X-ray Studies of Tri-*o*-thymotide Inclusion Compounds and Related Medium Ring Compounds

A Thesis submitted for the
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by

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ABSTRACT

The *X*-ray structures of ten compounds have been determined. Nine are macrocyclic and contain a central 12-membered ring. Each of these undergoes conformational interconversion between different chiral conformations in solution and some exhibit spontaneous resolution on crystallisation. The other compound is a cyclisation intermediate.

The first four compounds are different structural forms of tri-*o*-thymotide, two are cavity inclusion compounds, one a channel inclusion compound and the other the unsolvated structure. For the inclusion compounds the bounds and dimensions of the inclusion regions have been mapped. Comparisons have been made of the conformations of the tri-*o*-thymotide molecule in these different crystalline environments. These have shown that though the molecule always adopts a propeller conformation, this differs significantly in each of these structures and in all cases shows large deviations from C_3 symmetry.

Two disubstituted trianthranilides studied both adopt helical conformations. A different trans-annular hydrogen bond has been found in each of these structures. The *trans*-amide groups all show characteristic deformations, though in one case the degree of distortion is exceptional. One of these compounds (*N*,*N'*-dibenzyltrianthranilide) forms inclusion compounds and the bounds of the inclusion region have been mapped.

The analyses of two differently substituted trithiosalicylides have shown that they adopt significantly differing conformations in the solid state. This is attributed to packing requirements rather than to internal steric constraints.

The non-cyclised *N*-acylurea compound is a cyclisation intermediate whose structure has given insight into the cyclisation mechanism involved in the formation of differently substituted trianthranilides.

The final compound, a cyclic bislactam, adopts a distorted C_2-propeller conformation. Its failure to adopt C_2 symmetry is attributed to conformational constraints due to the *trans*-stilbenoid fragment of the molecule. Distortions of the amide groups in this and the previous compound have been noted.

Future lines of investigation are discussed.

ACKNOWLEDGEMENTS

Firstly, I wish to thank Professor D. Rogers but for whose foresight and guidance none of this would have been possible. Secondly, I must thank Professor H.M. Powell and Dr. David Lawton who introduced me to the tri-*o*-thymotide problem and who have maintained a keen interest in the progress of these studies. I am also grateful to Professor W.D. Ollis and Dr. Fraser Stoddart of the University of Sheffield for involving me in the studies of the trianthranilides and the trithiosalicylides. Dr. Fraser Stoddart has always been available at the end of the telephone to help and answer even the most trivial of questions and this has been greatly appreciated.

Thanks are also due to past and present members of the IC crystallography group, in particular those responsible for the implementation and maintenance of the program libraries without which nothing would be able to be done. For this I wish to thank in particular Dr. Andrew Quick both when he was here, and subsequently at ULCC.

I thank again Dr. Andrew Quick for his assistance with the structure analyses described in Chapters 7 and 10, and Mrs. Eldrys Gil of the University of Los Andes, Venezuela for help with those in Chapters 8 and 9.

I thank Mr. Glyn Millhouse for photographing the figures in this thesis, and the staffs of the Computer Units of Imperial College and the University of London for their cooperation.

Finally, I give many thanks to my wife for typing this manuscript.

A cautionary tale probably as true
now as when it was first written.

Tri-o-thymotide et al.

This brilliant Thesis is the work of Mister Ivan D.
Submitted 1951 for Honours B.Sc.
The author who, as well you know, is famed for many things,
Perhaps is most outstanding in the field of giant rings.

He synthesises compounds with a merciless intent
(The yields obtained have not as yet exceeded nought per cent).
His skill is quite exceptional - a fact which can't be missed -
Not everyone could work so well on things which don't exist.
And yet, because (one must assume) his modesty is great,
The work of others, in the main, this Thesis will relate.

The air with which he started work was confident and placid,
He took the meta analogue of salicylic acid.
He heated it with this and that, its acetate distilled,
In every case his methods were unquestionably skilled.
Unquestionably skilled, I said, and yet, I say, alack!
In every case he merely got the meta acid back.

Undaunted and unruffled, then he cheerfully began
A synthesis, which went, at first, according to the plan.
He tried to make a lactone (and in trying ne'er despaired)
Related to an isomer which Zealley had prepared.
His failure here so very slight, to only this extends,
He neither got the open chain, nor could he join the ends.

Undaunted still, he persevered, his spirit never waned,
And from dinitrobenzene he successfully obtained
With patient skill, for which he has such universal fame,
A very common compound - azobenzene was its name.

And so perforce we bring this introduction to an end,
And hope that it may warn all those who foolishly intend
In chemistry to make their name, and think it sailing plain,
Remember poor old Dunstan and perhaps you'll think again!

B. GILBERT (1951)

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CHAPTER 1

The crystal structure of the cavity inclusion compound formed by tri-*o*-thymotide with methylene iodide

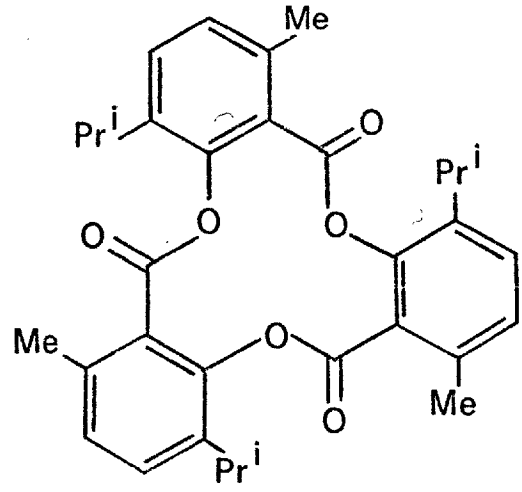
Summary

The title compound crystallises in the trigonal space group $P3_121$ with a = 13.655(5), c = 30.31(1)Å, Z = 6. The structure was solved by the heavy-atom method and refined by full-matrix least squares to R = 0.086 for the 1178 independent diffractometer measured reflections. The molecule (1) adopts a propeller conformation which deviates significantly from C_3 symmetry. The principal cavity in the structure has dimensions of ∿5.7 x 7.6 x 7.9Å and a maximum effective length of ∿9Å. The analysis has also revealed a secondary empty smaller cavity which may be just large enough to hold a small diatomic gas molecule.

Tri-*o*-thymotide, (TOT, $C_{33}H_{36}O_6$, (1)) forms molecular inclusion compounds with a wide range of substances.[1-6] More than 80 compounds have to date been characterised[5,6] and the potential for the formation of further compounds seems virtually limitless. Although these complexes represent a broad spectrum of structural types, (examples have been found in the triclinic, monoclinic, orthorhombic, trigonal and hexagonal crystal systems)[4,5] two principal structural configurations predominate. Complexes with straight chain or simple singly-branched straight chain molecules crystallise in the trigonal or hexagonal systems and, depending on the shape and length of the included molecule, form chiral, cavity or channel structures.[4] The framework of the structures of these two types has been shown to be virtually independent of the included molecules.[4]

The stoicheiometry of the cavity structures is 2 TOT molecules to 1 of guest. The asymmetric unit contains only one TOT molecule, and the requirement for an ordered arrangement of the guest molecule is that it possess a 2-fold axis of symmetry. Methylene iodide both fulfils this requirement and lies close to the maximum size limit for the formation of a cavity complex;[4] it should thus be fairly tightly bound.

We report here an *X*-ray determination of the solid-state conformation of the TOT molecule in the cavity complex formed with methylene iodide, also details of the dimensions and bounds of the cavity. Subsequent papers will describe the channel and unsolvated forms of TOT, also *X*-ray analyses of a range of related chiral medium-ring compounds, some of which also form inclusion compounds.[7] Like TOT, these are conformationally mobile in solution. Their conformational behaviour, in particular the dynamics of ring inversion, have been



(1)

studied by n.m.r. analysis and proposals made for their solid-state conformations.[8-13] It is hoped in the course of these studies to gain some insight into the reasons for the propensity of TOT to form such a wide range of inclusion compounds. A preliminary comparative account of the conformations of TOT in different crystalline environments has been reported.[14]

EXPERIMENTAL

As TOT has a great affinity for a wide range of molecules, including iodine, purity of the starting materials when crystallising the complexes is important.

Methylene iodide was purified by fractional distillation (b.p.182°) over activated copper turnings. Crystals of the complex were obtained by warming crystals of pure unsolvated TOT[2] in methylene iodide until fully dissolved, sealing, and allowing to cool slowly in the dark. Clear hexagonal prisms of the adduct formed readily. They were identified as being of the trigonal cavity form by their ready (001) cleavage, and by the presence of a transverse plane of symmetry in the diffraction pattern and a repeat distance of ~ 13.6Å in single-crystal oscillation photographs taken about a.[4]

Crystal Data[4] $C_{33}H_{36}O_6.\frac{1}{2}(CH_2I_2)$, M = 662.6, Trigonal, a = 13.655(5), c = 30.33(1)Å, U = 4898Å^3, D_m = 1.347gcm^{-3}, D_c = 1.347gcm^{-3}, Z = 6, $F(000)$ = 2034. Space-group $P3_121$(No. 152) or enantiomorphous $P3_221$ (No. 154), from the Laue symmetry and systematic absences. Cu-K_α radiation, $\bar{\lambda}$ = 1.54178Å, μ(Cu-K_α) = 82.3 cm^{-1}.

A crystal of dimensions 0.27 x 0.34 x 0.27 mm^3 was cut from a larger block and mounted along its a_2 axis. As this adduct, like other halogenated complexes, has a high overall temperature factor

(B estimated $\sim 8.7\text{Å}^2$) and suffers fairly rapid radiation damage, only a limited data set was collected. Data were measured on a Siemens off-line four-circle diffractometer using Ni-filtered Cu-K_α radiation. A total of 1178 independent reflections (an unique twelfth of reciprocal space), to $\theta = 40^\circ$, were measured using the $\theta - 2\theta$ scan technique with the 'five-value'[15] measuring procedure. Of these, 90 reflections had $I < 2.58\sigma(I)$ and were classed as unobserved.[15] The net count of the 300 reflection, measured as a reference every 50 reflections, did not alter significantly during the data collection (2 days), thus tending to indicate that there had been no significant deterioration. On the other hand a noticeable pink discolouration of the crystal had occurred. The reference reflection chosen was obviously insensitive to the decomposition taking place. The data were scaled and corrected for Lorentz and polarisation factors; no absorption corrections were applied at this stage.

Solution and Refinement of the Structure

The structure was solved by the conventional heavy-atom method. A three-dimensional, sharpened, origin-removed vector map gave sharp peaks corresponding to the vectors between symmetry related iodine atoms. The derived iodine position was refined ($R = 0.40$) and structure factors, phased on this position, (assuming the space-group to be $P3_121$) were used to compute an electron-density map. This, together with subsequent difference maps, gave the positions of all 39 non-hydrogen atoms of the TOT molecule, but failed to show up the carbon of the methylene iodide; this point will be discussed later. The 40 atoms were refined isotropically by full-matrix least-squares, reducing R to 0.137. At this stage allowance was made for the anomalous scattering due to the iodine atom. Refinement with the

complex component of the anomalous scattering factor (f'') for iodine positive increased R to 0.145; refinement with f'' negative resulted in a reduction of R to 0.122, clearly indicating that the crystal chosen contained the mirror molecule in the mirror space-group $P3_221$. (The coordinate list refers to $P3_121$). Further refinement allowing the iodine atom to refine anisotropically reduced R to 0.106.*

A difference map revealed two pairs of sharp peaks within the cavity of density $\sim 1.5 e\text{Å}^{-3}$ and distant ~ 1.5Å from the iodine. Their height and positions, in particular their closeness to the iodine atoms made it unlikely that they could be attributed to the missing methylene carbon. They lay well off the two-fold axis which the methylene iodide molecule straddles and in these positions, were they partial carbon atoms, could only be of 1/4 weight and thus incompatible with the observed electron density. Refinement, treating them as partial carbons caused their temperature factors to go negative, thus confirming this conclusion. They were thus interpreted as partial iodine atoms and estimated at 5% each. Refinement with iodines at fixed 5% occupancy in each position, and with a consequent reduction to 90% of the main iodine position, gave good convergence and resulted in realistic temperature factors for the partial atoms. (R fell to 0.086). A difference map then showed no peak in the cavity region greater than $0.5 e\text{Å}^{-3}$. Further refinement, attempting to interpret the residual electron density in terms of partial methylene carbons, was unsuccessful.

In view of the limited diffraction data none of the atoms of the TOT molecule was refined anisotropically, nor were hydrogens allowed for.

* In subsequent refinements the 0 0 3 reflection for which $|F_o| \ll |F_c|$, was suspected of being affected by extinction and was removed.

Inspection of the bond lengths at this stage revealed some particularly poor values, *e.g.* 1.29Å for the aromatic C(11)-C(16) bond in ring A. The data were corrected for absorption to see if this would bring about an improvement. The correction was performed by the method of Busing and Levy[16] with a Gaussian grid of 10 x 10 x 10 points, and with crystal path lengths determined by the procedure of Coppens *et al.*[17] Subsequent refinement, though not reducing R, did produce a small improvement in the bond lengths (*e.g.* C(11)-C(16) = 1.32Å, *cf.* 1.29Å), also an overall reduction of $\sim$ 3% in the positional e.s.d's. Refinement was terminated at a final R value of 0.086.

Unit weights were used throughout the refinements. Atomic scattering factors were taken from ref. 18. Anomalous scattering factors for iodine were taken from ref. 19. The computations were carried out on the Imperial College IBM 7094 and CDC 6400, and the University of London CDC 6600 and 7600 computers using, in the main, programs belonging to the *X*-ray 63 and 70 systems.[20]

RESULTS AND DISCUSSION

The observed and calculated structure factors are listed in Appendix I. The final fractional atomic coordinates and thermal parameters together with their estimated standard deviations are listed in Table 1. Figure 1 shows a stereo view of the TOT molecule (ORTEP[21]). Figures 2a, b show the bond lengths and angles, also the numbering scheme used. Figure 3 shows the values of the torsion angles around the central 12-membered ring, and Figure 4 the Newman projections[22] looking down each of the three aromatic-isopropyl bonds. Table 2 lists selected trans-annular and intramolecular distances, and Table 3 intermolecular contacts $\leq$ 3.6Å. Figure 5 shows a stereo view[21] of the packing of the host framework of TOT molecules in the

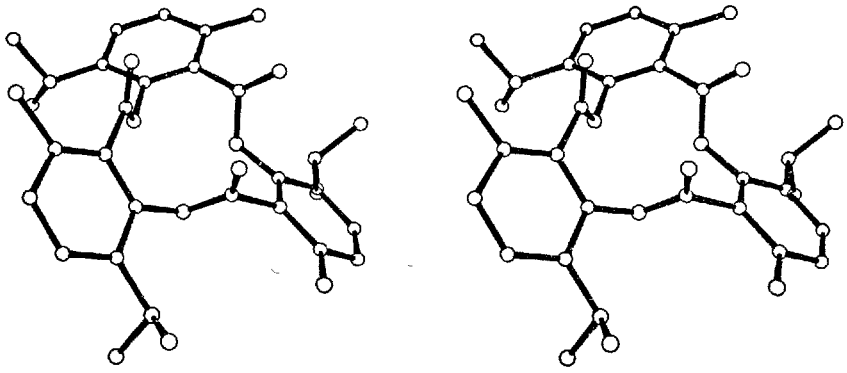


Figure 1. Stereo view of the tri-*o*-thymotide molecule.

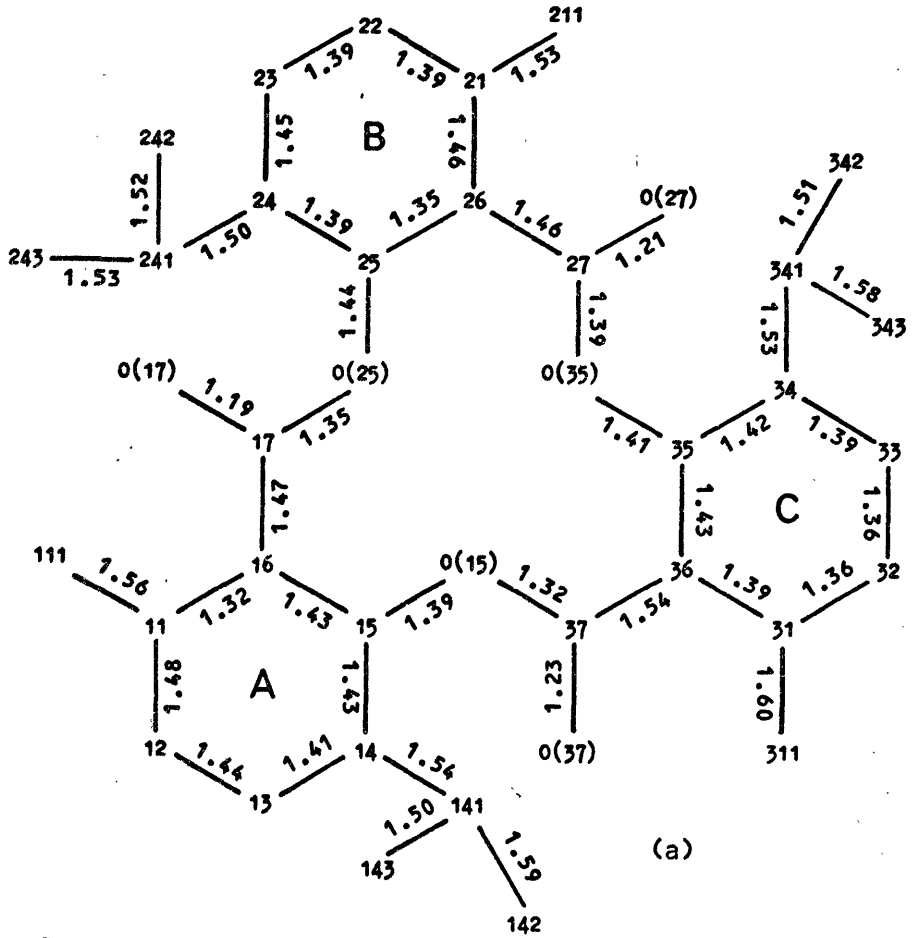


Figure 2(a) Bond lengths and numbering scheme (isopropyl methyl carbons nos. 142, 242 and 342 are on the same side of the central ring as the carbonyl oxygens); (b) valence angles. E.s.d's for bond lengths ∿.04Å, for angles ∿2.5°.

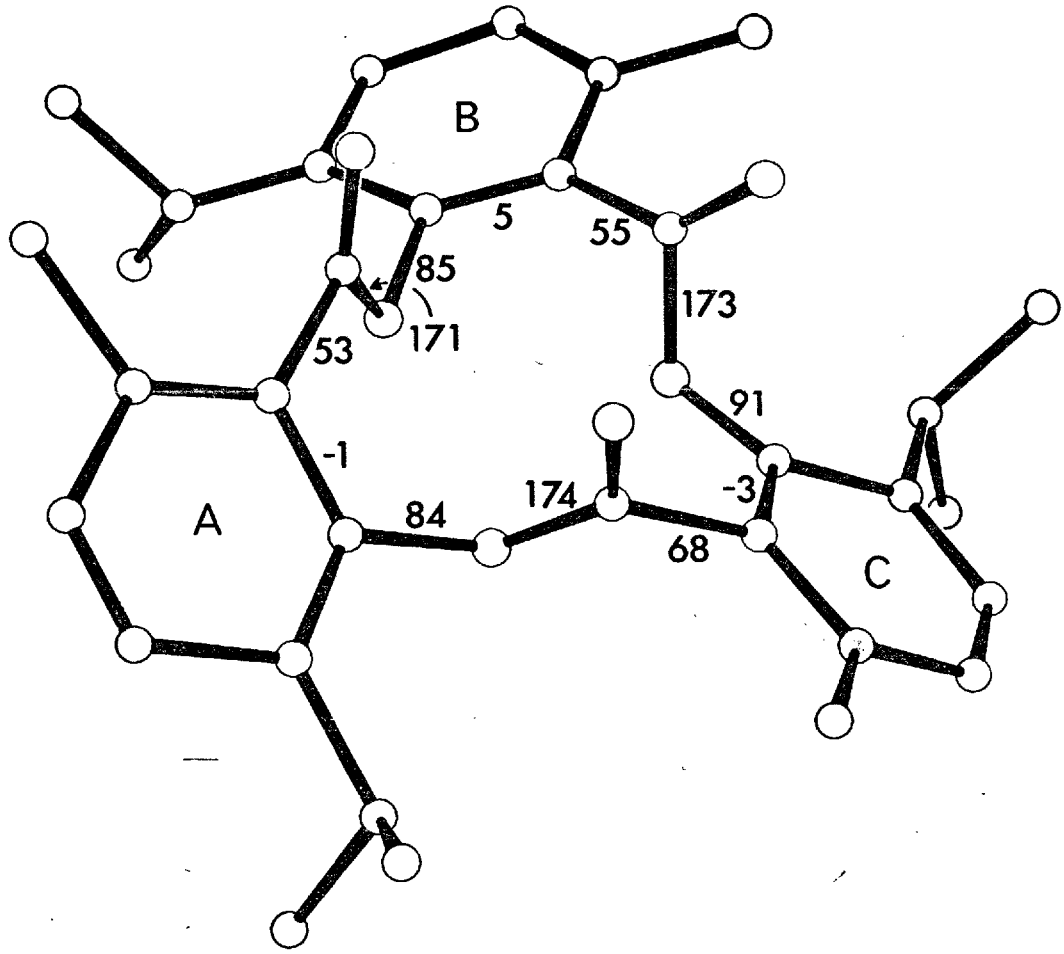


Figure 3. Torsion angles for the 12-membered ring.

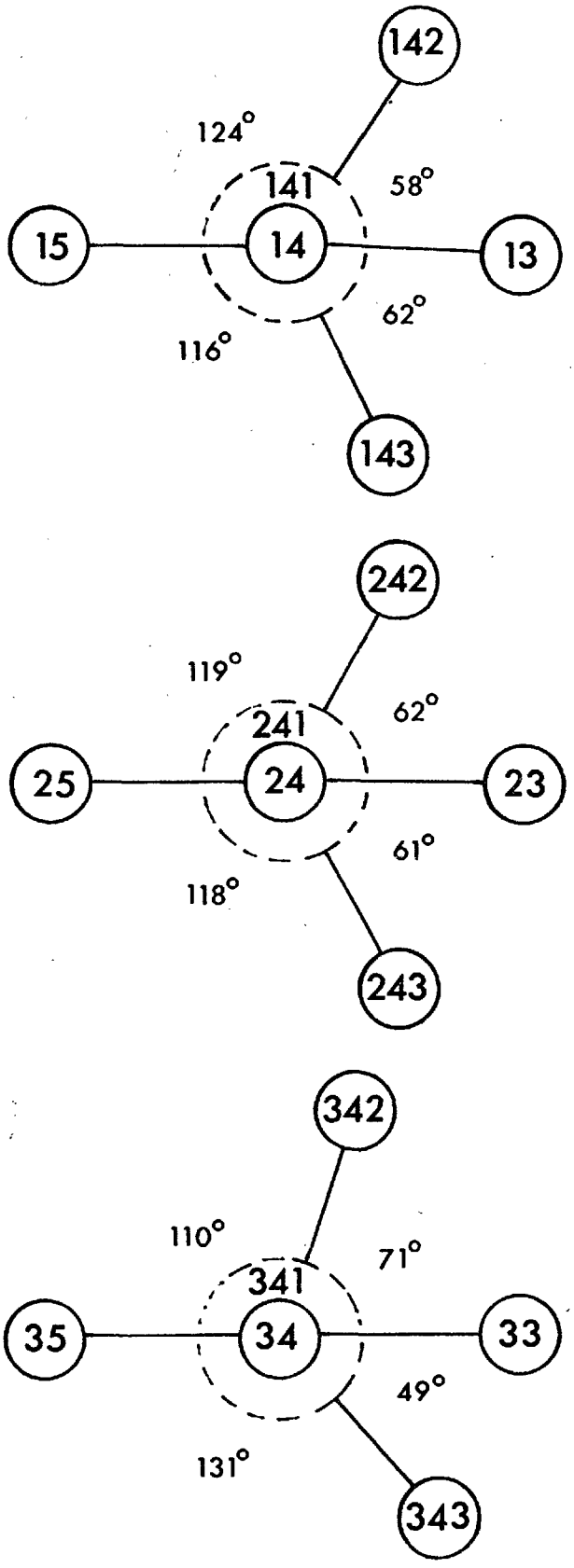


Figure 4. Newman projections down each of the three aromatic-isopropyl bonds.

unit cell.

The molecule adopts a propeller conformation (Fig.1), *i.e.* all three carbonyl oxygens lie on the same side of the central 12-membered ring. This confirms the conclusions of previous analyses which were based on dipole-moment measurements[23] and n.m.r. spectra.[8,9] The torsion angles (Figs.3 and 4) and trans-annular distances (Table 2) both show there are the characteristic departures from C_3 symmetry we have observed in other TOT structures,[14] though in this case the limitations of the data preclude detailed discussion.

The bond lengths and angles (Fig.2), though of limited accuracy, do not depart seriously from expected values, the majority being within 2σ. The reasons for the limitations of the accuracy are two-fold: (i) the low resolution of the data, and (ii) the dominance of the iodine atoms ($\Sigma Z_I^2/\Sigma Z_{C,O}^2 = 1.7$). The latter effect is aggravated by the fact that the iodines are the least well defined atoms in the structure. Errors occurring in the application of the absorption correction seem unlikely because of the simple hexagonal morphology.

The finding in the structure of partial iodine atoms does, however, pose a question of possible interpretations. The largest separation between any two partial atoms (2.99Å) is too short for them to belong to a differently oriented methylene iodide molecule. Two interpretations seem plausible: one, that they are due to free iodine which, despite the precautions, may have been present in small quantities in the starting solution and was trapped on crystallisation; the second, that they are iodine molecules produced by photochemical degradation of the methylene iodide brought about by the *X*-ray irradiation. We discount the former possibility because the inter-nuclear separation is too short, (I_2 has an I-I separation of 2.66Å)[25] and favour the latter, as it also explains the observed pink dis-

colouration of the crystal. A reaction of the type:-

$$CH_2I_2 + h\nu \rightarrow CH_2 + I_2$$

could be occurring, a likely product of which is the triplet state iodine $^3\Pi_{0u}^+$, which has a calculated nuclear separation of 3.016Å,[24] very similar to the value we observed. We think, however, that the lifetime of this state would be too short for it to be observed in the *X*-ray analysis and that it is likely that a more stable ionised form is present, the identity of which we have not been able to determine. Iodine-iodine distances ∿ 3Å have been found in ionised iodine compounds.[25] An embarrassing feature of one of these partial iodines is its close proximity to the carbonyl oxygen, O(37) (2.74Å). This, however, may not be a true separation in view of the high thermal parameter for the oxygen (U = 0.145Å^2). This value suggests that the oxygen atom may be disordered by being forced into a position of clearance in the ∿ 10% of cavities that contain 'free iodine'.

The packing of the TOT molecules of the framework, though involving two fairly short intermolecular contacts (C(13)...O(35) = 3.28Å and C(12)...O(35) = 3.04Å), is consistent with van der Waals interactions. Study of the three-dimensional arrangement of the TOT molecules does not give any immediate insight into how or why these molecules key together to produce a stable host structure. The environment of the guest molecule is discussed later.

Absolute Stereochemistry

An important feature of the TOT molecule is that, though it does not possess asymmetric centres, it is chiral, and in any one crystal of the complex the molecules are all of the same chirality. As described earlier, the anomalous scattering due to the iodine atoms was used to determine which of the two enantiomorphous space-groups

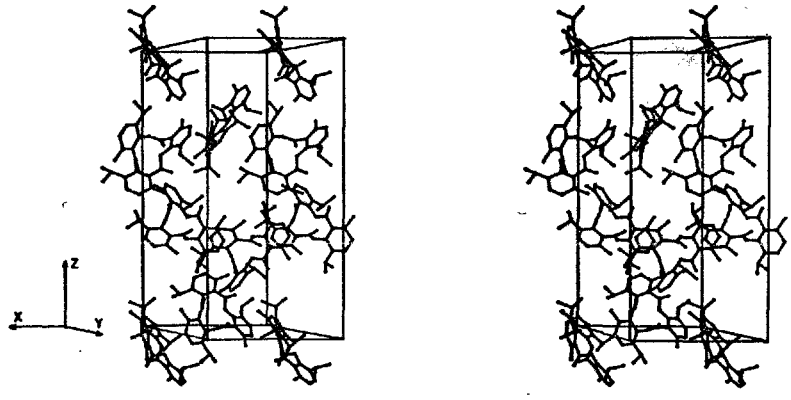


Figure 5. Stereo view of the packing of the host framework.

correctly described the particular crystal with which we were working. The determination of the chirality of the structure and hence that of the TOT molecules in the crystal studied, is of no chemical significance as, in both solution and in the unsolvated solid state TOT is a racemate. It is only resolved when it crystallises to form a complex. As the included molecule in this case was optically inactive, the chirality found was due solely to the TOT molecules and is thus merely a consequence of the crystal we happened to choose for the analysis, there being a likelihood of choosing one of either chirality. In the case of an optically active included molecule the analysis takes on a different significance, as the determination of the chirality of the structure then relates a particular chirality of host to that of the guest.[3,26]

The Cavity

The bounds of the cavity were determined by plotting, at $\frac{1}{2}$Å intervals up the *c* axis, the van der Waals sections of the atoms in the cell. Figure 6 shows the contour map thus derived (contours are at $\frac{1}{2}$Å intervals starting at Z = 0). Only half the cavity is shown, there being a crystallographic two-fold axis running as indicated through the cavity at Z = 0. Figure 7 shows the sectioned van der Waals spheres, at Z = 0, of all the atoms bounding the cavity, also the iodine atoms (broken circles). Figure 8 shows an outline of the largest section normal to the two-fold axis and gives selected dimensions. Figure 9 shows the corresponding sectioned van der Waals spheres of the iodines and the bounding atoms with their identities. Figure 10 shows the outline section in the plane parallel to the two-fold axis and perpendicular to that in Figure 7, and Figure 11 the corresponding sectioned contacts and iodine positions. From the

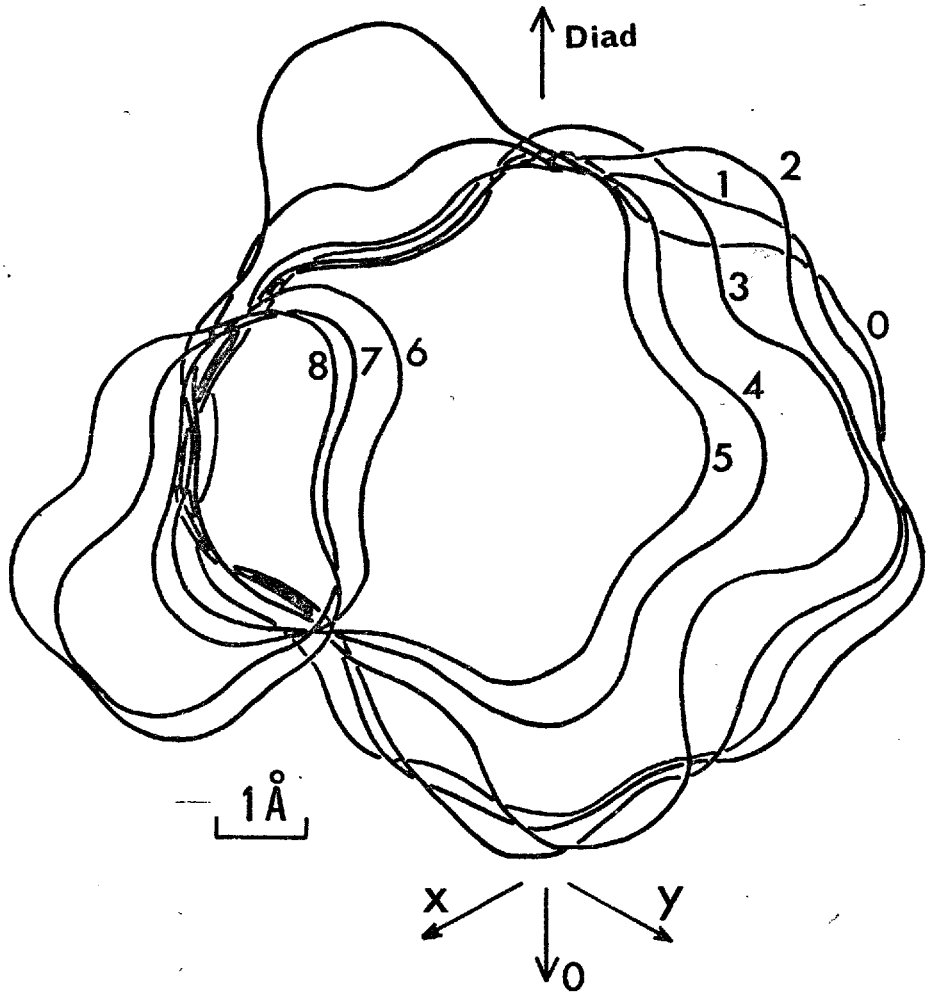


Figure 6. Contour map of the bounds of the cavity. Contours are at $\frac{1}{2}$Å intervals.

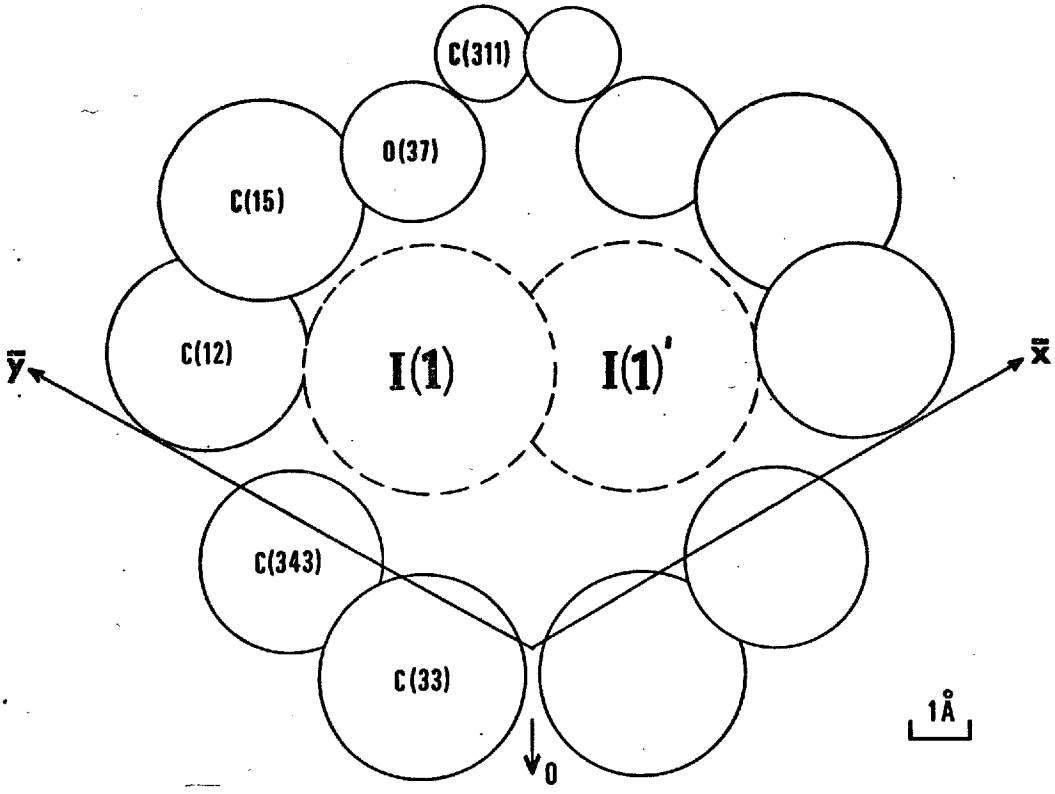


Figure 7. Identities and sectioned van der Waals spheres of the atoms bounding the cavity in the plane normal to c at $z = 0$.

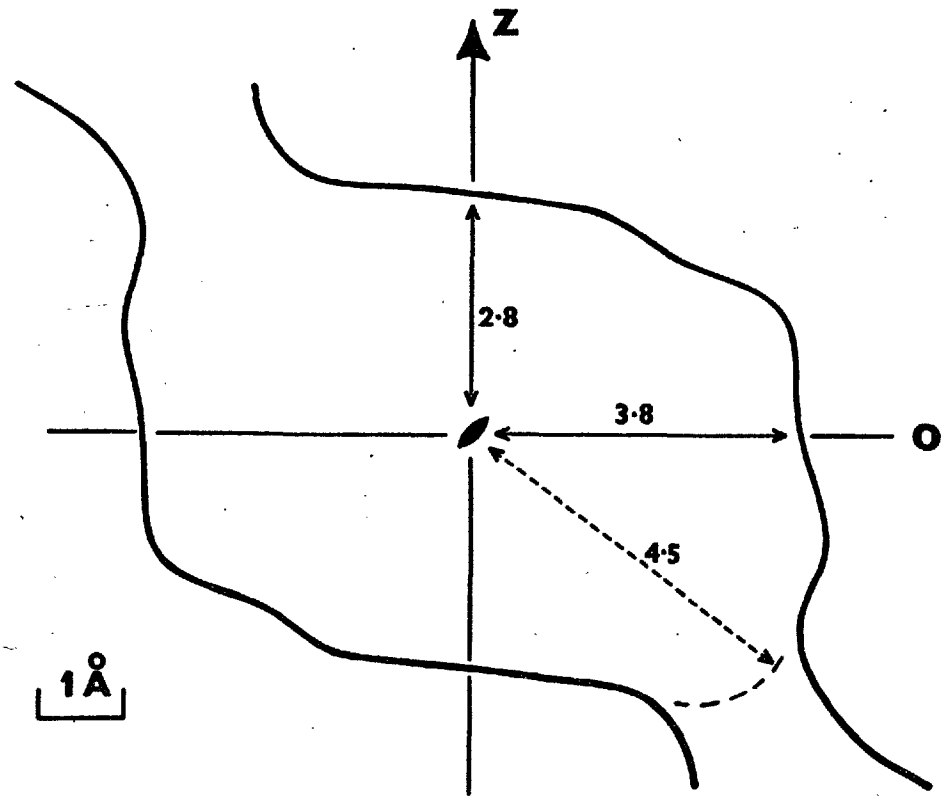


Figure 8. Outline section of cavity normal to the two-fold axis.

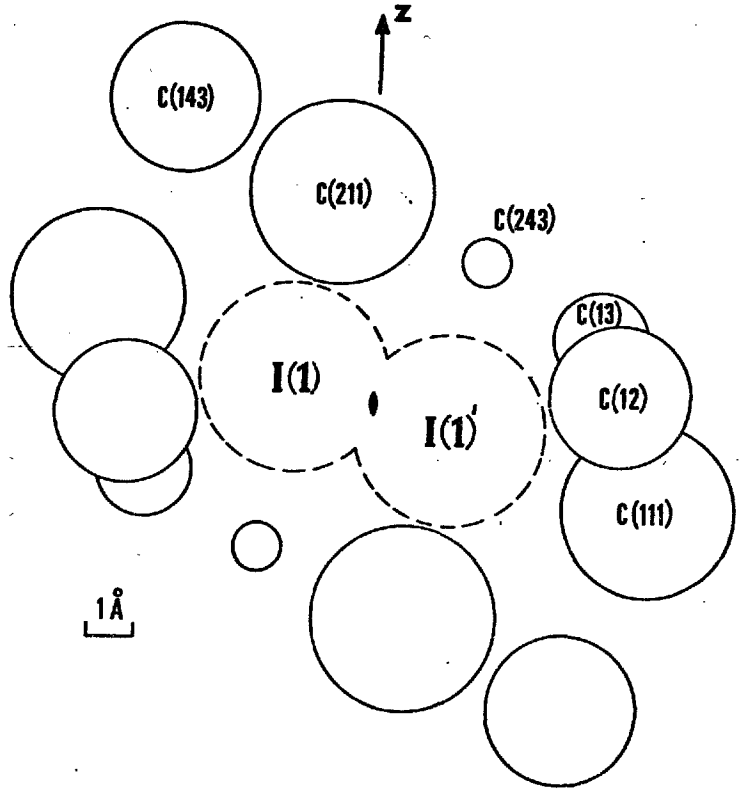


Figure 9. Identities and sectioned van der Waals spheres of the bounding atoms for the section shown in Figure 8.

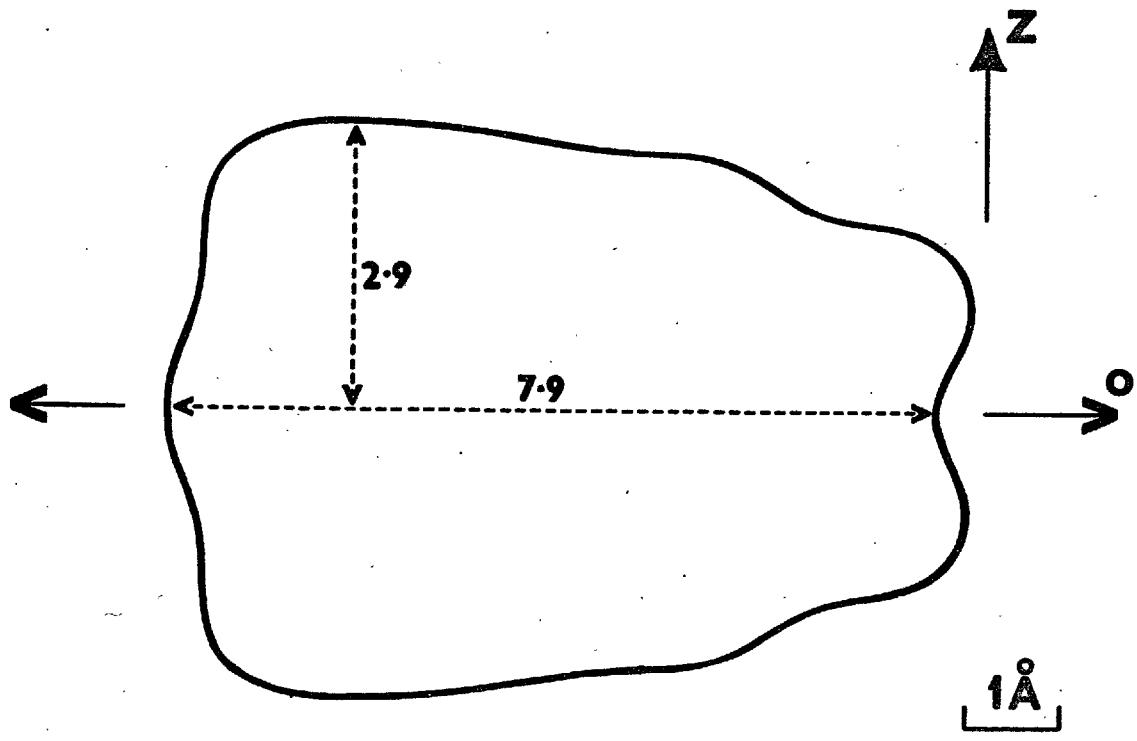


Figure 10. Outline section of cavity perpendicular to that shown in Figure 7.

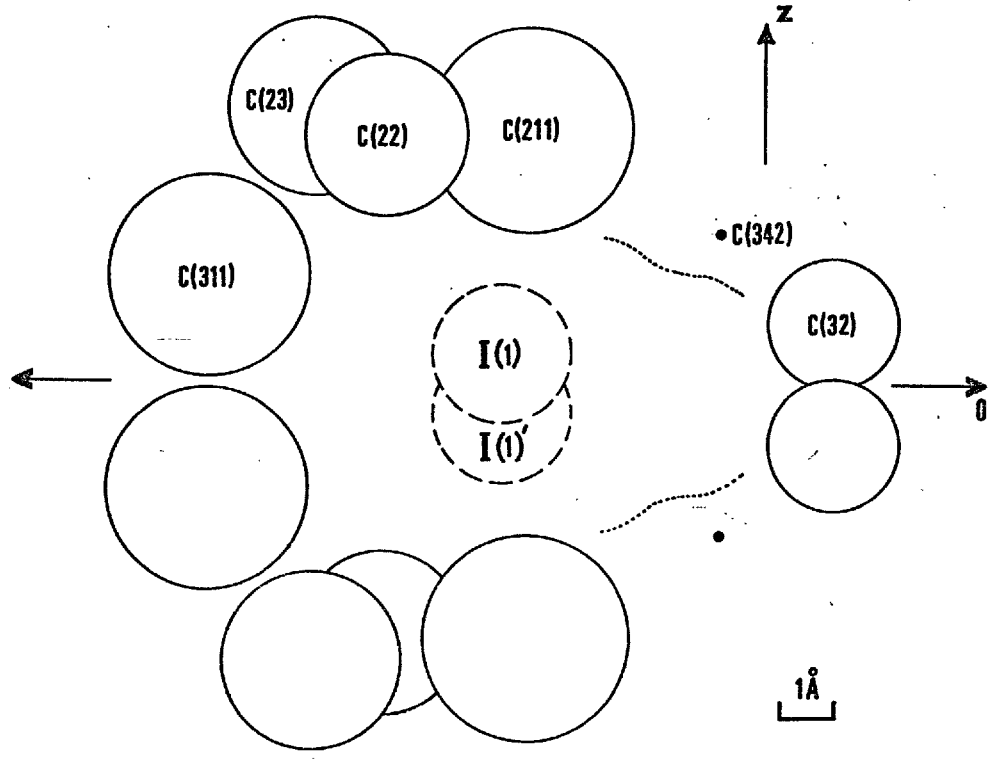


Figure 11. Identities and sectioned van der Waals spheres of the bounding atoms for the section shown in Figure 10.

above sections, the cavity can be seen to have height, width, and depth of ∿ 5.7, 7.6 and 7.9Å respectively, and a maximum effective length of ∿ 9Å which compares well with the value of 9.5Å estimated by Lawton and Powell.[4]

The major limiters of the cavity are: the aromatic ring C(11)-C(16) which by symmetry flanks two sides; the methyls and isopropyl methyls C(111), C(143), C(211), C(243), C(311), C(342) and C(343) which, together with the ring carbons C(22) and C(33), plug the top and bottom of the cavity, and the other two sides. The carbonyl oxygen O(37) also plays a major role in limiting, in one direction, the depth down the two-fold axis. This oxygen has the shortest contact to the iodine (3.62Å) and is noteworthy also in having, as mentioned earlier, a very much larger 'thermal' parameter than any of the other oxygens in the structure.

