7)	0.004	2970.8276(6)	4f ³ (⁴ I°)6s	(⁹ ₂ , ¹ ₂)° ₅	4f ³ (⁴ I°)6p	⁵ H ₄	30593.085	64243.914	
12	200	3.0×10^9	0.60	0.275	33660.364(12)	33660.354(8)	0.010	2969.9869(7)	4f ³ (⁴ I°)6s	(¹³ ₂ , ¹ ₂)° ₆	4f ³ (⁴ I°)6p	³ I ₆	34687.230	68347.584	
6	46	7.6×10^7	-1.00	0.214	33666.915(38)	33666.908(9)	0.007	2969.4087(8)	4f ³ (² H2°)5d	¹ H° ₅	4f ³ (⁴ I°)6p	⁵ H ₅	32605.894	66272.802	
8	90	1.6×10^9	0.32	0.229	33709.226(15)	33709.223(9)	0.003	2965.6811(8)	4f ³ (⁴ G°)5d	⁵ I° ₇	4f ³ (⁴ I°)6p	³ K ₈	36890.347	70599.570	
7	66	2.5×10^9	0.52	0.214	33736.413(18)	33736.410(8)	0.003	2963.2910(7)	4f ³ (⁴ I°)6s	(¹⁵ ₂ , ¹ ₂)° ₇	4f ³ (⁴ I°)6p	³ H ₆	37089.599	70826.009	
16	230	1.8×10^9	0.37	0.277	33757.726(9)	33757.727(6)	-0.001	2961.4197(5)	4f ³ (⁴ I°)6s	(⁹ ₂ , ¹ ₂)° ₅	4f ³ (⁴ I°)6p	³ I ₅	30593.085	64350.812	
15	170	2.8×10^9	0.56	0.219	33820.153(17)	33820.157(8)	-0.004	2955.9529(7)	4f ³ (⁴ I°)6s	(¹³ ₂ , ¹ ₂)° ₆	4f ³ (⁴ I°)6p	³ K ₇	34687.230	68507.387	
9	68	7.3×10^7	-1.02	0.168	33839.251(12)	33839.265(8)	-0.014	2954.2837(7)	4f ³ (² H2°)5d	¹ H° ₅	4f ³ (⁴ I°)6p	³ H ₄	32605.894	66445.159	
7	40	9.5×10^7	-0.91	0.124	33845.877(13)	33845.918(8)	-0.041	2953.7029(7)	4f ³ (² H2°)5d	¹ H° ₅	4f ³ (⁴ I°)6p	³ K ₆	32605.894	66451.812	B/W
5	46	7.7×10^5	-3.00	0.231	33856.227(27)	33856.221(5)	0.006	2952.8040(5)	4f ⁴	⁵ I ₅	4f ³ (² H2°)5d	³ H° ₅	1137.794	34994.015	
19	260	3.6×10^9	0.67	0.252	33925.977(14)	33925.991(9)	-0.014	2946.7312(8)	4f ³ (⁴ I°)6s	(¹³ ₂ , ¹ ₂)° ₆	4f ³ (⁴ I°)6p	³ H ₅	34687.230	68613.221	
13	160	2.1×10^9	0.44	0.240	33935.658(20)	33935.662(10)	-0.004	2945.8914(8)	4f ³ (⁴ G°)5d	⁵ I° ₇	4f ³ (⁴ I°)6p	³ H ₆	36890.347	70826.009	

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm ⁻¹)	σ (cm ⁻¹)	σ_{Ritz} (cm ⁻¹)	$\sigma - \sigma_{\text{Ritz}}$ (cm ⁻¹)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm ⁻¹)	E_u (cm ⁻¹)	Note
12	120	2.4×10^9	0.49	0.232	33963.072(20)	33963.073(10)	-0.001	2943.5137(8)	4f ³ (⁴ I°)6s	($\frac{11}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p	⁵ H ₅	32309.729	66272.802	
4	58	9.5×10^5	-2.91	0.370	34016.629(40)	34016.643(5)	-0.014	2938.8780(4)	4f ⁴	⁵ I ₅	4f ³ (⁴ F°)5d	³ H° ₆	1137.794	35154.437	
13	110	1.5×10^6	-2.71	0.202	34017.308(10)	34017.306(4)	0.002	2938.8207(3)	4f ⁴	⁵ I ₄	4f ³ (⁴ G°)5d	⁵ I° ₅	0.000	34017.306	
4	48	8.3×10^7	-0.97	0.284	34068.143(33)	34068.177(5)	-0.034	2934.4323(5)	4f ³ (⁴ F°)5d	⁵ H° ₅	4f ³ (⁴ I°)6p	⁵ H ₄	30175.737	64243.914	
22	190	2.9×10^9	0.57	0.210	34135.428(6)	34135.430(11)	-0.002	2928.6506(9)	4f ³ (⁴ I°)6s	($\frac{11}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p	³ H ₄	32309.729	66445.159	B/W
14	130	2.2×10^9	0.45	0.227	34142.083(9)	34142.083(8)	0.000	2928.0799(7)	4f ³ (⁴ I°)6s	($\frac{11}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p	³ K ₆	32309.729	66451.812	
9	56	3.0×10^8	-0.41	0.173	34175.085(13)	34175.075(5)	0.010	2925.2531(4)	4f ³ (⁴ F°)5d	⁵ H° ₅	4f ³ (⁴ I°)6p	³ I ₅	30175.737	64350.812	
11	140	1.3×10^9	0.22	0.318	34197.132(28)	34197.144(10)	-0.012	2923.3652(8)	4f ³ (⁴ I°)6s	($\frac{11}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p	⁵ H ₅	32075.658	66272.802	
33	410	6.9×10^9	0.94	0.418	34301.184(10)	34301.181(9)	0.003	2914.4981(8)	4f ³ (⁴ I°)6s	($\frac{15}{2}, \frac{1}{2}$)° ₈	4f ³ (⁴ I°)6p	⁵ K ₉	35839.828	70141.009	
5	34	8.4×10^4	-3.97	0.200	34305.530(24)	34305.512(12)	0.018	2914.1301(10)	4f ³ (⁴ I°)6p	³ H ₆	4f ³ (⁴ I°)7s	($\frac{11}{2}, \frac{1}{2}$)° ₆	70826.009	105131.521	
25	260	2.0×10^9	0.40	0.290	34370.689(12)	34370.692(7)	-0.003	2908.6036(6)	4f ³ (⁴ I°)6s	($\frac{9}{2}, \frac{1}{2}$)° ₄	4f ³ (⁴ I°)6p	⁵ H ₄	29873.222	64243.914	
17	170	2.0×10^9	0.40	0.272	34376.165(17)	34376.154(8)	0.011	2908.1414(7)	4f ³ (⁴ I°)6s	($\frac{11}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p	³ K ₆	32075.658	66451.812	
32	350	5.5×10^9	0.84	0.298	34396.521(9)	34396.521(8)	0.000	2906.4194(6)	4f ³ (⁴ I°)6s	($\frac{13}{2}, \frac{1}{2}$)° ₇	4f ³ (⁴ I°)6p	⁵ K ₈	33906.143	68302.664	
13	110	1.5×10^6	-2.72	0.184	34411.788(19)	34411.771(4)	0.017	2905.1313(3)	4f ⁴	⁵ I ₅	4f ³ (⁴ G°)5d	⁵ I° ₆	1137.794	35549.565	
25	250	3.3×10^9	0.62	0.319	34421.561(12)	34421.567(8)	-0.006	2904.3045(7)	4f ³ (⁴ I°)6s	($\frac{11}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p	⁵ I ₇	32075.658	66497.225	
33	260	3.1×10^9	0.59	0.235	34430.549(8)	34430.548(6)	0.001	2903.5469(5)	4f ³ (⁴ I°)6s	($\frac{9}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p	⁵ H ₆	30593.085	65023.633	
8	78	1.5×10^9	0.28	0.295	34441.432(17)	34441.441(9)	-0.009	2902.6285(8)	4f ³ (⁴ I°)6s	($\frac{13}{2}, \frac{1}{2}$)° ₇	4f ³ (⁴ I°)6p	³ I ₆	33906.143	68347.584	
30	300	2.6×10^9	0.52	0.299	34474.470(10)	34474.477(7)	-0.007	2899.8469(6)	4f ³ (⁴ I°)6s	($\frac{9}{2}, \frac{1}{2}$)° ₄	4f ³ (⁴ I°)6p	⁵ H ₃	29873.222	64347.699	
17	160	1.4×10^9	0.25	0.300	34477.598(9)	34477.590(6)	0.008	2899.5850(5)	4f ³ (⁴ I°)6s	($\frac{9}{2}, \frac{1}{2}$)° ₄	4f ³ (⁴ I°)6p	³ I ₅	29873.222	64350.812	
5	48	1.4×10^6	-2.75	0.348	34502.789(35)	34502.803(8)	-0.014	2897.4660(7)	4f ⁴	⁵ I ₆	4f ³ (⁴ G°)5d	⁵ I° ₇	2387.544	36890.347	
16	160	2.2×10^9	0.44	0.291	34601.241(18)	34601.244(9)	-0.003	2889.2223(7)	4f ³ (⁴ I°)6s	($\frac{13}{2}, \frac{1}{2}$)° ₇	4f ³ (⁴ I°)6p	³ K ₇	33906.143	68507.387	
7	98	1.6×10^9	0.30	0.463	34620.748(51)	34620.774(12)	-0.026	2887.5924(10)	4f ³ (⁴ I°)6s	($\frac{15}{2}, \frac{1}{2}$)° ₈	4f ³ (⁴ I°)6p	³ I ₇	35839.828	70460.602	
14	130	1.2×10^9	0.18	0.280	34641.835(20)	34641.855(9)	-0.020	2885.8351(7)	4f ³ (⁴ I°)6s	($\frac{11}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p	⁵ H ₇	32075.658	66717.513	
16	140	2.5×10^9	0.49	0.303	34759.736(19)	34759.742(11)	-0.006	2876.0474(9)	4f ³ (⁴ I°)6s	($\frac{15}{2}, \frac{1}{2}$)° ₈	4f ³ (⁴ I°)6p	³ K ₈	35839.828	70599.570	
8	44	1.5×10^6	-2.73	0.201	34803.218(15)	34803.225(4)	-0.007	2872.4539(3)	4f ⁴	⁵ I ₇	4f ³ (⁴ G°)5d	⁵ I° ₈	3714.548	38517.773	
4	16	3.2×10^7	-1.40	0.151	34846.519(25)	34846.491(6)	0.028	2868.8872(5)	4f ³ (² H ²)5d	³ I° ₅	4f ³ (⁴ I°)6p	⁵ H ₄	29397.423	64243.914	
14	66	3.5×10^8	-0.36	0.169	34847.905(16)	34847.896(5)	0.009	2868.7716(4)	4f ³ (⁴ F°)5d	⁵ H° ₅	4f ³ (⁴ I°)6p	⁵ H ₆	30175.737	65023.633	
526	2600	3.9×10^7	-1.32	0.189	34856.862(3)	34856.862(3)	0.000	2868.0336(2)	4f ⁴	⁵ I ₄	4f ³ (² G ¹)5d	³ G° ₃	0.000	34856.862	
566	2700	5.5×10^7	-1.17	0.191	35097.386(3)	35097.385(3)	0.001	2848.3780(2)	4f ⁴	⁵ I ₅	4f ³ (⁴ G°)5d	⁵ H° ₄	1137.794	36235.179	

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm ⁻¹)	σ (cm ⁻¹)	σ_{Ritz} (cm ⁻¹)	$\sigma - \sigma_{\text{Ritz}}$ (cm ⁻¹)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm ⁻¹)	E_u (cm ⁻¹)	Note
6	20	8.1×10^7	-1.01	0.144	35136.934(17)	35136.924(13)	0.010	2845.1726(11)	4f ³ (⁴ F°)5d	5G° ₆	4f ³ (⁴ I°)6p	3I ₆	33210.660	68347.584	B/W
825	3900	1.2×10^8	-0.84	0.202	35205.216(3)	35205.215(3)	0.001	2839.6533(2)	4f ⁴	5I ₆	4f ³ (⁴ G°)5d	5H° ₅	2387.544	37592.759	
12	62	1.3×10^7	-1.80	0.187	35223.022(19)	35223.028(9)	-0.006	2838.2171(7)	4f ⁴	5F ₄	4f ³ (⁴ D°)5d	5F° ₄	12181.327	47404.355	
6	22	1.2×10^8	-0.84	0.154	35272.316(16)	35272.324(12)	-0.008	2834.2503(10)	4f ³ (² H2°)5d	3I° ₇	4f ³ (⁴ I°)6p	3I ₇	35188.278	70460.602	
687	3300	1.4×10^8	-0.77	0.213	35343.724(3)	35343.726(3)	-0.002	2828.5242(2)	4f ⁴	5I ₇	4f ³ (⁴ G°)5d	5H° ₆	3714.548	39058.274	
324	1400	3.8×10^7	-1.34	0.196	35379.556(3)	35379.556(3)	0.000	2825.6595(2)	4f ⁴	5I ₅	4f ³ (² H2°)5d	1G° ₄	1137.794	36517.350	
7	22	4.6×10^7	-1.26	0.146	35402.559(15)	35402.561(12)	-0.002	2823.8233(10)	4f ³ (⁴ F°)5d	5G° ₆	4f ³ (⁴ I°)6p	3H ₅	33210.660	68613.221	
449	2200	1.5×10^8	-0.75	0.224	35411.826(3)	35411.825(3)	0.001	2823.0845(2)	4f ⁴	5I ₈	4f ³ (⁴ G°)5d	5H° ₇	5093.257	40505.082	
358	1500	3.5×10^7	-1.38	0.195	35435.076(3)	35435.076(3)	0.000	2821.2321(2)	4f ⁴	5I ₅	4f ³ (⁴ G°)5d	5G° ₄	1137.794	36572.870	
712	2900	6.9×10^7	-1.09	0.198	35576.327(3)	35576.326(3)	0.001	2810.0303(2)	4f ⁴	5I ₄	4f ³ (⁴ G°)5d	5H° ₃	0.000	35576.326	
122	510	1.7×10^7	-1.70	0.200	35590.099(3)	35590.097(3)	0.002	2808.9429(2)	4f ⁴	5I ₆	4f ³ (⁴ G°)5d	5G° ₅	2387.544	37977.641	
9	24	1.1×10^8	-0.89	0.130	35626.221(11)	35626.210(5)	0.011	2806.0954(4)	4f ³ (² H2°)5d	3I° ₅	4f ³ (⁴ I°)6p	5H ₆	29397.423	65023.633	
4	18	3.0×10^8	-0.46	0.273	35852.058(39)	35852.074(8)	-0.016	2788.4165(6)	4f ³ (⁴ I°)6s	($\frac{9}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p	3H ₄	30593.085	66445.159	
117	480	3.5×10^7	-1.39	0.215	35896.840(3)	35896.841(3)	-0.001	2784.9389(2)	4f ⁴	5I ₇	4f ³ (⁴ G°)5d	5G° ₆	3714.548	39611.389	
263	1100	6.5×10^7	-1.13	0.216	36166.770(2)	36166.770(2)	0.000	2764.1525(2)	4f ⁴	5I ₈	4f ³ (² K°)5d	3I° ₇	5093.257	41260.027	
50	210	4.5×10^6	-2.29	0.223	36235.176(5)	36235.179(4)	-0.003	2758.9338(3)	4f ⁴	5I ₄	4f ³ (⁴ G°)5d	5H° ₄	0.000	36235.179	
97	350	1.2×10^7	-1.87	0.204	36454.964(3)	36454.965(3)	-0.001	2742.2993(2)	4f ⁴	5I ₅	4f ³ (⁴ G°)5d	5H° ₅	1137.794	37592.759	
30	140	3.4×10^6	-2.42	0.258	36517.349(9)	36517.350(4)	-0.001	2737.6142(3)	4f ⁴	5I ₄	4f ³ (² H2°)5d	1G° ₄	0.000	36517.350	
29	130	2.6×10^6	-2.54	0.235	36572.872(9)	36572.870(4)	0.002	2733.4581(3)	4f ⁴	5I ₄	4f ³ (⁴ G°)5d	5G° ₄	0.000	36572.870	
58	210	9.6×10^6	-1.97	0.213	36670.732(5)	36670.730(4)	0.002	2726.1632(3)	4f ⁴	5I ₆	4f ³ (⁴ G°)5d	5H° ₆	2387.544	39058.274	
14	58	4.8×10^5	-3.27	0.304	36783.949(20)	36783.937(11)	0.012	2717.7727(8)	4f ³ (⁴ I°)6p	3I ₆	4f ³ (⁴ I°)7s ($\frac{11}{2}, \frac{1}{2}$)° ₆	($\frac{11}{2}, \frac{1}{2}$)° ₆	68347.584	105131.521	
21	74	6.4×10^6	-2.15	0.189	36790.531(6)	36790.534(4)	-0.003	2717.2853(3)	4f ⁴	5I ₇	4f ³ (⁴ G°)5d	5H° ₇	3714.548	40505.082	
18	74	2.4×10^6	-2.58	0.231	36839.837(14)	36839.847(4)	-0.010	2713.6478(3)	4f ⁴	5I ₅	4f ³ (⁴ G°)5d	5G° ₅	1137.794	37977.641	
4	14	3.2×10^7	-1.46	0.230	37180.083(34)	37180.095(5)	-0.012	2688.8129(4)	4f ³ (⁴ I°)5d	3K° ₈	4f ³ (⁴ I°)6p	5K ₇	27441.911	64622.006	
13	48	3.4×10^6	-2.43	0.213	37223.863(18)	37223.845(4)	0.018	2685.6525(3)	4f ⁴	5I ₆	4f ³ (⁴ G°)5d	5G° ₆	2387.544	39611.389	
2	6	6.4×10^7	-1.16	0.170	37326.829(52)	37326.835(12)	-0.006	2678.2420(9)	4f ³ (⁴ I°)6p	3K ₈	4f ³ (⁴ I°)6d	5K° ₈	70599.570	107926.405	
4	18	3.8×10^7	-1.39	0.286	37405.983(34)	37405.994(6)	-0.011	2672.5739(4)	4f ³ (⁴ I°)5d	3K° ₆	4f ³ (⁴ I°)6p	5K ₅	23120.073	60526.067	
21	78	2.8×10^6	-2.53	0.214	37545.482(12)	37545.479(3)	0.003	2662.6445(2)	4f ⁴	5I ₇	4f ³ (² K°)5d	3I° ₇	3714.548	41260.027	
20	58	4.7×10^8	-0.31	0.171	37914.700(11)	37914.703(7)	-0.003	2636.7134(5)	4f ³ (⁴ I°)5d	3L° ₉	4f ³ (⁴ I°)6p	5I ₈	28877.321	66792.024	

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm ⁻¹)	σ (cm ⁻¹)	σ_{Ritz} (cm ⁻¹)	$\sigma - \sigma_{\text{Ritz}}$ (cm ⁻¹)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Lower Level Term _J	Upper Level Config.	Upper Level Term _J	E_l (cm ⁻¹)	E_u (cm ⁻¹)	Note
77	240	2.7×10^8	-0.55	0.203	37945.292(2)	37945.321(9)	-0.029	2634.5857(6)	4f ³ (⁴ I°)5d	³ L° ₈	4f ³ (⁴ I°)6p	⁵ K ₇	26676.685	64622.006	B/W
10	28	1.3×10^8	-0.87	0.188	38023.476(12)	38023.481(6)	-0.005	2629.1698(4)	4f ³ (⁴ I°)5d	³ L° ₇	4f ³ (⁴ I°)6p	⁵ K ₆	24497.165	62520.646	
4	20	7.4×10^6	-2.12	0.288	38177.860(32)	38177.851(23)	0.009	2618.5383(16)	4f ³ (⁴ G°)5d	⁵ H° ₆	4f ³ (² H ² °)6p	¹ I ₆	39058.274	77236.125	
4	8	4.5×10^7	-1.34	0.111	38220.125(21)	38220.115(9)	0.010	2615.6425(6)	4f ³ (² H ² °)5d	¹ H° ₅	4f ³ (⁴ I°)6p	³ H ₆	32605.894	70826.009	B/W
9	30	2.8×10^6	-2.54	0.160	38269.063(23)	38269.079(12)	-0.016	2612.2957(8)	4f ³ (⁴ I°)6p	³ I ₇	4f ³ (⁴ I°)6d	³ K° ₇	70460.602	108729.681	
18	62	2.2×10^9	0.35	0.214	38311.840(7)	38311.836(6)	0.004	2609.3801(4)	4f ³ (⁴ I°)6p	⁵ H ₆	4f ³ (⁴ I°)7s	(⁹ ₂ , ¹ ₂)° ₅	65023.633	103335.469	
6	26	7.6×10^8	-0.11	0.283	38414.015(24)	38414.008(11)	0.007	2602.4394(7)	4f ³ (⁴ I°)6p	⁵ H ₇	4f ³ (⁴ I°)7s	(¹¹ ₂ , ¹ ₂)° ₆	66717.513	105131.521	
7	24	1.5×10^9	0.18	0.239	38468.583(19)	38468.575(11)	0.008	2598.7476(7)	4f ³ (⁴ I°)6p	³ K ₈	4f ³ (⁴ I°)7s	(¹⁵ ₂ , ¹ ₂)° ₈	70599.570	109068.145	
8	34	1.3×10^9	0.12	0.288	38550.940(18)	38550.960(9)	-0.020	2593.1936(6)	4f ³ (⁴ I°)6p	³ K ₇	4f ³ (⁴ I°)7s	(¹³ ₂ , ¹ ₂)° ₇	68507.387	107058.347	
11	46	2.7×10^9	0.43	0.211	38564.806(22)	38564.829(12)	-0.023	2592.2610(8)	4f ³ (⁴ I°)6p	³ H ₆	4f ³ (⁴ I°)7s	(¹⁵ ₂ , ¹ ₂)° ₇	70826.009	109390.838	
3	16	8.4×10^8	-0.07	0.317	38607.569(48)	38607.543(12)	0.026	2589.3928(8)	4f ³ (⁴ I°)6p	³ I ₇	4f ³ (⁴ I°)7s	(¹⁵ ₂ , ¹ ₂)° ₈	70460.602	109068.145	
11	48	2.3×10^9	0.36	0.247	38619.638(23)	38619.630(13)	0.008	2588.5824(9)	4f ³ (⁴ I°)6p	³ H ₅	4f ³ (⁴ I°)7s	(¹³ ₂ , ¹ ₂)° ₆	68613.221	107232.851	
12	46	2.0×10^9	0.30	0.245	38634.274(23)	38634.296(11)	-0.022	2587.5997(7)	4f ³ (⁴ I°)6p	⁵ I ₇	4f ³ (⁴ I°)7s	(¹¹ ₂ , ¹ ₂)° ₆	66497.225	105131.521	
2	8	2.4×10^8	-0.62	0.258	38671.451(76)	38671.445(8)	0.006	2585.1138(5)	4f ³ (⁴ I°)6p	⁵ H ₆	4f ³ (⁴ I°)6d	⁵ L° ₆	65023.633	103695.078	
8	28	1.2×10^9	0.08	0.237	38673.076(17)	38673.073(10)	0.003	2585.0049(7)	4f ³ (⁴ I°)6p	³ K ₆	4f ³ (⁴ I°)7s	(¹¹ ₂ , ¹ ₂)° ₅	66451.812	105124.885	
21	70	1.2×10^9	0.08	0.213	38679.725(6)	38679.709(11)	0.016	2584.5614(7)	4f ³ (⁴ I°)6p	³ K ₆	4f ³ (⁴ I°)7s	(¹¹ ₂ , ¹ ₂)° ₆	66451.812	105131.521	B/W
21	70	1.9×10^9	0.28	0.213	38679.725(6)	38679.726(11)	-0.001	2584.5603(7)	4f ³ (⁴ I°)6p	³ H ₄	4f ³ (⁴ I°)7s	(¹¹ ₂ , ¹ ₂)° ₅	66445.159	105124.885	B/W
4	14	7.9×10^8	-0.10	0.226	38710.735(30)	38710.763(9)	-0.028	2582.4879(6)	4f ³ (⁴ I°)6p	³ I ₆	4f ³ (⁴ I°)7s	(¹³ ₂ , ¹ ₂)° ₇	68347.584	107058.347	
7	34	1.7×10^9	0.23	0.289	38725.451(19)	38725.464(12)	-0.013	2581.5075(8)	4f ³ (⁴ I°)6p	³ K ₇	4f ³ (⁴ I°)7s	(¹³ ₂ , ¹ ₂)° ₆	68507.387	107232.851	
5	22	8.5×10^8	-0.07	0.256	38734.943(25)	38734.953(10)	-0.010	2580.8751(7)	4f ³ (⁴ I°)6p	³ I ₅	4f ³ (⁴ I°)7s	(⁹ ₂ , ¹ ₂)° ₄	64350.812	103085.765	
11	40	1.4×10^9	0.15	0.221	38738.062(11)	38738.066(9)	-0.004	2580.6677(6)	4f ³ (⁴ I°)6p	⁵ H ₃	4f ³ (⁴ I°)7s	(⁹ ₂ , ¹ ₂)° ₄	64347.699	103085.765	
19	80	3.3×10^9	0.52	0.219	38755.688(7)	38755.683(7)	0.005	2579.4945(4)	4f ³ (⁴ I°)6p	⁵ K ₈	4f ³ (⁴ I°)7s	(¹³ ₂ , ¹ ₂)° ₇	68302.664	107058.347	
8	36	2.2×10^9	0.34	0.289	38791.265(18)	38791.268(11)	-0.003	2577.1281(7)	4f ³ (⁴ I°)6p	³ K ₈	4f ³ (⁴ I°)7s	(¹⁵ ₂ , ¹ ₂)° ₇	70599.570	109390.838	
10	42	1.2×10^9	0.08	0.207	38841.868(23)	38841.851(10)	0.017	2573.7717(7)	4f ³ (⁴ I°)6p	⁵ H ₄	4f ³ (⁴ I°)7s	(⁹ ₂ , ¹ ₂)° ₄	64243.914	103085.765	
11	50	1.6×10^9	0.20	0.229	38852.077(11)	38852.083(9)	-0.006	2573.0938(6)	4f ³ (⁴ I°)6p	⁵ H ₅	4f ³ (⁴ I°)7s	(¹¹ ₂ , ¹ ₂)° ₅	66272.802	105124.885	
5	18	7.6×10^8	-0.12	0.226	38858.717(25)	38858.719(12)	-0.002	2572.6544(8)	4f ³ (⁴ I°)6p	⁵ H ₅	4f ³ (⁴ I°)7s	(¹¹ ₂ , ¹ ₂)° ₆	66272.802	105131.521	
8	28	1.9×10^9	0.28	0.236	38885.273(17)	38885.267(12)	0.006	2570.8979(8)	4f ³ (⁴ I°)6p	³ I ₆	4f ³ (⁴ I°)7s	(¹³ ₂ , ¹ ₂)° ₆	68347.584	107232.851	
17	66	4.2×10^9	0.62	0.191	38927.126(14)	38927.136(11)	-0.010	2568.1325(7)	4f ³ (⁴ I°)6p	⁵ K ₉	4f ³ (⁴ I°)7s	(¹⁵ ₂ , ¹ ₂)° ₈	70141.009	109068.145	
8	30	2.2×10^9	0.34	0.231	38930.244(15)	38930.236(11)	0.008	2567.9280(7)	4f ³ (⁴ I°)6p	³ I ₇	4f ³ (⁴ I°)7s	(¹⁵ ₂ , ¹ ₂)° ₇	70460.602	109390.838	

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm ⁻¹)	σ (cm ⁻¹)	σ_{Ritz} (cm ⁻¹)	$\sigma - \sigma_{\text{Ritz}}$ (cm ⁻¹)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm ⁻¹)	E_u (cm ⁻¹)	Note
9	36	1.4×10^9	0.14	0.263	38984.644(16)	38984.657(8)	-0.013	2564.3430(5)	4f ³ (4f ^o)6p	³ I ₅	4f ³ (4f ^o)7s	(⁹ / ₂ ; ¹ / ₂) ^o ₅	64350.812	103335.469	
4	20	6.6×10^8	-0.19	0.310	39091.547(37)	39091.555(8)	-0.008	2557.3303(5)	4f ³ (4f ^o)6p	⁵ H ₄	4f ³ (4f ^o)7s	(⁹ / ₂ ; ¹ / ₂) ^o ₅	64243.914	103335.469	
4	10	3.1×10^7	-1.52	0.157	39147.104(28)	39147.081(4)	0.023	2553.7027(3)	4f ³ (4f ^o)5d	³ H ^o ₄	4f ³ (4f ^o)6p	⁵ I ₄	21491.882	60638.963	
11	36	9.0×10^7	-1.06	0.167	39159.551(19)	39159.559(4)	-0.008	2552.8889(3)	4f ³ (4f ^o)5d	⁵ G ^o ₃	4f ³ (4f ^o)6p	⁵ I ₄	21479.404	60638.963	
4	8	1.2×10^9	0.07	0.143	39232.902(27)	39232.891(10)	0.011	2548.1169(6)	4f ³ (4f ^o)6p	³ K ₈	4f ³ (4f ^o)6d	⁵ K ^o ₉	70599.570	109832.461	
3	14	9.9×10^7	-1.02	0.317	39266.741(54)	39266.792(8)	-0.051	2545.9168(5)	4f ³ (² G1 ^o)5d	³ H ^o ₆	4f ³ (4f ^o)6p	³ H ₆	31559.217	70826.009	
6	22	1.7×10^8	-0.78	0.236	39275.612(22)	39275.602(5)	0.010	2545.3457(4)	4f ³ (4f ^o)5d	³ K ^o ₈	4f ³ (4f ^o)6p	⁵ H ₇	27441.911	66717.513	
19	78	1.6×10^9	0.19	0.209	39344.273(13)	39344.266(7)	0.007	2540.9033(5)	4f ³ (4f ^o)6p	³ I ₅	4f ³ (4f ^o)6d	⁵ L ^o ₆	64350.812	103695.078	
3	16	7.7×10^8	-0.13	0.310	39359.879(47)	39359.852(15)	0.027	2539.8970(10)	4f ³ (4f ^o)6p	⁵ H ₇	4f ³ (4f ^o)6d	⁵ K ^o ₇	66717.513	106077.365	
5	18	1.1×10^9	0.03	0.229	39360.314(25)	39360.302(21)	0.012	2539.8680(14)	4f ³ (4f ^o)6p	³ K ₈	4f ³ (4f ^o)6d	⁵ I ^o ₈	70599.570	109959.872	
9	22	1.4×10^9	0.13	0.161	39408.556(12)	39408.558(9)	-0.002	2536.7577(6)	4f ³ (4f ^o)6p	⁵ H ₄	4f ³ (4f ^o)6d	⁵ K ^o ₅	64243.914	103652.472	
3	12	7.4×10^8	-0.15	0.296	39413.697(54)	39413.729(15)	-0.032	2536.4249(10)	4f ³ (4f ^o)6p	³ H ₅	4f ³ (4f ^o)6d	⁵ I ^o ₆	68613.221	108026.950	
3	10	8.3×10^8	-0.10	0.202	39419.054(39)	39419.018(11)	0.036	2536.0845(7)	4f ³ (4f ^o)6p	³ K ₇	4f ³ (4f ^o)6d	⁵ K ^o ₈	68507.387	107926.405	
9	34	3.5×10^8	-0.47	0.227	39425.350(14)	39425.343(8)	0.007	2535.6776(5)	4f ³ (4f ^o)5d	³ L ^o ₉	4f ³ (4f ^o)6p	⁵ K ₈	28877.321	68302.664	
3	16	4.9×10^8	-0.33	0.306	39536.921(44)	39536.930(11)	-0.009	2528.5206(7)	4f ³ (4f ^o)6p	⁵ H ₆	4f ³ (4f ^o)6d	³ I ^o ₅	65023.633	104560.563	
9	26	2.1×10^9	0.30	0.151	39580.118(22)	39580.140(15)	-0.022	2525.7600(10)	4f ³ (4f ^o)6p	⁵ I ₇	4f ³ (4f ^o)6d	⁵ K ^o ₇	66497.225	106077.365	
12	34	2.4×10^9	0.36	0.164	39588.687(18)	39588.691(10)	-0.004	2525.2144(6)	4f ³ (4f ^o)6p	⁵ H ₆	4f ³ (4f ^o)6d	⁵ K ^o ₆	65023.633	104612.324	
3	12	9.2×10^8	-0.06	0.209	39603.397(36)	39603.423(32)	-0.026	2524.2750(20)	4f ³ (4f ^o)6p	⁵ K ₈	4f ³ (4f ^o)6d	⁵ I ^o ₇	68302.664	107906.087	B/W
4	14	1.1×10^9	0.02	0.211	39607.006(31)	39606.980(19)	0.026	2524.0483(12)	4f ³ (4f ^o)6p	³ H ₄	4f ³ (4f ^o)6d	⁵ I ^o ₅	66445.159	106052.139	B/W
13	52	4.4×10^9	0.62	0.217	39623.736(20)	39623.741(11)	-0.005	2522.9805(7)	4f ³ (4f ^o)6p	⁵ K ₈	4f ³ (4f ^o)6d	⁵ K ^o ₈	68302.664	107926.405	
8	22	8.7×10^7	-1.08	0.167	39629.810(14)	39629.816(9)	-0.006	2522.5938(6)	4f ³ (4f ^o)5d	⁵ G ^o ₄	4f ³ (4f ^o)6p	⁵ I ₅	23010.450	62640.266	
5	14	6.9×10^7	-1.18	0.190	39671.200(25)	39671.208(10)	-0.008	2519.9616(6)	4f ³ (4f ^o)5d	⁵ G ^o ₅	4f ³ (4f ^o)6p	⁵ I ₆	24878.412	64549.620	
16	72	6.2×10^9	0.77	0.219	39691.450(8)	39691.452(8)	-0.002	2518.6762(5)	4f ³ (4f ^o)6p	⁵ K ₉	4f ³ (4f ^o)6d	⁵ K ^o ₉	70141.009	109832.461	
13	34	2.5×10^9	0.38	0.106	39692.839(14)	39692.840(9)	-0.001	2518.5881(5)	4f ³ (4f ^o)6p	⁵ H ₇	4f ³ (4f ^o)6d	⁵ L ^o ₈	66717.513	106410.353	
6	34	4.7×10^7	-1.35	0.325	39726.740(24)	39726.718(6)	0.022	2516.4402(4)	4f ³ (4f ^o)5d	³ I ^o ₆	4f ³ (4f ^o)6p	⁵ K ₅	20799.349	60526.067	
31	100	7.2×10^9	0.83	0.189	39774.270(4)	39774.270(4)	0.000	2513.4315(3)	4f ³ (4f ^o)6p	⁵ H ₆	4f ³ (4f ^o)6d	⁵ L ^o ₇	65023.633	104797.903	
7	26	1.4×10^9	0.12	0.220	39782.705(18)	39782.705(13)	0.000	2512.8985(8)	4f ³ (4f ^o)6p	⁵ H ₃	4f ³ (4f ^o)6d	⁵ I ^o ₄	64347.699	104130.404	
4	20	8.3×10^7	-1.11	0.316	39817.843(39)	39817.869(5)	-0.026	2510.6792(3)	4f ³ (4f ^o)5d	⁵ I ^o ₇	4f ³ (4f ^o)6p	⁵ K ₆	22702.777	62520.646	
4	26	1.5×10^9	0.15	0.366	39818.834(39)	39818.863(22)	-0.029	2510.6165(14)	4f ³ (4f ^o)6p	⁵ K ₉	4f ³ (4f ^o)6d	⁵ I ^o ₈	70141.009	109959.872	

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm^{-1})	σ (cm^{-1})	σ_{Ritz} (cm^{-1})	$\sigma - \sigma_{\text{Ritz}}$ (cm^{-1})	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm^{-1})	E_u (cm^{-1})	Note
16	58	3.8×10^8	-0.44	0.172	39820.539(7)	39820.540(9)	-0.001	2510.5107(6)	4f ³ (4f ^o)5d	3L ^o ₈	4f ³ (4f ^o)6p	5I ₇	26676.685	66497.225	B/W
16	58	9.8×10^8	-0.03	0.172	39820.539(7)	39820.528(13)	0.011	2510.5115(8)	4f ³ (4f ^o)6p	3H ₄	4f ³ (4f ^o)6d	5H ^o ₄	66445.159	106265.687	B/W
3	14	1.8×10^9	0.23	0.255	39843.399(39)	39843.377(15)	0.022	2509.0717(9)	4f ³ (4f ^o)6p	3H ₆	4f ³ (4f ^o)6d	3I ^o ₇	70826.009	110669.386	
3	8	6.5×10^8	-0.21	0.136	39886.478(29)	39886.490(13)	-0.012	2506.3595(8)	4f ³ (4f ^o)6p	5H ₄	4f ³ (4f ^o)6d	5I ^o ₄	64243.914	104130.404	
35	120	1.3×10^{10}	1.09	0.196	39907.230(4)	39907.230(4)	0.000	2505.0568(2)	4f ³ (4f ^o)6p	5K ₈	4f ³ (4f ^o)6d	5L ^o ₉	68302.664	108209.894	
27	110	7.9×10^9	0.87	0.197	39913.128(9)	39913.128(8)	0.000	2504.6866(5)	4f ³ (4f ^o)6p	5I ₇	4f ³ (4f ^o)6d	5L ^o ₈	66497.225	106410.353	
5	10	1.4×10^9	0.12	0.135	39955.080(21)	39955.090(12)	-0.010	2502.0559(8)	4f ³ (4f ^o)6p	3H ₅	4f ³ (4f ^o)6d	5H ^o ₆	68613.221	108568.311	
37	130	1.7×10^{10}	1.20	0.192	39984.385(4)	39984.385(4)	0.000	2500.2227(2)	4f ³ (4f ^o)6p	5K ₉	4f ³ (4f ^o)6d	5L ^o ₁₀	70141.009	110125.394	
4	22	3.7×10^8	-0.46	0.317	39992.907(37)	39992.885(13)	0.022	2499.6912(8)	4f ³ (4f ^o)6p	5H ₅	4f ³ (4f ^o)6d	5H ^o ₄	66272.802	106265.687	
9	24	1.8×10^9	0.23	0.158	40032.238(12)	40032.221(110)	0.017	2497.2348(69)	4f ³ (4f ^o)6p	5H ₃	4f ³ (4f ^o)6d	5H ^o ₃	64347.699	104379.920	
13	46	3.0×10^8	-0.55	0.154	40040.832(17)	40040.828(9)	0.004	2496.6980(5)	4f ³ (4f ^o)5d	3L ^o ₈	4f ³ (4f ^o)6p	5H ₇	26676.685	66717.513	
7	38	1.8×10^8	-0.77	0.311	40047.062(21)	40047.052(8)	0.010	2496.3100(5)	4f ³ (4f ^o)5d	5G ^o ₆	4f ³ (4f ^o)6p	5H ₇	26670.461	66717.513	
6	22	1.8×10^9	0.23	0.194	40060.937(19)	40060.924(11)	0.013	2495.4455(7)	4f ³ (4f ^o)6p	3K ₇	4f ³ (4f ^o)6d	5H ^o ₆	68507.387	108568.311	
3	14	2.0×10^9	0.27	0.264	40069.799(43)	40069.816(15)	-0.017	2494.8917(9)	4f ³ (4f ^o)6p	3K ₈	4f ³ (4f ^o)6d	3I ^o ₇	70599.570	110669.386	
7	32	1.7×10^9	0.20	0.270	40109.115(21)	40109.095(9)	0.020	2492.4483(6)	4f ³ (4f ^o)6p	3K ₆	4f ³ (4f ^o)6d	5H ^o ₅	66451.812	106560.907	
4	22	9.0×10^8	-0.08	0.304	40115.747(36)	40115.748(10)	-0.001	2492.0349(6)	4f ³ (4f ^o)6p	3H ₄	4f ³ (4f ^o)6d	5H ^o ₅	66445.159	106560.907	
26	94	8.4×10^9	0.89	0.188	40148.647(5)	40148.648(5)	-0.001	2489.9926(3)	4f ³ (4f ^o)6p	3K ₆	4f ³ (4f ^o)6d	3L ^o ₇	66451.812	106600.460	
16	66	4.6×10^9	0.63	0.188	40151.999(14)	40151.993(12)	0.006	2489.7852(7)	4f ³ (4f ^o)6p	3K ₆	4f ³ (4f ^o)6d	3K ^o ₆	66451.812	106603.805	
11	50	5.2×10^9	0.68	0.242	40184.298(12)	40184.289(10)	0.009	2487.7840(6)	4f ³ (4f ^o)6p	3H ₆	4f ³ (4f ^o)6d	3H ^o ₆	70826.009	111010.298	
17	78	7.3×10^9	0.83	0.204	40208.783(14)	40208.784(13)	-0.001	2486.2683(8)	4f ³ (4f ^o)6p	3I ₇	4f ³ (4f ^o)6d	3I ^o ₇	70460.602	110669.386	
19	60	4.4×10^9	0.61	0.164	40209.753(12)	40209.751(10)	0.002	2486.2085(6)	4f ³ (4f ^o)6p	3I ₅	4f ³ (4f ^o)6d	3I ^o ₅	64350.812	104560.563	
16	62	6.3×10^9	0.77	0.166	40220.725(14)	40220.727(10)	-0.002	2485.5300(6)	4f ³ (4f ^o)6p	3I ₆	4f ³ (4f ^o)6d	5H ^o ₆	68347.584	108568.311	
14	60	5.0×10^9	0.67	0.219	40222.282(17)	40222.294(11)	-0.012	2485.4332(7)	4f ³ (4f ^o)6p	3K ₇	4f ³ (4f ^o)6d	3K ^o ₇	68507.387	108729.681	
24	120	4.2×10^9	0.59	0.229	40239.744(6)	40239.745(6)	-0.001	2484.3552(3)	4f ³ (4f ^o)6p	3H ₅	4f ³ (4f ^o)6d	3H ^o ₅	68613.221	108852.966	
4	18	8.7×10^8	-0.09	0.243	40248.244(31)	40248.283(7)	-0.039	2483.8282(4)	4f ³ (4f ^o)6p	5I ₆	4f ³ (4f ^o)6d	5L ^o ₇	64549.620	104797.903	B/W
21	78	4.7×10^9	0.64	0.191	40261.514(11)	40261.512(9)	0.002	2483.0120(6)	4f ³ (4f ^o)6p	3I ₅	4f ³ (4f ^o)6d	5K ^o ₆	64350.812	104612.324	
17	62	5.0×10^9	0.66	0.199	40288.102(7)	40288.105(7)	-0.003	2481.3729(4)	4f ³ (4f ^o)6p	5H ₅	4f ³ (4f ^o)6d	5H ^o ₅	66272.802	106560.907	
16	80	8.1×10^9	0.87	0.227	40312.009(16)	40312.009(16)	0.000	2479.9014(10)	4f ³ (4f ^o)6p	3H ₆	4f ³ (4f ^o)6d	3G ^o ₅	70826.009	111138.018	
10	32	3.1×10^9	0.46	0.190	40312.507(12)	40312.518(10)	-0.011	2479.8701(6)	4f ³ (4f ^o)6p	3H ₄	4f ³ (4f ^o)6d	5G ^o ₄	66445.159	106757.677	

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm^{-1})	σ (cm^{-1})	σ_{Ritz} (cm^{-1})	$\sigma - \sigma_{\text{Ritz}}$ (cm^{-1})	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm^{-1})	E_u (cm^{-1})	Note
10	50	2.6×10^9	0.38	0.167	40316.643(24)	40316.649(11)	-0.006	2479.6160(7)	4f ³ (4f ^o)6p	5H ₄	4f ³ (4f ^o)6d	3I ^o ₅	64243.914	104560.563	
9	38	5.5×10^9	0.71	0.228	40326.891(14)	40326.891(11)	0.000	2478.9862(7)	4f ³ (4f ^o)6p	3K ₈	4f ³ (4f ^o)6d	3K ^o ₈	70599.570	110926.461	
13	50	4.3×10^9	0.60	0.186	40330.995(18)	40331.003(12)	-0.008	2478.7334(7)	4f ³ (4f ^o)6p	5H ₅	4f ³ (4f ^o)6d	3K ^o ₆	66272.802	106603.805	
17	60	6.7×10^9	0.79	0.184	40338.513(13)	40338.513(13)	0.000	2478.2719(8)	4f ³ (4f ^o)6p	3H ₅	4f ³ (4f ^o)6d	3G ^o ₄	68613.221	108951.734	
22	84	9.4×10^9	0.94	0.178	40349.768(10)	40349.769(9)	-0.001	2477.5805(6)	4f ³ (4f ^o)6p	3K ₇	4f ³ (4f ^o)6d	3L ^o ₈	68507.387	108857.156	
3	8	1.5×10^7	-1.86	0.134	40353.918(32)	40353.906(6)	0.012	2477.3265(4)	4f ³ (4f ^o)5d	5H ^o ₇	4f ³ (4f ^o)6p	3K ₆	26097.906	66451.812	
15	62	5.4×10^9	0.70	0.217	40382.116(16)	40382.097(11)	0.019	2475.5970(7)	4f ³ (4f ^o)6p	3I ₆	4f ³ (4f ^o)6d	3K ^o ₇	68347.584	108729.681	
7	42	1.7×10^9	0.19	0.345	40402.698(23)	40402.686(15)	0.012	2474.3353(9)	4f ³ (4f ^o)6p	3I ₅	4f ³ (4f ^o)6d	3H ^o ₄	64350.812	104753.498	
14	46	5.2×10^9	0.68	0.188	40408.500(9)	40408.500(9)	0.000	2473.9793(5)	4f ³ (4f ^o)6p	3H ₄	4f ³ (4f ^o)6d	3G ^o ₃	66445.159	106853.659	
7	16	1.5×10^9	0.14	0.129	40445.498(14)	40445.496(12)	0.002	2471.7161(7)	4f ³ (4f ^o)6p	5H ₃	4f ³ (4f ^o)6d	5G ^o ₃	64347.699	104793.195	
16	82	3.8×10^9	0.54	0.207	40456.741(17)	40456.741(17)	0.000	2471.0291(10)	4f ³ (4f ^o)6p	5H ₃	4f ³ (4f ^o)6d	5G ^o ₂	64347.699	104804.440	
12	30	6.2×10^9	0.75	0.133	40465.859(16)	40465.859(11)	0.000	2470.4722(7)	4f ³ (4f ^o)6p	3I ₇	4f ³ (4f ^o)6d	3K ^o ₈	70460.602	110926.461	
18	78	3.6×10^9	0.52	0.205	40484.889(14)	40484.875(10)	0.014	2469.3118(6)	4f ³ (4f ^o)6p	5H ₅	4f ³ (4f ^o)6d	5G ^o ₄	66272.802	106757.677	
11	48	4.0×10^9	0.56	0.247	40505.397(25)	40505.382(10)	0.015	2468.0615(6)	4f ³ (4f ^o)6p	3I ₆	4f ³ (4f ^o)6d	3H ^o ₅	68347.584	108852.966	
15	86	3.7×10^9	0.53	0.244	40509.576(19)	40509.584(15)	-0.008	2467.8055(9)	4f ³ (4f ^o)6p	5H ₄	4f ³ (4f ^o)6d	3H ^o ₄	64243.914	104753.498	
43	160	1.1×10^9	0.00	0.178	40526.468(3)	40526.468(3)	0.000	2466.7773(2)	4f ³ (4f ^o)5d	3L ^o ₇	4f ³ (4f ^o)6p	5H ₆	24497.165	65023.633	
19	72	1.1×10^{10}	1.00	0.188	40547.182(6)	40547.182(6)	0.000	2465.5170(4)	4f ³ (4f ^o)6p	3K ₈	4f ³ (4f ^o)6d	3L ^o ₉	70599.570	111146.752	
12	46	3.2×10^9	0.47	0.171	40549.277(19)	40549.281(12)	-0.004	2465.3894(7)	4f ³ (4f ^o)6p	5H ₄	4f ³ (4f ^o)6d	5G ^o ₃	64243.914	104793.195	
7	22	4.5×10^9	0.61	0.160	40549.684(14)	40549.696(11)	-0.012	2465.3642(7)	4f ³ (4f ^o)6p	3I ₇	4f ³ (4f ^o)6d	3H ^o ₆	70460.602	111010.298	
5	16	1.2×10^9	0.03	0.171	40843.159(21)	40843.154(11)	0.005	2447.6492(7)	4f ³ (4f ^o)6p	5H ₆	4f ³ (4f ^o)6d	3I ^o ₆	65023.633	105866.787	
4	24	8.2×10^7	-1.13	0.326	40909.432(40)	40909.445(5)	-0.013	2443.6827(3)	4f ³ (4f ^o)5d	3I ^o ₅	4f ³ (4f ^o)6p	5K ₅	19616.622	60526.067	
51	190	9.3×10^8	-0.08	0.185	41045.869(3)	41045.869(3)	0.000	2435.5600(2)	4f ³ (4f ^o)5d	5H ^o ₃	4f ³ (4f ^o)6p	5I ₄	19593.094	60638.963	
7	24	2.0×10^9	0.25	0.224	41053.736(36)	41053.732(15)	0.004	2435.0935(9)	4f ³ (4f ^o)6p	5H ₆	4f ³ (4f ^o)6d	5K ^o ₇	65023.633	106077.365	
3	6	8.5×10^8	-0.12	0.110	41134.395(28)	41134.381(11)	0.014	2430.3189(7)	4f ³ (4f ^o)6p	5I ₈	4f ³ (4f ^o)6d	5K ^o ₈	66792.024	107926.405	
52	200	1.1×10^9	-0.01	0.196	41148.386(3)	41148.384(3)	0.002	2429.4918(2)	4f ³ (4f ^o)5d	3H ^o ₄	4f ³ (4f ^o)6p	5I ₅	21491.882	62640.266	
47	190	1.3×10^9	0.06	0.196	41201.900(3)	41201.899(3)	0.001	2426.3360(2)	4f ³ (4f ^o)5d	3H ^o ₅	4f ³ (4f ^o)6p	5I ₆	23347.721	64549.620	
8	30	2.2×10^8	-0.71	0.185	41230.733(14)	41230.739(5)	-0.006	2424.6387(3)	4f ³ (4f ^o)5d	3K ^o ₆	4f ³ (4f ^o)6p	3I ₅	23120.073	64350.812	
4	22	1.3×10^9	0.06	0.294	41408.833(38)	41408.862(31)	-0.029	2414.2081(18)	4f ³ (4f ^o)6p	5I ₇	4f ³ (4f ^o)6d	5I ^o ₇	66497.225	107906.087	B/W
4	32	2.1×10^9	0.26	0.426	41417.902(47)	41417.870(8)	0.032	2413.6830(4)	4f ³ (4f ^o)6p	5I ₈	4f ³ (4f ^o)6d	5L ^o ₉	66792.024	108209.894	