Figure 12 shows a stereo view[21] of the molecules surrounding the cavity, and the iodines of the included methylene iodide molecule. Figure 13 is a projection down the two-fold axes showing how the cavities spiral up the 3_1 screw axes. The linking neck between the bottom of one cavity and the top of another narrows to a window of ∿ 1.75Å by 3.75Å thereby preventing anything passing through the structure. Figure 14 shows the corresponding projection down *c*, the contours showing the points of maximum and minimum width together with their heights up *c* in Å. The link between the cavities can be seen to be well away from the three-fold axis. The narrow linking neck widens, as can be seen from these figures, to form a small secondary empty cavity centred on the two-fold axis at 1/6th in *c*. This cavity is found on inspection to be just large enough to accommodate two spheres of ∿ 2.5Å diameter about 1Å apart. It is debatable whether it would be possible to have this cavity filled as the only

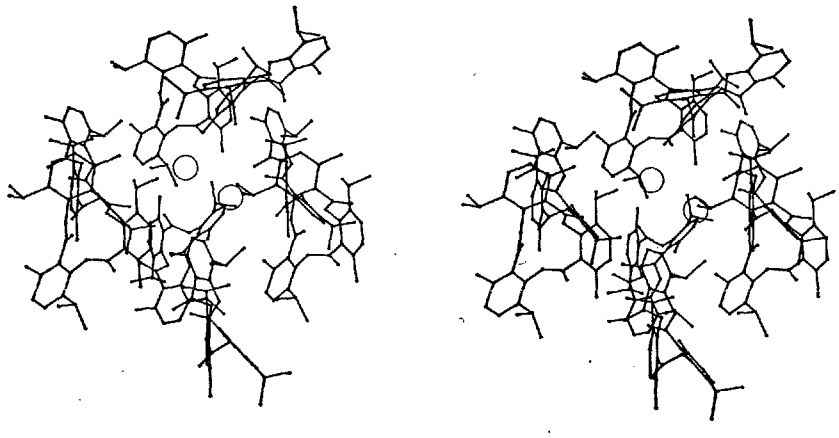


Figure 12. Stereo view of the molecules bounding the cavity, showing the environment of the iodines (large circles) of the included methylene iodide molecule.

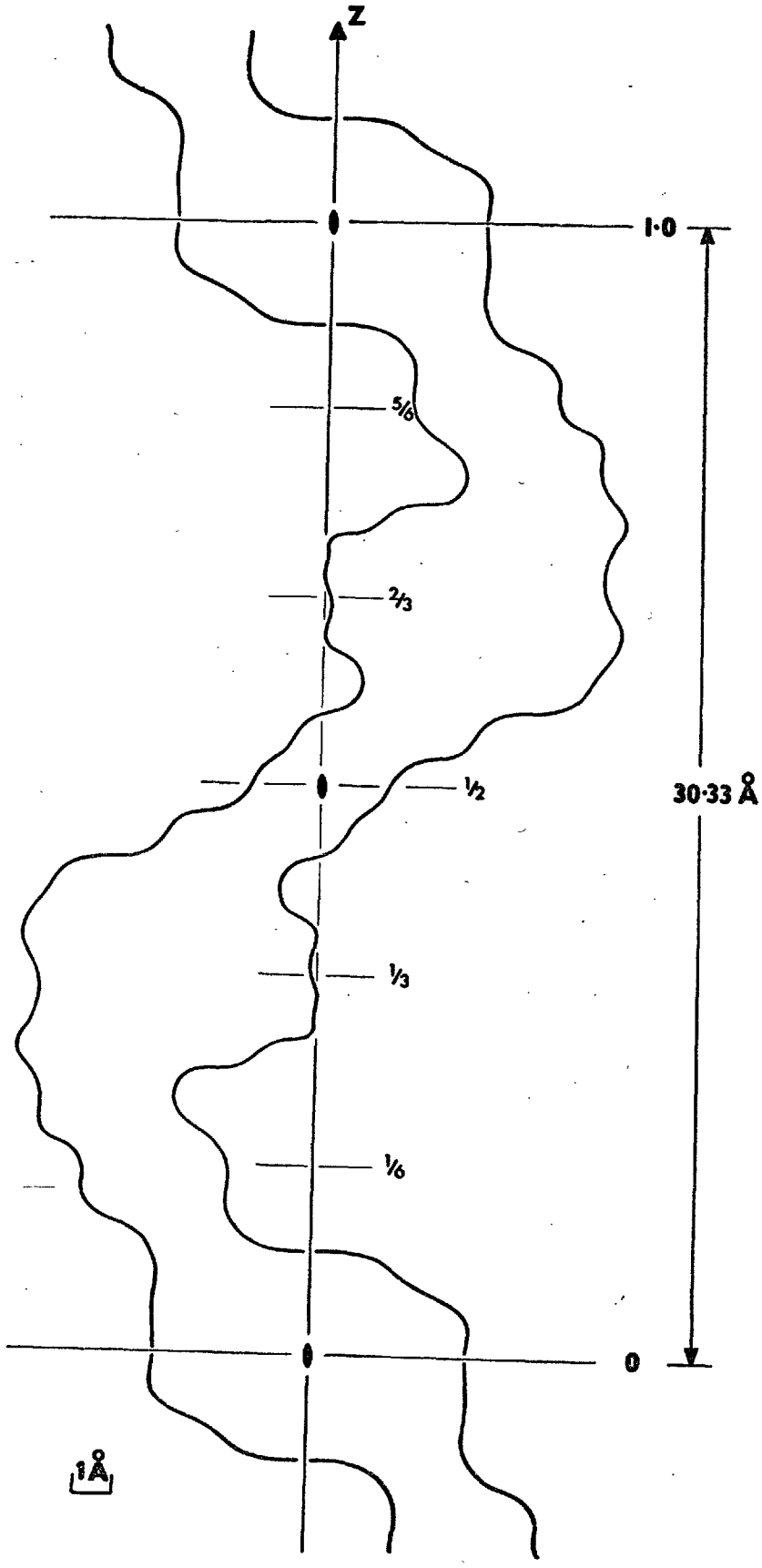


Figure 13. Projection of the system of cavities in the structure looking down the two-fold axes.

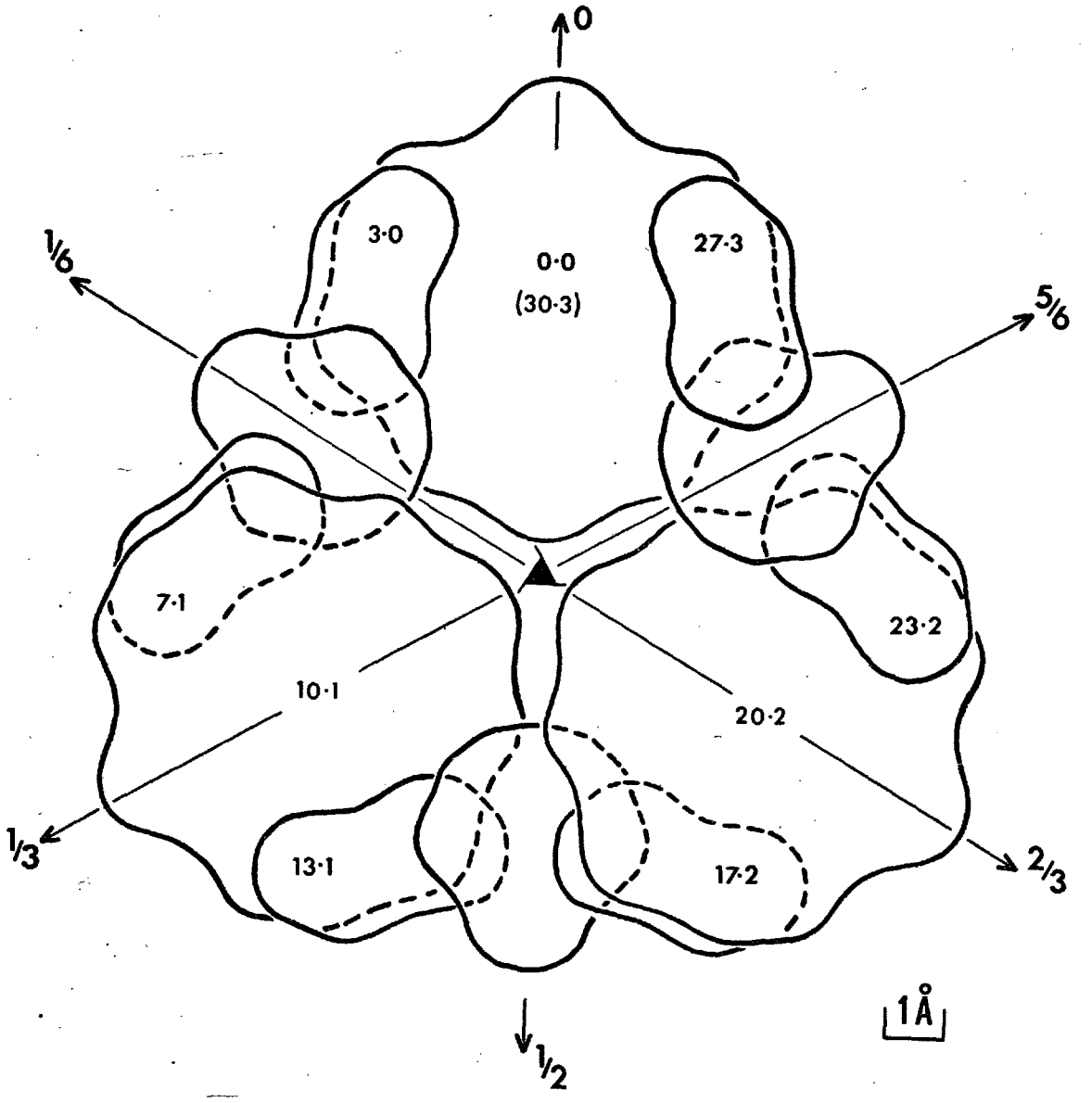


Figure 14. Projection down *c* of the system of cavities, the contours showing the maximum and minimum widths of the system and their heights in Å up the *c* axis.

molecules that would fit would be hydrogen, or possibly helium. These could not be included into a formed structure as they would be too large to pass through the window into the cavity, and their inclusion during the formation of the system would be difficult as complexes are formed from solution. We intend however to try to include hydrogen by a crystallisation, under a pressure of hydrogen, of the ethanol adduct.

Using the sectional plan shown in Figure 6 and by cutting, to a scale of $\frac{1}{2}$" = 1Å, correctly shaped holes in a series of sheets of perspex, we have built a three-dimensional model of the cavity. The model is constructed to come apart at the centre in the plane of the two-fold axis, thereby permitting space-filling models to be inserted to see how, or if, they will fit. Plate 1a shows a photograph of this model in its two parts, with a model of a methylene iodide molecule inserted. Plate 1b is a photograph of the model closed, containing the included molecule. On placing the methylene iodide molecule in the cavity the iodines were found to fit quite snugly so these atoms are not disordered, but it was immediately evident that it was possible, keeping the positions of the iodines fixed, to rotate the molecule in the cavity freely about the axis through the two iodines. This almost certainly explains why it was not possible to find the methylene carbon; it is probably smeared out over a complete circle.

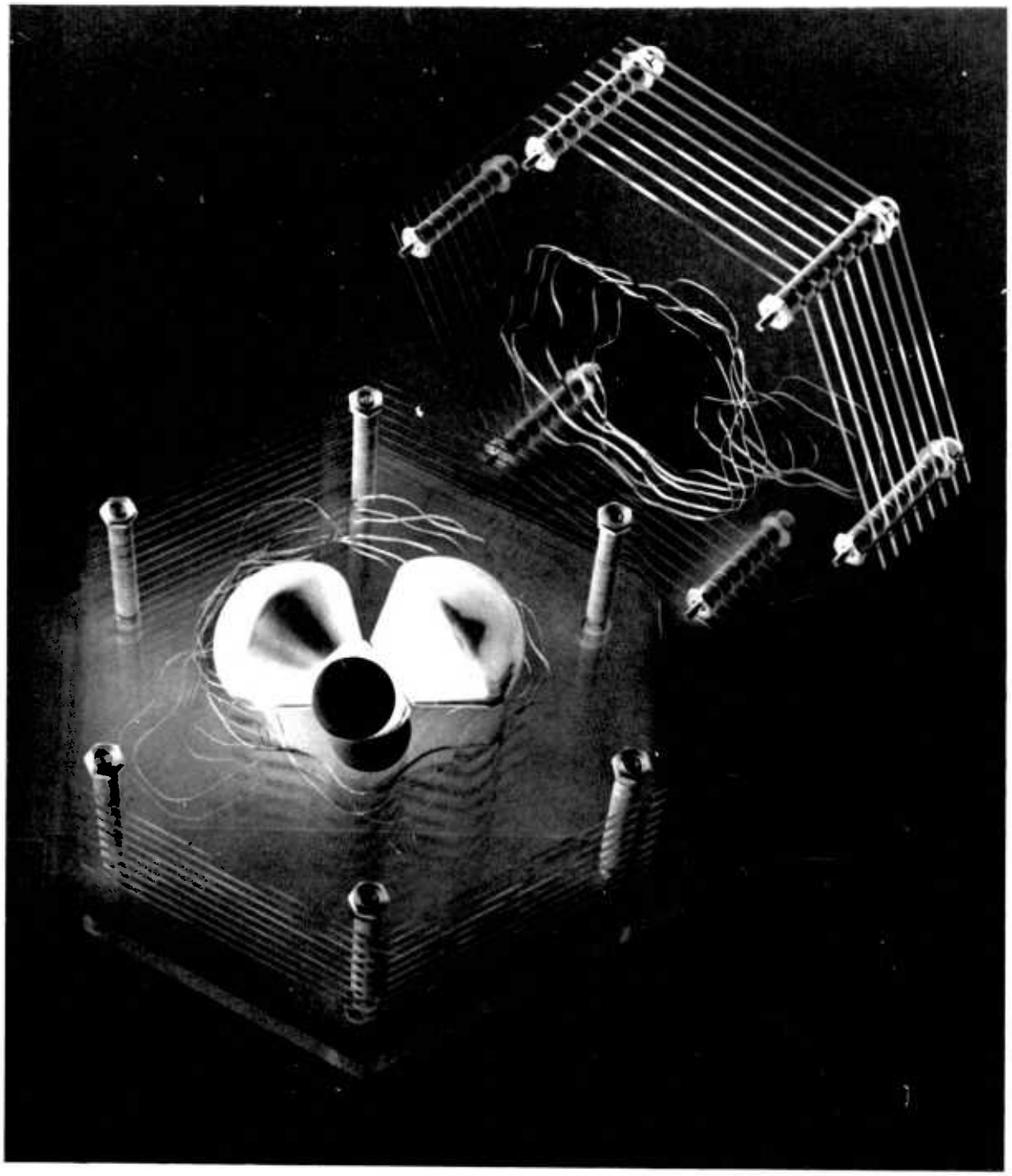


Plate 1(a) Photograph of the model of the cavity in its two parts with a space-filling model of methylene iodide inserted.

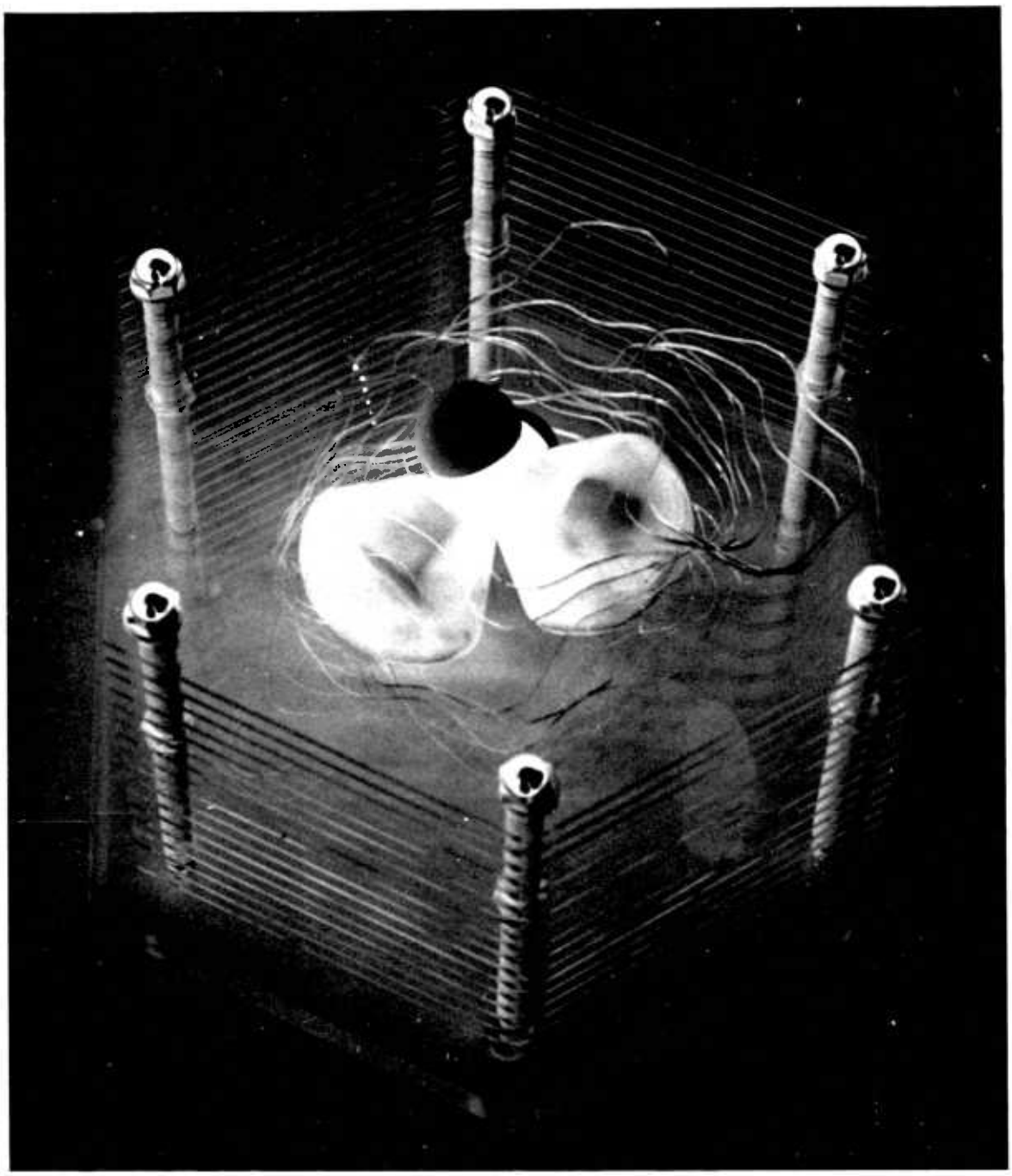


Plate 1(b) Photograph of the model closed, containing the included molecule.

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Table 1

Final fractional atomic coordinates (X 10^4) and isotropic thermal parameters (X 10^3) with estimated standard deviations in parentheses.

Atom	x	y	z	$U(\text{Å}^2)$
^{1}I(1)	7276(3)	5870(3)	175(1)	*
^{2}I(100)	5895(50)	5406(50)	129(15)	129(18)
^{2}I(101)	7768(50)	7076(53)	225(16)	128(18)
C(111)	8894(24)	3905(25)	723(8)	89(9)
C(11)	8075(26)	3547(26)	321(8)	86(9)
C(12)	8653(23)	4143(24)	-89(8)	77(9)
C(13)	7980(24)	3845(23)	-482(8)	77(9)
C(14)	6802(23)	3092(22)	-483(8)	68(8)
C(15)	6307(23)	2593(25)	-68(8)	71(8)
C(16)	6970(20)	2872(20)	324(7)	44(6)
C(17)	6421(21)	2294(22)	738(8)	61(8)
O(15)	5165(14)	1784(13)	-64(5)	61(5)
O(17)	6520(16)	2798(16)	1069(6)	92(6)
C(14)	6065(22)	2783(23)	-901(8)	76(9)
C(142)	6231(26)	3929(25)	-1100(8)	89(9)
C(143)	6442(27)	2205(26)	-1222(9)	104(11)
C(211)	2743(24)	-668(23)	1831(8)	89(9)
C(21)	3914(21)	-376(21)	1661(8)	68(8)
C(22)	4580(23)	-742(22)	1867(8)	72(9)
C(23)	5619(23)	-517(22)	1703(8)	71(8)
C(24)	6107(21)	144(22)	1309(7)	66(8)
C(25)	5408(20)	495(19)	1115(7)	50(7)
C(26)	4387(19)	293(19)	1262(7)	50(7)

Table 1 (contd.)

Atom	x	y	z	U(Å^2)
C(27)	3687(22)	639(21)	1020(8)	67(8)
O(25)	5849(12)	1156(13)	718(5)	54(4)
O(27)	3172(15)	1104(15)	1139(5)	84(6)
C(241)	7238(24)	402(23)	1134(8)	76(8)
C(242)	8206(29)	1092(30)	1452(10)	129(12)
C(243)	7263(27)	-673(28)	1011(9)	106(11)
C(311)	3045(24)	2397(23)	-628(8)	79(8)
C(31)	2550(23)	1291(23)	-324(8)	70(8)
C(32)	1463(24)	428(24)	-366(9)	79(9)
C(33)	1045(21)	-461(21)	-81(8)	63(8)
C(34)	1644(23)	-595(24)	263(8)	73(8)
C(35)	2785(22)	285(22)	300(8)	67(8)
C(36)	3217(23)	1240(23)	11(8)	66(8)
C(37)	4471(27)	2149(26)	57(9)	85(9)
O(35)	3532(13)	194(12)	598(5)	56(4)
O(37)	4772(22)	3094(23)	205(7)	145(9)
C(341)	1194(24)	-1579(24)	589(8)	86(9)
C(342)	372(26)	-1479(28)	892(9)	106(10)
C(343)	565(28)	-2750(29)	338(10)	115(11)

* Anisotropic thermal parameters U_{ij} (X 10^3 Å^2) with estimated standard deviations.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
[1]I(1)	137(3)	170(4)	139(2)	105(3)	17(2)	-5(2)

The form of the anisotropic temperature factor is:

$$\exp[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^* +2U_{13}hla^*c^*+2U_{23}klb^*c^*)]$$

[1] Estimated occupancy 90% [2] Estimated occupancy 5%

Table 2

Selected trans-annular and intramolecular contacts (Å)

O(15) ...O(25)	2.83	O(25) ...O(35)	2.78
O(35) ...O(15)	2.98	O(17) ...O(27)	3.96
O(27) ...O(37)	3.77	O(37) ...O(17)	3.70
O(15) ...C(17)	2.85	O(25) ...C(27)	2.82
O(35) ...C(37)	2.83	C(111)...O(17)	3.00
C(211)...O(27)	3.04	C(311)...O(37)	3.26

Table 3

Intermolecular distances* ≤ 3.6Å

I(100)...O(37)	2.74	I(1) ...I(1^{i})	3.49
I(101)...I(100^{i})	2.99	C(31) ...C(31^{i})	3.57
C(32) ...C(33^{i})	3.41	C(33) ...C(33^{i})	3.59
C(32) ...C(32^{i})	3.30	O(37) ...C(311^{i})	3.46
O(17) ...C(142^{ii})	3.59	C(12) ...C(35^{iii})	3.60
C(12) ...O(25^{iii})	3.58	C(12) ...O(35^{iii})	3.04
C(13) ...C(25^{iii})	3.56	C(13) ...O(35^{iii})	3.28
C(23) ...O(27^{iv})	3.60		

* Roman numeral superscripts denote the following equivalent positions relative to the reference molecule at x,y,z:

i $y,x,-z$ ii $1-y,x-y,1/3+z$ iii $1+y,x,-z$ iv $1-x,y-x,1/3-z$

CHAPTER 2

The crystal structure of the cavity inclusion compound formed by tri-*o*-thymotide with ethanol

Summary

The title compound crystallises in the trigonal space group $P3_121$ with a = 13.443(1), c = 30.143(2)Å, Z = 6. The structure, which is isostructural with that of the methylene iodide adduct, was refined by full-matrix least squares to R = 0.072 for the 3451 independent diffractometer measured reflections. The tri-*o*-thymotide molecule adopts a very similar conformation to that found in the methylene iodide adduct and again shows significant departures from C_3 symmetry. The angles between the planes of the three aromatic rings are 43°, 43° and 28°. The ethanol molecule is disordered and there is no evidence of host-guest hydrogen bonding.

Detailed analysis of the bounds of the cavity in the structure of the methylene iodide complex of tri-*o*-thymotide[1] revealed that two, symmetry related, carbonyl oxygen atoms form a significant portion of one of the end walls. This suggested a possible explanation for the apparently greater stability of the analogous cavity complex formed with ethanol. The stability of this complex has been evidenced both by *X*-ray photographs (high $\sin\theta/\lambda$ diffraction) and by experiments performed to remove the ethanol. In the latter, heating for 13h at 160°C and 1mm pressure, followed by a further 6h at 178° was necessary before all the ethanol was removed.[2]

As the packing of the host structure is governed by van der Waals forces, and the structural type (cavity or channel) depends on the shape and size of the included molecule,[3] ethanol, being very much smaller in volume (less than half) than the available space in the cavity, would be expected to form a physically less stable complex than one where the space was fully occupied. The stability of this complex may thus reflect the presence of host-guest interactions in the form of hydrogen bonds, linking the ethanol to the carbonyl oxygens mentioned above. An *X*-ray analysis of the ethanol complex was therefore undertaken to investigate this proposal, and to obtain more accurate details of the conformational geometry of the tri-*o*-thymotide molecule which had not been possible with the limited, heavy-atom dominated, data obtained for the methylene iodide complex.

EXPERIMENTAL

As has previously been reported tri-*o*-thymotide (TOT) forms inclusion compounds with a wide range of substances.[3-8] In some cases both an organic solvent and its impurities constitute

alternative potential guest species. A common impurity of ethanol is benzene with which TOT readily forms inclusion compounds. Thus for the preparation of the ethanol adduct, spectroscopic grade ethanol was used. The complex was prepared by dissolving pure unsolvated TOT[5] in warm ethanol (60°C) and allowing to cool slowly. Large clear hexagonal prisms (elongated along *c*) of the adduct formed readily and were identified from *X*-ray photographs as being of the trigonal form.

Crystal Data $C_{33}H_{36}O_6.\frac{1}{2}(C_2H_5OH)$, M = 551.7, Trigonal, a = 13.443(1), c = 30.143(2)Å, U = 4717Å^3, D_c = 1.165gcm^{-3}, Z = 6, $F(000)$ = 1770. Space-group $P3_121$(No. 152) or enantiomorphous $P3_221$(No. 154), from the Laue symmetry and systematic absences. Cu-K_α radiation, $\bar{\lambda}$ = 1.54178Å, μ(Cu-K_α) = 6.1cm^{-1}.

The lattice parameters were determined (at 10°C) from measurements of high-angle axial α_1 and α_2 reflections on a diffractometer using Cu-K_α radiation. They lie within the temperature dependent range of values previously reported.[3]

A crystal of dimensions 0.4 x 0.4 x 0.35mm^3 was cut from a longer needle and mounted along its a_1 direction. Data were measured on a Siemens off-line four-circle diffractometer using Ni-filtered Cu-K_α radiation. A total of 3451 independent reflections (an unique twelfth of reciprocal space) were measured (to θ = 71°) using the $\theta - 2\theta$ scan technique with the 'five value' measuring procedure.[9] Of these, 145 reflections had $I < 2.58\sigma(I)$ and were classed as unobserved.[9] The net count of the 0 4 $\bar{1}$ reflection, measured as a reference every 50 reflections, did not alter significantly during the data collection (*ca.* 7 days) indicating that no deterioration of the crystal had occurred. The data were brought to

a uniform arbitrary scale by use of this reflection,[9] and Lorentz and polarisation corrections were applied. No absorption corrections were applied.

Solution and Refinement of the Structure

Despite variations of up to 2% in the lattice parameters of different cavity adducts,[3] the complexes retain a common molecular framework, *i.e.* are isostructural. The ethanol complex was solved by re-refinement of the coordinates of the TOT molecule obtained from the analysis of the methylene iodide complex,[1] using the ethanol data.

The 39 atoms of the TOT molecule were refined anisotropically by full-matrix least-squares, to give a residual R = 0.104. A difference map contained peaks corresponding to all the hydrogen atoms of the TOT molecule, but no well defined peaks for the ethanol molecule. The cavity region of the map contained a diffuse cloud of electron density spreading over nearly the whole of the region. Only very small irregular peaks (the largest being only 0.9eÅ^{-3} on the two-fold axis) were discernable within this cloud, and it was not possible to rationalise these in terms of partial site occupancies of an ethanol molecule. All attempts at refinement of trial ethanol positions were unsuccessful.

The structure was further refined with the hydrogens fixed at optimised calculated positions corresponding to their observed positions in the difference map. The methyl hydrogens attached to C(211) were disordered and were allowed for by giving them $\frac{1}{2}$ weight in 6 equally staggered positions. Two reflections (the 101 and $10\bar{2}$) which had $|F_o| << |F_c|$ were suspected of being affected by extinction and therefore removed. The refinement was terminated at a final R value of 0.072. The maximum shift/error for the refined parameters

at this stage was 0.2 (for C(343)). A final difference map showed no improvement in resolution of the residual electron density in the cavity region; the maximum elsewhere was $0.2 e\text{Å}^{-3}$.

Unit weights were used throughout the refinements. Atomic scattering factors were taken from ref. 10 with the exception of those for hydrogen which were taken from ref. 11. The computations were carried out on the Imperial College CDC 6400 and the University of London CDC 6600 and 7600 computers using, in the main, programs belonging to the *X*-ray 70 and 72 systems.[12]

RESULTS AND DISCUSSION

The observed and calculated structure factors are listed in Appendix II. The final fractional atomic coordinates and anisotropic thermal parameters for the non-hydrogen atoms together with their estimated standard deviations are listed in Tables 1 and 2. Those for the hydrogen atoms with their isotropic temperature factors are given in Table 3. Figure 1 shows a stereo view of the molecule (ORTEP[13]). Figures 2a, b show the bond lengths and angles together with their estimated standard deviations and the numbering scheme used. Figure 3 shows the values of the torsion angles around the central 12-membered ring, also for comparison the values for the methylene iodide complex.[1] Figure 4 gives the Newman projections[14] looking down each of the aromatic-isopropyl bonds. Table 4 lists selected trans-annular and intramolecular distances, and Table 5 intermolecular contacts ≤ 3.6Å. Table 6 lists the equations of the least-squares planes for the three aromatic rings and the largest deviations of particular atoms from them. The photograph shows the bounds of the cavity region and the form of the electron density within it.

The molecule (Fig.1) adopts the predicted propeller conformation[15-17]

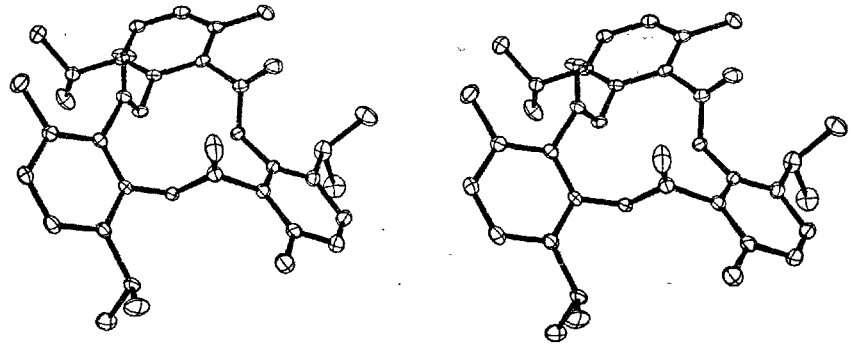


Figure 1. Stereo view of the tri-*o*-thymotide molecule.

found in the methylene iodide complex. Despite the overall greater stability of this complex, compared with that containing CH_2I_2 there is still appreciable thermal anisotropy present in the structure. This is confined mainly, however, to the isopropyl groups and the carbonyl oxygens. The anisotropy, though quite large, is for none of the atoms exceptional and there is no reason to suspect any disorder. It is, however, interesting to note that the directions of the principal axes of vibration of the three carbonyl oxygens are consistent with the proposed mechanism for conformational inversion,[15] also that in the solid state there is still significant conformational flexibility.

The accuracy achieved for the bond lengths, though very much better than in the methylene iodide complex, is not as great as that usually attained in light atom structures, and is a consequence of being unable to allow effectively (in refinement) for all the scattering material in the structure. The lengths do not deviate significantly from expected values. There is an internal difference between the 'equivalent' bonds C(15)-O(15) and C(25)-O(25), 1.387(7)Å and 1.428(7)Å respectively; this difference is $>4\sigma$ and therefore significant. There is a similar difference between these bonds in the methylene iodide complex. The three C(CO)O angles are all significantly less than 120° (111.1(5)° at C(17), 109.3(8)° at C(27) and 113.0(7)° at C(37)), the values being very similar to those observed in other structures containing carboxy groups, *e.g.* 108° in methyl *m*-bromocinnamate,[18] and 111° in acetylcholine bromide.[19] The acuteness of the angles is probably due to non-bonding interactions between the ether and carbonyl oxygens.

The torsion angles show that, in addition to the already reported departures from C_3 symmetry,[20] there are also significant differences

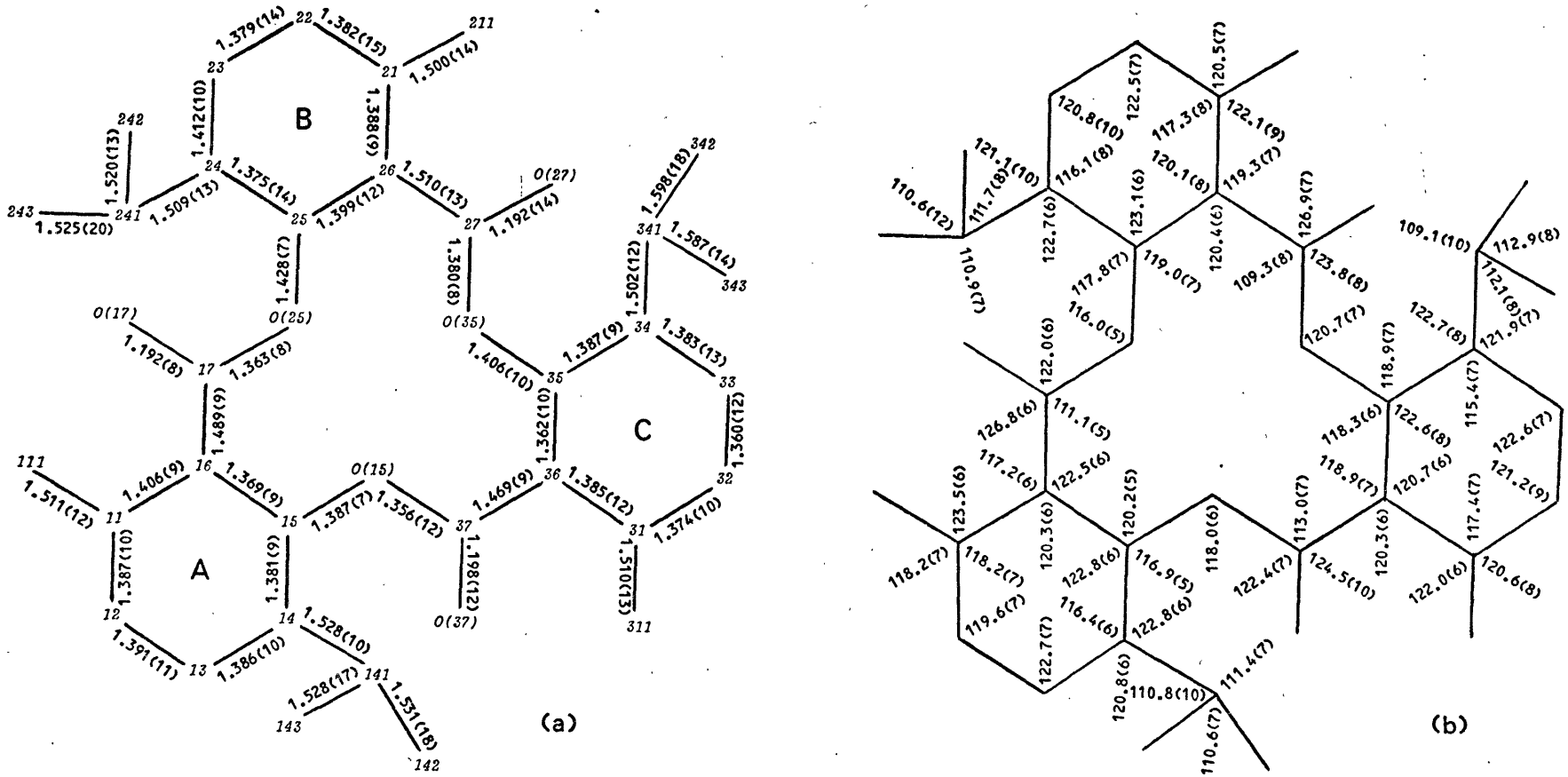


Figure 2(a) Bond lengths and numbering scheme (isopropyl methyl carbons nos. 142, 242 and 342 are on the same side of the central ring as the carbonyl oxygens); (b) valence angles. Standard deviations in parentheses.

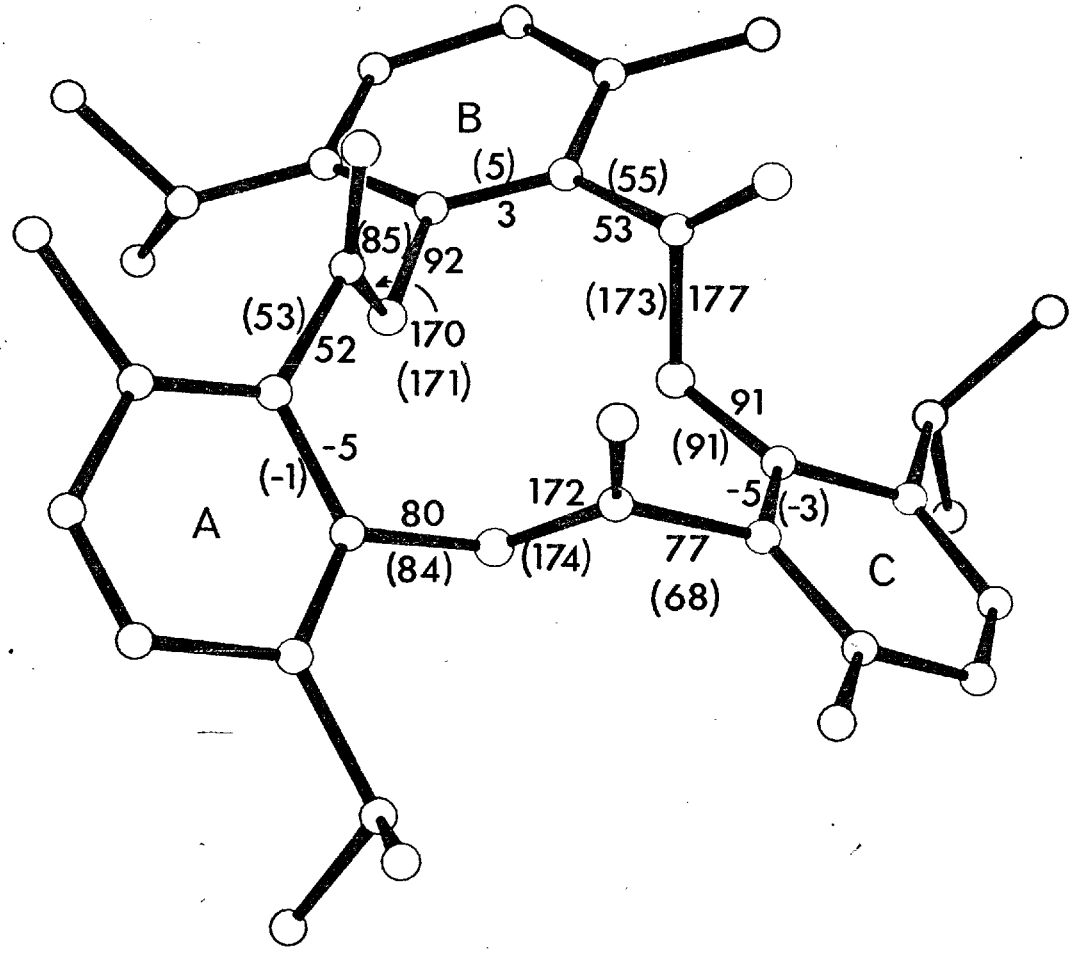


Figure 3. Torsion angles around the 12-membered ring with the values found in the methylene iodide complex in parentheses.

between the conformations of the 12-membered rings in the methylene iodide and ethanol complexes (Fig.3). There is, for example, a difference of 9° in the torsion angle about the C(36)-C(37) bond. Also, in the ethanol complex the departures from 'ideal' values[20] are greater, *e.g.* the C(35)C(36)C(37)O(15) angle being 17° greater than the 'ideal' value of 60°. For the 12-membered ring $\Sigma|\Delta\tau| = 75^{\circ}$ and $\Sigma\Delta\tau = 33^{\circ}$ * *cf.* 63° and 35° respectively in the methylene iodide complex. Thus the description of the cavity series of structures as isostructural must be qualified: clearly they are only approximately so.

The torsion angles between the isopropyl groups and their adjacent aromatic rings show (Fig.4) that for rings A and C these groups are rotated so that their terminal methyl carbons are asymmetrically disposed above and below the planes of the rings. The direction of rotation in each case is not the same. The rotations of the groups in this structure are in the same sense, but slightly larger, than those observed in the methylene iodide complex with the C(341), C(342), C(343) group again rotated significantly more than the other two (∿ 16° from a symmetric orientation).

Two of the trans-annular (ether) oxygen-oxygen distances are about equal to the sum of the van der Waals radii, and one (O(35)..
..O(15), 3.06Å) is somewhat larger. There are fairly close intra-molecular methyl-carbonyl oxygen contacts between C(111) and O(17) (2.96Å) and between C(211) and O(27) (3.03Å). The intermolecular contact distances show little change compared with those for the methylene iodide complex; the differences are small (∿ 0.1Å) and

* $\Delta\tau$ is the difference between the observed and 'ideal'[20] torsion angles.

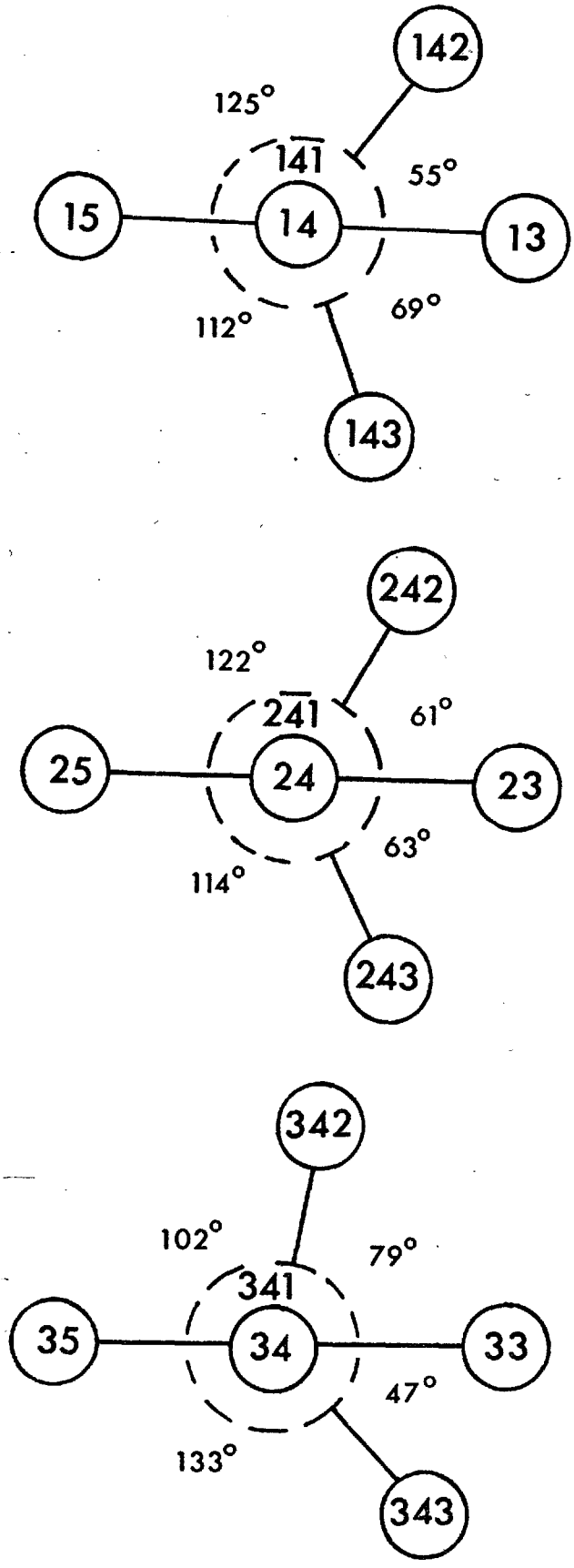


Figure 4. Newman projections down each of the three aromatic-isopropyl bonds.

the short C(12)...O(35) contact (3.06Å) is still present.

Departures from planarity in the three aromatic rings are small with the largest deviation (∿ 0.013Å) occurring with C(32) in ring C. Ring B is equally inclined to rings A and C (43° between normals) but the angle between rings A and C is significantly less (28°) thus emphasising the asymmetry in the molecule.

Finally, analysis of the residual electron density leads to the conclusion that the ethanol molecule is disordered, or probably more correctly, that it adopts widely differing orientations throughout the crystal. There is no evidence for host-guest hydrogen bonding. If such bonding were present, and even allowing for the likelihood of some motion of the molecule within the cavity, at least the oxygen atom of the ethanol should be resolvable, but it is not.

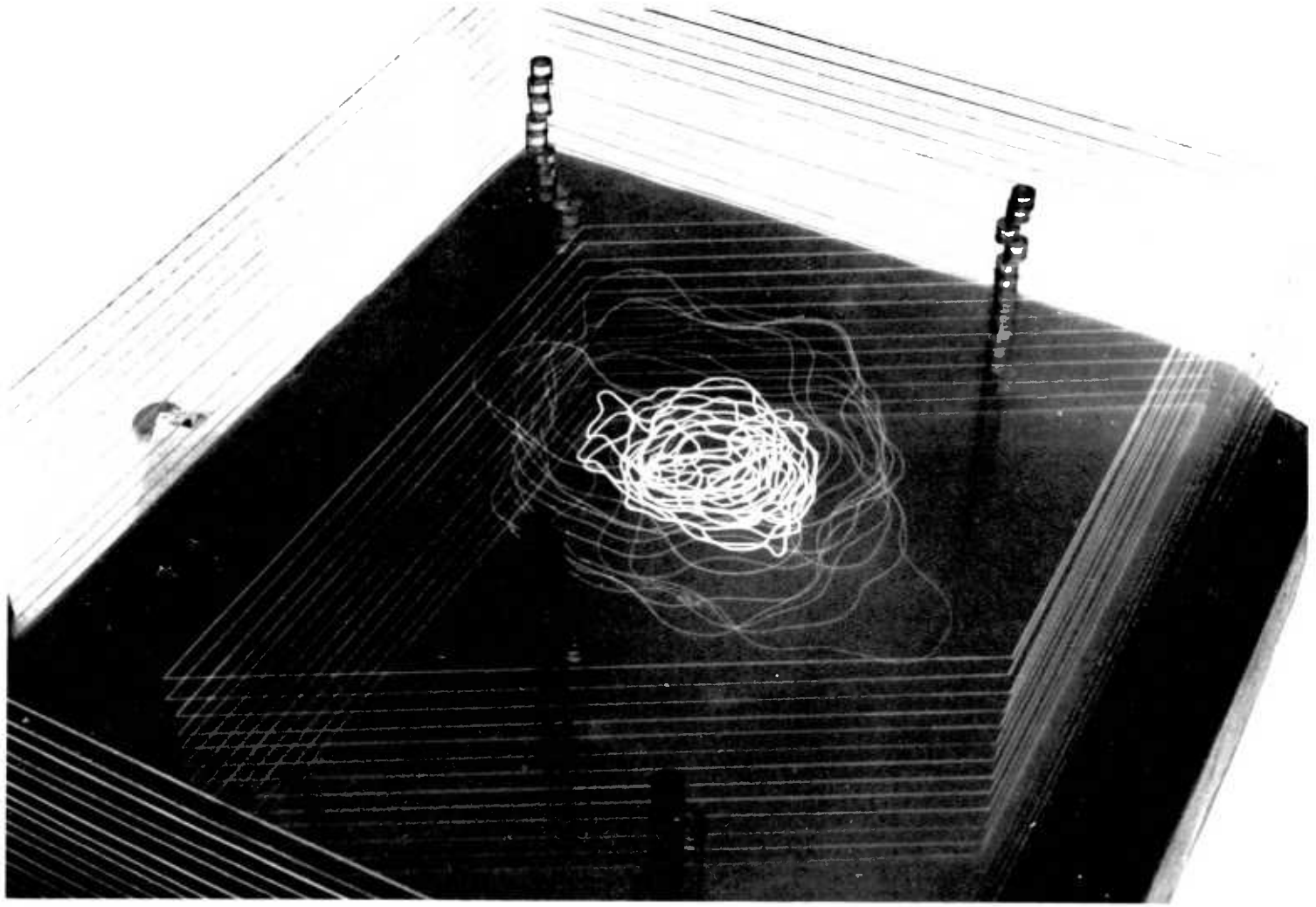


Plate. Bounds of the cavity (faint contours) and the form of the electron density within it (heavy contours).

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Table 1

Fractional coordinates (X 10^4) for the non-hydrogen atoms with estimated standard deviations in parentheses

Atom	x	y	z
C(111)	8914(8)	3868(8)	739(3)
C(11)	8150(7)	3616(7)	340(2)
C(12)	8656(7)	4148(7)	-57(3)
C(13)	7983(7)	3904(8)	-436(2)
C(14)	6814(7)	3115(7)	-439(2)
C(15)	6336(6)	2594(6)	-391(2)
C(16)	6967(6)	2817(6)	342(2)
C(17)	6441(6)	2276(6)	775(2)
O(15)	5179(4)	1771(4)	-41(1)
O(17)	6570(6)	2752(5)	1122(2)
C(141)	6115(7)	2860(8)	-865(2)
C(142)	6241(11)	3955(10)	-1073(3)
C(143)	6455(9)	2224(9)	-1199(3)
C(211)	2763(8)	-765(8)	1880(3)
C(21)	3925(7)	-428(7)	1696(2)
C(22)	4614(8)	-786(7)	1899(2)
C(23)	5670(8)	-531(7)	1732(2)
C(24)	6110(7)	136(6)	1343(2)
C(25)	5417(6)	486(6)	1144(2)
C(26)	4334(6)	208(6)	1309(2)
C(27)	3565(7)	515(6)	1048(2)
O(25)	5804(4)	1110(4)	737(1)
O(27)	3090(6)	1000(5)	1183(2)
C(241)	7255(8)	397(8)	1153(3)
C(242)	8227(10)	1064(13)	1478(3)

Table 1 (contd.)

Atom	x	y	z
C(243)	7231(11)	-697(11)	1008(4)
C(311)	3053(9)	2320(9)	-586(3)
C(31)	2567(7)	1271(7)	-293(2)
C(32)	1458(8)	392(8)	-350(2)
C(33)	988(7)	-530(8)	-73(3)
C(34)	1597(7)	-656(7)	272(3)
C(35)	2725(6)	221(6)	315(2)
C(36)	3197(6)	1166(6)	49(2)
C(37)	4424(7)	2070(7)	121(2)
O(35)	3441(4)	91(4)	622(1)
O(37)	4727(6)	2983(6)	292(3)
C(341)	1064(8)	-1683(8)	574(3)
C(342)	280(10)	-1514(11)	932(4)
C(343)	388(10)	-2853(9)	309(4)

Table 2

Anisotropic thermal parameters* (X 10^3 Å^2) for the non-hydrogen atoms with standard deviations in parentheses

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(111)	66(6)	75(6)	79(6)	15(5)	-20(5)	-4(5)
C(11)	57(5)	50(4)	53(4)	24(4)	2(4)	2(3)
C(12)	51(5)	61(5)	63(4)	23(4)	11(4)	7(4)
C(13)	59(5)	74(6)	57(4)	33(5)	22(4)	18(4)
C(14)	56(5)	63(5)	47(4)	35(4)	10(3)	11(3)
C(15)	44(4)	45(4)	39(3)	22(3)	11(3)	5(3)
C(16)	47(4)	43(4)	45(3)	21(3)	7(3)	5(3)
C(17)	55(4)	40(4)	46(3)	18(3)	1(3)	0(3)
O(15)	51(3)	48(3)	40(2)	26(2)	4(2)	-0(2)
O(17)	118(5)	52(3)	45(3)	20(4)	12(3)	-6(2)
C(141)	64(5)	101(7)	45(4)	45(5)	11(4)	21(4)
C(142)	154(12)	121(9)	65(5)	100(9)	-17(6)	5(6)
C(143)	94(8)	97(8)	64(5)	53(6)	-11(5)	-10(5)
C(211)	78(6)	74(6)	62(5)	33(5)	24(4)	14(5)
C(21)	64(5)	48(4)	40(3)	21(4)	5(3)	3(3)
C(22)	72(6)	54(5)	42(4)	23(4)	3(4)	11(3)
C(23)	74(6)	57(5)	48(4)	32(5)	-3(4)	7(4)
C(24)	59(5)	49(4)	43(3)	24(4)	-6(3)	2(3)
C(25)	53(4)	39(4)	34(3)	17(3)	-3(3)	-0(3)
C(26)	55(4)	42(4)	40(3)	20(3)	-5(3)	-3(3)
C(27)	55(5)	44(4)	49(4)	18(4)	-2(3)	-4(3)
O(25)	58(3)	39(2)	35(2)	18(2)	-0(2)	3(2)
O(27)	99(5)	88(4)	67(3)	67(4)	-10(3)	-21(3)
C(241)	63(5)	78(6)	54(4)	37(5)	1(4)	10(4)
C(242)	70(7)	185(14)	88(7)	48(9)	-8(6)	-18(8)

Table 2 (contd.)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(243)	129(11)	115(10)	114(8)	81(9)	48(8)	16(7)
C(311)	88(7)	92(7)	65(5)	60(6)	10(5)	17(5)
C(31)	60(5)	67(5)	54(4)	39(4)	3(4)	-0(4)
C(32)	64(5)	83(6)	58(4)	43(5)	-13(4)	-5(4)
C(33)	47(5)	72(6)	76(5)	25(4)	-12(4)	-5(5)
C(34)	44(4)	55(5)	63(4)	19(4)	0(4)	-4(4)
C(35)	48(4)	55(4)	43(3)	29(4)	-5(3)	-7(3)
C(36)	45(4)	52(4)	43(3)	24(4)	3(3)	-2(3)
C(37)	55(5)	60(5)	59(4)	32(4)	5(4)	-3(4)
O(35)	53(3)	55(3)	45(2)	31(3)	-6(2)	-7(2)
O(37)	63(4)	73(5)	187(7)	27(4)	6(5)	-59(5)
C(341)	59(5)	63(6)	97(6)	24(5)	-1(5)	6(5)
C(342)	94(8)	100(9)	109(8)	26(7)	37(7)	23(7)
C(343)	94(8)	56(6)	161(10)	23(6)	-0(8)	12(7)

* In the form: $\exp[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^*+2U_{13}hla^*c^*+2U_{23}klb^*c^*)]$

Table 3

Fractional coordinates and isotropic thermal parameters (X 10^3) for the hydrogen atoms*

Atom	x	y	z	U(Å^2)
H(12)	950	470	-7	63
H(13)	836	431	-72	63
H(1111)	972	446	66	89
H(1112)	863	416	99	89
H(1113)	890	315	84	89
H(141)	529	233	-80	76
H(1421)	602	436	-85	89
H(1422)	706	447	-116	89
H(1423)	573	375	-134	89
H(1431)	637	151	-106	89
H(1432)	595	202	-147	89
H(1433)	727	173	-129	89
H(22)	434	-125	218	63
H(23)	613	-82	189	63
^{1}H(2111)	263	-122	216	89
^{1}H(2112)	272	-6	195	89
^{1}H(2113)	216	-124	166	89
^{1}H(2114)	239	-43	169	89
^{1}H(2115)	228	-162	188	89
^{1}H(2116)	285	-47	219	89
H(241)	740	86	88	76
H(2421)	823	178	157	89
H(2422)	812	58	175	89
H(2423)	898	127	133	89
H(2431)	659	-112	80	89

Table 3 (contd.)

Atom	x	y	z	$U(\text{Å}^2)$
H(2432)	798	-50	86	89
H(2433)	712	-119	127	89
H(32)	99	43	-60	63
H(33)	17	-114	-12	63
H(3111)	247	223	-81	89
H(3112)	327	302	-40	89
H(3113)	375	241	-74	89
H(341)	168	-175	73	76
H(3421)	75	-77	109	89
H(3422)	-38	-152	78	89
H(3423)	-2	-216	115	89
H(3431)	92	-291	9	89
H(3432)	9	-351	52	89
H(3433)	-27	-287	15	89

[1] Occupancy 50%

* The numbering of the hydrogen atoms is that of the atoms to which they are bonded.

Table 4

Selected trans-annular and intramolecular distances (Å)

O(15) ...O(25)	2.78	O(35) ...O(15)	3.06
O(25) ...O(35)	2.78	O(17) ...O(27)	4.06
O(27) ...O(37)	3.65	O(17) ...O(37)	3.64
C(111)...O(17)	2.96	C(211)...O(27)	3.03
C(311)...O(37)	3.30	O(35) ...C(37)	2.76
O(25) ...C(27)	2.86	O(15) ...C(17)	2.87

Table 5

Intermolecular distances* ≤ 3.6Å

O(17) ...C(142^{i})	3.50	O(17) ...C(143^{i})	3.56
C(12) ...O(35^{ii})	3.06	C(12) ...O(25^{ii})	3.56
C(12) ...C(35^{ii})	3.56	C(13) ...O(35^{ii})	3.24
O(37) ...C(311^{iii})	3.40	C(32) ...C(32^{iii})	3.26
C(32) ...C(33^{iii})	3.40	C(33) ...C(33^{iii})	3.56
C(31) ...C(31^{iii})	3.50	O(27) ...C(23^{iv})	3.50

* Roman numeral superscripts denote the following equivalent positions relative to the reference molecule at x,y,z:

i $1-y,x-y,1/3+z$ ii $1+y,x,-z$ iii $y,x,-z$ iv $1-x,1-x+y,1/3-z$

Table 6

Equations of the least-squares planes (in direct space) for the three aromatic rings in the structure together with their standard deviations and the largest displacements from them.

A $-8.612x + 12.873y + 6.607z = -2.144$

$\sigma = 0.006$Å C(12) -0.009Å

B $0.150x + 9.679y + 16.451z = 2.429$

$\sigma = 0.007$Å C(26) -0.009Å

C $-8.441x + 9.724y + 18.637z = -1.488$

$\sigma = 0.011$Å C(32) -0.013Å

Dihedral angles between the planes of the rings:

A,B = 43° A,C = 28° B,C = 43°

CHAPTER 3

The crystal structure of the channel inclusion compound formed by tri-*o*-thymotide with *n*-cetyl alcohol

Summary

The title compound crystallises in the hexagonal space group $P6_1$ with a = 14.308(1), c = 29.016(2)Å, Z = 6. The structure was solved by direct methods and refined by full-matrix least squares to R = 0.076 for the 3332 independent diffractometer measured reflections. The tri-*o*-thymotide molecule, as in the cavity structures, adopts a propeller conformation which deviates significantly from C_3 symmetry. The angles between the planes of the three aromatic rings are 43°, 39° and 31°. The channel has a fairly uniform cross-section and presents an almost unhindered free passage of diameter ∿4.3Å running the length of the c direction. There is no evidence of ordering of the included molecule.

The inclusion compounds of tri-*o*-thymotide formed with straight chain or singly-branched straight-chain molecules have been shown to be of two major chiral structural types, cavity or channel, depending on the shape and size of the included molecule.[1] *X*-ray analyses have established the host-structural framework common to all the trigonal cavity complexes.[2,3] Here, the first of the channel structures is reported.

Unlike the cavity complexes which form stoicheiometric 2:1 host-guest compounds,[1,2] the channel complexes are, in most cases crystallographically non-stoicheiometric.[1] They differ too in that there is no apparent limit to the length of molecules that can be included, an example having been reported where an included molecule exceeds the unit-cell length.[1] The channel compounds, like the cavity compounds, undergo spontaneous resolution on crystallisation.[4,5] It has been concluded that the general space-group for the hexagonal channel series is $P6_1$ if one considers only the host structure, but that the observed space-group is sometimes of lower symmetry due to the imposition on a particular complex of the symmetry of packing of the guest molecules, and does not indicate a different host structure.[1]

Our first attempt was to determine the structure of the stoicheiometric, heavy-atom channel complex formed with *n*-pentyl iodide but, for reasons not yet determined, this was unsuccessful. An *X*-ray analysis was then undertaken of the stable, light-atom, non-stoicheiometric complex formed with *n*-cetyl alcohol ($C_{16}H_{33}OH$), both to determine the form, dimensions and bounds of the channel, and to obtain accurate details of the conformational geometry of the tri-*o*-thymotide molecule for comparison with those obtained (in a different crystalline environment) from the ethanol cavity complex.[3]

EXPERIMENTAL

Crystals of pure unsolvated TOT[5] were dissolved in 'AnalaR' grade *n*-cetyl alcohol heated above its melting point (50°C). Clear, well-formed, doubly-terminated hexagonal prisms of the complex (elongated along *c*) formed readily on slow cooling of the solution. They were identified as being of the hexagonal channel form from *X*-ray photographs. Lattice parameters were determined (at 10°C) from measurements of high-angle axial α_1 and α_2 reflections on a diffractometer using Cu-K_α radiation. They agree well, allowing for the temperature difference, with those previously reported.[1]

Crystal Data $C_{33}H_{36}O_6.0.22(C_{16}H_{33}OH)$, M = 581.9, Hexagonal, a = 14.308(1), c = 29.016(2)Å at 10°C, U = 5144Å^3, D_c = 1.127gcm^{-3}, Z = 6, $F(000)$ = 1874. Space-group $P6_1$(No. 169) or enantiomorphous $P6_5$(No. 170) from systematic absences. Cu-K_α radiation. $\bar{\lambda}$ = 1.54178Å, μ(Cu-K_α) = 5.7cm^{-1}.

A crystal of dimensions *ca.* 0.4 x 0.5 x 0.75 mm^3 was mounted along its a_1 direction. Data were measured on a Siemens off-line four-circle diffractometer using Ni-filtered Cu-K_α radiation. A total of 3332 independent reflections (an unique twelfth of reciprocal space) were measured (to θ = 70°) using the θ-2θ scan technique with the 'five value'[6] measuring procedure. Of these 363 reflections had $I < 2.58\sigma(I)$ and were classed as unobserved.[6] The net count of the 0 4 13 reflection, measured as a reference every 50 reflections, did not alter significantly during the data collection (4 days) indicating that no deterioration of the crystal had occurred. The data were brought to a uniform arbitrary scale by use of this reflection,[6] and Lorentz and polarisation corrections were applied. No absorption corrections were applied.

Solution and Refinement of the Structure

The structure was solved by direct methods by application of the program MULTAN[7] to 200 reflections with normalised structure factors (E's) > 1.67. Initial trials, using up to 400 reflections, had resulted in poor 'figures of merit' with maximum values of $\sim$ 0.9 and with very little difference between their values for the different phase sets. However, an E map based on 200 reflections, and computed for the phase solution with the highest 'combined figure of merit' gave plausible positions for all but 5 of the non-hydrogen atoms of the TOT molecule. The missing atoms were positioned on the basis of the expected molecular configuration.

The TOT molecule was refined isotropically by full-matrix least-squares to an R-value of 0.21. The refinement showed one methyl carbon to be wrongly placed, and inspection of the bond lengths showed that two other methyl carbon atoms belonging to one of the isopropyl groups had also been incorrectly positioned. These two atoms had not been found in the E map and had been placed in expected positions, assuming a symmetrical relationship between the group and the plane of the aromatic ring to which it was bonded. Though their refinement appeared reasonable they had clearly refined into false minima. The correct positions of these atoms were determined from a difference map and the structure was then refined anisotropically to an R-value of 0.11.

The isotropic temperature factors (B's) of two isopropyl methyl carbons C(342) and C(343) converged satisfactorily to values of 16 and 15 Å^2 respectively. These values, though large, were comparable with those for the other two isopropyl groups in the structure. However when they were refined anisotropically, unlike the other groups,

they assumed very much larger values, whilst still retaining a sensible internal geometry for the group. It is concluded that this indicates a probable dynamic disorder of this group. The packing, discussed later, is able to accommodate small rotations of this group.

Three reflections (the 006, 100 and 110) which had $|F_o| \ll |F_c|$ were suspected of being affected by extinction and therefore removed. Subsequent refinement with the hydrogen atoms fixed at calculated positions 1.0Å from their parent carbons (the orientation of the methyl hydrogens was determined from a difference map) reduced R to 0.076. A difference map gave no evidence for any ordering of the included molecule of cetyl alcohol, there being a column of more or less uniform electron density $\sim$ 0.55eÅ^3 running the full length along the c axis. No allowance was made for the scattering contribution of the included molecule and refinement was terminated at a final R value of 0.076. The maximum shift/error for the refined parameters at this stage was 0.3 (for C(342)).

Unit weights were used throughout the refinements. Atomic scattering factors were taken from ref. 8 with the exception of those for hydrogen which were taken from ref. 9. The computations were carried out on the Imperial College CDC 6400 and the University of London CDC 6600 and 7600 computers using, in the main, programs belonging to the *X*-ray 70 and 72 systems.[10]

RESULTS AND DISCUSSION

The observed and calculated structure factors are listed in Appendix III. The final fractional atomic coordinates and anisotropic thermal parameters for the non-hydrogen atoms together with their estimated standard deviations are listed in Tables 1 and 2. Those for the hydrogen atoms with their isotropic temperature factors are

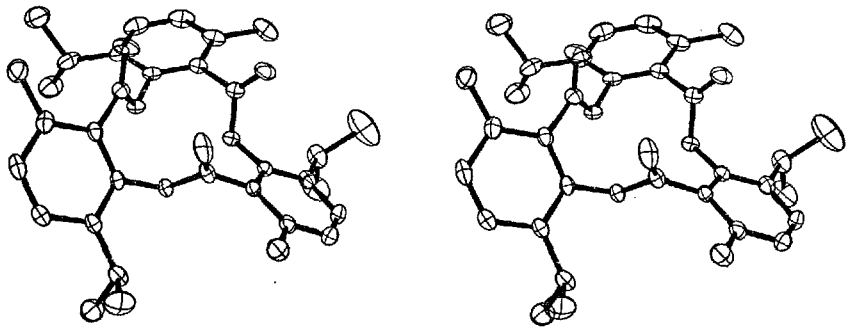


Figure 1. Stereo view of the tri-*o*-thymotide molecule.

given in Table 3. Figure 1 shows a stereo view of the molecule (ORTEP[11]). Figures 2a, b show the bond lengths and angles together with their estimated standard deviations and the numbering scheme used. Figure 3 shows the values of the torsion angles around the 12-membered ring, and Figure 4 the Newman projections[12] looking down each of the three aromatic-isopropyl bonds. Table 4 lists intermolecular contacts $\leq 3.6\mathring{A}$ and Table 5, selected trans-annular and intramolecular distances. Table 6 lists the equations of the least-squares planes for the three aromatic rings and the deviations of selected atoms from them. Figure 5 shows a stereo view[11] of the packing of the molecules in the cell.

The TOT molecule, as in the cavity complexes, adopts a propeller conformation in the solid state.[2,3] There is again pronounced thermal anisotropy present in the molecule, though as before this is confined mainly to the carbonyl oxygens, the methyls and the isopropyl groups. The amount of thermal motion in the isopropyl groups is very much greater than that observed for the ethanol cavity structure;[3] it is exceptionally large for the C(342) and C(343) methyl carbons.

The bond lengths, though slightly less accurate than those for the ethanol complex,[3] do not deviate significantly from expected values. Those around the 12-membered ring still show, however, significant internal inconsistencies with, for example, the C(26)-C(27) and C(36)-C(37) bonds differing by 5σ. The carboxy O(CO)O angles are again significantly less than 120°, with an average angle of 110°.

The torsion angles show that the conformation, though deviating significantly from C_3 symmetry,[13] is closer to 'ideal'[13] than that found in the ethanol complex. For the 12-membered ring $\Sigma|\Delta\tau| = 69^{\circ}$

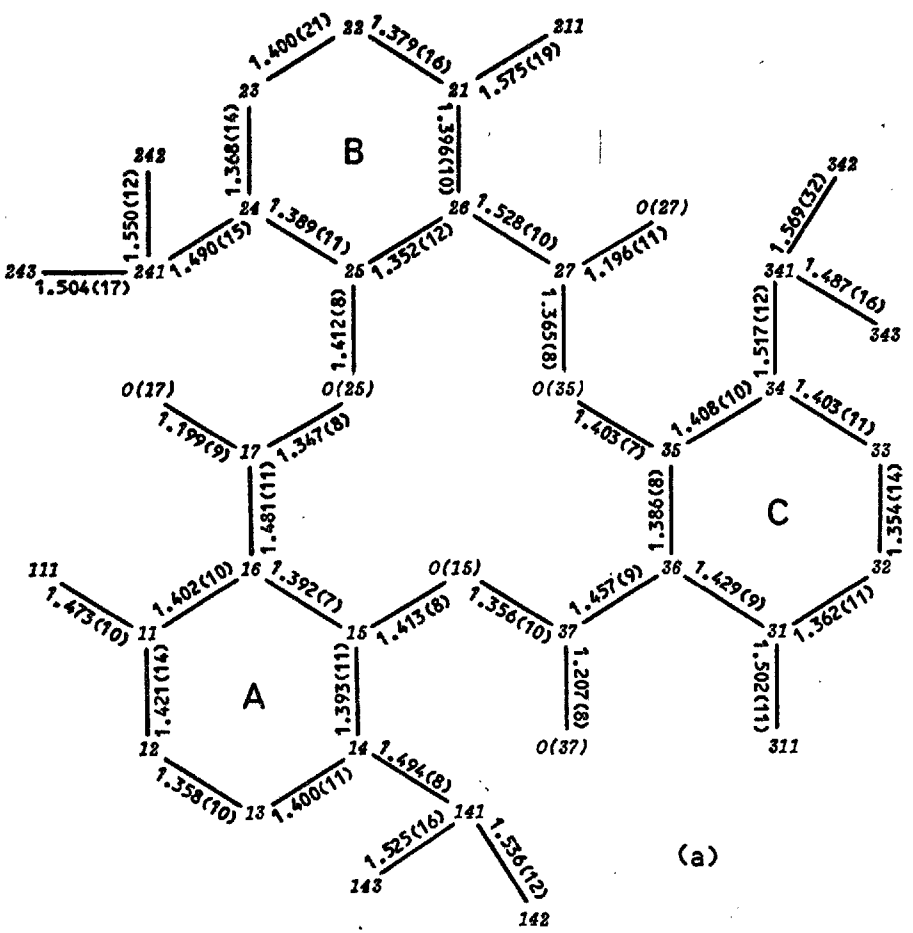


Figure 2(a) Bond lengths and numbering scheme (isopropyl methyl carbons nos. 142, 242 and 342 are on the same side of the central ring as the carbonyl oxygens); (b) valence angles. Standard deviations in parentheses.

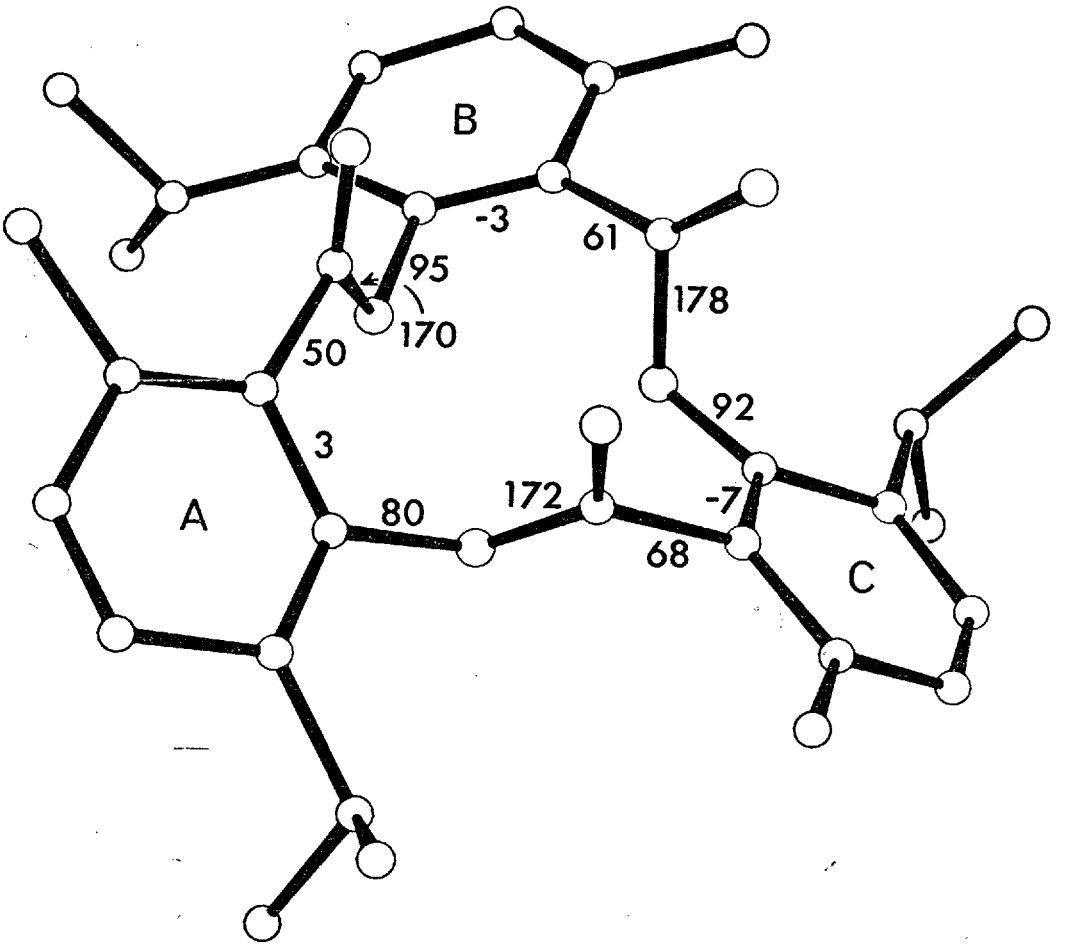


Figure 3. Torsion angles around the central 12-membered ring.

and $\Sigma\Delta\tau = 31^{o*}$ *cf.* 75^{o} and 33^{o} respectively in the ethanol complex.[3†] The isopropyl groups are rotated slightly with respect to the planes of their adjacent aromatic rings. The sense of rotation, unlike that in the ethanol and methylene iodide complexes, is the same for all three groups. The amount of rotation for each of the three groups is very similar and averages $\sim 4^{o}$.

The number of short intermolecular contacts is very nearly the same as in the cavity-type structures, though none is less than 3.3Å. The type of contact differs with, for example, five being between oxygens and methyl carbons compared with only two or three in the cavity structures. Two of the trans-annular (ether) oxygen-oxygen contacts are approximately equal to the sum of the van der Waals radii (2.8Å) and one (O(15)...O(35), 2.92Å) is slightly greater.

The departures from planarity in the three aromatic rings are greater than in the ethanol structure, with a maximum deviation of 0.030Å (for C(11)) occurring in ring A. The inclination of the rings with respect to each other are very similar to those in the ethanol cavity complex, the angles between rings A and B, A and C, and B and C being 43^{o}, 39^{o} and 31^{o} respectively (*cf.* 43^{o}, 28^{o} and 43^{o} in the ethanol complex[3]). This again emphasises both the asymmetry in the conformation and the similarity of the degree of deformation in each case.[13]

* $\Delta\tau$ is the difference between the observed and 'ideal'[13] torsion angles.

† To facilitate comparison with the cavity complexes, all torsion angle calculations are based on the coordinate set for the enantiomorph in $P6_5$ and not those listed, which are for $P6_1$. This is merely an accidental consequence of the crystals selected for study in each case.

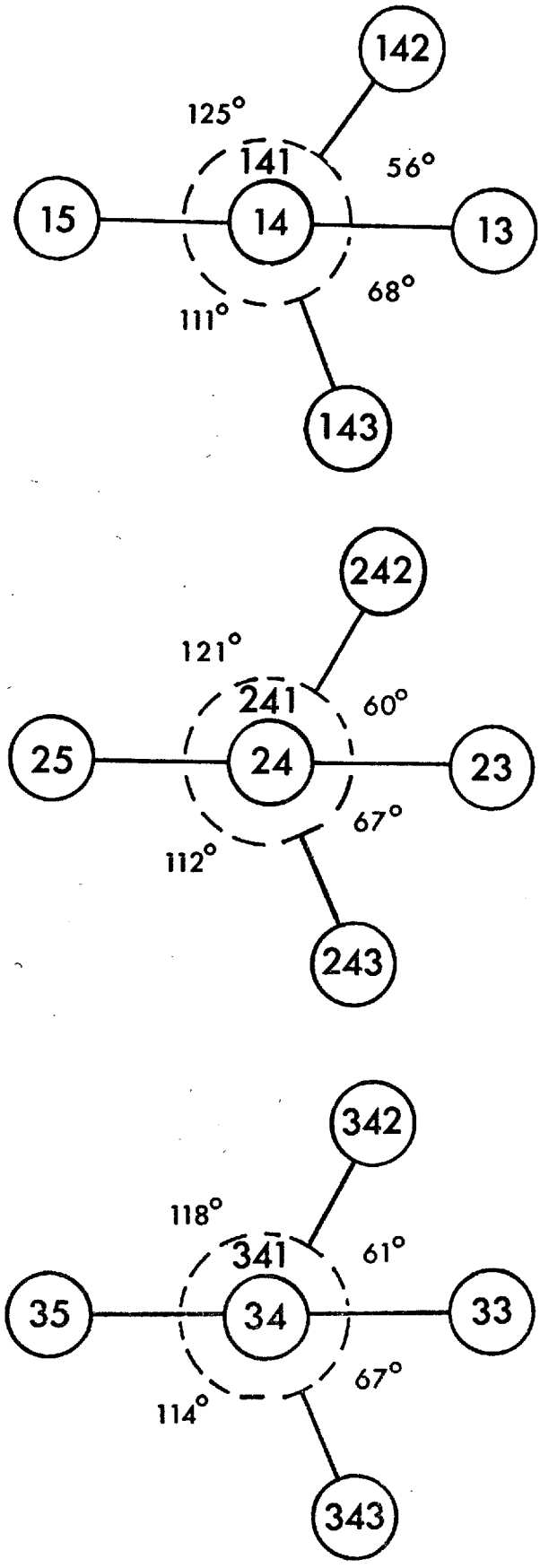


Figure 4. Newman projections down each of the three aromatic-isopropyl bonds.

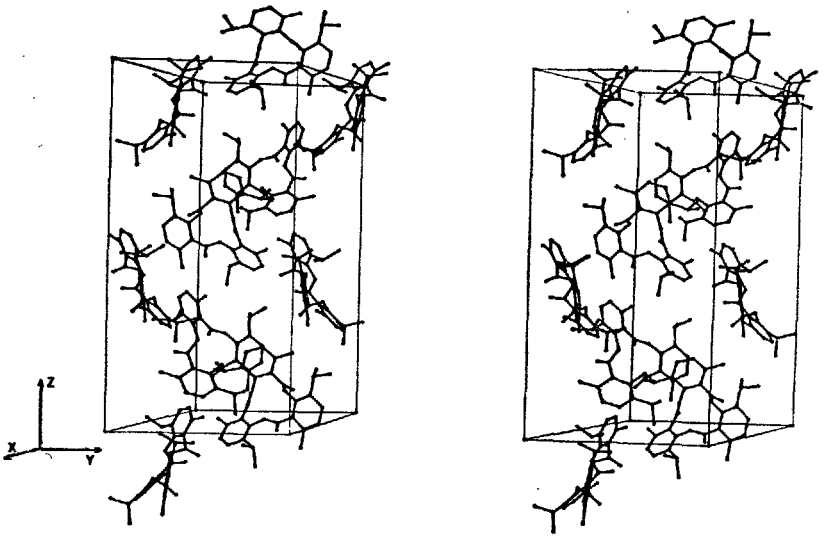


Figure 5. Stereo view of the packing of the molecules of the host framework.

The Channel

As in the cavity-type structure formed with methylene iodide,[2] the bounds of the inclusion region in the structure (the channel) have been mapped by plotting the van der Waals sections of the bounding atoms, at $\sim 1\mathring{A}$ intervals along the channel direction (c). Figure 6 shows the contour map thus derived. Only 1/6th of the length of the channel is illustrated, the rest being generated by the 6_1 screw. The channel is confined to the six-fold axis at the origin of the unit-cell: there are no voids associated with the three-fold axes. This confirms the conclusions of Lawton and Powell.[1] As can be seen, the channel has a fairly uniform cross-section and presents an almost unhindered free passage (of diameter $\sim 4.3\mathring{A}$) running the length of the c direction; there is no pronounced spiralling of the channel.

Figure 7 shows a section through the channel (in the plane of b and c) and illustrates how the channel walls are dominated by methyl and isopropyl groups. This can also be seen very clearly in Figure 8 which shows a plan view of the arrangement of the TOT molecules looking down c. (To avoid overlap, cell translated molecules have been omitted). To appreciate the overall dominance of the methyl and isopropyl groups along the full length of the channel, it is necessary to consider the environment around each of the four corners of the cell, to build up a composite picture.

The contour pattern shows the possibility of a secondary cavity, or recess, in the wall of the channel. However, as can be seen in Figure 9 which shows the section (Q, Fig.6) through what would be the window into the cavity, the entrance is completely blocked. It is interesting to note, however, that the methyls of the isopropyl group (C(342) and C(343)) which, as mentioned earlier display very large

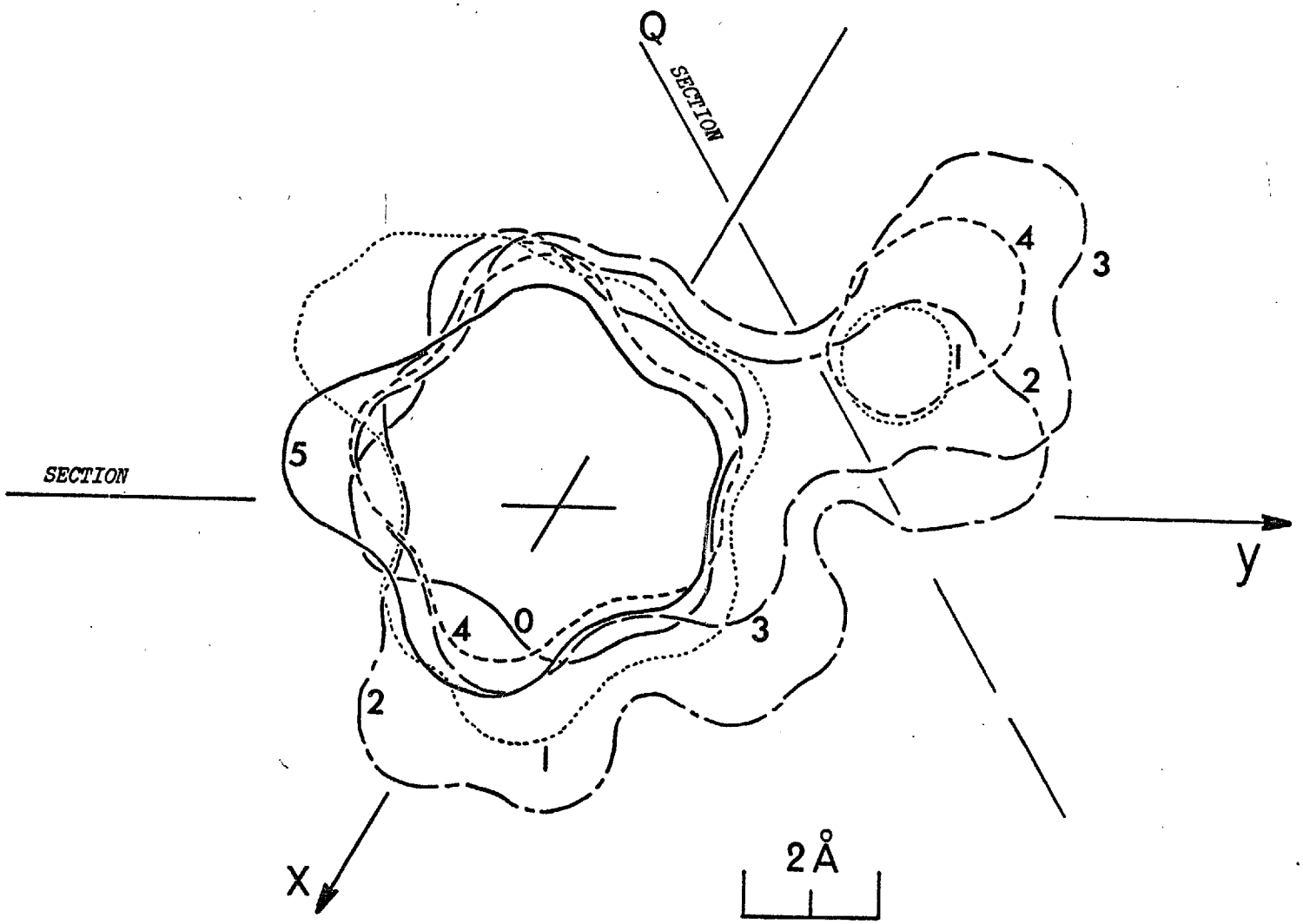


Figure 6. Contour map of the bounds of the channel with contours at ∿ 1Å intervals. 1/6th of the length of the channel is shown.

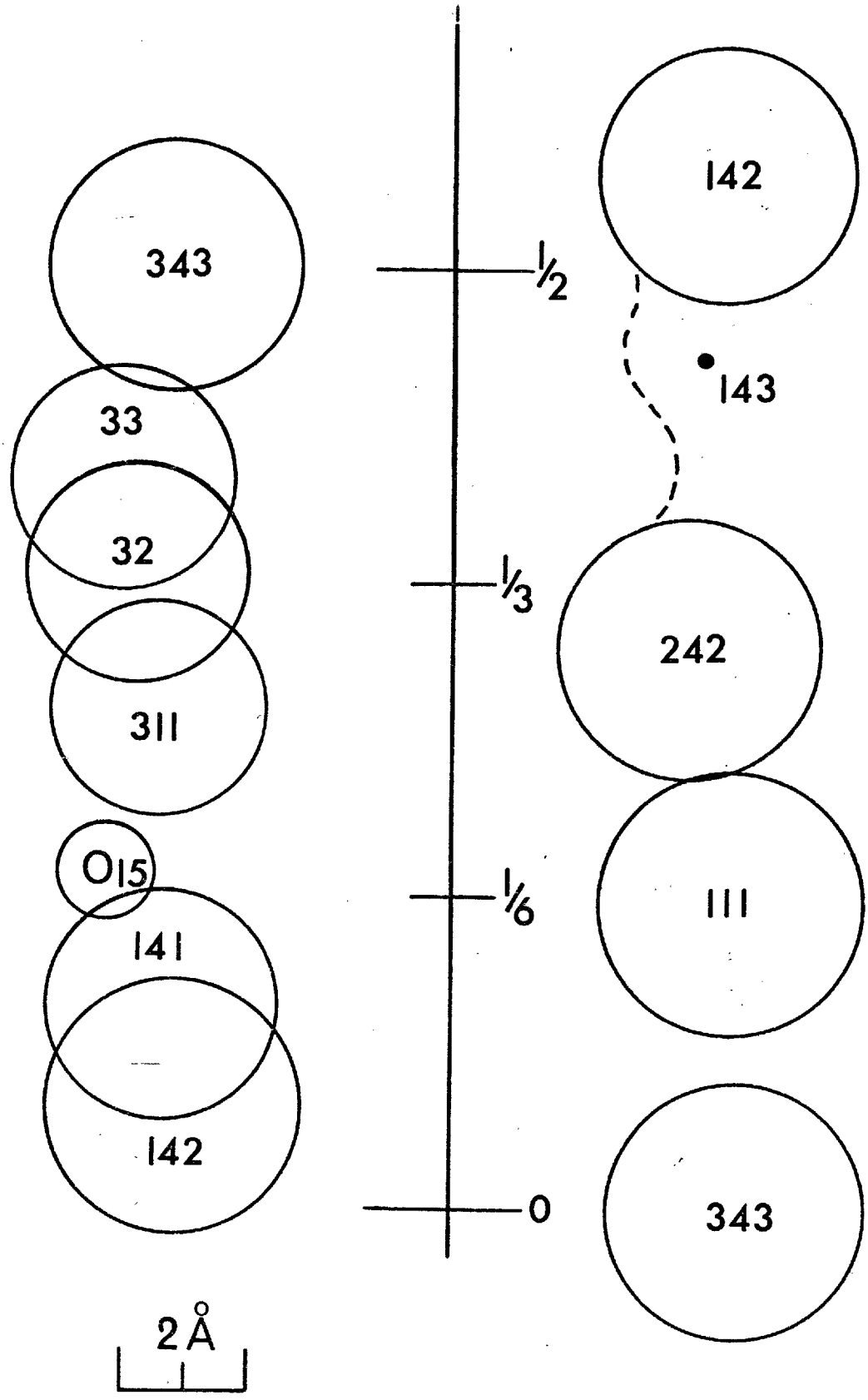


Figure 7. Sectioned van der Waals spheres of the atoms bounding the channel in the *bc* plane.

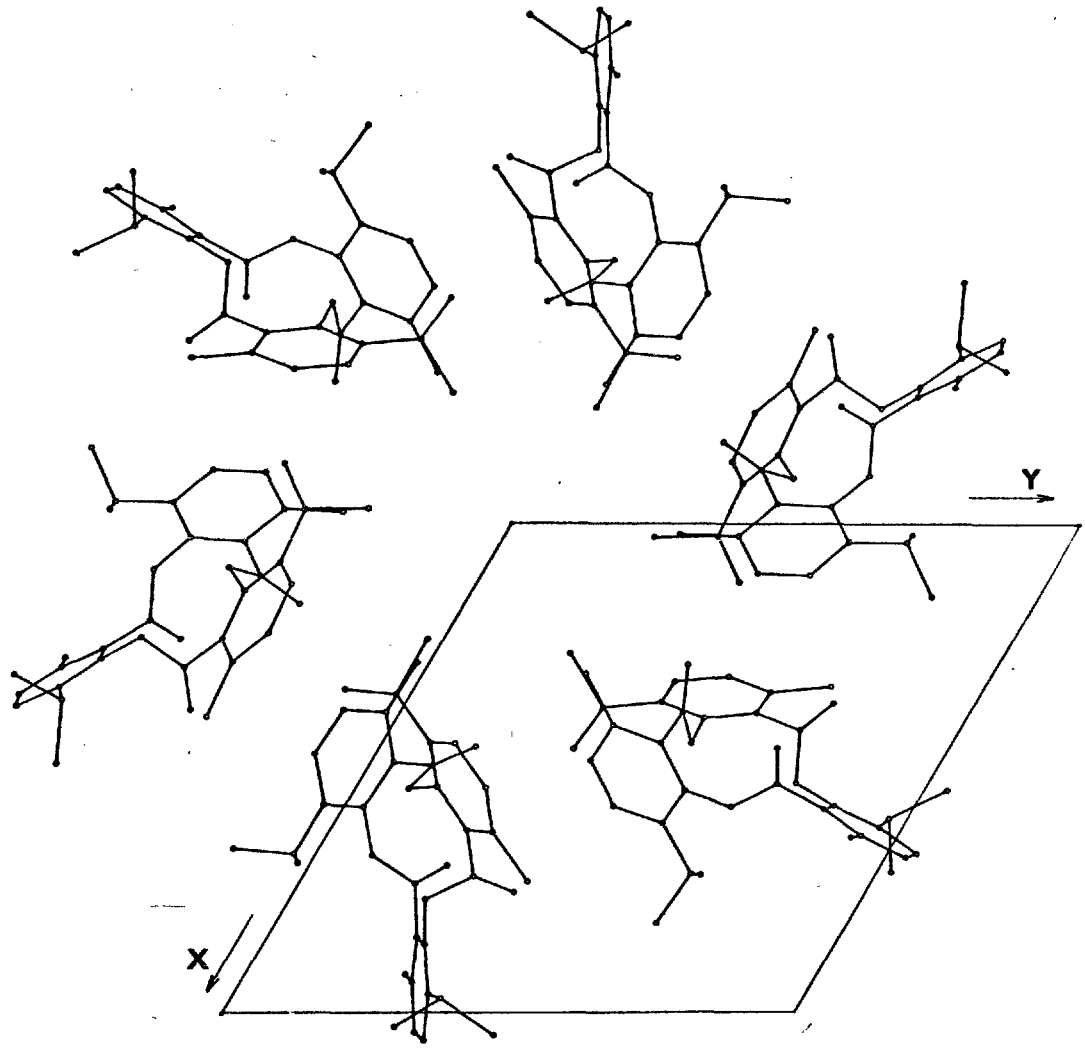


Figure 8. Arrangement of the tri-*o*-thymotide molecules looking down *c*. (Cell translated molecules have been omitted for clarity.)