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm ⁻¹)	σ (cm ⁻¹)	σ_{Ritz} (cm ⁻¹)	$\sigma - \sigma_{\text{Ritz}}$ (cm ⁻¹)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm ⁻¹)	E_u (cm ⁻¹)	Note
2	10	1.6×10^9	0.15	0.267	41429.177(73)	41429.180(11)	-0.003	2413.0241(6)	4f ³ (4f ^o)6p	5I ₇	4f ³ (4f ^o)6d	5K ^o ₈	66497.225	107926.405	
3	10	8.8×10^7	-1.11	0.160	41429.561(34)	41429.547(4)	0.014	2413.0027(2)	4f ³ (4f ^o)5d	3K ^o ₆	4f ³ (4f ^o)6p	5I ₆	23120.073	64549.620	
14	54	4.9×10^8	-0.37	0.187	41462.395(8)	41462.393(8)	0.002	2411.0910(4)	4f ³ (4f ^o)5d	3H ^o ₆	4f ³ (4f ^o)6p	5I ₇	25034.832	66497.225	B/W
3	8	1.0×10^8	-1.06	0.109	41472.413(27)	41472.445(7)	-0.032	2410.5065(4)	4f ³ (4f ^o)5d	3K ^o ₇	4f ³ (4f ^o)6p	5I ₈	25319.579	66792.024	B/W
5	16	8.8×10^8	-0.12	0.156	41516.005(44)	41515.975(12)	0.030	2407.9789(7)	4f ³ (4f ^o)6p	3I ₅	4f ³ (4f ^o)6d	3I ^o ₆	64350.812	105866.787	
3	18	4.6×10^8	-0.40	0.366	41529.714(96)	41529.725(14)	-0.011	2407.1816(8)	4f ³ (4f ^o)6p	5I ₇	4f ³ (4f ^o)6d	5I ^o ₆	66497.225	108026.950	B/W
3	16	5.2×10^8	-0.35	0.261	41576.870(46)	41576.827(7)	0.043	2404.4543(4)	4f ³ (4f ^o)6p	5H ₆	4f ³ (4f ^o)6d	3L ^o ₇	65023.633	106600.460	
22	92	3.4×10^8	-0.53	0.186	41642.389(11)	41642.398(5)	-0.009	2400.6679(3)	4f ³ (4f ^o)5d	5I ^o ₄	4f ³ (4f ^o)6p	5K ₅	18883.669	60526.067	
3	6	1.3×10^9	0.05	0.075	41657.239(23)	41657.208(22)	0.031	2399.8144(13)	4f ³ (4f ^o)6p	5K ₈	4f ³ (4f ^o)6d	5I ^o ₈	68302.664	109959.872	B/W
5	20	1.8×10^8	-0.81	0.191	41675.900(23)	41675.912(5)	-0.012	2398.7372(3)	4f ³ (4f ^o)5d	3H ^o ₅	4f ³ (4f ^o)6p	5H ₆	23347.721	65023.633	
30	130	1.4×10^9	0.08	0.182	41682.685(8)	41682.681(6)	0.004	2398.3477(4)	4f ³ (4f ^o)5d	3H ^o ₆	4f ³ (4f ^o)6p	5H ₇	25034.832	66717.513	
9	38	2.5×10^8	-0.67	0.187	41721.301(12)	41721.297(5)	0.004	2396.1277(3)	4f ³ (4f ^o)5d	3I ^o ₆	4f ³ (4f ^o)6p	5K ₆	20799.349	62520.646	
31	140	2.5×10^9	0.33	0.184	41722.248(4)	41722.249(4)	-0.001	2396.0730(2)	4f ³ (4f ^o)5d	3L ^o ₉	4f ³ (4f ^o)6p	3K ₈	28877.321	70599.570	
49	200	1.1×10^9	-0.02	0.180	41755.295(3)	41755.294(3)	0.001	2394.1766(2)	4f ³ (4f ^o)5d	5I ^o ₄	4f ³ (4f ^o)6p	5I ₄	18883.669	60638.963	
6	30	3.2×10^9	0.44	0.223	41788.348(20)	41788.347(9)	0.001	2392.2827(5)	4f ³ (4f ^o)6p	5K ₇	4f ³ (4f ^o)6d	5L ^o ₈	64622.006	106410.353	
34	160	2.1×10^9	0.26	0.191	41830.700(7)	41830.702(7)	-0.002	2389.8603(4)	4f ³ (4f ^o)5d	3L ^o ₈	4f ³ (4f ^o)6p	3K ₇	26676.685	68507.387	
5	20	1.2×10^8	-0.99	0.192	41840.911(25)	41840.917(4)	-0.006	2389.2768(2)	4f ³ (4f ^o)5d	3I ^o ₆	4f ³ (4f ^o)6p	5I ₅	20799.349	62640.266	
7	30	1.7×10^8	-0.84	0.198	41846.853(18)	41846.843(3)	0.010	2388.9384(2)	4f ³ (4f ^o)5d	5I ^o ₇	4f ³ (4f ^o)6p	5I ₆	22702.777	64549.620	
17	82	5.7×10^8	-0.31	0.168	41919.223(7)	41919.229(5)	-0.006	2384.8129(3)	4f ³ (4f ^o)5d	5I ^o ₇	4f ³ (4f ^o)6p	5K ₇	22702.777	64622.006	
31	130	1.5×10^9	0.11	0.189	41954.648(4)	41954.647(4)	0.001	2382.7995(2)	4f ³ (4f ^o)5d	3L ^o ₇	4f ³ (4f ^o)6p	3K ₆	24497.165	66451.812	
3	18	1.0×10^9	-0.07	0.317	41972.042(58)	41972.058(10)	-0.016	2381.8109(6)	4f ³ (4f ^o)6p	5I ₅	4f ³ (4f ^o)6d	5K ^o ₆	62640.266	104612.324	
15	84	7.6×10^8	-0.19	0.197	42125.248(8)	42125.254(5)	-0.006	2373.1484(3)	4f ³ (4f ^o)5d	5I ^o ₈	4f ³ (4f ^o)6p	5H ₇	24592.259	66717.513	
20	120	4.6×10^8	-0.41	0.210	42171.908(12)	42171.904(5)	0.004	2370.5230(3)	4f ³ (4f ^o)5d	5I ^o ₅	4f ³ (4f ^o)6p	5K ₆	20348.742	62520.646	
20	96	1.1×10^9	-0.03	0.208	42199.769(6)	42199.765(5)	0.004	2368.9578(3)	4f ³ (4f ^o)5d	5I ^o ₈	4f ³ (4f ^o)6p	5I ₈	24592.259	66792.024	
6	30	5.7×10^7	-1.32	0.213	42249.715(20)	42249.678(6)	0.037	2366.1589(3)	4f ³ (4f ^o)5d	5H ^o ₇	4f ³ (4f ^o)6p	3I ₆	26097.906	68347.584	B/W
4	20	1.3×10^8	-0.96	0.223	42251.246(33)	42251.271(4)	-0.025	2366.0697(2)	4f ³ (4f ^o)5d	5H ^o ₄	4f ³ (4f ^o)6p	5I ₅	20388.995	62640.266	
5	36	2.6×10^9	0.34	0.296	42276.140(28)	42276.121(11)	0.019	2364.6788(6)	4f ³ (4f ^o)6p	5I ₈	4f ³ (4f ^o)7s	(¹⁵ / ₂ , ¹ / ₂) ₈	66792.024	109068.145	
12	62	4.0×10^9	0.53	0.205	42277.258(21)	42277.257(7)	0.001	2364.6153(4)	4f ³ (4f ^o)6p	5K ₆	4f ³ (4f ^o)6d	5L ^o ₇	62520.646	104797.903	
51	240	1.3×10^9	0.04	0.197	42291.522(3)	42291.524(3)	-0.002	2363.8175(2)	4f ³ (4f ^o)5d	5I ^o ₅	4f ³ (4f ^o)6p	5I ₅	20348.742	62640.266	

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm ⁻¹)	σ (cm ⁻¹)	σ_{Ritz} (cm ⁻¹)	$\sigma - \sigma_{\text{Ritz}}$ (cm ⁻¹)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm ⁻¹)	E_u (cm ⁻¹)	Note
10	64	4.8×10^8	-0.40	0.227	42320.862(24)	42320.856(5)	0.006	2362.1791(3)	4f ³ (4f ^o)5d	5 ¹ I ₇	4f ³ (4f ^o)6p	5H ₆	22702.777	65023.633	
4	20	2.1×10^9	0.24	0.238	42350.607(37)	42350.632(11)	-0.025	2360.5181(6)	4f ³ (4f ^o)6p	5H ₇	4f ³ (4f ^o)7s	($\frac{15}{2}, \frac{1}{2}$) ^o ₈	66717.513	109068.145	
22	98	2.2×10^9	0.26	0.180	42385.973(11)	42385.962(8)	0.011	2358.5504(4)	4f ³ (4f ^o)5d	3G ^o ₅	4f ³ (4f ^o)6p	3H ₆	28440.047	70826.009	
4	32	2.0×10^9	0.22	0.366	42436.303(43)	42436.341(9)	-0.038	2355.7502(5)	4f ³ (4f ^o)6p	5K ₇	4f ³ (4f ^o)7s	($\frac{13}{2}, \frac{1}{2}$) ^o ₇	64622.006	107058.347	
4	26	1.0×10^9	-0.08	0.277	42446.793(36)	42446.802(10)	-0.009	2355.1696(5)	4f ³ (4f ^o)6p	5I ₄	4f ³ (4f ^o)7s	($\frac{9}{2}, \frac{1}{2}$) ^o ₄	60638.963	103085.765	
25	120	1.9×10^9	0.20	0.180	42472.997(5)	42472.996(5)	0.001	2353.7169(3)	4f ³ (4f ^o)5d	3G ^o ₄	4f ³ (4f ^o)6p	3H ₅	26140.225	68613.221	
4	18	1.0×10^9	-0.08	0.181	42484.658(51)	42484.619(10)	0.039	2353.0730(6)	4f ³ (4f ^o)6p	5I ₅	4f ³ (4f ^o)7s	($\frac{11}{2}, \frac{1}{2}$) ^o ₅	62640.266	105124.885	
7	50	1.9×10^9	0.20	0.276	42491.225(38)	42491.255(11)	-0.030	2352.7054(6)	4f ³ (4f ^o)6p	5I ₅	4f ³ (4f ^o)7s	($\frac{11}{2}, \frac{1}{2}$) ^o ₆	62640.266	105131.521	
9	48	4.2×10^8	-0.46	0.226	42494.001(14)	42494.000(6)	0.001	2352.5535(3)	4f ³ (4f ^o)5d	3I ^o ₇	4f ³ (4f ^o)6p	5I ₇	24003.225	66497.225	
5	32	2.2×10^9	0.26	0.254	42508.730(25)	42508.727(8)	0.003	2351.7384(5)	4f ³ (4f ^o)6p	5I ₆	4f ³ (4f ^o)7s	($\frac{13}{2}, \frac{1}{2}$) ^o ₇	64549.620	107058.347	
29	140	1.5×10^9	0.09	0.199	42553.932(8)	42553.933(7)	-0.001	2349.2398(4)	4f ³ (4f ^o)5d	3G ^o ₃	4f ³ (4f ^o)6p	3H ₄	23891.226	66445.159	
6	44	2.0×10^9	0.22	0.311	42559.713(24)	42559.698(10)	0.015	2348.9216(6)	4f ³ (4f ^o)6p	5K ₅	4f ³ (4f ^o)7s	($\frac{9}{2}, \frac{1}{2}$) ^o ₄	60526.067	103085.765	
40	200	1.5×10^9	0.09	0.195	42569.097(4)	42569.098(3)	-0.001	2348.4029(2)	4f ³ (4f ^o)5d	5I ^o ₆	4f ³ (4f ^o)6p	5I ₆	21980.522	64549.620	
6	50	7.7×10^8	-0.20	0.302	42570.964(50)	42570.920(12)	0.044	2348.3024(7)	4f ³ (4f ^o)6p	5I ₇	4f ³ (4f ^o)7s	($\frac{15}{2}, \frac{1}{2}$) ^o ₈	66497.225	109068.145	
3	24	2.0×10^9	0.22	0.317	42598.838(47)	42598.814(11)	0.024	2346.7645(6)	4f ³ (4f ^o)6p	5I ₈	4f ³ (4f ^o)7s	($\frac{15}{2}, \frac{1}{2}$) ^o ₇	66792.024	109390.838	
6	30	2.0×10^9	0.22	0.167	42604.263(34)	42604.239(11)	0.024	2346.4657(6)	4f ³ (4f ^o)6p	5K ₆	4f ³ (4f ^o)7s	($\frac{11}{2}, \frac{1}{2}$) ^o ₅	62520.646	105124.885	
8	44	1.5×10^9	0.09	0.218	42610.861(15)	42610.875(12)	-0.014	2346.1002(7)	4f ³ (4f ^o)6p	5K ₆	4f ³ (4f ^o)7s	($\frac{11}{2}, \frac{1}{2}$) ^o ₆	62520.646	105131.521	B/W
8	44	2.0×10^9	0.22	0.218	42610.861(15)	42610.845(13)	0.016	2346.1019(7)	4f ³ (4f ^o)6p	5K ₇	4f ³ (4f ^o)7s	($\frac{13}{2}, \frac{1}{2}$) ^o ₆	64622.006	107232.851	B/W
16	72	5.9×10^8	-0.31	0.194	42641.494(15)	42641.484(5)	0.010	2344.4160(3)	4f ³ (4f ^o)5d	5I ^o ₆	4f ³ (4f ^o)6p	5K ₇	21980.522	64622.006	
3	24	8.8×10^8	-0.14	0.385	42673.361(62)	42673.325(12)	0.036	2342.6666(7)	4f ³ (4f ^o)6p	5H ₇	4f ³ (4f ^o)7s	($\frac{15}{2}, \frac{1}{2}$) ^o ₇	66717.513	109390.838	
5	20	1.8×10^9	0.17	0.161	42696.498(21)	42696.506(8)	-0.008	2341.3946(4)	4f ³ (4f ^o)6p	5I ₄	4f ³ (4f ^o)7s	($\frac{9}{2}, \frac{1}{2}$) ^o ₅	60638.963	103335.469	
21	110	1.2×10^9	-0.01	0.195	42714.288(11)	42714.288(5)	0.000	2340.4198(3)	4f ³ (4f ^o)5d	3I ^o ₇	4f ³ (4f ^o)6p	5H ₇	24003.225	66717.513	
24	110	9.5×10^8	-0.11	0.169	42764.515(9)	42764.510(5)	0.005	2337.6710(3)	4f ³ (4f ^o)5d	5G ^o ₃	4f ³ (4f ^o)6p	5H ₄	21479.404	64243.914	
10	56	6.7×10^8	-0.26	0.233	42788.797(13)	42788.799(5)	-0.002	2336.3439(3)	4f ³ (4f ^o)5d	3I ^o ₇	4f ³ (4f ^o)6p	5I ₈	24003.225	66792.024	
4	18	9.7×10^8	-0.10	0.183	42809.413(28)	42809.402(9)	0.011	2335.2194(5)	4f ³ (4f ^o)6p	5K ₅	4f ³ (4f ^o)7s	($\frac{9}{2}, \frac{1}{2}$) ^o ₅	60526.067	103335.469	
3	24	1.3×10^8	-0.97	0.316	42858.947(50)	42858.930(5)	0.017	2332.5205(3)	4f ³ (4f ^o)5d	3H ^o ₄	4f ³ (4f ^o)6p	3I ₅	21491.882	64350.812	
11	48	5.1×10^8	-0.38	0.160	42868.286(19)	42868.295(7)	-0.009	2332.0109(4)	4f ³ (4f ^o)5d	5G ^o ₃	4f ³ (4f ^o)6p	5H ₃	21479.404	64347.699	
29	140	1.2×10^9	-0.01	0.191	42870.371(4)	42870.371(4)	0.000	2331.8980(2)	4f ³ (4f ^o)5d	5G ^o ₂	4f ³ (4f ^o)6p	5H ₃	21477.328	64347.699	
9	28	3.6×10^9	0.46	0.122	43013.510(10)	43013.509(8)	0.001	2324.1374(5)	4f ³ (4f ^o)6p	5I ₄	4f ³ (4f ^o)6d	5K ^o ₅	60638.963	103652.472	

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int. (arb.)	$g_u A$ (s^{-1})	$\log(g_l f)$	FWHM (cm^{-1})	σ (cm^{-1})	σ_{Ritz} (cm^{-1})	$\sigma - \sigma_{Ritz}$ (cm^{-1})	λ_{Ritz}^{air} ($\text{\AA}$)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm^{-1})	E_u (cm^{-1})	Note
15	78	1.5×10^9	0.08	0.205	43018.696(8)	43018.691(6)	0.005	2323.8574(3)	4f ³ (4f ^o)5d	3K ^o ₈	4f ³ (4f ^o)6p	3I ₇	27441.911	70460.602	
13	82	1.0×10^9	-0.09	0.213	43027.996(19)	43028.005(7)	-0.009	2323.3543(4)	4f ³ (4f ^o)5d	3K ^o ₇	4f ³ (4f ^o)6p	3I ₆	25319.579	68347.584	
8	44	7.7×10^9	0.79	0.208	43040.438(15)	43040.437(9)	0.001	2322.6832(5)	4f ³ (4f ^o)6p	5I ₈	4f ³ (4f ^o)6d	5K ^o ₉	66792.024	109832.461	
13	58	5.0×10^9	0.61	0.169	43126.407(9)	43126.405(10)	0.002	2318.0527(5)	4f ³ (4f ^o)6p	5K ₅	4f ³ (4f ^o)6d	5K ^o ₅	60526.067	103652.472	B/W
15	74	8.2×10^8	-0.18	0.178	43152.720(15)	43152.729(7)	-0.009	2316.6386(4)	4f ³ (4f ^o)5d	3K ^o ₆	4f ³ (4f ^o)6p	5H ₅	23120.073	66272.802	
14	70	1.5×10^9	0.08	0.193	43157.659(16)	43157.659(7)	0.000	2316.3739(4)	4f ³ (4f ^o)5d	3K ^o ₈	4f ³ (4f ^o)6p	3K ₈	27441.911	70599.570	
8	36	7.2×10^9	0.76	0.168	43167.872(13)	43167.848(22)	0.024	2315.8271(12)	4f ³ (4f ^o)6p	5I ₈	4f ³ (4f ^o)6d	5I ^o ₈	66792.024	109959.872	B/W
22	120	1.0×10^{10}	0.91	0.200	43169.009(6)	43169.011(6)	-0.002	2315.7647(3)	4f ³ (4f ^o)6p	5K ₅	4f ³ (4f ^o)6d	5L ^o ₆	60526.067	103695.078	
16	92	1.3×10^9	0.02	0.208	43187.806(8)	43187.808(6)	-0.002	2314.7567(3)	4f ³ (4f ^o)5d	3K ^o ₇	4f ³ (4f ^o)6p	3K ₇	25319.579	68507.387	
5	28	3.3×10^9	0.42	0.206	43226.520(22)	43226.521(11)	-0.001	2312.6835(6)	4f ³ (4f ^o)6p	5I ₅	4f ³ (4f ^o)6d	3I ^o ₆	62640.266	105866.787	
4	20	3.1×10^9	0.40	0.206	43242.400(69)	43242.359(22)	0.041	2311.8364(12)	4f ³ (4f ^o)6p	5H ₇	4f ³ (4f ^o)6d	5I ^o ₈	66717.513	109959.872	B/W
22	130	1.1×10^9	-0.05	0.194	43262.353(11)	43262.352(9)	0.001	2310.7679(5)	4f ³ (4f ^o)5d	5G ^o ₄	4f ³ (4f ^o)6p	5H ₅	23010.450	66272.802	
5	26	3.8×10^9	0.48	0.229	43265.518(28)	43265.536(17)	-0.018	2310.5978(9)	4f ³ (4f ^o)6p	5I ₈	4f ³ (4f ^o)6d	5H ^o ₇	66792.024	110057.560	
8	32	6.1×10^9	0.69	0.146	43284.061(12)	43284.081(31)	-0.020	2309.6078(17)	4f ³ (4f ^o)6p	5K ₇	4f ³ (4f ^o)6d	5I ^o ₇	64622.006	107906.087	B/W
8	44	6.7×10^9	0.73	0.197	43304.394(14)	43304.399(11)	-0.005	2308.5240(6)	4f ³ (4f ^o)6p	5K ₇	4f ³ (4f ^o)6d	5K ^o ₈	64622.006	107926.405	
19	100	1.2×10^9	-0.02	0.195	43331.729(13)	43331.739(6)	-0.010	2307.0673(3)	4f ³ (4f ^o)5d	3K ^o ₆	4f ³ (4f ^o)6p	3K ₆	23120.073	66451.812	
6	32	6.1×10^9	0.69	0.198	43340.057(20)	43340.047(16)	0.010	2306.6251(9)	4f ³ (4f ^o)6p	5H ₇	4f ³ (4f ^o)6d	5H ^o ₇	66717.513	110057.560	
8	38	5.2×10^9	0.62	0.186	43346.137(15)	43346.141(11)	-0.004	2306.3007(6)	4f ³ (4f ^o)6p	5K ₆	4f ³ (4f ^o)6d	3I ^o ₆	62520.646	105866.787	
4	24	3.2×10^9	0.41	0.225	43356.467(31)	43356.467(31)	0.000	2305.7514(16)	4f ³ (4f ^o)6p	5I ₆	4f ³ (4f ^o)6d	5I ^o ₇	64549.620	107906.087	
5	32	2.9×10^9	0.36	0.254	43404.958(27)	43404.944(14)	0.014	2303.1760(7)	4f ³ (4f ^o)6p	5K ₇	4f ³ (4f ^o)6d	5I ^o ₆	64622.006	108026.950	
10	66	5.7×10^9	0.66	0.197	43411.875(25)	43411.873(18)	0.002	2302.8084(10)	4f ³ (4f ^o)6p	5I ₅	4f ³ (4f ^o)6d	5I ^o ₅	62640.266	106052.139	
10	82	6.6×10^8	-0.28	0.256	43434.726(28)	43434.709(10)	0.017	2301.5975(5)	4f ³ (4f ^o)5d	5G ^o ₄	4f ³ (4f ^o)6p	3H ₄	23010.450	66445.159	
16	90	1.3×10^9	0.01	0.184	43469.174(14)	43469.172(10)	0.002	2299.7726(5)	4f ³ (4f ^o)6p	5I ₆	4f ³ (4f ^o)6d	3I ₆	24878.412	68347.584	
8	48	6.4×10^9	0.71	0.226	43477.328(15)	43477.330(13)	-0.002	2299.3411(7)	4f ³ (4f ^o)6p	5I ₆	4f ³ (4f ^o)6d	5I ^o ₆	64549.620	108026.950	
6	28	4.4×10^9	0.54	0.181	43491.447(19)	43491.441(13)	0.006	2298.5950(7)	4f ³ (4f ^o)6p	5I ₄	4f ³ (4f ^o)6d	5I ^o ₄	60638.963	104130.404	
5	24	2.2×10^9	0.24	0.189	43531.492(24)	43531.493(18)	-0.001	2296.4799(9)	4f ³ (4f ^o)6p	5K ₆	4f ³ (4f ^o)6d	5I ^o ₅	62520.646	106052.139	
18	140	8.5×10^8	-0.17	0.234	43551.460(15)	43551.463(5)	-0.003	2295.4268(3)	4f ³ (4f ^o)5d	3I ^o ₆	4f ³ (4f ^o)6p	3I ₅	20799.349	64350.812	
10	66	6.6×10^9	0.72	0.185	43556.734(23)	43556.719(15)	0.015	2295.1498(8)	4f ³ (4f ^o)6p	5K ₆	4f ³ (4f ^o)6d	5K ^o ₇	62520.646	106077.365	
4	12	1.5×10^9	0.07	0.081	43604.360(40)	43604.337(13)	0.023	2292.6432(7)	4f ³ (4f ^o)6p	5K ₅	4f ³ (4f ^o)6d	5I ^o ₄	60526.067	104130.404	B/W

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm^{-1})	σ (cm^{-1})	σ_{Ritz} (cm^{-1})	$\sigma - \sigma_{\text{Ritz}}$ (cm^{-1})	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm^{-1})	E_u (cm^{-1})	Note
13	82	1.7×10^9	0.13	0.170	43604.767(17)	43604.764(15)	0.003	2292.6207(8)	$4f^3(^2H_2^\circ)5d$	$3K^\circ_6$	$4f^3(^2H_2^\circ)6p$	$3I_5$	29643.186	73247.950	
10	56	6.3×10^9	0.70	0.196	43625.419(12)	43625.421(11)	-0.002	2291.5350(6)	$4f^3(^4I^\circ)6p$	$5I_5$	$4f^3(^4I^\circ)6d$	$5H^\circ_4$	62640.266	106265.687	
8	46	8.5×10^8	-0.18	0.208	43710.400(29)	43710.405(6)	-0.005	2287.0793(3)	$4f^3(^4I^\circ)5d$	$5I^\circ_8$	$4f^3(^4I^\circ)6p$	$5K_8$	24592.259	68302.664	
13	84	8.6×10^8	-0.17	0.239	43734.807(20)	43734.809(11)	-0.002	2285.8030(6)	$4f^3(^4I^\circ)5d$	$5G^\circ_5$	$4f^3(^4I^\circ)6p$	$3H_5$	24878.412	68613.221	
6	26	4.3×10^9	0.53	0.159	43740.937(17)	43740.957(110)	-0.020	2285.4817(57)	$4f^3(^4I^\circ)6p$	$5I_4$	$4f^3(^4I^\circ)6d$	$5H^\circ_3$	60638.963	104379.920	
5	34	3.2×10^8	-0.60	0.225	43749.025(23)	43749.035(5)	-0.010	2285.0597(3)	$4f^3(^4I^\circ)5d$	$5I^\circ_7$	$4f^3(^4I^\circ)6p$	$3K_6$	22702.777	66451.812	
13	80	1.5×10^9	0.07	0.182	43790.131(17)	43790.141(9)	-0.010	2282.9145(5)	$4f^3(^4I^\circ)5d$	$5G^\circ_6$	$4f^3(^4I^\circ)6p$	$3I_7$	26670.461	70460.602	
12	74	9.0×10^8	-0.15	0.210	43794.434(20)	43794.448(6)	-0.014	2282.6899(3)	$4f^3(^4I^\circ)5d$	$5I^\circ_7$	$4f^3(^4I^\circ)6p$	$5I_7$	22702.777	66497.225	
4	24	5.5×10^8	-0.37	0.211	43850.519(30)	43850.527(16)	-0.008	2279.7704(8)	$4f^3(^2H_2^\circ)5d$	$3I^\circ_5$	$4f^3(^2H_2^\circ)6p$	$3I_5$	29397.423	73247.950	
22	130	1.1×10^9	-0.07	0.184	43854.910(10)	43854.919(5)	-0.009	2279.5421(3)	$4f^3(^4I^\circ)5d$	$5H^\circ_4$	$4f^3(^4I^\circ)6p$	$5H_4$	20388.995	64243.914	
5	24	7.5×10^7	-1.23	0.184	43895.197(24)	43895.172(5)	0.025	2277.4515(3)	$4f^3(^4I^\circ)5d$	$5I^\circ_5$	$4f^3(^4I^\circ)6p$	$5H_4$	20348.742	64243.914	
4	30	1.9×10^8	-0.83	0.278	43958.704(36)	43958.704(7)	0.000	2274.1597(4)	$4f^3(^4I^\circ)5d$	$5H^\circ_4$	$4f^3(^4I^\circ)6p$	$5H_3$	20388.995	64347.699	
8	36	4.0×10^8	-0.51	0.163	43961.811(14)	43961.817(5)	-0.006	2273.9986(2)	$4f^3(^4I^\circ)5d$	$5H^\circ_4$	$4f^3(^4I^\circ)6p$	$3I_5$	20388.995	64350.812	
4	22	2.2×10^8	-0.77	0.188	44014.722(26)	44014.736(5)	-0.014	2271.2643(3)	$4f^3(^4I^\circ)5d$	$5I^\circ_7$	$4f^3(^4I^\circ)6p$	$5H_7$	22702.777	66717.513	
4	10	1.4×10^9	0.03	0.090	44079.835(22)	44079.814(8)	0.021	2267.9108(4)	$4f^3(^4I^\circ)6p$	$5K_6$	$4f^3(^4I^\circ)6d$	$3L^\circ_7$	62520.646	106600.460	
4	16	4.8×10^8	-0.43	0.161	44083.234(30)	44083.236(22)	-0.002	2267.7347(11)	$4f^3(^4F^\circ)5d$	$5H^\circ_5$	$4f^3(^4F^\circ)6p$	$5G_4$	30175.737	74258.973	
2	20	6.0×10^8	-0.33	0.296	44086.272(62)	44086.257(11)	0.015	2267.5793(6)	$4f^3(^4I^\circ)6p$	$5K_5$	$4f^3(^4I^\circ)6d$	$5K^\circ_6$	60526.067	104612.324	
3	8	3.7×10^7	-1.54	0.116	44089.243(33)	44089.247(5)	-0.004	2267.4255(3)	$4f^3(^4I^\circ)5d$	$5I^\circ_7$	$4f^3(^4I^\circ)6p$	$5I_8$	22702.777	66792.024	
20	120	1.4×10^9	0.03	0.211	44091.507(12)	44091.503(10)	0.004	2267.3095(5)	$4f^3(^4I^\circ)5d$	$5H^\circ_5$	$4f^3(^4I^\circ)6p$	$5H_5$	22181.299	66272.802	
5	36	8.1×10^8	-0.21	0.237	44155.542(24)	44155.548(10)	-0.006	2264.0206(5)	$4f^3(^4I^\circ)5d$	$5G^\circ_6$	$4f^3(^4I^\circ)6p$	$3H_6$	26670.461	70826.009	
6	42	3.5×10^8	-0.57	0.244	44211.113(22)	44211.109(5)	0.004	2261.1751(3)	$4f^3(^4I^\circ)5d$	$5K^\circ_8$	$4f^3(^4I^\circ)6p$	$5K_7$	20410.897	64622.006	B/W
17	110	1.1×10^9	-0.07	0.194	44224.267(14)	44224.284(5)	-0.017	2260.5014(3)	$4f^3(^4I^\circ)5d$	$3I^\circ_6$	$4f^3(^4I^\circ)6p$	$5H_6$	20799.349	65023.633	B/W
6	24	3.4×10^9	0.42	0.144	44235.151(17)	44235.150(10)	0.001	2259.9461(5)	$4f^3(^4I^\circ)6p$	$5K_7$	$4f^3(^4I^\circ)6d$	$3L^\circ_8$	64622.006	108857.156	
5	28	2.4×10^8	-0.74	0.204	44263.862(25)	44263.860(12)	0.002	2258.4801(6)	$4f^3(^4I^\circ)5d$	$5H^\circ_5$	$4f^3(^4I^\circ)6p$	$3H_4$	22181.299	66445.159	
6	32	4.5×10^8	-0.46	0.183	44270.504(19)	44270.513(11)	-0.009	2258.1407(6)	$4f^3(^4I^\circ)5d$	$5H^\circ_5$	$4f^3(^4I^\circ)6p$	$3K_6$	22181.299	66451.812	
17	110	1.7×10^9	0.11	0.226	44289.070(8)	44289.066(6)	0.004	2257.1946(3)	$4f^3(^4I^\circ)5d$	$5H^\circ_6$	$4f^3(^4I^\circ)6p$	$3I_6$	24058.518	68347.584	
4	18	2.0×10^8	-0.82	0.158	44344.350(26)	44344.359(6)	-0.009	2254.3799(3)	$4f^3(^4I^\circ)5d$	$3I^\circ_7$	$4f^3(^4I^\circ)6p$	$3I_6$	24003.225	68347.584	
4	22	4.4×10^9	0.53	0.210	44354.749(33)	44354.728(9)	0.021	2253.8528(5)	$4f^3(^4I^\circ)6p$	$5I_8$	$4f^3(^4I^\circ)6d$	$3L^\circ_9$	66792.024	111146.752	
14	90	1.9×10^9	0.16	0.219	44362.689(9)	44362.696(7)	-0.007	2253.4479(3)	$4f^3(^4I^\circ)5d$	$5H^\circ_7$	$4f^3(^4I^\circ)6p$	$3I_7$	26097.906	70460.602	B/W

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm ⁻¹)	σ (cm ⁻¹)	σ_{Ritz} (cm ⁻¹)	$\sigma - \sigma_{\text{Ritz}}$ (cm ⁻¹)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm ⁻¹)	E_u (cm ⁻¹)	Note
2	10	3.9×10^8	-0.53	0.179	44403.692(57)	44403.678(23)	0.014	2251.3679(12)	4f ³ (4F°)5d	5H° ₇	4f ³ (² H2°)6p	1I ₆	32832.447	77236.125	B/W
8	56	1.2×10^9	-0.04	0.251	44413.906(17)	44413.906(17)	0.000	2250.8494(9)	4f ³ (4F°)5d	5H° ₃	4f ³ (4F°)6p	5G ₂	27675.024	72088.930	
8	60	1.6×10^9	0.08	0.200	44433.505(31)	44433.505(31)	0.000	2249.8565(16)	4f ³ (4F°)5d	5H° ₆	4f ³ (4F°)6p	5G ₅	31146.457	75579.962	
7	42	6.3×10^8	-0.32	0.187	44448.877(19)	44448.869(6)	0.008	2249.0788(3)	4f ³ (4F°)5d	5H° ₆	4f ³ (4F°)6p	3K ₇	24058.518	68507.387	
9	68	1.4×10^9	0.03	0.187	44456.643(28)	44456.643(28)	0.000	2248.6854(14)	4f ³ (4F°)5d	5H° ₄	4f ³ (4F°)6p	5G ₃	28745.307	73201.950	
6	54	7.9×10^8	-0.22	0.271	44501.678(25)	44501.664(7)	0.014	2246.4103(3)	4f ³ (4F°)5d	5H° ₇	4f ³ (4F°)6p	3K ₈	26097.906	70599.570	
3	24	3.1×10^8	-0.63	0.266	44554.754(52)	44554.703(8)	0.051	2243.7359(4)	4f ³ (4F°)5d	5H° ₆	4f ³ (4F°)6p	3H ₅	24058.518	68613.221	
12	94	1.1×10^9	-0.08	0.215	44594.929(12)	44594.909(5)	0.020	2241.7127(3)	4f ³ (4F°)5d	5K° ₉	4f ³ (4F°)6p	5I ₈	22197.115	66792.024	B/W
14	110	7.2×10^8	-0.27	0.220	44627.288(11)	44627.292(5)	-0.004	2240.0859(3)	4f ³ (4F°)5d	3I° ₅	4f ³ (4F°)6p	5H ₄	19616.622	64243.914	
2	20	3.7×10^8	-0.56	0.293	44728.130(72)	44728.103(8)	0.027	2235.0366(4)	4f ³ (4F°)5d	5H° ₇	4f ³ (4F°)6p	3H ₆	26097.906	70826.009	
24	160	1.4×10^9	0.02	0.182	44734.181(11)	44734.190(5)	-0.009	2234.7324(2)	4f ³ (4F°)5d	3I° ₅	4f ³ (4F°)6p	3I ₅	19616.622	64350.812	
9	54	4.9×10^8	-0.44	0.185	44754.605(14)	44754.605(7)	0.000	2233.7130(4)	4f ³ (4F°)5d	5H° ₃	4f ³ (4F°)6p	5H ₃	19593.094	64347.699	
4	28	7.8×10^8	-0.24	0.213	44861.552(33)	44861.550(22)	0.002	2228.3875(11)	4f ³ (² H2°)5d	3I° ₅	4f ³ (4F°)6p	5G ₄	29397.423	74258.973	
4	24	1.6×10^9	0.08	0.177	44862.774(27)	44862.773(27)	0.001	2228.3268(13)	4f ³ (² H2°)5d	3K° ₇	4f ³ (² H2°)6p	3I ₆	31781.802	76644.575	
6	44	5.0×10^8	-0.43	0.238	44953.267(24)	44953.277(7)	-0.010	2223.8400(3)	4f ³ (4F°)5d	3H° ₄	4f ³ (4F°)6p	3H ₄	21491.882	66445.159	
47	310	1.3×10^9	-0.02	0.200	45263.631(5)	45263.630(5)	0.001	2208.5906(2)	4f ³ (4F°)5d	5K° ₅	4f ³ (4F°)6p	5K ₅	15262.437	60526.067	
6	30	5.0×10^8	-0.44	0.160	45265.483(19)	45265.500(8)	-0.017	2208.4994(4)	4f ³ (4F°)5d	3H° ₅	4f ³ (4F°)6p	3H ₅	23347.721	68613.221	
94	570	2.6×10^9	0.28	0.202	45367.914(5)	45367.913(5)	0.001	2203.5134(2)	4f ³ (4F°)5d	5L° ₆	4f ³ (4F°)6p	5K ₅	15158.154	60526.067	
30	180	1.0×10^9	-0.14	0.193	45376.521(6)	45376.526(4)	-0.005	2203.0951(2)	4f ³ (4F°)5d	5K° ₅	4f ³ (4F°)6p	5I ₄	15262.437	60638.963	
4	24	8.7×10^8	-0.20	0.207	45454.316(32)	45454.323(23)	-0.007	2199.3240(11)	4f ³ (² H2°)5d	3K° ₇	4f ³ (² H2°)6p	1I ₆	31781.802	77236.125	
8	38	3.4×10^8	-0.61	0.153	45464.044(14)	45464.030(7)	0.014	2198.8544(3)	4f ³ (4F°)5d	5I° ₄	4f ³ (4F°)6p	5H ₃	18883.669	64347.699	
5	32	4.7×10^8	-0.47	0.214	45548.738(26)	45548.750(8)	-0.012	2194.7642(4)	4f ³ (4F°)5d	5I° ₈	4f ³ (4F°)6p	5K ₉	24592.259	70141.009	
70	420	2.7×10^9	0.29	0.201	45567.813(5)	45567.811(5)	0.002	2193.8460(2)	4f ³ (4F°)5d	5L° ₇	4f ³ (4F°)6p	5K ₆	16952.835	62520.646	
37	230	1.4×10^9	0.00	0.202	45582.576(8)	45582.578(7)	-0.002	2193.1352(4)	4f ³ (4F°)5d	5K° ₆	4f ³ (4F°)6p	5K ₆	16938.068	62520.646	
28	160	1.0×10^9	-0.14	0.196	45702.194(10)	45702.198(7)	-0.004	2187.3943(3)	4f ³ (4F°)5d	5K° ₆	4f ³ (4F°)6p	5I ₅	16938.068	62640.266	
51	300	2.5×10^9	0.25	0.196	45760.941(5)	45760.942(5)	-0.001	2184.5861(2)	4f ³ (4F°)5d	5L° ₈	4f ³ (4F°)6p	5K ₇	18861.064	64622.006	
4	34	6.6×10^8	-0.33	0.275	45791.168(35)	45791.177(9)	-0.009	2183.1435(4)	4f ³ (4F°)5d	3H° ₆	4f ³ (4F°)6p	3H ₆	25034.832	70826.009	
2	14	2.5×10^8	-0.75	0.247	45804.566(67)	45804.610(6)	-0.044	2182.5032(3)	4f ³ (4F°)5d	5I° ₇	4f ³ (4F°)6p	3K ₇	22702.777	68507.387	
22	130	1.1×10^9	-0.11	0.211	45893.342(7)	45893.348(4)	-0.006	2178.2827(2)	4f ³ (4F°)5d	5K° ₇	4f ³ (4F°)6p	5I ₆	18656.272	64549.620	

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Table D.1: Nd III Transitions Classified from the Nd-Ar PDL FT Spectra (continued)

SNR	Int.	$g_u A$ (arb.)	$\log(g_l f)$	FWHM (cm ⁻¹)	σ (cm ⁻¹)	σ_{Ritz} (cm ⁻¹)	$\sigma - \sigma_{\text{Ritz}}$ (cm ⁻¹)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level Config.	Term _J	Upper Level Config.	Term _J	E_l (cm ⁻¹)	E_u (cm ⁻¹)	Note
25	140	1.8×10^9	0.11	0.201	45932.292(7)	45932.292(7)	0.000	2176.4356(3)	4f ³ (4f ^o)5d	5L ^o ₉	4f ³ (4f ^o)6p	5I ₈	20859.732	66792.024	
26	150	1.4×10^9	0.00	0.201	45965.740(7)	45965.734(5)	0.006	2174.8520(2)	4f ³ (4f ^o)5d	5K ^o ₇	4f ³ (4f ^o)6p	5K ₇	18656.272	64622.006	
3	20	4.5×10^8	-0.50	0.232	46007.325(47)	46007.311(6)	0.014	2172.8864(3)	4f ³ (4f ^o)5d	5I ^o ₈	4f ³ (4f ^o)6p	3K ₈	24592.259	70599.570	
22	140	1.6×10^9	0.05	0.222	46086.326(7)	46086.328(6)	-0.002	2169.1605(3)	4f ³ (4f ^o)5d	5K ^o ₈	4f ³ (4f ^o)6p	5I ₇	20410.897	66497.225	
6	28	3.4×10^8	-0.62	0.174	46096.438(21)	46096.417(7)	0.021	2168.6856(3)	4f ³ (4f ^o)5d	5I ^o ₅	4f ³ (4f ^o)6p	3H ₄	20348.742	66445.159	
12	78	1.2×10^9	-0.07	0.243	46105.560(24)	46105.549(7)	0.011	2168.2561(3)	4f ³ (4f ^o)5d	5K ^o ₉	4f ³ (4f ^o)6p	5K ₈	22197.115	68302.664	
6	34	1.9×10^9	0.13	0.212	46142.380(24)	46142.379(24)	0.001	2166.5252(11)	4f ³ (4f ^o)5d	5H ^o ₇	4f ³ (4f ^o)6p	5G ₆	32832.447	78974.826	
6	40	3.7×10^8	-0.59	0.247	46367.353(25)	46367.361(5)	-0.008	2156.0117(2)	4f ³ (4f ^o)5d	5K ^o ₇	4f ³ (4f ^o)6p	5H ₆	18656.272	65023.633	
13	86	1.0×10^9	-0.16	0.220	46381.118(21)	46381.127(6)	-0.009	2155.3717(3)	4f ³ (4f ^o)5d	5K ^o ₈	4f ³ (4f ^o)6p	5I ₈	20410.897	66792.024	
3	24	3.4×10^8	-0.63	0.317	46632.722(59)	46632.699(8)	0.023	2143.7427(4)	4f ³ (4f ^o)5d	5I ^o ₆	4f ³ (4f ^o)6p	3H ₅	21980.522	68613.221	
3	12	4.3×10^8	-0.53	0.116	46822.763(28)	46822.784(7)	-0.021	2135.0389(3)	4f ³ (4f ^o)5d	3I ^o ₇	4f ³ (4f ^o)6p	3H ₆	24003.225	70826.009	
39	260	6.0×10^9	0.61	0.211	47208.733(6)	47208.733(6)	0.000	2117.5821(2)	4f ³ (4f ^o)5d	5L ^o ₁₀	4f ³ (4f ^o)6p	5K ₉	22932.276	70141.009	
10	70	5.7×10^8	-0.42	0.193	47412.758(25)	47412.744(8)	0.014	2108.4693(4)	4f ³ (4f ^o)5d	5K ^o ₆	4f ³ (4f ^o)6p	3I ₅	16938.068	64350.812	
26	190	3.3×10^9	0.34	0.224	47442.932(7)	47442.932(7)	0.000	2107.1276(3)	4f ³ (4f ^o)5d	5L ^o ₉	4f ³ (4f ^o)6p	5K ₈	20859.732	68302.664	
15	140	1.4×10^9	-0.03	0.214	47636.162(10)	47636.161(8)	0.001	2098.5793(3)	4f ³ (4f ^o)5d	5L ^o ₈	4f ³ (4f ^o)6p	5I ₇	18861.064	66497.225	
7	56	5.7×10^8	-0.43	0.233	47795.548(20)	47795.540(6)	0.008	2091.5805(2)	4f ³ (4f ^o)5d	5K ^o ₇	4f ³ (4f ^o)6p	3K ₆	18656.272	66451.812	
3	28	2.8×10^8	-0.74	0.275	47840.961(53)	47840.953(6)	0.008	2089.5948(3)	4f ³ (4f ^o)5d	5K ^o ₇	4f ³ (4f ^o)6p	5I ₇	18656.272	66497.225	
7	42	4.8×10^8	-0.50	0.166	47856.459(17)	47856.449(7)	0.010	2088.9181(3)	4f ³ (4f ^o)5d	5L ^o ₈	4f ³ (4f ^o)6p	5H ₇	18861.064	66717.513	
8	64	1.1×10^9	-0.14	0.221	47891.776(17)	47891.767(7)	0.009	2087.3774(3)	4f ³ (4f ^o)5d	5K ^o ₈	4f ³ (4f ^o)6p	5K ₈	20410.897	68302.664	
13	110	2.5×10^9	0.21	0.193	47943.883(10)	47943.894(8)	-0.011	2085.1076(3)	4f ³ (4f ^o)5d	5K ^o ₉	4f ³ (4f ^o)6p	5K ₉	22197.115	70141.009	
13	90	9.2×10^8	-0.22	0.159	48070.793(10)	48070.798(7)	-0.005	2079.6024(3)	4f ³ (4f ^o)5d	5L ^o ₇	4f ³ (4f ^o)6p	5H ₆	16952.835	65023.633	
6	40	6.5×10^8	-0.38	0.179	48096.502(21)	48096.490(6)	0.012	2078.4914(3)	4f ³ (4f ^o)5d	5K ^o ₈	4f ³ (4f ^o)6p	3K ₇	20410.897	68507.387	
9	130	9.6×10^5	-3.21	0.361	48213.955(20)	48214.003(10)	-0.048	2073.4248(4)	4f ³ (4f ^o)6p	5I ₄	4f ³ (4f ^o)6d	3H ^o ₅	60638.963	108852.966	B/W
5	32	7.4×10^8	-0.32	0.158	48402.467(24)	48402.455(7)	0.012	2065.3510(3)	4f ³ (4f ^o)5d	5K ^o ₉	4f ³ (4f ^o)6p	3K ₈	22197.115	70599.570	
8	36	5.0×10^8	-0.51	0.177	48981.473(32)	48981.477(6)	-0.004	2040.9327(2)	4f ³ (4f ^o)5d	5K ^o ₅	4f ³ (4f ^o)6p	5H ₄	15262.437	64243.914	
5	68	6.1×10^8	-0.42	0.259	49192.654(29)	49192.658(8)	-0.004	2032.1699(3)	4f ³ (4f ^o)5d	5L ^o ₆	4f ³ (4f ^o)6p	3I ₅	15158.154	64350.812	
10	120	1.3×10^7	-2.14	0.251	51599.527(28)	51599.538(9)	-0.011	1937.3641(3)	4f ³ (4f ^o)5d	5L ^o ₈	4f ³ (4f ^o)6p	3I ₇	18861.064	70460.602	B/W