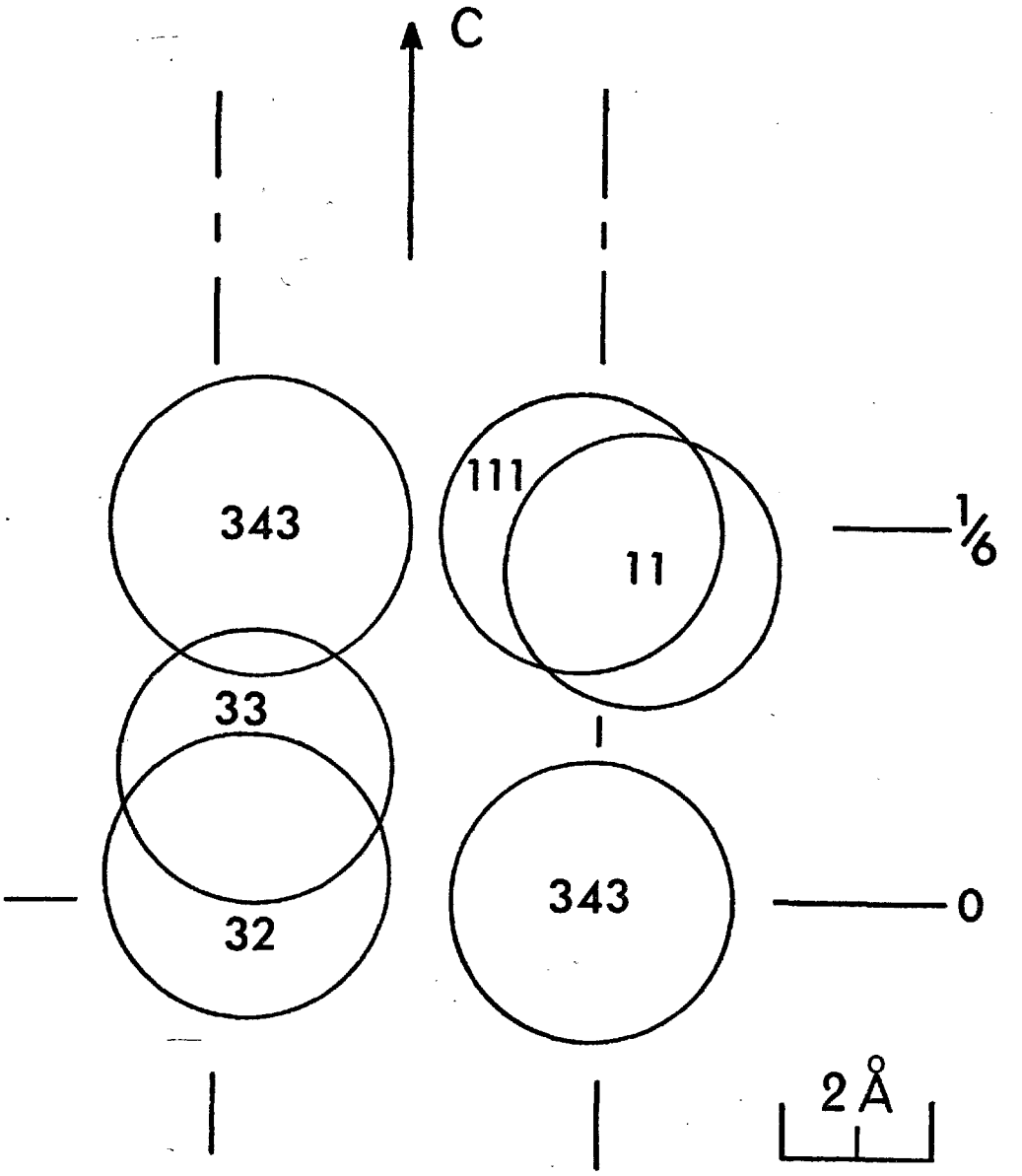


Figure 9. Sectioned van der Waals spheres corresponding to the section line Q in Figure 6, showing how the entrance to the secondary cavity in the wall of the channel is blocked.

motion, are major limiters to the side and entrance to this secondary cavity. Consequently they have the freedom to vary their orientation without affecting the rest of the structure and probably do so to allow the inclusion of singly-branched straight chain molecules.

There is no evidence from this analysis of an ordering of the stacking (in the *c* direction) of the CH_2 groups of the cetyl alcohol molecule. The residual electron density in the channel forms a more or less uniform column running the length of the *c* axis, with no indication of any systematic 'bunching'.

Finally, the constitutional formula: $C_{33}H_{36}O_6.0.22(C_{16}H_{33}OH)$, is that determined by Lawton and Powell[1] and has not been verified in this study. Their figure of 1.32 cetyl alcohol molecules/unit-cell, was derived from accurate unit-cell and density measurement. They used a gradient column to measure the densities of various adducts and found that in most cases (including cetyl alcohol) a sharply defined layer was formed for each complex, thus indicating a high constitutional consistency.[1] The cetyl alcohol molecule has a calculated packing length (allowing for end groups) of 23.2Å,[1] this when multiplied by 1.32 gives 30.6Å. Clearly some buckling or overlap of molecules is necessary to accommodate 1.32 molecules into the cell length of 29.02Å. Although there is no pronounced spiralling of the channel (Figs.6,7) its centre does precess about the axis, thereby reducing the projected length of the included molecule; also in parts of the channel wall there are recesses providing sufficient widening of the channel to permit some overlap between the ends of the included molecules.

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Table 1

Fractional coordinates (X 10^4) for the non-hydrogen atoms with estimated standard deviations in parentheses

Atom	*x*	*y*	*z*
C(111)	3096(7)	2883(7)	-55(4)
C(11)	4114(6)	3875(6)	-164(3)
C(12)	4823(7)	3837(7)	-497(3)
C(13)	5756(6)	4730(6)	-623(3)
C(14)	6101(5)	5743(5)	-425(2)
C(15)	5435(5)	5773(5)	-82(2)
C(16)	4476(5)	4870(5)	56(2)
C(17)	3838(5)	4938(5)	443(2)
O(15)	5787(3)	6777(3)	137(1)
O(17)	2883(4)	4592(5)	446(2)
C(141)	7127(6)	6721(6)	-569(3)
C(142)	7143(9)	6910(10)	-1091(3)
C(143)	8104(8)	6632(8)	-425(4)
C(211)	3307(8)	7262(10)	1931(3)
C(21)	3414(6)	6260(8)	1783(3)
C(22)	3107(8)	5386(11)	2070(3)
C(23)	3227(8)	4513(9)	1932(3)
C(24)	3641(5)	4470(7)	1513(3)
C(25)	3958(5)	5375(6)	1239(2)
C(26)	3850(5)	6230(6)	1356(2)
C(27)	4215(5)	7189(5)	1030(2)
O(25)	4461(3)	5402(3)	816(2)
O(27)	3665(4)	7525(5)	876(2)
C(241)	3753(6)	3528(7)	1375(3)
C(242)	2693(9)	2423(10)	1360(6)

Table 1 (contd.)

Atom	*x*	*y*	*z*
C(243)	4567(8)	3398(9)	1654(4)
C(311)	6434(8)	9242(7)	-602(3)
C(31)	6376(6)	9358(6)	-90(3)
C(32)	6827(6)	10349(6)	111(3)
C(33)	6747(7)	10484(5)	568(4)
C(34)	6203(6)	9608(6)	870(3)
C(35)	5769(5)	8579(5)	669(2)
C(36)	5832(5)	8431(5)	200(2)
C(37)	5319(5)	7353(5)	0
O(35)	5297(3)	7659(3)	950(1)
O(37)	4572(5)	6970(5)	-267(2)
C(341)	6055(8)	9733(7)	1380(3)
C(342)	5396(16)	10330(17)	1449(4)
C(343)	7081(10)	10232(11)	1646(5)

Table 2

Anisotropic thermal parameters* (X 10^3 Å^2) for the non-hydrogen atoms with standard deviations in parentheses

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(111)	93(6)	84(5)	136(8)	43(5)	-21(6)	-23(5)
C(11)	88(5)	69(4)	86(5)	45(4)	-24(4)	-14(4)
C(12)	113(6)	90(5)	88(5)	74(5)	-24(5)	-29(4)
C(13)	87(5)	88(5)	72(4)	60(4)	-0(4)	-9(4)
C(14)	77(4)	73(4)	60(4)	53(4)	-1(3)	-0(3)
C(15)	76(4)	63(4)	52(3)	47(3)	-9(3)	-4(3)
C(16)	68(4)	63(4)	65(4)	43(3)	-14(3)	-9(3)
C(17)	59(4)	72(4)	70(4)	35(3)	-8(3)	1(3)
O(15)	67(2)	62(2)	54(2)	42(2)	-5(2)	-4(2)
O(17)	62(3)	156(5)	83(3)	53(3)	-18(3)	-26(4)
C(141)	94(5)	99(5)	68(4)	67(5)	12(4)	7(4)
C(142)	133(8)	169(10)	81(6)	71(8)	22(6)	38(6)
C(143)	97(6)	113(7)	124(8)	54(6)	-8(5)	8(6)
C(211)	137(8)	203(11)	69(5)	113(8)	10(5)	-16(6)
C(21)	76(4)	144(8)	47(4)	55(5)	6(3)	7(4)
C(22)	99(6)	175(10)	53(4)	58(7)	23(4)	27(6)
C(23)	95(6)	125(8)	84(6)	27(6)	3(5)	45(6)
C(24)	63(4)	86(5)	80(5)	27(4)	-4(4)	24(4)
C(25)	44(3)	81(4)	58(4)	22(3)	-1(3)	9(3)
C(26)	59(4)	83(4)	49(3)	35(3)	2(3)	8(3)
C(27)	63(4)	83(4)	48(3)	35(4)	1(3)	-2(3)
O(25)	46(2)	73(3)	60(2)	24(2)	-2(2)	-1(2)
O(27)	69(3)	117(4)	112(4)	58(3)	9(3)	35(3)
C(241)	70(5)	81(5)	117(7)	16(4)	-10(5)	34(5)
C(242)	106(8)	120(9)	272(16)	41(7)	-2(10)	23(10)

Table 2 (contd.)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(243)	105(7)	132(8)	159(10)	52(6)	-25(7)	24(7)
C(311)	131(7)	121(6)	82(5)	88(6)	37(5)	47(5)
C(31)	84(5)	76(4)	80(5)	57(4)	19(4)	22(4)
C(32)	83(5)	64(4)	120(7)	39(4)	23(5)	29(5)
C(33)	87(5)	48(4)	135(7)	30(4)	5(5)	-5(4)
C(34)	74(4)	81(5)	82(5)	46(4)	-9(4)	-20(4)
C(35)	54(3)	61(3)	57(3)	32(3)	0(3)	2(3)
C(36)	64(3)	61(3)	55(3)	40(3)	5(3)	5(3)
C(37)	83(4)	78(4)	47(3)	57(4)	-4(3)	1(3)
O(35)	53(2)	75(3)	50(2)	34(2)	1(2)	6(2)
O(37)	148(5)	115(4)	101(4)	101(4)	-65(4)	-34(3)
C(341)	122(7)	111(6)	85(5)	65(6)	-23(5)	-45(5)
C(342)	349(22)	405(26)	106(9)	300(22)	-13(12)	-71(13)
C(343)	148(10)	223(14)	148(10)	104(10)	-54(8)	-86(10)

* In the form: $\exp[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^*+2U_{13}hla^*c^*+2U_{23}klb^*c^*)]$

Table 3

Fractional coordinates and isotropic thermal parameters (X 10^3) for the hydrogen atoms*

Atom	x	y	z	U(Å^2)
H(12)	463	313	-64	63
H(13)	622	466	-87	63
H(1111)	301	228	-26	114
H(1112)	310	269	28	114
H(1113)	248	301	-11	114
H(141)	720	737	-40	89
H(1421)	650	697	-118	114
H(1422)	782	759	-118	114
H(1423)	712	629	-126	114
H(1431)	808	651	-9	114
H(1432)	808	601	-59	114
H(1433)	878	731	-51	114
H(22)	279	537	238	63
H(23)	300	390	215	63
H(2111)	298	714	225	114
H(2112)	404	793	194	114
H(2113)	284	737	171	114
H(241)	408	368	106	89
H(2421)	214	249	117	114
H(2422)	284	187	121	114
H(2423)	242	219	168	114
H(2431)	526	411	167	114
H(2432)	429	316	197	114
H(2433)	470	285	151	114
H(32)	724	1100	-9	63

Table 3 (contd.)

Atom	x	y	z	U(Å^2)
H(33)	709	1124	70	63
H(3111)	684	997	-75	114
H(3112)	681	882	-67	114
H(3113)	569	884	-73	114
H(341)	566	900	153	89
H(3421)	471	995	127	114
H(3422)	521	1031	178	114
H(3423)	583	1109	135	114
H(3431)	747	983	159	114
H(3432)	754	1100	154	114
H(3433)	692	1022	198	114

* The numbering of the hydrogen atoms is that of the atoms to which they are bonded.

Table 4

Intermolecular distances* ≤ 3.6Å

C(211)...O(37^{i})	3.38	C(32) ...C(25^{ii})	3.50
C(311)...O(15^{ii})	3.54	C(32) ...O(35^{ii})	3.47
O(27) ...C(243^{ii})	3.32	C(311)...O(25^{ii})	3.49
C(12) ...O(17^{iii})	3.58	C(12) ...C(21^{iii})	3.51
C(13) ...O(27^{iii})	3.37	C(12) ...C(26^{iii})	3.59
C(343)...O(17^{iv})	3.56		

* Roman numeral superscripts denote the following equivalent positions relative to the reference molecule at x,y,z:

i $1-y,1+x-y,1/3+z$ ii $y,1-x+y,-1/6+z$ iii $y,-x+y,-1/6+z$

iv $-1+y,-x+y,-1/6+z$

Table 5

Selected trans-annular and intramolecular distances (Å)

C(111)...O(17)	2.99	O(15) ...O(25)	2.76
C(211)...O(27)	3.09	O(15) ...O(35)	2.92
C(311)...O(37)	3.15	O(25) ...O(35)	2.85
O(17) ...O(27)	3.97	O(17) ...O(37)	3.67
O(27) ...O(37)	3.79	O(15) ...C(17)	2.86
O(25) ...C(27)	2.82	O(35) ...C(37)	2.79

Table 6

Equations of the least-squares planes (in direct space) for the three aromatic rings in the structure together with their standard deviations and the largest displacements from them.

A $9.795x - 7.513y + 20.245z = 0.817$

$\sigma = 0.020$Å C(11) -0.030Å

B $11.476x - 0.274y + 11.691z = 5.834$

$\sigma = 0.006$Å C(24) -0.009Å

C $14.144x - 7.083y + 4.379z = 2.364$

$\sigma = 0.011$Å C(34) -0.014Å

Dihedral angles between the planes of the rings:

A,B = 43° A,C = 39° B,C = 31°

CHAPTER 4

The crystal structure of unsolvated tri-*o*-thymotide

Summary

The title compound crystallises in the orthorhombic space group $Pna2_1$, with a = 16.049(2), b = 13.424(2), c = 13.969(2)Å, Z = 4. The structure was solved by direct methods and refined by full-matrix least squares to R = 0.043 for the 3039 independent diffractometer measured reflections. The tri-*o*-thymotide molecule, as in the solvated forms, adopts a propeller conformation which deviates significantly from C_3 symmetry. The deviations are larger than in the solvated structures. The angles between the planes of the three aromatic rings are 31°, 48° and 37°.

Tri-*o*-thymotide (TOT) as well as forming a wide range of crystalline, chiral inclusion compounds,[1-4] also crystallises in an unsolvated form.[2] This, whilst still crystallising in a non-centrosymmetric space-group, adopts one that contains glide planes and is consequently a racemate, unlike the majority of solvated forms of TOT. An *X*-ray analysis of the unsolvated form was undertaken to determine whether crystallisation as a racemate and the consequent different molecular packing, is accompanied by significant changes in the conformational geometry of the TOT molecule, compared with that found in the chiral, channel[5] and cavity[6,7] structures.

Preliminary accounts of this investigation[8] and of an independent determination[9] have been reported.

EXPERIMENTAL

Crystals suitable for analysis were prepared by recrystallisation of pure unsolvated TOT[2] from methanol. The unsolvated form crystallises as long clear needles with an approximately square cross-section. Accurate lattice parameters were determined (at 10°C) from measurements of high angle α_1 and α_2 reflections on a diffractometer using Cu-K_α radiation.

Crystal Data $C_{33}H_{36}O_6$, M = 528.6, Orthorhombic, a = 16.049(2), b = 13.424(2), c = 13.969(2)Å, U = 3010Å^3, D_c = 1.166gcm^{-3}, Z = 4, $F(000)$ = 1128. Space-group $Pna2_1$ (No. 33),† from systematic absences; *Pnam* is ruled out by cell contents. Cu-K_α radiation, $\bar{\lambda}$ = 1.54178Å, μ(Cu-K_α) = 6.1cm^{-1}.

† This space-group, though non-centrosymmetric, contains glide planes and consequently equal numbers of molecules of both chiralities.

A crystal *ca.* 0.25 x 0.25 x 0.55 mm^3 was cut from a longer needle and mounted along its *c* direction. Data were measured on a Siemens off-line four-circle diffractometer using Ni-filtered Cu-K_α radiation. A total of 3039 independent reflections were measured (to $\theta = 71^\circ$) using the θ-2θ scan technique with the 'five value'[10] measuring procedure. Of these 93 reflections had $I < 2.58\sigma(I)$ and were classed as unobserved.[10] The net count of the 7 1 0 reflection, measured as a reference every 50 reflections, did not alter significantly during the data collection (*ca.* 6 days) indicating that no deterioration of the crystal had occurred. The data were brought to a uniform arbitrary scale by use of this reflection,[10] and Lorentz and polarisation corrections were applied. No absorption corrections were applied.

Solution and Refinement of the Structure

The structure was solved by direct methods by application of the program MULTAN[11] to 200 reflections with normalised structure factors (E's) > 1.67. Initial runs using up to 400 reflections failed to give good 'figures of merit' for any of the phase solutions. An E map computed for the phase solution (200 reflections) with the highest 'combined figure of merit' gave plausible positions for 33 of the 39 non-hydrogen atoms. The remaining atoms were positioned on the basis of the expected molecular configuration.

Isotropic (full-matrix) refinement gave an R-value of 0.143 and showed that two of the isopropyl methyl carbons had not, as had been assumed, positions symmetrically related to their associated aromatic ring. Their correct positions were determined from a difference map and the structure was refined anisotropically (by full-matrix least-squares) to $R = 0.066$. A difference map revealed the positions of

all the hydrogen atoms which, for subsequent refinements, were fixed at calculated positions 1.0Å from their parent carbons. No reflections were judged to have been significantly affected by extinction. Refinement was terminated at a final *R*-value of 0.043. The maximum shift/error for all the refined parameters was 0.3, and the maximum residual electron density in the final difference map was $<0.2 e Å^{-3}$.

Unit weights were used throughout the refinements. Atomic scattering factors were taken from ref. 12 with the exception of those for hydrogen which were taken from ref. 13. The computations were carried out on the Imperial College CDC 6400 and the University of London CDC 6600 and 7600 computers using, in the main, programs belonging to the *X*-ray 70 and 72 systems.[14]

RESULTS AND DISCUSSION

The observed and calculated structure factors are listed in Appendix IV. The final fractional atomic coordinates and anisotropic thermal parameters for the non-hydrogen atoms together with their estimated standard deviations are listed in Tables 1 and 2. Those for the hydrogen atoms with their isotropic temperature factors are given in Table 3. Figure 1 shows a stereo view of the molecule (ORTEP[15]). Figures 2a, b show the bond lengths and angles together with their estimated standard deviations and the numbering scheme used. Figure 3 shows the values of the torsion angles around the central 12-membered ring. Figure 4 gives the Newman projections[16] looking down each of the three aromatic-isopropyl bonds. Table 4 lists selected trans-annular and intramolecular distances and Table 5 intermolecular contacts ≤ 3.7Å. Figure 5 shows a stereo view[15] of the packing of the molecules in the structure. Table 6 lists the equations of the least-squares planes for the three aromatic

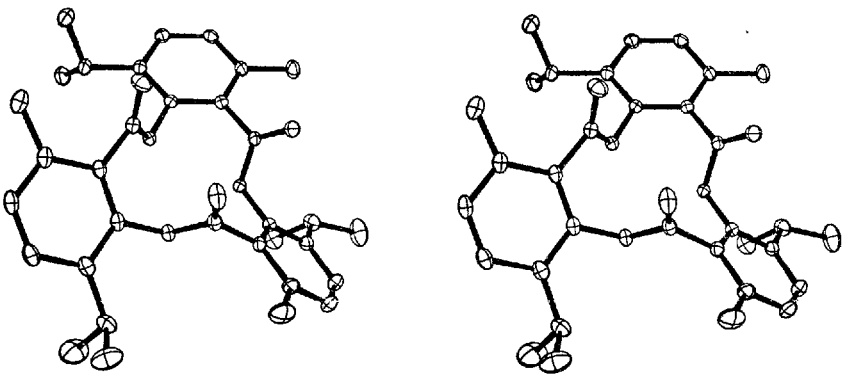


Figure 1. Stereo view of the tri-*o*-thymotide molecule.

rings in the structure and the deviations of particular atoms from them.

The molecule, as in the other two principal structural environments (cavity and channel), adopts a propeller conformation.[5-8] It is reasonable to assume, therefore, that this will be the conformation in all crystalline environments and that the intermediate helical conformation[17,18] is confined to solution.

The molecule again displays notable thermal anisotropy in the methyl and isopropyl groups, but to a lesser degree than in the cetyl alcohol, channel, complex.[5] The accuracy achieved for the bond lengths and angles shows a significant improvement over the values obtained for the adducts, the estimated standard deviations being half those obtained for the ethanol adduct.[7] The internal consistency of the bond lengths is good, and for the 12-membered ring, equivalent distances are all within 2σ. The three carboxy C(C=O)O angles show characteristic reductions from a normal trigonal value, with an average angle of 110.6°.

The torsion angles show, that as well as the already reported departures from C_3 symmetry,[8] there are significant differences between the conformation of the 12-membered ring here and in the solvated structures. In this structure we see the largest difference, so far, between equivalent torsion angles: 31° between the torsion angles about the O(15)-C(15) and O(25)-C(25) bonds. However, the overall deviations from 'ideal'[8] values are very similar to those in the ethanol adduct with $\Sigma|\Delta\tau| = 74^{\circ}$ and $\Sigma\Delta\tau = 32^{\circ}$ (*cf.* 75° and 33° respectively in the ethanol adduct[7]).

The torsion angles between the isopropyl groups and their adjacent aromatic rings, again show these groups to be rotated from a symmetric orientation. For rings A and B the rotations are small ($\sim 4^{\circ}$), but for ring C it is vastly greater than that observed in any

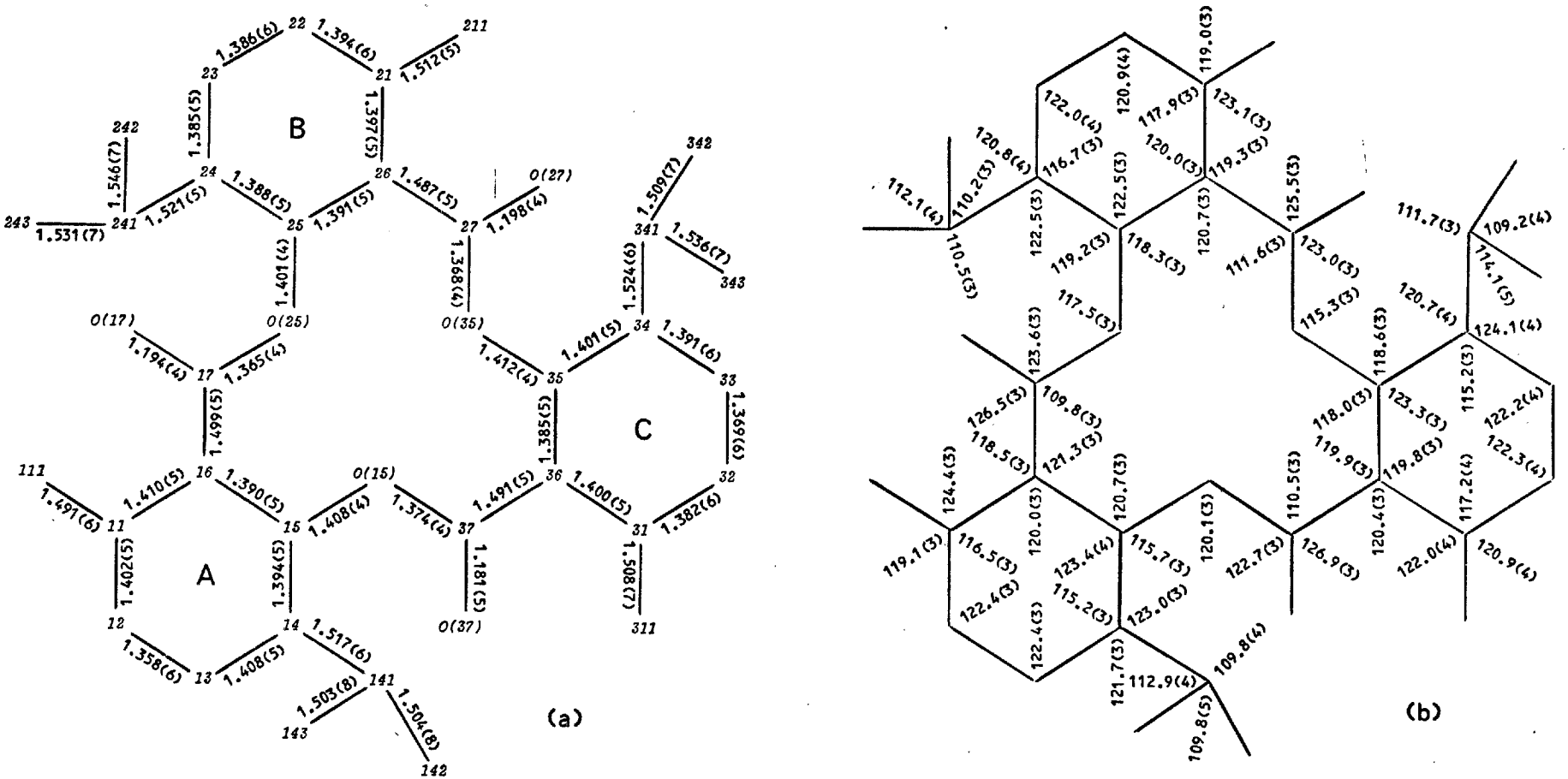


Figure 2(a) Bond lengths and numbering scheme (isopropyl methyl carbons nos. 142, 242 and 342 are on the same side of the central ring as the carbonyl oxygens); (b) valence angles. Standard deviations in parentheses.

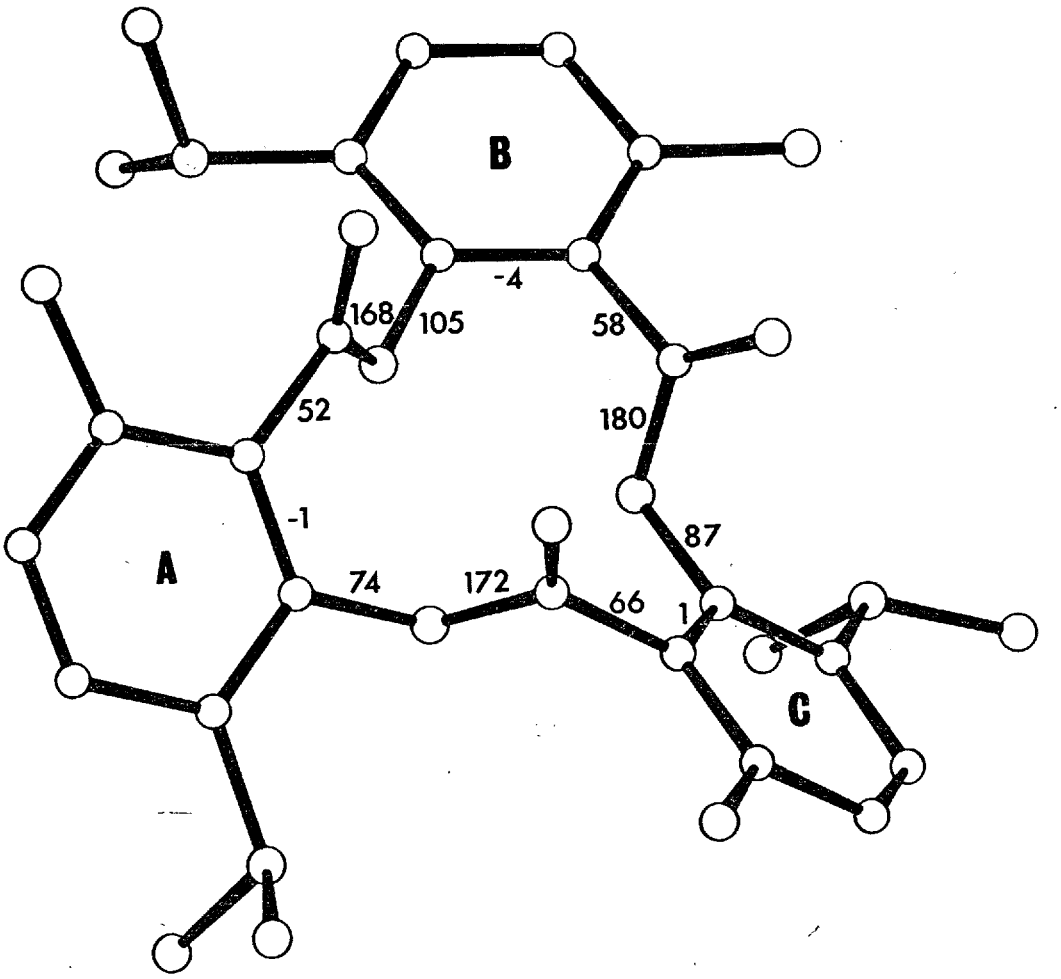


Figure 3. Torsion angles around the central 12-membered ring.

of the other structures, the group being rotated by 42° from a symmetric orientation.

The trans-annular (ether) oxygen-oxygen distances are very similar to those in the ethanol complex,[7] with two (O(15)...O(25) and O(25)...O(35), 2.79 and 2.80Å respectively) about equal to the sum of the van der Waals radii, and the third (O(35)...O(15), 2.94Å) slightly longer. There are again fairly close methyl...carbonyl oxygen contacts between C(111) and O(17) (3.06Å), and between C(211) and O(27) (3.08Å); that between C(311) and O(37) is 3.21Å.

Analysis of the intermolecular contacts shows the packing of the TOT molecules to be very much looser than in the solvated forms. There is only one intermolecular contact of less than 3.5Å, and eight of less than 3.7Å. This compares with eleven contacts of less than 3.6Å in the cetyl alcohol adduct,[5] and twelve in the ethanol one.[7] There is however no evidence of any cavities or channels in the present structure. The inability of the molecule to achieve a more tightly packed arrangement (in the unsolvated structure) may be a contributary factor in its preference for forming inclusion compounds.

The deviations from planarity in the three aromatic rings are small, with a maximum deviation from the least-squares planes of only 0.009Å for C(24) in ring B. The angles between the normals to these planes differ significantly from the values observed in the solvated structures, and show a wider spread of values. The angles between rings A and B, A and C, and B and C are 31°, 48° and 37° respectively, emphasising again the asymmetry of the molecule.[8]

A comparison of these results and those of the independent determination[9†] does not reveal any significant differences between the

† The first reports of these two analyses were at the H.M. Powell Symposium, Oxford, 9th April 1974.

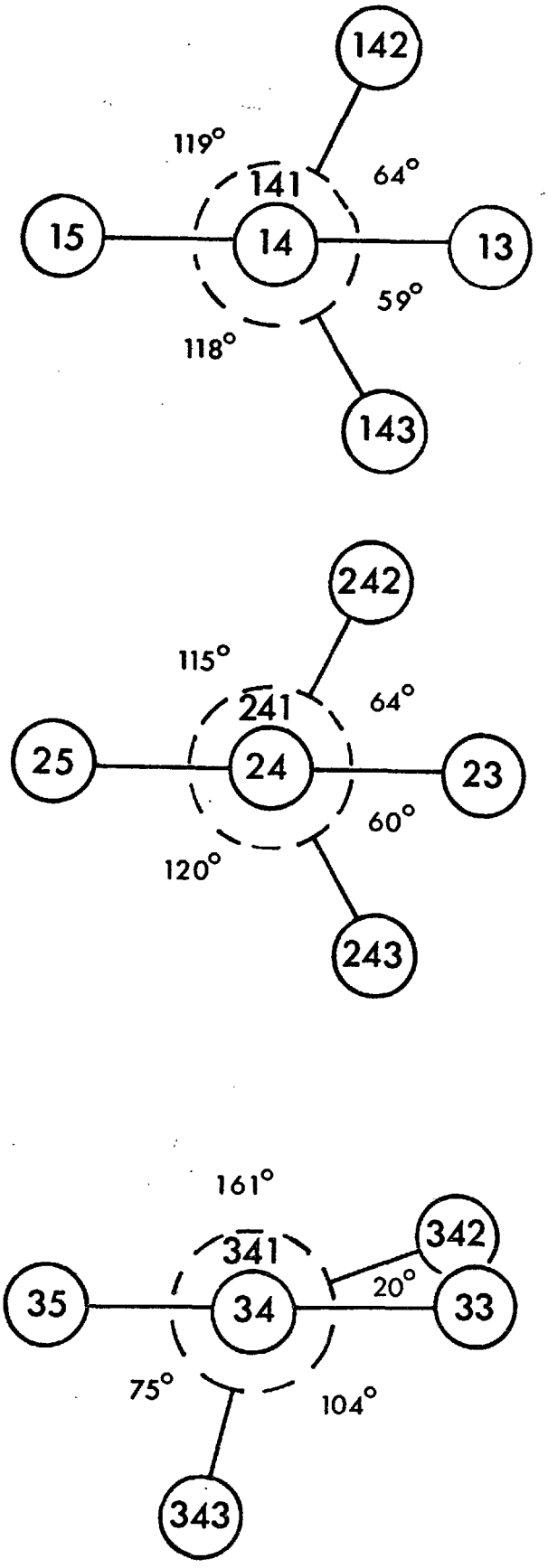


Figure 4. Newman projections down each of the three aromatic-isopropyl bonds.

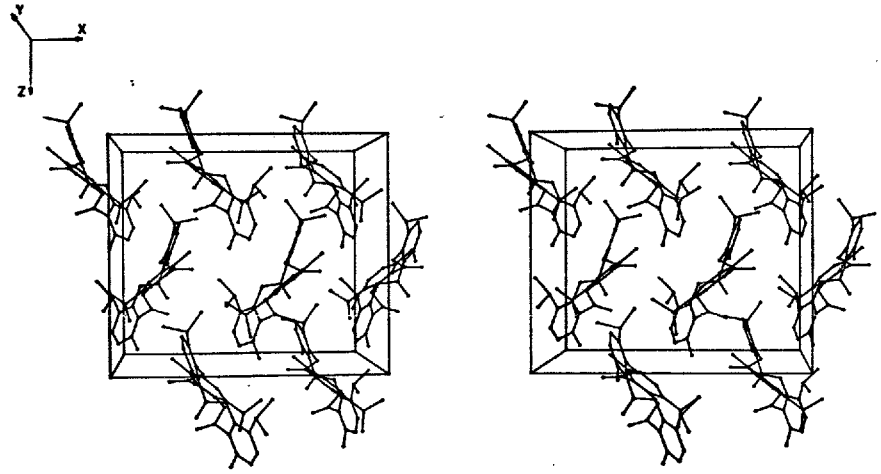


Figure 5. Stereo view of the packing of the molecules in the cell.

structures. The report of the other determination contains some minor errors: the labelling in their figure of atoms C(9) and C(10) is reversed, also that of rings A and C. Standard deviations quoted for C-H distances (which are less than those for C-C) are meaningless, as the hydrogen atoms were in fixed positions.

The determination was based on only 1327 reflections (there are 2054 independent reflections in the Cu sphere up to the quoted value of $\theta = 56^{o}$), 290 of which were classed as unobserved, and a further 50 removed for extinction. The structure, which was refined anisotropically, contains, together with a scale factor, 352 variable parameters. This results, at best, in a ratio of observations to variable parameters of 3.8, or at worst 2.8, depending on how many of the unobserved and extinct reflections contributed to the final least-squares matrix; In both cases these are unusually low figures. Anomalies in the relative standard deviations for different atoms (*e.g.* the values for the methyl carbon C(29) are the same as those for the ether oxygen atoms) are probably a consequence of this. It is interesting to note that the overall effect of using a reduced data set is manifest, not in the final R value which is similar to that we have obtained, but in an approximately 3-fold increase in the estimated positional standard deviations. This represents a serious weakness of an otherwise good analysis.

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Table 1

Fractional coordinates (X 10^4) for the non-hydrogen atoms with estimated standard deviations in parentheses

Atom	x	y	z
C(111)	7831(3)	7445(4)	5000(3)
C(11)	7130(2)	7385(3)	5698
C(12)	6700(3)	8258(3)	5942(3)
C(13)	6034(3)	8257(3)	6541(3)
C(14)	5732(2)	7380(3)	6971(3)
C(15)	6154(2)	6510(2)	6723(2)
C(16)	6836(2)	6493(2)	6109(3)
C(17)	7231(2)	5530(2)	5811(3)
O(15)	5805(1)	5618(2)	7068(2)
O(17)	7957(2)	5339(2)	5823(2)
C(141)	4976(3)	7389(3)	7624(3)
C(142)	5113(4)	7985(5)	8522(5)
C(143)	4234(4)	7789(6)	7092(5)
C(211)	6994(3)	1235(3)	5432(3)
C(21)	7082(2)	2255(3)	4986(3)
C(22)	7380(3)	2331(3)	4051(3)
C(23)	7437(3)	3248(3)	3600(3)
C(24)	7196(2)	4123(3)	4047(3)
C(25)	6911(2)	4042(2)	4982(3)
C(26)	6850(2)	3133(2)	5454(3)
C(27)	6561(2)	3084(2)	6464(3)
O(25)	6637(1)	4900(2)	5460(2)
O(27)	6938(2)	2717(2)	7115(2)
C(241)	7248(3)	5116(3)	3525(3)
C(242)	8166(3)	5371(3)	3296(4)

Table 1 (contd.)

Atom	*x*	*y*	*z*
C(243)	6705(3)	5101(4)	2624(4)
C(311)	5563(3)	5092(4)	9744(3)
C(31)	5359(2)	4264(3)	9053(3)
C(32)	4853(3)	3481(4)	9324(3)
C(33)	4647(3)	2724(3)	8711(3)
C(34)	4942(2)	2686(3)	7775(3)
C(35)	5463(2)	3476(3)	7508(3)
C(36)	5668(2)	4253(3)	8116(2)
C(37)	6208(2)	5081(3)	7765(3)
O(35)	5786(1)	3493(2)	6568(2)
O(37)	6888(2)	5276(2)	8029(2)
C(341)	4722(2)	1867(3)	7063(4)
C(342)	4411(4)	920(4)	7521(5)
C(343)	4084(3)	2225(3)	6320(4)

Table 2

Anisotropic thermal parameters* (X 10^3 Å^2) for the non-hydrogen atoms with standard deviations in parentheses

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(111)	89(3)	68(3)	79(3)	-24(2)	1(3)	16(2)
C(11)	67(2)	47(2)	52(2)	-11(2)	-12(2)	7(2)
C(12)	91(3)	37(2)	60(2)	-11(2)	-19(2)	6(2)
C(13)	86(3)	38(2)	68(3)	0(2)	-17(3)	-6(2)
C(14)	68(2)	42(2)	52(2)	1(2)	-15(2)	-7(2)
C(15)	60(2)	37(2)	42(2)	-5(1)	-14(2)	2(1)
C(16)	54(2)	37(2)	51(2)	-4(2)	-11(2)	3(1)
C(17)	56(2)	46(2)	49(2)	-2(2)	0(2)	8(2)
O(15)	50(1)	38(1)	49(1)	-2(1)	-8(1)	4(1)
O(17)	54(2)	69(2)	95(2)	5(1)	-10(2)	-4(2)
C(141)	67(2)	54(2)	85(3)	7(2)	-3(3)	-13(2)
C(142)	105(4)	162(6)	87(4)	-15(4)	21(4)	-42(4)
C(143)	75(3)	201(7)	137(6)	20(4)	-9(4)	20(6)
C(211)	101(3)	41(2)	65(2)	13(2)	9(3)	6(2)
C(21)	60(2)	40(2)	53(2)	11(2)	4(2)	4(2)
C(22)	77(3)	49(2)	55(2)	20(2)	13(2)	-2(2)
C(23)	82(3)	61(2)	48(2)	18(2)	20(2)	4(2)
C(24)	67(2)	47(2)	52(2)	10(2)	15(2)	10(2)
C(25)	49(2)	37(2)	49(2)	5(1)	11(2)	1(1)
C(26)	47(2)	43(2)	43(2)	5(1)	3(2)	4(1)
C(27)	49(2)	35(1)	46(2)	0(1)	3(2)	4(2)
O(25)	50(1)	35(1)	51(1)	2(1)	9(1)	2(1)
O(27)	64(2)	85(2)	51(1)	21(2)	5(1)	19(2)
C(241)	88(3)	53(2)	61(2)	14(2)	29(2)	20(2)
C(242)	101(4)	70(3)	93(4)	7(3)	44(3)	22(3)

Table 2 (contd.)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(243)	107(4)	79(3)	74(3)	28(3)	18(3)	28(3)
C(311)	102(4)	120(4)	51(2)	9(3)	5(3)	-26(3)
C(31)	64(2)	67(2)	42(2)	13(2)	4(2)	-0(2)
C(32)	72(3)	91(3)	49(2)	11(3)	21(2)	19(2)
C(33)	64(2)	67(3)	77(3)	-1(2)	24(2)	24(2)
C(34)	48(2)	44(2)	67(2)	2(2)	7(2)	9(2)
C(35)	44(2)	42(2)	45(2)	5(1)	5(2)	5(1)
C(36)	49(2)	43(2)	41(2)	4(2)	-1(2)	5(1)
C(37)	62(2)	38(2)	42(2)	2(2)	-5(2)	-3(1)
O(35)	44(1)	40(1)	38(1)	1(1)	3(1)	3(1)
O(37)	76(2)	62(2)	95(2)	-22(1)	-44(2)	22(2)
C(341)	59(2)	42(2)	103(3)	-8(2)	7(2)	-2(2)
C(342)	151(5)	55(3)	161(6)	-33(3)	-32(5)	22(3)
C(343)	95(3)	73(3)	100(4)	-10(3)	-19(3)	-10(3)

* In the form: $\exp[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^*+2U_{13}hla^*c^*+2U_{23}klb^*c^*)]$

Table 3

Fractional coordinates and isotropic thermal parameters ($\times 10^3$) for the hydrogen atoms*

Atom	x	y	z	U(Å^2)
H(12)	689	891	567	63
H(13)	575	891	668	63
H(1111)	792	816	482	89
H(1112)	835	718	530	89
H(1113)	769	705	442	89
H(141)	484	669	781	76
H(1421)	560	772	888	89
H(1422)	521	870	835	89
H(1423)	460	794	894	89
H(1431)	415	738	649	89
H(1432)	373	774	750	89
H(1433)	433	850	691	89
H(22)	755	172	370	63
H(23)	766	328	293	63
H(2111)	720	72	497	89
H(2112)	733	120	603	89
H(2113)	640	111	558	89
H(241)	700	565	394	76
H(2421)	850	537	390	89
H(2422)	840	486	285	89
H(2423)	820	605	299	89
H(2431)	612	494	281	89
H(2432)	672	578	232	89
H(2433)	692	459	217	89
H(32)	463	347	999	63

Table 3 (contd.)

Atom	x	y	z	$U(\text{Å}^2)$
H(33)	427	218	894	63
H(3111)	528	496	1037	89
H(3112)	617	513	984	89
H(3113)	535	573	948	89
H(341)	523	170	669	76
H(3421)	482	68	801	89
H(3422)	386	105	784	89
H(3423)	434	40	702	89
H(3431)	429	285	601	89
H(3432)	402	170	582	89
H(3433)	354	235	664	89

* The numbering of the hydrogen atoms is that of the atoms to which they are bonded.

Table 4

Selected trans-annular and intramolecular distances (Å)

O(35) ...O(15)	2.94	O(27) ...O(17)	4.28
O(25) ...O(15)	2.79	O(37) ...O(17)	3.53
O(35) ...O(25)	2.80	O(37) ...O(27)	3.67
C(111)...O(17)	3.06	C(211)...O(27)	3.08
C(311)...O(37)	3.21	C(17) ...O(15)	2.89
C(27) ...O(25)	2.82	C(37) ...O(35)	2.80

Table 5

Intermolecular distances* $\leq$ 3.7Å

C(32) ...C(16^{i})	3.68	C(32) ...O(25^{i})	3.60
C(311)...O(25^{i})	3.67	C(143)...C(23^{i})	3.68
O(37) ...C(22^{ii})	3.32	C(242)...O(27^{iii})	3.56
C(111)...C(143^{iv})	3.70	O(17) ...C(143^{iv})	3.70
O(27) ...C(343^{v})	3.62		

* Roman numeral superscripts denote the following equivalent positions relative to the reference molecule at x,y,z:

i $1-x,1-y,\frac{1}{2}+z$ ii $1\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z$ iii $1\frac{1}{2}-x,\frac{1}{2}+y,-\frac{1}{2}+z$

iv $\frac{1}{2}+x,1\frac{1}{2}-y,z$ v $\frac{1}{2}+x,\frac{1}{2}-y,z$

Table 6

Equations of the least-squares planes (in direct space) for the three aromatic rings in the structure together with their standard deviations and the largest displacements from them.

A $9.861x + 1.800y + 10.861z = 14.546$

$\sigma = 0.004$Å C(14) 0.006Å

B $14.958x + 1.499y + 4.816z = 13.339$

$\sigma = 0.006$Å C(24) -0.009Å

C $12.843x - 6.895y + 4.325z = 7.860$

$\sigma = 0.004$Å C(35) 0.006Å

Dihedral angles between the planes of the rings:

A,B = 31° A,C = 48° B,C = 37°

CHAPTER 5

The crystal structure of 5,11-dibenzyltribenzo[*b*,*f*,*j*][1,5,9]triazacyclododecine-6(5*H*),12(11*H*),18(17*H*)-trione (*N*,*N*'-dibenzyltrianthranilide)

Summary

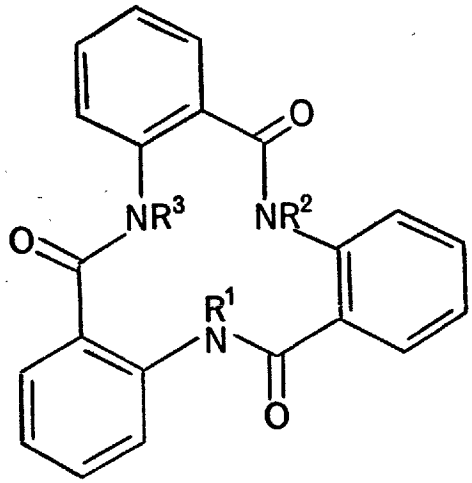
The title compound (1a) crystallises in the monoclinic space group $P2_1/a$ with a = 14.304(1), b = 14.090(1), c = 15.237(1)Å, β = 96.53(1)°, Z = 4. The structure was solved by direct methods and refined by full-matrix least squares to R = 0.061 for the 4550 independent diffractometer measured reflections. The molecule adopts a helical conformation and the angles between the planes of the three macrocyclic aromatic rings are 3°, 14° and 14°. The 12-membered ring is stabilised by a trans annular amide-amide NH...O hydrogen bond (2.935(3)Å). The structure contains a trapped toluene molecule which has been located and bounds of the cavity have been mapped. Evidence has been found of possible zeolitic properties.

Differently substituted trianthranilides (1)[1-3] form a new group of chiral medium-ring compounds that are conformationally mobile in solution. They have been shown to undergo conformational inversion via defined conformational itineraries[2,3] to give racemic mixtures in solution (*i.e.* a mixture of enantiomers of two discrete conformations: helix and propeller).

They are a natural progression from the trisalicylides which have been the subject of extensive study for more than a decade.[1,4] The conformational behaviour, in particular the dynamics of ring inversion, of these and related medium-ring systems[5,6] have already been investigated by n.m.r. line-shape analysis, and conclusions have been drawn regarding both the relative populations of conformers in solution and the probable solid-state conformations. An *X*-ray analysis has shown that one of these compounds, (1b),[7] like tri-*o*-thymotide,[4] exhibits spontaneous resolution on crystallisation.

The n.m.r. analyses have indicated that *N,N'*-dibenzyltrianthranilide (1a) adopts a helical conformation in the solid-state[3] (*i.e.* two carbonyl oxygens lie on one side of the 12-membered ring and one on the other).† An *X*-ray analysis has been carried out both to verify this conclusion and to determine accurately the molecule's conformational geometry.

† It should be noted that whilst with a chemically symmetric molecule where $R_1 = R_2 = R_3$, (1), there is only one possible helical conformation (and its enantiomorph), when one substituent differs from the others, *e.g.* $R_1 = R_2 \neq R_3$ there become possible three non-equivalent helical conformations (and their enantiomorphs). The significance of this to the n.m.r. analysis has been discussed elsewhere.[8]



(1)

a; R^1=H, R^2=R^3=CH_2Ph

b; R^1=H, R^2=R^3=Me

EXPERIMENTAL

The title compound crystallises from toluene as large clear rectangular blocks. Accurate lattice parameters were obtained by least-squares refinement of 18 high-angle reflections measured (at 12°C) on a diffractometer using Cu-K_α radiation.

Crystal Data $C_{35}H_{27}N_3O_3.\frac{1}{2}(C_7H_8)$, M = 583.7, Monoclinic, a = 14.3041(7), b = 14.0898(7), c = 15.2371(7)Å, β = 96.534(5)°, U = 3051Å^3, D_c = 1.27gcm^{-3}, Z = 4, $F(000)$ = 1228. Space-group $P2_1/a$ (No. 14),† uniquely determined from systematic absences. Cu-K_α radiation, $\bar{\lambda}$ = 1.54178Å, μ(Cu-K_α) = 6.1cm^{-1}.

A crystal *ca.* 0.65 x 0.75 x 0.5 mm^3 was mounted along its b direction. Data were measured on a Siemens off-line four-circle diffractometer using Ni-filtered Cu-K_α radiation. As several of the low-angle reflections were exceptionally strong the data were collected as two concentric spheres, the lower angle sphere (up to θ = 40°) being measured with reduced X-ray tube current. A total of 4550 independent reflections were measured (to θ = 60°) using the θ-2θ scan technique with the 'five value'[9] measuring procedure. Of these 209 reflections had $I < 2.58\sigma(I)$ and were classed as unobserved.[9] The net count of the 2 0 $\bar{9}$ reflection, measured as a reference every 50 reflections, did not alter significantly during the data collection (*ca.* 9 days) indicating that no deterioration of the crystal had occurred. The data were brought to a uniform arbitrary scale by use

† This space-group contains 2D and 2L molecules; the compound is thus a racemate both in solution and in the solid state.

of this reflection,[9] and Lorentz and polarisation corrections were applied. No absorption corrections were applied.

Solution and Refinement of the Structure

The structure was solved by direct methods by application of the program MULTAN[10] to 400 reflections with normalised structure factors (E's) > 1.70. An E map calculated for the phase solution with the highest 'combined figure of merit', gave plausible positions for all 41 non-hydrogen atoms of the trianthranilide molecule. These atoms were refined anisotropically (R = 0.277) and a difference map computed which revealed 4 pairs of peaks arranged about the crystallographic centre of symmetry at 0, ½, 0; one pair was approximately half the height of the others. They were interpreted as being due to the presence of an included molecule of the solvent of crystallisation, toluene, disordered about the centre of symmetry. All 45 atoms were refined anisotropically by full-matrix least squares, and with the toluene methyl carbon at half-weight, to give an R-value of 0.12. All the hydrogen atoms of the trianthranilide molecule were clearly located in a difference map and with the exception of the amide hydrogen H(17) (which was refined isotropically), were, for subsequent refinements, fixed at calculated positions 1.0Å from their parent carbons. Eighteen strong low-angle reflections which had $|F_o| << |F_c|$ were suspected of being affected by extinction and therefore removed. Subsequent refinement, including the hydrogens of the trapped toluene molecule in fixed positions (the most probable orientation of the methyl hydrogens was determined from a difference map), reduced R to a final value of 0.061. A final difference map still showed small amounts of residual electron density ($\sim$ 0.3eÅ^{-3}) in the region of the toluene molecule, possibly reflecting some additional disorder in its

orientation throughout the crystal. (For compliance with the crystallographic requirement of a centre of symmetry in the centre of the toluene molecule, 50% occupancy of two orientations of the molecule rotated by 180° to each other, and with the rings overlapping, had been assumed; this is probably just a good approximation.)

Unit weights were used throughout the refinements. Atomic scattering factors were taken from ref. 11 with the exception of those for hydrogen which were taken from ref. 12. The computations were carried out on the Imperial College CDC 6400 and the University of London CDC 6600 and 7600 computers using, in the main, programs belonging to the *X*-ray 70 and 72 systems.[13]

RESULTS AND DISCUSSION

The observed and calculated structure factors are listed in Appendix V. The final fractional atomic coordinates and anisotropic thermal parameters for the non-hydrogen atoms together with their estimated standard deviations are listed in Tables 1 and 2. Those for the hydrogen atoms with their isotropic temperature factors are given in Table 3. Figure 1 shows a stereo view of the molecule (ORTEP[14]). Figures 2a, b show the bond lengths and angles together with their estimated standard deviations and the numbering scheme used. Table 4 lists selected intra- and intermolecular contacts ≤ 3.5Å. Figure 3 shows the torsion angles around the central 12-membered ring, and Figure 4 the Newman projections[15] for the three amide groups. Table 5 lists the equations of some selected least-squares planes and the deviations of particular atoms from them. Figure 5 shows a contour pattern of the bounds of the inclusion region in the structure. Figure 6 shows a stereo view[14] of the packing of both the host (trianthranilide) and guest (toluene) molecules in the structure.

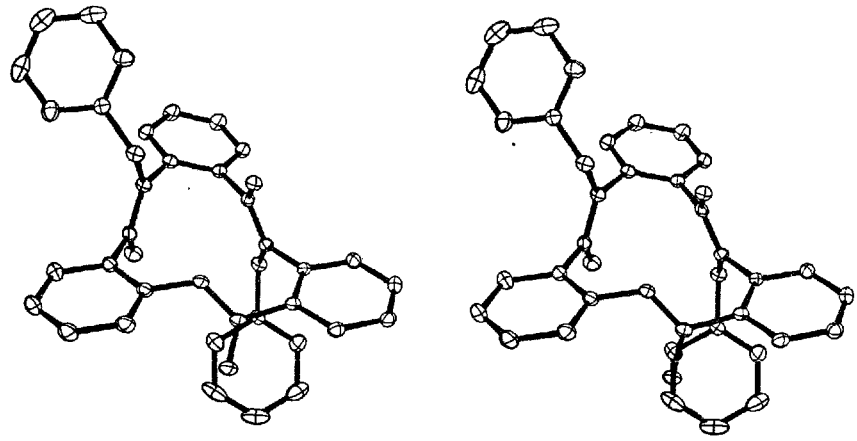


Figure 1. Stereo view of the *N,N'*-dibenzyltrianthranilide molecule.

The molecular conformation is, in accordance with the n.m.r. conclusions,[3] helical with the benzyl groups lying on opposite sides of the 12-membered ring (Fig.1). Rings A and C (Fig.3) are nearly parallel (3° between normals) and ring B is inclined equally to rings A and C (14° between normals). The planes of the *trans* amide linkages between rings A and B and between B and C are approximately normal to their adjacent rings (*i.e.* minimum conjugation), whilst that linking rings A and C is inclined at only ∿43° to the mean plane of these rings (*i.e.* more than 45° from the normal). Consequently, as the nitrogen (N(17)) has normal sp^2 geometry, the N-H bond is directed toward the opposite amide carbonyl oxygen (O(6)) and ring stabilisation is achieved by the formation of a trans-annular N-H...O hydrogen bond (2.935(3)Å). The NHO angle is 159°. The benzyls, D and E, adopt different orientations with respect to the planes of the amides, the C-Ph bonds being inclined by ∿45° (ring D) and ∿60° (ring E). The planes of the phenyl rings are, in turn, rotated with respect to their linking N-C bonds by ∿86° (D) and ∿70° (E).

The bond lengths (Fig.2a) do not deviate appreciably from expected values. There are, however, some notable internal differences: for example, C(16a)-N(17), (1.419(4)Å) is significantly shorter (by more than 5σ) than C(10a)-N(11), (1.450(4)Å) and C(4a)-N(5), (1.449(4)Å). The apparently rather short value for the aromatic bond C(113)-C(114), (1.348(8)Å, ring E) is undoubtedly due to foreshortening effects caused by anisotropic motion of the ring. The amide C-N bonds show a characteristic shortening reflecting their partial double-bond nature, and there is a small accompanying increase in the carbonyl C=O bond lengths. The degree of bond modification is not as large as that sometimes associated with delocalisation effects, nor is there any correlation between the observed shortening of the C-N bond lengths and the increase in their associated C=O lengths. This is

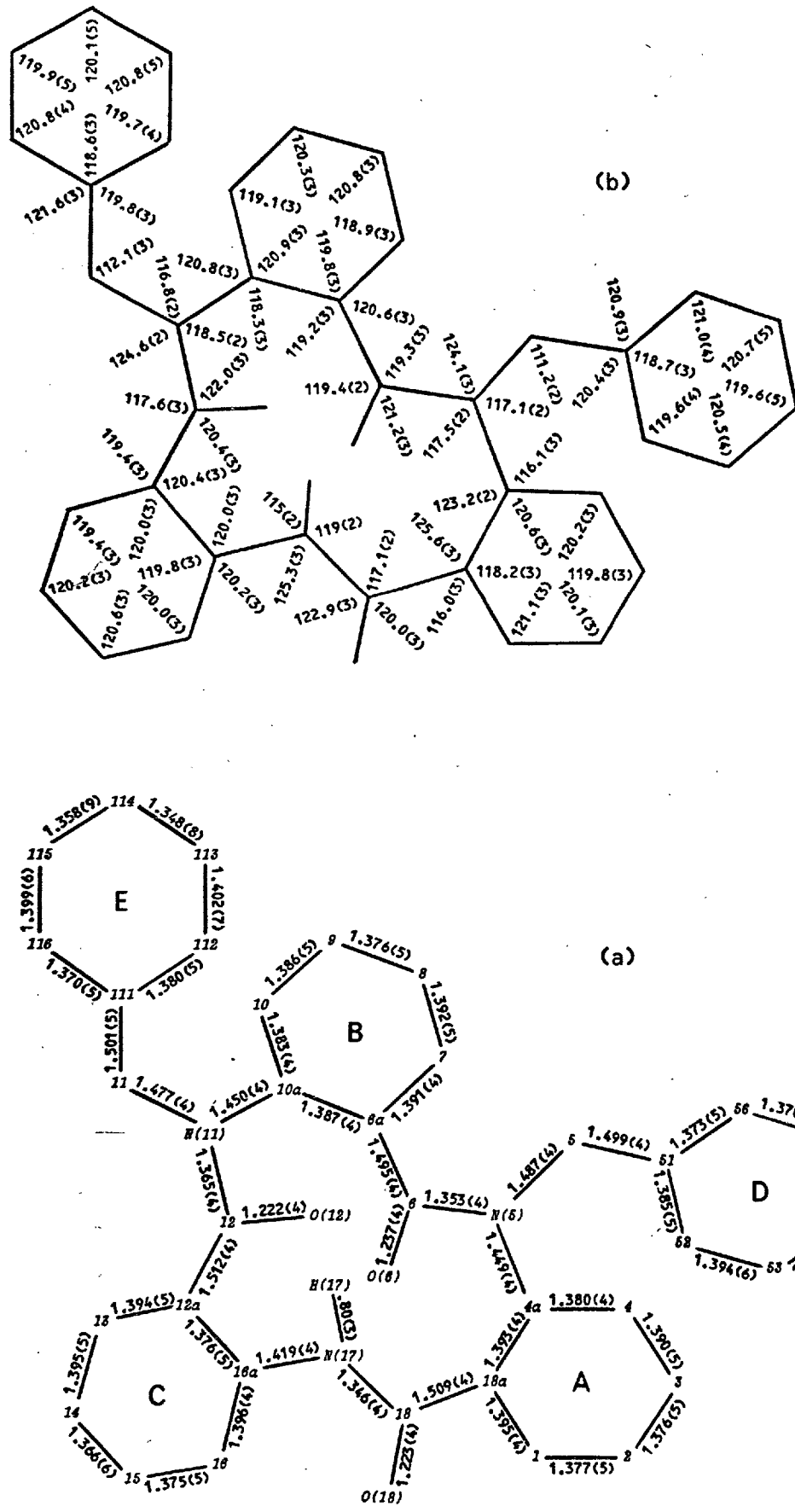


Figure 2(a) Bond lengths and numbering scheme; (b) valence angles. Standard deviations in parentheses.

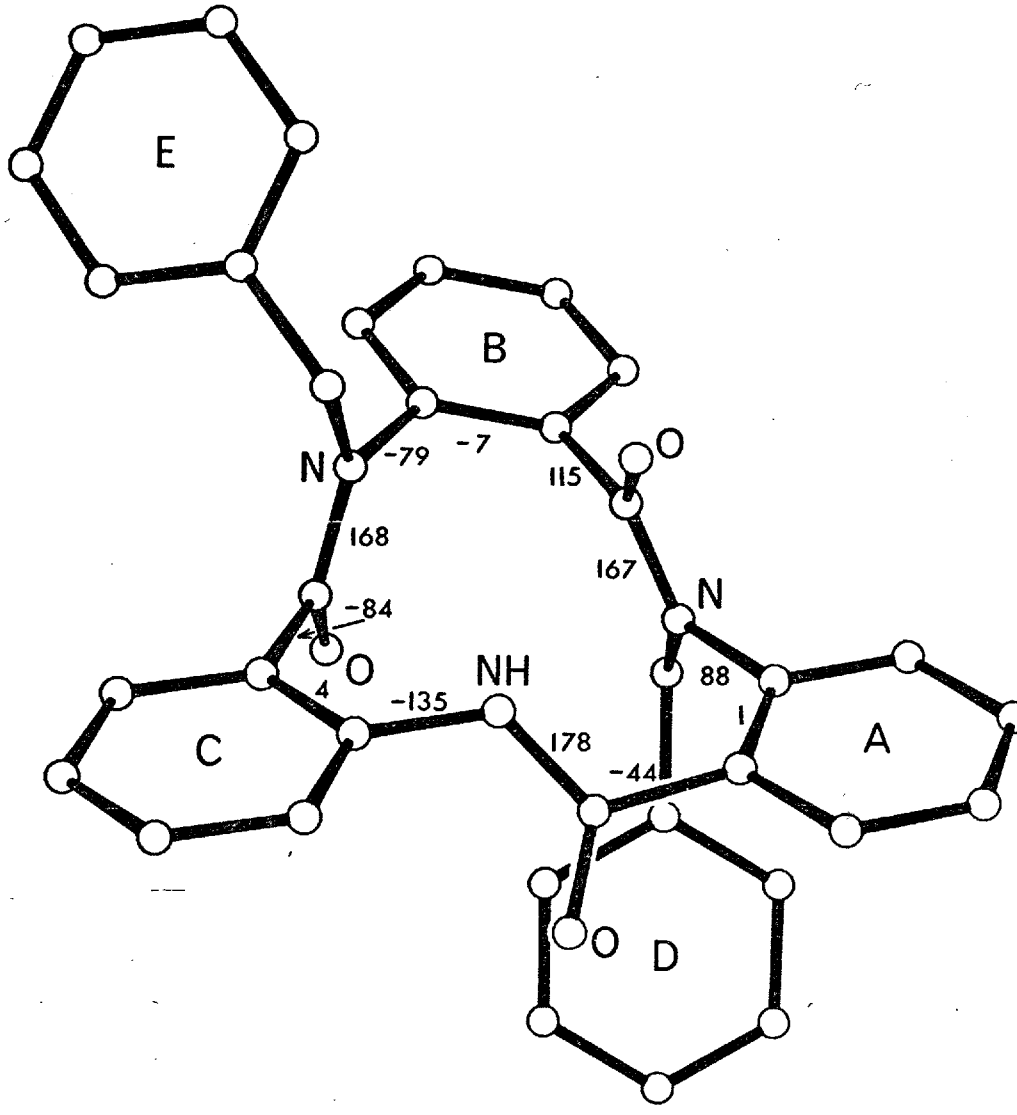


Figure 3. Torsion angles around the central 12-membered ring.

particularly apparent from a comparison of the amide linking rings B and C with that linking A and C; here the C-N bond lengths differ significantly (*i.e.* by more than 3σ) whilst there is no difference between the C=O lengths.

None of the amide groups are planar (Fig.4), however, the degree of distortion is in each case fairly small with the deformation taking the form principally of a combination of a torsional twist about the C-N bond, and an out-of-plane bending at the nitrogen. The out-of-plane bending at the carbon is in each case very small. Distortions of the above type are quite common and have been discussed previously, and a notation for describing them defined.[16,17] For the amide group linking rings B and C the deformation is primarily a rotational one; but with those linking A and B and A and C it is a combination of both effects, the largest distortion being in that linking A and B where the out-of-plane deformation parameters are: $\chi_C = 2^\circ$, $\chi_N = 13^\circ$, and $\tau = 172^\circ$. The values of these parameters for the other two amides are given with the Newman projections (Fig.4).

Of the five aromatic rings (A-E) none show significant departures from planarity. This shows that strains imposed on the rings (A-C) by the non-zero torsion angles along the common edges with the 12-membered ring are not transmitted to the rings. The largest deviation from planarity is in ring A which has the smallest torsion angle and *vice versa* for ring B.

As has been mentioned in the experimental section, the structure has been found to contain included solvent molecules. The presence of these molecules had been suggested before the structure determination was started. The first batch of crystals of the compound investigated had been crystallised from toluene, but subsequently dried. All but one of these crystals were unsuitable for *X*-ray analysis,

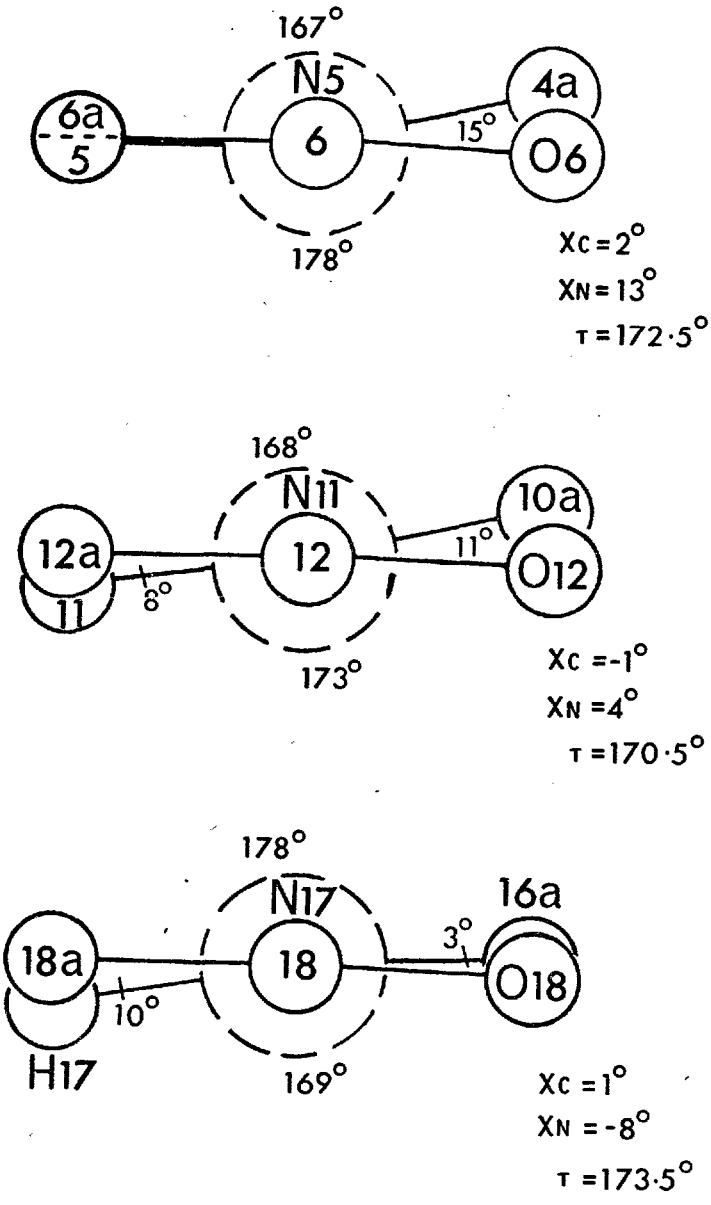


Figure 4. Newman projections and out-of-plane bending parameters for the three *trans* amide groups.

having become opaque and powdery. The remaining crystal was a slightly milky colour, but gave photographs adequate for the determination of preliminary unit-cell and space-group details. It was not possible, having just this one crystal, to measure its density and hence to determine the molecular weight of the compound. A second batch of crystals again crystallised from toluene, but this time not dried, were of excellent quality and were found to have approximately the same unit-cell dimensions and the same space-group as before, but gave large differences in the intensities of a few of the reflections. A crystal from this second batch was used for the above structure analysis. It has been concluded that the crystal from the original batch represented a partially desorbed structure, the implication being that it may be possible to remove all the toluene from the structure without destroying the host framework (*i.e.* it has zeolitic properties). For this to occur the structure must contain continuous channels or linked cavities.

Figure 5 shows the contour pattern of the bounds of the inclusion region in the structure. This is derived from a three-dimensional analysis of the van der Waals radii of the host structure. The contours are at 1Å intervals in the *b* direction; only half the region is shown, there being a crystallographic centre of symmetry, as shown, in the zero contour level.

As can be seen, the inclusion region is totally enclosed thus posing a problem as to how a trapped molecule might escape. However, inspection of the three-dimensional packing diagram (Fig.6) gives some insight as to a possible mechanism whereby this could happen. The cavity regions in the structure are the areas around the centres of symmetry at $(\frac{1}{2},0,0)$ and $(0,\frac{1}{2},0)$, *i.e.* at the boundaries between cells in the *c* direction. (These are the top and bottom edges in the

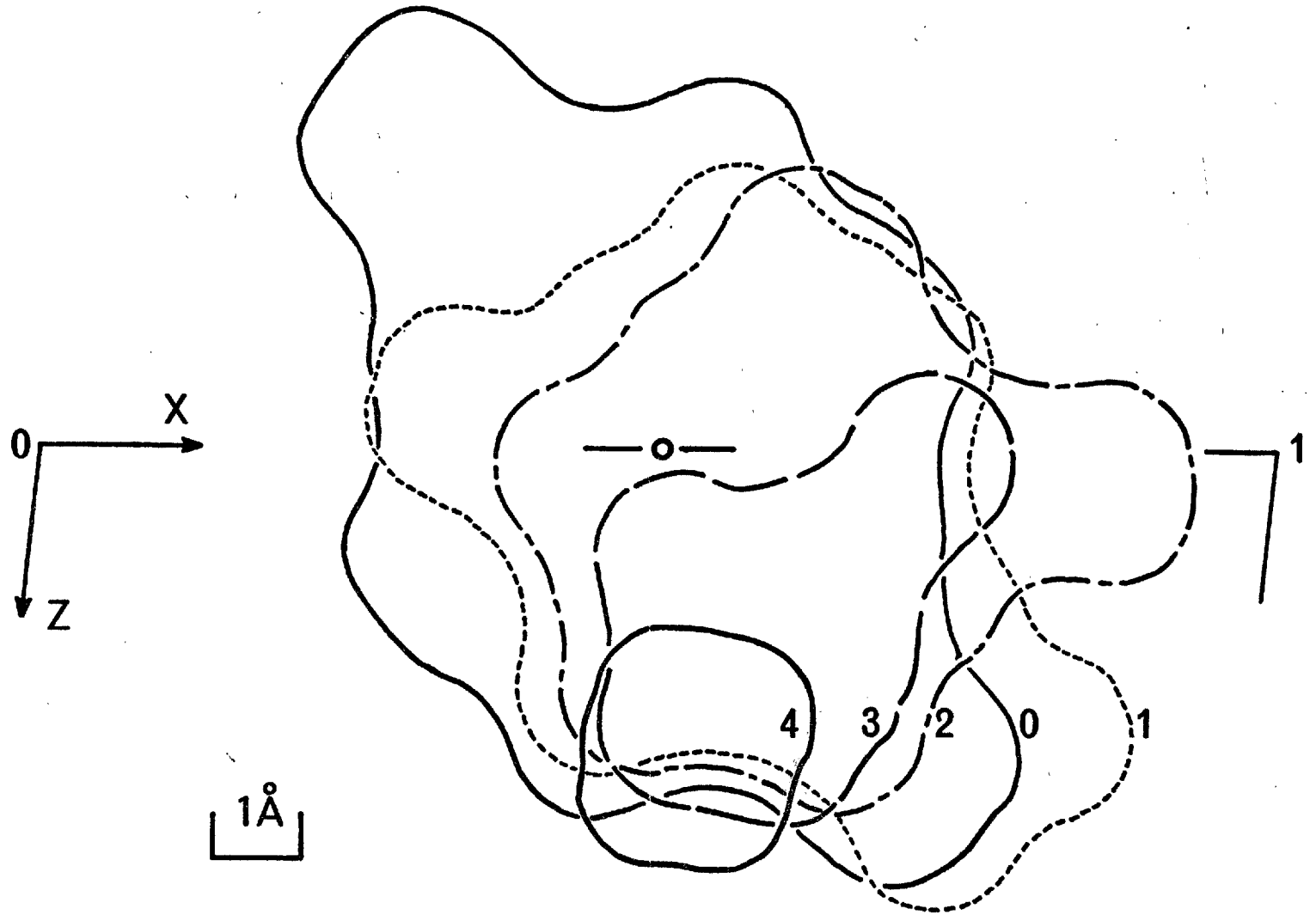


Figure 5. Contour pattern of the inclusion region in the structure. Contours at 1Å intervals.

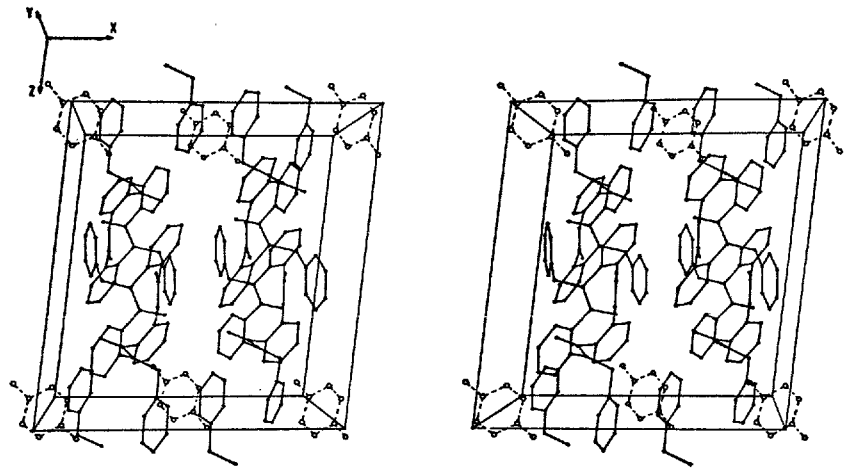


Figure 6. Stereo view of the packing of the host and guest (broken bonds) molecules in the structure.

diagram.) As can be seen, these areas are bounded in the x and y directions by one of the benzyl groups (ring E) and its symmetry related partners. These groups are chemically free to rotate, and may do so, hinging like a louvre or venetian blind, thus allowing the trapped molecule to escape from the crystal. Such a structural modification is compatible with the perturbations in the unit-cell parameters observed for a different adduct; these occur primarily in the a and b dimensions, there being little change in c.

The included molecule is not very tightly trapped in the cavity, there being only one host-guest intermolecular contact of less than 3.5Å. This is one of 3.39Å in the c direction between C(100) and C(10). The closest contact to the benzyl ring is 3.76Å between C(103) and C(112), and the shortest distance between the benzyl ring and the toluene ring is 3.92Å between C(102) and C(113). The remainder of the structure is fairly tightly packed with seven contacts under 3.5Å, the shortest being 3.38Å between O(6) and C(54) (Table 4).

Finally, the inclusion of a molecule of toluene in the lattice disordered symmetrically in two orientations results in an arrangement the same as if a molecule of p-xylene were included. Crystallisation of dried material from xylene resulted in the ready formation of good crystals which were found from X-ray photography, to have the same space-group and structure as those of the toluene adduct, but slightly different lattice parameters (Δa = +0.070, Δb = +0.019, Δc = +0.001Å, $\Delta\beta$ = -0.35°). This difference indicates that the assumed overlap of the two half toluene molecules cannot be perfect.

Clearly N,N'-dibenzyltrianthranilide has the potential to include a range of other possible guests, or even to resolve mixed isomers. This will be the subject of further study.

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Table 1

Fractional coordinates (X 10^4) for the non-hydrogen atoms with estimated standard deviations in parentheses

Atom	*x*	*y*	*z*
C(1)	4075(2)	4461(2)	4238(2)
C(2)	4109(2)	5154(3)	3605(2)
C(3)	3634(3)	5995(3)	3673(2)
C(4)	3132(2)	6149(2)	4390(2)
C(4a)	3113(2)	5462(2)	5032(2)
N(5)	2543(2)	5672(2)	5736(2)
C(5)	1504(2)	5653(2)	5509(2)
C(51)	1203(2)	4808(2)	4949(2)
C(52)	1023(2)	3948(3)	5338(3)
C(53)	735(3)	3173(3)	4805(4)
C(54)	33(3)	3256(4)	3906(4)
C(55)	810(4)	4102(5)	3530(3)
C(56)	1082(3)	4874(3)	4044(2)
C(6)	2983(2)	6044(2)	6491(2)
O(6)	3850(1)	6014(1)	6656(1)
C(6a)	2409(2)	6467(2)	7153(2)
C(7)	1946(2)	7238(2)	6984(2)
C(8)	1510(3)	7754(2)	7654(2)
C(9)	1537(3)	7338(3)	8474(2)
C(10)	1989(2)	6475(2)	8640(2)
C(10a)	2425(2)	6048(2)	7978(2)
N(11)	2914(2)	5152(2)	8130(2)
C(11)	3888(2)	5193(2)	8569(2)
C(111)	3933(2)	5577(2)	9492(2)

Table 1 (contd.)

Atom	*x*	*y*	*z*
C(112)	4314(3)	6463(3)	9683(3)
C(113)	4347(3)	6824(3)	10543(4)
C(114)	4006(4)	6319(5)	11188(3)
C(115)	3620(3)	5450(5)	11007(3)
C(116)	3593(3)	5072(3)	10155(2)
C(12)	2472(2)	4341(2)	7816(2)
O(12)	1639(2)	4331(2)	7527(2)
C(12a)	3058(2)	3448(2)	7812(2)
C(13)	3012(3)	2776(2)	8476(2)
C(14)	3519(3)	1933(3)	8451(3)
C(15)	4049(3)	1765(2)	7776(3)
C(16)	4082(3)	2419(2)	7110(2)
C(16a)	3583(2)	3269(2)	7127(2)
N(17)	3627(2)	3952(2)	6450(2)
C(18)	3540(2)	3765(2)	5578(2)
O(18)	3450(2)	2960(2)	5279(2)
C(18a)	3574(2)	4599(2)	4962(2)
C(100)	-144(5)	4862(6)	869(5)
C(101)	595(5)	4469(5)	525(6)
C(102)	733(5)	4600(5)	-357(5)
[1]C(103)	1176(13)	3973(10)	1069(10)

[1] Occupancy 50%.

Table 2

Anisotropic thermal parameters* (X 10^3 Å^2) for the non-hydrogen atoms with standard deviations in parentheses

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	45(2)	50(2)	52(2)	-3(1)	10(1)	-13(1)
C(2)	53(2)	66(2)	49(2)	-11(2)	18(1)	-12(2)
C(3)	78(2)	58(2)	51(2)	-9(2)	21(2)	4(2)
C(4)	68(2)	43(2)	55(2)	1(2)	16(2)	2(1)
C(4a)	25(2)	39(2)	43(2)	-3(1)	10(1)	-6(1)
N(5)	43(1)	37(1)	47(1)	4(1)	11(1)	-3(1)
C(5)	43(2)	48(2)	62(2)	8(1)	8(1)	-3(2)
C(51)	36(2)	43(2)	60(2)	8(1)	5(1)	1(1)
C(52)	54(2)	60(2)	87(3)	-4(2)	-13(2)	17(2)
C(53)	61(2)	44(2)	169(5)	-2(2)	-30(3)	7(3)
C(54)	66(3)	87(3)	152(5)	13(3)	-15(3)	-61(4)
C(55)	102(4)	134(5)	71(3)	-12(3)	0(2)	-38(3)
C(56)	77(3)	77(3)	61(2)	-8(2)	3(2)	2(2)
C(6)	56(2)	32(1)	48(2)	5(1)	14(1)	3(1)
O(6)	45(1)	50(1)	57(1)	1(1)	9(1)	-8(1)
C(6a)	49(2)	39(2)	47(2)	6(1)	9(1)	-4(1)
C(7)	75(2)	45(2)	52(2)	16(2)	11(2)	0(1)
C(8)	80(2)	51(2)	67(2)	28(2)	13(2)	-4(2)
C(9)	69(2)	64(2)	61(2)	21(2)	19(2)	-10(2)
C(10)	56(2)	59(2)	49(2)	11(2)	13(1)	-3(2)
C(10a)	43(2)	39(2)	52(2)	5(1)	6(1)	-3(1)
N(11)	42(1)	40(1)	53(1)	7(1)	4(1)	1(1)
C(11)	43(2)	49(2)	65(2)	7(1)	2(1)	-2(2)
C(111)	43(2)	53(2)	56(2)	9(1)	-1(1)	1(2)
C(112)	63(2)	63(2)	78(3)	2(2)	-3(2)	-7(2)

Table 2 (contd.)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(113)	87(3)	88(3)	103(4)	10(3)	-19(3)	-39(3)
C(114)	96(4)	147(5)	67(3)	35(4)	-6(3)	-21(3)
C(115)	83(3)	149(5)	60(3)	24(3)	7(2)	26(3)
C(116)	69(2)	79(3)	67(2)	6(2)	-1(2)	15(2)
C(12)	55(2)	47(2)	44(2)	1(1)	11(1)	5(1)
O(12)	52(1)	59(1)	75(2)	-1(1)	-4(1)	-1(1)
C(12a)	58(2)	37(2)	53(2)	-1(1)	1(1)	3(1)
C(13)	84(3)	49(2)	65(2)	-3(2)	10(2)	9(2)
C(14)	118(3)	42(2)	72(2)	-2(2)	-4(2)	14(2)
C(15)	108(3)	38(2)	72(2)	15(2)	-7(2)	-0(2)
C(16)	83(2)	41(2)	61(2)	13(2)	-0(2)	-6(2)
C(16a)	56(2)	34(2)	51(2)	1(1)	-0(1)	-2(1)
N(17)	57(2)	31(1)	50(2)	3(1)	6(1)	-6(1)
C(18)	40(2)	39(2)	54(2)	3(1)	7(1)	-7(1)
O(18)	90(2)	37(1)	61(1)	0(1)	4(1)	-11(1)
C(18a)	37(1)	40(2)	46(2)	-4(1)	6(1)	-9(1)
C(100)	105(5)	136(6)	157(6)	-61(4)	55(5)	-67(5)
C(101)	132(6)	115(5)	175(8)	-66(5)	33(5)	-49(5)
C(102)	129(6)	135(6)	133(6)	-59(5)	65(5)	-57(5)
C(103)	213(16)	102(10)	153(13)	-38(10)	11(11)	-13(9)

* In the form: $\exp[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^*+2U_{13}hla^*c^*+2U_{23}klb^*c^*)]$

Table 3

Fractional coordinates and isotropic thermal parameters (X 10^3) for the hydrogen atoms with estimated standard deviations (for those refined) in parentheses*

Atom	x	y	z	U(Å^2)
H(1)	442	335	418	70
H(2)	448	504	310	70
H(3)	364	649	321	70
H(4)	278	676	444	70
H(501)	119	563	606	70
H(502)	130	625	518	70
H(52)	110	389	600	70
H(53)	59	255	510	70
H(54)	43	268	355	70
H(55)	74	414	288	70
H(56)	119	550	375	70
H(7)	193	764	639	70
H(8)	117	837	753	70
H(9)	122	766	895	70
H(10)	200	617	923	70
H(1101)	416	454	860	70
H(1102)	427	561	822	70
H(112)	457	684	920	70
H(113)	463	747	1068	70
H(114)	404	659	1180	70
H(115)	336	509	1149	70
H(116)	333	442	1003	70
H(13)	262	290	897	70
H(14)	350	145	893	70

Table 3 (contd.)

Atom	x	y	z	$U(\text{Å}^2)$
H(15)	442	116	777	70
H(16)	447	228	661	70
H(17)	378(2)	447(2)	662(2)	53(10)
H(100)	-25	474	153	127
[1]H(101)	108	405	93	127
H(102)	128	428	-62	127
[1]H(1031)	173	370	75	127
[1]H(1032)	150	437	158	127
[1]H(1033)	88	341	134	127

[1] Occupancy 50%

* The numbering of the hydrogen atoms is that of the atoms to which they are bonded.

Table 4

Selected intra- and intermolecular* contacts ≤ 3.5 Å

N(5) ...N(17)	3.01	O(6) ...N(17)	2.94
O(6) ...N(11)	3.00	N(11)...N(17)	3.32
O(12)...N(17)	3.48		
C(1) ...O(6^{i})	3.47	C(2) ...O(6^{i})	3.42
C(2) ...N(17^{i})	3.48	C(10)...C(100^{ii})	3.39
C(4) ...C(53^{ii})	3.44	C(4) ...O(18^{iii})	3.49
C(5) ...O(18^{iii})	3.47	O(6) ...C(54^{iii})	3.38

* Roman numeral superscripts denote the following equivalent positions relative to the reference molecule at x,y,z:

i $1-x,1-y,1-z$ ii $-x,1-y,1-z$ iii $\frac{1}{2}-x,\frac{1}{2}+y,1-z$

Table 5

Equations of the least squares planes (in direct space) for the five aromatic rings in the structure together with their standard deviations and the largest displacements from them.

A $10.924x + 5.506y + 6.455z = 9.646$

$\sigma = 0.007$Å C(4a) 0.010Å

B $11.699x + 6.865y + 3.216z = 9.555$

$\sigma = 0.004$Å C(9) 0.006Å

C $10.522x + 6.066y + 6.642z = 10.489$

$\sigma = 0.006$Å C(12a) 0.008Å

D $13.795x - 3.716y - 1.969z = -1.107$

$\sigma = 0.005$Å C(56) -0.008Å

E $12.554x - 5.875y + 2.056z = 3.613$

$\sigma = 0.005$Å C(115) -0.008Å

Dihedral angles between the planes of the rings:

A,B = 14° A,C = 3° B,C = 14°

CHAPTER 6

The crystal structure of 5,11-dimethyltribenzo[*b*,*f*,*j*][1,5,9]triazacyclododecine-6(5*H*),12(11*H*),18(17*H*)-trione (*N*,*N*'-dimethyltrianthranilide)

Summary

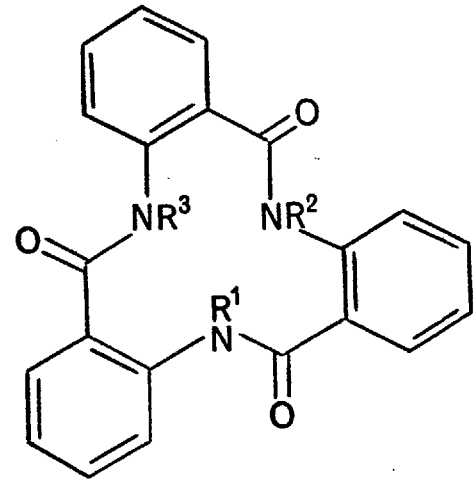
The title compound (1b) crystallises in the monoclinic space group $P2_1$ with a = 11.422(1), b = 12.594(1), c = 6.537(1)Å, β = 101.32°, Z = 2. The structure was solved by direct methods and refined by full-matrix least squares to R = 0.050 for the 1871 independent diffractometer measured reflections. The molecule adopts a helical conformation with angles of 5°, 19° and 14° between the planes of the three aromatic rings. The 12-membered ring is stabilised by a trans-annular amide-amide NH...N hydrogen bond (2.960(5)Å) which involves a severely distorted *trans*-amide group.

An *X*-ray analysis[1,2] has confirmed the n.m.r. conclusion,[3] that the molecule (1a) adopts a helical conformation in the solid state. The analysis revealed, however, the presence of an unsuspected stabilising feature in the structure; a trans-annular amide-amide N-H...O bond. N.m.r. analysis of the conformational behaviour of *N,N'*-dimethyl, trianthranilide (1b)[4] indicated that this molecule too adopts a helical conformation in the solid state.† As (1b) crystallises to give well formed single crystals an *X*-ray analysis was undertaken to establish its solid-state conformation; also to determine whether the replacement of the rather bulky benzyl groups in (1a) by methyls (1b), influences in any way the conformation and thereby the form of any trans-annular ring stabilisation that may be present.

EXPERIMENTAL

The title compound crystallises from dioxane as clear well formed plates. Accurate lattice parameters were obtained by least-squares refinement of 19 high-angle reflections measured (at 12°C) on a diffractometer using Cu-K_α radiation.

† *N.B.* (1b), like (1a) is chemically non-symmetric (*i.e.* $R_1 = R_2 \neq R_3$) and consequently there are three possible non-equivalent helical conformations (and their enantiomorphs). The significance of this to the n.m.r. analysis has been discussed elsewhere.[4]



(1)

a; R^1=H, R^2=R^3=CH_2Ph
b; R^1=H, R^2=R^3=Me

Crystal Data $C_{23}H_{19}N_3O_3$, M = 385.4, Monoclinic, a = 11.4219(5), b = 12.5937(6), c = 6.5373(3)Å, β = 101.318(5)°, U = 922Å^3, D_c = 1.39gcm^{-3}, Z = 2, $F(000)$ = 404. Space-group $P2_1$(No. 4)† from systematic absences and cell contents. Cu-K_α radiation, $\bar{\lambda}$ = 1.54178Å, μ(Cu-K_α) = 7.2cm^{-1}.

A crystal *ca.* 0.15 x 0.4 x 0.5 mm^3 was mounted along its c direction. Data were measured on a Siemens off-line four-circle diffractometer using Ni-filtered Cu-K_α radiation. A total of 1871 independent reflections were measured (to θ = 71°) using the θ-2θ scan technique with the 'five-value'[5] measuring procedure. Of these, 53 reflections had $I < 2.58\sigma(I)$ and were classed as unobserved.[5] The net count of the 5 7 0 reflection, measured as a reference every 50 reflections, did not alter significantly during the data collection (2 days) indicating that no deterioration of the crystal had occurred. The data were brought to a uniform arbitrary scale by use of this reflection,[5] and Lorentz and polarisation corrections were applied. No absorption corrections were applied.

Solution and Refinement of the Structure

The structure was solved by direct methods by application of the program MULTAN[6] to 250 reflections with normalised structure factors (E's) $\geq$ 1.40. An initial run resulted in a very flat profile for the 'figures of merit' with no one phase set standing out above the rest. A second run, using renormalised structure factors, taking into account the spherical scattering for a possible molecular configuration

† This space group contains molecules of one chirality only; the compound, being a racemate in solution, thus exhibits spontaneous resolution on crystallisation.

for the macrocycle,[7] gave appreciably better discrimination. An *E* map calculated for the phase solution with the highest 'combined figure of merit', though giving some multiple imaging of part of the structure, revealed 25 atoms that could be attributed to the main framework of the molecule. These atoms were refined isotropically (as carbons) giving $R = 0.30$, and a difference map computed which revealed the remaining non-hydrogen atoms. The different atom identities were assigned on the basis of bond lengths, thermal parameters, and chemical information.