Table D.2: Classified Nd III Transitions Observed Only from the Nd VS Spectra

Int.	$g_u A$ (10^6 s^{-1})	$\log(g_l f)$	λ (Å)	λ_{Ritz} (Å)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level	Upper Level	E_l (cm^{-1})	E_u (cm^{-1})
1	3100	-0.34	993.794	993.793(3)		$4f^3(^4I^\circ)5d^5K^\circ_7$	$4f^3(^4I^\circ)5f^5I_6$	18656.272	119280.8
1	2800	-0.38	994.019	994.019(3)		$4f^3(^4I^\circ)5d^5K^\circ_6$	$4f^3(^4I^\circ)5f^5I_5$	16938.068	117539.8
0	2000	-0.53	994.138	994.137(3)		$4f^3(^4I^\circ)5d^5K^\circ_5$	$4f^3(^4I^\circ)5f^5I_4$	15262.437	115852.2
3	2400	-0.45	997.327	997.322(3)		$4f^3(^4I^\circ)5d^5K^\circ_7$	$4f^3(^4I^\circ)5f^3L_8$	18656.272	118924.8
5	4600	-0.16	997.916	997.915(4)		$4f^3(^4I^\circ)5d^5L^\circ_8$	$4f^3(^4I^\circ)5f^3M_9$	18861.064	119070.0
20	6600	0.00	1002.162	1002.162(4)		$4f^3(^4I^\circ)5d^5L^\circ_7$	$4f^3(^4I^\circ)5f^3M_8$	16952.835	116737.1
1	1700	-0.59	1002.891	1002.889(3)		$4f^3(^4I^\circ)5d^5K^\circ_6$	$4f^3(^4I^\circ)5f^3L_7$	16938.068	116650.0
4	2700	-0.39	1003.114	1003.112(3)		$4f^3(^4I^\circ)5d^5K^\circ_7$	$4f^3(^4I^\circ)5f^3I_7$	18656.272	118346.0
4	3400	-0.29	1004.592	1004.590(3)		$4f^3(^4I^\circ)5d^5K^\circ_7$	$4f^3(^4I^\circ)5f^5K_8$	18656.272	118199.4
1	2300	-0.46	1005.000	1004.998(3)		$4f^3(^4I^\circ)5d^5K^\circ_8$	$4f^3(^4I^\circ)5f^5K_9$	20410.897	119913.6
12	6500	-0.01	1005.070	1005.068(3)		$4f^3(^4I^\circ)5d^5K^\circ_6$	$4f^3(^4I^\circ)5f^5K_7$	16938.068	116433.8
3	2700	-0.39	1005.219	1005.217(3)		$4f^3(^4I^\circ)5d^5L^\circ_7$	$4f^3(^4I^\circ)5f^5K_7$	16952.835	116433.8
2	4100	-0.21	1005.480	1005.479(3)		$4f^3(^4I^\circ)5d^5K^\circ_9$	$4f^3(^4I^\circ)5f^5I_8$	22197.115	121652.2
3	3800	-0.24	1006.411	1006.410(3)		$4f^3(^4I^\circ)5d^5L^\circ_7$	$4f^3(^4I^\circ)5f^5L_8$	16952.835	116315.9
1	1700	-0.59	1006.662	1006.661(3)		$4f^3(^4I^\circ)5d^5L^\circ_8$	$4f^3(^4I^\circ)5f^5K_8$	18861.064	118199.4
3	3100	-0.33	1007.785	1007.783(4)		$4f^3(^4I^\circ)5d^5L^\circ_8$	$4f^3(^4I^\circ)5f^5L_9$	18861.064	118088.8
10	5000	-0.12	1008.013	1008.011(3)		$4f^3(^4I^\circ)5d^5K^\circ_6$	$4f^3(^4I^\circ)5f^3I_6$	16938.068	116143.3
1	2100	-0.49	1008.528	1008.533(4)		$4f^3(^4I^\circ)5d^5L^\circ_9$	$4f^3(^4I^\circ)5f^5L_{10}$	20859.732	120013.7
100	27500	0.63	1011.562	1011.563(5)		$4f^3(^4I^\circ)5d^5L^\circ_6$	$4f^3(^4I^\circ)5f^5M_7$	15158.154	114015.1
30	9700	0.17	1012.570	1012.567(4)		$4f^3(^4I^\circ)5d^5K^\circ_5$	$4f^3(^4I^\circ)5f^5K_5$	15262.437	114021.3
40	17000	0.42	1012.618	1012.618(6)		$4f^3(^4I^\circ)5d^5K^\circ_5$	$4f^3(^4I^\circ)5f^5L_6$	15262.437	114016.4
1	5300	-0.09	1014.414	1014.415(4)		$4f^3(^4F^\circ)5d^5H^\circ_6$	$4f^3(^4F^\circ)5f^3I_7$	31146.457	129725.4
5	6000	-0.03	1014.449	1014.450(6)		$4f^3(^4F^\circ)5d^5H^\circ_4$	$4f^3(^4F^\circ)5f^5H_5$	28745.307	127320.9
5	2500	-0.41	1020.476	1020.473(3)		$4f^3(^4I^\circ)5d^5K^\circ_7$	$4f^3(^4I^\circ)5f^3L_7$	18656.272	116650.0
1	2100	-0.48	1021.085	1021.078(4)		$4f^3(^4I^\circ)5d^5I^\circ_4$	$4f^3(^4I^\circ)5f^3G_4$	18883.669	116819.4
15	5900	-0.03	1021.362	1021.359(3)		$4f^3(^4I^\circ)5d^5K^\circ_6$	$4f^3(^4I^\circ)5f^5K_6$	16938.068	114846.8
50	21300	0.52	1021.674	1021.675(3)		$4f^3(^4I^\circ)5d^5L^\circ_7$	$4f^3(^4I^\circ)5f^5M_8$	16952.835	114831.3
40	27300	0.63	1022.321	1022.322(4)		$4f^3(^4I^\circ)5d^5K^\circ_9$	$4f^3(^4I^\circ)5f^5L_{10}$	22197.115	120013.7
30	11700	0.26	1022.405	1022.404(3)		$4f^3(^4I^\circ)5d^5K^\circ_6$	$4f^3(^4I^\circ)5f^5L_7$	16938.068	114746.8
20	4300	-0.17	1022.547	1022.558(3)		$4f^3(^4I^\circ)5d^5L^\circ_7$	$4f^3(^4I^\circ)5f^5L_7$	16952.835	114746.8
30	12500	0.29	1022.616	1022.615(3)		$4f^3(^4I^\circ)5d^5K^\circ_8$	$4f^3(^4I^\circ)5f^5K_8$	20410.897	118199.4
20	6900	0.03	1022.730	1022.730(3)		$4f^3(^4I^\circ)5d^5K^\circ_7$	$4f^3(^4I^\circ)5f^5K_7$	18656.272	116433.8
2	8700	0.14	1022.949	1022.951(4)		$4f^3(^2H_2^\circ)5d^3I^\circ_5$	$4f^3(^4F^\circ)5f^5I_6$	29397.423	127153.8
1	100	-1.80	1023.015	1023.014(4)		$4f^3(^2G_1^\circ)5d^3H^\circ_6$	$4f^3(^4F^\circ)5f^5H_7$	31559.217	129309.6
1	4000	-0.20	1023.301	1023.300(3)		$4f^3(^2H_2^\circ)5d^3I^\circ_5$	$4f^3(^2H_2^\circ)5f^3K_6$	29397.423	127120.5
40	15400	0.38	1023.367	1023.369(3)		$4f^3(^4I^\circ)5d^5K^\circ_9$	$4f^3(^4I^\circ)5f^5K_9$	22197.115	119913.6
50	19900	0.50	1023.772	1023.773(4)		$4f^3(^4I^\circ)5d^5K^\circ_8$	$4f^3(^4I^\circ)5f^5L_9$	20410.897	118088.8
40	14400	0.35	1023.965	1023.965(3)		$4f^3(^4I^\circ)5d^5K^\circ_7$	$4f^3(^4I^\circ)5f^5L_8$	18656.272	116315.9
15	9300	0.17	1024.416	1024.416(6)		$4f^3(^4F^\circ)5d^5H^\circ_4$	$4f^3(^4F^\circ)5f^5I_5$	28745.307	126361.9
60	27400	0.64	1025.340	1025.338(4)		$4f^3(^4I^\circ)5d^5L^\circ_8$	$4f^3(^4I^\circ)5f^5M_9$	18861.064	116389.9
1	2100	-0.48	1025.530	1025.529(4)		$4f^3(^2H_2^\circ)5d^3K^\circ_6$	$4f^3(^4F^\circ)5f^5I_6$	29643.186	127153.8
10	6000	-0.02	1026.118	1026.116(3)		$4f^3(^4I^\circ)5d^5L^\circ_8$	$4f^3(^4I^\circ)5f^5L_8$	18861.064	116315.9
20	20500	0.51	1027.606	1027.605(6)		$4f^3(^2H_2^\circ)5d^3K^\circ_6$	$4f^3(^2H_2^\circ)5f^3L_7$	29643.186	126956.8
20	14400	0.36	1027.748	1027.746(3)		$4f^3(^4I^\circ)5d^5I^\circ_6$	$4f^3(^4I^\circ)5f^5I_6$	21980.522	119280.8

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Table D.2: Classified Nd III Transitions Observed Only from the Nd VS Spectra (continued)

Int.	$g_u A$ (10^6 s^{-1})	$\log(g_l f)$	λ (Å)	λ_{Ritz} (Å)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level	Upper Level	E_l (cm^{-1})	E_u (cm^{-1})
40	34200	0.73	1027.827	1027.828(4)		$4f^3(^4I^\circ)5d^5L^\circ_9$	$4f^3(^4I^\circ)5f^5M_{10}$	20859.732	118152.3
20	7900	0.10	1028.502	1028.499(4)		$4f^3(^4I^\circ)5d^5L^\circ_9$	$4f^3(^4I^\circ)5f^5L_9$	20859.732	118088.8
20	11800	0.27	1028.903	1028.901(3)		$4f^3(^4I^\circ)5d^5I^\circ_5$	$4f^3(^4I^\circ)5f^5I_5$	20348.742	117539.8
50	42400	0.83	1029.826	1029.826(6)		$4f^3(^4I^\circ)5d^5L^\circ_{10}$	$4f^3(^4I^\circ)5f^5M_{11}$	22932.276	120036.1
20db	1200	-0.72	1029.875	1029.871(3)		$4f^3(^4I^\circ)5d^5H^\circ_5$	$4f^3(^4I^\circ)5f^5I_6$	22181.299	119280.8
20db	7500	0.08	1029.875	1029.875(3)		$4f^3(^4I^\circ)5d^3I^\circ_7$	$4f^3(^4I^\circ)5f^5G_6$	24003.225	121102.4
20	10600	0.23	1030.064	1030.063(4)		$4f^3(^4I^\circ)5d^5L^\circ_{10}$	$4f^3(^4I^\circ)5f^5L_{10}$	22932.276	120013.7
5	1200	-0.72	1030.112	1030.110(5)		$4f^3(^4I^\circ)5d^5K^\circ_6$	$4f^3(^4I^\circ)5f^5M_7$	16938.068	114015.1
5	1100	-0.76	1030.112	1030.106(3)		$4f^3(^4I^\circ)5d^5I^\circ_6$	$4f^3(^4I^\circ)5f^3K_7$	21980.522	119057.9
30	13900	0.34	1030.289	1030.291(3)		$4f^3(^4I^\circ)5d^5I^\circ_8$	$4f^3(^4I^\circ)5f^5I_8$	24592.259	121652.2
20	10200	0.21	1030.496	1030.497(3)		$4f^3(^4I^\circ)5d^3I^\circ_7$	$4f^3(^4I^\circ)5f^3K_8$	24003.225	121043.8
8	3500	-0.25	1031.162	1031.161(4)		$4f^3(^4F^\circ)5d^5H^\circ_5$	$4f^3(^4F^\circ)5f^5I_6$	30175.737	127153.8
10	8100	0.11	1031.262	1031.262(3)		$4f^3(^4I^\circ)5d^5I^\circ_4$	$4f^3(^4I^\circ)5f^5I_4$	18883.669	115852.2
8	14400	0.36	1031.457	1031.462(6)		$4f^3(^4F^\circ)5d^5H^\circ_6$	$4f^3(^4F^\circ)5f^5I_7$	31146.457	128096.2
5	10600	0.23	1031.514	1031.515(3)		$4f^3(^4F^\circ)5d^5H^\circ_5$	$4f^3(^2H2^\circ)5f^3K_6$	30175.737	127120.5
30	14700	0.37	1032.200	1032.200(6)		$4f^3(^4I^\circ)5d^3I^\circ_7$	$4f^3(^4I^\circ)5f^5I_7$	24003.225	120883.7
10	6200	0.00	1032.637	1032.637(4)		$4f^3(^4I^\circ)5d^5I^\circ_6$	$4f^3(^4I^\circ)5f^5G_5$	21980.522	118820.0
1	2000	-0.49	1033.691	1033.694(3)		$4f^3(^4I^\circ)5d^3I^\circ_6$	$4f^3(^4I^\circ)5f^5I_5$	20799.349	117539.8
1	2200	-0.45	1035.982	1035.983(3)		$4f^3(^4I^\circ)5d^3I^\circ_5$	$4f^3(^4I^\circ)5f^3I_6$	19616.622	116143.3
30db	22000	0.55	1036.426	1036.428(9)		$4f^3(^4F^\circ)5d^5H^\circ_7$	$4f^3(^4F^\circ)5f^5I_8$	32832.447	129317.7
30db	2700	-0.36	1036.426	1036.421(5)		$4f^3(^2H2^\circ)5d^1I^\circ_6$	$4f^3(^4F^\circ)5f^5H_7$	32823.701	129309.6
5	4600	-0.13	1036.588	1036.585(4)		$4f^3(^4I^\circ)5d^5I^\circ_5$	$4f^3(^4I^\circ)5f^3G_4$	20348.742	116819.4
3	5700	-0.04	1036.792	1036.790(3)		$4f^3(^4I^\circ)5d^5I^\circ_8$	$4f^3(^4I^\circ)5f^3K_8$	24592.259	121043.8
10	6500	0.02	1037.716	1037.716(3)		$4f^3(^4I^\circ)5d^5I^\circ_6$	$4f^3(^4I^\circ)5f^3I_7$	21980.522	118346.0
3	1300	-0.68	1037.823	1037.828(3)		$4f^3(^4I^\circ)5d^5I^\circ_7$	$4f^3(^4I^\circ)5f^3K_7$	22702.777	119057.9
5	2000	-0.49	1038.077	1038.070(3)		$4f^3(^4I^\circ)5d^3K^\circ_7$	$4f^3(^4I^\circ)5f^5I_8$	25319.579	121652.2
8	1800	-0.54	1038.408	1038.407(5)		$4f^3(^4F^\circ)5d^5H^\circ_6$	$4f^3(^2H2^\circ)5f^3K_7$	31146.457	127447.8
3	3400	-0.26	1038.864	1038.863(3)		$4f^3(^4I^\circ)5d^5H^\circ_3$	$4f^3(^4I^\circ)5f^5I_4$	19593.094	115852.2
1	1700	-0.56	1039.112	1039.117(3)		$4f^3(^4I^\circ)5d^3I^\circ_5$	$4f^3(^4I^\circ)5f^5I_4$	19616.622	115852.2
1	1900	-0.51	1039.623	1039.624(3)		$4f^3(^4I^\circ)5d^3I^\circ_6$	$4f^3(^4I^\circ)5f^3K_6$	20799.349	116988.0
10	2800	-0.34	1039.772	1039.771(3)		$4f^3(^4I^\circ)5d^5K^\circ_7$	$4f^3(^4I^\circ)5f^5M_8$	18656.272	114831.3
20db	4100	-0.18	1040.594	1040.581(4)		$4f^3(^4I^\circ)5d^3H^\circ_6$	$4f^3(^4I^\circ)5f^3G_5$	25034.832	121135.0
20db	13000	0.32	1040.594	1040.594(5)		$4f^3(^4F^\circ)5d^5G^\circ_6$	$4f^3(^4F^\circ)5f^5H_7$	33210.660	129309.6
30	10200	0.22	1040.934	1040.934(3)		$4f^3(^4I^\circ)5d^3H^\circ_6$	$4f^3(^4I^\circ)5f^5G_6$	25034.832	121102.4
3	5700	-0.03	1041.012	1041.013(4)		$4f^3(^2H2^\circ)5d^3K^\circ_8$	$4f^3(^2H2^\circ)5f^3K_8$	34534.549	130594.8
10	4900	-0.10	1041.077	1041.077(7)		$4f^3(^4I^\circ)5d^5H^\circ_3$	$4f^3(^4I^\circ)5f^5G_2$	19593.094	115647.5
2	3400	-0.26	1041.145	1041.147(3)		$4f^3(^4I^\circ)5d^3H^\circ_4$	$4f^3(^4I^\circ)5f^5I_5$	21491.882	117539.8
10	3600	-0.23	1041.893	1041.895(5)		$4f^3(^4I^\circ)5d^5K^\circ_8$	$4f^3(^4I^\circ)5f^5M_9$	20410.897	116389.9
5	2900	-0.33	1042.155	1042.153(5)		$4f^3(^4I^\circ)5d^5K^\circ_9$	$4f^3(^4I^\circ)5f^5M_{10}$	22197.115	118152.3
5	3600	-0.23	1042.392	1042.393(3)		$4f^3(^4I^\circ)5d^3H^\circ_5$	$4f^3(^4I^\circ)5f^5I_6$	23347.721	119280.8
15	1900	-0.51	1042.806	1042.806(4)		$4f^3(^4I^\circ)5d^5H^\circ_3$	$(115488)5f_2$	19593.094	115488.2
20	15400	0.40	1042.877	1042.877(5)		$4f^3(^2G1^\circ)5d^3H^\circ_6$	$4f^3(^2H2^\circ)5f^3K_7$	31559.217	127447.8
20	27100	0.65	1043.037	1043.036(7)		$4f^3(^2H2^\circ)5d^3K^\circ_8$	$4f^3(^2H2^\circ)5f^3L_9$	34534.549	130408.5
15	12600	0.31	1043.138	1043.138(4)		$4f^3(^4I^\circ)5d^3H^\circ_6$	$4f^3(^4I^\circ)5f^5F_5$	25034.832	120899.4

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Table D.2: Classified Nd III Transitions Observed Only from the Nd VS Spectra (continued)

Int.	$g_u A$ (10^6 s^{-1})	$\log(g_l f)$	λ (Å)	λ_{Ritz} (Å)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level	Upper Level	E_l (cm^{-1})	E_u (cm^{-1})
20	7400	0.08	1043.900	1043.901(3)		$4f^3(^4I^\circ)5d\ ^5I^\circ_5$	$4f^3(^4I^\circ)5f\ ^3I_6$	20348.742	116143.3
1	3000	-0.31	1044.031	1044.029(3)		$4f^3(^4I^\circ)5d\ ^3K^\circ_7$	$4f^3(^4I^\circ)5f\ ^5G_6$	25319.579	121102.4
20	9900	0.21	1044.709	1044.709(4)		$4f^3(^4I^\circ)5d\ ^3H^\circ_5$	$4f^3(^4I^\circ)5f\ ^5G_4$	23347.721	119068.2
20	9800	0.21	1045.314	1045.314(4)		$4f^3(^4I^\circ)5d\ ^3H^\circ_4$	$4f^3(^4I^\circ)5f\ ^5G_3$	21491.882	117156.9
20	22800	0.57	1045.470	1045.470(5)		$4f^3(^2H2^\circ)5d\ ^3K^\circ_7$	$4f^3(^2H2^\circ)5f\ ^3L_8$	31781.802	127432.6
20	10400	0.23	1045.552	1045.552(3)		$4f^3(^4I^\circ)5d\ ^5I^\circ_7$	$4f^3(^4I^\circ)5f\ ^3I_7$	22702.777	118346.0
20	8600	0.15	1045.647	1045.648(3)		$4f^3(^4I^\circ)5d\ ^3I^\circ_6$	$4f^3(^4I^\circ)5f\ ^5K_7$	20799.349	116433.8
5	3900	-0.19	1046.209	1046.211(4)		$4f^3(^4I^\circ)5d\ ^3H^\circ_5$	$4f^3(^4I^\circ)5f\ ^5F_4$	23347.721	118930.7
10	8100	0.12	1046.531	1046.525(3)		$4f^3(^4I^\circ)5d\ ^5H^\circ_7$	$4f^3(^4I^\circ)5f\ ^5I_8$	26097.906	121652.2
20	11100	0.26	1047.151	1047.157(3)		$4f^3(^4I^\circ)5d\ ^5I^\circ_7$	$4f^3(^4I^\circ)5f\ ^5K_8$	22702.777	118199.4
10	9300	0.18	1047.425	1047.424(4)		$4f^3(^4I^\circ)5d\ ^3H^\circ_5$	$4f^3(^4I^\circ)5f\ ^5G_5$	23347.721	118820.0
10	14300	0.37	1048.148	1048.146(4)		$4f^3(^2H2^\circ)5d\ ^3I^\circ_7$	$4f^3(^2H2^\circ)5f\ ^3K_8$	35188.278	130594.8
15	6600	0.04	1048.263	1048.264(4)		$4f^3(^4I^\circ)5d\ ^5H^\circ_7$	$4f^3(^4I^\circ)5f\ ^3H_6$	26097.906	121493.7
10	6800	0.05	1048.834	1048.834(3)		$4f^3(^4I^\circ)5d\ ^3I^\circ_6$	$4f^3(^4I^\circ)5f\ ^3I_6$	20799.349	116143.3
3	100	-1.78	1048.885	1048.892(4)		$4f^3(^2H2^\circ)5d\ ^3K^\circ_7$	$4f^3(^2H2^\circ)5f\ ^3K_6$	31781.802	127120.5
40db	6500	0.03	1049.011	1049.015(4)		$4f^3(^4I^\circ)5d\ ^3H^\circ_4$	$4f^3(^4I^\circ)5f\ ^3G_4$	21491.882	116819.4
40db	6200	0.01	1049.011	1049.017(5)		$4f^3(^4I^\circ)5d\ ^5H^\circ_6$	$4f^3(^4I^\circ)5f\ ^3H_5$	24058.518	119385.9
30	14800	0.39	1049.087	1049.083(4)		$4f^3(^4I^\circ)5d\ ^5I^\circ_8$	$4f^3(^4I^\circ)5f\ ^5K_9$	24592.259	119913.6
3	4100	-0.17	1049.246	1049.247(4)		$4f^3(^4I^\circ)5d\ ^5I^\circ_4$	$4f^3(^4I^\circ)5f\ ^5H_3$	18883.669	114190.1
5	4500	-0.13	1050.010	1050.010(4)		$4f^3(^4I^\circ)5d\ ^5H^\circ_5$	$4f^3(^4I^\circ)5f\ ^3H_4$	22181.299	117418.5
15	9400	0.19	1050.085	1050.087(3)		$4f^3(^4I^\circ)5d\ ^3I^\circ_5$	$4f^3(^4I^\circ)5f\ ^5K_6$	19616.622	114846.8
3	2400	-0.40	1050.133	1050.134(3)		$4f^3(^4I^\circ)5d\ ^3K^\circ_6$	$4f^3(^4I^\circ)5f\ ^3I_7$	23120.073	118346.0
15	9900	0.21	1050.535	1050.536(4)		$4f^3(^4I^\circ)5d\ ^3I^\circ_5$	$4f^3(^4I^\circ)5f\ ^3I_5$	19616.622	114806.1
20	10000	0.22	1051.106	1051.109(4)		$4f^3(^4I^\circ)5d\ ^5I^\circ_4$	$4f^3(^4I^\circ)5f\ ^5K_5$	18883.669	114021.3
2	2800	-0.33	1052.579	1052.582(3)		$4f^3(^4I^\circ)5d\ ^5H^\circ_7$	$4f^3(^4I^\circ)5f\ ^5G_6$	26097.906	121102.4
15	8900	0.17	1052.638	1052.638(3)		$4f^3(^4I^\circ)5d\ ^5H^\circ_6$	$4f^3(^4I^\circ)5f\ ^3K_7$	24058.518	119057.9
2	3400	-0.25	1053.232	1053.231(3)		$4f^3(^4I^\circ)5d\ ^5H^\circ_7$	$4f^3(^4I^\circ)5f\ ^3K_8$	26097.906	121043.8
10	2900	-0.32	1053.497	1053.501(3)		$4f^3(^4I^\circ)5d\ ^3I^\circ_7$	$4f^3(^4I^\circ)5f\ ^3L_8$	24003.225	118924.8
10	9900	0.22	1054.596	1054.594(4)		$4f^3(^4I^\circ)5d\ ^5G^\circ_6$	$4f^3(^4I^\circ)5f\ ^3H_6$	26670.461	121493.7
20db	4000	-0.18	1054.783	1054.788(5)		$4f^3(^4I^\circ)5d\ ^5H^\circ_4$	$4f^3(^4I^\circ)5f\ ^3G_3$	20388.995	115194.8
20db	7800	0.11	1054.783	1054.778(3)		$4f^3(^4I^\circ)5d\ ^5H^\circ_5$	$4f^3(^4I^\circ)5f\ ^3K_6$	22181.299	116988.0
3	3900	-0.19	1056.307	1056.307(3)		$4f^3(^4I^\circ)5d\ ^5I^\circ_6$	$4f^3(^4I^\circ)5f\ ^3L_7$	21980.522	116650.0
8	6800	0.06	1057.118	1057.116(4)		$4f^3(^4I^\circ)5d\ ^5H^\circ_3$	$4f^3(^4I^\circ)5f\ ^5H_3$	19593.094	114190.1
5	6100	0.01	1057.407	1057.407(4)		$4f^3(^4I^\circ)5d\ ^3H^\circ_6$	$4f^3(^4I^\circ)5f\ ^3I_7$	35154.437	129725.4
15	10300	0.24	1058.120	1058.117(5)		$4f^3(^4I^\circ)5d\ ^5G^\circ_5$	$4f^3(^4I^\circ)5f\ ^3H_5$	24878.412	119385.9
8	2100	-0.45	1058.223	1058.223(3)		$4f^3(^4I^\circ)5d\ ^5I^\circ_5$	$4f^3(^4I^\circ)5f\ ^5K_6$	20348.742	114846.8
5db	1600	-0.57	1058.597	1058.586(3)		$4f^3(^4I^\circ)5d\ ^5I^\circ_8$	$4f^3(^4I^\circ)5f\ ^3K_7$	24592.259	119057.9
5db	4400	-0.13	1058.597	1058.598(4)		$4f^3(^4I^\circ)5d\ ^5G^\circ_6$	$4f^3(^4I^\circ)5f\ ^3G_5$	26670.461	121135.0
15	6800	0.06	1059.130	1059.130(4)		$4f^3(^4I^\circ)5d\ ^5H^\circ_4$	$4f^3(^4I^\circ)5f\ ^3I_5$	20388.995	114806.1
15	8300	0.14	1059.232	1059.232(4)		$4f^3(^4I^\circ)5d\ ^5G^\circ_4$	$4f^3(^4I^\circ)5f\ ^3H_4$	23010.450	117418.5
1	1400	-0.63	1059.548	1059.541(4)		$4f^3(^4I^\circ)5d\ ^5I^\circ_5$	$4f^3(^4I^\circ)5f\ ^5H_4$	20348.742	114729.2
20	12000	0.31	1059.874	1059.875(5)		$4f^3(^4I^\circ)5d\ ^5H^\circ_6$	$4f^3(^4I^\circ)5f\ ^5H_6$	24058.518	118409.3
40db	7600	0.11	1059.986	1059.993(4)		$4f^3(^4I^\circ)5d\ ^5H^\circ_4$	$4f^3(^4I^\circ)5f\ ^5H_4$	20388.995	114729.2
40db	12300	0.32	1059.986	1059.986(4)		$4f^3(^4I^\circ)5d\ ^5H^\circ_7$	$4f^3(^4I^\circ)5f\ ^5H_7$	26097.906	120438.8

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Table D.2: Classified Nd III Transitions Observed Only from the Nd VS Spectra (continued)

Int.	$g_u A$ (10^6 s^{-1})	$\log(g_l f)$	λ (Å)	λ_{Ritz} (Å)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level	Upper Level	E_l (cm^{-1})	E_u (cm^{-1})
1	1400	-0.63	1060.614	1060.612(3)		$4f^3(^4I^\circ)5d \ ^5I^\circ_7$	$4f^3(^4I^\circ)5f \ ^3K_6$	22702.777	116988.0
10	8200	0.14	1061.245	1061.245(4)		$4f^3(^4I^\circ)5d \ ^5G^\circ_6$	$4f^3(^4I^\circ)5f \ ^5F_5$	26670.461	120899.4
5	5300	-0.05	1061.453	1061.455(3)		$4f^3(^4I^\circ)5d \ ^3K^\circ_8$	$4f^3(^4I^\circ)5f \ ^5I_8$	27441.911	121652.2
2	1000	-0.77	1062.180	1062.175(4)		$4f^3(^4I^\circ)5d \ ^5G^\circ_4$	$4f^3(^4I^\circ)5f \ ^5G_3$	23010.450	117156.9
20	10000	0.23	1062.394	1062.394(3)		$4f^3(^4I^\circ)5d \ ^5H^\circ_5$	$4f^3(^4I^\circ)5f \ ^5H_5$	22181.299	116308.3
15	10100	0.23	1063.239	1063.238(4)		$4f^3(^4I^\circ)5d \ ^5G^\circ_5$	$4f^3(^4I^\circ)5f \ ^5F_4$	24878.412	118930.7
8	2300	-0.41	1063.295	1063.293(3)		$4f^3(^4I^\circ)5d \ ^3I^\circ_6$	$4f^3(^4I^\circ)5f \ ^5K_6$	20799.349	114846.8
5	1600	-0.57	1063.709	1063.707(4)		$4f^3(^4I^\circ)5d \ ^5G^\circ_2$	(115488)5f $_2$	21477.328	115488.2
15	6500	0.04	1064.423	1064.425(4)		$4f^3(^4I^\circ)5d \ ^3I^\circ_6$	$4f^3(^4I^\circ)5f \ ^5L_7$	20799.349	114746.8
15	8400	0.16	1065.327	1065.327(3)		$4f^3(^4I^\circ)5d \ ^3K^\circ_6$	$4f^3(^4I^\circ)5f \ ^3K_6$	23120.073	116988.0
15	7800	0.12	1065.429	1065.430(4)		$4f^3(^4I^\circ)5d \ ^5G^\circ_4$	$4f^3(^4I^\circ)5f \ ^5F_3$	23010.450	116869.3
3	3100	-0.28	1066.458	1066.458(4)		$4f^3(^4I^\circ)5d \ ^5G^\circ_6$	$4f^3(^4I^\circ)5f \ ^5H_7$	26670.461	120438.8
30	21300	0.56	1066.728	1066.728(4)		$4f^3(^4I^\circ)5d \ ^3K^\circ_8$	$4f^3(^4I^\circ)5f \ ^3L_9$	27441.911	121186.5
20	11400	0.29	1066.799	1066.800(3)		$4f^3(^4I^\circ)5d \ ^3K^\circ_7$	$4f^3(^4I^\circ)5f \ ^3K_7$	25319.579	119057.9
10	5900	0.00	1067.063	1067.061(5)		$4f^3(^4I^\circ)5d \ ^5G^\circ_3$	$4f^3(^4I^\circ)5f \ ^3G_3$	21479.404	115194.8
20db	2500	-0.37	1067.546	1067.534(6)		$4f^3(^4I^\circ)5d \ ^5G^\circ_2$	$4f^3(^4I^\circ)5f \ ^5F_2$	21477.328	115151.2
20db	6300	0.03	1067.546	1067.557(6)		$4f^3(^4I^\circ)5d \ ^5G^\circ_3$	$4f^3(^4I^\circ)5f \ ^5F_2$	21479.404	115151.2
8	5300	-0.04	1068.227	1068.226(3)		$4f^3(^4I^\circ)5d \ ^5I^\circ_7$	$4f^3(^4I^\circ)5f \ ^5L_8$	22702.777	116315.9
20	13600	0.37	1068.317	1068.316(3)		$4f^3(^4I^\circ)5d \ ^3K^\circ_7$	$4f^3(^4I^\circ)5f \ ^3L_8$	25319.579	118924.8
10	7500	0.11	1068.354	1068.355(3)		$4f^3(^4I^\circ)5d \ ^3K^\circ_8$	$4f^3(^4I^\circ)5f \ ^3K_8$	27441.911	121043.8
30db	12400	0.33	1069.175	1069.177(3)		$4f^3(^4I^\circ)5d \ ^3K^\circ_6$	$4f^3(^4I^\circ)5f \ ^3L_7$	23120.073	116650.0
30db	4600	-0.10	1069.175	1069.166(5)		$4f^3(^4I^\circ)5d \ ^5G^\circ_5$	$4f^3(^4I^\circ)5f \ ^5H_6$	24878.412	118409.3
20	5700	-0.01	1069.535	1069.535(6)		$4f^3(^4I^\circ)5d \ ^5G^\circ_2$	$4f^3(^4I^\circ)5f \ ^5F_1$	21477.328	114975.9
5	4500	-0.11	1071.837	1071.836(3)		$4f^3(^4I^\circ)5d \ ^5G^\circ_4$	$4f^3(^4I^\circ)5f \ ^5H_5$	23010.450	116308.3
15	9300	0.20	1072.028	1072.028(6)		$4f^3(^4I^\circ)5d \ ^3G^\circ_3$	$4f^3(^4I^\circ)5f \ ^3F_2$	23891.226	117172.4
5	4000	-0.16	1072.397	1072.388(4)		$4f^3(^4I^\circ)5d \ ^5G^\circ_3$	$4f^3(^4I^\circ)5f \ ^5H_4$	21479.404	114729.2
1	1300	-0.65	1073.099	1073.097(3)		$4f^3(^4I^\circ)5d \ ^3K^\circ_6$	$4f^3(^4I^\circ)5f \ ^5H_5$	23120.073	116308.3
20	13000	0.35	1074.350	1074.351(6)		$4f^3(^4I^\circ)5d \ ^3G^\circ_4$	$4f^3(^4I^\circ)5f \ ^3F_3$	26140.225	119219.7
1	2900	-0.30	1075.305	1075.305(4)		$4f^3(^4I^\circ)5d \ ^3K^\circ_8$	$4f^3(^4I^\circ)5f \ ^5H_7$	27441.911	120438.8
3	4500	-0.11	1075.524	1075.522(4)		$4f^3(^4I^\circ)5d \ ^3G^\circ_3$	$4f^3(^4I^\circ)5f \ ^5F_3$	23891.226	116869.3
20	15800	0.44	1075.690	1075.689(6)		$4f^3(^4I^\circ)5d \ ^3G^\circ_5$	$4f^3(^4I^\circ)5f \ ^3F_4$	28440.047	121403.7
8	5500	-0.02	1076.102	1076.102(4)		$4f^3(^4I^\circ)5d \ ^3G^\circ_4$	$4f^3(^4I^\circ)5f \ ^5G_4$	26140.225	119068.2
8	8100	0.15	1078.807	1078.807(4)		$4f^3(^4I^\circ)5d \ ^3G^\circ_5$	$4f^3(^4I^\circ)5f \ ^3G_5$	28440.047	121135.0
40	34600	0.78	1080.949	1080.949(6)		$4f^3(^4I^\circ)5d \ ^3L^\circ_9$	$4f^3(^4I^\circ)5f \ ^3M_{10}$	28877.321	121388.6
40	29100	0.71	1082.328	1082.329(4)		$4f^3(^4I^\circ)5d \ ^3L^\circ_8$	$4f^3(^4I^\circ)5f \ ^3M_9$	26676.685	119070.0
5	8300	0.16	1083.318	1083.316(4)		$4f^3(^4I^\circ)5d \ ^3L^\circ_9$	$4f^3(^4I^\circ)5f \ ^3L_9$	28877.321	121186.5
30	6500	0.06	1084.030	1084.033(3)		$4f^3(^4I^\circ)5d \ ^3L^\circ_8$	$4f^3(^4I^\circ)5f \ ^3L_8$	26676.685	118924.8
40	22700	0.60	1084.129	1084.129(4)		$4f^3(^4I^\circ)5d \ ^3L^\circ_7$	$4f^3(^4I^\circ)5f \ ^3M_8$	24497.165	116737.1
2	4000	-0.15	1085.156	1085.154(3)		$4f^3(^4I^\circ)5d \ ^3L^\circ_7$	$4f^3(^4I^\circ)5f \ ^3L_7$	24497.165	116650.0
8	6300	0.06	1107.003	1107.001(4)		$4f^3(^4I^\circ)5d \ ^3L^\circ_7$	$4f^3(^4I^\circ)5f \ ^5M_8$	24497.165	114831.3
32	160	-1.06	1904.916	1904.9130(7)	1904.2801	$4f^3(^4I^\circ)5d \ ^5H^\circ_3$	$4f^3(^4F^\circ)6p \ ^5G_2$	19593.094	72088.930
39	210	-0.94	1906.218	1906.2183(11)	1905.5852	$4f^3(^4I^\circ)5d \ ^3K^\circ_6$	$4f^3(^4F^\circ)6p \ ^5G_5$	23120.073	75579.962
7	65	-1.44	1933.861	1933.8594(11)	1933.2223	$4f^3(^4I^\circ)5d \ ^3H^\circ_4$	$4f^3(^4F^\circ)6p \ ^5G_3$	21491.882	73201.950
10	55	-1.50	1950.555	1950.5562(6)	1949.9165	$4f^3(^4I^\circ)5d \ ^5I^\circ_6$	$4f^3(^2H^\circ_2)6p \ ^3I_5$	21980.522	73247.950

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Table D.2: Classified Nd III Transitions Observed Only from the Nd VS Spectra (continued)

Int.	$g_u A$ (10^6 s^{-1})	$\log(g_l f)$	λ (Å)	λ_{Ritz} (Å)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level	Upper Level	E_l (cm^{-1})	E_u (cm^{-1})
11	97	-1.25	1977.631	1977.6266(10)	1976.9825	$4f^3(^4I^\circ)5d\ ^5G^\circ_6$	$4f^3(^2H2^\circ)6p\ ^1I_6$	26670.461	77236.125
16	160	-1.03	1978.375	1978.3697(11)	1977.7255	$4f^3(^4I^\circ)5d\ ^5H^\circ_7$	$4f^3(^2H2^\circ)6p\ ^3I_6$	26097.906	76644.575
37	250	-0.83	1994.897	1994.8980(6)	1994.2509	$4f^3(^4I^\circ)5d\ ^3K^\circ_6$	$4f^3(^2H2^\circ)6p\ ^3I_5$	23120.073	73247.950
13	81	-1.31	1998.012	1998.0138(3)	1997.3662	$4f^3(^4I^\circ)5d\ ^5K^\circ_8$	$4f^3(^4I^\circ)6p\ ^3I_7$	20410.897	70460.602
25	130	-1.11	2005.397	2005.3954(3)	2004.7465	$4f^3(^4I^\circ)5d\ ^5L^\circ_6$	$4f^3(^4I^\circ)6p\ ^5H_6$	15158.154	65023.633
12	51	-1.51	2009.458	2009.4574(4)	2008.8078	$4f^3(^4I^\circ)5d\ ^5L^\circ_7$	$4f^3(^4I^\circ)6p\ ^5H_7$	16952.835	66717.513
26	71	-1.37	2009.596	2009.5980(2)	2008.9484	$4f^3(^4I^\circ)5d\ ^5K^\circ_5$	$4f^3(^4I^\circ)6p\ ^5H_6$	15262.437	65023.633
32	160	-1.01	2012.418	2012.4242(3)	2011.7741	$4f^3(^4I^\circ)5d\ ^5K^\circ_7$	$4f^3(^4I^\circ)6p\ ^3I_6$	18656.272	68347.584
23	88	-1.27	2014.248	2014.2451(3)	2013.5946	$4f^3(^4I^\circ)5d\ ^5K^\circ_7$	$4f^3(^4I^\circ)6p\ ^5K_8$	18656.272	68302.664
23	40	-1.61	2014.248	2014.2479(3)	2013.5974	$4f^3(^4I^\circ)5d\ ^5L^\circ_8$	$4f^3(^4I^\circ)6p\ ^3K_7$	18861.064	68507.387
12	55	-1.47	2017.792	2017.7906(4)	2017.1395	$4f^3(^4I^\circ)5d\ ^5K^\circ_6$	$4f^3(^4I^\circ)6p\ ^5I_7$	16938.068	66497.225
24	110	-1.17	2018.392	2018.3920(4)	2017.7408	$4f^3(^4I^\circ)5d\ ^5L^\circ_7$	$4f^3(^4I^\circ)6p\ ^5I_7$	16952.835	66497.225
32	130	-1.10	2020.241	2020.2438(3)	2019.5923	$4f^3(^4I^\circ)5d\ ^5L^\circ_7$	$4f^3(^4I^\circ)6p\ ^3K_6$	16952.835	66451.812
29	180	-0.96	2022.589	2022.5883(4)	2021.9364	$4f^3(^4I^\circ)5d\ ^5L^\circ_8$	$4f^3(^4I^\circ)6p\ ^5K_8$	18861.064	68302.664
42	270	-0.78	2026.971	2026.9695(4)	2026.3168	$4f^3(^4I^\circ)5d\ ^5K^\circ_6$	$4f^3(^4I^\circ)6p\ ^5H_5$	16938.068	66272.802
30	150	-1.03	2029.167	2029.1682(5)	2028.5151	$4f^3(^4I^\circ)5d\ ^5L^\circ_9$	$4f^3(^4I^\circ)6p\ ^5K_9$	20859.732	70141.009
27	100	-1.21	2032.957	2032.9570(7)	2032.3032	$4f^3(^4I^\circ)5d\ ^5H^\circ_6$	$4f^3(^2H2^\circ)6p\ ^3I_5$	24058.518	73247.950
42	170	-0.96	2079.633	2079.6262(3)	2078.9637	$4f^3(^4I^\circ)5d\ ^5K^\circ_6$	$4f^3(^4I^\circ)6p\ ^5H_6$	16938.068	65023.633
42	190	-0.91	2080.680	2080.6787(2)	2080.0160	$4f^3(^4I^\circ)5d\ ^5K^\circ_7$	$4f^3(^4I^\circ)6p\ ^5H_7$	18656.272	66717.513
17	44	-1.54	2086.332	2086.3342(4)	2085.6704	$4f^3(^4I^\circ)5d\ ^5L^\circ_8$	$4f^3(^4I^\circ)6p\ ^5I_8$	18861.064	66792.024
23	47	-1.51	2087.816	2087.8225(3)	2087.1584	$4f^3(^4I^\circ)5d\ ^5I^\circ_7$	$4f^3(^4I^\circ)6p\ ^3K_8$	22702.777	70599.570
44	310	-0.69	2090.811	2090.8093(11)	2090.1447	$4f^3(^4F^\circ)5d\ ^5H^\circ_6$	$4f^3(^4F^\circ)6p\ ^5G_6$	31146.457	78974.826
21	39	-1.59	2093.901	2093.8977(3)	2093.2324	$4f^3(^4I^\circ)5d\ ^5I^\circ_7$	$4f^3(^4I^\circ)6p\ ^3I_7$	22702.777	70460.602
34	63	-1.38	2097.782	2097.7919(4)	2097.1259	$4f^3(^4I^\circ)5d\ ^5L^\circ_7$	$4f^3(^4I^\circ)6p\ ^5K_7$	16952.835	64622.006
39	87	-1.24	2100.976	2100.9822(3)	2100.3156	$4f^3(^4I^\circ)5d\ ^5L^\circ_7$	$4f^3(^4I^\circ)6p\ ^5I_6$	16952.835	64549.620
48	390	-0.59	2101.146	2101.1520(10)	2100.4853	$4f^3(^2H2^\circ)5d\ ^3K^\circ_6$	$4f^3(^2H2^\circ)6p\ ^1I_6$	29643.186	77236.125
34	82	-1.26	2103.118	2103.1275(3)	2102.4604	$4f^3(^4I^\circ)5d\ ^3I^\circ_6$	$4f^3(^4I^\circ)6p\ ^3I_6$	20799.349	68347.584
22	49	-1.48	2111.370	2111.3754(4)	2110.7067	$4f^3(^4I^\circ)5d\ ^5L^\circ_6$	$4f^3(^4I^\circ)6p\ ^5K_6$	15158.154	62520.646
21	33	-1.65	2116.028	2116.0345(3)	2115.3649	$4f^3(^4I^\circ)5d\ ^5K^\circ_5$	$4f^3(^4I^\circ)6p\ ^5K_6$	15262.437	62520.646
47	350	-0.63	2118.956	2118.9572(11)	2118.2871	$4f^3(^2H2^\circ)5d\ ^3K^\circ_7$	$4f^3(^4F^\circ)6p\ ^5G_6$	31781.802	78974.826
16	52	-1.45	2135.140	2135.1467(3)	2134.4733	$4f^3(^4I^\circ)5d\ ^3I^\circ_5$	$4f^3(^4I^\circ)6p\ ^3K_6$	19616.622	66451.812
47	120	-1.08	2143.332	2143.3388(3)	2142.6637	$4f^3(^4I^\circ)5d\ ^3I^\circ_5$	$4f^3(^4I^\circ)6p\ ^5H_5$	19616.622	66272.802
12	83	-1.24	2146.959	2146.9599(8)	2146.2841	$4f^3(^4I^\circ)5d\ ^5G^\circ_6$	$4f^3(^2H2^\circ)6p\ ^3I_5$	26670.461	73247.950
44	230	-0.80	2152.510	2152.5107(3)	2151.8338	$4f^3(^4I^\circ)5d\ ^3I^\circ_7$	$4f^3(^4I^\circ)6p\ ^3I_7$	24003.225	70460.602
19	42	-1.53	2155.070	2155.0756(3)	2154.3982	$4f^3(^4I^\circ)5d\ ^5H^\circ_6$	$4f^3(^4I^\circ)6p\ ^3I_7$	24058.518	70460.602
24	54	-1.42	2166.081	2166.0829(6)	2165.4032	$4f^3(^4I^\circ)5d\ ^5H^\circ_5$	$4f^3(^4I^\circ)6p\ ^3I_6$	22181.299	68347.584
47	260	-0.74	2166.797	2166.7944(12)	2166.1146	$4f^3(^2H2^\circ)5d\ ^1I^\circ_6$	$4f^3(^4F^\circ)6p\ ^5G_6$	32823.701	78974.826
77	1900	0.13	2167.202	2167.2051(11)	2166.5252	$4f^3(^4F^\circ)5d\ ^5H^\circ_7$	$4f^3(^4F^\circ)6p\ ^5G_6$	32832.447	78974.826
18	82	-1.24	2169.691	2169.6837(11)	2169.0032	$4f^3(^4F^\circ)5d\ ^5H^\circ_6$	$4f^3(^2H2^\circ)6p\ ^1I_6$	31146.457	77236.125
31	81	-1.24	2177.790	2177.7874(3)	2177.1053	$4f^3(^4I^\circ)5d\ ^3I^\circ_6$	$4f^3(^4I^\circ)6p\ ^5H_7$	20799.349	66717.513
29	61	-1.36	2179.415	2179.4181(3)	2178.7357	$4f^3(^4I^\circ)5d\ ^5H^\circ_4$	$4f^3(^4I^\circ)6p\ ^5H_5$	20388.995	66272.802
58	640	-0.34	2185.126	2185.1158(13)	2184.4321	$4f^3(^4F^\circ)5d\ ^5G^\circ_6$	$4f^3(^4F^\circ)6p\ ^5G_6$	33210.660	78974.826
53	110	-1.10	2188.273	2188.2855(3)	2187.6012	$4f^3(^4I^\circ)5d\ ^3I^\circ_6$	$4f^3(^4I^\circ)6p\ ^5I_7$	20799.349	66497.225
37	330	-0.63	2189.297	2189.2900(11)	2188.6056	$4f^3(^2G1^\circ)5d\ ^3H^\circ_6$	$4f^3(^2H2^\circ)6p\ ^1I_6$	31559.217	77236.125

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Table D.2: Classified Nd III Transitions Observed Only from the Nd VS Spectra (continued)