These atoms were refined anisotropically by full-matrix least squares, to give an *R*-value of 0.078. A difference map contained sharp peaks corresponding to all the hydrogen atoms. The aromatic and methyl hydrogen atoms were fixed at optimised calculated positions corresponding to their observed positions in the difference map, and only the amide hydrogen (H(17)) allowed to vary. One reflection (the $\bar{2}01$) which had $|F_o| << |F_c|$ was suspected of being affected by extinction and therefore removed. Subsequent refinement, the amide hydrogen isotropically, the remaining non-hydrogen atoms anisotropically, reduced *R* to a final value of 0.050. The maximum shift/error for all the refined parameters at the termination of refinement was 0.5. The maximum residual electron density in the final difference map was $0.2e\text{Å}^{-3}$. Unit weights were used throughout the refinements. Atomic scattering factors were taken from ref. 8 with the exception of those for hydrogen which were taken from ref. 9.

The computations were carried out on the Imperial College CDC 6400 and the University of London CDC 6600 and 7600 computers using, in the main, programs belonging to the *X*-ray 70 and 72 systems.[10]

RESULTS AND DISCUSSION

The observed and calculated structure factors are listed in Appendix VI. The final fractional atomic coordinates and anisotropic thermal parameters for the non-hydrogen atoms together with their estimated standard deviations are listed in Tables 1 and 2. Those for the hydrogen atoms with their isotropic temperature factors are given in Table 3. Figure 1 shows a stereo view of the molecule (ORTEP[11]). Figures 2a, b show the bond lengths and angles together with their estimated standard deviations, and the numbering scheme used. Table 4 lists selected intra- and intermolecular contacts $\leq 3.5\text{Å}$. Figure 3 shows the torsion angles around the central 12-membered ring and for comparison those for the related *N,N'*-dibenzyl molecule (1a).[1,2] Figure 4 shows the Newman projections[12] for the three *trans* amide groups. Table 5 lists the equations of the least-squares planes for the three aromatic rings in the structure and the largest deviants from them. Figure 5 shows a stereo view[11] of the packing of the molecules in the structure.

The molecular conformation is, in accordance with the n.m.r. conclusions,[3] helical with the methyl groups lying on opposite sides of the 12-membered ring (Fig.1). Rings A and C (Fig.3) are nearly parallel (5° between normals) and ring B is inclined to rings A and C by 19° and 14° respectively. The planes of the *trans* amide linkages between rings A and B and between A and C are approximately normal to their adjacent rings (*i.e.* minimum conjugation), whilst that linking rings A and C is inclined at only $\sim 37^\circ$ to the mean plane of these rings (*i.e.* rotated by more than 50° from the normal). The conformation is very similar to that found for the analogous *N,N'*-dibenzyl compound (1a),[1,2] but there is one very significant difference.

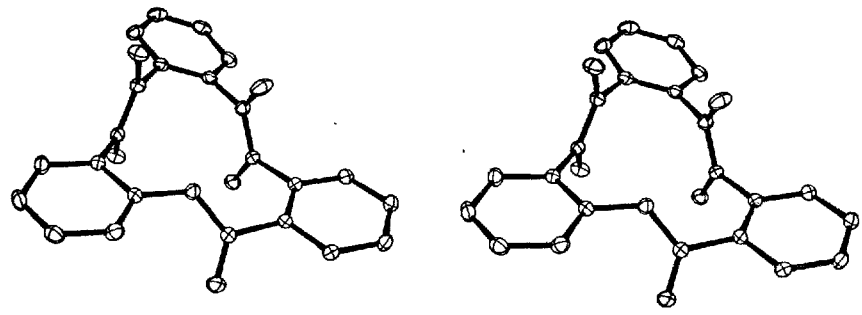


Figure 1. Stereo view of the *N,N'*-dimethyltrianthranilide molecule.

Location of the hydrogen atom attached to N(17) and successful refinement of its position has shown that, unlike in (1a) where the geometry at this nitrogen is normal sp^2, here it is pyramidal with CNH angles of 108° and 111° and CNC of 125° (Fig.2b). The associated OCNH torsion angle is -138° (Fig.4). The effect of this distortion is to direct the N-H bond down into the macrocycle, the bond running nearly parallel to the planes of rings A and C, thus enabling ring stabilisation to be achieved by the formation of a trans-annular N-H...N hydrogen bond (2.960(5)Å) to the opposite amide nitrogen N(5), (*cf* to O(6) in (1a)[1,2]). The N(17)-O(6) distance in the structure is 3.26Å.

The effect of this change of hydrogen bonding is reflected in small, but marked, differences between the conformational angles in the arms of the molecules involved (A-B and A-C, Fig.3). As can be seen in the figure, one of the most noticeable differences between the structures is the 'swinging outwards' of the carbonyl C(6)=O(6) with respect to the plane of ring B in (1b) compared with its orientation in (1a). This produces a decrease in the N(5) C(6) C(6a) C(10a) torsion angle of 7°. Similar complementary differences can be seen to occur in the other angles.

The bond lengths (Fig.2a) do not deviate appreciably from expected values, and there is fairly good internal consistency between equivalent bonds. One noticeable difference, however, is between the amide C-N bond lengths N(11)-C(12) (1.364(6)Å) and N(17)-C(18) (1.338(6)Å) where the difference is greater than 3σ; a similar difference was observed between these bonds in (1a).[2] As in (1a) the amides show characteristic, but small, degrees of bond modification associated with delocalisation effects in the groups. The very small increase in the C(12)=O(12) bond length is probably a reflection of errors in this length due to anisotropic motion of O(12).

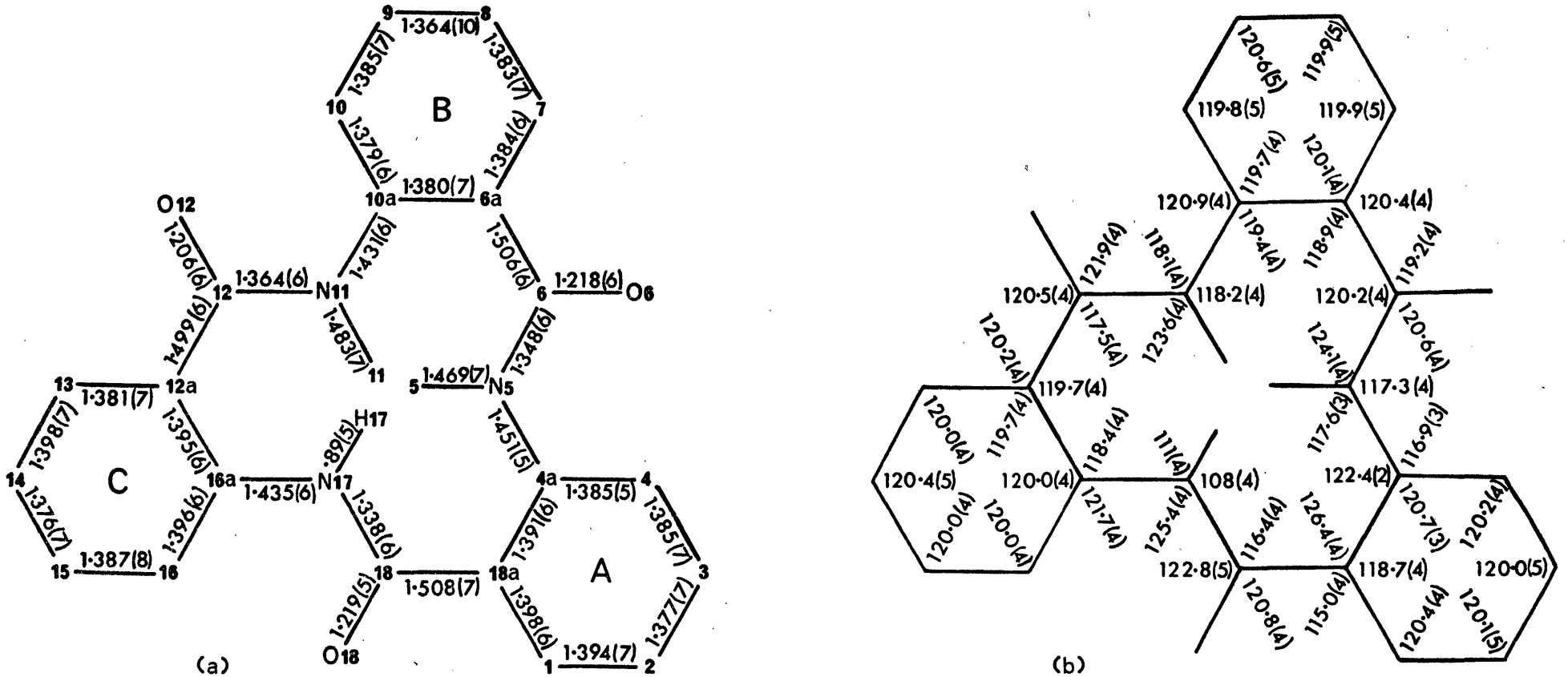


Figure 2(a) Bond lengths and numbering scheme; (b) valence angles. Standard deviations in parentheses.

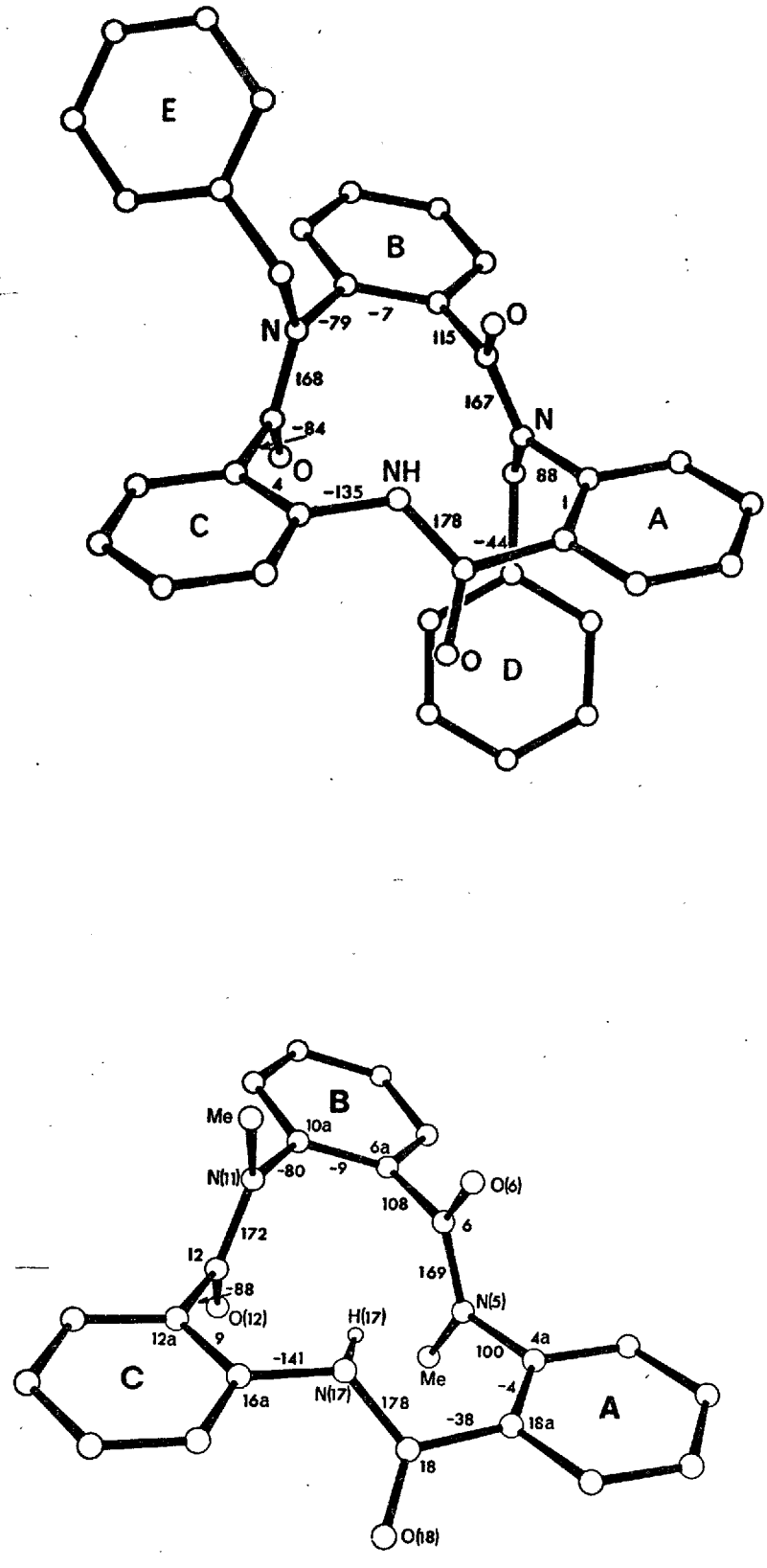


Figure 3. Torsion angles for the central 12-membered ring with (above), for comparison, those for *N,N'*-dibenzyltrianthranilide.

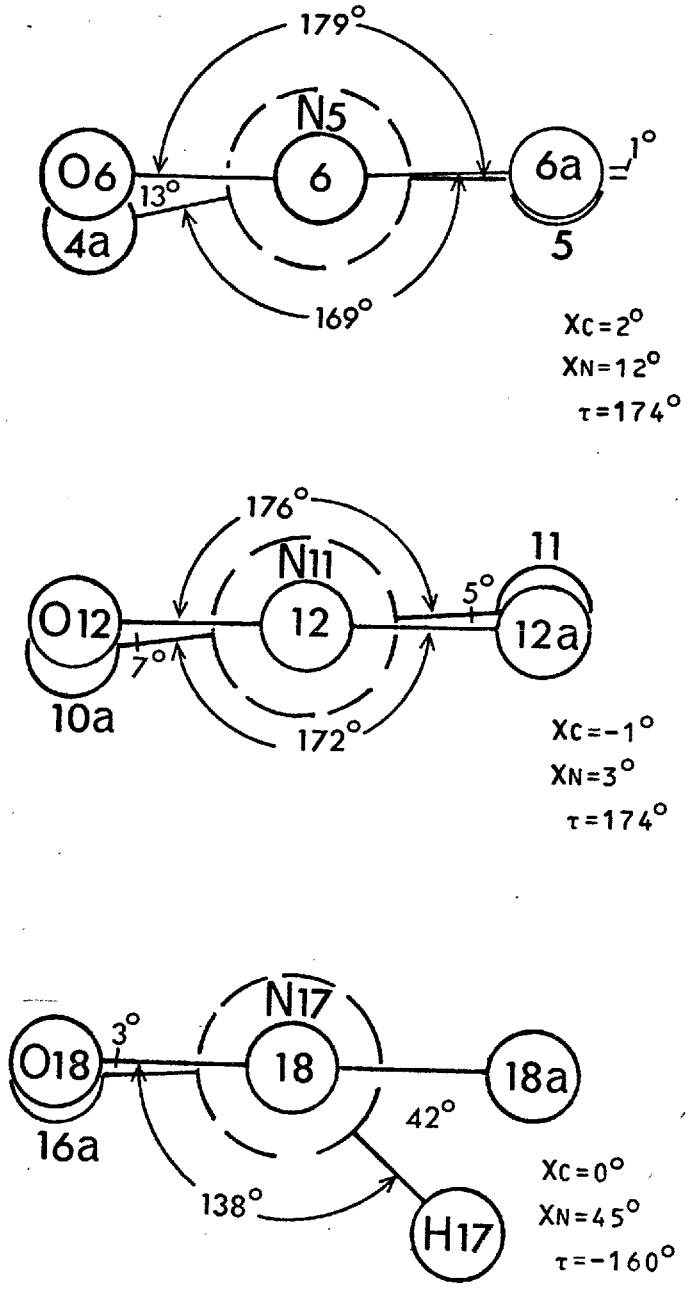


Figure 4. Newman projections and out-of-plane bending parameters for the three *trans* amide groups.

As in (1a)[2] none of the amide groups is planar. The out-of-plane deformation parameters[13,14] for the amides linking rings A and B and B and C are fairly small (Fig.4), the distortions being similar in magnitude to those found for (1a).[2] However, the deformation in the amide linking rings A and C is exceptionally large with an out-of-plane bending at the nitrogen χ_N, of 45°. As reported previously[14] distortion of amide groups is fairly common, but in the majority of cases the deformations are small; they certainly do not approach the degree of distortion observed here (a notable exception is an out-of-plane rotation of ∿ 30° of one of the substituents on each nitrogen in the structure of *N,N'*-diethyl-*N,N'*-diphenyl-urea[15]). This current result lends further support to the deduction that the force resisting out-of-plane deformation in amides must be small.[16,17]

None of the aromatic rings shows significant departures from planarity (Table 5) indicating that, as in (1a),[2] the strains imposed by the presence of non-zero torsion angles along the common edges between the 12- and 6-membered rings are not relieved by bending of the aromatics. Ring C, whose 12-membered substituents are rotated with respect to each other by 9° along the C(12a)-C(16a) bond, is the flattest of the three rings with a maximum deviation from planarity of 0.004Å.

The structure is quite tightly packed (Fig.5) with eight intermolecular contacts of under 3.5Å. The shortest of these is one of 3.31Å between C(1) and C(15) (Table 4). The packing is consistent with van der Waals interactions.

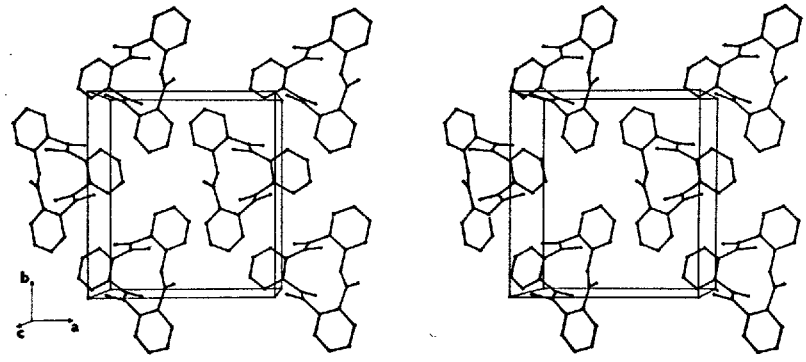


Figure 5. Stereo view of the packing of the molecules.

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Table 1

Fractional coordinates (X 10^4) for the non-hydrogen atoms with estimated standard deviations in parentheses

Atom	*x*	*y*	*z*
C(1)	5745(4)	3489(4)	2166(7)
C(2)	6016(5)	2416(4)	2489(7)
C(3)	7107(5)	2114(4)	3641(7)
C(4)	7946(4)	2876(4)	4442(7)
C(4a)	7678(4)	3944	4141(6)
N(5)	8619(3)	4694(3)	4957(5)
C(5)	9472(4)	4968(4)	3626(7)
C(6)	8765(4)	4951(4)	6993(7)
O(6)	8011(3)	4714(4)	7998(5)
C(6a)	9847(4)	5570(4)	8035(6)
C(7)	10927(4)	5061(4)	8717(8)
C(8)	11856(4)	5593(5)	9978(8)
C(9)	11708(4)	6622(6)	10528(7)
C(10)	10641(4)	7146(5)	9807(7)
C(10a)	9708(4)	6617(4)	8562(6)
N(11)	8589(3)	7135(3)	7829(5)
C(11)	7727(5)	7194(5)	9252(8)
C(12)	8354(4)	7506(4)	5831(7)
O(12)	9097(3)	7496(3)	4750(5)
C(12a)	7120(4)	7910(3)	4988(6)
C(13)	6891(4)	8988(4)	4933(8)
C(14)	5779(5)	9370(4)	3913(8)
C(15)	4904(4)	8678(4)	2980(7)
C(16)	5124(4)	7595(4)	3033(7)
C(16a)	6235(4)	7208(4)	4031(7)

Table 1 (contd.)

Atom	x	y	z
N(17)	6495(3)	6092(3)	4140(6)
C(18)	6155(4)	5395(4)	2593(7)
O(18)	5540(4)	5641(3)	919(5)
C(18a)	6572(4)	4266(4)	3021(6)

Table 2

Anisotropic thermal parameters* ($X10^3$ Å^2) for the non-hydrogen atoms with standard deviations in parentheses

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	56(3)	45(3)	40(2)	-5(2)	-0(2)	-4(2)
C(2)	74(3)	43(3)	48(3)	-16(2)	12(2)	-12(2)
C(3)	73(3)	39(2)	52(3)	-1(2)	13(2)	-4(2)
C(4)	55(3)	41(2)	48(2)	4(2)	6(2)	1(2)
C(4a)	45(2)	39(2)	37(2)	-4(2)	6(2)	-1(2)
N(5)	47(2)	42(2)	40(2)	-4(2)	2(1)	-1(2)
C(5)	57(3)	56(3)	48(2)	-10(2)	12(2)	4(2)
C(6)	44(2)	45(3)	49(2)	-3(2)	2(2)	-1(2)
O(6)	73(2)	98(3)	56(2)	-41(2)	21(2)	-25(2)
C(6a)	45(2)	49(3)	39(2)	-3(2)	-1(2)	6(2)
C(7)	54(3)	57(3)	57(3)	3(2)	1(2)	14(2)
C(8)	47(3)	81(4)	50(3)	5(3)	-0(2)	17(3)
C(9)	46(3)	98(5)	45(3)	-16(3)	-5(2)	-4(3)
C(10)	54(3)	62(3)	51(3)	-13(2)	3(2)	-10(2)
C(10a)	42(2)	52(3)	37(2)	-3(2)	2(2)	6(2)
N(11)	49(2)	47(2)	42(2)	1(2)	5(2)	3(2)
C(11)	66(3)	78(4)	47(3)	10(3)	17(2)	9(3)
C(12)	45(2)	37(2)	46(2)	-6(2)	0(2)	-3(2)
O(12)	47(2)	73(2)	47(2)	5(2)	8(1)	9(2)
C(12a)	47(2)	40(2)	40(2)	1(2)	2(2)	0(2)
C(13)	59(3)	37(2)	64(3)	-3(2)	9(2)	1(2)
C(14)	71(3)	40(3)	65(3)	12(2)	16(3)	12(2)
C(15)	54(3)	61(3)	46(2)	17(2)	8(2)	8(2)
C(16)	48(3)	57(3)	46(2)	2(2)	2(2)	-8(2)
C(16a)	47(2)	39(2)	40(2)	0(2)	3(2)	2(2)

Table 2 (contd.)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(17)	48(2)	40(2)	51(2)	2(2)	-8(2)	-4(2)
C(18)	55(3)	41(2)	43(2)	-2(2)	3(2)	0(2)
O(18)	141(4)	53(2)	54(2)	25(3)	-33(2)	-6(2)
C(18a)	53(3)	37(2)	36(2)	-3(2)	7(2)	1(2)

* In the form: $\exp[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^*+2U_{13}hla^*c^*+2U_{23}klb^*c^*)]$

Table 3

Fractional coordinates and isotropic thermal parameters (X 10^3) for the hydrogen atoms with estimated standard deviations (for those refined) in parentheses*

Atom	x	y	z	U(Å^2)
H(1)	495	370	132	63
H(2)	542	186	188	63
H(3)	729	134	390	63
H(4)	875	265	524	63
H(51)	1007	549	437	82
H(52)	989	431	331	82
H(53)	903	529	230	82
H(7)	1103	431	830	63
H(8)	1263	523	1049	63
H(9)	1238	700	1146	63
H(10)	1055	791	1019	63
H(111)	699	758	854	82
H(112)	751	646	963	82
H(113)	810	759	1055	82
H(13)	752	950	562	63
H(14)	562	1015	386	63
H(15)	411	896	226	63
H(16)	444	709	236	63
H(17)	726(4)	597(5)	470(8)	85(17)

* The numbering of the hydrogen atoms is that of the atoms to which they are bonded.

Table 4

Selected intra- and intermolecular* contacts ≤ 3.5 Å

N(5) ...N(17)	2.96	C(6) ...N(17)	3.22
O(6) ...N(17)	3.26	N(11)...O(6)	3.13
C(11)...O(6)	3.26	C(12)...C(6)	3.32
O(12)...C(5)	3.32		
C(4) ...O(12^{i})	3.35	C(9) ...C(3^{i})	3.33
C(8) ...C(3^{i})	3.43	C(15)...C($18a^{ii}$)	3.46
C(15)...C(1^{ii})	3.41	C(2) ...C(16^{ii})	3.44
C(2) ...O(18^{iii})	3.40	C(1) ...C(15^{iii})	3.31

* Roman numeral superscripts denote the following equivalent positions relative to the reference molecule at x,y,z:

i $2-x,\frac{1}{2}+y,1-z$ ii $1-x,\frac{1}{2}+y,1-z$ iii $1-x,\frac{1}{2}+y,-z$

Table 5

Equations of the least squares planes (in direct space) for the three aromatic rings in the structure together with their standard deviations and the largest displacements from them.

A $6.226x - 0.200y - 6.072z = 2.183$

$\sigma = 0.010$Å C(31),C(18a) -0.012Å

B $5.678x + 3.824y - 5.848z = 3.033$

$\sigma = 0.008$Å C(6a) -0.011Å

C $-5.878x - 0.907y + 6.137z = -1.842$

$\sigma = 0.003$Å C(14) -0.004Å

Dihedral angles between the planes of the rings:

A,B = 19° A,C = 5° B,C = 14°

CHAPTER 7

The crystal structure of 4,10,16-trimethyltribenzo[*b*,*f*,*j*][1,5,9] trithiacyclododecine-6,12,18-trione (Tri-3-methylthiosalicylide)

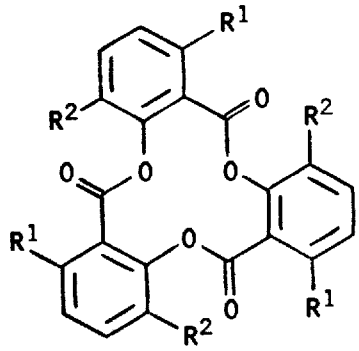
Summary

The title compound (7) crystallises in the monoclinic space group $P2_1/c$ with a = 18.772(1), b = 7.465(1), c = 16.303(1)Å, β = 109.59°, Z = 4. The structure was solved by direct methods and refined by full-matrix least squares to R = 0.046 for the 4081 independent diffractometer measured reflections. The molecule adopts a helical conformation with angles of 6°, 31° and 30° between the planes of the three aromatic rings. The average S-C(sp^2) distance is 1.780Å.

Studies of the conformational behaviour of the trisalicylides (1)-(3),[1,2] and the related medium-ring compounds (4)-(6),[3,4] have suggested that the barrier heights for conformational changes in the 12-membered rings depend on the nature of the substituent atoms, or groups, at the *ortho* positions of the aromatic rings. As a continuation of these studies attempts have been made to prepare the thia analogue of tri-*o*-thymotide (tri-thiothymotide)[5] to enable investigation of its conformational behaviour, also to see if it too, exhibits the same exceptional inclusion compound forming properties. These attempts have resulted in the successful formation of the chiral intermediate, thiosalicylide (7), which n.m.r. analysis has shown undergoes conformational inversion in solution. It has been proposed that (7) adopts a helical conformation in the solid state (*i.e.* two carbonyl oxygens lie on one side of the 12-membered ring and one on the other). The *X*-ray analysis reported here has been carried out to establish the solid state conformation and to provide accurate details of the conformational geometry. A crystal structure determination has shown (6) to have a helical conformation.[6]

EXPERIMENTAL

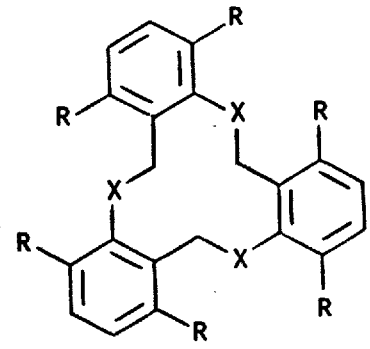
The title compound crystallises as colourless laths elongated along *b*. Accurate lattice parameters were obtained by least squares refinement of 25 high-angle reflections measured (at 12°C) on a diffractometer using Cu-K_α radiation.



(1) $R^1=R^2=CH_3$

(2) $R^1=CH_3$, $R^2=CH(CH_3)_2$

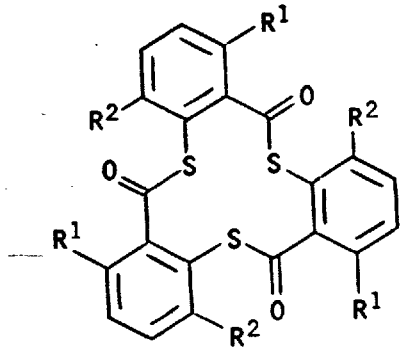
(3) $R^1=CH(CH_3)_2$, $R^2=CH_3$



(4) R=H, $X=CH_2$

(5) $R=CH_3$, $X=CH_2$

(6) R=H, X=S



(7) $R^1=H$, $R^2=CH_3$

Crystal Data $C_{24}H_{18}S_3O_3$, M = 450.6; Monoclinic, a = 18.7720(8), b = 7.4651(5), c = 16.3028(8)Å, β = 109.590(4)°, U = 2152Å^3, D_c = 1.39gcm^{-3}, D_m = 1.37(2)gcm^{-3} (by flotation), Z = 4, $F(000)$ = 936. Space-group $P2_1/c$ (No. 14)† uniquely determined from systematic absences. Cu-K_α radiation, $\bar{\lambda}$ = 1.54178Å, μ(Cu-K_α) = 32.8cm^{-1}.

A crystal *ca.* 0.2 x 0.7 x 0.4 mm^3 was mounted along its b direction. Data were measured on a Siemens off-line four-circle diffractometer using Ni-filtered Cu-K_α radiation. A total of 4081 independent reflections were measured (to θ = 70°) using the θ-2θ scan technique with the 'five value'[7] measuring procedure. Of these, 231 reflections had $I < 2.58\sigma(I)$ and were classed as unobserved.[7] The net count of the 12 0 $\bar{6}$ reflection, measured as a reference every 50 reflections, did not alter significantly during the data collection (*ca.* 8 days) indicating that no deterioration of the crystal had occurred. The data were brought to a uniform arbitrary scale by use of this reflection,[7] and Lorentz and polarisation corrections were applied. No absorption corrections were applied at this stage.

Solution and Refinement of the Structure

The structure was solved by direct methods by application of the program MULTAN[8] to 250 reflections with normalised structure factors (E's) > 1.50. An E map computed for the phase solution with the highest 'combined figure of merit' gave plausible positions for all

† This space-group contains equal numbers of molecules of both chiralities; the compound is thus a racemate both in solution and in the solid state.

of the non-hydrogen atoms of the structure.

These atoms were refined anisotropically by full-matrix least squares to give a residual R = 0.087. A difference map contained sharp peaks corresponding to all the hydrogen atoms, which for subsequent refinement, were fixed at optimised calculated positions 1.0Å from their parent carbon atoms. R fell to 0.082. The data were then corrected for absorption using the method of Busing and Levy[9] with a Gaussian grid of 12 x 12 x 12 points, and with crystal path lengths determined by the procedure of Coppens, Leiserowitz and Rabinovich.[10] Refinement with the absorption corrected data reduced R to 0.068. Fifteen low-angle reflections which had $|F_o| << |F_c|$ were suspected of being affected by extinction and therefore removed. Subsequent refinement with allowance made for the anomalous scattering due to the sulphur atoms reduced R to a final value of 0.046. The maximum shift/error for the refined parameters was 0.4 and the maximum residual electron density in the final difference map was < 0.2eÅ^{-3}.

Unit weights were used throughout the refinements. Atomic scattering factors were taken from ref. 11 with the exception of those for hydrogen which were taken from ref. 12. Anomalous scattering factors for sulphur were taken from ref. 13. The computations were carried out on the Imperial College CDC 6400 and the University of London CDC 6600 and 7600 computers using, in the main, programs belonging to the *X*-ray 70 and 72 systems.[14]

RESULTS AND DISCUSSION

The observed and calculated structure factors are listed in Appendix VII. The final fractional atomic coordinates and anisotropic thermal parameters for the non-hydrogen atoms together with their estimated standard deviations are listed in Tables 1 and 2. Those for

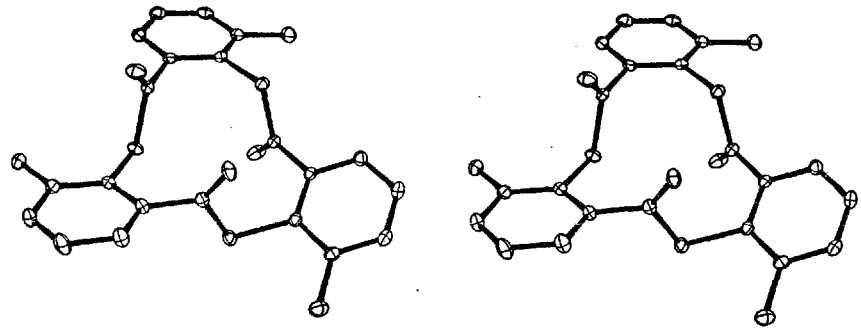


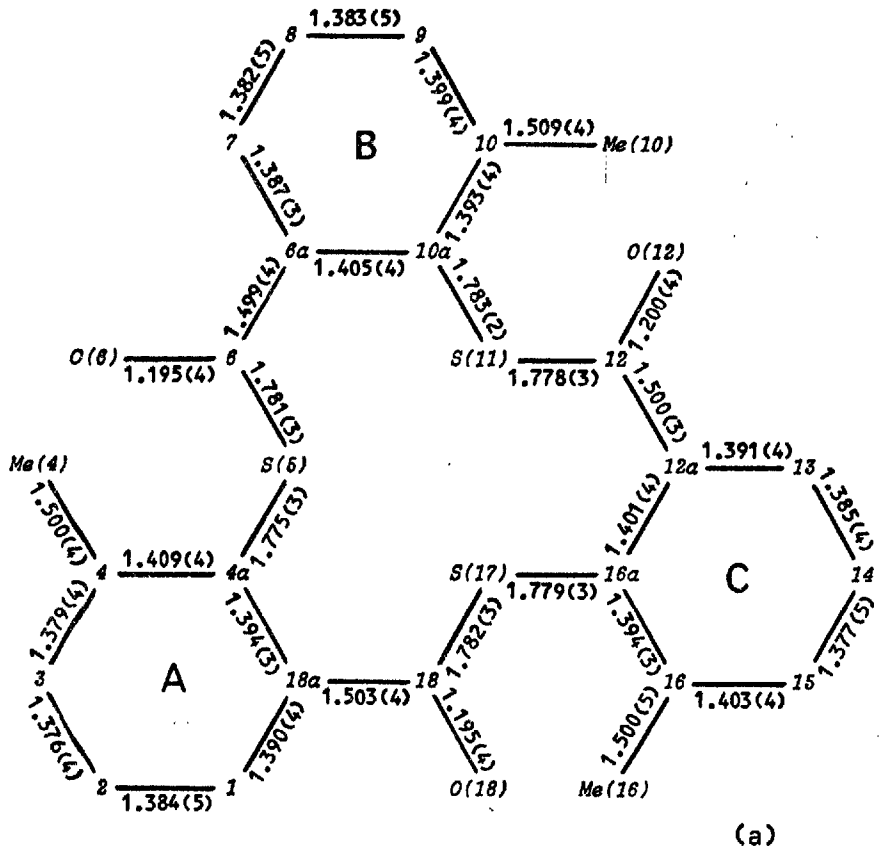
Figure 1. Stereo view of the molecule.

the hydrogen atoms with their isotropic temperature factors are given in Table 3. Figure 1 shows a stereo view of the molecule (ORTEP[15]). Figures 2a, b show the bond lengths and angles together with their estimated standard deviations, also the numbering scheme used. Table 4 lists selected intra- and intermolecular contacts ≤ 3.6Å. Figure 3 shows the torsion angles around the central 12-membered ring and for comparison, the values reported for (6)[6] (in parentheses). Table 5 lists the equations of the least-squares planes for the three aromatic rings and the largest deviants from each of them. Figure 4 shows a stereo view of the packing of the molecules in the structure.[15]

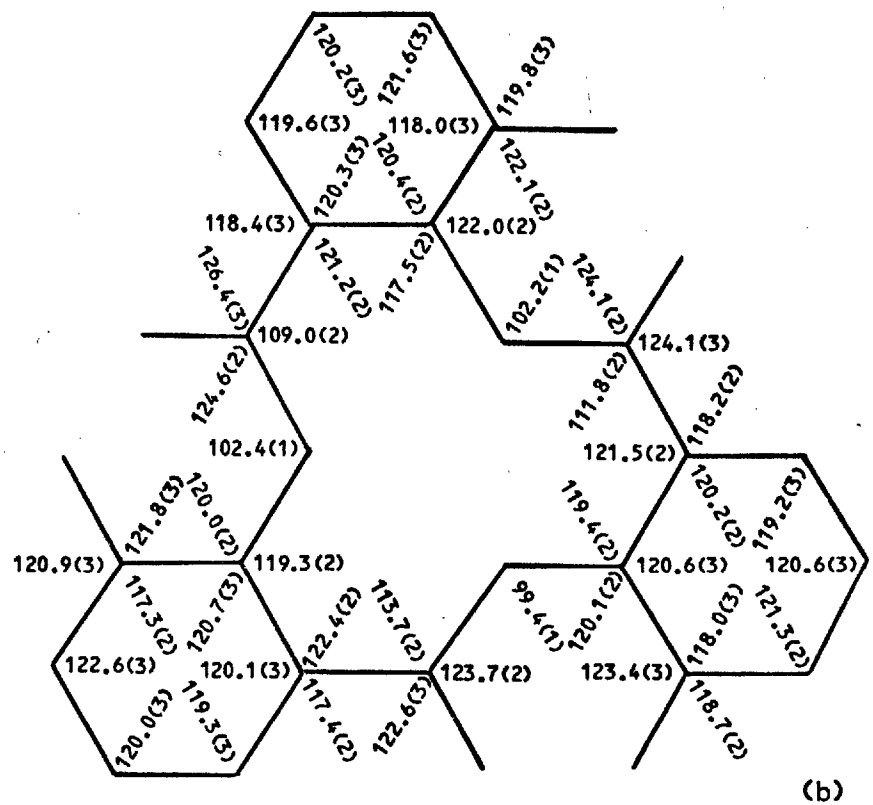
The molecule adopts a helical conformation (Fig.1), thus confirming the n.m.r. predictions.[5] Rings A and B are nearly parallel to each other (6° between normals) and ring C is almost equally inclined to both rings A and B (31° and 30° respectively). The almost planar thiocarboxy linking arms are approximately normal to the mean planes of their adjacent rings. The conformation mirrors very closely that found for (6) where the angles between the rings A and B, A and C, and B and C were 1°, 28° and 28° respectively.[6] This similarity extends also to the torsion angles for the 12-membered ring where, with two minor exceptions (the torsional twists about C(6a)-C(10a) and S(5)-C(6)), they are within 5° of the values we have found for (7) (Fig.3).

Comparisons were made,[6] for (6), between the observed torsion angles and the supposedly 'ideal' values of $\pm\frac{n\pi}{2}$, (n=1,2). However, we consider such comparisons to be unrealistic in a closed system which by its nature can never achieve them.

All six S-C(sp^2) distances are, within 3σ, the same, ranging between 1.775(3) and 1.783(2)Å, with an average bond length of 1.780Å. This value is slightly, but not significantly, larger than the average



(a)



(b)

Figure 2(a) Bond lengths and numbering scheme; (b) valence angles. Standard deviations in parentheses.

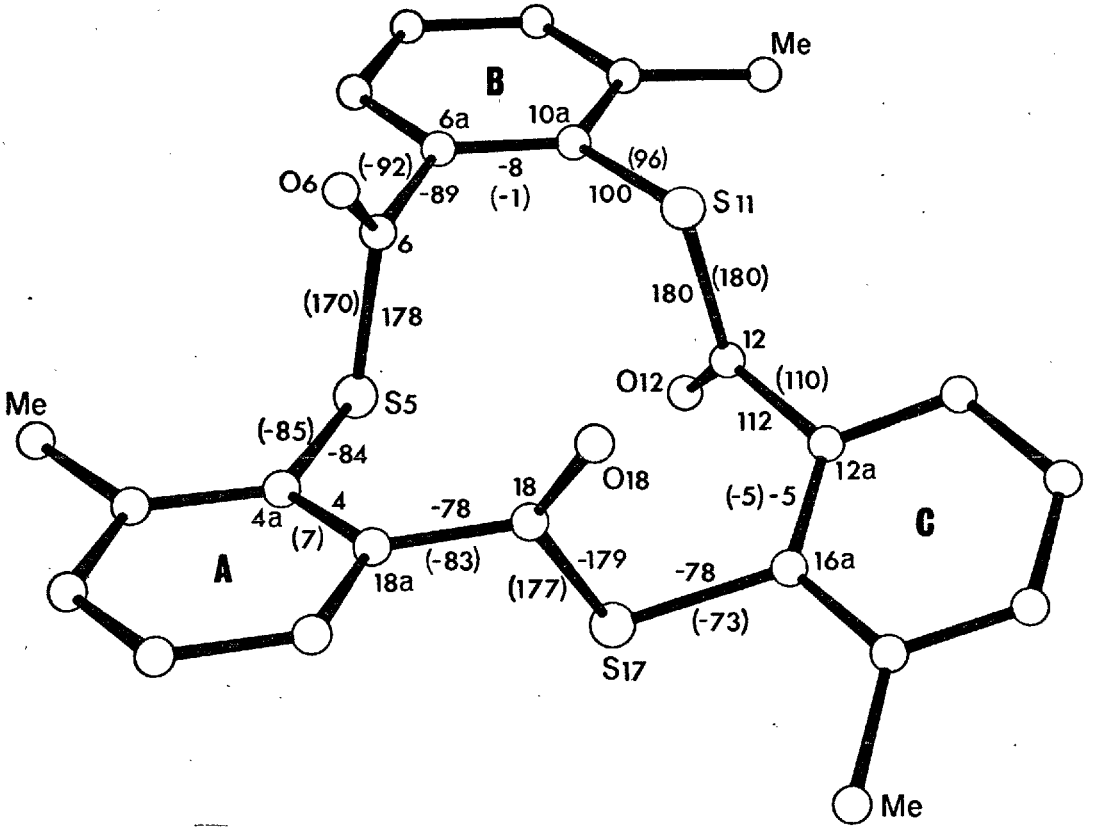


Figure 3. Torsion angles around the central 12-membered ring with, in parentheses, those for (6).

(1.771Å) found for (6).[6] The value agrees well with those found in the structure of 2,2'-diaminodiphenyl disulphide,[14] and is in accordance with the expected value.[17] The bond angles at the sulphurs differ significantly from each other with that at S(5) being 3° greater than at S(17); a similar difference occurs in (6). A more notable feature of the bond angles is the acuteness of the thiocarboxy S(CO)C angles. These are all significantly less than 120°, the smallest being 109.0(2)° at C(6). But this does not reflect any loss of planarity in these groups as the difference is made up in the other two angles, the sum of the angles at each carbon being 360°. A similar value is found in the structure of thiphenamil hydrochloride[18] where the S(CO)C angle is 112°. This reduction in these angles is probably a consequence, within the group, of non-bonding interactions between the sulphur and oxygen atoms analogous to that observed between the ether and carbonyl oxygens in carboxy groups, where the O(CO)C angles are similarly reduced. Very similar values have been observed for the carboxy O(CO)C angles in tri-*o*-thymotide.[19]

The trans-annular S...S, S...O and O...O contacts range from 3.31Å to > 5Å, six of them being under 3.6Å (Table 4). All the S...O contacts are greater than the sum of the van der Waals radii for these atoms (3.25Å). The shortest S...S distance (3.53Å) is, however, less than twice the van der Waals radius for sulphur (3.7Å).

Departures from planarity in the three aromatic rings are small with maximum deviations from the least-squares planes of 0.012 (C(1)), 0.009 (C(10a)) and 0.016Å (C(13)) for rings A, B and C respectively. Clearly the strain imposed (on ring B) by the fairly large (8°) torsional twist about the C(6a)-C(10a) bond in the 12-membered ring is not relieved by buckling of the aromatic ring.

The structure is fairly tightly packed (Fig.4) with five

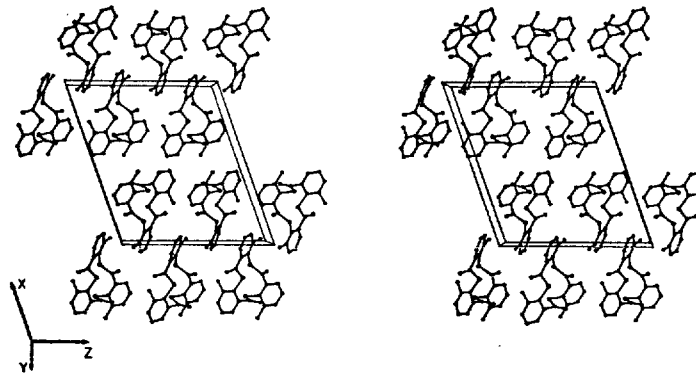


Figure 4. Stereo view of the packing of the molecules.

intermolecular contacts (all involving carbonyl oxygen atoms) of less than 3.5Å. The shortest of these is 3.26Å between O(12) and C(2) (Table 4). The packing is consistent with van der Waals interactions.

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19. See chapters 2-4.

Table 1

Fractional coordinates (X 10^4) for the non-hydrogen atoms with estimated standard deviations in parentheses

Atom	*x*	*y*	*z*
C(1)	2381(2)	1001(5)	631(2)
C(2)	2938(2)	-200(5)	614(2)
C(3)	3597(2)	-316(4)	1313(2)
C(4)	3732(2)	722(4)	2050(2)
Me(4)	4465(2)	579(5)	2792(2)
C(4a)	3155(2)	1905(4)	2076(2)
S(5)	3276(0)	3239(1)	3013(0)
C(6)	3612(1)	5299(4)	2729(2)
O(6)	3747(1)	5548(3)	2073(2)
C(6a)	3723(2)	6611(4)	3458(2)
C(7)	4414(2)	6631(4)	4127(2)
C(8)	4519(2)	7768(5)	4828(2)
C(9)	3935(2)	8855(4)	4866(2)
C(10)	3232(2)	8862(4)	4202(2)
Me(10)	2600(2)	10016(5)	4287(2)
C(10a)	3134(1)	7739(4)	3489(2)
S(11)	2293(0)	7773(1)	2562(0)
C(12)	1682(2)	6348(4)	2895(2)
O(12)	1853(1)	5630(4)	3593(1)
C(12a)	922(1)	6181(4)	2205(2)
C(13)	445(2)	7663(4)	2032(2)
C(14)	-284(2)	7497(5)	1452(2)
C(15)	-529(2)	5903(5)	1025(2)
C(16)	-51(2)	4407(4)	1163(2)

Table 1 (contd.)

Atom	*x*	*y*	*z*
Me(16)	-349(2)	2718(5)	668(2)
C(16a)	676(2)	4563(4)	1765(2)
S(17)	1307(0)	2707(1)	1974(1)
C(18)	1878(2)	3368(4)	1346(2)
O(18)	1776(1)	4709(3)	923(1)
C(18a)	2486(2)	2042(4)	1369(2)

Table 2

Anisotropic thermal parameters* (X 10^3 Å^2) for the non-hydrogen atoms with standard deviations in parentheses

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	57(2)	52(2)	38(2)	12(2)	6(1)	-7(1)
C(2)	75(2)	54(2)	44(2)	19(2)	13(2)	-16(2)
C(3)	54(2)	44(2)	51(2)	15(1)	21(1)	-3(1)
C(4)	40(1)	35(1)	43(2)	1(1)	14(1)	3(1)
Me(4)	37(2)	53(2)	59(2)	5(1)	9(1)	-1(2)
C(4a)	41(1)	18(1)	36(1)	-0(1)	14(1)	-1(1)
S(5)	54(0)	34(0)	36(0)	-4(0)	16(0)	-3(0)
C(6)	30(1)	37(1)	43(1)	0(1)	11(1)	-1(1)
O(6)	79(2)	52(1)	58(1)	-16(1)	40(1)	-6(1)
C(6a)	34(1)	31(1)	41(1)	-5(1)	10(1)	-2(1)
C(7)	37(1)	39(2)	53(2)	-0(1)	5(1)	-0(1)
C(8)	48(2)	50(2)	45(2)	-12(1)	-0(1)	-0(1)
C(9)	62(2)	41(2)	39(2)	-15(1)	14(1)	-7(1)
C(10)	49(2)	35(1)	46(2)	-7(1)	23(1)	-3(1)
Me(10)	70(2)	52(2)	72(2)	2(2)	42(2)	-10(2)
C(10a)	35(1)	33(1)	38(1)	-6(1)	14(1)	1(1)
S(11)	35(0)	46(0)	41(0)	-1(0)	10(0)	6(0)
C(12)	33(1)	42(2)	39(1)	-0(1)	11(1)	0(1)
O(12)	48(1)	81(2)	44(1)	-18(1)	6(1)	20(1)
C(12a)	30(1)	44(2)	37(1)	-0(1)	13(1)	4(1)
C(13)	42(2)	45(2)	46(2)	4(1)	15(1)	-3(1)
C(14)	39(2)	56(2)	47(2)	15(1)	12(1)	4(1)
C(15)	31(1)	64(2)	43(2)	2(1)	9(1)	7(1)
C(16)	39(1)	48(2)	38(1)	-6(1)	15(1)	2(1)
Me(16)	57(2)	59(2)	58(2)	-13(2)	11(2)	-7(2)

Table 2 (contd.)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(16a)	32(1)	40(2)	40(1)	2(1)	15(1)	5(1)
S(17)	49(0)	40(0)	65(0)	8(0)	25(0)	14(0)
C(18)	39(1)	39(2)	30(1)	4(1)	5(1)	-3(1)
O(18)	60(1)	50(1)	51(1)	20(1)	27(1)	17(1)
C(18a)	43(1)	33(1)	37(1)	6(1)	13(1)	-0(1)

* In the form: $\exp[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^*+2U_{13}hla^*c^*+2U_{23}klb^*c^*)]$

Table 3

Fractional coordinates and isotropic thermal parameters ($X\ 10^3$) for the hydrogen atoms*

Atom	x	y	z	$U(\text{Å}^2)$
H(1)	191	112	12	63
H(2)	286	-98	9	63
H(3)	399	-119	129	63
H(41)	480	-33	265	82
H(42)	473	177	289	82
H(43)	437	20	333	82
H(7)	483	583	410	63
H(8)	502	781	531	63
H(9)	402	966	538	63
H(101)	278	1072	484	82
H(102)	242	1086	378	82
H(103)	217	924	429	82
H(13)	63	884	233	63
H(14)	-64	855	134	63
H(15)	-106	581	61	63
H(161)	-88	291	27	82
H(162)	-3	238	31	82
H(163)	-34	173	109	82

* The numbering of the hydrogen atoms is that of the atoms to which they are bonded

Table 4

Selected intra- and intermolecular* contacts ≤ 3.6Å

Me(4) ...S(5)	3.10	Me(10)...S(11)	3.16
Me(16)...S(17)	3.12	S(11) ...O(18)	3.40
S(17) ...O(12)	3.31	S(11) ...O(6)	3.51
S(17) ...S(5)	3.53	S(5) ...O(12)	3.59
O(18) ...O(6)	3.60		
O(6) ...C(3^{i})	3.30	C(6a) ...Me(4^{i})	3.59
O(18) ...C(13^{ii})	3.29	Me(16)...O(18^{ii})	3.60
O(6) ...Me(4^{iii})	3.29	O(12) ...C(1^{iv})	3.36
O(12) ...C(2^{iv})	3.26	C(13) ...C(16^{v})	3.52
Me(10)...O(18^{vi})	3.51		

* Roman numeral superscripts denote the following equivalent positions relative to the reference molecule at x,y,z:

i $x,1+y,z$ ii $-x,1-y,-z$ iii $1-x,\frac{1}{2}+y,\frac{1}{2}-z$ iv $x,\frac{1}{2}-y,\frac{1}{2}+z$
v $-x,\frac{1}{2}+y,\frac{1}{2}-z$ vi $x,1\frac{1}{2}-y,\frac{1}{2}+z$

Table 5

Equations of the least squares planes (in direct space) for the three aromatic rings in the structure together with their standard deviations and the largest displacements from them.

A $10.835x + 5.322y - 9.272z = 2.515$

$\sigma = 0.009$Å C(1) 0.012Å

B $-9.543x - 5.385y + 10.003z = -3.659$

$\sigma = 0.007$Å C(10a) -0.009Å

C $-11.474x - 2.175y + 14.644z = 0.815$

$\sigma = 0.012$Å C(13) -0.016Å

Dihedral angles between the planes of the rings:

A,B = 6° A,C = 31° B,C = 30°

CHAPTER 8

The crystal structure of 1,7,13-trimethyltribenzo[*b*,*f*,*j*][1,5,9] trithiacyclododecine-6,12,18-trione (Tri-6-methylthiosalicylide)

Summary

The title compound (2) crystallises in the orthorhombic space group $P2_12_12_1$ with a = 8.298(1), b = 15.852(1), c = 16.327(1)Å, Z = 4. The structure was solved by direct methods and refined by full-matrix least squares to R = 0.026 for the 2379 independent diffractometer measured reflections. The molecule adopts a helical conformation with angles of 8°, 18° and 20° between the planes of the three aromatic rings. The conformation differs significantly from that found for the analogous 4,10,16-trimethyl compound (1). The average S-C(sp^2) distance is 1.782Å.

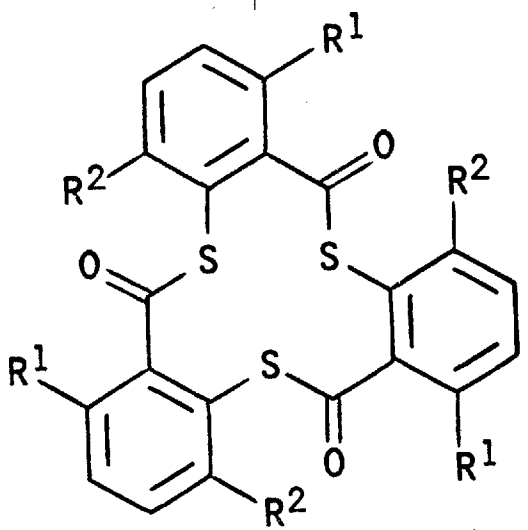
Attempts to prepare the thia analogue of tri-*o*-thymotide, tri-thiothymotide[1] have resulted in the successful synthesis of two intermediate, chiral, methyl substituted, thiosalicylides (1), (2).[2] N.m.r. analyses have shown that both compounds undergo conformational inversion via defined conformational itineraries[2,3] to give racemic mixtures in solution. The solid-state conformations of both these molecules have been deduced as being helical[2] (*i.e.* with two carbonyl oxygens lying on one side of the 12-membered ring and one on the other). An *X*-ray analysis of (1)[4] has confirmed the n.m.r. conclusion of a helical solid-state conformation. In view of the different steric constraints associated with the alternative siting of the methyl groups in (2), *cf* (1) an *X*-ray analysis of (2) was undertaken to determine whether the change in these constraints affect in any way the solid-state conformational geometry.

EXPERIMENTAL

The title compound crystallises as large well formed yellow blocks. Accurate lattice parameters were determined (at 12°C) from measurements of high-angle axial α_1 and α_2 reflections on a diffractometer using Cu-K_α radiation.

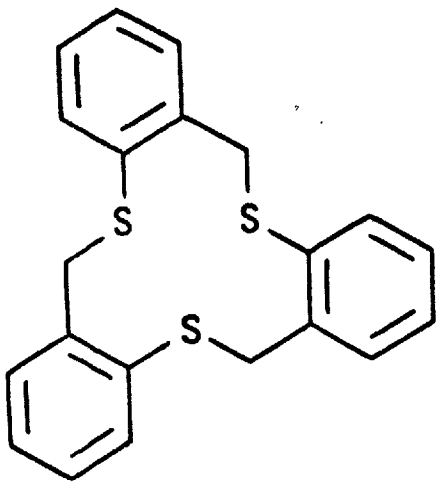
Crystal Data $C_{24}H_{18}S_3O_3$, M = 450.6; Orthorhombic, a = 8.298(1), b = 15.852(1), c = 16.327(1)Å, U = 2148Å^3, D_c = 1.39gcm^{-3}, Z = 4 $F(000)$ = 936. Space-group $P2_12_12_1$ (No. 19),† uniquely determined from systematic absences. Cu-K_α radiation. $\bar{\lambda}$ = 1.54178Å, μ(Cu-K_α) = 32.8cm^{-1}.

† This space-group contains molecules of one chirality only; the compound, being a racemate in solution, thus exhibits spontaneous resolution on crystallisation.



(1) $R^1=H$, $R^2=CH_3$

(2) $R^1=CH_3$, $R^2=H$



(3)

A crystal *ca.* 0.4 x 0.25 x 0.35 mm^3 was cut from a larger block and mounted along its a direction. Data were measured on a Siemens off-line four-circle diffractometer using Ni-filtered Cu-K_α radiation. A total of 2379 independent reflections were measured (to $\theta = 71^\circ$) using the θ-2θ scan technique with the 'five-value'[5] measuring procedure. Of these, 53 reflections had $I < 2.58\sigma(I)$ and were classed as unobserved.[5] The net count of the 0 9 3 reflection, measured as a reference every 50 reflections, did not alter significantly during the data collection (4 days) indicating that no deterioration of the crystal had occurred. The data were brought to a uniform arbitrary scale by use of this reflection,[5] and Lorentz and polarisation corrections were applied. No absorption corrections were applied at this stage.

Solution and Refinement of the Structure

The structure was solved by direct methods by application of the program MULTAN[6] to 300 reflections with normalised structure factors (E's) ≥ 1.45. An E map calculated for the phase solution with the highest 'combined figure of merit' gave plausible positions for all the non-hydrogen atoms of the structure.

These atoms were refined anisotropically by full-matrix least squares to give a residual $R = 0.057$. A difference map contained sharp peaks corresponding to all the hydrogen atoms, and these for subsequent refinement were fixed at optimised calculated positions 1.0Å from their parent carbon atoms; R fell to 0.042. The data were then corrected for absorption using the method of Busing and Levy[7] with a Gaussian grid of 12 x 12 x 12 points and with crystal path lengths determined by the procedure of Coppens, Leiserowitz and Rabinovich.[8] Refinement with the absorption corrected data reduced

R to 0.031. Two reflections (the 002 and 020) which had $|F_o| << |F_c|$ were suspected of being affected by extinction and therefore removed: R dropped to 0.030. Finally allowance was made for the anomalous scattering due to the sulphur atoms. Refinement with the complex component of the anomalous scattering factor (f") for sulphur positive, reduced R to 0.026; refinement with f" negative resulted in an increase of R to 0.042. The coordinate set thus relates to the correct absolute configuration for the molecules in the crystal selected. Refinement was terminated at this final R value of 0.026. The maximum shift/error for the refined parameters was 0.4 and the maximum residual electron density in a final difference map was < 0.15eÅ^{-3}.

Unit weights were used throughout the refinements. Atomic scattering factors were taken from ref. 9 with the exception of those for hydrogen which were taken from ref. 10. Anomalous scattering factors for sulphur were taken from ref. 11. The computations were carried out on the Imperial College CDC 6400 and the University of London CDC 6600 and 7600 computers using, in the main, programs belonging to the X-ray 70 and 72 systems.[12]

RESULTS AND DISCUSSION

The observed and calculated structure factors are listed in Appendix VIII. The final fractional atomic coordinates and anisotropic thermal parameters for the non-hydrogen atoms together with their estimated standard deviations are listed in Tables 1 and 2. Those for the hydrogen atoms with their isotropic temperature factors are given in Table 3. Figure 1 shows a stereo view of the molecule (ORTEP[13]). Figures 2a, b show the bond lengths and angles together with their estimated standard deviations; also the numbering scheme used. Figure 3 shows the torsion angles around the central

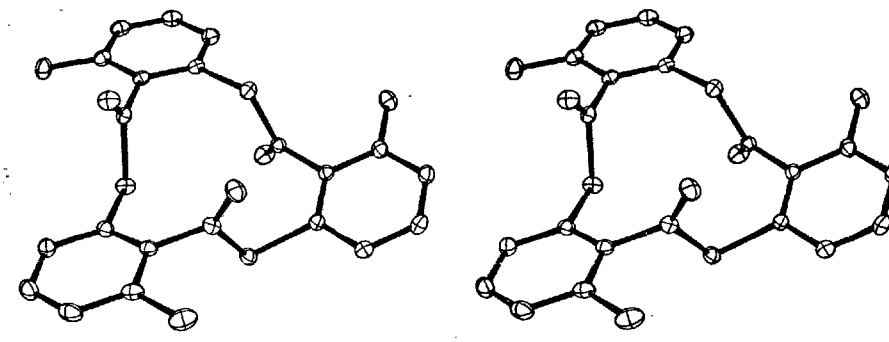


Figure 1. Stereo view of the molecule.

12-membered ring and for comparison the conformational arrangement and torsion angles for (1).[4] Table 4 lists selected intra- and inter-molecular contacts of less than 3.6Å and Figure 4 shows the comparative values for some of the trans-annular S...S, S...O and O...O distances in (1) and (2). Table 5 lists the equations of the least-squares planes for the three aromatic rings and the largest deviants from them. Figure 5 shows a stereo view[13] of the packing of the molecules in the structure.

As predicted by the n.m.r. analyses[2] the molecule adopts a helical conformation in the solid state (Fig.1). Ring A is inclined to ring B by 8°, and ring C is inclined to rings A and B by 18° and 20° respectively. The arrangement of these rings is thus somewhat flatter than that observed for (1)[4] and (3)[14] where ring C is at approximately 30° to A and B. The almost planar thiocarboxy linking arms are, as in (1) approximately normal to the mean planes of their adjacent rings.

The S-C(sp^2) bond distances, unlike those in (1)[4], fall into two groups, with the S-Ph distances all slightly shorter than those for S-CO; the mean values are 1.776Å and 1.787Å respectively. This difference is near the margin of significance, and the overall mean for both sets (1.782Å) is very close to the mean found for (1) (1.780Å).[4] The angles at the sulphur atoms show a narrower spread of values (Δ max = 1.2°) than is observed in (1)[4] or (3)[14] (Δ max = 4.5°). The S(CO)C angles are, as in (1) significantly less than 120° with values of 109.6, 109.5 and 112.9° at C(6), C(12) and C(18) respectively. This does not, however, reflect any out-of-plane distortion of the geometry at these carbon atoms, the difference (from 360°) being made up in each case nearly symmetrically by the other two angles.

A comparison of the torsion angles (Fig.3) for the 12-membered

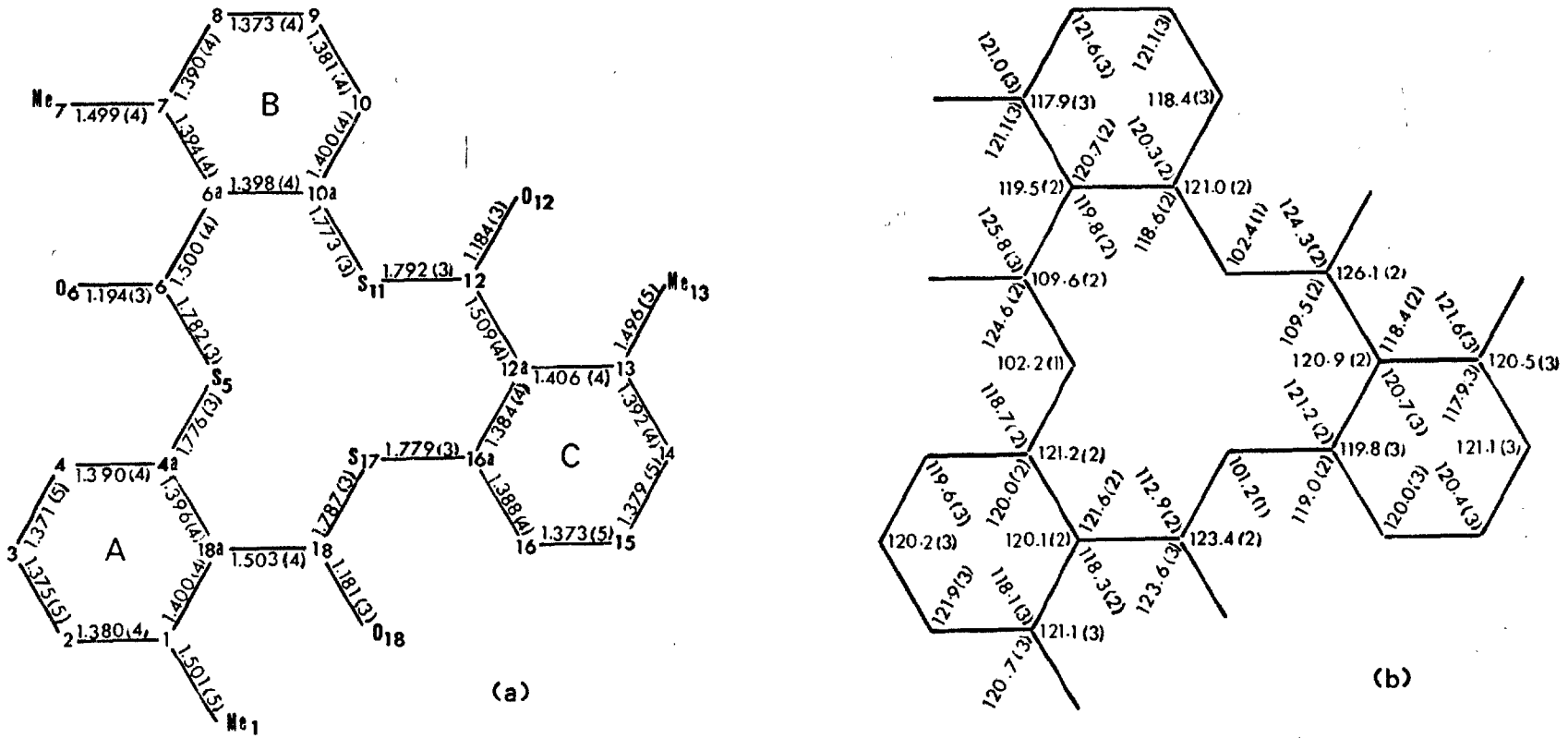


Figure 2(a) Bond lengths and numbering scheme; (b) valence angles. Standard deviations in parentheses.

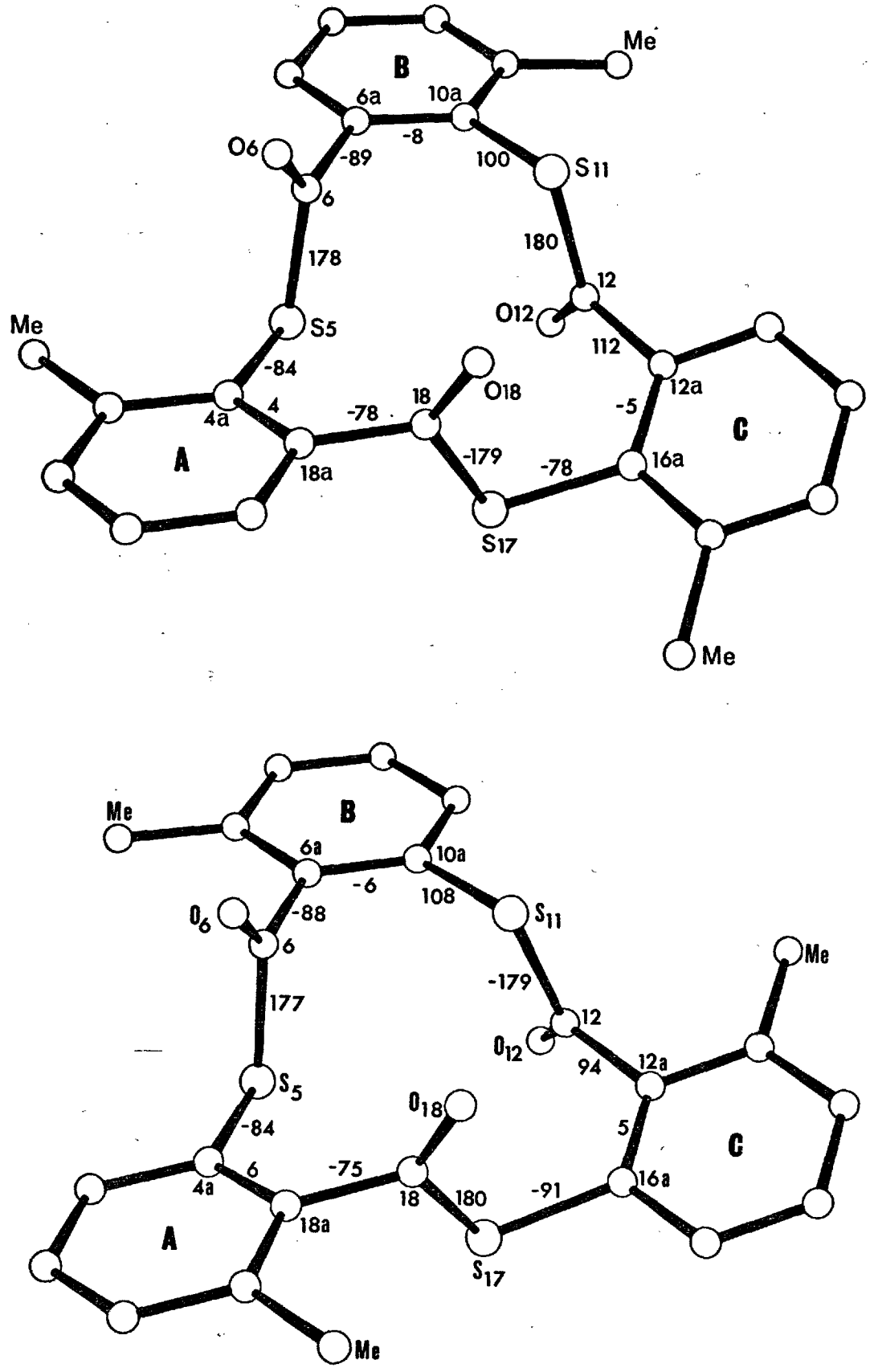
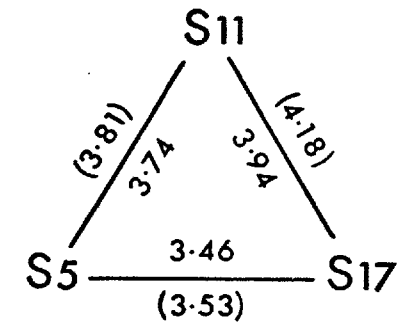


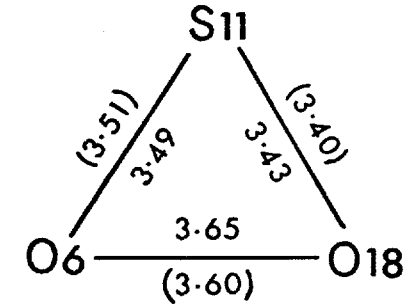
Figure 3. Torsion angles around the central 12-membered ring with (above), for comparison, those for (1).

rings in (1) and (2) immediately shows the very significant differences between them which accompany the change of tilt of ring C with respect to rings A and B. These differences, however, are confined primarily to changes in rotation about the two bonds immediately adjacent to ring C and to a change of sign for the rotation about the edge of the ring (C(12a)-C(16a)). The changes are 18°, 10° and 13° about C(12)-C(12a), C(12a)-C(16a) and C(16a)-S(17) respectively, the remaining torsion angles in the ring, with the exception of that about C(10a)-S(11) (an 8° difference), being very similar to those for (1). We conclude that the changes in conformation are not a consequence of satisfying any internal steric requirements associated with the change from a 4,10,16 Me to a 1,7,13 Me configuration, (or *vice versa*) but that they are due to the different packing requirements. Analysis of the short intermolecular contacts (Table 4) bears out this conclusion, with the shortest contact (3.163Å between Me(13) and O(12)), (*cf.* 3.44Å intra-) being shorter than any of the intramolecular Me...O distances. Another of the short intermolecular contacts (3.399Å) is between O(12) and S(17) and this is shorter than any of the trans-annular S...O distances. In (1) too, intermolecular contacts are shorter than trans-annular ones. It is interesting to note that despite the conformational and packing changes, both (1) and (2) achieve virtually identical packing densities (U(1) = 2148Å^3, U(2) = 2152Å^3).

The deviations from planarity in the three aromatic rings are very similar to those for (1)[4] with, as in (1), the largest deviations, 0.015Å (C(4a)) and 0.017Å (C(12a)) occurring in rings A and C respectively. Ring B does not depart significantly from planar (Δ max = 0.002Å).

As has been mentioned earlier, (2) is a racemate in solution, but exhibits spontaneous resolution on crystallisation. The determination





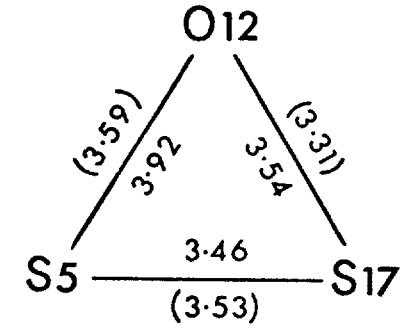


Figure 4. Trans-annular distances for (2) with, in parentheses, the corresponding distances for (1).

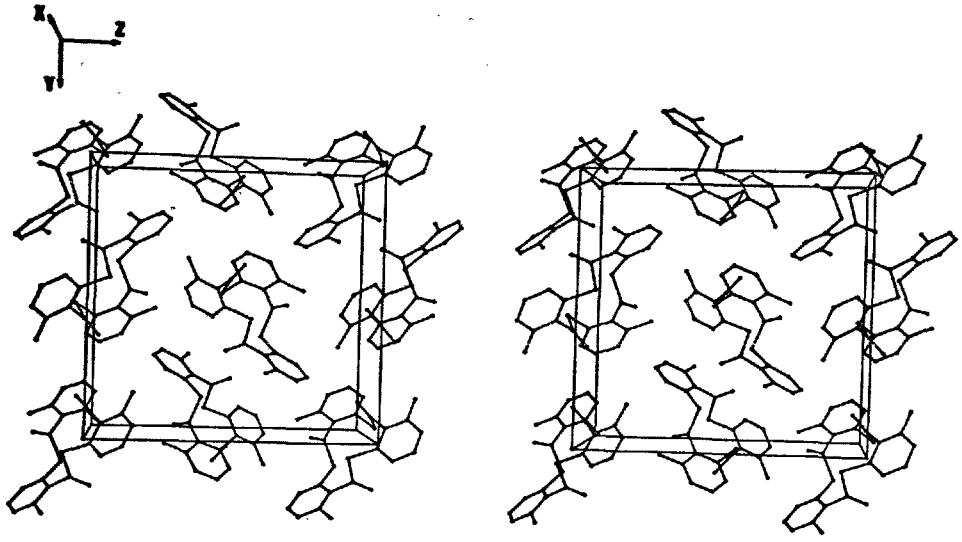


Figure 5. Stereo view of the packing of the molecules.

of the absolute configuration (described in the experimental section) is thus of no immediate interest as it relates only to the molecules in the crystal selected. However, an analysis of the calculated structure factors for both configurations has shown that, whilst in the majority of cases the effect is small, several reflections do exhibit quite large Bijvoet differences.[15] This means that for a particular crystal only a few reflections need be accurately measured to determine the configuration of the molecules present. As the compound crystallises to give large well formed crystals it may thus be possible, either using a crystal of sufficient size, or by using a smaller one of known configuration as a seed to produce a batch, to obtain a correlation between the absolute configuration and optical rotation. It is proposed to investigate this possibility further.

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Table 1

Fractional coordinates (X 10^4) for the non-hydrogen atoms with estimated standard deviations in parentheses

Atom	*x*	*y*	*z*
C(1)	433(3)	-731(2)	-1448(2)
Me(1)	7(5)	-386(2)	-2276(2)
C(2)	-485(4)	-1358(2)	-1093(2)
C(3)	-147(4)	-1670(2)	-326(3)
C(4)	1120(4)	-1352(2)	115(2)
C(4a)	2044(3)	-702(2)	-211(2)
S(5)	3560(1)	-237(0)	410(0)
C(6)	5335(3)	-763(2)	67(2)
O(6)	5354(3)	-1318(1)	-427(1)
C(6a)	6776(3)	-411(2)	504(1)
C(7)	7282(3)	-777(2)	1236(2)
Me(7)	6453(5)	-1540(2)	1577(2)
C(8)	8597(4)	-421(2)	1634(2)
C(9)	9380(4)	272(2)	1323(2)
C(10)	8895(3)	640(2)	598(2)
C(10a)	7575(3)	292(2)	184(1)
S(11)	6972(1)	683(0)	-786(0)
C(12)	5948(3)	1640(2)	-521(2)
O(12)	5842(3)	1908(1)	153(1)
C(12a)	5322(3)	2057(2)	-1289(2)
C(13)	6359(4)	2597(2)	-1724(2)
Me(13)	8019(4)	2794(2)	-1423(2)
C(14)	5793(4)	2950(2)	-2450(2)
C(15)	4256(5)	2785(2)	-2728(2)
C(16)	3235(4)	2282(2)	-2282(2)

Table 1 (contd.)

Atom	x	y	z
C(16a)	3764(3)	1915(2)	-1558(2)
S(17)	2391(1)	1296(0)	-975(0)
C(18)	2750(3)	269(2)	-1387(2)
O(18)	3659(3)	136(1)	-1929(1)
C(18a)	1723(3)	-401(1)	-997(2)

Table 2

Anisotropic thermal parameters* (X10^3 Å^2) for the non-hydrogen atoms with standard deviations in parentheses

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	42(1)	52(2)	61(2)	7(1)	-5(1)	-14(1)
Me(1)	70(2)	89(3)	67(2)	15(2)	-21(2)	-17(2)
C(2)	44(2)	57(2)	92(2)	-6(2)	-8(2)	-20(2)
C(3)	57(2)	48(2)	99(3)	-9(2)	13(2)	-3(2)
C(4)	55(2)	48(2)	65(2)	1(2)	9(2)	9(2)
C(4a)	38(1)	46(1)	49(1)	1(1)	4(1)	-3(1)
S(5)	49(0)	60(0)	44(0)	4(0)	-2(0)	-9(0)
C(6)	49(1)	41(1)	40(1)	2(1)	-3(1)	6(1)
O(6)	59(1)	58(1)	61(1)	3(1)	-5(1)	-20(1)
C(6a)	43(1)	43(1)	40(1)	7(1)	-6(1)	-5(1)
C(7)	52(2)	53(2)	41(1)	8(1)	-6(1)	0(1)
Me(7)	81(2)	64(2)	59(2)	-3(2)	-13(2)	18(2)
C(8)	55(2)	66(2)	44(1)	12(2)	-10(1)	-4(1)
C(9)	50(2)	71(2)	54(2)	4(2)	-15(1)	-15(2)
C(10)	50(2)	51(2)	60(2)	-2(1)	-3(1)	-4(1)
C(10a)	43(1)	45(1)	43(1)	7(1)	-4(1)	-2(1)
S(11)	56(0)	46(0)	41(0)	7(0)	1(0)	-0(0)
C(12)	42(1)	42(1)	44(1)	1(1)	4(1)	-2(1)
O(12)	83(2)	72(1)	46(1)	18(1)	2(1)	-9(1)
C(12a)	47(1)	37(1)	44(1)	4(1)	6(1)	1(1)
C(13)	55(2)	35(1)	53(2)	-2(1)	6(1)	-3(1)
Me(13)	63(2)	62(2)	71(2)	-18(2)	5(2)	0(2)
C(14)	63(2)	43(1)	62(2)	5(2)	13(1)	12(2)
C(15)	69(2)	73(2)	66(2)	15(2)	0(2)	30(2)
C(16)	48(2)	72(2)	70(2)	3(2)	-6(2)	22(2)

Table 2 (contd.)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(16a)	47(2)	42(1)	52(2)	4(1)	7(1)	6(1)
S(17)	49(0)	45(0)	60(0)	1(0)	11(0)	1(0)
C(18)	44(1)	51(1)	43(1)	0(1)	-0(1)	-2(1)
O(18)	69(1)	67(1)	54(1)	-5(1)	21(1)	-6(1)
C(18a)	37(1)	42(1)	48(1)	3(1)	1(1)	-6(1)

* In the form: $\exp[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^*+2U_{13}hla^*c^*+2U_{23}klb^*c^*)]$

Table 3

Fractional coordinates and isotropic thermal parameters ($\times 10^3$) for the hydrogen atoms*

Atom	x	y	z	U(Å^2)
H(11)	-95	-70	-250	76
H(12)	-28	23	-222	76
H(13)	94	-45	-265	76
H(2)	-142	-158	-141	63
H(3)	-81	-215	-10	63
H(4)	136	-158	68	63
H(71)	701	-171	210	76
H(72)	531	-141	169	76
H(73)	654	-201	118	76
H(8)	901	-67	216	63
H(9)	1032	52	163	63
H(10)	947	115	37	63
H(131)	856	319	-182	76
H(132)	794	307	-87	76
H(133)	865	226	-138	76
H(14)	650	335	-277	63
H(15)	390	303	-326	63
H(16)	210	219	-247	63

* The numbering of the hydrogen atoms is that of the atoms to which they are bonded

Table 4

Selected intra- and intermolecular* contacts ≤ 3.6Å

Me(13)...O(12)	3.44	Me(7) ...O(6)	3.41
Me(1) ...O(18)	3.19	S(5) ...S(17)	3.46
S(11) ...O(6)	3.49	S(11) ...O(18)	3.43
S(17) ...O(12)	3.54		
C(8) ...O(18^{i})	3.30	C(9) ...O(18^{i})	3.35
Me(7) ...C(14^{i})	3.57	Me(13)...O(12^{ii})	3.16
O(12) ...S(17^{ii})	3.40	C(9) ...C(14^{ii})	3.56
O(6) ...C(3^{iii})	3.44	C(15) ...O(6^{iv})	3.35
C(6a) ...C(5^{v})	3.51	C(8) ...C(4^{v})	3.56
C(9) ...C(4^{v})	3.55	C(7) ...Me(1^{vi})	3.59

* Roman numeral superscripts denote the following equivalent positions relative to the reference molecule at x,y,z:

i $1\frac{1}{2}-x,-y,\frac{1}{2}+z$ ii $\frac{1}{2}+x,\frac{1}{2}-y,-z$ iii $\frac{1}{2}+x,-\frac{1}{2}-y,-z$ iv $1-x,\frac{1}{2}+y,-\frac{1}{2}-z$
v $1+x,y,z$ vi $\frac{1}{2}-x,-y,\frac{1}{2}+z$

Table 5

Equations of the least squares planes (in direct space) for the three aromatic rings in the structure together with their standard deviations and the largest displacements from them.

A $-5.063x + 10.858y + 6.500z = -1.949$

σ = 0.010Å C(4a) 0.015Å

B $-5.112x + 9.545y + 8.291z = -3.440$

σ = 0.002Å C(8),C(9) 0.002Å

C $-2.748x + 12.559y + 8.367z = 0.060$

σ = 0.012Å C(12a) -0.017Å

Dihedral angles between the planes of the rings:

A,B = 8° A,C = 18° B,C = 20°

CHAPTER 9

The crystal structure of 1,3-dicyclohexyl-1-[*N*-methyl-*N*-(*N*-anthraniloyl-*N*-methylanthraniloyl)anthraniloyl] urea - a cyclisation intermediate produced in the formation of *N,N'*-dimethyltrianthranilide

Summary

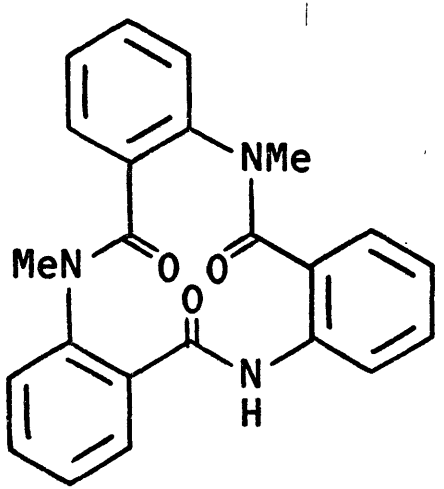
The title compound crystallises in the monoclinic space group $P2_1/n$ with a = 11.749(1), b = 15.063(1), c = 18.994(1)Å, β = 98.44(1)°, Z = 4. The structure was solved by direct methods and refined by full-matrix least squares to R = 0.041 for the 4948 independent diffractometer measured reflections. The compound, a cyclisation intermediate, has given insight into the mechanisms involved in the cyclisation process. The trianthranilide portion of the molecule contains both *cis* and *trans*-amide linkages, and the molecule as a whole is stabilised by a strong intramolecular amide-amide NH...O hydrogen bond (2.853(2)Å) between the cyclohexylurea and trianthranilide portions.

X-ray examination of an initial batch of crystals thought to be *N,N'*-dimethyltrianthranilide (1) revealed a substantial discrepancy between the observed (606) and calculated (385) molecular weights. The difference (221) was too large to be attributed to included solvent molecules. It was deduced from a chemical analysis, mass spectra, and n.m.r. spectra, that the crystals contained, in addition to (1), molecules of *N,N'*-dicyclohexylurea (2), a by-product of the cyclisation process. The observed molecular weight was consistent with a 1:1 adduct of (1) and (2). The objective at that stage was to verify the n.m.r. conclusion of a helical solid-state conformation for (1),[1] and it was considered that the presence of this additional molecule, representing an extra 16 non-hydrogen atoms, would unnecessarily complicate the analysis. There was also the possibility that (2) might form intermolecular hydrogen bonds with (1) thereby influencing the conformation of (1) and thus invalidating comparison between the *X*-ray and the n.m.r. analyses.

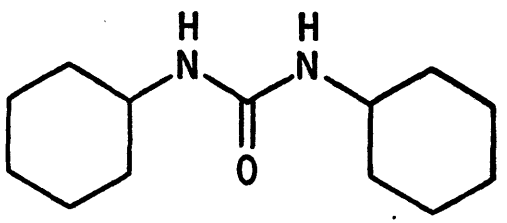
Subsequent *X*-ray analysis of a pure sample of (1) revealed a trans-annular N-H...N hydrogen bond involving an unusually distorted *trans* amide geometry.[2,3] In view of this an *X*-ray analysis of the adduct, (1) + (2), was undertaken to ascertain whether, in a different crystalline environment, (1) still retained the same conformation and the same N-H...N hydrogen bond.

EXPERIMENTAL

The adduct crystallises from ethanol as large clear well formed blocks. Accurate lattice parameters were obtained by least-squares refinement of 20 high-angle reflections measured (at 12°C) on a



(1)



(2)

diffractometer using Cu-K_α radiation.

Crystal Data $C_{36}H_{43}N_5O_4$, M = 609.8, Monoclinic, a = 11.7488(6), b = 15.0631(7), c = 18.9944(7)Å, β = 98.439(5)°, U = 3325Å^3, D_c = 1.22gcm^{-3}, D_m = 1.21gcm^{-3} (by flotation), Z = 4, $F(000)$ = 1304. Space-group $P2_1/n$ (No. 14), uniquely determined from systematic absences. Cu-K_α radiation, $\bar{\lambda}$ = 1.54178Å, μ(Cu-K_α) = 6.1cm^{-1}.

A crystal *ca.* 0.5 x 0.35 x 0.25 mm^3 was mounted along its a direction. Data were measured on a Siemens off-line four-circle diffractometer using Ni-filtered Cu-K_α radiation. A total of 4948 independent reflections were measured (to θ = 60°) using the θ-2θ scan technique with the 'five-value'[4] measuring procedure. Of these, 566 reflections had $I < 2.58\sigma(I)$ and were classed as unobserved.[4] The net count of the 0 6 10 reflection, measured as a reference every 50 reflections, did not alter significantly during the data collection (5 days) indicating that no deterioration of the crystal had occurred. The data were brought to a uniform arbitrary scale by use of this reflection,[4] and Lorentz and polarisation corrections were applied. No absorption corrections were applied.

Solution and Refinement of the Structure

The structure was solved by direct methods by application of the program MULTAN[5] to 400 reflections with normalised structure factors (E's) $\geq$ 1.76. An E map calculated for the phase solution with the highest 'combined figure of merit' gave plausible positions for 37 of the 45 non-hydrogen atoms; the positions of the atoms of one of the cyclohexane rings were not resolved. These 37 atoms were refined isotropically (as carbons) giving R = 0.35, and a difference map then revealed the remaining non-hydrogen atoms. The different atom iden-

tities were assigned on the basis of bond lengths, thermal parameters, and chemical information.

In view of the large data set, initial refinements were carried out using an 'inner core' of data comprising ~ 3000 reflections. Anisotropic refinement by full-matrix least squares reduced R to 0.092. The hydrogen atoms were located from a difference map and, with the exception of those involved in hydrogen bonding, were for subsequent refinements fixed at optimised calculated positions; the hydrogens of the two methyl groups were observed to have partial occupancy in two orientations and were in each case fixed at half weight in 6 equally staggered positions. Eight reflections which had $|F_o| << |F_c|$ were suspected of being affected by extinction and therefore removed. Subsequent refinement, the hydrogen-bonded hydrogens isotropically, the remaining non-hydrogen atoms anisotropically, reduced R to a final value of 0.041 for the full data. The final ratios of shift/error for the refined hydrogens were of the same order as for the other atoms. The maximum residual electron density in the final difference map was < 0.25eÅ^{-3}.

Unit weights were used throughout the refinements. Atomic scattering factors were taken from ref. 6 with the exception of those for hydrogen which were taken from ref. 7. The computations were carried out on the Imperial College CDC 6400 and the University of London CDC 6600 and 7600 computers using, in the main, programs belonging to the *X*-ray 70 and 72 systems.[8]

RESULTS AND DISCUSSION

The observed and calculated structure factors are listed in Appendix IX. The final fractional coordinates and anisotropic thermal parameters for the non-hydrogen atoms together with their estimated

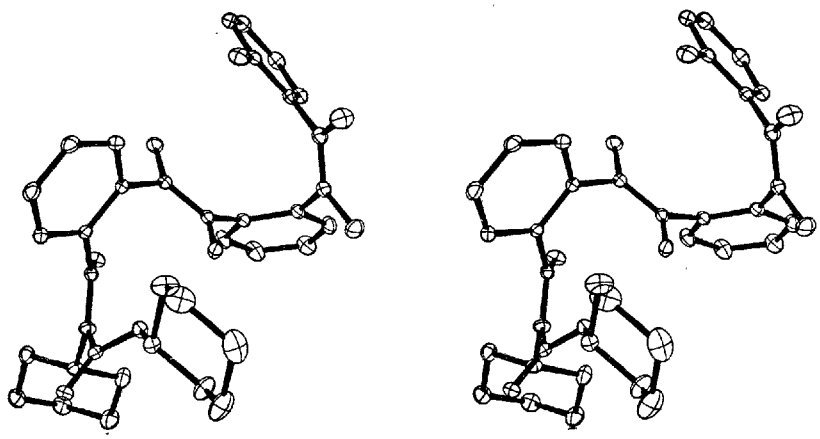
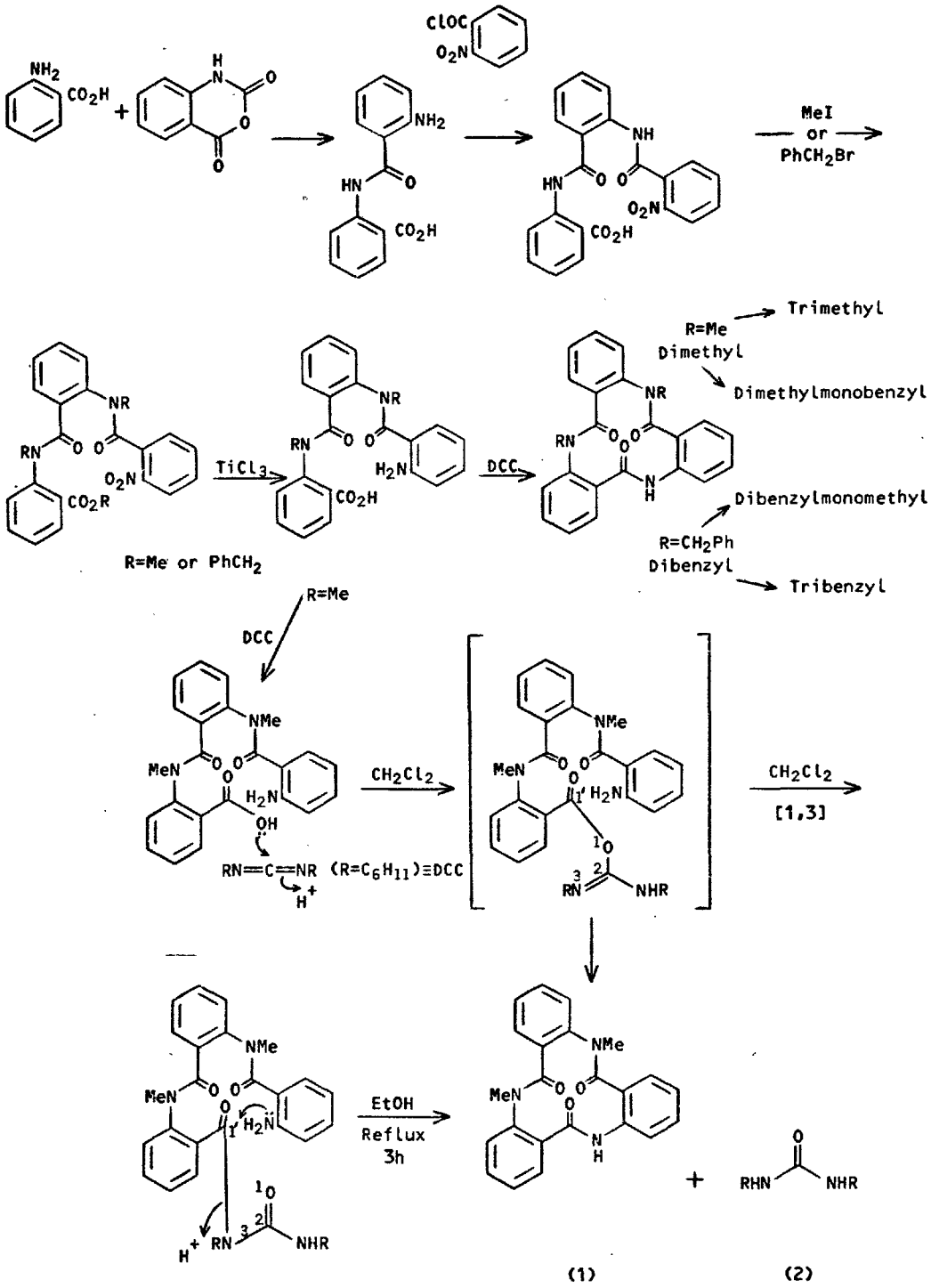


Figure 1. Stereo view of the molecule.

standard deviations are listed in Tables 1 and 2. Those for the hydrogen atoms with their isotropic temperature factors are given in Table 3. Figure 1 shows a stereo view of the molecule (ORTEP[9]). Figure 2 shows the geometry of the NH_2 group attached to ring A. Figures 3a, b show the bond lengths and angles together with their estimated standard deviations, and the numbering scheme used. Table 4 lists selected intra- and intermolecular contacts ≤ 3.5Å. Figure 4 shows the torsion angles for the 'backbone' of the molecule and Figure 5 the Newman projections[10] and out-of-plane bending parameters[11,12] for the amides in the structure. Table 5 lists the least-squares planes for the aromatic rings in the structure and the largest deviants from them. Figure 6 shows a stereo view[9] of the packing of the molecules in the structure.