Int.	$g_u A$ (10^6 s^{-1})	$\log(g_l f)$	λ (Å)	λ_{Ritz} (Å)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level	Upper Level	E_l (cm^{-1})	E_u (cm^{-1})
54	210	-0.82	2190.464	2190.4623(3)	2189.7776	$4f^3(^4I^\circ)5d\ ^3I^\circ_6$	$4f^3(^4I^\circ)6p\ ^3K_6$	20799.349	66451.812
50	250	-0.74	2192.987	2192.9879(3)	2192.3026	$4f^3(^4I^\circ)5d\ ^5I^\circ_7$	$4f^3(^4I^\circ)6p\ ^5K_8$	22702.777	68302.664
25	95	-1.16	2197.146	2197.1423(11)	2196.4562	$4f^3(^4F^\circ)5d\ ^5H^\circ_4$	$4f^3(^4F^\circ)6p\ ^5G_4$	28745.307	74258.973
19	42	-1.52	2199.090	2199.0853(3)	2198.3987	$4f^3(^4I^\circ)5d\ ^3I^\circ_6$	$4f^3(^4I^\circ)6p\ ^5H_5$	20799.349	66272.802
18	38	-1.56	2199.395	2199.3904(2)	2198.7039	$4f^3(^4I^\circ)5d\ ^5I^\circ_4$	$4f^3(^4I^\circ)6p\ ^3I_5$	18883.669	64350.812
80	200	-0.84	2202.294	2202.3031(2)	2201.6159	$4f^3(^4I^\circ)5d\ ^3I^\circ_5$	$4f^3(^4I^\circ)6p\ ^5H_6$	19616.622	65023.633
38	110	-1.10	2204.573	2204.5736(3)	2203.8860	$4f^3(^4I^\circ)5d\ ^5I^\circ_4$	$4f^3(^4I^\circ)6p\ ^5H_4$	18883.669	64243.914
34	57	-1.38	2208.483	2208.4810(4)	2207.7925	$4f^3(^4I^\circ)5d\ ^3K^\circ_7$	$4f^3(^4I^\circ)6p\ ^3K_8$	25319.579	70599.570
34	130	-1.02	2218.111	2218.1106(14)	2217.4201	$4f^3(^4F^\circ)5d\ ^5D^\circ_3$	$4f^3(^4F^\circ)6p\ ^5G_3$	28118.535	73201.950
23	54	-1.40	2222.224	2222.2290(3)	2221.5376	$4f^3(^4I^\circ)5d\ ^3H^\circ_5$	$4f^3(^4I^\circ)6p\ ^3I_6$	23347.721	68347.584
25	79	-1.23	2231.748	2231.7492(8)	2231.0557	$4f^3(^4I^\circ)5d\ ^3G^\circ_5$	$4f^3(^2H2^\circ)6p\ ^3I_5$	28440.047	73247.950
30	150	-0.95	2240.634	2240.6337(12)	2239.9384	$4f^3(^2H2^\circ)5d\ ^1H^\circ_5$	$4f^3(^2H2^\circ)6p\ ^1I_6$	32605.894	77236.125
31	85	-1.19	2246.982	2246.9809(3)	2246.2842	$4f^3(^4I^\circ)5d\ ^3I^\circ_7$	$4f^3(^4I^\circ)6p\ ^3K_7$	24003.225	68507.387
31	89	-1.17	2248.644	2248.6418(3)	2247.9447	$4f^3(^4I^\circ)5d\ ^5I^\circ_6$	$4f^3(^4I^\circ)6p\ ^3K_6$	21980.522	66451.812
65	1600	0.08	2250.554	2250.5539(16)	2249.8565	$4f^3(^4F^\circ)5d\ ^5H^\circ_6$	$4f^3(^4F^\circ)6p\ ^5G_5$	31146.457	75579.962
73	1200	-0.04	2251.547	2251.5471(9)	2250.8494	$4f^3(^4F^\circ)5d\ ^5H^\circ_3$	$4f^3(^4F^\circ)6p\ ^5G_2$	27675.024	72088.930
53	200	-0.82	2257.735	2257.7298(4)	2257.0308	$4f^3(^4I^\circ)5d\ ^5I^\circ_6$	$4f^3(^4I^\circ)6p\ ^5H_5$	21980.522	66272.802
22	51	-1.41	2262.407	2262.3985(2)	2261.6985	$4f^3(^4I^\circ)5d\ ^5I^\circ_5$	$4f^3(^4I^\circ)6p\ ^5I_6$	20348.742	64549.620
21	370	-0.55	2263.457	2263.4645(6)	2262.7643	$4f^3(^4I^\circ)6p\ ^5I_6$	$4f^3(^4I^\circ)6d\ ^3K^\circ_7$	64549.620	108729.681
49	770	-0.23	2264.787	2264.7886(7)	2264.0881	$4f^3(^4I^\circ)6p\ ^5I_4$	$4f^3(^4I^\circ)6d\ ^5G^\circ_3$	60638.963	104793.195
7	430	-0.48	2270.948	2270.9469(6)	2270.2450	$4f^3(^4I^\circ)6p\ ^5K_5$	$4f^3(^4I^\circ)6d\ ^3I^\circ_5$	60526.067	104560.563
39	120	-1.03	2277.117	2277.1196(3)	2276.4165	$4f^3(^4I^\circ)5d\ ^5I^\circ_8$	$4f^3(^4I^\circ)6p\ ^3K_7$	24592.259	68507.387
30	75	-1.23	2279.754	2279.7544(3)	2279.0507	$4f^3(^4I^\circ)5d\ ^5K^\circ_7$	$4f^3(^4I^\circ)6p\ ^5K_6$	18656.272	62520.646
23	490	-0.42	2282.008	2282.0175(15)	2281.3132	$4f^3(^2H2^\circ)5d\ ^1I^\circ_6$	$4f^3(^2H2^\circ)6p\ ^3I_6$	32823.701	76644.575
52	550	-0.37	2282.475	2282.4730(15)	2281.7687	$4f^3(^4F^\circ)5d\ ^5H^\circ_7$	$4f^3(^2H2^\circ)6p\ ^3I_6$	32832.447	76644.575
38	2200	0.24	2295.671	2295.6665(9)	2294.9592	$4f^3(^4I^\circ)6p\ ^5I_7$	$4f^3(^4I^\circ)6d\ ^5H^\circ_7$	66497.225	110057.560
19	920	-0.14	2300.828	2300.8263(12)	2300.1179	$4f^3(^4I^\circ)6p\ ^5I_7$	$4f^3(^4I^\circ)6d\ ^5I^\circ_8$	66497.225	109959.872
53	110	-1.06	2305.357	2305.3611(3)	2304.6518	$4f^3(^4I^\circ)5d\ ^3K^\circ_6$	$4f^3(^4I^\circ)6p\ ^5I_7$	23120.073	66497.225
44	120	-1.01	2319.978	2319.9654(3)	2319.2529	$4f^3(^4I^\circ)5d\ ^3H^\circ_5$	$4f^3(^4I^\circ)6p\ ^3K_6$	23347.721	66451.812
51	250	-0.69	2321.690	2321.6824(8)	2320.9695	$4f^3(^4F^\circ)5d\ ^5H^\circ_5$	$4f^3(^2H2^\circ)6p\ ^3I_5$	30175.737	73247.950
8	610	-0.31	2325.403	2325.4020(8)	2324.6883	$4f^3(^4I^\circ)6p\ ^5H_6$	$4f^3(^4I^\circ)6d\ ^5I^\circ_6$	65023.633	108026.950
45	160	-0.89	2326.497	2326.4966(4)	2325.7826	$4f^3(^4I^\circ)5d\ ^3K^\circ_7$	$4f^3(^4I^\circ)6p\ ^5K_8$	25319.579	68302.664
26	65	-1.28	2326.979	2326.9847(17)	2326.2706	$4f^3(^2H2^\circ)5d\ ^1H^\circ_5$	$4f^3(^4F^\circ)6p\ ^5G_5$	32605.894	75579.962
17	340	-0.56	2331.345	2331.3494(7)	2330.6344	$4f^3(^4I^\circ)6p\ ^5I_7$	$4f^3(^4I^\circ)7s\ (\frac{15}{2}, \frac{1}{2})^\circ_7$	66497.225	109390.838
55	56	-1.34	2334.132	2334.1399(6)	2333.4242	$4f^3(^4I^\circ)5d\ ^5H^\circ_5$	$4f^3(^4I^\circ)6p\ ^5H_6$	22181.299	65023.633
2	2000	0.22	2346.820	2346.8204(7)	2346.1019	$4f^3(^4I^\circ)6p\ ^5K_7$	$4f^3(^4I^\circ)7s\ (\frac{13}{2}, \frac{1}{2})^\circ_6$	64622.006	107232.851
21	28	-1.63	2355.788	2355.7910(3)	2355.0705	$4f^3(^4I^\circ)5d\ ^3I^\circ_7$	$4f^3(^4I^\circ)6p\ ^3K_6$	24003.225	66451.812
24	66	-1.26	2356.040	2356.0431(18)	2355.3225	$4f^3(^2H2^\circ)5d\ ^3G^\circ_4$	$4f^3(^4F^\circ)6p\ ^5G_5$	33135.917	75579.962
35	110	-1.04	2356.340	2356.3395(3)	2355.6188	$4f^3(^4I^\circ)5d\ ^5H^\circ_6$	$4f^3(^4I^\circ)6p\ ^5I_7$	24058.518	66497.225
24	16	-1.87	2358.860	2358.8636(3)	2358.1424	$4f^3(^4I^\circ)5d\ ^5H^\circ_6$	$4f^3(^4I^\circ)6p\ ^3K_6$	24058.518	66451.812
27	99	-1.08	2360.209	2360.1994(19)	2359.4779	$4f^3(^4F^\circ)5d\ ^5G^\circ_6$	$4f^3(^4F^\circ)6p\ ^5G_5$	33210.660	75579.962
47	150	-0.90	2360.257	2360.2540(6)	2359.5325	$4f^3(^4I^\circ)5d\ ^5H^\circ_5$	$4f^3(^4I^\circ)6p\ ^5I_6$	22181.299	64549.620
39	57	-1.32	2366.880	2366.8819(4)	2366.1589	$4f^3(^4I^\circ)5d\ ^5H^\circ_7$	$4f^3(^4I^\circ)6p\ ^3I_6$	26097.906	68347.584
35	77	-1.19	2371.380	2371.3814(6)	2370.6574	$4f^3(^4I^\circ)5d\ ^5H^\circ_5$	$4f^3(^4I^\circ)6p\ ^3I_5$	22181.299	64350.812

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Table D.2: Classified Nd III Transitions Observed Only from the Nd VS Spectra (continued)

Int.	$g_u A$ (10^6 s^{-1})	$\log(g_l f)$	λ (Å)	λ_{Ritz} (Å)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level	Upper Level	E_l (cm^{-1})	E_u (cm^{-1})
19	840	-0.15	2373.060	2373.0623(6)	2372.3380	$4f^3(^4I^\circ)6p\ ^5H_7$	$4f^3(^4I^\circ)6d\ ^3L^\circ_8$	66717.513	108857.156
27	450	-0.42	2377.873	2377.8846(7)	2377.1592	$4f^3(^4I^\circ)6p\ ^5I_6$	$4f^3(^4I^\circ)6d\ ^3K^\circ_6$	64549.620	106603.805
14	460	-0.41	2378.071	2378.0738(4)	2377.3483	$4f^3(^4I^\circ)6p\ ^5I_6$	$4f^3(^4I^\circ)6d\ ^3L^\circ_7$	64549.620	106600.460
25	110	-1.03	2378.243	2378.2431(15)	2377.5175	$4f^3(^2H2^\circ)5d\ ^3I^\circ_7$	$4f^3(^2H2^\circ)6p\ ^1I_6$	35188.278	77236.125
25	40	-1.47	2380.946	2380.9490(4)	2380.2228	$4f^3(^4I^\circ)5d\ ^3L^\circ_7$	$4f^3(^4I^\circ)6p\ ^5I_7$	24497.165	66497.225
59	140	-0.92	2382.271	2382.2868(18)	2381.5603	$4f^3(^4F^\circ)5d\ ^5F^\circ_4$	$4f^3(^4F^\circ)6p\ ^5G_5$	33603.488	75579.962
27	66	-1.25	2390.235	2390.2330(5)	2389.5047	$4f^3(^4I^\circ)5d\ ^5G^\circ_6$	$4f^3(^4I^\circ)6p\ ^3K_7$	26670.461	68507.387
38	110	-1.02	2394.075	2394.0701(13)	2393.3409	$4f^3(^4F^\circ)5d\ ^5F^\circ_3$	$4f^3(^4F^\circ)6p\ ^5G_4$	32489.101	74258.973
26	55	-1.32	2400.785	2400.7829(13)	2400.0523	$4f^3(^2H2^\circ)5d\ ^1H^\circ_5$	$4f^3(^4F^\circ)6p\ ^5G_4$	32605.894	74258.973
24	46	-1.40	2402.351	2402.3459(5)	2401.6149	$4f^3(^4I^\circ)5d\ ^3L^\circ_8$	$4f^3(^4I^\circ)6p\ ^5K_8$	26676.685	68302.664
32	320	-0.56	2405.279	2405.2837(8)	2404.5520	$4f^3(^4I^\circ)6p\ ^3K_6$	$4f^3(^4I^\circ)6d\ ^5I^\circ_6$	66451.812	108026.950
27	520	-0.34	2408.036	2408.0287(9)	2407.2964	$4f^3(^4I^\circ)6p\ ^5I_6$	$4f^3(^4I^\circ)6d\ ^5K^\circ_7$	64549.620	106077.365
33	45	-1.41	2409.535	2409.5263(3)	2408.7937	$4f^3(^4I^\circ)5d\ ^3K^\circ_6$	$4f^3(^4I^\circ)6p\ ^5K_7$	23120.073	64622.006
35	860	-0.12	2412.222	2412.2334(9)	2411.5001	$4f^3(^4I^\circ)6p\ ^5K_7$	$4f^3(^4I^\circ)6d\ ^5K^\circ_7$	64622.006	106077.365
42	48	-1.38	2413.786	2413.7923(5)	2413.0587	$4f^3(^2H2^\circ)5d\ ^3I^\circ_5$	$4f^3(^4I^\circ)6p\ ^3H_6$	29397.423	70826.009
46	75	-1.18	2415.576	2415.5795(4)	2414.8455	$4f^3(^4I^\circ)5d\ ^3K^\circ_7$	$4f^3(^4I^\circ)6p\ ^5H_7$	25319.579	66717.513
26	26	-1.64	2415.786	2415.7863(7)	2415.0522	$4f^3(^4I^\circ)5d\ ^5G^\circ_5$	$4f^3(^4I^\circ)6p\ ^5H_5$	24878.412	66272.802
43	69	-1.22	2418.952	2418.9435(6)	2418.2087	$4f^3(^4I^\circ)5d\ ^5G^\circ_4$	$4f^3(^4I^\circ)6p\ ^3I_5$	23010.450	64350.812
36	100	-1.06	2420.527	2420.5199(17)	2419.7847	$4f^3(^4F^\circ)5d\ ^5F^\circ_2$	$4f^3(^4F^\circ)6p\ ^5G_3$	31888.511	73201.950
34	40	-1.45	2425.214	2425.2146(6)	2424.4784	$4f^3(^4I^\circ)5d\ ^5G^\circ_4$	$4f^3(^4I^\circ)6p\ ^5H_4$	23010.450	64243.914
22	200	-0.75	2426.659	2426.6607(7)	2425.9242	$4f^3(^4I^\circ)6p\ ^5H_7$	$4f^3(^4I^\circ)6d\ ^5K^\circ_8$	66717.513	107926.405
38	79	-1.16	2428.502	2428.5021(4)	2427.7652	$4f^3(^4I^\circ)5d\ ^3K^\circ_7$	$4f^3(^4I^\circ)6p\ ^5I_7$	25319.579	66497.225
45	120	-0.97	2428.907	2428.9037(10)	2428.1667	$4f^3(^4F^\circ)5d\ ^3H^\circ_4$	$4f^3(^2H2^\circ)6p\ ^3I_5$	32077.113	73247.950
32	50	-1.35	2431.185	2431.1833(4)	2430.4458	$4f^3(^4I^\circ)5d\ ^3K^\circ_7$	$4f^3(^4I^\circ)6p\ ^3K_6$	25319.579	66451.812
34	89	-1.10	2434.939	2434.9399(19)	2434.2014	$4f^3(^4F^\circ)5d\ ^5F^\circ_5$	$4f^3(^4F^\circ)6p\ ^5G_5$	34511.186	75579.962
21	100	-1.05	2435.767	2435.7681(4)	2435.0295	$4f^3(^4I^\circ)6p\ ^5I_5$	$4f^3(^4I^\circ)6d\ ^5L^\circ_6$	62640.266	103695.078
29	29	-1.59	2437.695	2437.6961(2)	2436.9570	$4f^3(^4I^\circ)5d\ ^3I^\circ_5$	$4f^3(^4I^\circ)6p\ ^5I_4$	19616.622	60638.963
28	37	-1.48	2441.102	2441.1014(3)	2440.3616	$4f^3(^4I^\circ)5d\ ^5H^\circ_6$	$4f^3(^4I^\circ)6p\ ^5H_6$	24058.518	65023.633
30	70	-1.20	2449.943	2449.9346(4)	2449.1927	$4f^3(^2H2^\circ)5d\ ^3K^\circ_6$	$4f^3(^4I^\circ)6p\ ^3I_7$	29643.186	70460.602
17	210	-0.72	2450.101	2450.0903(5)	2449.3484	$4f^3(^4I^\circ)6p\ ^5K_6$	$4f^3(^4I^\circ)7s\ (\frac{9}{2}, \frac{1}{2})^\circ_5$	62520.646	103335.469
43	70	-1.20	2457.355	2457.3576(3)	2456.6140	$4f^3(^4I^\circ)5d\ ^5H^\circ_7$	$4f^3(^4I^\circ)6p\ ^5I_8$	26097.906	66792.024
29	110	-1.00	2460.496	2460.5054(10)	2459.7612	$4f^3(^2H2^\circ)5d\ ^1H^\circ_5$	$4f^3(^2H2^\circ)6p\ ^3I_5$	32605.894	73247.950
57	80	-1.14	2461.879	2461.8653(3)	2461.1207	$4f^3(^4I^\circ)5d\ ^5H^\circ_7$	$4f^3(^4I^\circ)6p\ ^5H_7$	26097.906	66717.513
37	48	-1.36	2465.267	2465.2712(3)	2464.5258	$4f^3(^4I^\circ)5d\ ^5H^\circ_6$	$4f^3(^4I^\circ)6p\ ^5K_7$	24058.518	64622.006
21	25	-1.64	2469.678	2469.6784(2)	2468.9320	$4f^3(^4I^\circ)5d\ ^5H^\circ_6$	$4f^3(^4I^\circ)6p\ ^5I_6$	24058.518	64549.620
24	35	-1.49	2471.646	2471.6400(7)	2470.8931	$4f^3(^4I^\circ)5d\ ^5H^\circ_5$	$4f^3(^4I^\circ)6p\ ^5I_5$	22181.299	62640.266
28	67	-1.21	2473.692	2473.6846(19)	2472.9373	$4f^3(^4F^\circ)5d\ ^3H^\circ_6$	$4f^3(^4F^\circ)6p\ ^5G_5$	35154.437	75579.962
46	42	-1.41	2478.971	2478.9692(7)	2478.2207	$4f^3(^4I^\circ)5d\ ^5H^\circ_5$	$4f^3(^4I^\circ)6p\ ^5K_6$	22181.299	62520.646
22	15	-1.86	2481.864	2481.8642(3)	2481.1149	$4f^3(^4I^\circ)5d\ ^5H^\circ_6$	$4f^3(^4I^\circ)6p\ ^3I_5$	24058.518	64350.812
23	36	-1.48	2484.475	2484.4740(2)	2483.7242	$4f^3(^4I^\circ)5d\ ^5H^\circ_4$	$4f^3(^4I^\circ)6p\ ^5I_4$	20388.995	60638.963
24	30	-1.55	2491.460	2491.4623(3)	2490.7108	$4f^3(^4I^\circ)5d\ ^5H^\circ_4$	$4f^3(^4I^\circ)6p\ ^5K_5$	20388.995	60526.067
11	260	-0.62	2493.357	2493.3565(8)	2492.6046	$4f^3(^4I^\circ)6p\ ^5I_7$	$4f^3(^4I^\circ)6d\ ^3K^\circ_6$	66497.225	106603.805
37	530	-0.31	2493.556	2493.5644(5)	2492.8125	$4f^3(^4I^\circ)6p\ ^5I_7$	$4f^3(^4I^\circ)6d\ ^3L^\circ_7$	66497.225	106600.460
54	83	-1.11	2498.143	2498.1422(3)	2497.3892	$4f^3(^4I^\circ)5d\ ^5I^\circ_8$	$4f^3(^4I^\circ)6p\ ^5K_7$	24592.259	64622.006

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Table D.2: Classified Nd III Transitions Observed Only from the Nd VS Spectra (continued)

Int.	$g_u A$ (10^6 s^{-1})	$\log(g_l f)$	λ (Å)	λ_{Ritz} (Å)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level	Upper Level	E_l (cm^{-1})	E_u (cm^{-1})
37	30	-1.55	2510.874	2510.8743(6)	2510.1184	$4f^3(^4I^\circ)5d \ ^5G^\circ_6$	$4f^3(^4I^\circ)6p \ ^5I_7$	26670.461	66497.225
17	300	-0.55	2513.869	2513.8679(12)	2513.1113	$4f^3(^4I^\circ)6p \ ^5H_5$	$4f^3(^4I^\circ)6d \ ^5I^\circ_5$	66272.802	106052.139
60	46	-1.36	2518.628	2518.6345(4)	2517.8767	$4f^3(^4I^\circ)5d \ ^3K^\circ_7$	$4f^3(^4I^\circ)6p \ ^5H_6$	25319.579	65023.633
18	320	-0.51	2530.395	2530.3924(9)	2529.6318	$4f^3(^4I^\circ)6p \ ^3K_7$	$4f^3(^4I^\circ)6d \ ^5I^\circ_6$	68507.387	108026.950
14	570	-0.26	2534.343	2534.3410(11)	2533.5795	$4f^3(^4I^\circ)6p \ ^3K_8$	$4f^3(^4I^\circ)6d \ ^5H^\circ_7$	70599.570	110057.560
22	550	-0.27	2538.156	2538.1548(20)	2537.3925	$4f^3(^4I^\circ)6p \ ^3K_7$	$4f^3(^4I^\circ)6d \ ^5I^\circ_7$	68507.387	107906.087
31	59	-1.24	2541.293	2541.2888(4)	2540.5257	$4f^3(^4I^\circ)5d \ ^3K^\circ_8$	$4f^3(^4I^\circ)6p \ ^5I_8$	27441.911	66792.024
19	25	-1.61	2545.017	2545.0120(2)	2544.2481	$4f^3(^4I^\circ)5d \ ^3H^\circ_5$	$4f^3(^4I^\circ)6p \ ^5I_5$	23347.721	62640.266
11	540	-0.28	2548.977	2548.9688(12)	2548.2039	$4f^3(^4I^\circ)6p \ ^3H_6$	$4f^3(^4I^\circ)6d \ ^5H^\circ_7$	70826.009	110057.560
35	58	-1.24	2570.600	2570.6026(4)	2569.8326	$4f^3(^2G^\circ)5d \ ^3H^\circ_6$	$4f^3(^4I^\circ)6p \ ^3I_7$	31559.217	70460.602
2	1200	0.08	2574.542	2574.5426(7)	2573.7717	$4f^3(^4I^\circ)6p \ ^5H_4$	$4f^3(^4I^\circ)7s \ (\frac{9}{2}, \frac{1}{2})^\circ_4$	64243.914	103085.765
10	23	-1.62	2652.530	2652.5303(5)	2651.7409	$4f^3(^4F^\circ)5d \ ^5H^\circ_4$	$4f^3(^4I^\circ)6p \ ^3H_4$	28745.307	66445.159
33	26	-1.55	2688.097	2688.0949(5)	2687.2970	$4f^3(^4I^\circ)5d \ ^3K^\circ_7$	$4f^3(^4I^\circ)6p \ ^5K_6$	25319.579	62520.646
15	82	-1.04	2708.562	2708.5689(8)	2707.7660	$4f^3(^4I^\circ)6s \ (\frac{13}{2}, \frac{1}{2})^\circ_7$	$4f^3(^4I^\circ)6p \ ^3H_6$	33906.143	70826.009
8	180	-0.70	2711.225	2711.2279(6)	2710.4244	$4f^3(^4I^\circ)6p \ ^3K_6$	$4f^3(^4I^\circ)7s \ (\frac{9}{2}, \frac{1}{2})^\circ_5$	66451.812	103335.469
40	50	-1.26	2716.756	2716.7545(4)	2715.9496	$4f^3(^2H^\circ)5d \ ^3K^\circ_6$	$4f^3(^4I^\circ)6p \ ^3K_6$	29643.186	66451.812
21	39	-1.36	2722.901	2722.8974(6)	2722.0911	$4f^3(^2H^\circ)5d \ ^3K^\circ_7$	$4f^3(^4I^\circ)6p \ ^3K_7$	31781.802	68507.387
33	170	-0.72	2736.909	2736.9094(8)	2736.0997	$4f^3(^4I^\circ)6s \ (\frac{11}{2}, \frac{1}{2})^\circ_6$	$4f^3(^4I^\circ)6p \ ^3H_5$	32075.658	68613.221
10	26	-1.53	2738.166	2738.1610(6)	2737.3510	$4f^3(^2H^\circ)5d \ ^3K^\circ_7$	$4f^3(^4I^\circ)6p \ ^5K_8$	31781.802	68302.664
9	71	-1.09	2756.950	2756.9531(7)	2756.1385	$4f^3(^4I^\circ)6s \ (\frac{11}{2}, \frac{1}{2})^\circ_6$	$4f^3(^4I^\circ)6p \ ^3I_6$	32075.658	68347.584
40	190	-0.66	2772.765	2772.7698(6)	2771.9513	$4f^3(^2H^\circ)5d \ ^3K^\circ_8$	$4f^3(^4I^\circ)6p \ ^3K_8$	34534.549	70599.570
23	41	-1.32	2783.492	2783.4953(6)	2782.6743	$4f^3(^2H^\circ)5d \ ^3K^\circ_8$	$4f^3(^4I^\circ)6p \ ^3I_7$	34534.549	70460.602
34	14	-1.79	2794.116	2794.1140(7)	2793.2904	$4f^3(^2H^\circ)5d \ ^1I^\circ_6$	$4f^3(^4I^\circ)6p \ ^3H_5$	32823.701	68613.221
61	160	-0.72	2802.715	2802.7128(7)	2801.8871	$4f^3(^4I^\circ)6s \ (\frac{9}{2}, \frac{1}{2})^\circ_5$	$4f^3(^4I^\circ)6p \ ^5H_5$	30593.085	66272.802
45	110	-0.89	2803.084	2803.0881(5)	2802.2623	$4f^3(^4F^\circ)5d \ ^5H^\circ_7$	$4f^3(^4I^\circ)6p \ ^3K_7$	32832.447	68507.387
21	49	-1.24	2803.347	2803.3528(7)	2802.5269	$4f^3(^4F^\circ)5d \ ^3H^\circ_6$	$4f^3(^4I^\circ)6p \ ^3H_6$	35154.437	70826.009
72	43	-1.29	2806.015	2806.0148(10)	2805.1882	$4f^3(^2H^\circ)5d \ ^3I^\circ_7$	$4f^3(^4I^\circ)6p \ ^3H_6$	35188.278	70826.009
10	19	-1.65	2817.013	2817.0119(4)	2816.1827	$4f^3(^4F^\circ)5d \ ^5H^\circ_4$	$4f^3(^4I^\circ)6p \ ^5H_4$	28745.307	64243.914
82	35	-1.38	2823.948	2823.9580(10)	2823.1270	$4f^3(^2H^\circ)5d \ ^3I^\circ_7$	$4f^3(^4I^\circ)6p \ ^3K_8$	35188.278	70599.570
13	32	-1.42	2826.419	2826.4199(4)	2825.5884	$4f^3(^2H^\circ)5d \ ^3K^\circ_6$	$4f^3(^4I^\circ)6p \ ^5H_6$	29643.186	65023.633
28	34	-1.39	2828.793	2828.7929(5)	2827.9607	$4f^3(^4F^\circ)5d \ ^5H^\circ_6$	$4f^3(^4I^\circ)6p \ ^5I_7$	31146.457	66497.225
56	25	-1.52	2833.123	2833.1239(10)	2832.2907	$4f^3(^4F^\circ)5d \ ^5G^\circ_6$	$4f^3(^4I^\circ)6p \ ^3K_7$	33210.660	68507.387
27	31	-1.42	2844.772	2844.7724(3)	2843.9364	$4f^3(^2H^\circ)5d \ ^3I^\circ_5$	$4f^3(^4I^\circ)6p \ ^5I_6$	29397.423	64549.620
15	26	-1.50	2846.867	2846.8661(6)	2846.0295	$4f^3(^4F^\circ)5d \ ^5H^\circ_6$	$4f^3(^4I^\circ)6p \ ^5H_5$	31146.457	66272.802
60	26	-1.50	2860.962	2860.9529(4)	2860.1129	$4f^3(^2H^\circ)5d \ ^3I^\circ_5$	$4f^3(^4I^\circ)6p \ ^3I_5$	29397.423	64350.812
23	56	-1.16	2862.406	2862.4006(6)	2861.5602	$4f^3(^2H^\circ)5d \ ^3K^\circ_7$	$4f^3(^4I^\circ)6p \ ^5H_7$	31781.802	66717.513
36	41	-1.29	2881.222	2881.2112(4)	2880.3662	$4f^3(^2H^\circ)5d \ ^3K^\circ_6$	$4f^3(^4I^\circ)6p \ ^3I_5$	29643.186	64350.812
92	310	-0.39	2944.939	2944.9412(5)	2944.0805	$4f^3(^4I^\circ)6s \ (\frac{9}{2}, \frac{1}{2})^\circ_5$	$4f^3(^4I^\circ)6p \ ^5I_6$	30593.085	64549.620
26	28	-1.44	2950.291	2950.2912(4)	2949.4292	$4f^3(^4F^\circ)5d \ ^5H^\circ_4$	$4f^3(^4I^\circ)6p \ ^5I_5$	28745.307	62640.266
29	46	-1.22	2969.689	2969.6922(7)	2968.8253	$4f^3(^2H^\circ)5d \ ^1I^\circ_6$	$4f^3(^4I^\circ)6p \ ^5I_7$	32823.701	66497.225
31	14	-1.73	2973.711	2973.7026(7)	2972.8347	$4f^3(^2H^\circ)5d \ ^1I^\circ_6$	$4f^3(^4I^\circ)6p \ ^3K_6$	32823.701	66451.812
49	160	-0.67	2988.761	2988.7518(8)	2987.8802	$4f^3(^4F^\circ)5d \ ^3H^\circ_6$	$4f^3(^4I^\circ)6p \ ^3H_5$	35154.437	68613.221
11	87	-0.93	2998.231	2998.2355(7)	2997.3616	$4f^3(^4F^\circ)5d \ ^3H^\circ_6$	$4f^3(^4I^\circ)6p \ ^3K_7$	35154.437	68507.387
35	27	-1.44	3004.210	3004.2151(12)	3003.3396	$4f^3(^4F^\circ)5d \ ^5G^\circ_6$	$4f^3(^4I^\circ)6p \ ^5I_7$	33210.660	66497.225

Continued on next page...

Table D.2: Classified Nd III Transitions Observed Only from the Nd VS Spectra (continued)

Int.	$g_u A$ (10^6 s^{-1})	$\log(g_l f)$	λ (Å)	λ_{Ritz} (Å)	$\lambda_{\text{Ritz}}^{\text{air}}$ (Å)	Lower Level	Upper Level	E_l (cm^{-1})	E_u (cm^{-1})
20	25	-1.47	3019.839	3019.8355(12)	3018.9562	$4f^3(^2H^{\circ})5d \ ^3I^{\circ}_7$	$4f^3(^4I^{\circ})6p \ ^5K_8$	35188.278	68302.664
96	390	-0.27	3035.091	3035.0879(8)	3034.2047	$4f^3(^4I^{\circ})6s \ (\frac{11}{2}, \frac{1}{2})^{\circ}_6$	$4f^3(^4I^{\circ})6p \ ^5H_6$	32075.658	65023.633
98	560	-0.11	3040.814	3040.8186(8)	3039.9340	$4f^3(^4I^{\circ})6s \ (\frac{13}{2}, \frac{1}{2})^{\circ}_7$	$4f^3(^4I^{\circ})6p \ ^5I_8$	33906.143	66792.024
32	47	-1.18	3047.737	3047.7240(8)	3046.8377	$4f^3(^4I^{\circ})6s \ (\frac{13}{2}, \frac{1}{2})^{\circ}_7$	$4f^3(^4I^{\circ})6p \ ^5H_7$	33906.143	66717.513
35	95	-0.87	3061.148	3061.1409(12)	3060.2512	$4f^3(^4I^{\circ})6s \ (\frac{15}{2}, \frac{1}{2})^{\circ}_8$	$4f^3(^4I^{\circ})6p \ ^3K_7$	35839.828	68507.387
89	290	-0.38	3079.387	3079.3902(8)	3078.4959	$4f^3(^4I^{\circ})6s \ (\frac{11}{2}, \frac{1}{2})^{\circ}_6$	$4f^3(^4I^{\circ})6p \ ^5I_6$	32075.658	64549.620
94	480	-0.17	3080.445	3080.4456(12)	3079.5511	$4f^3(^4I^{\circ})6s \ (\frac{15}{2}, \frac{1}{2})^{\circ}_8$	$4f^3(^4I^{\circ})6p \ ^5K_8$	35839.828	68302.664
47	54	-1.11	3091.678	3091.6767(5)	3090.7793	$4f^3(^4F^{\circ})5d \ ^5H^{\circ}_5$	$4f^3(^4I^{\circ})6p \ ^5K_6$	30175.737	62520.646
58	110	-0.80	3098.354	3098.3586(8)	3097.4596	$4f^3(^4I^{\circ})6s \ (\frac{11}{2}, \frac{1}{2})^{\circ}_6$	$4f^3(^4I^{\circ})6p \ ^3I_5$	32075.658	64350.812
7	51	-1.13	3107.235	3107.2340(7)	3106.3328	$4f^3(^2H^{\circ})5d \ ^3K^{\circ}_8$	$4f^3(^4I^{\circ})6p \ ^5H_7$	34534.549	66717.513
90	240	-0.46	3120.397	3120.3993(6)	3119.4947	$4f^3(^4I^{\circ})6s \ (\frac{9}{2}, \frac{1}{2})^{\circ}_5$	$4f^3(^4I^{\circ})6p \ ^5I_5$	30593.085	62640.266
56	220	-0.49	3120.987	3120.9931(9)	3120.0884	$4f^3(^4I^{\circ})6s \ (\frac{11}{2}, \frac{1}{2})^{\circ}_5$	$4f^3(^4I^{\circ})6p \ ^3I_5$	32309.729	64350.812
80	190	-0.56	3122.044	3122.0455(8)	3121.1405	$4f^3(^4I^{\circ})6s \ (\frac{13}{2}, \frac{1}{2})^{\circ}_6$	$4f^3(^4I^{\circ})6p \ ^5H_7$	34687.230	66717.513
100	630	-0.03	3132.083	3132.0902(7)	3131.1827	$4f^3(^4I^{\circ})6s \ (\frac{9}{2}, \frac{1}{2})^{\circ}_5$	$4f^3(^4I^{\circ})6p \ ^5K_6$	30593.085	62520.646
18	53	-1.10	3143.670	3143.6660(8)	3142.7556	$4f^3(^4I^{\circ})6s \ (\frac{13}{2}, \frac{1}{2})^{\circ}_6$	$4f^3(^4I^{\circ})6p \ ^5I_7$	34687.230	66497.225
34	21	-1.51	3144.826	3144.8217(7)	3143.9110	$4f^3(^2H^{\circ})5d \ ^1I^{\circ}_6$	$4f^3(^4I^{\circ})6p \ ^5K_7$	32823.701	64622.006
61	98	-0.84	3148.152	3148.1604(9)	3147.2489	$4f^3(^4I^{\circ})6s \ (\frac{13}{2}, \frac{1}{2})^{\circ}_6$	$4f^3(^4I^{\circ})6p \ ^3K_6$	34687.230	66451.812
66	36	-1.27	3150.113	3150.1105(8)	3149.1985	$4f^3(^2H^{\circ})5d \ ^1H^{\circ}_5$	$4f^3(^4I^{\circ})6p \ ^3I_5$	32605.894	64350.812
24	22	-1.48	3151.998	3151.9970(6)	3151.0845	$4f^3(^2H^{\circ})5d \ ^1I^{\circ}_6$	$4f^3(^4I^{\circ})6p \ ^5I_6$	32823.701	64549.620
80	44	-1.18	3164.178	3164.1819(12)	3163.2663	$4f^3(^2H^{\circ})5d \ ^3I^{\circ}_7$	$4f^3(^4I^{\circ})6p \ ^5I_8$	35188.278	66792.024
6	38	-1.24	3166.003	3166.0025(10)	3165.0865	$4f^3(^4I^{\circ})6s \ (\frac{13}{2}, \frac{1}{2})^{\circ}_6$	$4f^3(^4I^{\circ})6p \ ^5H_5$	34687.230	66272.802
47	29	-1.36	3171.659	3171.6596(12)	3170.7421	$4f^3(^2H^{\circ})5d \ ^3I^{\circ}_7$	$4f^3(^4I^{\circ})6p \ ^5H_7$	35188.278	66717.513
27	100	-0.82	3183.463	3183.4646(10)	3182.5442	$4f^3(^4G^{\circ})5d \ ^5I^{\circ}_7$	$4f^3(^4I^{\circ})6p \ ^5K_8$	36890.347	68302.664
76	44	-1.17	3183.563	3183.5630(13)	3182.6426	$4f^3(^4F^{\circ})5d \ ^5G^{\circ}_6$	$4f^3(^4I^{\circ})6p \ ^5K_7$	33210.660	64622.006
63	32	-1.31	3190.919	3190.9164(12)	3189.9940	$4f^3(^4F^{\circ})5d \ ^5G^{\circ}_6$	$4f^3(^4I^{\circ})6p \ ^5I_6$	33210.660	64549.620
50	34	-1.28	3200.866	3200.8665(5)	3199.9417	$4f^3(^2H^{\circ})5d \ ^3I^{\circ}_5$	$4f^3(^4I^{\circ})6p \ ^5I_4$	29397.423	60638.963
39	17	-1.58	3212.476	3212.4753(6)	3211.5475	$4f^3(^2H^{\circ})5d \ ^3I^{\circ}_5$	$4f^3(^4I^{\circ})6p \ ^5K_5$	29397.423	60526.067
69	190	-0.53	3213.624	3213.6268(9)	3212.6987	$4f^3(^4I^{\circ})6s \ (\frac{13}{2}, \frac{1}{2})^{\circ}_7$	$4f^3(^4I^{\circ})6p \ ^5H_6$	33906.143	65023.633

Appendix E

Unclassified Nd III Line List of Dr H. M. Crosswhite

This is a list of 643 lines Dr Hannah M. Crosswhite had classified and observed as belonging to Nd III in her grating spectra, which likely comes from her works in [84,85] and possibly circulates within the astrophysical community [63]. I think this table would be useful for others if it were within a locatable document. A scan of this table is attached after the digital Table E.1, which was provided to Dr Tanya Ryabchikova by Prof. Charles Cowley, the handwritten notes are those of Dr Tanya Ryabchikova, who has kindly allowed me to include this document in my thesis. A tolerance of $\pm 0.3 \text{ cm}^{-1}$ was used to match this list with the observed wavenumbers from the Nd-Ar PDL spectra. A total of 428 lines were found common between her line list and the Nd-Ar PDL FT spectra line list under this tolerance, 224 of which are classified as Nd III lines in the Nd-Ar PDL FT spectra (Table D.1) and 204 of which were observed but remain unclassified in the Nd-Ar PDL FT spectra. In her line list, 66 lines were also unobserved in the Nd-Ar PDL FT spectra but matched with Ritz wavenumbers of transitions of classified Nd III levels allowed by the E1 selection rules ($\Delta J = 0, \pm 1$, but not $J = 0 \leftrightarrow 0$ and change of parity).

The first two columns of Table E.1 are the raw data from the scan - likely relative intensity on the same scale and vacuum wavelength. Columns 4-6 are the observed SNR, relative intensity, and wavenumber observed in the Nd-Ar PDL spectra, where zero SNR and intensity imply unobserved in the PDL and any non-zero observed wavenumbers in this case are Ritz wavenumbers. Column 7 is the difference between the Nd-Ar PDL FT spectra's and Dr Cross-

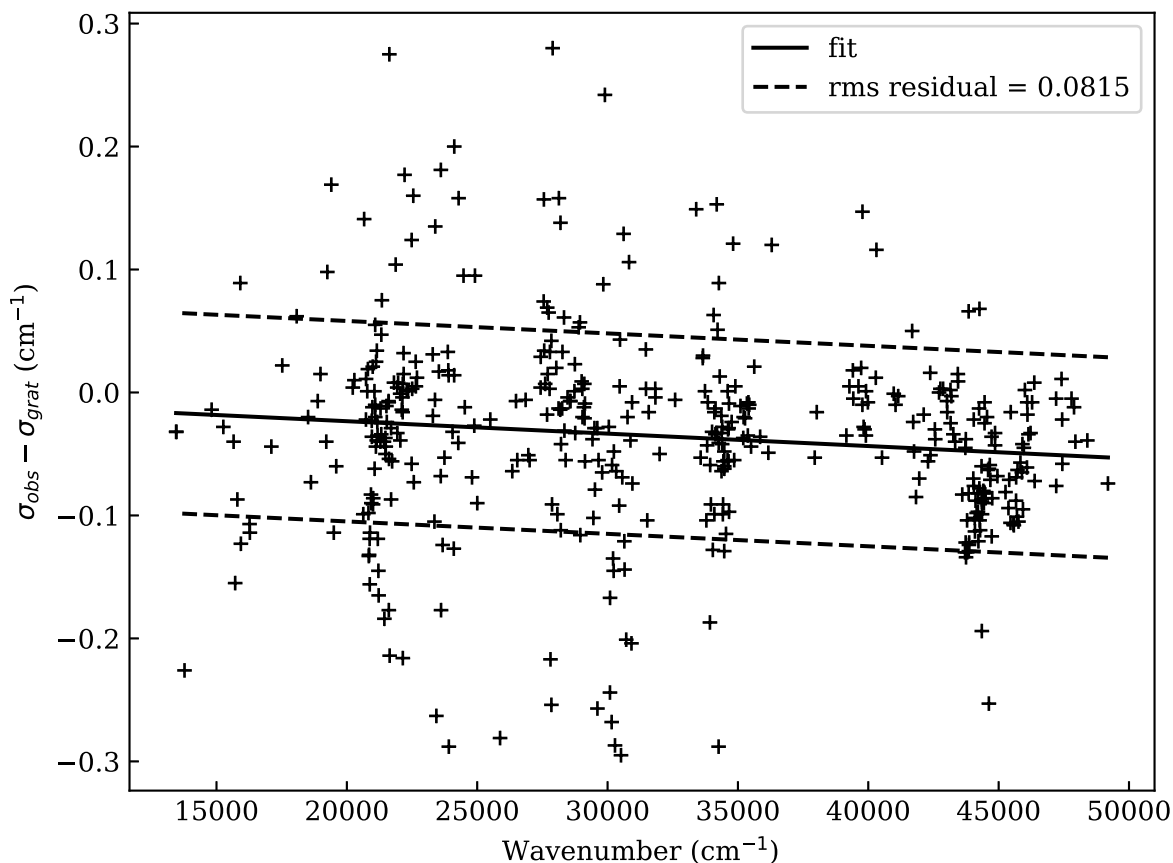


Figure E.1: Difference between Nd-Ar PDL FT spectra and Dr Crosswhite’s wavenumbers that were common to both line lists, plotted against wavenumber. The linear fit of gradient 1.0×10^{-6} and intercept $-3.2 \times 10^{-3} \text{ cm}^{-1}$ is shown with one rms deviation from the fit in dashed.

white’s wavenumbers. Columns 8-11 are level information of the transitions, where unclassified but observed lines in the PDL are given the label ‘U’, and unclassified and unobserved lines are labelled ‘-’. The final column is a crude calibration of wavenumbers of column 3 by me, where a linear fit was carried out on the difference between the observed wavenumbers of Dr Crosswhite’s line list and of the Nd-Ar FT spectra against the wavenumber (see Figure E.1). The deviations in Figure E.1 helped to gauge uncertainties of Dr Crosswhite’s line list, which also led to the choice of $\pm 0.3 \text{ cm}^{-1}$ as the tolerance for wavenumber matching between the two line lists.

I would like to note that the digital table was converted from the scan by hand over one long afternoon, zero mistakes are not guaranteed but 99% of the data are expected to be correctly transcribed.

Table E.1: Unclassified Nd III Line List of Dr H. M. Crosswhite Compared with the Nd-Ar PDL Line List of this Thesis

Int. (arb.)	λ (Å)	σ_{grat} (cm ⁻¹)	SNR	PDL Int. (arb.)	σ_{obs} (cm ⁻¹)	Diff. (cm ⁻¹)	L1	L2	E1 (cm ⁻¹)	E2 (cm ⁻¹)	σ_{cal} (cm ⁻¹)
150	1894.7284	52760.420	0	0	0	0	-	-	-	-	52760.413
150	1994.2518	50127.852	0	0	50127.877	0.025	4f ³ (⁴ I°)5d ³ K° ₆	4f ³ (² H2°)6p ³ I° ₅	23120.073	73247.950	50127.799
150	2004.7459	49865.491	0	0	49865.479	-0.012	4f ³ (⁴ I°)5d ⁵ L° ₆	4f ³ (⁴ I°)6p ⁵ H° ₆	15158.154	65023.633	49865.438
150	2008.9480	49761.203	0	0	49761.196	-0.007	4f ³ (⁴ I°)5d ⁵ K° ₅	4f ³ (⁴ I°)6p ⁵ H° ₆	15262.437	65023.633	49761.150
325	2011.7730	49691.337	0	0	49691.311	-0.026	4f ³ (⁴ I°)5d ⁵ K° ₇	4f ³ (⁴ I°)6p ³ I° ₆	18656.273	68347.584	49691.284
325	2013.4369	49650.278	0	0	0	0	-	-	-	-	49650.271
325	2013.5948	49646.385	0	0	49646.391	0.006	4f ³ (⁴ I°)5d ⁵ K° ₇	4f ³ (⁴ I°)6p ⁵ K° ₈	18656.273	68302.664	49646.333
325	2017.7393	49544.425	0	0	49544.390	-0.035	4f ³ (⁴ I°)5d ⁵ L° ₇	4f ³ (⁴ I°)6p ⁵ I° ₇	16952.835	66497.225	49544.373
150	2019.5911	49499.003	0	0	49498.977	-0.026	4f ³ (⁴ I°)5d ⁵ L° ₇	4f ³ (⁴ I°)6p ³ K° ₆	16952.835	66451.812	49498.951
150	2021.9348	49441.635	0	0	49441.600	-0.035	4f ³ (⁴ I°)5d ⁵ L° ₈	4f ³ (⁴ I°)6p ⁵ K° ₈	18861.064	68302.664	49441.583
325	2026.3139	49334.801	0	0	49334.734	-0.067	4f ³ (⁴ I°)5d ⁵ K° ₆	4f ³ (⁴ I°)6p ⁵ H° ₅	16938.068	66272.802	49334.749
150	2028.5096	49281.408	0	0	49281.277	-0.131	4f ³ (⁴ I°)5d ⁵ L° ₉	4f ³ (⁴ I°)6p ⁵ K° ₉	20859.732	70141.009	49281.356
700	2032.1669	49192.728	5	68	49192.654	-0.074	4f ³ (⁴ I°)5d ⁵ L° ₆	4f ³ (⁴ I°)6p ³ I ₅	15158.154	64350.812	49192.676
325	2032.3032	49189.430	0	0	49189.432	0.003	4f ³ (⁴ I°)5d ⁵ H° ₆	4f ³ (² H2°)6p ³ I° ₅	24058.518	73247.950	49189.378
50	2055.5863	48632.349	0	0	0	0	-	-	-	-	48632.342
150	2056.1505	48619.007	0	0	0	0	-	-	-	-	48619.000
150	2056.3441	48614.430	0	0	0	0	-	-	-	-	48614.423
150	2058.6856	48559.144	0	0	0	0	-	-	-	-	48559.137
50	2062.9457	48458.880	0	0	0	0	-	-	-	-	48458.873
150	2063.3889	48448.473	0	0	0	0	-	-	-	-	48448.466
325	2065.3487	48402.506	5	32	48402.467	-0.039	4f ³ (⁴ I°)5d ⁵ K° ₉	4f ³ (⁴ I°)6p ³ K ₈	22197.115	70599.570	48402.455
100	2066.0476	48386.135	0	0	0	0	-	-	-	-	48386.128
100	2066.0993	48384.924	0	0	0	0	-	-	-	-	48384.917
50	2067.0424	48362.851	0	0	0	0	-	-	-	-	48362.844
100	2067.8580	48343.779	0	0	0	0	-	-	-	-	48343.772
325	2070.5762	48280.322	0	0	0	0	-	-	-	-	48280.315
325	2085.1063	47943.923	13	110	47943.883	-0.04	4f ³ (⁴ I°)5d ⁵ K° ₉	4f ³ (⁴ I°)6p ⁵ K ₉	22197.115	70141.009	47943.872
150	2087.3764	47891.788	8	64	47891.776	-0.012	4f ³ (⁴ I°)5d ⁵ K° ₈	4f ³ (⁴ I°)6p ⁵ K ₈	20410.897	68302.664	47891.737
150	2087.9275	47879.149	0	0	0	0	-	-	-	-	47879.142
150	2091.5798	47795.553	7	56	47795.548	-0.005	4f ³ (⁴ I°)5d ⁵ K° ₇	4f ³ (⁴ I°)6p ³ K ₆	18656.272	66451.812	47795.502
700	2107.1249	47442.990	26	190	47442.932	-0.058	4f ³ (⁴ I°)5d ⁵ L° ₉	4f ³ (⁴ I°)6p ⁵ K ₈	20859.732	68302.664	47442.940
150	2107.4001	47436.795	7	50	47436.773	-0.022	U	U	U	U	47436.745
150	2108.4691	47412.747	10	70	47412.758	0.011	4f ³ (⁴ I°)5d ⁵ K° ₆	4f ³ (⁴ I°)6p ³ I ₅	16938.068	64350.812	47412.697
325	2117.5786	47208.809	39	260	47208.733	-0.076	4f ³ (⁴ I°)5d ⁵ L° ₁₀	4f ³ (⁴ I°)6p ⁵ K ₉	22932.276	70141.009	47208.759
150	2117.7569	47204.835	4	22	47204.830	-0.005	U	U	U	U	47204.785
50	2140.3042	46707.607	0	0	0	0	-	-	-	-	46707.600
150	2154.5736	46398.305	0	0	0	0	-	-	-	-	46398.298
325	2155.3687	46381.191	13	86	46381.118	-0.072	4f ³ (⁴ I°)5d ⁵ K° ₈	4f ³ (⁴ I°)6p ⁵ I ₈	20410.897	66792.024	46381.141
150	2156.0124	46367.344	6	40	46367.353	0.008	4f ³ (⁴ I°)5d ⁵ K° ₇	4f ³ (⁴ I°)6p ⁵ H ₆	18656.272	65023.633	46367.294
150	2159.9193	46283.484	5	34	46283.475	-0.008	U	U	U	U	46283.435
150	2160.1787	46277.926	0	0	0	0	-	-	-	-	46277.919
150	2162.5438	46227.319	0	0	0	0	-	-	-	-	46227.312
150	2162.6826	46224.353	6	20	46224.320	-0.033	U	U	U	U	46224.304
150	2164.5914	46183.595	0	0	0	0	-	-	-	-	46183.588
150	2164.7645	46179.903	0	0	0	0	-	-	-	-	46179.896
150	2166.2281	46148.705	0	0	0	0	-	-	-	-	46148.698
325	2166.5235	46142.413	6	34	46142.380	-0.034	4f ³ (⁴ F°)5d ⁵ H° ₇	4f ³ (⁴ F°)6p ⁵ G ₆	32832.447	78974.826	46142.364
150	2167.8011	46115.222	0	0	0	0	-	-	-	-	46115.215
150	2168.2546	46105.578	12	78	46105.560	-0.018	4f ³ (⁴ I°)5d ⁵ K° ₉	4f ³ (⁴ I°)6p ⁵ K ₈	22197.115	68302.664	46105.529
150	2168.6842	46096.446	6	28	46096.438	-0.008	4f ³ (⁴ I°)5d ⁵ I° ₅	4f ³ (⁴ I°)6p ³ H ₄	20348.742	66445.159	46096.397
700	2169.1576	46086.387	22	140	46086.326	-0.061	4f ³ (⁴ I°)5d ⁵ K° ₈	4f ³ (⁴ I°)6p ⁵ I ₇	20410.897	66497.225	46086.338
325	2170.5577	46056.662	0	0	0	0	-	-	-	-	46056.655
150	2172.8857	46007.323	3	20	46007.325	0.002	4f ³ (⁴ I°)5d ⁵ I° ₈	4f ³ (⁴ I°)6p ³ K ₈	24592.259	70599.570	46007.274
700	2174.8495	45965.785	26	150	45965.740	-0.045	4f ³ (⁴ I°)5d ⁵ K° ₇	4f ³ (⁴ I°)6p ⁵ K ₇	18656.272	64622.006	45965.736
700	2176.4310	45932.388	25	144	45932.292	-0.095	4f ³ (⁴ I°)5d ⁵ L° ₉	4f ³ (⁴ I°)6p ⁵ I ₈	20859.732	66792.024	45932.339
150	2177.4042	45911.860	3	20	45911.818	-0.042	U	U	U	U	45911.811
325	2178.2798	45893.407	22	132	45893.342	-0.065	4f ³ (⁴ I°)5d ⁵ K° ₇	4f ³ (⁴ I°)6p ⁵ I ₆	18656.272	64549.620	45893.358
150	2178.9355	45879.598	0	0	0	0	-	-	-	-	45879.591
150	2180.5435	45845.768	0	0	0	0	-	-	-	-	45845.761

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Table E.1: Unclassified Nd III Line List of Dr H. M. Crosswhite Compared with the Nd-Ar PDL Line List of this Thesis (continued)

Int. (arb.)	λ (Å)	σ_{grat} (cm ⁻¹)	SNR	PDL Int. (arb.)	σ_{obs} (cm ⁻¹)	Diff. (cm ⁻¹)	L1	L2	E1 (cm ⁻¹)	E2 (cm ⁻¹)	σ_{cal} (cm ⁻¹)
325	2181.0213	45835.726	21	126	45835.669	-0.057	U	U	U	U	45835.677
1000	2184.5810	45761.046	51	302	45760.941	-0.105	4f ³ (⁴ I°)5d ⁵ L° ₈	4f ³ (⁴ I°)6p ⁵ K ₇	18861.064	64622.006	45760.997
150	2184.9958	45752.360	0	0	0	0	-	-	-	-	45752.353
150	2185.4713	45742.406	0	0	0	0	-	-	-	-	45742.399
150	2186.3232	45724.585	4	20	45724.522	-0.063	U	U	U	U	45724.536
325	2187.3896	45702.295	28	162	45702.194	-0.101	4f ³ (⁴ I°)5d ⁵ K° ₆	4f ³ (⁴ I°)6p ⁵ I ₅	16938.068	62640.266	45702.246
150	2188.8423	45671.967	4	36	45671.898	-0.069	U	U	U	U	45671.918
150	2189.0380	45667.884	6	36	45667.796	-0.088	U	U	U	U	45667.835
150	2192.3025	45599.888	0	0	45599.887	-0.002	4f ³ (⁴ I°)5d ⁵ I° ₇	4f ³ (⁴ I°)6p ⁵ K° ₈	22702.777	68302.664	45599.839
1000	2193.1300	45582.685	37	230	45582.576	-0.108	4f ³ (⁴ I°)5d ⁵ K° ₆	4f ³ (⁴ I°)6p ⁵ K ₆	16938.068	62520.646	45582.636
700	2193.8407	45567.919	70	422	45567.813	-0.107	4f ³ (⁴ I°)5d ⁵ L° ₇	4f ³ (⁴ I°)6p ⁵ K ₆	16952.835	62520.646	45567.870
150	2198.8529	45464.060	8	38	45464.044	-0.016	4f ³ (⁴ I°)5d ⁵ I° ₄	4f ³ (⁴ I°)6p ⁵ H ₃	18883.669	64347.699	45464.011
150	2199.3192	45454.422	4	24	45454.316	-0.106	4f ³ (² H2°)5d ³ K° ₇	4f ³ (² H2°)6p ¹ I ₆	31781.802	77236.125	45454.373
150	2201.6941	45405.396	4	26	45405.325	-0.071	U	U	U	U	45405.347
150	2202.6527	45385.638	0	0	45385.441	-0.197	4f ³ (⁴ I°)6p ⁵ K° ₆	4f ³ (⁴ I°)6d ⁵ I° ₇	62520.647	107906.087	45385.589
150	2202.9588	45379.332	0	0	0	0	-	-	-	-	45379.325
150	2203.0907	45376.616	30	180	45376.521	-0.094	4f ³ (⁴ I°)5d ⁵ K° ₅	4f ³ (⁴ I°)6p ⁵ I ₄	15262.437	60638.963	45376.567
325	2204.2052	45353.674	0	0	0	0	-	-	-	-	45353.667
150	2208.5865	45263.713	47	306	45263.631	-0.081	4f ³ (⁴ I°)5d ⁵ K° ₅	4f ³ (⁴ I°)6p ⁵ K ₅	15262.437	60526.067	45263.665
150	2220.7604	45015.608	0	0	0	0	-	-	-	-	45015.601
150	2223.8371	44953.335	6	44	44953.267	-0.068	4f ³ (⁴ I°)5d ³ H° ₄	4f ³ (⁴ I°)6p ³ H ₄	21491.882	66445.159	44953.287
150	2228.3245	44862.817	4	24	44862.774	-0.043	4f ³ (² H2°)5d ³ K° ₇	4f ³ (² H2°)6p ³ I ₆	31781.802	76644.575	44862.769
150	2228.3857	44861.585	4	28	44861.552	-0.033	4f ³ (² H2°)5d ³ I° ₅	4f ³ (⁴ F°)6p ⁵ G ₄	29397.423	74258.973	44861.537
325	2229.1749	44845.704	0	0	0	0	-	-	-	-	44845.697
150	2230.2517	44824.054	0	0	0	0	-	-	-	-	44824.047
325	2233.7086	44754.691	9	54	44754.605	-0.086	4f ³ (⁴ I°)5d ⁵ H° ₃	4f ³ (⁴ I°)6p ⁵ H ₃	19593.094	64347.699	44754.643
150	2234.1449	44745.952	0	0	0	0	-	-	-	-	44745.945
700	2234.7270	44734.297	24	162	44734.181	-0.117	4f ³ (⁴ I°)5d ³ I° ₅	4f ³ (⁴ I°)6p ³ I ₅	19616.622	64350.812	44734.249
325	2235.0334	44728.165	3	20	44728.130	-0.036	4f ³ (⁴ I°)5d ⁵ H° ₇	4f ³ (⁴ I°)6p ³ H ₆	26097.906	70826.009	44728.117
325	2237.3124	44682.608	4	36	44682.538	-0.071	U	U	U	U	44682.560
325	2238.4341	44660.220	4	20	44660.160	-0.059	U	U	U	U	44660.172
150	2238.6611	44655.691	0	0	0	0	-	-	-	-	44655.684
150	2239.5575	44637.819	0	0	0	0	-	-	-	-	44637.812
325	2240.0829	44627.351	14	106	44627.288	-0.062	4f ³ (⁴ I°)5d ³ I° ₅	4f ³ (⁴ I°)6p ⁵ H ₄	19616.622	64243.914	44627.303
150	2240.1882	44625.253	0	0	44625.220	-0.033	U	U	U	U	44625.205
700	2241.7085	44594.992	12	94	44594.929	-0.063	4f ³ (⁴ I°)5d ⁵ K° ₉	4f ³ (⁴ I°)6p ⁵ I ₈	22197.115	66792.024	44594.944
325	2242.2065	44585.088	0	0	0	0	-	-	-	-	44585.081
150	2243.1033	44567.265	0	0	0	0	-	-	-	-	44567.258
325	2243.7322	44554.774	3	24	44554.754	-0.02	4f ³ (⁴ I°)5d ⁵ H° ₆	4f ³ (⁴ I°)6p ³ H ₅	24058.518	68613.221	44554.726
325	2244.0037	44549.384	0	0	0	0	-	-	-	-	44549.377
150	2244.0965	44547.542	0	0	0	0	-	-	-	-	44547.535
325	2246.4052	44501.763	6	54	44501.678	-0.086	4f ³ (⁴ I°)5d ⁵ H° ₇	4f ³ (⁴ I°)6p ³ K ₈	26097.906	70599.570	44501.715
150	2247.0321	44489.349	0	0	0	0	-	-	-	-	44489.342
150	2247.9426	44471.331	0	0	44471.289	-0.042	4f ³ (⁴ I°)5d ⁵ I° ₆	4f ³ (⁴ I°)6p ³ K° ₆	21980.522	66451.812	44471.283
150	2248.4583	44461.132	4	14	44461.124	-0.008	U	U	U	U	44461.084
150	2248.5796	44458.734	4	22	44458.709	-0.025	U	U	U	U	44458.686
325	2248.6812	44456.725	9	68	44456.643	-0.082	4f ³ (⁴ F°)5d ⁵ H° ₄	4f ³ (⁴ F°)6p ⁵ G ₃	28745.307	73201.950	44456.677
325	2249.0742	44448.958	7	42	44448.877	-0.081	4f ³ (⁴ I°)5d ⁵ H° ₆	4f ³ (⁴ I°)6p ³ K ₇	24058.518	68507.387	44448.910
325	2249.5665	44439.231	0	0	0	0	-	-	-	-	44439.224
325	2249.8519	44433.595	8	60	44433.505	-0.09	4f ³ (⁴ F°)5d ⁵ H° ₆	4f ³ (⁴ F°)6p ⁵ G ₅	31146.457	75579.962	44433.547
700	2250.8453	44413.986	8	56	44413.906	-0.08	4f ³ (⁴ F°)5d ⁵ H° ₃	4f ³ (⁴ F°)6p ⁵ G ₂	27675.024	72088.930	44413.938
150	2251.3630	44403.774	2	10	44403.692	-0.082	4f ³ (⁴ F°)5d ⁵ H° ₇	4f ³ (² H2°)6p ¹ I ₆	32832.447	77236.125	44403.726
700	2253.4432	44362.788	13	90	44362.689	-0.099	4f ³ (⁴ I°)5d ⁵ H° ₇	4f ³ (⁴ I°)6p ³ I ₇	26097.906	70460.602	44362.740
150	2253.5540	44360.607	3	22	44360.518	-0.089	U	U	U	U	44360.559
150	2253.8418	44354.943	4	22	44354.749	-0.194	4f ³ (⁴ I°)6p ⁵ I ₈	4f ³ (⁴ I°)6d ³ L° ₉	66792.024	111146.752	44354.895
150	2254.1127	44349.613	3	24	44349.526	-0.087	U	U	U	U	44349.565
150	2254.3772	44344.410	4	18	44344.350	-0.06	4f ³ (⁴ I°)5d ³ I° ₇	4f ³ (⁴ I°)6p ³ I ₆	24003.225	68347.584	44344.362
150	2257.0269	44292.355	0	0	44292.280	-0.075	4f ³ (⁴ I°)5d ⁵ I° ₆	4f ³ (⁴ I°)6p ⁵ H° ₅	21980.522	66272.802	44292.307
325	2257.1886	44289.183	17	108	44289.070	-0.112	4f ³ (⁴ I°)5d ⁵ H° ₆	4f ³ (⁴ I°)6p ³ I ₆	24058.518	68347.584	44289.135
150	2258.1357	44270.609	6	32	44270.504	-0.104	4f ³ (⁴ I°)5d ⁵ H° ₅	4f ³ (⁴ I°)6p ³ K ₆	22181.299	66451.812	44270.561

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Table E.1: Unclassified Nd III Line List of Dr H. M. Crosswhite Compared with the Nd-Ar PDL Line List of this Thesis (continued)

Int. (arb.)	λ (Å)	σ_{grat} (cm ⁻¹)	SNR	PDL Int. (arb.)	σ_{obs} (cm ⁻¹)	Diff. (cm ⁻¹)	L1	L2	E1 (cm ⁻¹)	E2 (cm ⁻¹)	σ_{cal} (cm ⁻¹)
150	2258.4834	44263.794	5	28	44263.862	0.068	4f ³ (⁴ I°)5d ⁵ H° ₅	4f ³ (⁴ I°)6p ³ H ₄	22181.299	66445.159	44263.746
325	2258.6943	44259.661	6	20	44259.583	-0.078	U	U	U	U	44259.613
150	2259.2285	44249.197	4	24	44249.184	-0.013	U	U	U	U	44249.149
150	2259.8150	44237.714	0	0	0	0	-	-	-	-	44237.707
150	2260.2198	44229.792	0	0	0	0	-	-	-	-	44229.785
325	2260.4960	44224.388	17	106	44224.267	-0.121	4f ³ (⁴ I°)5d ³ I° ₆	4f ³ (⁴ I°)6p ⁵ H ₆	20799.349	65023.633	44224.340
150	2261.1706	44211.195	6	42	44211.113	-0.082	4f ³ (⁴ I°)5d ⁵ K° ₈	4f ³ (⁴ I°)6p ⁵ K ₇	20410.897	64622.006	44211.147
100	2261.4877	44204.997	4	28	44204.899	-0.097	U	U	U	U	44204.949
150	2262.7487	44180.364	0	0	0	0	-	-	-	-	44180.357
150	2262.8980	44177.449	0	0	0	0	-	-	-	-	44177.442
150	2263.3626	44168.382	0	0	0	0	-	-	-	-	44168.375
150	2264.0158	44155.640	5	36	44155.542	-0.098	4f ³ (⁴ I°)5d ⁵ G° ₆	4f ³ (⁴ I°)6p ³ H ₆	26670.461	70826.009	44155.593
150	2266.1699	44113.672	3	46	44113.584	-0.088	U	U	U	U	44113.625
700	2267.3034	44091.620	20	118	44091.507	-0.113	4f ³ (⁴ I°)5d ⁵ H° ₅	4f ³ (⁴ I°)6p ⁵ H ₅	22181.299	66272.802	44091.573
150	2267.7295	44083.336	3	16	44083.234	-0.102	4f ³ (⁴ F°)5d ⁵ H° ₅	4f ³ (⁴ F°)6p ⁵ G ₄	30175.737	74258.973	44083.289
150	2269.3855	44051.171	3	10	44051.095	-0.076	U	U	U	U	44051.124
150	2269.6963	44045.139	3	22	44045.117	-0.022	U	U	U	U	44045.092
150	2269.8234	44042.673	0	0	0	0	-	-	-	-	44042.666
150	2269.9499	44040.219	0	0	44040.260	0.041	4f ³ (⁴ I°)6p ⁵ K° ₆	4f ³ (⁴ I°)6d ⁵ H° ₅	62520.647	106560.907	44040.172
150	2270.5515	44028.551	3	42	44028.481	-0.070	U	U	U	U	44028.504
150	2270.9604	44020.625	0	0	44020.745	0.120	4f ³ (² G1°)5d ³ H° ₆	4f ³ (⁴ F°)6p ⁵ G° ₅	31559.217	75579.962	44020.578
150	2272.6216	43988.450	0	0	0	0	-	-	-	-	43988.443
150	2278.7515	43870.131	3	16	43870.009	-0.122	U	U	U	U	43870.084
150	2279.2762	43860.033	4	24	43859.909	-0.124	U	U	U	U	43859.986
325	2279.5358	43855.038	22	126	43854.910	-0.129	4f ³ (⁴ I°)5d ⁵ H° ₄	4f ³ (⁴ I°)6p ⁵ H ₄	20388.995	64243.914	43854.991
150	2279.7665	43850.601	4	24	43850.519	-0.082	4f ³ (² H2°)5d ³ I° ₅	4f ³ (² H2°)6p ³ I ₅	29397.423	73247.950	43850.554
150	2279.8177	43849.616	2	14	43849.682	0.066	U	U	U	U	43849.569
150	2282.6838	43794.564	12	74	43794.434	-0.13	4f ³ (⁴ I°)5d ⁵ I° ₇	4f ³ (⁴ I°)6p ⁵ I ₇	22702.777	66497.225	43794.517
325	2282.9095	43790.235	13	80	43790.131	-0.104	4f ³ (⁴ I°)5d ⁵ G° ₆	4f ³ (⁴ I°)6p ³ I ₇	26670.461	70460.602	43790.188
150	2285.0531	43749.159	5	34	43749.025	-0.134	4f ³ (⁴ I°)5d ⁵ I° ₇	4f ³ (⁴ I°)6p ³ K ₆	22702.777	66451.812	43749.112
150	2285.4807	43740.975	5	26	43740.937	-0.038	4f ³ (⁴ I°)6p ⁵ I ₄	4f ³ (⁴ I°)6d ⁵ H° ₃	60638.963	104379.920	43740.928
150	2285.7967	43734.928	13	84	43734.807	-0.122	4f ³ (⁴ I°)5d ⁵ G° ₅	4f ³ (⁴ I°)6p ³ H ₅	24878.412	68613.221	43734.881
150	2286.3689	43723.984	5	24	43723.939	-0.045	U	U	U	U	43723.937
325	2287.0727	43710.530	10	46	43710.400	-0.13	4f ³ (⁴ I°)5d ⁵ I° ₈	4f ³ (⁴ I°)6p ⁵ K ₈	24592.259	68302.664	43710.483
325	2292.6161	43604.850	13	82	43604.767	-0.083	4f ³ (² H2°)5d ³ K° ₆	4f ³ (² H2°)6p ³ I ₅	29643.186	73247.950	43604.803
150	2301.1038	43444.027	6	22	43444.036	0.009	U	U	U	U	43443.980
325	2301.5974	43434.710	10	82	43434.726	0.015	4f ³ (⁴ I°)5d ⁵ G° ₄	4f ³ (⁴ I°)6p ³ H ₄	23010.450	66445.159	43434.663
150	2306.6790	43339.032	0	0	0	0	-	-	-	-	43339.025
325	2307.0657	43331.769	19	102	43331.729	-0.04	4f ³ (⁴ I°)5d ³ K° ₆	4f ³ (⁴ I°)6p ³ K ₆	23120.073	66451.812	43331.722
325	2310.7660	43262.386	22	132	43262.353	-0.034	4f ³ (⁴ I°)5d ⁵ G° ₄	4f ³ (⁴ I°)6p ⁵ H ₅	23010.450	66272.802	43262.339
700	2314.7566	43187.809	16	92	43187.806	-0.003	4f ³ (⁴ I°)5d ³ K° ₇	4f ³ (⁴ I°)6p ³ K ₇	25319.579	68507.387	43187.762
325	2316.3725	43157.684	14	70	43157.659	-0.025	4f ³ (⁴ I°)5d ³ K° ₈	4f ³ (⁴ I°)6p ³ K ₈	27441.911	70599.570	43157.637
150	2316.6391	43152.718	15	74	43152.720	0.002	4f ³ (⁴ I°)5d ³ K° ₆	4f ³ (⁴ I°)6p ⁵ H ₅	23120.073	66272.802	43152.671
150	2317.3454	43139.567	0	0	0	0	-	-	-	-	43139.560
325	2323.3539	43028.012	12	82	43027.996	-0.016	4f ³ (⁴ I°)5d ³ K° ₇	4f ³ (⁴ I°)6p ³ I ₆	25319.579	68347.584	43027.966
325	2323.8567	43018.703	15	78	43018.696	-0.007	4f ³ (⁴ I°)5d ³ K° ₈	4f ³ (⁴ I°)6p ³ I ₇	27441.911	70460.602	43018.657
325	2331.8981	42870.368	29	136	42870.371	0.003	4f ³ (⁴ I°)5d ⁵ G° ₂	4f ³ (⁴ I°)6p ⁵ H ₃	21477.328	64347.699	42870.322
150	2333.4123	42842.551	0	0	42842.334	-0.217	4f ³ (⁴ I°)5d ⁵ H° ₅	4f ³ (⁴ I°)6p ⁵ H° ₆	22181.299	65023.633	42842.505
150	2337.6708	42764.512	24	112	42764.515	0.003	4f ³ (⁴ I°)5d ⁵ G° ₃	4f ³ (⁴ I°)6p ⁵ H ₄	21479.404	64243.914	42764.466
150	2340.4197	42714.288	0	0	42714.287	0.000	4f ³ (⁴ I°)5d ³ I° ₇	4f ³ (⁴ I°)6p ⁵ H° ₇	24003.225	66717.513	42714.242
150	2348.4008	42569.134	40	204	42569.097	-0.038	4f ³ (⁴ I°)5d ⁵ I° ₆	4f ³ (⁴ I°)6p ⁵ I ₆	21980.522	64549.620	42569.088
150	2349.2382	42553.962	29	140	42553.932	-0.03	4f ³ (⁴ I°)5d ³ G° ₃	4f ³ (⁴ I°)6p ³ H ₄	23891.226	66445.159	42553.916
150	2358.5469	42386.024	22	98	42385.973	-0.051	4f ³ (⁴ I°)5d ³ G° ₅	4f ³ (⁴ I°)6p ³ H ₆	28440.047	70826.009	42385.978
150	2359.1649	42374.921	5	26	42374.937	0.016	U	U	U	U	42374.875
150	2363.8144	42291.579	51	240	42291.522	-0.056	4f ³ (⁴ I°)5d ⁵ I° ₅	4f ³ (⁴ I°)6p ⁵ I ₅	20348.742	62640.266	42291.533
150	2373.1476	42125.266	15	84	42125.248	-0.018	4f ³ (⁴ I°)5d ⁵ I° ₈	4f ³ (⁴ I°)6p ⁵ H ₇	24592.259	66717.513	42125.220
150	2382.7954	41954.717	31	130	41954.648	-0.07	4f ³ (⁴ I°)5d ³ L° ₇	4f ³ (⁴ I°)6p ³ K ₆	24497.165	66451.812	41954.672
150	2389.8555	41830.785	34	156	41830.700	-0.085	4f ³ (⁴ I°)5d ³ L° ₈	4f ³ (⁴ I°)6p ³ K ₇	26676.685	68507.387	41830.740
150	2394.1737	41755.343	49	202	41755.295	-0.048	4f ³ (⁴ I°)5d ⁵ I° ₄	4f ³ (⁴ I°)6p ⁵ I ₄	18883.669	60638.963	41755.298
150	2396.0716	41722.272	31	144	41722.248	-0.024	4f ³ (⁴ I°)5d ³ L° ₉	4f ³ (⁴ I°)6p ³ K ₈	28877.321	70599.570	41722.227

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Table E.1: Unclassified Nd III Line List of Dr H. M. Crosswhite Compared with the Nd-Ar PDL Line List of this Thesis (continued)

Int. (arb.)	λ (Å)	σ_{grat} (cm ⁻¹)	SNR	PDL Int. (arb.)	σ_{obs} (cm ⁻¹)	Diff. (cm ⁻¹)	L1	L2	E1 (cm ⁻¹)	E2 (cm ⁻¹)	σ_{cal} (cm ⁻¹)
150	2398.3503	41682.634	30	130	41682.685	0.05	4f ³ (⁴ I°)5d ³ H° ₆	4f ³ (⁴ I°)6p ⁵ H ₇	25034.832	66717.513	41682.589
150	2429.4914	41148.389	52	204	41148.386	-0.003	4f ³ (⁴ I°)5d ³ H° ₄	4f ³ (⁴ I°)6p ⁵ I ₅	21491.882	62640.266	41148.344
325	2435.5594	41045.879	51	194	41045.869	-0.01	4f ³ (⁴ I°)5d ⁵ H° ₃	4f ³ (⁴ I°)6p ⁵ I ₄	19593.094	60638.963	41045.834
150	2439.7221	40975.851	4	14	40975.850	-0.001	U	U	U	U	40975.806
700	2466.7740	40526.521	43	158	40526.468	-0.053	4f ³ (⁴ I°)5d ³ L° ₇	4f ³ (⁴ I°)6p ⁵ H ₆	24497.165	65023.633	40526.477
150	2479.8779	40312.391	10	32	40312.507	0.116	4f ³ (⁴ I°)6p ³ H ₄	4f ³ (⁴ I°)6d ⁵ G° ₄	66445.159	106757.677	40312.347
150	2481.3738	40288.090	17	62	40288.102	0.012	4f ³ (⁴ I°)6p ⁵ H ₅	4f ³ (⁴ I°)6d ⁵ H° ₅	66272.802	106560.907	40288.046
325	2500.2221	39984.393	37	134	39984.385	-0.008	4f ³ (⁴ I°)6p ⁵ K ₉	4f ³ (⁴ I°)6d ⁵ L° ₁₀	70141.009	110125.394	39984.349
150	2504.6866	39913.128	27	114	39913.128	0.001	4f ³ (⁴ I°)6p ⁵ I ₇	4f ³ (⁴ I°)6d ⁵ L° ₈	66497.225	106410.353	39913.084
150	2505.0546	39907.265	35	116	39907.230	-0.035	4f ³ (⁴ I°)6p ⁵ K ₈	4f ³ (⁴ I°)6d ⁵ L° ₉	68302.664	108209.894	39907.221
150	2508.1225	39858.454	4	6	39858.424	-0.030	U	U	U	U	39858.410
325	2510.5090	39820.567	16	58	39820.539	-0.028	4f ³ (⁴ I°)5d ³ L° ₈	4f ³ (⁴ I°)6p ⁵ I ₇	26676.685	66497.225	39820.523
150	2513.2741	39776.759	8	52	39776.906	0.147	U	U	U	U	39776.715
150	2513.4308	39774.280	31	100	39774.270	-0.01	4f ³ (⁴ I°)6p ⁵ H ₆	4f ³ (⁴ I°)6d ⁵ L° ₇	65023.633	104797.903	39774.236
150	2516.4400	39726.720	6	34	39726.740	0.02	4f ³ (⁴ I°)5d ³ I° ₆	4f ³ (⁴ I°)6p ⁵ K ₅	20799.349	60526.067	39726.677
150	2517.8712	39704.140	0	0	39704.054	-0.086	4f ³ (⁴ I°)5d ³ K° ₇	4f ³ (⁴ I°)6p ⁵ H° ₆	25319.579	65023.633	39704.097
150	2519.5048	39678.399	0	0	0	0	-	-	-	-	39678.392
150	2522.5941	39629.810	0	0	39629.815	0.006	4f ³ (⁴ I°)5d ⁵ G° ₄	4f ³ (⁴ I°)6p ⁵ I° ₅	23010.450	62640.266	39629.767
150	2522.9811	39623.731	13	52	39623.736	0.005	4f ³ (⁴ I°)6p ⁵ K ₈	4f ³ (⁴ I°)6d ⁵ K° ₈	68302.664	107926.405	39623.688
150	2534.1802	39448.637	0	0	0	0	-	-	-	-	39448.630
700	2535.6768	39425.355	9	34	39425.350	-0.005	4f ³ (⁴ I°)5d ³ L° ₉	4f ³ (⁴ I°)6p ⁵ K ₈	28877.321	68302.664	39425.312
150	2536.7589	39408.539	9	22	39408.556	0.018	4f ³ (⁴ I°)6p ⁵ H ₄	4f ³ (⁴ I°)6d ⁵ K° ₅	64243.914	103652.472	39408.496
150	2541.1895	39339.834	0	0	0	0	-	-	-	-	39339.827
150	2542.4018	39321.077	0	0	0	0	-	-	-	-	39321.070
150	2545.3453	39275.608	6	22	39275.612	0.005	4f ³ (⁴ I°)5d ³ K° ₈	4f ³ (⁴ I°)6p ⁵ H ₇	27441.911	66717.513	39275.565
150	2552.8871	39159.586	11	36	39159.551	-0.035	4f ³ (⁴ I°)5d ⁵ G° ₃	4f ³ (⁴ I°)6p ⁵ I ₄	21479.404	60638.963	39159.543
150	2618.7008	38175.481	0	0	0	0	-	-	-	-	38175.474
150	2629.1690	38023.492	10	28	38023.476	-0.016	4f ³ (⁴ I°)5d ³ L° ₇	4f ³ (⁴ I°)6p ⁵ K ₆	24497.165	62520.646	38023.450
325	2634.5840	37945.345	75	242	37945.292	-0.053	4f ³ (⁴ I°)5d ³ L° ₈	4f ³ (⁴ I°)6p ⁵ K ₇	26676.685	64622.006	37945.303
50	2754.2956	36296.194	6	56	36296.314	0.120	U	U	U	U	36296.154
50	2764.1487	36166.819	263	1058	36166.770	-0.049	4f ⁴ ⁵ I ₈	4f ³ (² K°)5d ³ I° ₇	5093.257	41260.027	36166.779
50	2771.9483	36065.060	0	0	36065.021	-0.039	4f ³ (² H2°)5d ³ K° ₈	4f ³ (⁴ I°)6p ³ K° ₈	34534.549	70599.570	36065.020
50	2772.6263	36056.241	0	0	0	0	-	-	-	-	36056.234
50	2788.4149	35852.094	4	18	35852.058	-0.036	4f ³ (⁴ I°)6s ($\frac{9}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p ³ H ₄	30593.085	66445.159	35852.054
50	2793.2923	35789.495	0	0	35789.520	0.025	4f ³ (² H2°)5d ¹ I° ₆	4f ³ (⁴ I°)6p ³ H° ₅	32823.701	68613.221	35789.455
50	2797.6006	35734.382	0	0	0	0	-	-	-	-	35734.375
50	2802.2620	35674.943	0	0	35674.940	-0.003	4f ³ (⁴ F°)5d ⁵ H° ₇	4f ³ (⁴ I°)6p ³ K° ₇	32832.447	68507.387	35674.903
50	2805.1869	35637.748	0	0	35637.730	-0.017	4f ³ (² H2°)5d ³ I° ₇	4f ³ (⁴ I°)6p ³ H° ₆	35188.278	70826.009	35637.708
50	2806.0962	35626.200	9	24	35626.221	0.021	4f ³ (² H2°)5d ³ I° ₅	4f ³ (⁴ I°)6p ⁵ H ₆	29397.423	65023.633	35626.160
50	2806.5222	35620.793	0	0	0	0	-	-	-	-	35620.786
50	2811.0231	35563.761	0	0	0	0	-	-	-	-	35563.754
50	2815.7488	35504.077	5	34	35504.032	-0.044	U	U	U	U	35504.037
50	2821.2312	35435.086	358	1530	35435.076	-0.01	4f ⁴ ⁵ I ₅	4f ³ (⁴ G°)5d ⁵ G° ₄	1137.794	36572.870	35435.046
50	2823.0834	35411.839	449	2214	35411.826	-0.013	4f ⁴ ⁵ I ₈	4f ³ (⁴ G°)5d ⁵ H° ₇	5093.257	40505.082	35411.799
50	2823.1232	35411.340	0	0	35411.292	-0.048	4f ³ (² H2°)5d ³ I° ₇	4f ³ (⁴ I°)6p ³ K° ₈	35188.278	70599.570	35411.300
50	2823.8228	35402.567	7	22	35402.559	-0.008	4f ³ (⁴ F°)5d ⁵ G° ₆	4f ³ (⁴ I°)6p ³ H ₅	33210.660	68613.221	35402.527
50	2825.6567	35379.591	324	1416	35379.556	-0.035	4f ⁴ ⁵ I ₅	4f ³ (² H2°)5d ¹ G° ₄	1137.794	36517.350	35379.551
150	2828.5236	35343.733	687	3300	35343.724	-0.009	4f ⁴ ⁵ I ₇	4f ³ (⁴ G°)5d ⁵ H° ₆	3714.548	39058.274	35343.694
50	2830.9776	35313.098	0	0	0	0	-	-	-	-	35313.091
50	2831.5187	35306.350	0	0	35306.165	-0.184	4f ³ (⁴ F°)5d ³ H° ₆	4f ³ (⁴ I°)6p ³ I° ₇	35154.437	70460.602	35306.311
50	2832.2920	35296.710	0	0	35296.727	0.017	4f ³ (⁴ F°)5d ⁵ G° ₆	4f ³ (⁴ I°)6p ³ K° ₇	33210.660	68507.387	35296.671
100	2834.2492	35272.337	6	22	35272.316	-0.021	4f ³ (² H2°)5d ³ I° ₇	4f ³ (⁴ I°)6p ³ I ₇	35188.278	70460.602	35272.298
100	2838.6793	35217.293	5	46	35217.273	-0.020	U	U	U	U	35217.254
50	2838.7385	35216.559	0	0	0	0	-	-	-	-	35216.552
150	2839.6502	35205.253	825	3936	35205.216	-0.037	4f ⁴ ⁵ I ₆	4f ³ (⁴ G°)5d ⁵ H° ₅	2387.544	37592.759	35205.214
50	2848.3770	35097.397	566	2652	35097.386	-0.011	4f ⁴ ⁵ I ₅	4f ³ (⁴ G°)5d ⁵ H° ₄	1137.794	36235.179	35097.358
50	2864.3417	34901.787	4	32	34901.792	0.005	U	U	U	U	34901.748
50	2868.0291	34856.917	526	2648	34856.862	-0.055	4f ⁴ ⁵ I ₄	4f ³ (² G1°)5d ³ G° ₃	0.000	34856.862	34856.878
150	2871.4328	34815.600	4	42	34815.721	0.121	U	U	U	U	34815.561
50	2876.0459	34759.760	16	140	34759.736	-0.024	4f ³ (⁴ I°)6s ($\frac{15}{2}, \frac{1}{2}$)° ₈	4f ³ (⁴ I°)6p ³ K ₈	35839.828	70599.570	34759.721

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Table E.1: Unclassified Nd III Line List of Dr H. M. Crosswhite Compared with the Nd-Ar PDL Line List of this Thesis (continued)

Int. (arb.)	λ (Å)	σ_{grat} (cm ⁻¹)	SNR	PDL Int. (arb.)	σ_{obs} (cm ⁻¹)	Diff. (cm ⁻¹)	L1	L2	E1 (cm ⁻¹)	E2 (cm ⁻¹)	σ_{cal} (cm ⁻¹)
150	2883.7965	34666.342	0	0	0	0	-	-	-	-	34666.335
50	2884.3607	34659.562	162	1148	34659.465	-0.097	U	U	U	U	34659.523
50	2884.6290	34656.338	4	20	34656.329	-0.009	U	U	U	U	34656.299
50	2885.3058	34648.209	0	0	0	0	-	-	-	-	34648.202
50	2885.6471	34644.112	6	40	34644.082	-0.029	U	U	U	U	34644.073
150	2885.8321	34641.891	14	126	34641.835	-0.056	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ⁵ H ₇	32075.658	66717.513	34641.852
150	2887.5920	34620.779	7	98	34620.748	-0.03	4f ³ (⁴ I°)6s ($\frac{15}{2}, \frac{1}{2}$)° ₈	4f ³ (⁴ I°)6p ³ I ₇	35839.828	70460.602	34620.740
50	2888.7792	34606.551	4	44	34606.552	0.001	U	U	U	U	34606.512
50	2889.2179	34601.297	16	156	34601.241	-0.055	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₇	4f ³ (⁴ I°)6p ³ K ₇	33906.143	68507.387	34601.258
50	2894.1206	34542.684	6	98	34542.569	-0.115	U	U	U	U	34542.645
50	2899.4593	34479.084	3	42	34479.023	-0.062	U	U	U	U	34479.045
150	2899.5803	34477.646	17	160	34477.598	-0.048	4f ³ (⁴ I°)6s ($\frac{9}{2}, \frac{1}{2}$)° ₄	4f ³ (⁴ I°)6p ³ I ₅	29873.222	64350.812	34477.607
100	2899.6410	34476.924	6	66	34476.864	-0.060	U	U	U	U	34476.885
200	2899.8366	34474.599	30	298	34474.470	-0.129	4f ³ (⁴ I°)6s ($\frac{9}{2}, \frac{1}{2}$)° ₄	4f ³ (⁴ I°)6p ⁵ H ₃	29873.222	64347.699	34474.560
100	2902.6245	34441.488	8	78	34441.432	-0.056	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₇	4f ³ (⁴ I°)6p ³ I ₆	33906.143	68347.584	34441.449
200	2903.5391	34430.640	31	264	34430.549	-0.091	4f ³ (⁴ I°)6s ($\frac{9}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p ⁵ H ₆	30593.085	65023.633	34430.601
200	2904.2966	34421.660	25	250	34421.561	-0.099	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ⁵ I ₇	32075.658	66497.225	34421.621
100	2906.1202	34400.061	3	20	34400.034	-0.028	U	U	U	U	34400.022
325	2906.4158	34396.563	32	350	34396.521	-0.042	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₇	4f ³ (⁴ I°)6p ⁵ K ₈	33906.143	68302.664	34396.524
200	2908.1377	34376.197	17	168	34376.165	-0.033	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ³ K ₆	32075.658	66451.812	34376.158
200	2908.5984	34370.753	25	258	34370.689	-0.064	4f ³ (⁴ I°)6s ($\frac{9}{2}, \frac{1}{2}$)° ₄	4f ³ (⁴ I°)6p ⁵ H ₄	29873.222	64243.914	34370.714
50	2908.9663	34366.406	6	74	34366.387	-0.019	U	U	U	U	34366.367
700	2914.4989	34301.171	33	406	34301.184	0.013	4f ³ (⁴ I°)6s ($\frac{15}{2}, \frac{1}{2}$)° ₈	4f ³ (⁴ I°)6p ⁵ K ₉	35839.828	70141.009	34301.132
200	2917.2500	34268.825	3	54	34268.914	0.089	U	U	U	U	34268.787
50	2917.6446	34264.191	4	68	34264.150	-0.041	U	U	U	U	34264.153
50	2918.0759	34259.127	7	62	34258.838	-0.288	U	U	U	U	34259.089
50	2921.4718	34219.306	6	36	34219.357	0.051	U	U	U	U	34219.268
150	2923.3634	34197.165	11	140	34197.132	-0.033	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ⁵ H ₅	32075.658	66272.802	34197.127
50	2924.3116	34186.077	4	40	34186.230	0.153	U	U	U	U	34186.039
150	2928.0788	34142.096	14	134	34142.083	-0.013	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p ³ K ₆	32309.729	66451.812	34142.058
250	2928.6478	34135.463	20	192	34135.428	-0.034	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p ³ H ₄	32309.729	66445.159	34135.425
50	2931.9810	34096.658	2	8	34096.559	-0.099	U	U	U	U	34096.620
50	2932.1703	34094.457	9	92	34094.441	-0.016	U	U	U	U	34094.419
50	2934.4406	34068.080	4	48	34068.143	0.063	4f ³ (⁴ F°)5d ⁵ H° ₅	4f ³ (⁴ I°)6p ⁵ H ₄	30175.737	64243.914	34068.042
50	2937.1026	34037.204	3	62	34037.076	-0.128	U	U	U	U	34037.166
50	2938.4638	34021.438	3	20	34021.203	-0.235	U	U	U	U	34021.400
150	2938.5024	34020.991	5	26	34020.940	-0.051	U	U	U	U	34020.953
150	2938.5438	34020.511	3	32	34020.556	0.044	U	U	U	U	34020.473
150	2939.5536	34008.825	4	48	34008.793	-0.032	U	U	U	U	34008.787
50	2941.1770	33990.055	0	0	0	0	-	-	-	-	33990.048
200	2943.5059	33963.163	12	124	33963.072	-0.091	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p ⁵ H ₅	32309.729	66272.802	33963.125
325	2945.8866	33935.717	13	160	33935.658	-0.059	4f ³ (⁴ G°)5d ⁵ I° ₇	4f ³ (⁴ I°)6p ³ H ₆	36890.347	70826.009	33935.679
50	2945.9851	33934.582	0	0	0	0	-	-	-	-	33934.575
325	2946.6757	33926.630	0	0	0	0	-	-	-	-	33926.623
325	2946.7162	33926.163	19	262	33925.977	-0.187	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ³ H ₅	34687.230	68613.221	33926.125
50	2953.7444	33845.442	3	24	33845.435	-0.008	U	U	U	U	33845.404
325	2955.9495	33820.195	15	166	33820.153	-0.043	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ³ K ₇	34687.230	68507.387	33820.157
50	2958.6130	33789.750	4	64	33789.645	-0.104	U	U	U	U	33789.712
200	2958.7877	33787.755	0	0	0	0	-	-	-	-	33787.748
50	2963.2908	33736.412	7	66	33736.413	0.001	4f ³ (⁴ I°)6s ($\frac{15}{2}, \frac{1}{2}$)° ₇	4f ³ (⁴ I°)6p ³ H ₆	37089.599	70826.009	33736.374
50	2966.8539	33695.898	0	0	0	0	-	-	-	-	33695.891
325	2969.9886	33660.335	12	198	33660.364	0.03	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ³ I ₆	34687.230	68347.584	33660.297
150	2970.8297	33650.805	8	106	33650.833	0.028	4f ³ (⁴ I°)6s ($\frac{9}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p ⁵ H ₄	30593.085	64243.914	33650.767
325	2977.9571	33570.269	8	64	33570.216	-0.053	4f ³ (⁴ G°)5d ⁵ I° ₇	4f ³ (⁴ I°)6p ³ I ₇	36890.347	70460.602	33570.231
325	2988.1673	33455.569	0	0	0	0	-	-	-	-	33455.562
50	2993.1929	33399.399	72	822	33399.548	0.149	U	U	U	U	33399.361
150	3034.2021	32948.003	0	0	32947.975	-0.028	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ⁵ H° ₆	32075.658	65023.633	32947.966
150	3039.9301	32885.923	0	0	32885.881	-0.042	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₇	4f ³ (⁴ I°)6p ⁵ I° ₈	33906.143	66792.024	32885.886
150	3057.3384	32698.680	0	0	0	0	-	-	-	-	32698.673
100	3057.3884	32698.146	0	0	0	0	-	-	-	-	32698.139

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Table E.1: Unclassified Nd III Line List of Dr H. M. Crosswhite Compared with the Nd-Ar PDL Line List of this Thesis (continued)

Int. (arb.)	λ (Å)	σ_{grat} (cm ⁻¹)	SNR	PDL Int. (arb.)	σ_{obs} (cm ⁻¹)	Diff. (cm ⁻¹)	L1	L2	E1 (cm ⁻¹)	E2 (cm ⁻¹)	σ_{cal} (cm ⁻¹)
150	3067.4317	32591.091	4	138	32591.085	-0.006	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₇	4f ³ (⁴ I°)6p ⁵ I ₇	33906.143	66497.225	32591.054
150	3071.6462	32546.375	0	0	32546.349	-0.027	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ⁵ K° ₇	32075.658	64622.006	32546.338
100	3078.4944	32473.978	0	0	32473.962	-0.016	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ⁵ I° ₆	32075.658	64549.620	32473.941
100	3079.5510	32462.836	0	0	32462.836	-0.001	4f ³ (⁴ I°)6s ($\frac{15}{2}, \frac{1}{2}$)° ₈	4f ³ (⁴ I°)6p ⁵ K° ₈	35839.828	68302.664	32462.799
100	3095.1229	32299.519	0	0	32299.686	0.168	4f ⁴ ⁵ I° ₆	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₆	2387.544	34687.231	32299.482
50	3097.4566	32275.185	0	0	32275.155	-0.030	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ³ I° ₅	32075.658	64350.812	32275.148
100	3119.4922	32047.207	0	0	32047.180	-0.026	4f ³ (⁴ I°)6s ($\frac{9}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p ⁵ I° ₅	30593.086	62640.266	32047.171
150	3121.1391	32030.297	0	0	32030.282	-0.015	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ⁵ H° ₇	34687.231	66717.513	32030.261
150	3124.4475	31996.382	6	208	31996.332	-0.05	4f ⁴ ⁵ I ₈	4f ³ (⁴ I°)6s ($\frac{15}{2}, \frac{1}{2}$)° ₇	5093.257	37089.599	31996.346
150	3130.3227	31936.332	0	0	0	0	-	-	-	-	31936.325
325	3131.1820	31927.568	0	0	31927.561	-0.007	4f ³ (⁴ I°)6s ($\frac{9}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p ⁵ K° ₆	30593.086	62520.647	31927.532
325	3135.5094	31883.505	0	0	31883.571	0.066	4f ³ (² H°)6p ³ I° ₅	4f ³ (⁴ I°)7s ($\frac{11}{2}, \frac{1}{2}$)° ₆	73247.950	105131.521	31883.469
150	3140.2837	31835.033	14	490	31835.030	-0.004	4f ⁴ ⁵ I ₇	4f ³ (⁴ G°)5d ⁵ I° ₆	3714.548	35549.565	31834.997
100	3140.9260	31828.524	3	138	31828.527	0.003	U	U	U	U	31828.488
50	3147.2390	31764.682	0	0	31764.581	-0.100	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ³ K° ₆	34687.231	66451.812	31764.646
50	3149.1962	31744.941	0	0	31744.918	-0.023	4f ³ (² H°)5d ¹ H° ₅	4f ³ (⁴ I°)6p ³ I° ₅	32605.894	64350.812	31744.905
50	3159.4139	31642.280	0	0	0	0	-	-	-	-	31642.273
150	3163.2624	31603.785	0	0	31603.745	-0.039	4f ³ (² H°)5d ³ I° ₇	4f ³ (⁴ I°)6p ⁵ I° ₈	35188.278	66792.024	31603.749
50	3165.8271	31578.183	4	82	31578.167	-0.016	U	U	U	U	31578.147
50	3166.1917	31574.547	0	0	0	0	-	-	-	-	31574.540
150	3171.3863	31522.831	9	256	31522.726	-0.104	U	U	U	U	31522.795
50	3176.3349	31473.721	15	542	31473.724	0.003	4f ⁴ ⁵ I ₇	4f ³ (² H°)5d ³ I° ₇	3714.548	35188.278	31473.685
150	3176.9026	31468.097	8	120	31468.133	0.035	4f ⁴ ⁵ I ₅	4f ³ (² H°)5d ¹ H° ₅	1137.794	32605.894	31468.061
50	3182.3607	31414.128	0	0	0	0	-	-	-	-	31414.121
100	3182.4063	31413.678	0	0	0	0	-	-	-	-	31413.671
250	3182.6427	31411.344	0	0	31411.346	0.002	4f ³ (⁴ F°)5d ⁵ G° ₆	4f ³ (⁴ I°)6p ⁵ K° ₇	33210.660	64622.006	31411.308
50	3189.9932	31338.968	0	0	31338.960	-0.008	4f ³ (⁴ F°)5d ⁵ G° ₆	4f ³ (⁴ I°)6p ⁵ I° ₆	33210.660	64549.620	31338.932
150	3196.6363	31273.843	0	0	0	0	-	-	-	-	31273.836
200	3200.3447	31237.606	0	0	0	0	-	-	-	-	31237.599
250	3201.6450	31224.920	0	0	0	0	-	-	-	-	31224.913
150	3203.2076	31209.688	0	0	0	0	-	-	-	-	31209.681
150	3212.6967	31117.510	0	0	31117.490	-0.019	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₇	4f ³ (⁴ I°)6p ⁵ H° ₆	33906.143	65023.633	31117.474
100	3215.6679	31088.759	0	0	0	0	-	-	-	-	31088.752
50	3219.8191	31048.679	0	0	0	0	-	-	-	-	31048.672
50	3220.4467	31042.628	0	0	0	0	-	-	-	-	31042.621
50	3220.8771	31038.480	0	0	0	0	-	-	-	-	31038.473
50	3225.7460	30991.633	0	0	0	0	-	-	-	-	30991.626
100	3228.0881	30969.148	0	0	0	0	-	-	-	-	30969.141
325	3229.8464	30952.289	5	144	30952.215	-0.074	4f ³ (⁴ I°)6s ($\frac{15}{2}, \frac{1}{2}$)° ₈	4f ³ (⁴ I°)6p ⁵ I ₈	35839.828	66792.024	30952.254
50	3231.1991	30939.332	15	420	30939.324	-0.008	4f ⁴ ⁵ I ₅	4f ³ (⁴ F°)5d ³ H° ₄	1137.794	32077.113	30939.297
100	3232.9704	30922.381	0	0	0	0	-	-	-	-	30922.374
100	3233.4982	30917.334	27	684	30917.130	-0.204	U	U	U	U	30917.299
100	3234.1744	30910.870	0	0	0	0	-	-	-	-	30910.863
100	3236.4044	30889.572	0	0	0	0	-	-	-	-	30889.565
325	3237.6448	30877.738	5	152	30877.699	-0.039	4f ³ (⁴ I°)6s ($\frac{15}{2}, \frac{1}{2}$)° ₈	4f ³ (⁴ I°)6p ⁵ H ₇	35839.828	66717.513	30877.703
50	3239.1135	30863.738	0	0	0	0	-	-	-	-	30863.731
100	3243.3939	30823.007	13	378	30823.113	0.106	4f ⁴ ⁵ I ₆	4f ³ (⁴ F°)5d ⁵ G° ₆	2387.544	33210.660	30822.972
150	3245.3365	30804.558	0	0	0	0	-	-	-	-	30804.551
50	3247.1348	30787.499	0	0	0	0	-	-	-	-	30787.492
50	3247.6422	30782.689	0	0	0	0	-	-	-	-	30782.682
250	3249.4250	30765.800	5	138	30765.780	-0.02	4f ³ (⁴ I°)6s ($\frac{9}{2}, \frac{1}{2}$)° ₄	4f ³ (⁴ I°)6p ⁵ I ₄	29873.222	60638.963	30765.765
325	3254.6892	30716.041	4	60	30715.840	-0.201	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₇	4f ³ (⁴ I°)6p ⁵ K ₇	33906.143	64622.006	30716.006
150	3256.4353	30699.571	0	0	0	0	-	-	-	-	30699.564
250	3260.9144	30657.405	0	0	30657.397	-0.008	4f ³ (⁴ I°)6s ($\frac{15}{2}, \frac{1}{2}$)° ₈	4f ³ (⁴ I°)6p ⁵ I° ₇	35839.828	66497.225	30657.370
325	3261.3844	30652.987	10	336	30652.843	-0.144	4f ³ (⁴ I°)6s ($\frac{9}{2}, \frac{1}{2}$)° ₄	4f ³ (⁴ I°)6p ⁵ K ₅	29873.222	60526.067	30652.952
325	3262.3819	30643.615	6	246	30643.494	-0.121	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₇	4f ³ (⁴ I°)6p ⁵ I ₆	33906.143	64549.620	30643.580
150	3265.3849	30615.434	182	3756	30615.564	0.129	U	U	U	U	30615.399
100	3266.3072	30606.790	0	0	0	0	-	-	-	-	30606.783
50	3268.1107	30589.900	0	0	0	0	-	-	-	-	30589.893
325	3270.8078	30564.677	6	200	30564.608	-0.069	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ⁵ I ₅	32075.658	62640.266	30564.642

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Table E.1: Unclassified Nd III Line List of Dr H. M. Crosswhite Compared with the Nd-Ar PDL Line List of this Thesis (continued)

Int. (arb.)	λ (Å)	σ_{grat} (cm ⁻¹)	SNR	PDL Int. (arb.)	σ_{obs} (cm ⁻¹)	Diff. (cm ⁻¹)	L1	L2	E1 (cm ⁻¹)	E2 (cm ⁻¹)	σ_{cal} (cm ⁻¹)
150	3273.3999	30540.474	0	0	0	0	-	-	-	-	30540.467
150	3276.0972	30515.330	104	2208	30515.035	-0.295	U	U	U	U	30515.295
200	3277.1976	30505.085	0	0	0	0	-	-	-	-	30505.078
150	3279.2023	30486.436	0	0	0	0	-	-	-	-	30486.429
325	3280.2608	30476.599	8	272	30476.642	0.043	U	U	U	U	30476.564
100	3281.4212	30465.822	0	0	0	0	-	-	-	-	30465.815
100	3281.7016	30463.219	8	330	30463.224	0.005	4f ³ (⁴ F°)5d ⁵ H° ₅	4f ³ (⁴ I°)6p ⁵ I ₄	30175.737	60638.963	30463.184
325	3283.6547	30445.100	8	252	30445.008	-0.092	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ⁵ K ₆	32075.658	62520.646	30445.065
200	3287.4804	30409.672	0	0	0	0	-	-	-	-	30409.665
100	3290.1424	30385.069	0	0	0	0	-	-	-	-	30385.062
100	3291.4245	30373.233	0	0	0	0	-	-	-	-	30373.226
150	3292.4500	30363.773	0	0	0	0	-	-	-	-	30363.766
150	3293.9040	30350.371	0	0	30350.331	-0.040	4f ³ (⁴ F°)5d ⁵ H° ₅	4f ³ (⁴ I°)6p ⁵ K° ₅	30175.737	60526.067	30350.336
150	3296.0529	30330.584	3	92	30330.520	-0.064	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p ⁵ I ₅	32309.729	62640.266	30330.549
50	3298.0639	30312.090	0	0	0	0	-	-	-	-	30312.083
50	3301.0151	30284.992	6	276	30284.704	-0.287	U	U	U	U	30284.957
150	3301.9955	30276.000	0	0	0	0	-	-	-	-	30275.993
150	3304.9089	30249.311	0	0	0	0	-	-	-	-	30249.304
100	3304.9764	30248.694	0	0	0	0	-	-	-	-	30248.687
50	3305.8435	30240.760	8	192	30240.712	-0.048	U	U	U	U	30240.725
100	3306.4822	30234.918	0	0	0	0	-	-	-	-	30234.911
100	3306.6515	30233.371	8	142	30233.226	-0.145	U	U	U	U	30233.336
325	3309.0943	30211.053	5	120	30210.918	-0.135	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p ⁵ K ₆	32309.729	62520.646	30211.018
100	3313.0683	30174.816	0	0	0	0	-	-	-	-	30174.809
100	3313.2435	30173.220	0	0	0	0	-	-	-	-	30173.213
100	3313.2863	30172.831	6	176	30172.772	-0.059	U	U	U	U	30172.796
50	3314.4523	30162.216	0	0	0	0	-	-	-	-	30162.209
150	3314.6048	30160.829	0	0	0	0	-	-	-	-	30160.822
150	3314.9939	30157.289	8	168	30157.021	-0.268	U	U	U	U	30157.254
150	3321.8363	30095.172	64	2016	30095.005	-0.167	4f ⁴ ⁵ I ₈	4f ³ (² H2°)5d ³ I° ₇	5093.257	35188.278	30095.137
50	3322.2075	30091.810	9	234	30091.566	-0.244	U	U	U	U	30091.775
100	3322.9856	30084.764	0	0	0	0	-	-	-	-	30084.757
150	3327.0240	30048.247	13	398	30048.219	-0.028	U	U	U	U	30048.212
100	3328.5578	30034.402	0	0	30034.371	-0.030	4f ³ (² H2°)5d ¹ H° ₅	4f ³ (⁴ I°)6p ⁵ I° ₅	32605.894	62640.266	30034.367
100	3331.6382	30006.633	0	0	0	0	-	-	-	-	30006.626
50	3333.5900	29989.065	0	0	0	0	-	-	-	-	29989.058
50	3338.5599	29944.424	0	0	0	0	-	-	-	-	29944.417
150	3339.6328	29934.804	0	0	29934.776	-0.028	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ⁵ K° ₇	34687.231	64622.006	29934.769
250	3343.3264	29901.734	0	0	29901.676	-0.058	4f ³ (⁴ G°)5d ⁵ I° ₇	4f ³ (⁴ I°)6p ⁵ I° ₈	36890.348	66792.024	29901.699
50	3343.8208	29897.313	19	458	29897.555	0.242	U	U	U	U	29897.278
100	3347.2284	29866.877	0	0	0	0	-	-	-	-	29866.870
150	3347.7282	29862.419	0	0	29862.389	-0.029	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p ⁵ I° ₆	34687.231	64549.620	29862.385
150	3349.3897	29847.605	0	0	0	0	-	-	-	-	29847.598
150	3349.9864	29842.289	0	0	0	0	-	-	-	-	29842.282
100	3350.6731	29836.173	5	104	29836.261	0.088	U	U	U	U	29836.139
50	3352.9787	29815.658	0	0	0	0	-	-	-	-	29815.651
50	3355.5531	29792.784	3	20	29792.719	-0.065	U	U	U	U	29792.750
100	3361.6012	29739.183	0	0	0	0	-	-	-	-	29739.176
100	3365.7588	29702.449	0	0	29702.425	-0.024	4f ³ (⁴ I°)6s ($\frac{15}{2}, \frac{1}{2}$)° ₇	4f ³ (⁴ I°)6p ⁵ I° ₈	37089.599	66792.024	29702.415
325	3371.3063	29653.575	16	408	29653.520	-0.055	U	U	U	U	29653.541
100	3376.1231	29611.269	8	210	29611.011	-0.257	U	U	U	U	29611.235
150	3376.6192	29606.918	3	42	29606.889	-0.029	4f ³ (⁴ G°)5d ⁵ I° ₇	4f ³ (⁴ I°)6p ⁵ I ₇	36890.347	66497.225	29606.884
50	3384.9650	29533.923	0	0	0	0	-	-	-	-	29533.916
325	3387.0366	29515.860	65	1530	29515.781	-0.079	U	U	U	U	29515.826
50	3389.3005	29496.145	44	1112	29496.117	-0.029	4f ⁴ ⁵ I ₇	4f ³ (⁴ F°)5d ⁵ G° ₆	3714.548	33210.660	29496.111
325	3393.9744	29455.527	61	1604	29455.425	-0.102	4f ⁴ ³ K ₂₇	4f ³ (⁴ G°)5d ³ I° ₆	15153.807	44609.232	29455.493
325	3397.8765	29421.701	16	344	29421.664	-0.038	U	U	U	U	29421.667
50	3423.3347	29202.909	0	0	0	0	-	-	-	-	29202.902
325	3431.4675	29133.698	59	1422	29133.642	-0.056	4f ⁴ ³ K ₂₈	4f ³ (⁴ G°)5d ³ I° ₇	16459.136	45592.778	29133.664
100	3431.6184	29132.417	4	82	29132.408	-0.009	U	U	U	U	29132.383

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Table E.1: Unclassified Nd III Line List of Dr H. M. Crosswhite Compared with the Nd-Ar PDL Line List of this Thesis (continued)

Int. (arb.)	λ (Å)	σ_{grat} (cm ⁻¹)	SNR	PDL Int. (arb.)	σ_{obs} (cm ⁻¹)	Diff. (cm ⁻¹)	L1	L2	E1 (cm ⁻¹)	E2 (cm ⁻¹)	σ_{cal} (cm ⁻¹)
150	3433.3267	29117.922	34	718	29117.901	-0.021	4f ⁴ 5I ₇	4f ³ (⁴ F°)5d 5H° ₇	3714.548	32832.447	29117.888
50	3433.4828	29116.599	0	0	0	0	-	-	-	-	29116.592
50	3434.3613	29109.151	31	784	29109.158	0.007	4f ⁴ 5I ₇	4f ³ (² H2°)5d 1I° ₆	3714.548	32823.701	29109.117
100	3436.4615	29091.361	23	480	29091.350	-0.012	4f ⁴ 5G ₅	4f ³ (⁴ D°)5d 5F° ₄	18313.004	47404.355	29091.327
325	3442.7808	29037.965	80	2008	29037.945	-0.02	4f ⁴ 5I ₅	4f ³ (⁴ F°)5d 5H° ₅	1137.794	30175.737	29037.931
50	3443.4771	29032.094	0	0	29032.362	0.269	4f ³ (⁴ F°)6p 5G° ₅	4f ³ (⁴ I°)6d 5K° ₆	75579.962	104612.324	29032.060
325	3446.6032	29005.762	16	362	29005.771	0.009	U	U	U	U	29005.728
150	3452.6549	28954.923	7	258	28954.807	-0.116	U	U	U	U	28954.889
100	3454.3612	28940.621	6	70	28940.678	0.057	U	U	U	U	28940.587
100	3460.1548	28892.165	5	50	28892.218	0.053	U	U	U	U	28892.131
150	3476.1837	28758.945	52	1038	28758.912	-0.033	4f ⁴ 5I ₆	4f ³ (⁴ F°)5d 5H° ₆	2387.544	31146.457	28758.912
150	3477.8342	28745.298	80	1956	28745.320	0.023	4f ⁴ 5I ₄	4f ³ (⁴ F°)5d 5H° ₄	0.000	28745.307	28745.265
200	3479.7872	28729.165	16	280	28729.166	0.001	U	U	U	U	28729.132
50	3492.6720	28623.183	0	0	28622.959	-0.224	4f ³ (⁴ G°)5d 5I° ₅	4f ³ (⁴ I°)6p 5I° ₅	34017.306	62640.266	28623.150
50	3498.3461	28576.760	13	270	28576.753	-0.007	U	U	U	U	28576.727
100	3500.6080	28558.296	16	298	28558.288	-0.007	U	U	U	U	28558.263
100	3512.1826	28464.183	8	158	28464.179	-0.004	U	U	U	U	28464.150
50	3521.1588	28391.624	7	132	28391.568	-0.055	U	U	U	U	28391.591
100	3524.9519	28361.073	0	0	28361.110	0.037	4f ⁴ 5I° ₇	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₆	3714.548	32075.658	28361.040
150	3526.9456	28345.042	23	428	28345.011	-0.031	U	U	U	U	28345.009
150	3528.9137	28329.234	0	0	28329.233	-0.001	4f ³ (⁴ I°)6s ($\frac{11}{2}, \frac{1}{2}$)° ₅	4f ³ (⁴ I°)6p 5I° ₄	32309.729	60638.962	28329.201
150	3536.3589	28269.593	8	146	28269.627	0.033	U	U	U	U	28269.560
150	3537.6066	28259.623	20	440	28259.610	-0.013	4f ⁴ 5I ₅	4f ³ (² H2°)5d 3I° ₅	1137.794	29397.423	28259.590
250	3543.3128	28214.114	18	232	28214.072	-0.042	U	U	U	U	28214.081
325	3544.3756	28205.655	41	1948	28205.543	-0.112	4f ⁴ 5I ₆	4f ³ (⁴ I°)6s ($\frac{9}{2}, \frac{1}{2}$)° ₅	2387.544	30593.085	28205.622
250	3545.8636	28193.819	78	2060	28193.956	0.138	U	U	U	U	28193.786
250	3547.1034	28183.964	20	400	28183.950	-0.014	U	U	U	U	28183.931
100	3553.6124	28132.343	22	446	28132.500	0.158	U	U	U	U	28132.310
150	3555.3558	28118.548	72	1748	28118.535	-0.013	4f ⁴ 5I ₄	4f ³ (⁴ F°)5d 5D° ₃	0.000	28118.535	28118.515
150	3559.0794	28089.130	0	0	0	0	-	-	-	-	28089.123
100	3560.9790	28074.147	18	628	28074.048	-0.099	U	U	U	U	28074.114
150	3566.1989	28033.055	5	56	28033.075	0.02	4f ³ (² H2°)5d 1H° ₅	4f ³ (⁴ I°)6p 5I ₄	32605.894	60638.963	28033.022
50	3580.6182	27920.168	0	0	27920.173	0.005	4f ³ (² H2°)5d 1H° ₅	4f ³ (⁴ I°)6p 5K° ₅	32605.894	60526.067	27920.135
100	3584.0119	27893.731	0	0	27893.770	0.039	U	U	U	U	27893.698
100	3587.0709	27869.945	5	210	27869.853	-0.091	U	U	U	U	27869.912
100	3590.2164	27845.528	11	190	27845.273	-0.254	U	U	U	U	27845.495
700	3590.3324	27844.628	314	6594	27844.670	0.042	4f ⁴ 5I ₇	4f ³ (² G1°)5d 3H° ₆	3714.548	31559.217	27844.595
100	3591.7816	27833.394	0	0	27833.416	0.022	4f ³ (⁴ I°)6s ($\frac{13}{2}, \frac{1}{2}$)° ₆	4f ³ (⁴ I°)6p 5K° ₆	34687.231	62520.647	27833.361
100	3594.7386	27810.499	39	740	27810.282	-0.217	U	U	U	U	27810.466
700	3597.6287	27788.158	679	15156	27788.191	0.033	4f ⁴ 5I ₆	4f ³ (⁴ F°)5d 5H° ₅	2387.544	30175.737	27788.125
325	3599.1554	27776.371	14	242	27776.374	0.003	U	U	U	U	27776.338
100	3603.8340	27740.312	53	826	27740.377	0.065	U	U	U	U	27740.279
150	3608.4584	27704.763	22	630	27704.778	0.015	U	U	U	U	27704.730
50	3611.0435	27684.930	4	26	27684.999	0.069	U	U	U	U	27684.898
50	3611.7169	27679.768	12	216	27679.750	-0.018	U	U	U	U	27679.736
150	3612.1317	27676.590	0	0	0	0	-	-	-	-	27676.583
325	3621.1707	27607.506	1161	21148	27607.514	0.007	4f ⁴ 5I ₅	4f ³ (⁴ F°)5d 5H° ₄	1137.794	28745.307	27607.474
150	3626.1211	27569.817	5	70	27569.851	0.034	U	U	U	U	27569.785
100	3627.7631	27557.339	73	1400	27557.496	0.157	U	U	U	U	27557.307
100	3628.8384	27549.174	8	162	27549.247	0.074	U	U	U	U	27549.142
150	3643.8378	27435.774	9	312	27435.803	0.029	U	U	U	U	27435.742
700	3644.3517	27431.905	648	13330	27431.909	0.004	4f ⁴ 5I ₇	4f ³ (⁴ F°)5d 5H° ₆	3714.548	31146.457	27431.873
150	3661.6353	27302.425	0	0	27302.254	-0.171	4f ⁴ 5I° ₅	4f ³ (⁴ I°)5d 3G° ₅	1137.794	28440.047	27302.393
150	3701.2882	27009.934	416	8786	27009.879	-0.055	4f ⁴ 5I ₆	4f ³ (² H2°)5d 3I° ₅	2387.544	29397.423	27009.902
150	3708.0785	26960.474	27	898	26960.423	-0.051	U	U	U	U	26960.442
150	3722.3414	26857.173	34	550	26857.167	-0.006	U	U	U	U	26857.141
150	3767.2414	26537.082	70	1644	26537.027	-0.055	U	U	U	U	26537.051
325	3774.2086	26488.096	61	1178	26488.089	-0.007	U	U	U	U	26488.065
150	3794.6327	26345.531	60	1214	26345.467	-0.064	U	U	U	U	26345.500
50	3863.3681	25876.813	4951	89824	25876.532	-0.281	U	U	U	U	25876.782

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Table E.1: Unclassified Nd III Line List of Dr H. M. Crosswhite Compared with the Nd-Ar PDL Line List of this Thesis (continued)

Int. (arb.)	λ (Å)	σ_{grat} (cm ⁻¹)	SNR	PDL Int. (arb.)	σ_{obs} (cm ⁻¹)	Diff. (cm ⁻¹)	L1	L2	E1 (cm ⁻¹)	E2 (cm ⁻¹)	σ_{cal} (cm ⁻¹)
100	3920.1639	25501.916	28	1298	25501.893	-0.022	U	U	U	U	25501.885
150	3998.4683	25002.507	30	1804	25002.418	-0.09	4f ⁴ 5I ₅	4f ³ (⁴ I°)5d ³ G° ₄	1137.794	26140.225	25002.477
150	4012.7965	24913.234	8	670	24913.329	0.095	U	U	U	U	24913.204
150	4016.9010	24887.778	5	138	24887.752	-0.027	U	U	U	U	24887.748
150	4030.9636	24800.956	12	394	24800.886	-0.069	4f ⁴ ³ K2 ₈	4f ³ (² K°)5d ³ I° ₇	16459.136	41260.027	24800.926
100	4048.4914	24693.583	0	0	0	0	-	-	-	-	24693.576
150	4059.7968	24624.820	0	0	0	0	-	-	-	-	24624.813
150	4076.6271	24523.159	16	1072	24523.147	-0.012	U	U	U	U	24523.129
325	4084.5991	24475.297	35	1848	24475.392	0.095	U	U	U	U	24475.267
100	4116.3530	24286.497	125	6290	24286.654	0.158	U	U	U	U	24286.468
150	4118.5399	24273.601	9	304	24273.560	-0.041	U	U	U	U	24273.572
150	4141.0644	24141.572	0	0	0	0	-	-	-	-	24141.565
150	4144.7899	24119.873	6	164	24120.073	0.200	U	U	U	U	24119.844
100	4145.4985	24115.750	2	108	24115.764	0.014	U	U	U	U	24115.721
100	4147.9434	24101.536	37	1600	24101.409	-0.127	U	U	U	U	24101.507
100	4156.1627	24053.874	13	750	24053.841	-0.032	4f ⁴ ⁵ F ₄	4f ³ (⁴ G°)5d ⁵ H° ₄	12181.327	36235.179	24053.845
325	4180.9461	23911.292	14	1518	23911.004	-0.288	U	U	U	U	23911.263
150	4182.1412	23904.459	15	612	23904.473	0.014	4f ⁴ ³ K2 ₇	4f ³ (⁴ G°)5d ⁵ H° ₆	15153.807	39058.274	23904.430
100	4184.4608	23891.209	48	1960	23891.226	0.018	4f ⁴ ⁵ I ₄	4f ³ (⁴ I°)5d ³ G° ₃	0.000	23891.226	23891.180
150	4187.7321	23872.546	16	888	23872.579	0.033	U	U	U	U	23872.517
100	4190.6544	23855.899	0	0	0	0	-	-	-	-	23855.892
100	4204.0664	23779.794	0	0	0	0	-	-	-	-	23779.787
150	4210.5938	23742.931	7	860	23742.878	-0.053	U	U	U	U	23742.902
100	4211.0029	23740.624	0	0	23740.619	-0.006	4f ⁴ ⁵ I° ₅	4f ³ (⁴ I°)5d ⁵ G° ₅	1137.794	24878.412	23740.595
50	4213.3558	23727.367	0	0	23727.364	-0.003	4f ⁴ ⁵ I° ₇	4f ³ (⁴ I°)5d ³ K° ₈	3714.548	27441.911	23727.338
150	4221.8277	23679.754	0	0	0	0	-	-	-	-	23679.747
150	4222.8437	23674.057	5	194	23673.933	-0.124	U	U	U	U	23674.028
50	4233.5939	23613.944	0	0	0	0	-	-	-	-	23613.937
150	4233.7955	23612.819	25	1378	23612.642	-0.177	U	U	U	U	23612.790
150	4235.1702	23605.155	81	4086	23605.335	0.181	U	U	U	U	23605.126
150	4235.7588	23601.875	13	742	23601.807	-0.068	U	U	U	U	23601.846
50	4239.6003	23580.490	0	0	0	0	-	-	-	-	23580.483
50	4246.5273	23542.025	0	0	0	0	-	-	-	-	23542.018
150	4248.8370	23529.228	7	258	23529.245	0.017	U	U	U	U	23529.199
50	4248.9708	23528.487	0	0	23528.482	-0.005	4f ⁴ ³ K2° ₆	4f ³ (⁴ G°)5d ⁵ H° ₅	14064.277	37592.759	23528.458
100	4249.8655	23523.534	0	0	0	0	-	-	-	-	23523.527
150	4266.1824	23433.565	10	370	23433.301	-0.263	U	U	U	U	23433.536
150	4273.9846	23390.788	21	878	23390.922	0.135	U	U	U	U	23390.759
100	4275.8956	23380.334	13	380	23380.328	-0.006	U	U	U	U	23380.305
150	4279.7383	23359.341	5	496	23359.236	-0.105	U	U	U	U	23359.312
150	4281.5691	23349.353	0	0	0	0	-	-	-	-	23349.346
250	4290.8108	23299.063	23	996	23299.045	-0.019	U	U	U	U	23299.034
150	4291.8146	23293.614	12	512	23293.645	0.031	U	U	U	U	23293.585
50	4295.5720	23273.239	0	0	0	0	-	-	-	-	23273.232
100	4336.3041	23054.631	0	0	0	0	-	-	-	-	23054.624
50	4367.7969	22888.405	0	0	0	0	-	-	-	-	22888.398
150	4406.1470	22689.193	9	360	22689.205	0.012	U	U	U	U	22689.165
325	4414.3002	22647.287	26	1240	22647.292	0.005	4f ⁴ ⁵ I ₆	4f ³ (⁴ I°)5d ³ H° ₆	2387.544	25034.832	22647.259
150	4415.5947	22640.648	2	52	22640.673	0.025	U	U	U	U	22640.620
150	4429.9458	22567.303	29	1530	22567.230	-0.073	U	U	U	U	22567.275
50	4433.7874	22547.750	6	196	22547.910	0.160	U	U	U	U	22547.722
150	4442.0536	22505.792	8	258	22505.795	0.003	U	U	U	U	22505.764
100	4445.9935	22485.848	6	276	22485.973	0.124	U	U	U	U	22485.820
100	4446.2335	22484.635	5	298	22484.576	-0.058	U	U	U	U	22484.607
50	4449.3464	22468.904	0	0	0	0	-	-	-	-	22468.897
150	4473.2872	22348.654	111	4638	22348.654	0.001	4f ⁴ ⁵ I ₈	4f ³ (⁴ I°)5d ³ K° ₈	5093.257	27441.911	22348.626
150	4483.4350	22298.071	16	610	22298.072	0.002	U	U	U	U	22298.043
150	4500.4367	22213.835	26	1178	22214.012	0.177	U	U	U	U	22213.807
150	4507.5333	22178.862	13	488	22178.877	0.015	4f ⁴ ⁵ F ₃	4f ³ (⁴ F°)5d ⁵ F° ₄	11424.605	33603.488	22178.835
100	4508.3785	22174.704	3	152	22174.736	0.032	U	U	U	U	22174.677

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Table E.1: Unclassified Nd III Line List of Dr H. M. Crosswhite Compared with the Nd-Ar PDL Line List of this Thesis (continued)

Int. (arb.)	λ (Å)	σ_{grat} (cm ⁻¹)	SNR	PDL Int. (arb.)	σ_{obs} (cm ⁻¹)	Diff. (cm ⁻¹)	L1	L2	E1 (cm ⁻¹)	E2 (cm ⁻¹)	σ_{cal} (cm ⁻¹)
150	4514.0790	22146.702	116	3840	22146.486	-0.216	U	U	U	U	22146.675
150	4514.6879	22143.715	21	708	22143.722	0.007	U	U	U	U	22143.688
150	4515.4042	22140.202	24	976	22140.186	-0.016	U	U	U	U	22140.175
150	4517.1934	22131.433	26	800	22131.429	-0.004	4f ⁴ 5F ₂	4f ³ (⁴ S°)5d 5D° ₂	10773.962	32905.369	22131.406
100	4522.2714	22106.582	10	732	22106.569	-0.014	U	U	U	U	22106.555
150	4524.7322	22094.560	0	0	0	0	-	-	-	-	22094.553
100	4533.4033	22052.300	20	466	22052.261	-0.039	U	U	U	U	22052.273
150	4534.9413	22044.821	36	1318	22044.820	-0.001	U	U	U	U	22044.794
150	4551.1525	21966.299	18	666	21966.307	0.008	U	U	U	U	21966.272
150	4557.4709	21935.845	7	294	21935.813	-0.033	4f ⁴ 3K ₂₇	4f ³ (⁴ I°)6s (¹⁵ / ₂ , ¹ / ₂)° ₇	15153.807	37089.599	21935.818
150	4558.1680	21932.491	13	772	21932.495	0.004	U	U	U	U	21932.464
50	4563.1070	21908.752	0	0	0	0	-	-	-	-	21908.745
50	4563.3953	21907.368	0	0	0	0	-	-	-	-	21907.361
50	4563.8781	21905.050	0	0	0	0	-	-	-	-	21905.043
150	4570.6596	21872.550	75	2528	21872.654	0.104	4f ⁴ 5I ₅	4f ³ (⁴ I°)5d 5G° ₄	1137.794	23010.450	21872.523
150	4584.5123	21806.460	12	612	21806.469	0.008	U	U	U	U	21806.433
150	4599.2552	21736.561	3	40	21736.505	-0.056	4f ⁴ 3K ₂₇	4f ³ (⁴ G°)5d 5I° ₇	15153.807	36890.347	21736.534
50	4607.7057	21696.697	5	332	21696.610	-0.087	U	U	U	U	21696.670
150	4607.8264	21696.129	5	318	21696.100	-0.029	U	U	U	U	21696.102
50	4613.5943	21669.005	0	0	0	0	-	-	-	-	21668.998
50	4619.3789	21641.870	8	186	21641.656	-0.214	U	U	U	U	21641.843
50	4621.7407	21630.811	0	0	0	0	-	-	-	-	21630.804
150	4621.9963	21629.615	258	10102	21629.890	0.275	U	U	U	U	21629.588
100	4624.9646	21615.733	73	2882	21615.679	-0.054	4f ⁴ 5I ₆	4f ³ (⁴ I°)5d 3I° ₇	2387.544	24003.225	21615.706
100	4626.3129	21609.433	3	184	21609.256	-0.177	U	U	U	U	21609.406
325	4627.2544	21605.037	33	1670	21605.029	-0.008	4f ⁴ 5I ₇	4f ³ (⁴ I°)5d 3K° ₇	3714.548	25319.579	21605.010
325	4628.2479	21600.399	49	1806	21600.392	-0.007	4f ⁴ 5F ₂	4f ³ (⁴ S°)5d 5D° ₁	10773.962	32374.355	21600.372
150	4642.9726	21531.897	25	1136	21531.872	-0.024	U	U	U	U	21531.870
50	4646.1404	21517.216	5	162	21517.206	-0.011	U	U	U	U	21517.189
150	4651.6087	21491.921	91	4618	21491.877	-0.044	4f ⁴ 5I ₄	4f ³ (⁴ I°)5d 3H° ₄	0.000	21491.882	21491.894
150	4654.0140	21480.814	72	2660	21480.764	-0.05	4f ⁴ 5F ₃	4f ³ (⁴ S°)5d 5D° ₂	11424.605	32905.369	21480.787
150	4654.3115	21479.441	154	4992	21479.404	-0.037	4f ⁴ 5I ₄	4f ³ (⁴ I°)5d 5G° ₃	0.000	21479.404	21479.414
50	4656.8284	21467.832	0	0	21467.794	-0.038	4f ³ (⁴ G°)5d 5H° ₆	4f ³ (⁴ I°)6p 5K° ₅	39058.274	60526.067	21467.805
50	4663.0482	21439.198	6	266	21439.014	-0.184	U	U	U	U	21439.171
150	4666.7484	21422.199	38	1982	21422.159	-0.04	4f ⁴ 5F ₄	4f ³ (⁴ F°)5d 5F° ₄	12181.327	33603.488	21422.172
50	4684.1803	21342.479	4	86	21342.554	0.075	U	U	U	U	21342.452
100	4688.6899	21321.952	4	212	21321.999	0.047	U	U	U	U	21321.925
150	4689.0517	21320.307	77	2444	21320.273	-0.034	4f ⁴ 5I ₇	4f ³ (⁴ I°)5d 3H° ₆	3714.548	25034.832	21320.280
150	4695.4145	21291.416	59	1582	21291.403	-0.013	U	U	U	U	21291.389
100	4696.2051	21287.832	9	296	21287.791	-0.040	U	U	U	U	21287.805
150	4711.2926	21219.660	221	5484	21219.496	-0.165	4f ⁴ 5F ₄	4f ³ (⁴ S°)5d 5D° ₃	12181.327	33400.822	21219.633
150	4713.4954	21209.744	212	4954	21209.599	-0.145	4f ⁴ 5F ₅	4f ³ (⁴ S°)5d 5D° ₄	13210.278	34419.877	21209.717
150	4718.4238	21187.590	15	658	21187.472	-0.119	U	U	U	U	21187.563
150	4720.7398	21177.196	20	572	21177.161	-0.035	U	U	U	U	21177.169
100	4722.8456	21167.754	14	580	21167.729	-0.024	4f ⁴ 5G ₃	4f ³ (² H ² °)5d 1G° ₄	15349.601	36517.350	21167.727
50	4726.8754	21149.708	189	4552	21149.741	0.034	U	U	U	U	21149.681
50	4727.6310	21146.327	18	380	21146.289	-0.039	4f ⁴ 5G ₄	4f ³ (⁴ G°)5d 5G° ₅	16831.344	37977.641	21146.300
50	4733.5494	21119.888	4	28	21119.913	0.025	U	U	U	U	21119.861
150	4734.7311	21114.617	91	1892	21114.573	-0.044	4f ⁴ 5F ₂	4f ³ (⁴ F°)5d 5F° ₂	10773.962	31888.511	21114.590
100	4740.2194	21090.171	12	398	21090.151	-0.02	4f ⁴ 3K ₂₆	4f ³ (⁴ F°)5d 3H° ₆	14064.277	35154.437	21090.145
100	4740.6637	21088.194	26	534	21088.184	-0.010	U	U	U	U	21088.168
325	4741.0145	21086.634	9	278	21086.689	0.055	U	U	U	U	21086.608
325	4745.9835	21064.557	139	2680	21064.495	-0.062	4f ⁴ 5F ₃	4f ³ (⁴ F°)5d 5F° ₃	11424.605	32489.101	21064.531
150	4747.4125	21058.216	19	462	21058.217	0.001	U	U	U	U	21058.190
100	4757.6755	21012.791	13	628	21012.705	-0.086	U	U	U	U	21012.765
150	4759.4993	21004.740	492	8822	21004.649	-0.091	4f ⁴ 5I ₈	4f ³ (⁴ I°)5d 5H° ₇	5093.257	26097.906	21004.714
150	4762.4196	20991.860	7	134	20991.881	0.021	U	U	U	U	20991.834
100	4765.2610	20979.343	49	902	20979.331	-0.012	U	U	U	U	20979.317
150	4769.6102	20960.213	264	3982	20960.177	-0.036	4f ⁴ 5I ₆	4f ³ (⁴ I°)5d 3H° ₅	2387.544	23347.721	20960.187
150	4770.8845	20954.615	63	1186	20954.592	-0.023	4f ⁴ 5F ₄	4f ³ (² H ² °)5d 3G° ₄	12181.327	33135.917	20954.589

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Table E.1: Unclassified Nd III Line List of Dr H. M. Crosswhite Compared with the Nd-Ar PDL Line List of this Thesis (continued)

Int. (arb.)	λ (Å)	σ_{grat} (cm ⁻¹)	SNR	PDL Int. (arb.)	σ_{obs} (cm ⁻¹)	Diff. (cm ⁻¹)	L1	L2	E1 (cm ⁻¹)	E2 (cm ⁻¹)	σ_{cal} (cm ⁻¹)
50	4774.6846	20937.938	6	110	20937.848	-0.090	U	U	U	U	20937.912
150	4777.6056	20925.136	31	562	20925.053	-0.083	U	U	U	U	20925.110
50	4786.2033	20887.548	9	128	20887.434	-0.114	U	U	U	U	20887.522
100	4788.4228	20877.867	167	2524	20877.711	-0.156	4f ⁴ 5I ₇	4f ³ (⁴ I°)5d 5I° ₈	3714.548	24592.259	20877.841
50	4789.2724	20874.163	24	396	20874.031	-0.132	U	U	U	U	20874.137
50	4794.2239	20852.604	53	922	20852.473	-0.132	U	U	U	U	20852.578
100	4796.4650	20842.861	326	5276	20842.729	-0.133	4f ⁴ 5I ₅	4f ³ (⁴ I°)5d 5I° ₆	1137.794	21980.522	20842.835
100	4799.8874	20828.000	86	1488	20827.903	-0.098	U	U	U	U	20827.974
50	4800.6661	20824.622	0	0	0	0	-	-	-	-	20824.615
50	4804.7188	20807.057	19	294	20807.075	0.019	4f ⁴ 5F ₅	4f ³ (⁴ G°)5d 5I° ₅	13210.278	34017.306	20807.031
150	4810.3694	20782.616	76	1330	20782.616	0.001	4f ⁴ 5I ₇	4f ³ (⁴ I°)5d 3L° ₇	3714.548	24497.165	20782.590
150	4821.1124	20736.306	50	770	20736.317	0.011	U	U	U	U	20736.280
100	4821.9858	20732.550	65	794	20732.528	-0.022	4f ⁴ 5I ₆	4f ³ (⁴ I°)5d 3K° ₆	2387.544	23120.073	20732.524
50	4838.2175	20662.996	17	436	20663.136	0.141	U	U	U	U	20662.970
100	4845.8354	20630.513	16	158	20630.414	-0.099	4f ⁴ 3K ₂₈	4f ³ (⁴ I°)6s ($\frac{15}{2}, \frac{1}{2}$)° ₇	16459.136	37089.599	20630.487
50	4927.4841	20288.669	1949	22590	20288.679	0.01	4f ⁴ 5I ₇	4f ³ (⁴ I°)5d 3I° ₇	3714.548	24003.225	20288.643
150	4942.6733	20226.321	555	7818	20226.325	0.004	4f ⁴ 5I ₈	4f ³ (⁴ I°)5d 3K° ₇	5093.257	25319.579	20226.295
325	5102.4302	19593.044	3871	42290	19592.984	-0.06	4f ⁴ 5I ₆	4f ³ (⁴ I°)5d 5I° ₆	2387.544	21980.522	19593.019
325	5127.0087	19499.117	4150	49616	19499.003	-0.114	4f ⁴ 5I ₈	4f ³ (⁴ I°)5d 5I° ₈	5093.257	24592.259	19499.092
50	5152.2924	19403.431	110	1258	19403.600	0.169	U	U	U	U	19403.406
150	5193.0613	19251.103	1443	18180	19251.201	0.098	4f ⁴ 5I ₅	4f ³ (⁴ I°)5d 5H° ₄	1137.794	20388.995	19251.078
325	5203.9058	19210.986	4868	57016	19210.946	-0.04	4f ⁴ 5I ₅	4f ³ (⁴ I°)5d 5I° ₅	1137.794	20348.742	19210.961
325	5264.9589	18988.216	2366	35920	18988.231	0.015	4f ⁴ 5I ₇	4f ³ (⁴ I°)5d 5I° ₇	3714.548	22702.777	18988.191
150	5294.1062	18883.675	4677	68190	18883.669	-0.007	4f ⁴ 5I ₄	4f ³ (⁴ I°)5d 5I° ₄	0.000	18883.669	18883.651
150	5368.5814	18621.716	29	590	18621.643	-0.073	U	U	U	U	18621.692
50	5400.0792	18513.100	9	220	18513.080	-0.020	U	U	U	U	18513.076
50	5530.8599	18075.351	124	2868	18075.412	0.062	4f ⁴ 3K ₂₈	4f ³ (² H2°)5d 3K° ₈	16459.136	34534.549	18075.327
150	5705.2382	17522.890	23	936	17522.913	0.022	U	U	U	U	17522.867
150	5844.9990	17103.901	310	10944	17103.858	-0.044	4f ⁴ 5I ₈	4f ³ (⁴ I°)5d 5K° ₉	5093.257	22197.115	17103.878
100	6141.0521	16279.349	5	274	16279.236	-0.114	U	U	U	U	16279.327
200	6145.0208	16268.835	341	13220	16268.729	-0.107	4f ⁴ 5I ₆	4f ³ (⁴ I°)5d 5K° ₇	2387.544	18656.272	16268.813
150	6273.6734	15935.217	21	1356	15935.094	-0.123	U	U	U	U	15935.195
150	6282.5665	15912.661	26	2730	15912.750	0.089	U	U	U	U	15912.639
50	6327.2200	15800.360	378	16330	15800.273	-0.087	4f ⁴ 5I ₅	4f ³ (⁴ I°)5d 5K° ₆	1137.794	16938.068	15800.338
150	6361.0420	15716.350	11	830	15716.194	-0.155	U	U	U	U	15716.328
100	6363.3298	15710.699	0	0	0	0	-	-	-	-	15710.692
150	6385.4094	15656.375	15	754	15656.335	-0.040	U	U	U	U	15656.353
150	6550.2121	15262.465	312	20566	15262.437	-0.028	4f ⁴ 5I ₄	4f ³ (⁴ I°)5d 5K° ₅	0.000	15262.437	15262.444
50	6748.7410	14813.489	4	266	14813.475	-0.014	U	U	U	U	14813.468
50	7225.3275	13836.390	0	0	0	0	-	-	-	-	13836.383
50	7258.1658	13773.790	4	218	13773.564	-0.226	U	U	U	U	13773.770
150	7427.2534	13460.220	11	2526	13460.188	-0.032	4f ⁴ 5F ₅	4f ³ (⁴ I°)5d 5G° ₆	13210.278	26670.461	13460.200
50	7432.5212	13450.680	4	510	13450.648	-0.032	U	U	U	U	13450.660
50	8454.6726	11824.530	0	0	11824.554	0.024	4f ⁴ 5F° ₅	4f ³ (⁴ I°)5d 3H° ₆	13210.278	25034.832	11824.512

150	1894.7284
150	1994.2518
150	2004.7459
150	2008.9480
325	2011.7730
325	2013.4369
325	2013.5948
325	2017.7393
150	2019.5911
150	2021.9348
325	2026.3139
150	2028.5096
700	2032.1669
325	2032.3032
50	2055.5863
150	2056.1505
150	2056.3441
100	2058.5598
150	2058.6856
50	2062.9457
150	2063.3889
325	2065.3487
100	2066.0476
100	2066.0993
50	2067.0424
100	2067.8580
325	2070.5762
325	2085.1063
150	2087.3764
150	2087.9275
150	2091.5798
700	2107.1249
150	2107.4001
150	2108.4691
325	2117.5786
150	2117.7569
50	140.3042
150	2154.5736
325	2155.3687
150	2156.0124
150	2159.9193
150	2160.1787
150	2162.5438
150	2162.6826
150	2164.5914
150	2164.7645
150	2166.2281
325	2166.5235
150	2167.8011
150	2168.2546
150	2168.6842
700	2169.1576
325	2170.5577
150	2172.8857
700	2174.8495
700	2176.4310
150	2177.4042
325	2178.2798
150	2178.9355
150	2180.5435

Ndm → Crosswhite.

0.62 : 4569.246

4516.652 - 2.46

4500.543

4940.583 con →
high excid.

8737.434 0.7

8632.347

8533.964

8341.78

6626.688

pub/get/cowley

udata.inc
con

4160.657 - 190

4145.137 - 2.11

4927.86

0.62 → 0.69
5.5 → 4.5

325	2181.0213
1000	2184.5810
150	2184.9958
150	2185.4713
150	2186.3232
325	2187.3896
150	2188.8423
150	2189.0380
150	2192.3025
1000	2193.1300
700	2193.8407
150	2198.8529
150	2199.3192
150	2202.6527
150	2202.9588
150	201.6941
150	2203.0907
325	2204.2052
150	2208.5865
150	2220.7604
150	2223.8371
150	2228.3245
150	2228.3857
325	2229.1749
150	2230.2517
325	2233.7086
150	2234.1449
700	2234.7270
325	2235.0334
325	2237.3124
325	2238.4341
150	2238.6611
150	2239.5575
325	2240.0829
150	2240.1882
700	2241.7085
325	2242.2065
150	2243.1033
325	2243.7322
325	2244.0037
150	2244.0965
325	2246.4052
150	2247.0231
150	2247.9426
150	2248.4583
150	2248.5796
325	2248.6812
325	2249.0742
325	2249.5665
325	2249.8519
700	2250.8453
150	2251.3630
700	2253.4432
150	2253.5540
150	2253.8418
150	2254.1127
150	2254.3772
150	2257.0269
325	2257.1886
150	2258.1357

150	2258.4834
325	2258.6943
150	2259.2285
150	2259.8150
150	2260.2198
325	2260.4960
150	2261.1706
100	2261.4877
150	2262.7487
150	2262.8980
150	2263.3626
150	2264.0158
150	2266.1699
700	2267.3034
150	2267.7295
150	2269.3855
150	2269.6963
150	2269.8234
150	2269.9499
150	2270.5515
150	2270.9604
150	2272.6216
150	2278.7515
150	2279.2762
325	2279.5358
150	2279.7665
150	2279.8177
150	2282.6838
325	2282.9095
150	2285.0531
150	2285.4807
150	2285.7967
150	2286.3689
325	2287.0727
325	2292.6161
150	2301.1038
325	2301.5974
150	2306.6790
325	2307.0657
325	2310.7660
700	2314.7566
325	2316.3725
150	2316.6391
150	2317.3454
325	2323.3539
325	2323.8567
325	2331.8981
150	2333.4123
150	2337.6708
150	2340.4197
150	2348.4008
150	2349.2382
150	2358.5469
150	2359.1649
150	2363.8144
150	2373.1476
150	2382.7954
150	2389.8555
150	2394.1737
150	2396.0716

150	2398.3503
150	2429.4914
325	2435.5594
150	2439.7221
700	2466.7740
150	2479.8779
150	2481.3738
325	2500.2221
150	2504.6866
150	2505.0546
150	2508.1225
325	2510.5090
150	2513.2741
150	2513.4308
150	2516.4400
150	2517.8712
150	2519.5048
150	2522.5941
150	2522.9811
150	2534.1802
700	2535.6768
150	2536.7589
150	2541.1895
150	2542.4018
150	2545.3453
150	2552.8871
150	2618.7008
150	2629.1690
325	2634.5840
50	2754.2956
50	2764.1487
50	2771.9483
50	2772.6263
50	2788.4149
50	2793.2923
50	2797.6006
50	2802.2620
50	2805.1869
50	2806.0962
50	2806.5222
50	2811.0231
50	2815.7488
50	2821.2312
50	2823.0834
50	2823.1232
50	2823.8228
50	2825.6567
150	2828.5236
50	2830.9776
50	2831.5187
50	2832.2920
100	2834.2492
100	2838.6793
50	2838.7385
150	2839.6502
50	2848.3770
50	2864.3417
50	2868.0291
150	2871.4328
50	2876.0459

150	2883.7965
50	2884.3607
50	2884.6290
50	2885.3058
50	2885.6471
150	2885.8321
150	2887.5920
50	2888.7792
50	2889.2179
50	2894.1206
50	2899.4593
150	2899.5803
100	2899.6410
200	2899.8366
100	2902.6245
200	2903.5391
200	2904.2966
100	2906.1202
325	2906.4158
200	2908.1377
200	2908.5984
50	2908.9663
700	2914.4989
200	2917.2500
50	2917.6446
50	2918.0759
50	2921.4718
150	2923.3634
50	2924.3116
150	2928.0788
250	2928.6478
50	2931.9810
50	2932.1703
50	2934.4406
50	2937.1026
50	2938.4638
150	2938.5024
150	2938.5438
150	2939.5536
50	2941.1770
200	2943.5059
325	2945.8866
50	2945.9851
325	2946.6757
325	2946.7162
50	2953.7444
325	2955.9495
50	2958.6130
200	2958.7877
50	2963.2908
50	2966.8539
325	2969.9886
150	2970.8297
325	2977.9571
325	2988.1673
50	2993.1929
150	3034.2021
150	3039.9301
150	3057.3384
100	3057.3884

150	3067.4317	67.46	53.5	733.9
150	3071.6462	.61 Ce II, perfect fit without Nd III		
100	3078.4944	78.45	25	81. Fe I 78.43, Fe II 78.44
100	3079.5510	еск, no blended with strong Nd II, Co I blend		
100	3095.1229	blend with strong 2nd 95.07		
50	3097.4566	blend Fe II 97.45		
100	3119.4922	19.50 strongly blended with Fe I 19.49 (but room exist!)		
150	3121.1391	V II 21.14		
150	3124.4475	24.43 $\geq 12.3 \rightarrow$ good weak line (25)		
150	3130.3227	30.34 Ce II		
325	3131.1820	in strong blend with Tm II 31.25		
325	3135.5094	$\rightarrow$ no еск, no memory 22 common sun II Ce II 35.49		
150	3140.2837	40.29 32 (20)		
100	3140.9260	40.95 25.3 slightly blended with V II 40.93 (21.3)		
50	3147.2390	blended		
50	3149.1962	defect		
50	3159.4139	unknown blend		
150	3163.2624	63.21 19.5 63.27 $\rightarrow$ weaker line, may be		
50	3165.8271	blend		
50	3166.1917	66.13 13.5 $\rightarrow$ or. cadans gungusone		
150	3171.3863	71.36 blended with Fe I 71.35		
50	3176.3349	76.33 22.3 (33)		
150	3176.9026	76.90 38 (42)		
50	3182.3607	$\rightarrow$ no line at all 82.53 Ce II		
100	3182.4063	very weak		
250	3182.6427	82.67 19 - V II 82.67 + Ce II 82.66		
50	3189.9932	89.97 23.0 чутк да. Mn I, Fe I		
150	3196.6363	96.70 15.29		
200	3200.3447	V II 3200.27, Fe I 3200.32		
250	3201.6450	чтo-то еск, но в бленде, воспримет от галыко наводе		
150	3203.2076	чтo-то еск, но в бленде.		
150	3212.6967	12.69 Dy II 12.68 + Ti II 12.70		
100	3215.6679	чтo-то еск, но бленда. Nb II 15.59		
50	3219.8191	19.80 Fe I		
50	3220.4467	20.44 Dy II		
50	3220.8771	20.89 Ce II		
50	3225.7460	25.79 25.78 Fe I		
100	3228.0881	28.08 Mn I		
325	3229.8464	опред, еск, м.д. селенка, но бленда. Ag II 29.94-37		
50	3231.1991	Геленр, Ce II 21.24 $\rightarrow$ нет		
100	3232.9704	да. Ni I 32.93 нескы ниско скарот		
100	3233.4982	б бленда		
100	3234.1744	бленда		
100	3236.4044	Nb II 36.40		
325	3237.6448	37.69 18.5 41		
50	3239.1135	нет		
100	3243.3939	43.37 Ce II		
150	3245.3365	нет миним		
50	3247.1348	бленда		
50	3247.6422	бленда		
250	3249.4250	Ce II 49.427		
325	3254.6892	вск, но бленду разделить наводе V II 54.76		
150	3256.4353	56.42 $\rightarrow$ бленда ~ 24 W		
250	3260.9144	Ce II 60.97		
325	3261.3844	61.38 64		
325	3262.3819	62.39 ~ 24		
150	3265.3849	Nd II 65.366 + Ce II 65.42		
100	3266.3072	бленда		
50	3268.1107	68.10 ~ 22 (30) но да.		
325	3270.8078	70.80 44 да. чутк Mn I 70.78 + Mn II 70.78		

62.70

988
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150	3273.3999	сеп. 6 д. сеп.
150	3276.0972	46.12 VII
200	3277.1976	47.19 Fe. NiT Nd
150	3279.2023	сеп. м. д. сеп., но в кр. сеп. сеп.
325	3280.2608	80.22 ErII + 80.26 FeI
100	3281.4212	81.48, 18 p.p.p.p. NdII 81.48
100	3281.7016	81.75 d. d. d. 81.75 + VII. 81.75
325	3283.6547	2387.60 - 3283.60 83.40 Сильно д. сеп. с CeII 83.68 и CoI 83.76
200	3287.4804	м. д. сеп., но м. д. не сеп.
100	3290.1424	90.06 28 ? 280 280 ?
100	3291.4245	91.46 (15) и 91.47 (9)
150	3292.4500	92.47 (10)
150	3293.9040	→ в сеп. сеп. с сеп. 93.88
150	3296.0529	96.05 (14) м. д. сеп. VII 96.05 (по раск. сеп., 28 д. сеп.)
50	3298.0639	д. сеп.
50	3301.0151	01.06 (19)
150	3301.9955	в сеп. сеп. с сеп.
150	3304.9089	нет
100	3304.9764	м. д. сеп.
50	3305.8435	05.85 (4) (19)
100	3306.4822	FeI 3306.48
100	3306.6515	CeII 06.65
325	3309.0943	09.12 (28) д. сеп. CeII 09.13
100	3313.0683	
100	3313.2435	
100	3313.2863	нет
50	3314.4523	14.43 ErII
150	3314.6048	14.62 → трудно сеп.
150	3314.9939	14.96 ErII 14.94 (по раск.)
150	3321.8363	21.85 EuII
50	3322.2075	22.21 CoI
100	3322.9856	→ 22.97 + TiII 22.94, 22.99
150	3327.0240	27.02 → трудно сеп. с CoI 26.99
100	3328.5578	28.55 (16) 28.55 CeII
100	3331.6382	31.64 FeI 31.64
50	3333.5900	33.54 ~ 38
50	3338.5599	38.61 ~ 38 FeI 38.62
150	3339.6328	39.62 ~ 30 ок
250	3343.3264	сеп. TiII, Cu
50	3343.8208	28.82
100	3347.2284	м. д. сеп. SmII 47.30
150	3347.7282	ErII 47.73
150	3349.3897	CrII 49.35, TiII 49.41
150	3349.9864	CeII 49.98
100	3350.6731	50.68 24 CeII 50.68
50	3352.9787	CeII 52.98
50	3355.5531	55.58 (15)
100	3361.6012	no line (between two other lines)
100	3365.7588	65.76 NiI → not needed NdII
325	3371.3063	71.30 (29)
100	3376.1231	76.09 ErII
150	3376.6192	76.61 DyII
50	3384.9650	85.00 TiII + 85.01 DyII
325	3387.0366	87.04 (31) CoI 87.06
50	3389.3005	89.32 SmII
325	3393.9774	93.92 CeII + 93.98 DyII
325	3397.8765	97.88 (14)
50	3423.3347	no line
325	3431.4675	31.48 → CeII 31.49
100	3431.6184	NiI 31.62

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✓ 150	3433.3267	.35 3714.9 - 2732.6	Strongly blended with Cr II	33.28
50	3433.4828	no line	N I	
50	3434.3613	34.37 Dy II		
100	3436.4615	36.46 23		
325	3442.7808	42.48 48		
50	3443.4771	43.47 Dy II		
325	3446.6032	46.61 16	→ blended with Ni I and Ca II	32.02
150	3452.6549	52.65 ~ 42		
100	3454.3612	54.38 Ce III (38)	Na II 54.36	
100	3460.1548	60.16 Ce II		
150	3476.1837	3476.19 seen 2388 - 31146.429	46.19 (34)	
+ ✓ 150	3477.8342	- 20 - 28745.3	77.84 50	81. Co I 77.85, Fe I 77.85
200	3479.7872	49.48 ~ 31		
50	3492.6720	no line	Sm II 92.62	
50	3498.3461	98.34 ~ 15		
100	3500.6080	00.60 → 170-10	сerb, no tripple group	
100	3512.1826	12.22 Gd II		
50	3521.1588	21.16 →	сerb, also good, but blended with Ni I and Ca II	
100	3524.9519	24.91 Er II + 24.93 Dy II		
48 24.10 50 mm. 150	3526.9456	26.90 Dy II		
47 28.48 150	3528.9137	28.90 Dy II		
150	3536.3589	36.35 ~ 28		
✓ 150	3537.6066	Blended with strong Dy II	37.66 37.61	
250	3543.3128	34 Nd II		
325	3544.3756	44.38 → 48	дленга с Dy II 44.35 (30000-10 Dy II отлит и отлит)	
250	3545.8636	45.90 →	в смеске дленга Ce II 45.90	
47.55 → 0.1 mm. 250	3547.1034	44.10 17		
100	3553.6124	no line		
✓ 150	3555.3558	→ сerb, blend	55.35 36	
150	3559.0794	59.10 Sm II		
100	3560.9790	no line		
150	3566.1989	66.17 V II		
80.76 → хор. 50	3580.6182	80.62 Gd II		
81.42 → хор. 100	3584.0119	83.98 28		
100	3587.0709	нет миним, 20-10 групп (меньше блан)		
100	3590.2164	→ 170-10, 10-10, 10-10	сerb, 90.21 ~ 10 Ce II	
✓ 700	3590.3324	сerb, blend	30000, 90.33 59	
100	3591.7816	91.72 Sm II, 91.81 Dy II, 91.45 Co I		
100	3594.7386	94.74 18		
✓ 700	3597.6287	0.60 - 27788.2	97.63 ~ 50	
325	3599.1554	-99.16 - 25	blended with Tm II 99.16, Ce II 99.13	
100.98 150	3603.8340	3603.98 0.1 mm	50	
50	3608.4584	08.48 → Mn II		
50	3611.0435	V II 11.04		
50	3611.7169	11.70 Co I 11.69 + Ce II 11.73		
150 12.32 150	3612.1317	?		
W= 49 325	3621.1707	21.17 81. Sm II 21.21 + Co II 21.22	W=	
наполнению 150	3626.1211	→ как-то меньше миним	26.11 W=10	
оды, а также 100	3627.7631	Co I 27.75		
Лай 12.34 100	3628.8384	La II 28.82		
Сей 12.35, 12.29 150	3643.8378	43.83 26	7(67)	
Тм II 12.36 700	3644.3517	35.17 3715 - 31146.429	31383, 10	
150	3661.6353	→ 250 бланка 3653.407 W=		
✓ 150	3701.2882			
150	3708.0785			
150	3722.3414			
150	3767.2414			
325	3774.2086			
150	3794.6327			
50	3863.3681	.41 Fe II		

100	3920.1639	Nd
150	3998.4683	.45 (3-4) u
150	4012.7965	.75 (5d) u 12.80 33
150	4016.9010	.50 (4) u 16.90 39
150	4030.9636	.47 (3) u 30.98 39
100	4048.4914	.52 (3) u 48.52 → менше от 48
150	4059.7968	.72 (4d) u 48.78 Erit 59.78
150	4076.6271	.62 (4) .64 Fe II .61 Sm II 46.62 + Fe II 76.62
325 .25L	4084.5991	.60 (5) u 84.22(2) u 84.65 → del. Sm II 84.68
100	4116.3530	.31 (3) u 16.83 Nd II 16.32
150	4118.5399	.53 (5) .55 Sm II → 18.55
150	4141.0644	.01 (3d) u 41.006 d II 41.05 M II
150	4144.7899	.50 (2) u 44.86 издано проверено Hb
100	4145.4985	.49 .52 2387.6 - 26503.2 24
100	4147.9434	.43 (2-3) u .94 28 4148.16 (52) → 94
100	4156.1627	.19 .24 3u + .16 → менше от 16
325	4180.9461	.46 (4) u 80.96 → del. Fe II 80.98 (34)
150	4182.1412	.13 (3-4) u 82.19 → 82.15 (3d) Ce II 82.22
100	4184.4608	.47 (3-4) u 84.47 (48)
150	4187.7321	.15 (4) u 87.49 - Fe II 87.78
100	4190.6544	.66 (1-2) u 90.64 Ce II 90.62
100	4204.0664	.01 (2d) .44 Fe II .02, La II 04.04
150	4210.5938	.60 (2) .62 3u не меньше от 60
100	4211.0029	.01 (2-3) u 11.01 48 27.63 (28)
50	4213.3558	u II? - 13.36 25? 15
150	4221.8277	→ 21.86 Sm II
150	4222.8437	.88 (2-3) .85 Ce II что-то есть, но там же Ce II 23.82 Ce II
50	4233.5939	.60 (1) .61 Fe I .60 → Fe I
150	4233.7955	.19 (1) u 33.88 16
150	4235.1702	.16 (3) u 35.15 35.14 M II
150	4235.7588	.81 (3d) u .44 4 II 35.73
50	4239.6003	.55 (1-2d) u и 8. Ce II, но в крыше делен
50	4246.5273	.55 (3) u .57 Gd II ? .83 10
150	4248.8370	.47 (2-3) u 49.00 48? Ce II 96, Ce II 98, Ce II
50	4248.9708	.86 (2) u .83 → erupce
100	4249.8655	.17 (1-2d) u .18 Ce II от асбаста
150	4266.1824	.00 (3) u .98 28
150	4273.9846	и 8. Ce II, но в крыше асбаста?
100	4275.8956	.70 (4) .75 Sm II, .68 Sm II Nd II не меньше
150	4279.7383	.54 (3) u .55 ~ 26 31 81.52
150	4281.5691	.83 ~ 30 38
250	4290.8108	.83 ~ 30 асб. V 91.81
150	4291.8146	что-то есть, но в делен
50	4295.5720	около дора Hb 36.24 Ce II + 36.28 Ce II
100	4336.3041	.78 ~ 14 277 Nd II не меньше
50	4367.7969	.14 24
150	4406.1470	.30 47
325	4414.3002	.60 → и что-то есть, но делен. Ce II 15.56
150	4415.5947	.92 La II 29.90 + Ce II 29.99 La II hfs
150	4429.9458	.45 Ce II 33.74 + Fe II 33.78
50	4433.7874	.05 24
150	4442.0536	.99 → что-то есть, трудно и мерить менше
100	4445.9935	.26 → 12? сильными делен
100	4446.2335	.33 Ce II 49.33
50	4449.3464	.29 56
150	4473.2872	.42 56
150	4483.4350	.50 → 5093.3 - 27391.4 Gd II 83.33
150	4500.4367	.50 → 130 деленная делен Ce II 83.31
150	4507.5333	.53 u = 0.750 26 → Ce II 4500.49 H-
100	4508.3785	del. Fe II 08.29

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использовано провер.

село 21.73 33

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13	150	64	4514.0790	д. Сат, FeI	14 - 66?
68	150	32	4514.6879	• 69 → 0.51	
	150		4515.4042	д. FeI 15.34 → 8.70-рресс	
18	150	~60	4517.1934	д. Сат, FeI	16 Сат 17.09 + Sm II 17.21 + Ce II 17.31
	100		4522.2714	Всплеск, б. с. л. а. н.	
	150		4524.7322	Fe II 24.68	
	100		4533.4033	д. - то с. н. б. д. л. е. н. e	40 0.812 19
94	150	52	4534.9413	• 95 → 0.702 35	
24	150	?	4551.1525	• 16 0.690 → 0.737 +	
45	150	40	4557.4709	• 43 0.637 → 0.637	Сел 57.04 + 57.41 + 57.44 + 57.45
17	150	45	4558.1680	• 11 0.526 д. 6 d II 58.08 → 0.526	Сел 58.07 +
	50		4563.1070	д. л. e. н. e 63.05 0.860	
	50		4563.3953	63.37 0.558 Сел 63.36 (2 мин)	+ +
	50		4563.8781	→ канал - то д. н. т. о. л. e. n. e	
66	150	51 (94)	4570.6596	• 64 0.594 → 0.51	51 +
56	150		4584.5123	→ 0.510 - то с. н. б. д. л. e. n. e	0.818 20 - 41
26	150	11	4599.2552	• 25 → 0.870 → 0.870	Сел 99.26 +
	150		4607.8264	д. - то д. н. т. o. л. e. n. e	
	50		4607.7057	д. - то д. н. т. o. л. e. n. e	
	50		4613.5943	д. - то д. н. т. o. л. e. n. e	
35	50	62?	4619.3789	→ 0.870 - то с. н. б. д. л. e. n. e	
	50		4621.7407	→ 0.870 - то с. н. б. д. л. e. n. e	
	150		4621.9963	→ 0.870 - то с. н. б. д. л. e. n. e	
100			4624.9646	→ 0.870 - то с. н. б. д. л. e. n. e	
100			4626.3129	д. - то с. н. б. д. л. e. n. e	
27	325	52?	4627.2544	27.28 0.07 27.23 35.6 45	
19	325	107?	4628.2479	д. - то с. н. б. д. л. e. n. e	
98	150	35	4642.9726	42.98 д. с. Тм II 42.85 + Сел 42.96	
16	50	45	4646.1404	д. - то с. н. б. д. л. e. n. e	
62	150	40	4651.6087	Сел? 62.0466 д. Р II 51.50	84
03	150		4654.0140	54.09 50 0.624 → 0.624	
30	150		4654.3115	54.28 Сел 54.28	но можно и добавить 54.30 (4)
87	50		4656.8284	→ 0.624 - то с. н. б. д. л. e. n. e	
04	50	30	4663.0482	• 06 д. с. н. б. д. л. e. n. e	
al II →	150		4666.7484	Fe II 4666.758	66.75 66.71
17	50	14	4684.1803	4684.16 → 0.624	66.75 66.71
66	100	23	4688.6899	88.65 7-0.75 88.64 W=38	
05	150	63	4689.0517	89.04 7=? 89.05 7=0.602 W=54	
SI? 48	150	28	4695.4145	95.41 д. SI 95.40 + 2 мин Сел	но 0.56
SI? 24	100	с. н. б. д. л. e. n. e	4696.2051	96.20 → с. н. б. д. л. e. n. e	
32	150	71	4711.2926	11.33 11.33 W=60	→ 0.624 - то с. н. б. д. л. e. n. e
51	150	44	4713.4954	13.53 13.53 W=58	→ 0.624 - то с. н. б. д. л. e. n. e
39	150	84	4718.4238	18.42 18.42 W=18, 7=838	
73	150	24	4720.7398	20.46 20.46 W=18, 7=838	
85	100	44	4722.8456	22.89 22.89 W=38	7=0.704 → 0.704
	50	нет	4726.8754	нет Сел 26.85	
	50	нет	4727.6310	Сел 24.65	
52	50	25	4733.5494	Сел 33.54 → 0.624 - то с. н. б. д. л. e. n. e	
75	150	64	4734.7311	34.76 → 0.678 → 0.678	35-75
24	100	40	4740.2194	40.27 40.27 W=18, 7=838	
65	100	22	4740.6637	40.53 40.53 W=18, 7=838	
325			4741.0145	41.02 41.02 W=18, 7=838	
99	325	69	4745.9835	45.99 45.99 W=18, 7=838	
40	150	7	4747.4125	47.43 47.43 W=18, 7=838	
	100		4757.6755	47.43 47.43 W=18, 7=838	
54	150	78	4759.4993	59.52 59.52 W=18, 7=838	
88	150		4762.4196	62.30 62.30 W=18, 7=838	
28	100	41	4765.2610	65.28 65.28 W=18, 7=838	
61	150	86	4769.6102	69.63 69.63 W=18, 7=838	
	150	д. н. т. o. л. e. n. e	4770.8845	70.88 70.88 W=18, 7=838	

Сел 4660.656 → нечетная lfs!!!

50	красн. кет	4774.6846	44.73	HD122970 - кет
150	селега	4777.6056	селега	
50		4786.2033	86.23(21)	Fe II
46 100	66	4788.4228	88.46	88.47 HD122970 - кетоний, 95
50	Fe	4789.2724		
50	Fe	4794.2239	94.24 HD122970	
49 100	102	4796.4650	96.47	94.25 + селега, HD
90 100	66	4799.8874	81	96.50 HD122970 → кетоний, 96
66 50	47	4800.6661	64 (16)	81 99.88 (41)
73 50	22	4804.7188		Fe II 80.65
37 150	41	4810.3694	10.36 (55)	84.72 HD122970 → кетоний
12 150	30	4821.1124	21.12	10.37 HD122970 - кетоний
99 100	61	4821.9858	22.00	21.12 → селега
150	селега	4838.2175		21.99 HD122970 - кетоний, 98
81 100	селега	4845.8354	45.84	красн. кет
48 50	98	4927.4841	42.60	→ селега
150	119	4942.6733	81.44	красн. кет
✓ 325		5102.4302	5093.3 - 25062.37	42.63 HD
✓ 325		5127.0087	5093.3 - 24686.4	
50		5152.2924		
✓ 150		5193.0613		
✓ 325		5203.9058		
✓ 325		5264.9589		
✓ 150		5294.1062		
150		5368.5814	68.56	68.57 HD122970 Fe II 68.53
50	Fe II	5400.0792	селега	
50		5530.8599		
150		5705.2382	05.24	30.82 HD122970 Co II 30.74
✓ 150		5844.9990		05.24 HD122970
100		6141.0521		
✓ 200		6145.0208		→ Fe II 6141.033
150		6273.6734	43.40	43.70 HD122970 Fe II 43.75 → селега
150	Fe II	6282.5665		
✓ 50		6327.2200		
150		6361.0420		
100		6363.3298		→ Ca 61.07 HD122970
150	Fe II	6385.4094	63.31 → селега	Ca II 63.33 HD122970
✓ 150		6550.2121		85.43 HD122970 Fe II 85.45
SI? 50		6748.7410	68.70.713	селега
50		7225.3275		81.51
50		7258.1658		красн. кет
150		7427.2534		58.14 HD121522
50		7432.5212		селега HD121522
50		8454.6726		? в поле HD кет

TABLE 1

HB LINES STRONG IN A MILD SPARK

INT C WAVELENGTH ION ENERGY LEVELS

12	80	2088.329		
11	90 B	2326.374		
10	80 B	2349.620	III	25558 - 68105
9	90	2357.264		
8	75 B	2369.814		
7	75	2374.378		
6	75	2375.543		
5	90	2385.108		
4	75	2387.059		
3	75 C	2396.977		

Use Mc 6 lamp
Do > 100

Appendix F

Co II Magnetic Interaction Hyperfine Structure Constants

The lists of HFS A constants for even and odd energy levels of Co II are presented in [Table F.1](#) and [Table F.2](#) respectively [171]. The configuration label, term label, J value, and energy of each level [100–102] are the first four columns, the energies were corrected by 6.7 parts in 10^8 to conform with the revised wavenumber scale [184]. The fifth and sixth column are the A constants and their uncertainties ($1 \text{ mK} = 0.001 \text{ cm}^{-1} = 30 \text{ MHz}$). The number of line profiles used to determine the A constants is in the seventh column N . Where available, previous measurements of the A constants are given in the final column (LF [97] and BP [64]). The $3d^7 5d$ levels (except for the $3d^7(^4F)5d \ ^5G$ term) and $3d^7 5g$ levels have been omitted as no A constants were determined for them.

Table F.1: HFS A Constants of Even Energy Levels of Co II

Configuration	Term	J	Energy (cm^{-1})	A (mK)	A err (mK)	N	Previous Work (mK)
$3d^8$	a^3F	4	0.000	13.0	5.0	2	
$3d^8$	a^3F	3	950.324	17.0	5.0	2	
$3d^8$	a^3F	2	1597.197	33.0	4.0	1	
$3d^7(^4F)4s$	a^5F	5	3350.494	34.4	1.0	7	LF(33.8 ± 0.8)
$3d^7(^4F)4s$	a^5F	4	4028.988	29.5	1.8	9	LF(29.9 ± 0.8)
$3d^7(^4F)4s$	a^5F	3	4560.789	25.4	2.2	6	LF(25.0 ± 0.8)
$3d^7(^4F)4s$	a^5F	2	4950.062	17.1	2.0	8	LF(17.6 ± 0.8)
$3d^7(^4F)4s$	a^5F	1	5204.698	-8.4	1.2	5	LF(-9.2 ± 1.0)
$3d^7(^4F)4s$	b^3F	4	9812.860	2.9	1.3	12	LF(2.2 ± 0.8)
$3d^7(^4F)4s$	b^3F	3	10708.331	17.4	1.2	4	LF(15.2 ± 0.9)
$3d^7(^4F)4s$	b^3F	2	11321.860	53.0	1.0	6	LF(50.1 ± 0.9)
$3d^8$	a^1D	2	11651.277	18.0	2.0	1	
$3d^8$	a^3P	2	13260.688	16.9	1.7	3	
$3d^8$	a^3P	1	13404.321	-3.0	5.0	2	
$3d^8$	a^3P	0	13593.288	0.0	0.0		
$3d^7(^4P)4s$	a^5P	3	17771.507	40.6	1.4	15	LF(40.2 ± 0.8), BP(40 ± 3)
$3d^7(^4P)4s$	a^5P	2	18031.427	50.3	2.3	12	LF(49.4 ± 0.8), BP(49.9 ± 1.5)
$3d^7(^4P)4s$	a^5P	1	18338.640	59.5	0.9	10	LF(59.1 ± 0.6), BP(60 ± 2)
$3d^8$	a^1G	4	18973.727	23.6	1.4	4	
$3d^7(^2G)4s$	a^3G	5	21624.528	40.8	0.7	13	
$3d^7(^2G)4s$	a^3G	4	22009.344	22.7	0.4	17	
$3d^7(^2G)4s$	a^3G	3	22414.431	6.9	0.9	11	
$3d^7(^4P)4s$	b^3P	2	24074.420	-9.6	1.2	3	
$3d^7(^4P)4s$	b^3P	1	24267.382	-10.6	1.9	6	
$3d^7(^4P)4s$	b^3P	0	24411.479	0.0	0.0		
$3d^7(^2P)4s$	c^3P	2	24886.400	51.8	1.0	14	
$3d^7(^2P)4s$	c^3P	1	25317.517	35.5	0.6	10	
$3d^7(^2P)4s$	c^3P	0	25861.322	0.0	0.0		
$3d^7(^2G)4s$	b^1G	4	25147.233	29.7	0.7	17	
$3d^7(^2H)4s$	a^3H	6	27105.744	39.5	0.7	5	
$3d^7(^2H)4s$	a^3H	5	27468.988	23.2	1.0	7	
$3d^7(^2H)4s$	a^3H	4	27902.161	9.5	1.9	4	
$3d^7(a^2D)4s$	a^3D	3	27484.373	52.6	1.0	15	
$3d^7(a^2D)4s$	a^3D	2	28111.872	24.4	2.0	6	
$3d^7(a^2D)4s$	a^3D	1	29268.777	-0.3	2.0	6	
$3d^7(^2P)4s$	a^1P	1	27585.138	26.4	0.9	4	
$3d^7(^2H)4s$	a^1H	5	30567.173	29.9	1.3	10	
$3d^7(a^2D)4s$	b^1D	2	31199.412	41.9	1.5	6	
d^6s^2	a^5D	4	40695.028				
d^6s^2	a^5D	3	41314.150				
d^6s^2	a^5D	2	41738.151				
$3d^7(^2F)4s$	c^3F	2	40771.113	1.0	5.0	3	
$3d^7(^2F)4s$	c^3F	3	40879.602				

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Table F.1: HFS A Constants of Even Energy Levels of Co II (continued)

Configuration	Term	J	Energy (cm ⁻¹)	A (mK)	A err (mK)	N	Previous Work (mK)
3d ⁷ (² F)4s	c ³ F	4	41047.334				
3d ⁷ (⁴ F)5s	e ⁵ F	5	84014.181	16.6	1.7	7	
3d ⁷ (⁴ F)5s	e ⁵ F	4	84586.868	13.6	1.1	5	
3d ⁷ (⁴ F)5s	e ⁵ F	3	85167.645	13.4	1.4	3	
3d ⁷ (⁴ F)5s	e ⁵ F	2	85596.170	19.0	1.5	5	
3d ⁷ (⁴ F)5s	e ⁵ F	1	85876.271	38.1	1.8	3	
3d ⁷ (⁴ F)5s	e ³ F	4	85481.689	16.2	2.0	2	
3d ⁷ (⁴ F)5s	e ³ F	3	86346.705	22.6	1.6	5	
3d ⁷ (⁴ F)5s	e ³ F	2	86940.150	41.7	2.2	3	
3d ⁷ (⁴ F)4d	f ⁵ F	5	89931.466	8.3	2.4	2	
3d ⁷ (⁴ F)4d	f ⁵ F	4	90199.163	14.0	2.0	4	
3d ⁷ (⁴ F)4d	f ⁵ F	3	90753.266	12.3	1.6	3	
3d ⁷ (⁴ F)4d	f ⁵ F	2	90967.590	25.9	0.7	11	
3d ⁷ (⁴ F)4d	f ⁵ F	1	91358.992	49.9	2.7	6	
3d ⁷ (⁴ F)4d	e ⁵ G	6	90302.776	8.8	2.1	3	
3d ⁷ (⁴ F)4d	e ⁵ G	5	90697.464	6.0	3.0	5	
3d ⁷ (⁴ F)4d	e ⁵ G	4	91352.880	6.0	3.0	3	
3d ⁷ (⁴ F)4d	e ⁵ G	3	91667.338	13.6	1.6	4	
3d ⁷ (⁴ F)4d	e ⁵ G	2	91928.989	23.0	1.1	5	
3d ⁷ (⁴ F)4d	e ⁵ P	3	90464.589	18.0	2.0	1	
3d ⁷ (⁴ F)4d	e ⁵ P	2	91424.773	10.5	2.8	2	
3d ⁷ (⁴ F)4d	e ⁵ P	1	91932.084	0.3	1.7	3	
3d ⁷ (⁴ F)4d	e ⁵ H	7	90667.894	9.1	2.3	3	
3d ⁷ (⁴ F)4d	e ⁵ H	6	90975.540	8.0	3.0	2	
3d ⁷ (⁴ F)4d	e ⁵ H	5	91646.447	11.0	2.0	4	
3d ⁷ (⁴ F)4d	e ⁵ H	4	92120.640	15.5	2.6	4	
3d ⁷ (⁴ F)4d	e ⁵ H	3	92405.999	21.8	1.4	3	
3d ⁷ (⁴ F)4d	e ⁵ D	4	91049.431	10.5	2.3	3	
3d ⁷ (⁴ F)4d	e ⁵ D	3	91958.369	3.0	4.0	1	
3d ⁷ (⁴ F)4d	e ⁵ D	0	92285.510	0.0	0.0		
3d ⁷ (⁴ F)4d	e ⁵ D	2	92317.368	2.0	2.0	4	
3d ⁷ (⁴ F)4d	e ⁵ D	1	92403.200	-28.7	0.9	3	
3d ⁷ (⁴ F)4d	e ³ G	5	91326.932	9.8	0.7	3	
3d ⁷ (⁴ F)4d	e ³ G	4	91918.200	10.5	3.5	5	
3d ⁷ (⁴ F)4d	e ³ G	3	92519.979	23.3	1.8	7	
3d ⁷ (⁴ F)4d	e ³ D	3	91408.494	9.5	1.8	7	
3d ⁷ (⁴ F)4d	e ³ D	2	92044.913	17.0	2.7	4	
3d ⁷ (⁴ F)4d	e ³ D	1	92639.846	41.5	2.6	3	
3d ⁷ (⁴ F)4d	e ³ H	6	91623.455	12.0	4.0	5	
3d ⁷ (⁴ F)4d	e ³ H	5	92359.180	11.6	1.6	3	
3d ⁷ (⁴ F)4d	e ³ H	4	92889.417	18.4	0.9	4	
3d ⁷ (⁴ F)4d	e ³ P	2	93678.422	11.5	1.8	3	
3d ⁷ (⁴ F)4d	e ³ P	1	94405.533	13.0	2.2	3	
3d ⁷ (⁴ F)4d	e ³ P	0	94720.916	0.0	0.0		

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Table F.1: HFS A Constants of Even Energy Levels of Co II (continued)

Configuration	Term	J	Energy (cm ⁻¹)	A (mK)	A err (mK)	N	Previous Work (mK)
3d ⁷ (⁴ F)4d	f ³ F	4	93738.788	10.9	1.9	4	
3d ⁷ (⁴ F)4d	f ³ F	3	94368.585	13.0	3.0	3	
3d ⁷ (⁴ F)4d	f ³ F	2	94743.698	28.7	1.1	4	
3d ⁷ (⁴ P)5s	⁵ P	3	99022.528	9.0	4.0	1	
3d ⁷ (⁴ P)5s	⁵ P	2	99235.161	6.0	6.0	1	
3d ⁷ (⁴ P)5s	⁵ P	1	99552.560	17.0	6.0	1	
3d ⁷ (⁴ P)5s	³ P	2	100331.391	-3.0	4.0	2	
3d ⁷ (⁴ P)5s	³ P	1	100596.386				
3d ⁷ (⁴ P)5s	³ P	0	100886.787	0.0	0.0		
3d ⁷ (² G)5s	f ³ G	5	101233.605	23.3	1.1	2	
3d ⁷ (² G)5s	f ³ G	4	101451.074	18.8	1.6	3	
3d ⁷ (² G)5s	f ³ G	3	102020.364	28.2	1.1	3	
3d ⁷ (² G)5s	e ¹ G	4	102371.610	31.5	2.2	4	
3d ⁷ (² P)5s	³ P	2	104412.631	24.0	4.0	2	
3d ⁷ (² P)5s	³ P	1	104678.460	0.0	4.0	2	
3d ⁷ (⁴ P)4d	⁵ P	1	104587.191				
3d ⁷ (⁴ P)4d	⁵ P	2	104676.623				
3d ⁷ (⁴ P)4d	⁵ P	3	104835.774				
3d ⁷ (⁴ P)4d	⁵ F	5	105308.135				
3d ⁷ (⁴ P)4d	⁵ F	4	105395.118				
3d ⁷ (⁴ P)4d	⁵ F	3	105504.380				
3d ⁷ (⁴ P)4d	⁵ F	2	105625.153				
3d ⁷ (⁴ P)4d	⁵ F	1	105739.760	33.0	4.0	1	
3d ⁷ (² P)5s	¹ P	1	105430.432	31.0	5.0	2	
d ⁶ s ²	¹ G	4	105591.110				
3d ⁷ (⁴ P)4d	³ F	4	106221.878	5.0	4.0	1	
3d ⁷ (⁴ P)4d	³ F	3	106316.344	5.0	5.0	1	
3d ⁷ (⁴ P)4d	³ F	2	106502.120				
3d ⁷ (⁴ P)4d	⁵ D	4	106428.864	2.0	7.0	1	
3d ⁷ (⁴ P)4d	⁵ D	0	106454.196	0.0	0.0		
3d ⁷ (⁴ P)4d	⁵ D	1	106516.641				
3d ⁷ (⁴ P)4d	⁵ D	3	106586.233				
3d ⁷ (⁴ P)4d	⁵ D	2	106647.186				
3d ⁷ (² H)5s	³ H	6	106905.104	24.2	1.3	1	
3d ⁷ (² H)5s	³ H	5	107116.009	21.0	2.0	1	
3d ⁷ (² H)5s	³ H	4	107624.640	27.0	3.0	1	
3d ⁷ (⁴ P)4d	³ P	0	106914.988	0.0	0.0		
3d ⁷ (⁴ P)4d	³ P	2	106918.224	0.0	5.0	2	
3d ⁷ (⁴ P)4d	³ D	3	106939.007	5.0	5.0	1	
3d ⁷ (⁴ P)4d	³ D	1	107224.636				
3d ⁷ (⁴ P)4d	³ D	2	107409.476				
3d ⁷ (a ² D)5s	³ D	3	107154.877	24.0	3.0	1	
3d ⁷ (a ² D)5s	³ D	2	107535.612	21.0	3.0	1	
3d ⁷ (a ² D)5s	³ D	1	108500.862	-7.0	3.0	2	

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Table F.1: HFS A Constants of Even Energy Levels of Co II (continued)

Configuration	Term	J	Energy (cm ⁻¹)	A (mK)	A err (mK)	N	Previous Work (mK)
3d ⁷ (² G)4d	³ D	3	107451.187	16.8	2.6	3	
3d ⁷ (² G)4d	³ D	2	107713.738				
3d ⁷ (² G)4d	³ I	6	107473.341				
3d ⁷ (² G)4d	³ I	5	108217.126	22.7	2.0	1	
3d ⁷ (² G)4d	³ G	5	107543.564				
3d ⁷ (² G)4d	³ G	4	107790.221				
3d ⁷ (² G)4d	³ G	3	108268.086	33.0	4.0	1	
3d ⁷ (² G)4d	³ H	5	107646.450	20.9	1.3	4	
3d ⁷ (² G)4d	³ H	6	107703.321				
3d ⁷ (² G)4d	³ H	4	108388.822	18.3	2.1	5	
3d ⁷ (² G)4d	¹ F	3	107671.856				
3d ⁷ (² H)5s	¹ H	5	108021.200	29.2	1.5	4	
3d ⁷ (² G)4d	¹ I	6	108347.492				
3d ⁷ (⁴ F)6s	⁵ F	5	108474.366	15.0	3.0	2	
3d ⁷ (⁴ F)6s	⁵ F	4	109442.072	16.0	1.9	3	
3d ⁷ (⁴ F)6s	⁵ F	3	109528.229	12.9	1.8	3	
3d ⁷ (⁴ F)6s	⁵ F	2	110022.927	22.0	3.0	1	
3d ⁷ (⁴ F)6s	⁵ F	1	110338.346	46.0	2.0	2	
3d ⁷ (² G)4d	³ F	4	108475.120	22.7	1.0	4	
3d ⁷ (² G)4d	³ F	3	108830.066	23.7	0.9	5	
3d ⁷ (² G)4d	³ F	2	109242.450	42.0	4.0	1	
3d ⁷ (² G)4d	¹ H	5	108600.173	21.0	3.0	4	
3d ⁷ (a ² D)5s	¹ D	2	108730.572	36.0	5.0	1	
3d ⁷ (⁴ F)6s	³ F	4	108819.860	11.3	1.2	4	
3d ⁷ (⁴ F)6s	³ F	3	110172.603	22.5	3.0	2	
3d ⁷ (⁴ F)6s	³ F	2	110698.567	38.9	2.4	3	
3d ⁷ (² G)4d	¹ D	2	108912.599	34.4	1.1	3	
3d ⁷ (² G)4d	¹ G	4	109312.083	23.7	2.3	1	
3d ⁷ (² P)4d	³ D	1	110443.236				
3d ⁷ (² P)4d	³ D	2	110523.375	7.0	7.0	4	
3d ⁷ (² P)4d	³ D	3	110576.482				
3d ⁷ (² P)4d	³ F	4	110725.407				
3d ⁷ (² P)4d	³ F	2	111493.638				
3d ⁷ (² P)4d	³ F	3	111541.364				
3d ⁷ (² P)4d	³ P	1	110859.436				
3d ⁷ (² P)4d	³ P	0	110863.529	0.0	0.0		
3d ⁷ (² P)4d	³ P	2	111332.473				
3d ⁷ (² P)4d	¹ F	3	110884.498				
3d ⁷ (⁴ F)5d	⁵ G	2	112917.704	21.0	4.0	1	
111436		3	111436.337				
3d ⁷ (² P)4d	¹ P	1	111707.192				
3d ⁷ (² P)4d	¹ D	2	112350.469				
3d ⁷ (² H)4d	³ K	7	112820.099	20.0	3.0	1	
3d ⁷ (² H)4d	³ K	6	113434.873	25.0	2.0	1	

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Table F.1: HFS A Constants of Even Energy Levels of Co II (continued)

Configuration	Term	J	Energy (cm ⁻¹)	A (mK)	A err (mK)	N	Previous Work (mK)
3d ⁷ (² H)4d	¹ F	3	112966.982				
3d ⁷ (² H)4d	³ G	5	112993.881				
3d ⁷ (² H)4d	³ G	4	113275.001	16.7	1.4	3	
3d ⁷ (² H)4d	³ G	3	113724.572	34.5	2.4	1	
113191		3	113191.686	26.0	3.0	1	
3d ⁷ (a ² D)4d	³ F	4	113253.946				
3d ⁷ (a ² D)4d	³ F	3	113355.633				
3d ⁷ (a ² D)4d	³ F	2	113821.511				
3d ⁷ (a ² D)4d	³ D	3	113523.218				
3d ⁷ (a ² D)4d	³ D	2	114260.795	11.0	4.0	3	
3d ⁷ (a ² D)4d	³ D	1	114854.335				
3d ⁷ (² H)4d	³ I	7	113707.636	19.0	3.0	2	
3d ⁷ (² H)4d	³ I	6	113803.548	20.2	1.9	3	
3d ⁷ (² H)4d	³ I	5	114376.722	24.5	1.1	1	
3d ⁷ (a ² D)4d	³ G	4	113829.007				
3d ⁷ (a ² D)4d	³ G	3	114926.979				
3d ⁷ (a ² D)4d	¹ P	1	113857.840	18.0	2.0	2	
3d ⁷ (² H)4d	¹ H	5	113864.592	23.3	0.8	5	
3d ⁷ (² H)4d	³ H	6	113945.285	19.0	2.1	3	
3d ⁷ (² H)4d	³ H	4	114528.951	28.6	2.0	1	
3d ⁷ (² H)4d	³ H	5	114559.108	22.0	3.0	3	
3d ⁷ (a ² D)4d	³ S	1	114251.937				
3d ⁷ (a ² D)4d	¹ F	3	114385.369	18.0	3.0	2	
3d ⁷ (² H)4d	¹ I	6	114763.695	21.0	2.0	1	
3d ⁷ (a ² D)4d	¹ G	4	114974.320				
3d ⁷ (a ² D)4d	³ P	2	115148.384	3.0	4.0	2	
3d ⁷ (a ² D)4d	³ P	0	115785.544	0.0	0.0		
3d ⁷ (a ² D)4d	³ P	1	115948.283				
3d ⁷ (² H)4d	³ F	4	115484.871	15.2	2.0	2	
3d ⁷ (² H)4d	³ F	3	116132.380	20.0	3.0	2	
3d ⁷ (² H)4d	³ F	2	116382.663				
3d ⁷ (a ² D)4d	¹ D	2	117416.558	17.0	7.0	1	
3d ⁷ (² H)4d	¹ G	4	117535.245				

Table F.2: HFS A Constants of Odd Energy Levels of Co II

Configuration	Term	J	Energy (cm ⁻¹)	A (mK)	A err (mK)	N	Previous Work (mK)
3d ⁷ (⁴ F)4p	z^5F	5	45197.711	12.1	1.5	5	LF(10.9 ± 0.8)
3d ⁷ (⁴ F)4p	z^5F	4	45378.754	8.5	1.5	6	LF(9.3 ± 0.8)
3d ⁷ (⁴ F)4p	z^5F	3	45972.036	13.8	3.1	4	LF(11.5 ± 0.8)
3d ⁷ (⁴ F)4p	z^5F	2	46452.700	18.6	1.0	4	

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Table F.1: HFS A Constants of Odd Energy Levels of Co II (continued)

Configuration	Term	J	Energy (cm^{-1})	A (mK)	A err (mK)	N	Previous Work (mK)
$3d^7(^4F)4p$	z^5F	1	46786.409	45.6	1.0	1	
$3d^7(^4F)4p$	z^5D	4	46320.832	8.8	1.7	3	LF(8.8 ± 0.8), BP(9 ± 2)
$3d^7(^4F)4p$	z^5D	3	47039.105	8.1	2.2	5	LF(7.8 ± 0.8), BP(8 ± 20)
$3d^7(^4F)4p$	z^5D	2	47537.365	8.0	2.6	3	LF(9.0 ± 0.8)
$3d^7(^4F)4p$	z^5D	1	47848.781	2.0	4.0	3	LF(5.5 ± 0.7), BP(5 ± 5)
$3d^7(^4F)4p$	z^5D	0	47995.594	0.0	0.0		
$3d^7(^4F)4p$	z^5G	6	47078.494	11.0	2.1	1	LF(9.9 ± 0.8)
$3d^7(^4F)4p$	z^5G	5	47345.845	13.0	2.0	5	LF(11.8 ± 0.8)
$3d^7(^4F)4p$	z^5G	4	47807.493	16.8	1.9	1	LF(15.0 ± 1.0)
$3d^7(^4F)4p$	z^5G	3	48150.940	19.9	1.2	3	
$3d^7(^4F)4p$	z^5G	2	48388.442	39.9	1.0	6	
$3d^7(^4F)4p$	z^3G	5	48556.052	13.9	1.2	6	LF(13.1 ± 0.8)
$3d^7(^4F)4p$	z^3G	4	49348.304	17.0	1.4	4	LF(16.7 ± 0.8)
$3d^7(^4F)4p$	z^3G	3	50036.348	26.9	1.0	4	LF(25.6 ± 0.9)
$3d^7(^4F)4p$	z^3F	4	49697.683	16.5	2.2	4	LF(13.6 ± 0.9)
$3d^7(^4F)4p$	z^3F	3	50381.724	20.9	1.9	6	LF(18.4 ± 0.9)
$3d^7(^4F)4p$	z^3F	2	50914.325	33.9	2.4	4	LF(31.3 ± 1.0)
$3d^7(^4F)4p$	z^3D	3	51512.268	12.3	3.2	4	
$3d^7(^4F)4p$	z^3D	2	52229.725	19.1	1.8	3	
$3d^7(^4F)4p$	z^3D	1	52684.634	46.7	1.2	6	
$3d^7(^4P)4p$	z^5S	2	56010.475	-7.7	1.3	6	LF(-8.7 ± 0.7)
$3d^7(^4P)4p$	y^5D	3	61240.746	8.4	1.6	4	
$3d^7(^4P)4p$	y^5D	2	61260.319	10.2	2.5	4	
$3d^7(^4P)4p$	y^5D	1	61350.268	11.0	3.0	1	
$3d^7(^4P)4p$	y^5D	4	61388.250	4.0	2.0	1	
$3d^7(^4P)4p$	y^5D	0	61458.124	0.0	0.0		
$3d^7(^4P)4p$	z^3S	1	62440.078	-11.1	1.9	7	
$3d^7(^2G)4p$	z^3H	5	63306.686	22.1	0.7	7	
$3d^7(^2G)4p$	z^3H	6	63597.396	16.0	2.0	1	
$3d^7(^2G)4p$	z^3H	4	63792.717	31.5	0.9	17	
$3d^7(^4P)4p$	z^5P	3	63344.333	1.9	2.3	5	
$3d^7(^4P)4p$	z^5P	2	63367.333	-3.6	2.2	4	
$3d^7(^4P)4p$	z^5P	1	63665.192	-15.8	1.0	5	
$3d^7(^2G)4p$	y^3F	4	63510.180	18.2	1.0	6	
$3d^7(^2G)4p$	y^3F	3	64360.050	26.2	1.3	4	
$3d^7(^2G)4p$	y^3F	2	65016.915	40.6	1.8	7	
$3d^7(^4P)4p$	y^3D	3	63586.987	5.6	1.0	8	
$3d^7(^4P)4p$	y^3D	2	63615.990	8.3	1.7	7	
$3d^7(^4P)4p$	y^3D	1	63865.170	36.6	0.9	4	
$3d^7(^2G)4p$	z^1G	4	64401.359	22.2	1.1	8	
$3d^7(^2G)4p$	y^3G	5	64601.778	18.7	0.8	7	
$3d^7(^2G)4p$	y^3G	4	65154.041	24.3	1.8	11	
$3d^7(^2G)4p$	y^3G	3	65174.661	30.8	1.9	4	
$3d^7(^2P)4p$	z^3P	0	64605.527	0.0	0.0		

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Table F.1: HFS A Constants of Odd Energy Levels of Co II (continued)

Configuration	Term	J	Energy (cm^{-1})	A (mK)	A err (mK)	N	Previous Work (mK)
$3d^7(^2P)4p$	z^3P	1	65028.512	5.1	0.7	5	
$3d^7(^2P)4p$	z^3P	2	65408.365	7.5	1.1	14	
$3d^7(^4P)4p$	y^3P	2	64914.630	10.1	1.1	12	
$3d^7(^4P)4p$	y^3P	0	65511.991	0.0	0.0		
$3d^7(^4P)4p$	y^3P	1	65657.249	-3.5	1.6	4	
$3d^7(^2G)4p$	z^1H	5	64957.482	22.5	0.7	7	
$3d^7(^2G)4p$	z^1F	3	66017.647	26.4	1.0	6	
$3d^7(^2P)4p$	z^1D	2	67209.258	17.0	0.7	6	
$3d^7(^2P)4p$	x^3D	3	67524.021	10.5	1.5	3	
$3d^7(^2P)4p$	x^3D	1	67824.389	27.0	1.0	3	
$3d^7(^2P)4p$	x^3D	2	67939.370	10.9	1.2	4	
$3d^7(^2P)4p$	1S	0	67910.933	0.0	0.0		
$3d^7(^2H)4p$	x^3G	5	68203.012	20.4	1.4	4	
$3d^7(^2H)4p$	x^3G	4	68843.428	26.1	0.8	5	
$3d^7(^2H)4p$	x^3G	3	69356.240	35.2	1.8	4	
$3d^7(^2H)4p$	z^3I	6	68311.113	23.4	1.0	5	
$3d^7(^2H)4p$	z^3I	7	68614.222	19.5	1.9	1	
$3d^7(^2H)4p$	z^3I	5	68829.451	29.9	1.8	6	
$3d^7(a^2D)4p$	w^3D	3	69059.933	17.0	2.0	2	
$3d^7(a^2D)4p$	w^3D	1	69317.077	22.2	0.7	1	
$3d^7(a^2D)4p$	w^3D	2	69637.023	18.0	2.0	3	
$3d^7(^2H)4p$	z^1I	6	69617.495	24.0	2.0	1	
$3d^7(a^2D)4p$	x^3F	4	70185.955	13.2	1.1	2	
$3d^7(a^2D)4p$	x^3F	3	70457.538	18.3	1.3	3	
$3d^7(a^2D)4p$	x^3F	2	70774.869	28.6	1.0	3	
$3d^7(^2P)4p$	y^3S	1	70265.915	-6.7	2.0	2	
$3d^7(^2P)4p$	z^1P	1	70857.053	23.2	2.3	5	
$3d^7(^2H)4p$	y^3H	6	71403.644	20.0	2.2	1	
$3d^7(^2H)4p$	y^3H	5	71702.960	23.2	0.9	4	
$3d^7(^2H)4p$	y^3H	4	72008.912	29.7	1.4	4	
$3d^7(a^2D)4p$	x^3P	2	71846.441	12.8	1.5	1	
$3d^7(a^2D)4p$	x^3P	1	73144.338	19.0	5.0	3	
$3d^7(a^2D)4p$	x^3P	0	73472.531	0.0	0.0		
$3d^7(a^2D)4p$	y^1F	3	72535.108	25.5	2.1	3	
$3d^7(a^2D)4p$	y^1D	2	72654.127	21.0	3.0	1	
$3d^7(^2H)4p$	y^1G	4	73147.041	27.8	1.3	1	
$3d^7(^2H)4p$	y^1H	5	74376.792	25.0	2.0	4	
$3d^7(a^2D)4p$	y^1P	1	74522.916	35.9	1.7	3	
$3d^7(^2F)4p$	w^3G	3	83110.662	35.0	4.0	1	
$3d^7(^2F)4p$	w^3G	4	83398.699				
$3d^7(^2F)4p$	w^3G	5	83877.863				
$3d^7(^2F)4p$	w^3F	3	83862.843				
$3d^7(^2F)4p$	w^3F	4	84140.653				
$3d^7(^2F)4p$	v^3D	3	84216.738				

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Table F.1: HFS A Constants of Odd Energy Levels of Co II (continued)

Configuration	Term	J	Energy (cm ⁻¹)	A (mK)	A err (mK)	N	Previous Work (mK)
3d ⁷ (² F)4p	v ³ D	2	84394.608				
3d ⁷ (² F)4p	v ³ D	1	84419.585	50.0	7.0	2	
3d ⁷ (⁴ F)5p	⁵ D	4	95036.155	9.0	3.0	2	
3d ⁷ (⁴ F)5p	⁵ D	3	95683.364	7.0	6.0	2	
3d ⁷ (⁴ F)5p	⁵ D	2	96205.841				
3d ⁷ (⁴ F)5p	⁵ F	5	95456.047	11.5	1.0	4	
3d ⁷ (⁴ F)5p	⁵ F	4	95976.579	11.7	0.8	2	
3d ⁷ (⁴ F)5p	⁵ F	3	96496.103	13.0	1.1	4	
3d ⁷ (⁴ F)5p	⁵ F	2	96890.966	19.1	1.3	1	
3d ⁷ (⁴ F)5p	⁵ F	1	97153.739	47.0	2.0	1	
3d ⁷ (⁴ F)5p	⁵ G	6	95998.735	12.9	1.3	4	
3d ⁷ (⁴ F)5p	⁵ G	4	96882.310	12.7	0.9	4	
3d ⁷ (⁴ F)5p	⁵ G	5	96942.130	13.5	1.7	4	
3d ⁷ (⁴ F)5p	⁵ G	3	97335.685	18.9	0.9	4	
3d ⁷ (⁴ F)5p	⁵ G	2	97628.434	29.0	2.0	1	
3d ⁷ (⁴ F)5p	³ G	5	96236.594	10.7	2.1	1	
3d ⁷ (⁴ F)5p	³ G	4	97705.056	16.5	1.6	3	
3d ⁷ (⁴ F)5p	³ G	3	98278.565	22.7	1.6	3	
3d ⁷ (⁴ F)5p	³ F	4	97062.844	14.9	0.9	3	
3d ⁷ (⁴ F)5p	³ F	3	97967.697	18.6	1.8	5	
3d ⁷ (⁴ F)5p	³ F	2	98287.640	30.0	2.0	1	
3d ⁷ (⁴ F)5p	³ D	3	97496.428	20.2	1.9	3	
3d ⁷ (⁴ F)5p	³ D	2	98648.516	22.2	1.4	3	
3d ⁷ (⁴ F)4f	(4.5)[6.5]	6	110008.482	18.7	1.7	5	
3d ⁷ (⁴ F)4f	(4.5)[6.5]	7	110096.458				
3d ⁷ (⁴ F)4f	(4.5)[5.5]	6	110070.208				
3d ⁷ (⁴ F)4f	(4.5)[5.5]	5	110094.056				
3d ⁷ (⁴ F)4f	(4.5)[4.5]	5	110077.560	9.0	3.0	2	
3d ⁷ (⁴ F)4f	(4.5)[4.5]	4	110099.385	11.4	1.8	3	
3d ⁷ (⁴ F)4f	(4.5)[3.5]	4	110129.926	8.9	2.5	3	
3d ⁷ (⁴ F)4f	(4.5)[3.5]	3	110130.164	12.9	1.6	2	
3d ⁷ (⁴ F)4f	(4.5)[7.5]	7	110148.061	9.0	2.5	2	
3d ⁷ (⁴ F)4f	(4.5)[7.5]	8	110158.673	7.5	2.0	1	
3d ⁷ (⁴ F)4f	(4.5)[2.5]	3	110162.781	15.0	2.0	2	
3d ⁷ (⁴ F)4f	(4.5)[2.5]	2	110163.094	19.1	2.9	1	
3d ⁷ (⁴ F)4f	(4.5)[1.5]	2	110194.244				
3d ⁷ (⁴ F)4f	(4.5)[1.5]	1	110199.790	34.5	1.2	2	
3d ⁷ (⁴ F)4f	(3.5)[4.5]	5	110926.337				
3d ⁷ (⁴ F)4f	(3.5)[4.5]	4	110927.845	7.0	5.0	3	
3d ⁷ (⁴ F)4f	(3.5)[5.5]	6	110932.343	7.6	1.9	3	
3d ⁷ (⁴ F)4f	(3.5)[5.5]	5	110940.775	9.1	1.1	4	
3d ⁷ (⁴ F)4f	(3.5)[3.5]	3	110934.611	11.0	2.0	1	
3d ⁷ (⁴ F)4f	(3.5)[3.5]	4	110942.715	7.7	1.2	4	
3d ⁷ (⁴ F)4f	(3.5)[2.5]	2	110970.554	15.7	1.2	3	

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Table F.1: HFS A Constants of Odd Energy Levels of Co II (continued)

Configuration	Term	J	Energy (cm ⁻¹)	A (mK)	A err (mK)	N	Previous Work (mK)
3d ⁷ (⁴ F)4f	(3.5)[2.5]	3	110976.722	9.0	2.0	3	
3d ⁷ (⁴ F)4f	(3.5)[6.5]	6	110980.867	10.4	2.0	2	
3d ⁷ (⁴ F)4f	(3.5)[6.5]	7	110986.083	7.8	2.0	4	
3d ⁷ (⁴ P)5p	⁵ D	4	110993.189	4.0	3.0	3	
3d ⁷ (⁴ P)5p	⁵ D	3	111005.925	7.3	1.4	1	
3d ⁷ (⁴ P)5p	⁵ D	2	111049.924				
3d ⁷ (⁴ F)4f	(3.5)[1.5]	2	110996.275	10.4	2.0	3	
3d ⁷ (⁴ F)4f	(3.5)[1.5]	1	111000.225	26.2	1.7	3	
3d ⁷ (⁴ F)4f	(3.5)[0.5]	1	111014.319	18.9	2.0	1	
3d ⁷ (⁴ F)4f	(2.5)[4.5]	5	111538.779	5.6	1.5	3	
3d ⁷ (⁴ F)4f	(2.5)[4.5]	4	111543.201	6.5	1.2	3	
3d ⁷ (⁴ F)4f	(2.5)[3.5]	3	111550.344	10.0	2.0	3	
3d ⁷ (⁴ F)4f	(2.5)[3.5]	4	111555.701	10.5	1.6	2	
3d ⁷ (⁴ F)4f	(2.5)[2.5]	2	111556.446	9.3	1.4	4	
3d ⁷ (⁴ F)4f	(2.5)[2.5]	3	111572.695	6.0	3.0	2	
3d ⁷ (⁴ F)4f	(2.5)[1.5]	1	111562.737	8.1	1.4	3	
3d ⁷ (⁴ F)4f	(2.5)[1.5]	2	111602.201	1.7	3.5	4	
3d ⁷ (⁴ F)4f	(2.5)[5.5]	6	111586.397	10.0	2.0	1	
3d ⁷ (⁴ F)4f	(2.5)[5.5]	5	111586.830	11.3	1.7	2	
3d ⁷ (⁴ F)4f	(2.5)[0.5]	1	111622.997	-16.2	0.6	2	
3d ⁷ (⁴ P)5p	³ D	2	111866.302	10.0	4.0	1	
3d ⁷ (⁴ F)4f	(1.5)[3.5]	4	111940.524	9.0	2.0	2	
3d ⁷ (⁴ F)4f	(1.5)[3.5]	3	111949.701	8.9	1.8	3	
3d ⁷ (⁴ F)4f	(1.5)[2.5]	2	111981.033	-0.5	2.8	4	
3d ⁷ (⁴ F)4f	(1.5)[2.5]	3	111984.575	2.8	0.9	1	
3d ⁷ (⁴ F)4f	(1.5)[4.5]	5	112000.519	13.7	1.0	3	
3d ⁷ (⁴ F)4f	(1.5)[4.5]	4	112007.833	15.9	1.6	2	
3d ⁷ (⁴ F)4f	(1.5)[1.5]	2	112036.179	-14.4	1.4	4	
3d ⁷ (⁴ F)4f	(1.5)[1.5]	1	112041.595	-32.5	0.9	4	

Appendix G

Nd-Ar PDL FT Spectra Plots

This appendix contains plots of the Nd-Ar PDL FT spectra of [Table 4.6](#), from lowest wavenumber to highest wavenumber. The x -axis gives wavenumber and the spectrum name is indicated in the x -axis label. The y -axis indicates SNR and any SNR above 40 was placed on the log scale. Each section has a width of 1000 cm^{-1} for spectra A, B, C, and D, and each section has a width of 2000 cm^{-1} for spectra E and F. The total spectral range displayed for each spectrum covers regions with observed spectral lines, this is to demonstrate the choices of PMT and filter combinations list in [Table 4.6](#) to avoid repeated spectrum overlaps when measuring in the second alias ([subsection 3.3.2](#)). The Nd-Ar PDL FT spectra were used for wavenumber measurements of 577 transitions and 188 energy levels of the $4f^3(4f + 5d + 6s + 6p + 7s + 6d)$ configurations of Nd III. To locate a line from [Table D.1](#) in these plots, the spectrum containing its measured wavenumber is indicated by the spectral ranges in [Table 4.6](#). This is because of the line lists merging process ([section 5.6](#)).

As frequently described in the thesis, the spectral regions below $30\,000\text{ cm}^{-1}$ (above 333 nm) are extremely line-rich and high in relative intensity, containing strong transitions of Nd I-III. The spectral regions above $30\,000\text{ cm}^{-1}$ (below 333 nm) are relatively line-sparse and lower in intensities, which mainly consisted of a relatively much smaller number of lines, from Ar I-III, Fe I-II, and transitions between higher-lying configurations of Nd III.

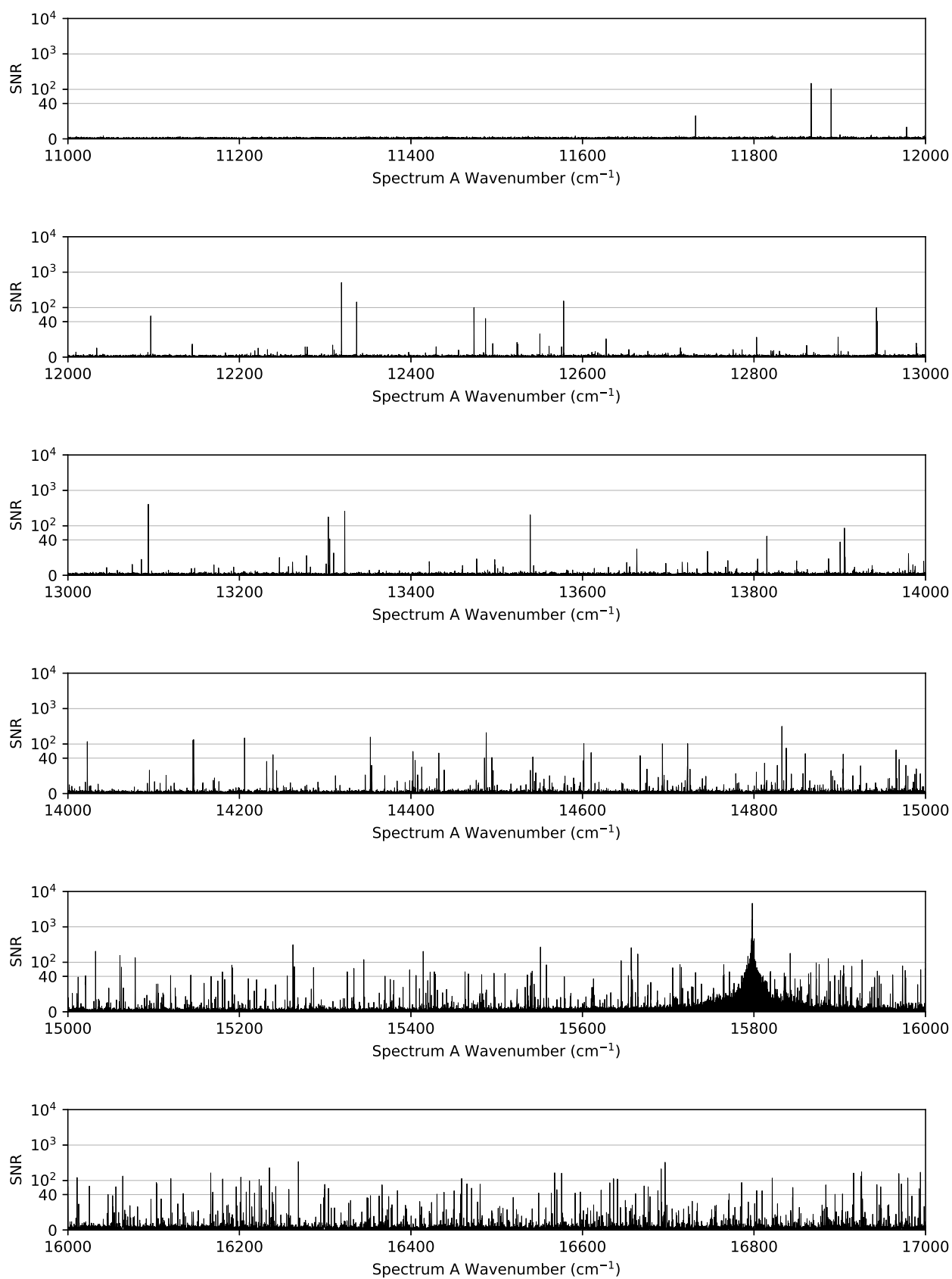


Figure G.1: Nd-Ar PDL FT Spectra Part 1

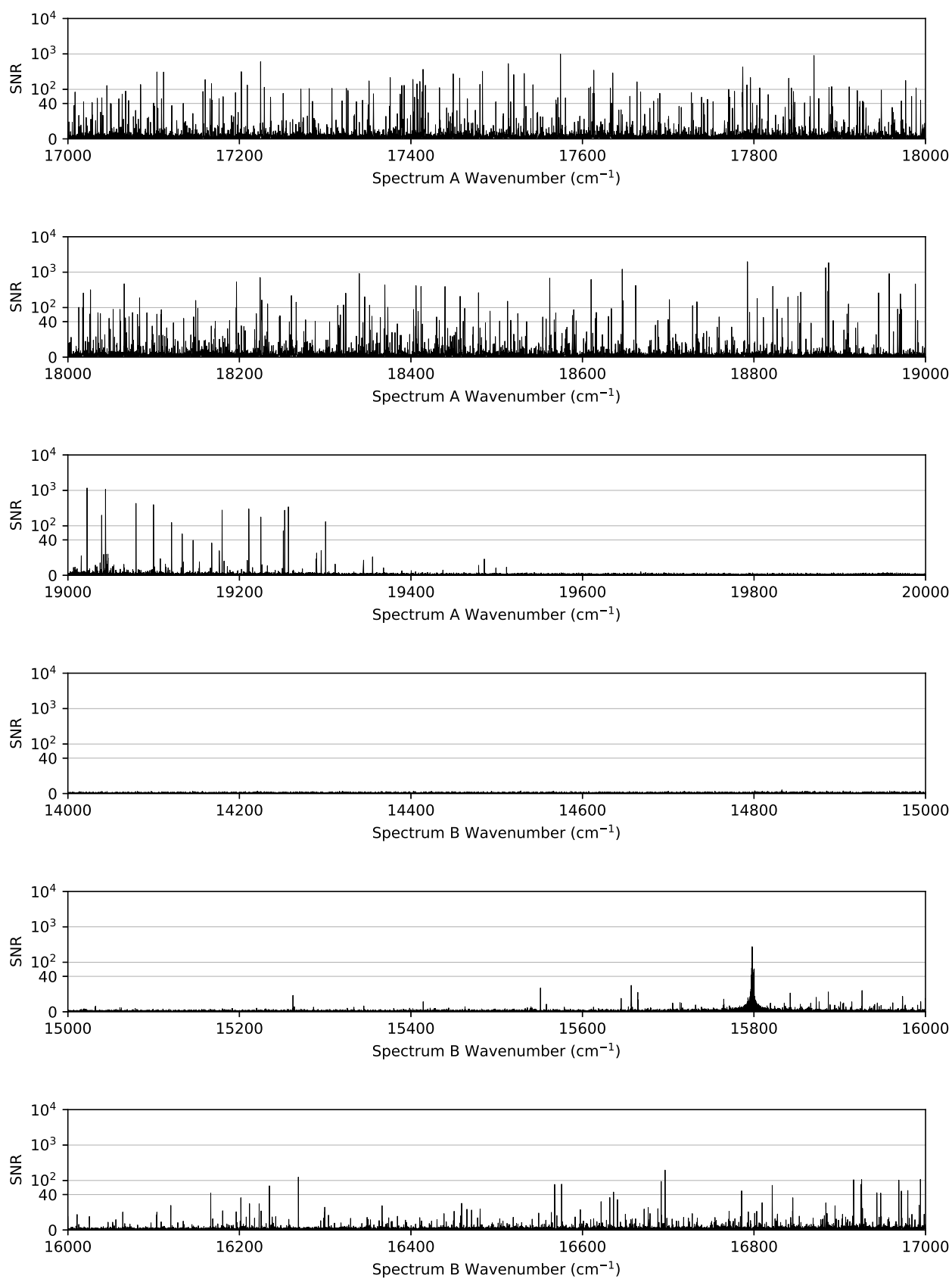


Figure G.2: Nd-Ar PDL FT Spectra Part 2

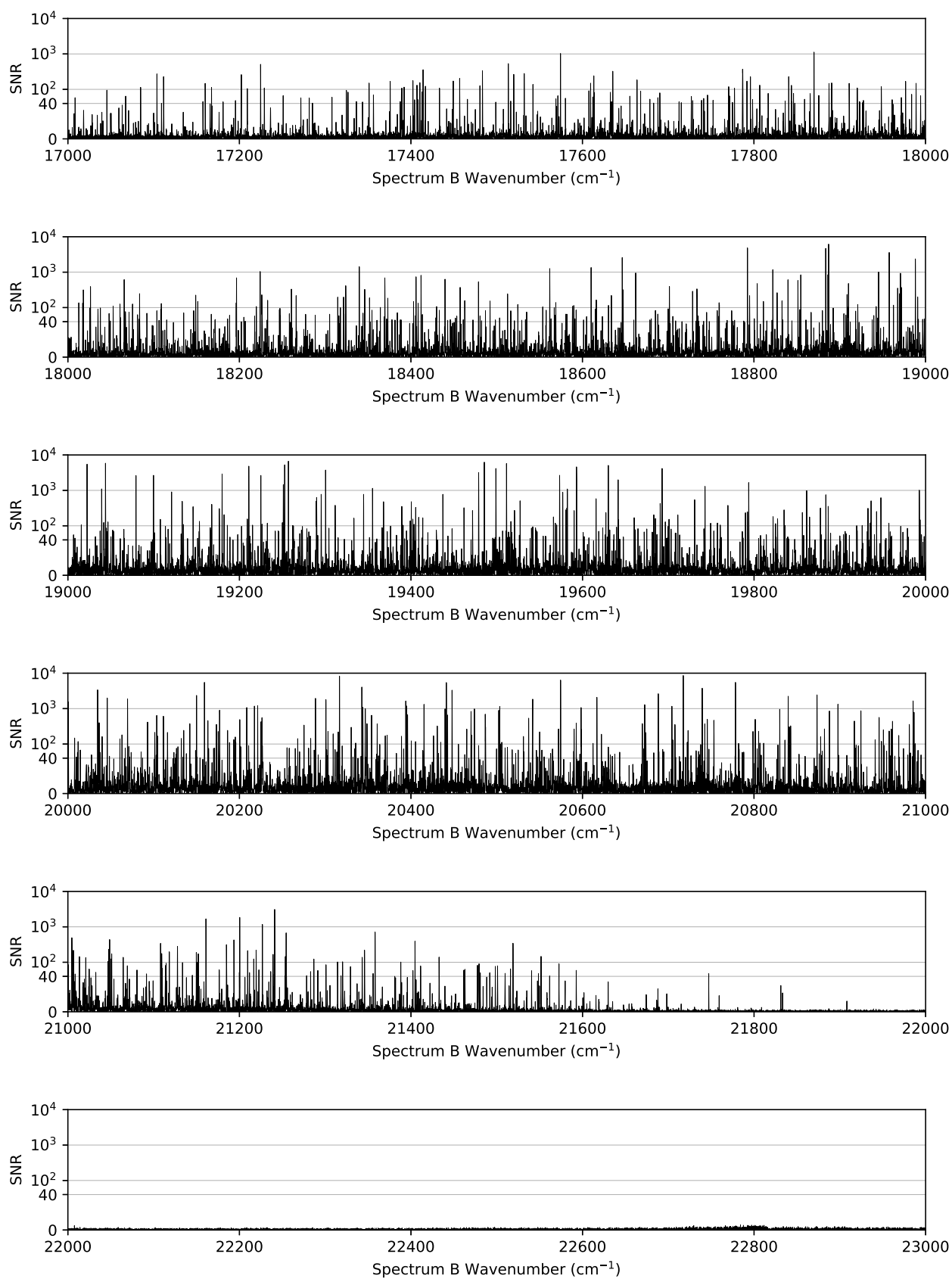


Figure G.3: Nd-Ar PDL FT Spectra Part 3

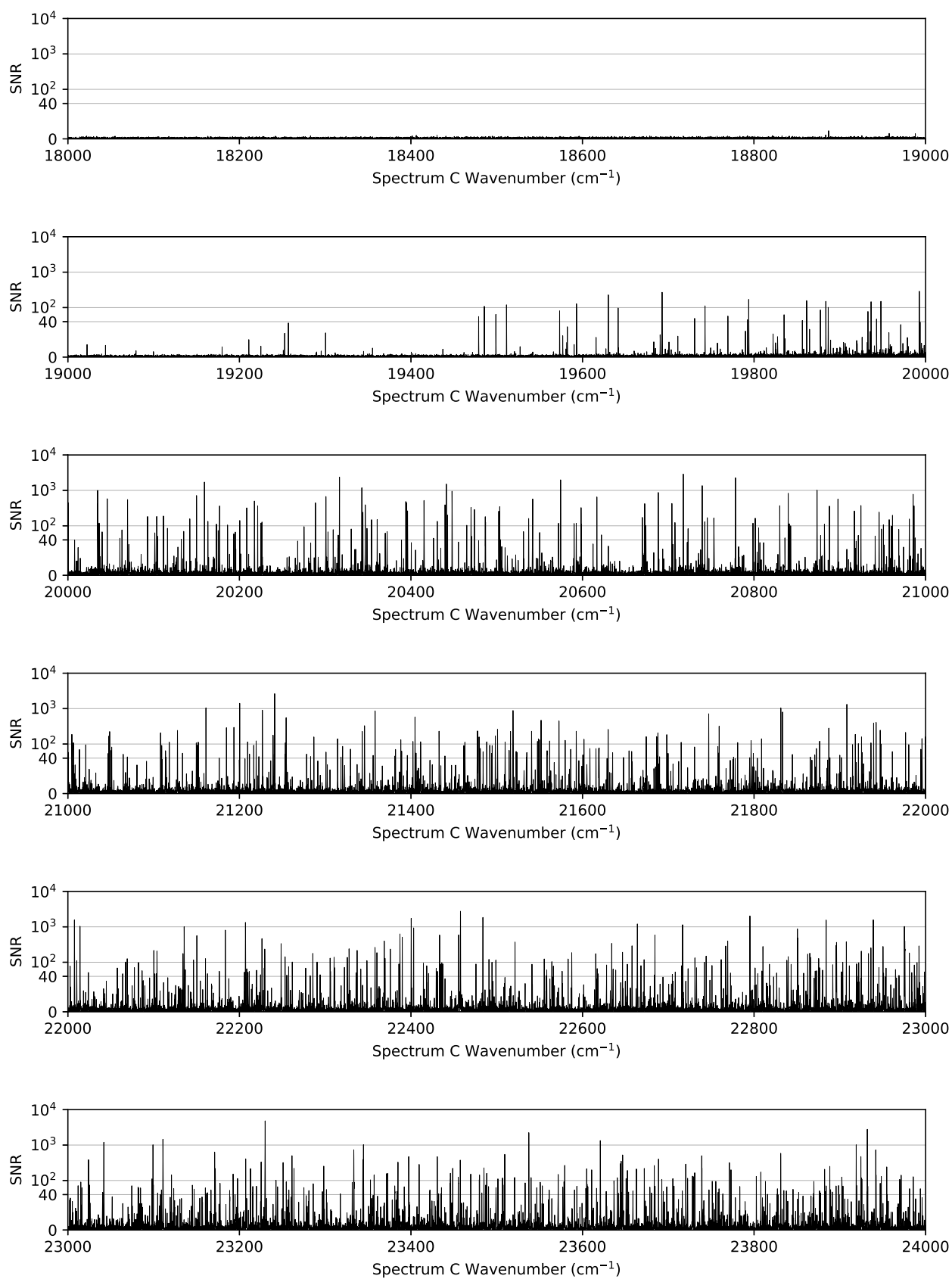


Figure G.4: Nd-Ar PDL FT Spectra Part 4

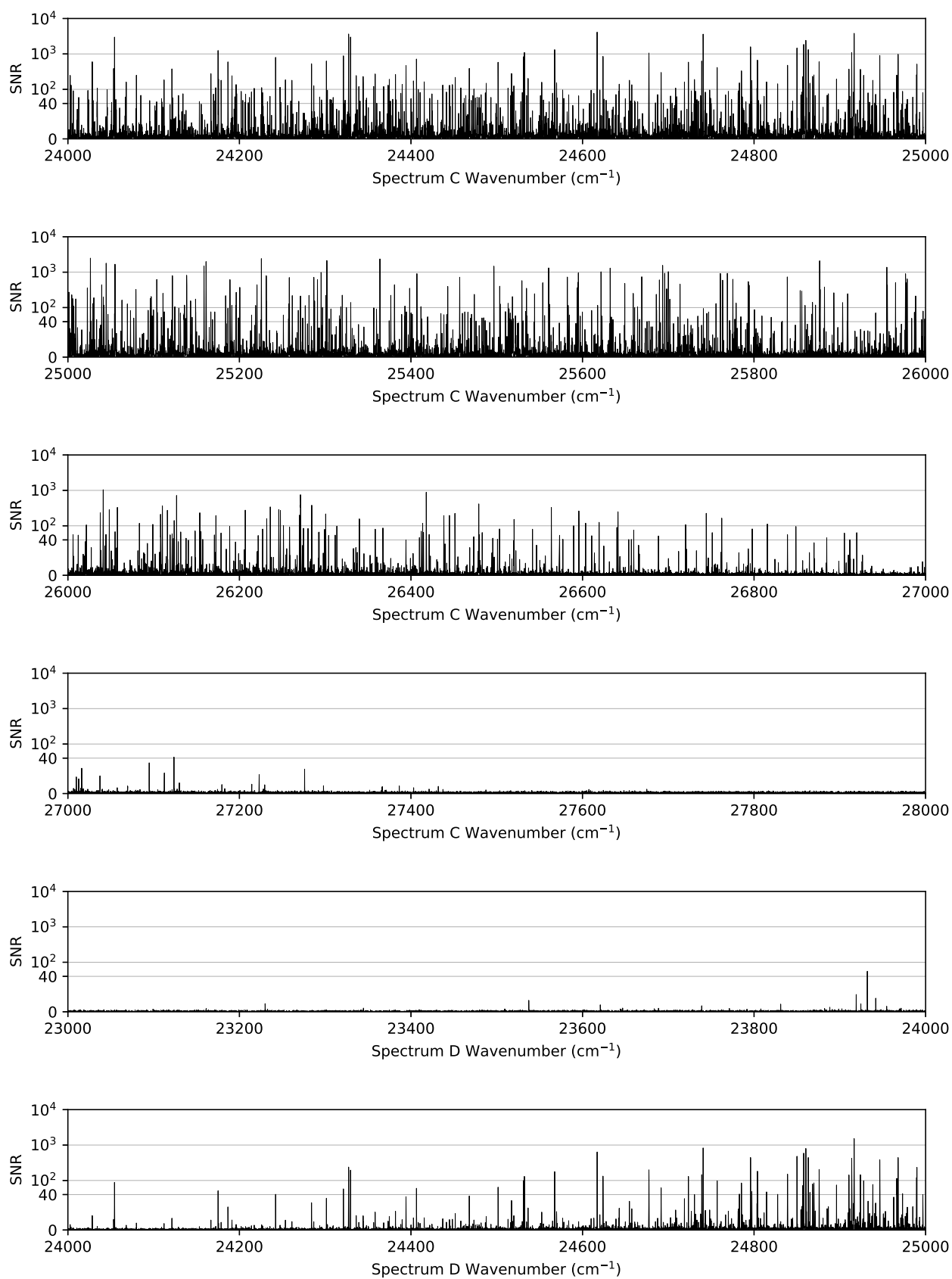


Figure G.5: Nd-Ar PDL FT Spectra Part 5

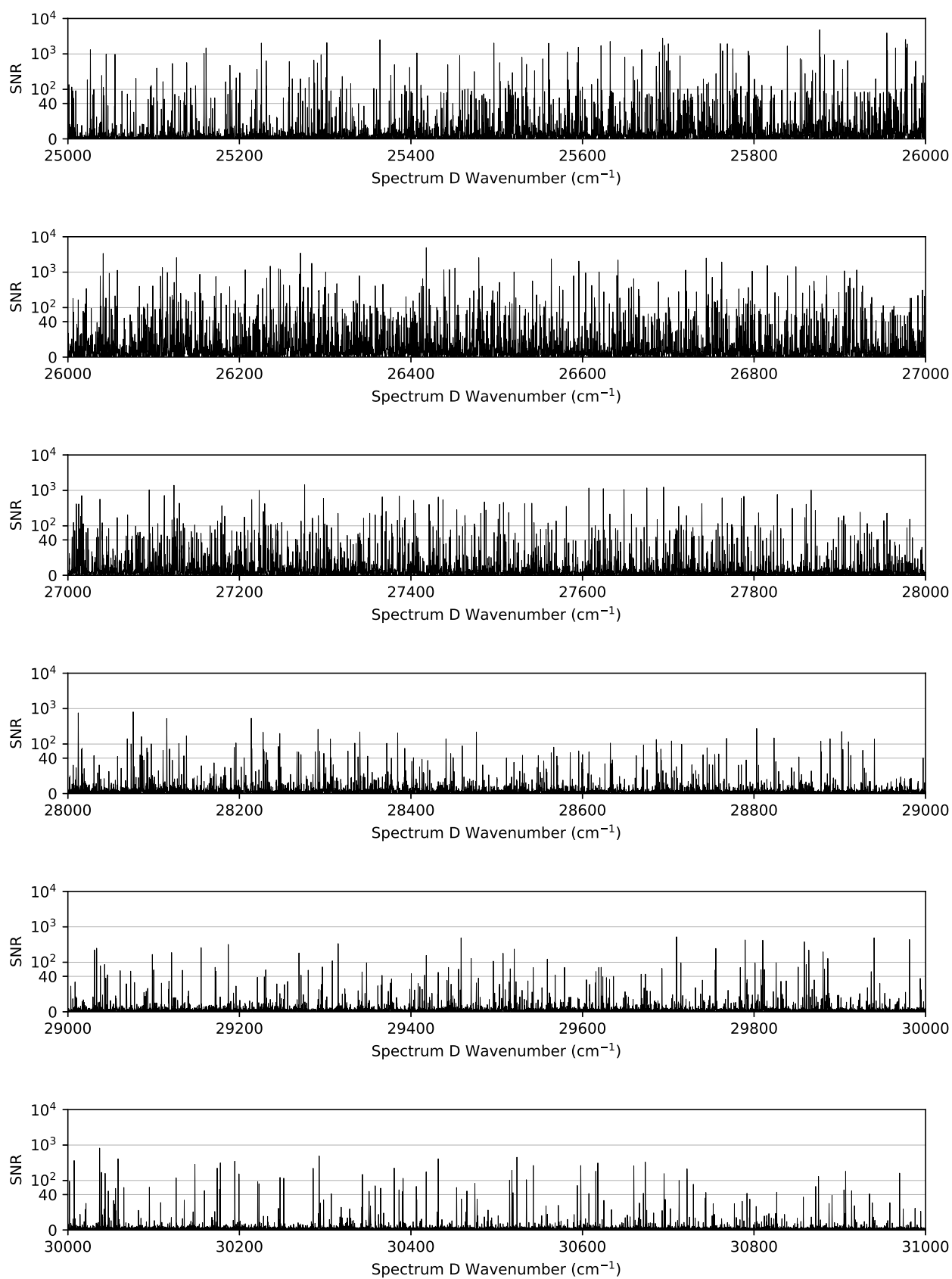


Figure G.6: Nd-Ar PDL FT Spectra Part 6

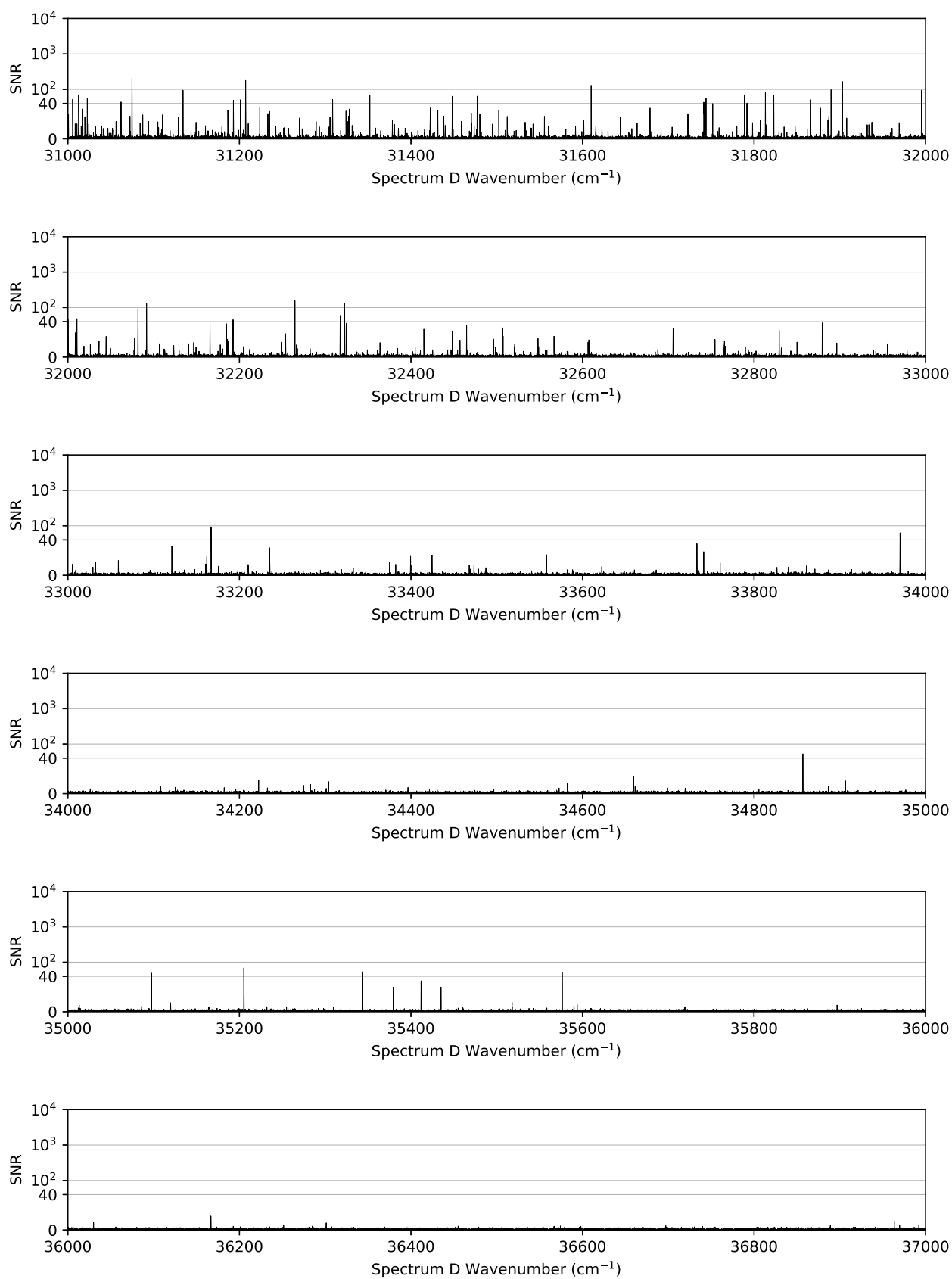


Figure G.7: Nd-Ar PDL FT Spectra Part 7

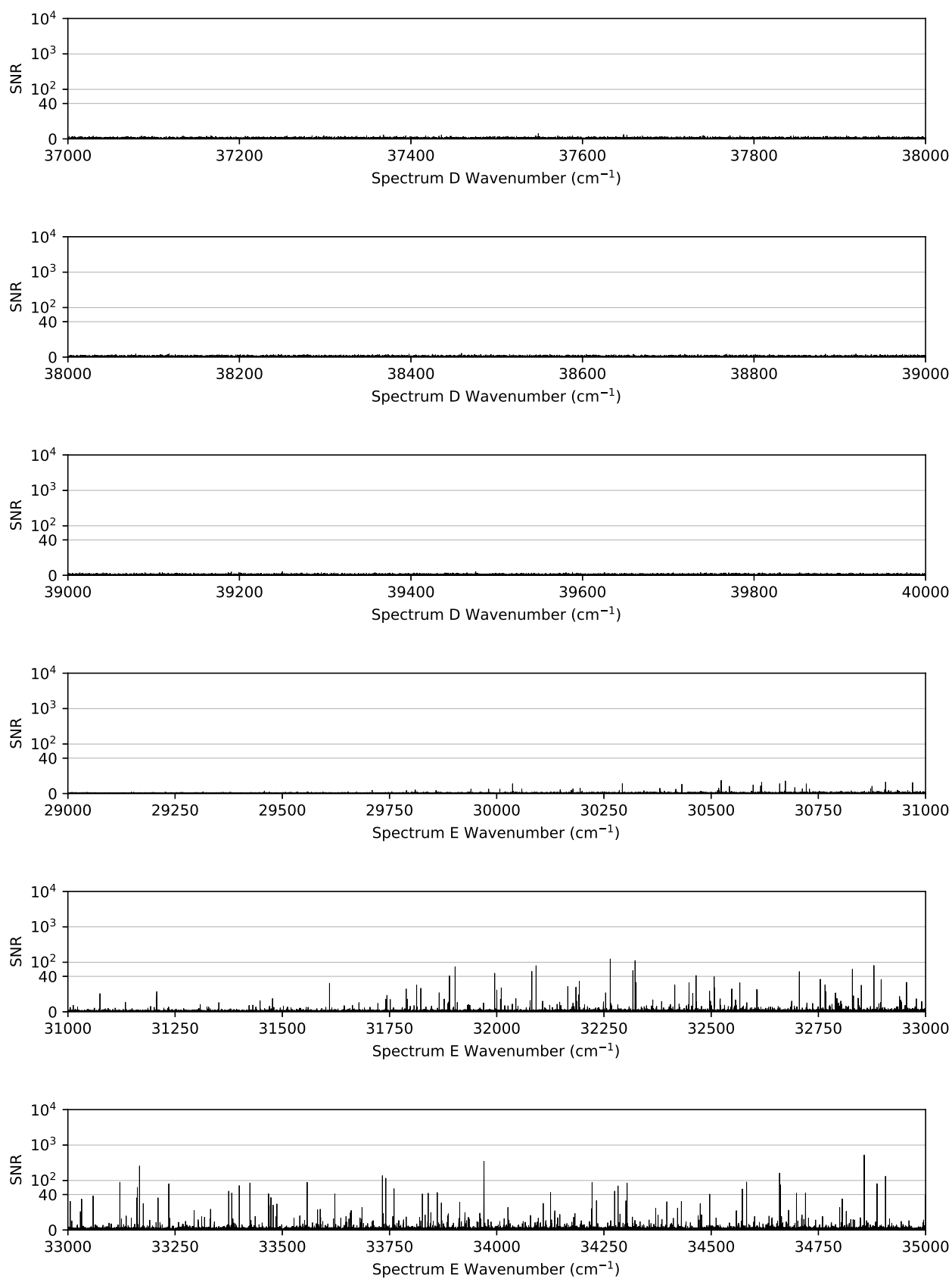


Figure G.8: Nd-Ar PDL FT Spectra Part 8

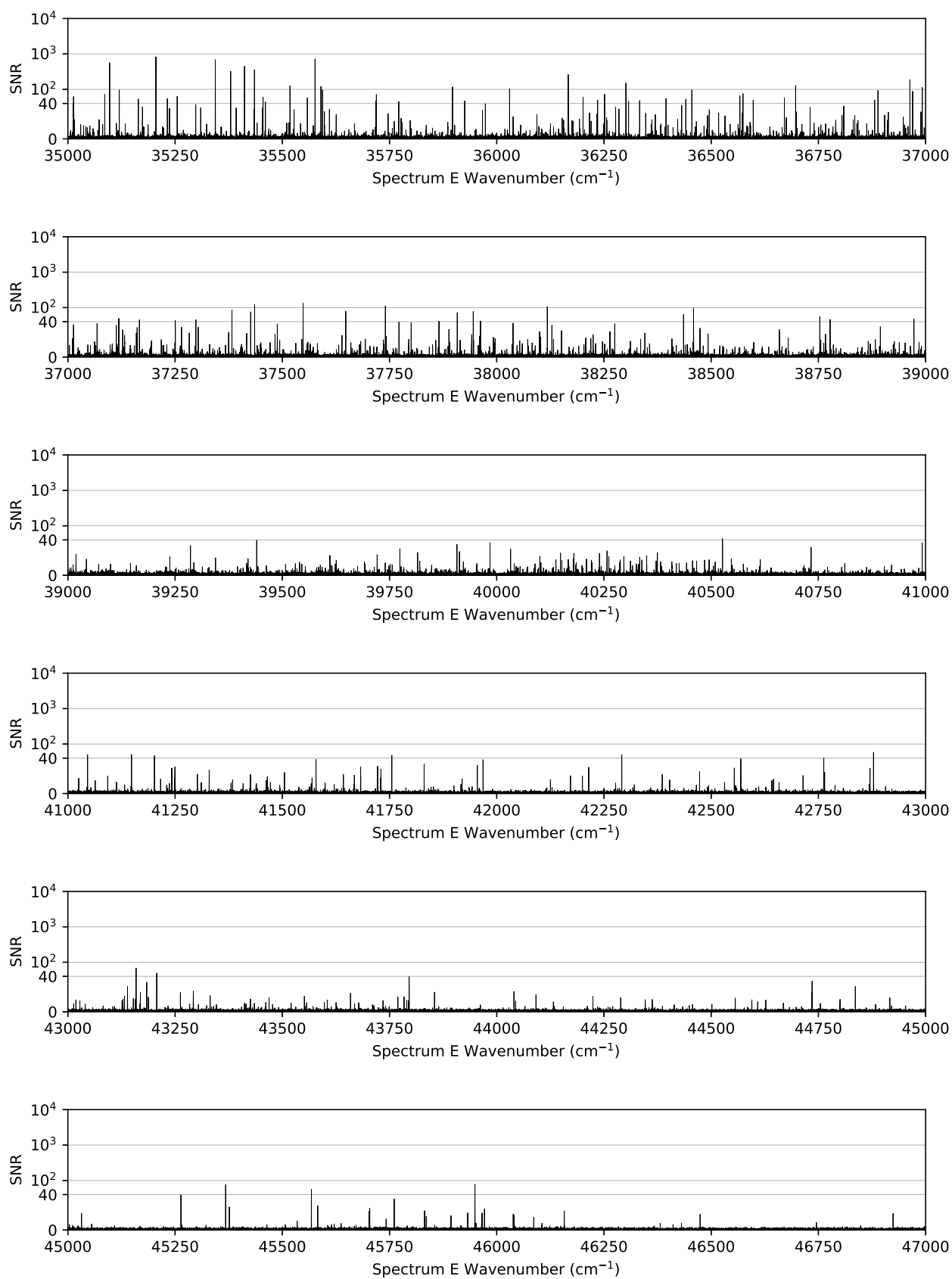


Figure G.9: Nd-Ar PDL FT Spectra Part 9

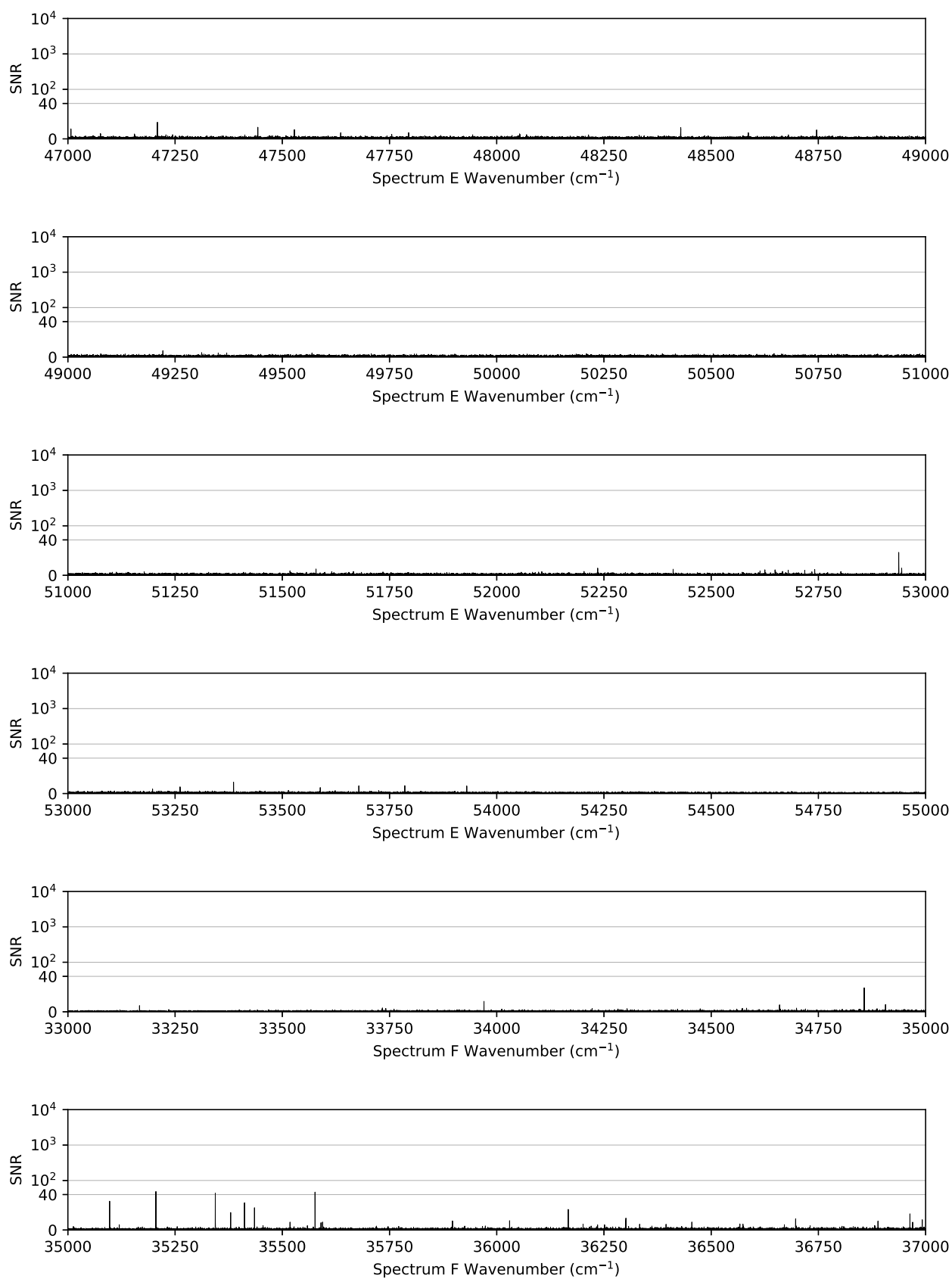


Figure G.10: Nd-Ar PDL FT Spectra Part 10

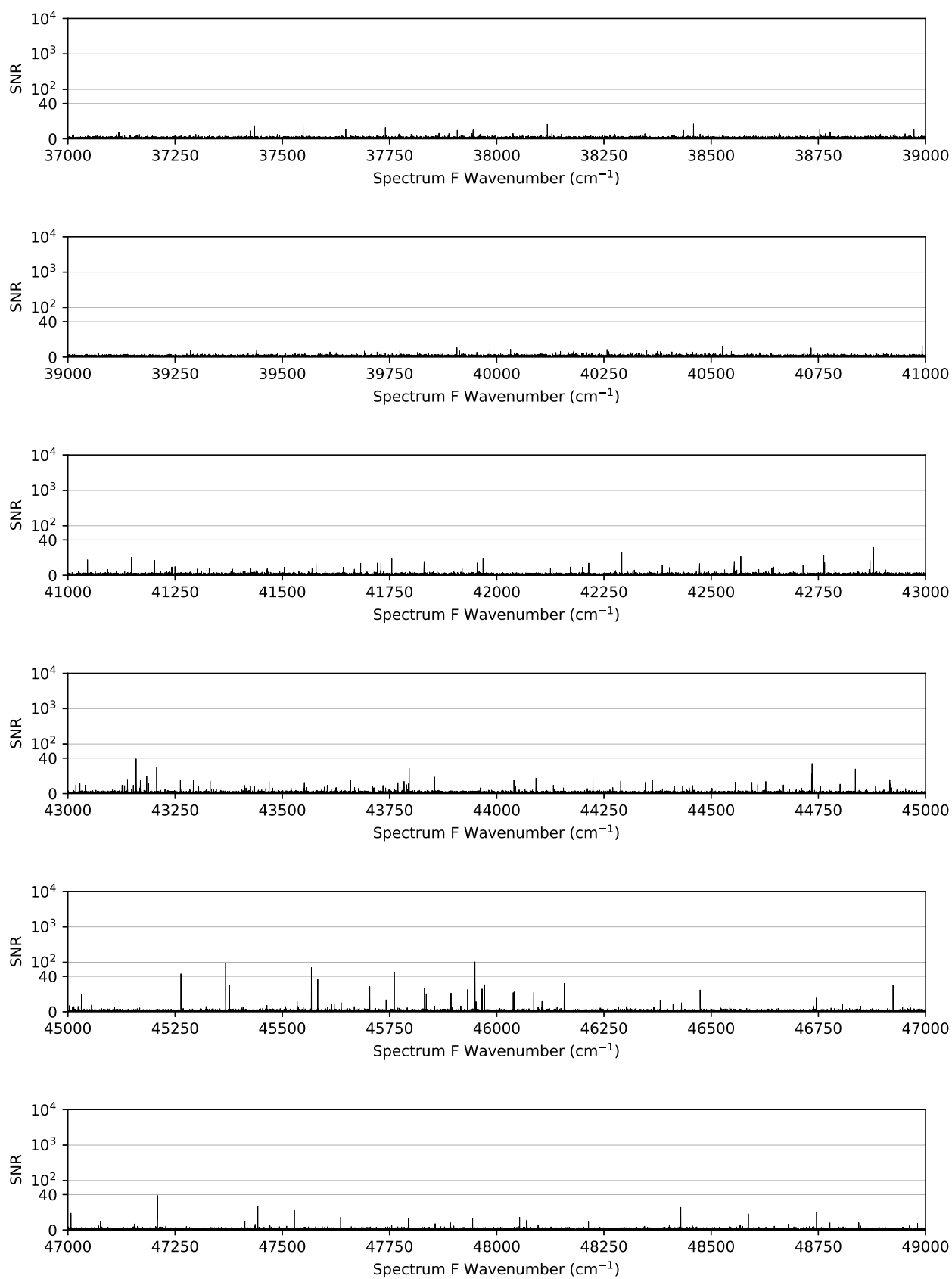


Figure G.11: Nd-Ar PDL FT Spectra Part 11

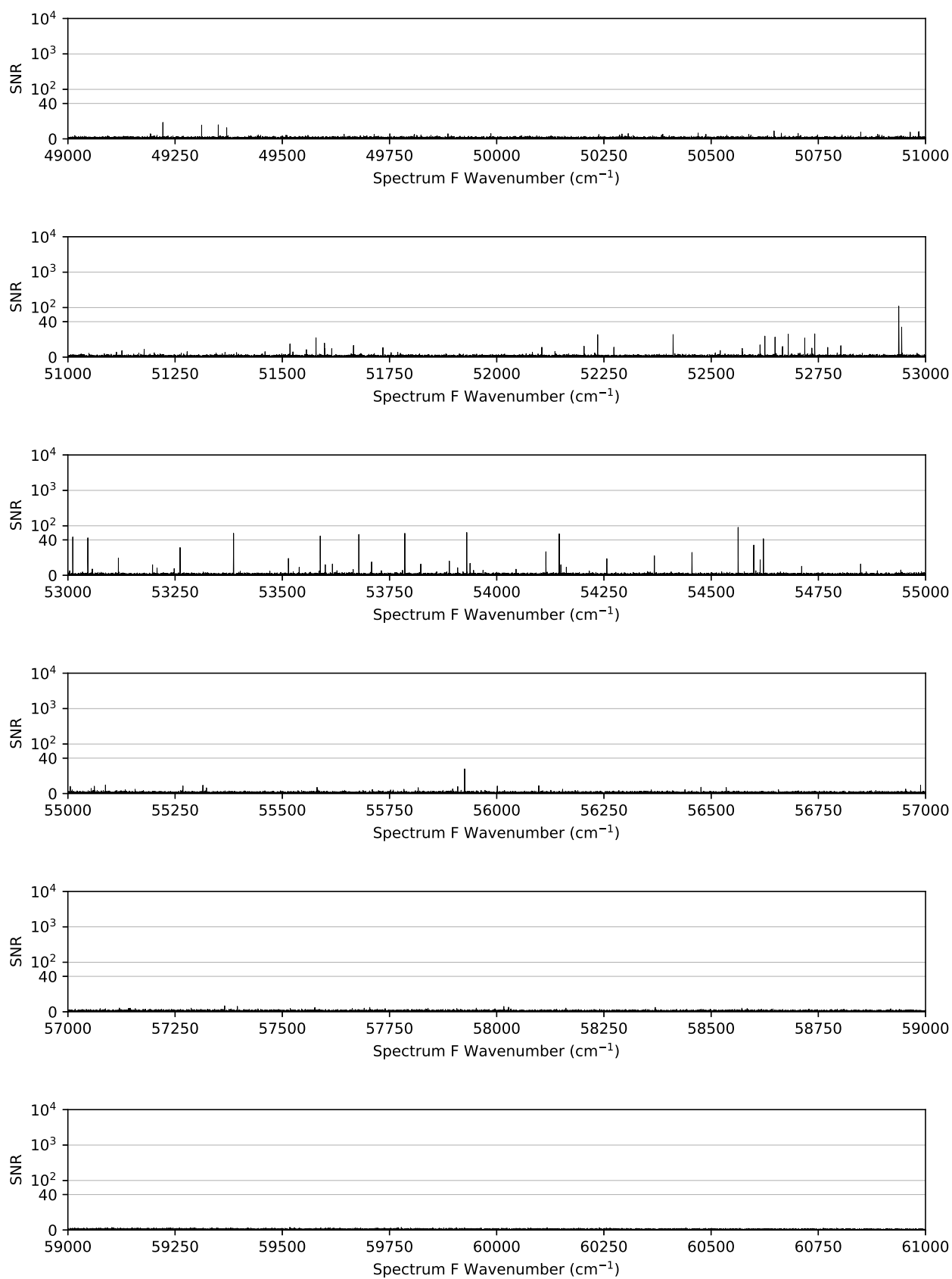


Figure G.12: Nd-Ar PDL FT Spectra Part 12