The analysis has revealed, not as originally expected a co-crystallisation of (1) and (2), but a new non-cyclic compound representing a reaction intermediate in the process of the cyclisation of (1). This has given new insight into the mechanism involved in the cyclisation process that 'stitches up the ends of an unwound trianthranilide molecule'. The scheme shows the route adopted by the Sheffield group for producing a range of substituted trianthranilides, and the mechanism they have proposed for the cyclisation of (1) via this new compound ('X') as an intermediate.[13]

The 'trianthranilide' portion of the molecule is in an 'unwound' state with a *cis* amide linkage between rings A and B and with a *trans* amide linking rings B and C. This portion is linked via a second amide link to the dicyclohexylurea unit. The overall conformation (Fig.1) can probably best be described as 'loosely coiled'. The apparently 'floppy' arrangement is stabilised by two strong intramolecular N-H...O hydrogen bonds N(1)-O(7) (2.779(3)Å) and N(32)-O(15)


ClOC
O2N
NH2
CO2H
MeI
or
PhCH2Br
TiCl3
DCC
R=Me or PhCH2
R=Me
Trimethyl
Dimethyl
Dimethylmonobenzyl
Dibenzylmonomethyl
R=CH2Ph
Dibenzyl
Tribenzyl
CH2Cl2
[1,3]
RN=C=NR (R=C6H11)≡DCC
EtOH
Reflux
3h
('X')
(1)
(2)

SCHEME

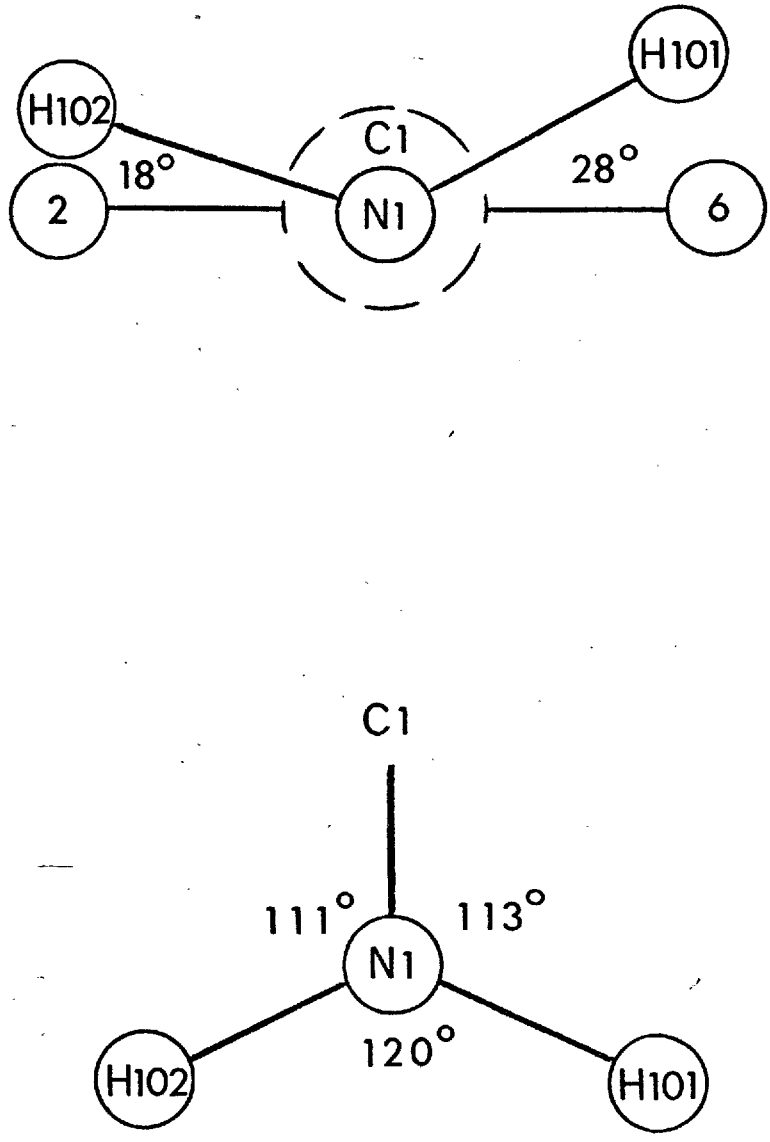


Figure 2. Geometry of the NH_2 group attached to ring A with, (above) the Newman projection down the N(1)-C(1) bond.

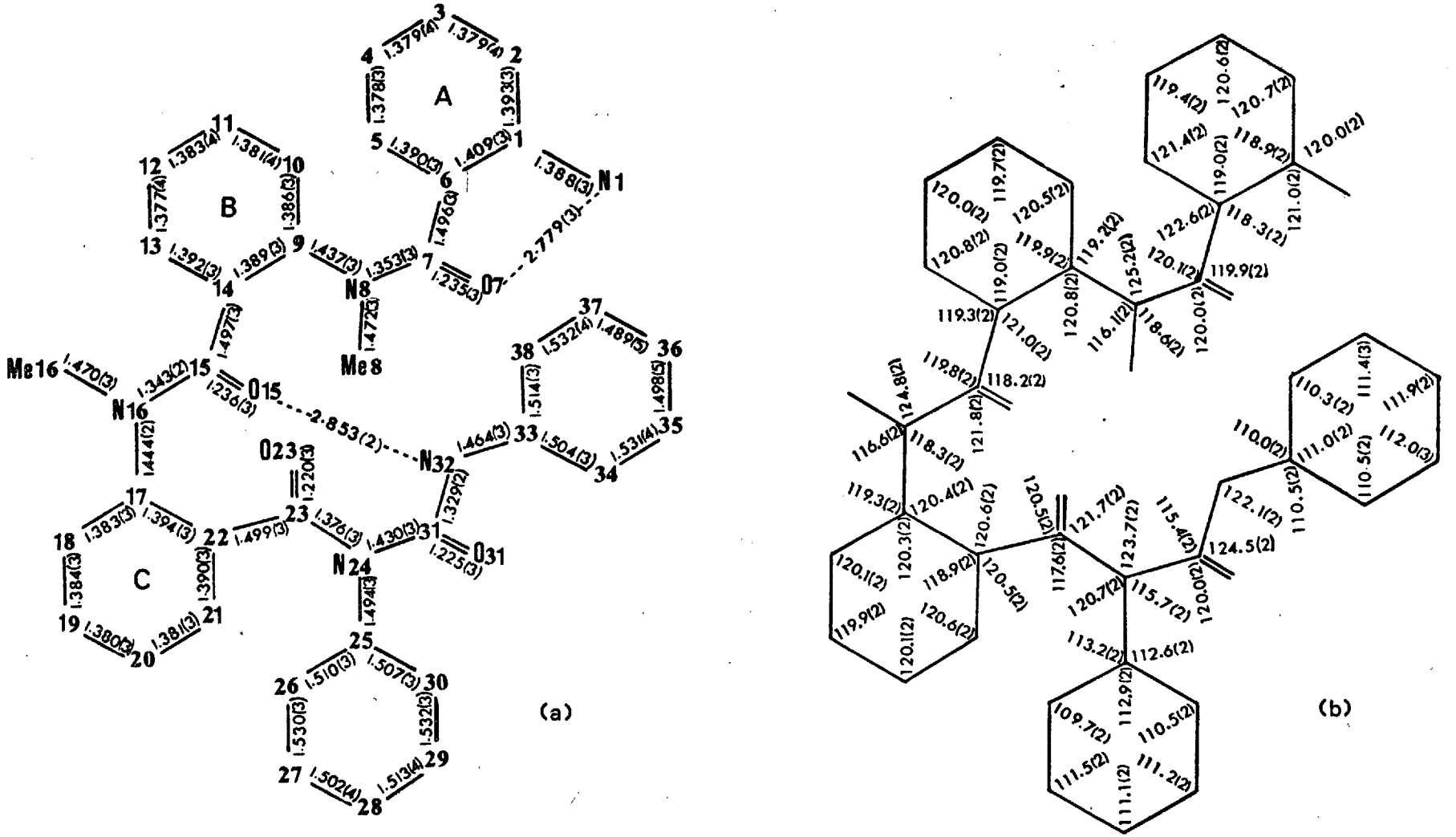


Figure 3(a) Bond lengths and numbering scheme; (b) valence angles. Standard deviations in parentheses.

(2.853(2)Å) and a slightly weaker intermolecular N-H...O hydrogen bond between N(1) and O(31) (2.912(2)Å). The N(1)-O(7) hydrogen bond is facilitated by a significant tetrahedral distortion of the NH_2 group, the N-H bond being deflected 28° out of the plane of ring A towards O(7) (Fig.2). The amide links throughout the structure are inclined so as to minimise conjugation with the aromatic rings.

There are significant variations in the lengths of the amide C-N bond (Fig.3a), these being similar to those observed in other trianthranilide structures.[3,14] Also as observed previously there is no correlation between the shortening of the C-N distance and the increase in the associated C=O length. It is worth noting, however, that the bond lengths in the methyl substituted *cis* and *trans* groups (between rings A and B, and B and C) are, within statistical significance, the same. All the amides show significant departures from planarity, comprising both a torsional twist about the C-N bond and out-of-plane bending at both the carbon and nitrogen atoms. This latter distortion occurs mainly at the nitrogen though with values of χ_N (Fig.5) slightly smaller than those previously observed in trianthranilide structures.[3,14]

The formation of an amide link (C(23)-N(24)) between the two main parts of the molecule destroys the symmetry of the dicyclohexylurea portion.[15] Moreover, the planarity of the urea moiety (C-N-CO-N-C) is prevented, partly by the N(32)-H...O(15) hydrogen bond, but more especially by numerous non-bonded interactions between N(32) and ring C. These result in a torsional twist of 42° around the N(24)-C(31) bond (Fig.4) with a consequent loss of conjugation which is manifest in its exceptional bond length (1.430(3)Å), which is a typical C-N single bond value. There is also a significant difference between the lengths of the bonds between the nitrogens (N(32) and

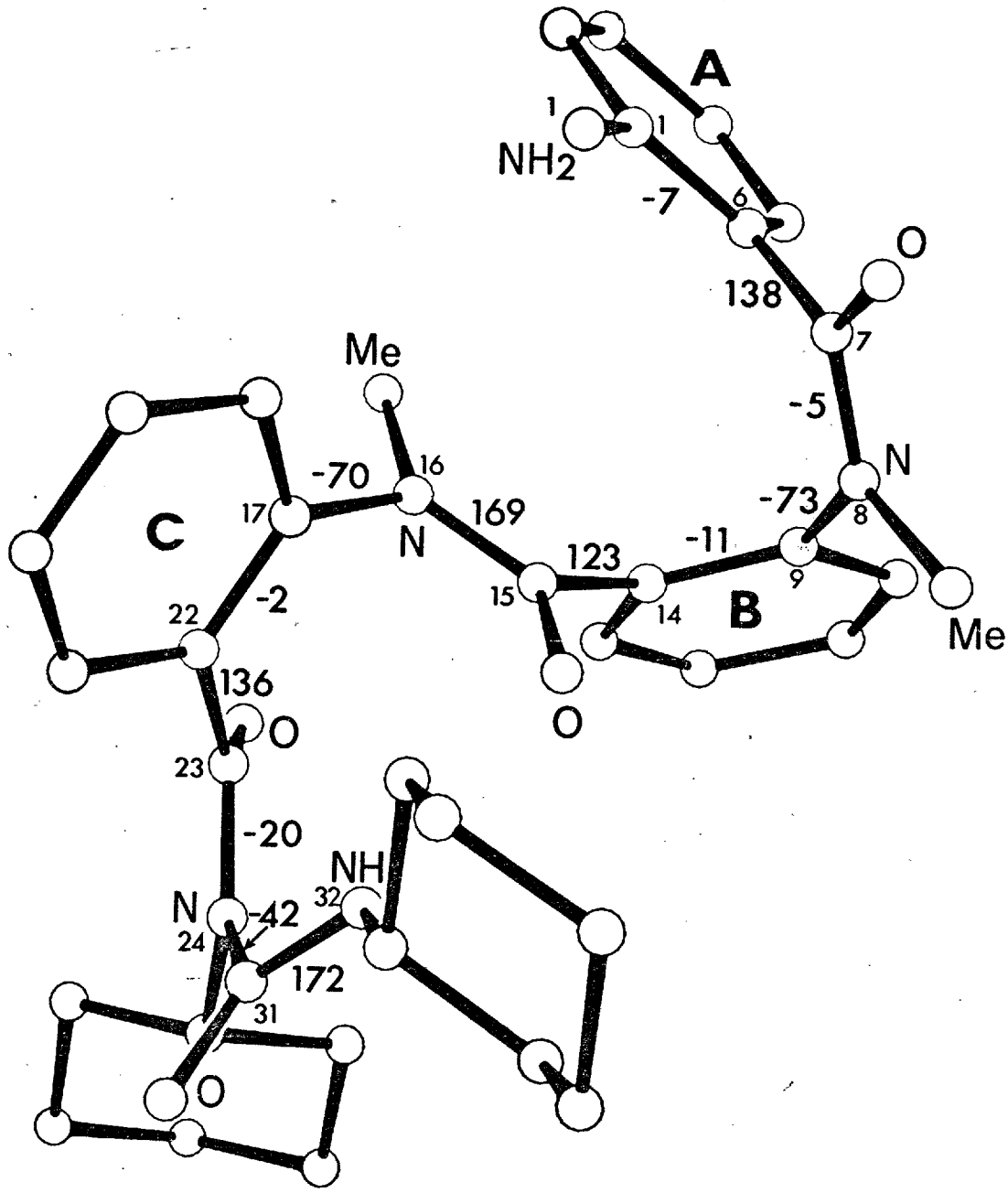


Figure 4. Torsion angles for the main chain.

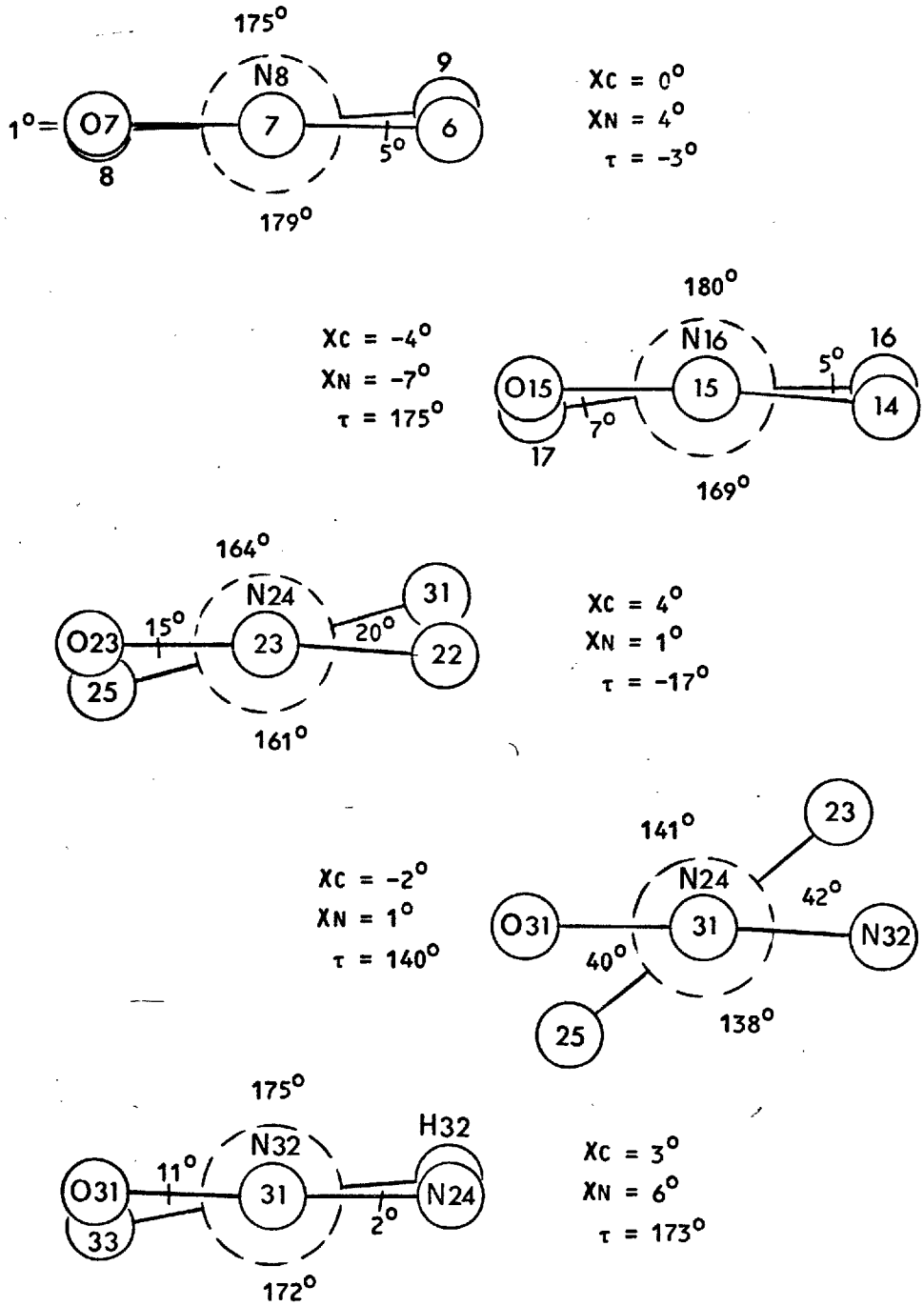


Figure 5. Newman projections and out-of-plane bending parameters for the amide groups.

N(24)) and the cyclohexyl rings, (1.464(3) and 1.494(3)Å respectively) the N(24)-C(25) distance being appreciably longer than that found in the structure of *N,N'*-dicyclohexylurea (1.444(5)Å).[15]

None of the aromatic rings display large departures from planarity (Table 5), though ring B is significantly less flat than either A or C. The maximum deviation from the least-squares plane for ring B is 0.021Å (C(14)) compared with values of 0.006 and 0.009Å for A and C respectively. The larger deviations in ring B are probably due to relief of the strain caused by the 11° external torsion angle about C(9)-C(14) (Fig.4). The structure is loosely packed (Fig.6) and apart from the N(1)-O(31) hydrogen bond, there are only three intermolecular contacts under 3.5Å (Table 4).

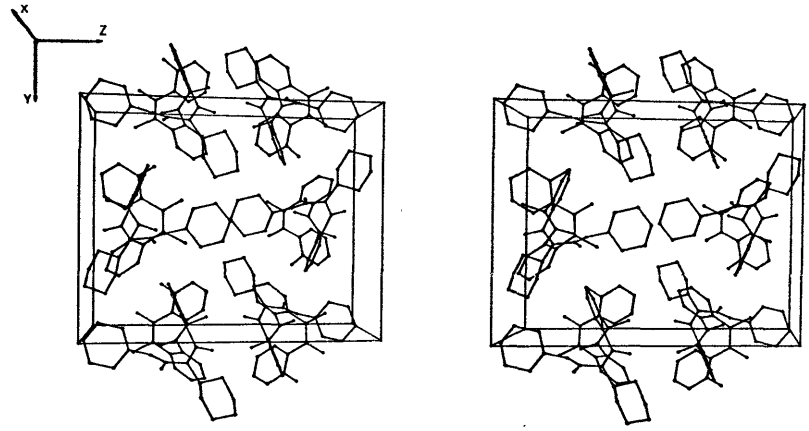


Figure 6. Stereo view of the packing of the molecules.

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Table 1

Fractional coordinates (X 10^4) for the non-hydrogen atoms with estimated standard deviations in parentheses

Atom	*x*	*y*	*z*
N(1)	5778(2)	2115(1)	7399(1)
C(1)	6383(2)	1699(1)	6918(1)
C(2)	6585(2)	2142(1)	6305(1)
C(3)	7150(2)	1727(2)	5810(1)
C(4)	7527(2)	862(2)	5913(1)
C(5)	7335(2)	416(1)	6517(1)
C(6)	6758(2)	813(1)	7023(1)
C(7)	6603(2)	366(1)	7705(1)
O(7)	6811(2)	774(1)	8273(1)
N(8)	6229(1)	-485(1)	7700(1)
Me(8)	6102(2)	-908(2)	8382(1)
C(9)	5867(2)	-1003(1)	7072(1)
C(10)	6547(2)	-1705(2)	6911(1)
C(11)	6212(2)	-2226(2)	6319(2)
C(12)	5202(2)	-2032(2)	5874(1)
C(13)	4514(2)	-1344(2)	6037(1)
C(14)	4825(2)	-834(1)	6645(1)
C(15)	3957(2)	-223(1)	6890(1)
O(15)	3531(1)	-424(1)	7434(1)
N(16)	3585(1)	488(1)	6495(1)
Me(16)	4030(2)	768(2)	5846(1)
C(17)	2604(2)	970(1)	6674(1)
C(18)	2761(2)	1809(1)	6968(1)
C(19)	1826(2)	2288(1)	7128(1)
C(20)	737(2)	1925(1)	6999(1)

Table 1 (contd.)

Atom	x	y	z
C(21)	579(2)	1081(1)	6718(1)
C(22)	1508(2)	593(1)	6552(1)
C(23)	1327(2)	-305(1)	6213(1)
O(23)	1730(1)	-480(1)	5674(1)
N(24)	629(1)	-893(1)	6504(1)
C(25)	109(2)	-1669(1)	6085(1)
C(26)	-558(2)	-1411(2)	5373(1)
C(27)	-1147(2)	-2232(2)	5010(1)
C(28)	-294(2)	-2956(2)	4935(1)
C(29)	369(2)	-3209(2)	5650(1)
C(30)	966(2)	-2400(2)	6029(1)
C(31)	362(2)	-820(1)	7213(1)
O(31)	-610(1)	-989(1)	7333(1)
N(32)	1237(1)	-597(1)	7706(1)
C(33)	1078(2)	-378(1)	8436(1)
C(34)	1461(2)	-1137(2)	8930(1)
C(35)	1323(3)	-898(2)	9696(1)
C(36)	1930(3)	-52(3)	9935(1)
C(37)	1569(3)	695(2)	9439(2)
C(38)	1728(3)	463(2)	8674(1)

Table 2

Anisotropic thermal parameters* (X 10^3 Å^2) for the non-hydrogen atoms with standard deviations in parentheses

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(1)	60(1)	44(1)	82(1)	-3(1)	22(1)	-19(1)
C(1)	35(1)	43(1)	56(1)	-8(1)	4(1)	-11(1)
C(2)	48(1)	47(1)	69(2)	-7(1)	0(1)	3(1)
C(3)	52(1)	76(2)	50(1)	-15(1)	3(1)	7(1)
C(4)	47(1)	75(2)	49(1)	-6(1)	12(1)	-11(1)
C(5)	39(1)	52(1)	52(1)	0(1)	4(1)	-9(1)
C(6)	34(1)	44(1)	42(1)	-5(1)	0(1)	-9(1)
C(7)	46(1)	51(1)	45(1)	-11(1)	1(1)	-7(1)
O(7)	113(1)	68(1)	43(1)	-19(1)	3(1)	-13(1)
N(8)	42(1)	50(1)	43(1)	-4(1)	-3(1)	1(1)
Me(8)	89(2)	71(2)	52(1)	-14(1)	-6(1)	13(1)
C(9)	37(1)	40(1)	49(1)	-3(1)	2(1)	-3(1)
C(10)	40(1)	55(1)	78(2)	10(1)	1(1)	-5(1)
C(11)	59(2)	57(2)	97(2)	10(1)	17(1)	-24(1)
C(12)	62(2)	68(2)	80(2)	0(1)	7(1)	-36(1)
C(13)	43(1)	60(1)	63(1)	0(1)	-2(1)	-19(1)
C(14)	33(1)	38(1)	46(1)	-2(1)	4(1)	-5(1)
C(15)	30(1)	40(1)	40(1)	-2(1)	-1(1)	-3(1)
O(15)	44(1)	56(1)	45(1)	10(1)	10(1)	12(1)
N(16)	33(1)	40(1)	39(1)	-1(1)	5(1)	2(1)
Me(16)	45(1)	62(1)	46(1)	-5(1)	11(1)	7(1)
C(17)	36(1)	35(1)	37(1)	1(1)	3(1)	5(1)
C(18)	46(1)	37(1)	52(1)	-5(1)	3(1)	0(1)
C(19)	65(2)	34(1)	63(1)	2(1)	9(1)	-2(1)
C(20)	53(1)	43(1)	65(1)	13(1)	14(1)	6(1)

Table 2 (contd.)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(21)	37(1)	46(1)	51(1)	3(1)	4(1)	8(1)
C(22)	38(1)	34(1)	34(1)	-1(1)	2(1)	6(1)
C(23)	35(1)	43(1)	34(1)	-2(1)	-2(1)	2(1)
O(23)	34(1)	61(1)	41(1)	-15(1)	15(1)	-10(1)
N(24)	47(1)	39(1)	33(1)	-11(1)	4(1)	-2(1)
C(25)	53(1)	38(1)	39(1)	-10(1)	3(1)	-4(1)
C(26)	55(1)	52(1)	55(1)	0(1)	-15(1)	-4(1)
C(27)	60(1)	66(2)	56(1)	-9(1)	-12(1)	-11(1)
C(28)	77(2)	66(2)	58(1)	-12(1)	3(1)	-23(1)
C(29)	86(2)	44(1)	80(2)	7(1)	-6(1)	-13(1)
C(30)	72(2)	47(1)	65(2)	9(1)	-19(1)	-7(1)
C(31)	44(1)	30(1)	38(1)	-1(1)	6(1)	2(1)
O(31)	42(1)	46(1)	50(1)	-8(1)	10(1)	0(1)
N(32)	38(1)	53(1)	33(1)	-2(1)	6(1)	-1(1)
C(33)	45(1)	52(1)	32(1)	2(1)	8(1)	-1(1)
C(34)	97(2)	63(2)	45(1)	17(1)	15(1)	10(1)
C(35)	131(3)	103(2)	43(1)	33(2)	22(2)	22(2)
C(36)	90(2)	150(3)	42(1)	10(2)	1(1)	-22(2)
C(37)	108(2)	93(2)	65(2)	-18(2)	24(2)	-34(2)
C(38)	102(2)	63(2)	55(1)	-20(2)	24(1)	-16(1)

* In the form: $\exp[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^*+2U_{13}hla^*c^*+2U_{23}klb^*c^*)]$

Table 3

Fractional coordinates and isotropic thermal parameters (X 10^3) for the hydrogen atoms with estimated standard deviations (for those refined) in parenthes*

Atom	x	y	z	U(Å^2)
HN(101)	598(2)	187(2)	788(1)	110(10)
HN(102)	574(2)	269(2)	734(1)	76(7)
H(2)	631	277	622	63
H(3)	729	205	537	63
H(4)	794	57	555	63
H(5)	762	-21	659	63
^{1}H(81)	638	-49	878	89
^{1}H(82)	527	-106	839	89
^{1}H(83)	657	-147	844	89
^{1}H(84)	582	-153	830	89
^{1}H(85)	686	-92	870	89
^{1}H(86)	554	-57	862	89
H(10)	729	-184	722	63
H(11)	669	-274	621	63
H(12)	497	-239	543	63
H(13)	378	-121	572	63
^{1}H(161)	470	39	577	89
^{1}H(162)	341	70	542	89
^{1}H(163)	427	140	589	89
^{1}H(164)	362	132	565	89
^{1}H(165)	487	90	596	89
^{1}H(166)	390	28	548	89
H(18)	-21	82	663	63
H(19)	6	228	711	63

Table 3 (contd.)

Atom	x	y	z	$U(\text{Å}^2)$
H(20)	194	290	734	63
H(21)	356	207	707	63
H(25)	-45	-188	640	63
H(261)	-116	-96	545	89
H(262)	-2	-116	507	89
H(271)	-173	-246	531	89
H(272)	-155	-206	453	89
H(281)	-72	-349	472	89
H(282)	25	-274	462	89
H(291)	-17	-347	595	89
H(292)	97	-366	557	89
H(301)	133	-258	652	89
H(302)	157	-218	575	89
H(32)	192(2)	-53(1)	759(1)	50(6)
H(33)	23	-28	843	63
H(341)	99	-167	878	89
H(342)	229	-127	891	89
H(351)	48	-83	972	89
H(352)	164	-139	1002	89
H(361)	176	11	1042	89
H(362)	278	-14	995	89
H(371)	73	83	945	89
H(372)	203	124	959	89
H(381)	143	96	835	89
H(382)	256	37	865	89

[1] Occupancy 50% * The numbering of the hydrogen atoms is that of the atoms to which they are bonded.

Table 4

Selected intra- and intermolecular* contacts ≤ 3.5Å

N(1) ...O(7)	2.78	Me(8) ...O(15)	3.34
O(15) ...N(32)	2.85	O(15) ...C(23)	3.23
Me(16)...C(1)	3.48	Me(16)...O(23)	3.27
N(16) ...O(23)	2.88	C(15) ...O(23)	3.25
C(13) ...O(23)	3.49	C(26) ...O(23)	3.01
C(5) ...O(31^{i})	3.41	C(10) ...O(31^{i})	3.49
O(23) ...C(4^{ii})	3.31	N(1) ...O(31^{iii})	2.91

* Roman numeral superscripts denote the following equivalent positions relative to the reference molecule at x,y,z:

i $1+x,y,z$ ii $1-x,-y,1-z$ iii $\frac{1}{2}-x,\frac{1}{2}+y,1\frac{1}{2}-z$

Table 5

Equations of the least squares planes (in direct space) for the three aromatic rings in the structure together with their standard deviations and the largest displacements from them:

A $9.545x + 4.955y + 6.781z = 11.622$

σ = 0.004Å C(6) -0.006Å

B $-6.676x - 9.364y + 11.713z = 5.322$

σ = 0.015Å C(14) 0.021Å

C $-0.013x - 5.882y + 17.300z = 10.981$

σ = 0.006Å C(17) -0.009Å

CHAPTER 10

The crystal structure of 5,18-dimethyl-5,18-dihydrotribenzo[*b*,*f*,*j*][1,4]diazacyclododecine-6,17-dione

Summary

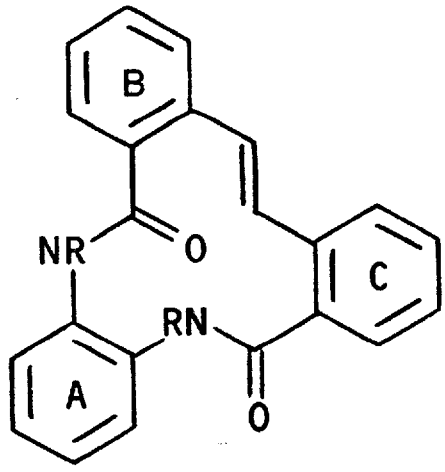
The title compound (2) crystallises in the orthorhombic space group $Pna2_1$ with a = 10.708(1), b = 28.233(2), c = 6.197(1)Å, Z = 4. The structure was solved by direct methods and refined by full-matrix least squares to R = 0.049 for the 1993 independent diffractometer measured reflections. The molecule adopts a distorted C_2 propeller conformation with angles of 35°, 33° and 14° between the planes of the three aromatic rings.

N.m.r. analyses of the conformational mobility in solution,[1,2] and *X*-ray determinations[3-5] of the solid-state conformations, of differently substituted trianthranilides have been reported recently. As a continuation of investigations of the conformational behaviour of medium-ring systems,[6-8] analyses have been made of the temperature dependent n.m.r. spectra of *N*,*N'*-dimethyl-(2) and *N*,*N'*-dibenzyl-(3) derivatives of the 12-membered olefinic bis-lactam (1).[9]

From a consideration of the three possible chiral conformations (4), (5) and (6), that retain the *trans*-11,12-olefinic bond and the two *trans*-amide linkages, it was concluded from the n.m.r. analyses that the most probable solid-state conformation was one of the two C_2 conformations (4) or (5) in both of which the plane of the olefinic group is approximately normal to the C_2 axis. The C_2-P conformation (4) is characterised by an approximately parallel alignment of the *trans*-olefinic bond with ring A, whilst in the C_2-H conformation (5) this bond is approximately orthogonal to ring A. As it was not possible to determine by n.m.r. which of these two possibilities represents the true solid-state conformation, an *X*-ray analysis of the bis-lactam (2) was undertaken. A preliminary account of this investigation has been reported.[9]

EXPERIMENTAL

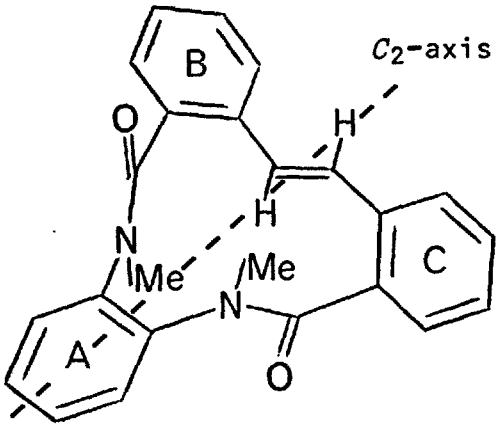
The title compound crystallises from methanol as large well-formed parallelopipeds. Accurate lattice parameters were determined (at 12°C) from measurements of high-angle axial α_1 and α_2 reflections on a diffractometer using Cu-K_α radiation.



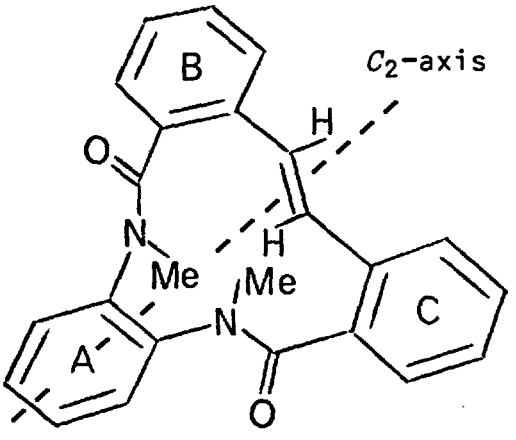
(1) R=H

(2) R=Me

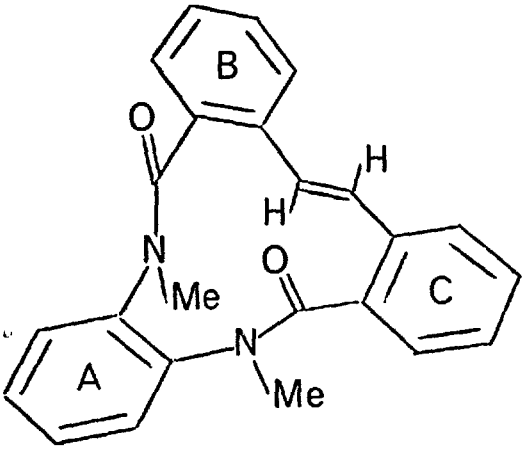
(3) R=CH_2Ph



(4) C_2-Propeller



(5) C_2-Helix



(6) C_1-Helix

Crystal Data $C_{24}H_{20}N_2O_2$, M = 368.4, Orthorhombic, a = 10.708(1), b = 28.233(2), c = 6.197(1)Å, U = 1874Å^3, D_c = 1.31gcm^{-3}, D_m = 1.30(2)gcm^{-3} (by flotation), Z = 4, $F(000)$ = 776. Space-group $Pna2_1$ (No. 33), from systematic absences and cell contents. Cu-K_α radiation, $\bar{\lambda}$ = 1.54178Å, μ(Cu-K_α) = 6.8cm^{-1}.

A crystal *ca.* 0.5 x 0.4 x 0.6 mm^3 was mounted along its c direction. Data were measured on a Siemens off-line four-circle diffractometer using Ni-filtered Cu-K_α radiation. A total of 1993 independent reflections were measured (to θ = 71°) using the θ-2θ scan technique with the 'five-value'[10] measuring procedure. Of these, 18 reflections had $I < 2.58\sigma(I)$ and were classed as unobserved.[10] The net count of the 4 18 0 reflection, measured as a reference every 50 reflections, did not alter significantly during the data collection (*ca.* 3 days) indicating that no deterioration of the crystal had occurred. The data were brought to a uniform arbitrary scale by use of this reflection,[10] and Lorentz and polarisation corrections were applied. No absorption corrections were applied.

Solution and Refinement of the Structure

The structure was solved by direct methods by application of the program MULTAN[11] to 225 reflections with normalised structure factors (E's) > 1.50. An E map calculated for the phase solution with the highest 'combined figure of merit' gave plausible positions for all the non-hydrogen atoms of the structure.

These atoms were refined anisotropically by full-matrix least squares to give a residual R = 0.090. A difference map contained sharp peaks corresponding to all the hydrogen atoms. These, with the exception of the *trans* olefinic hydrogens H(11) and H(12), were for

subsequent refinements fixed at calculated positions 1.0Å from their parent carbon atoms. Nine reflections which had $|F_o| << |F_c|$ were suspected of being affected by extinction and therefore removed. Further refinement, the olefinic hydrogens isotropically, the remaining non-hydrogen atoms anisotropically, reduced R to a final value of 0.049. The maximum residual electron density in the final difference map was $0.2 e Å^{-3}$.

Unit weights were used throughout the refinements. Atomic scattering factors were taken from ref. 12 with the exception of those for hydrogen which were taken from ref. 13. The computations were carried out on the Imperial College CDC 6400 and the University of London CDC 6600 and 7600 computers using, in the main, programs belonging to the *X*-ray 70 and 72 systems.[14]

RESULTS AND DISCUSSION

The observed and calculated structure factors are listed in Appendix X. The final fractional atomic coordinates and anisotropic thermal parameters for the non-hydrogen atoms together with their estimated standard deviations, are listed in Tables 1 and 2. Those for the hydrogen atoms with their isotropic temperature factors are given in Table 3. Figure 1 shows a stereo view of the molecule (ORTEP[15]). Figures 2a, b show the bond lengths and angles together with their estimated standard deviations and the numbering scheme used. Table 4 lists selected intra- and intermolecular contacts ≤ 3.5Å. Figure 3 shows the torsion angles around the central 12-membered ring and some of the short intramolecular contacts. Figure 4 shows the Newman projections[16] for the two amide groups. Figure 5 shows a stereo view of the packing of the molecules in the structure.[15] Table 5 lists the equations of some selected least-squares planes and

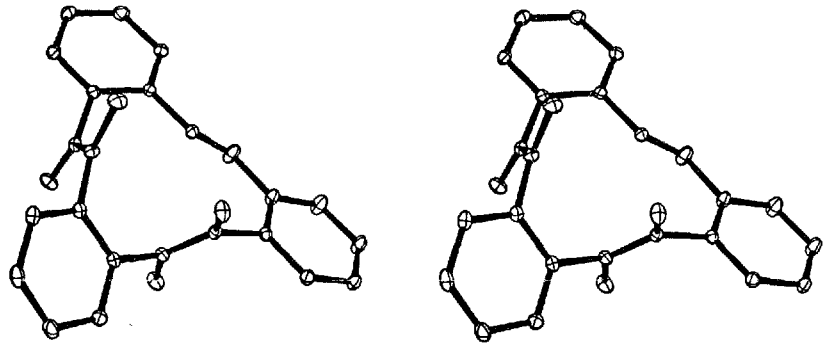


Figure 1. Stereo view of the molecule.

the deviations of particular atoms from them.

The molecule can be seen (Fig.1) to adopt a distorted C_2-P conformation (4) with ring A inclined to rings B and C by 35° and 33° respectively, and with ring B inclined to ring C by 14°. The *trans* amides linking rings A and B, and A and C are approximately normal to the mean planes of their adjacent rings (*i.e.* minimum conjugation) and have their *N*-methyl groups on opposite sides of the 12-membered ring. But the *trans* olefinic linkage between rings B and C is inclined at only 32° and 17° to rings B and C respectively, and this destroys the C_2 axis. This causes the olefinic carbon C(11) to protrude into the 12-membered ring so as to be nearly equidistant from N(5) and N(18) (3.16 and 3.23Å respectively) and only 2.96Å from the carbonyl carbon C(17). Furthermore H(11), which is very much better defined than H(12), is deflected slightly out of the C(10)C(11)C(12) plane toward C(17), so that the H(11)...C(17) distance is only 2.07(5)Å compared with 2.35Å to N(18). As such short trans-annular distances are not apparently due, in this molecule, to attractive forces such as hydrogen bonding or electrostatic interactions,† we conclude that they represent the best attempt to achieve the conjugational stability of a planar stilbenoid grouping for rings B and C. These are prevented by the trans-annular contacts from getting closer than 32° and 17° respectively from coplanarity and in so doing introduce torsional twists of +171° and -172° into the two amide groups. Apart from these distortions

† It is noteworthy from Figure 4 that small, but significant, departures from planar sp^2 geometries occur at C(17) and N(18) so that these atoms deviate toward H(11). The deformation of the amide group is weaker, but not unlike that which occurs with olefins in metal complexes. We record this as an observation without postulating a π complex type of attraction.

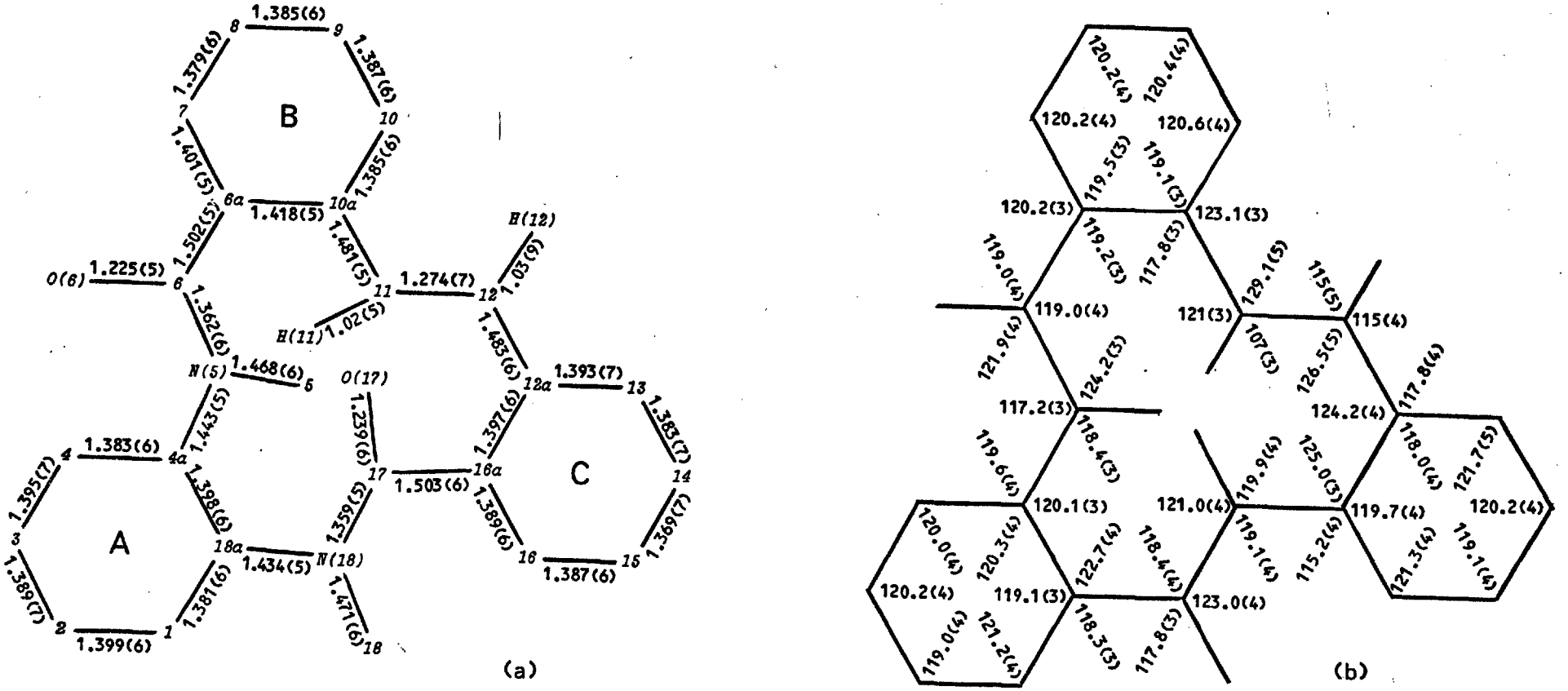


Figure 2(a) Bond lengths and numbering scheme; (b) valence angles. Standard deviations in parentheses.

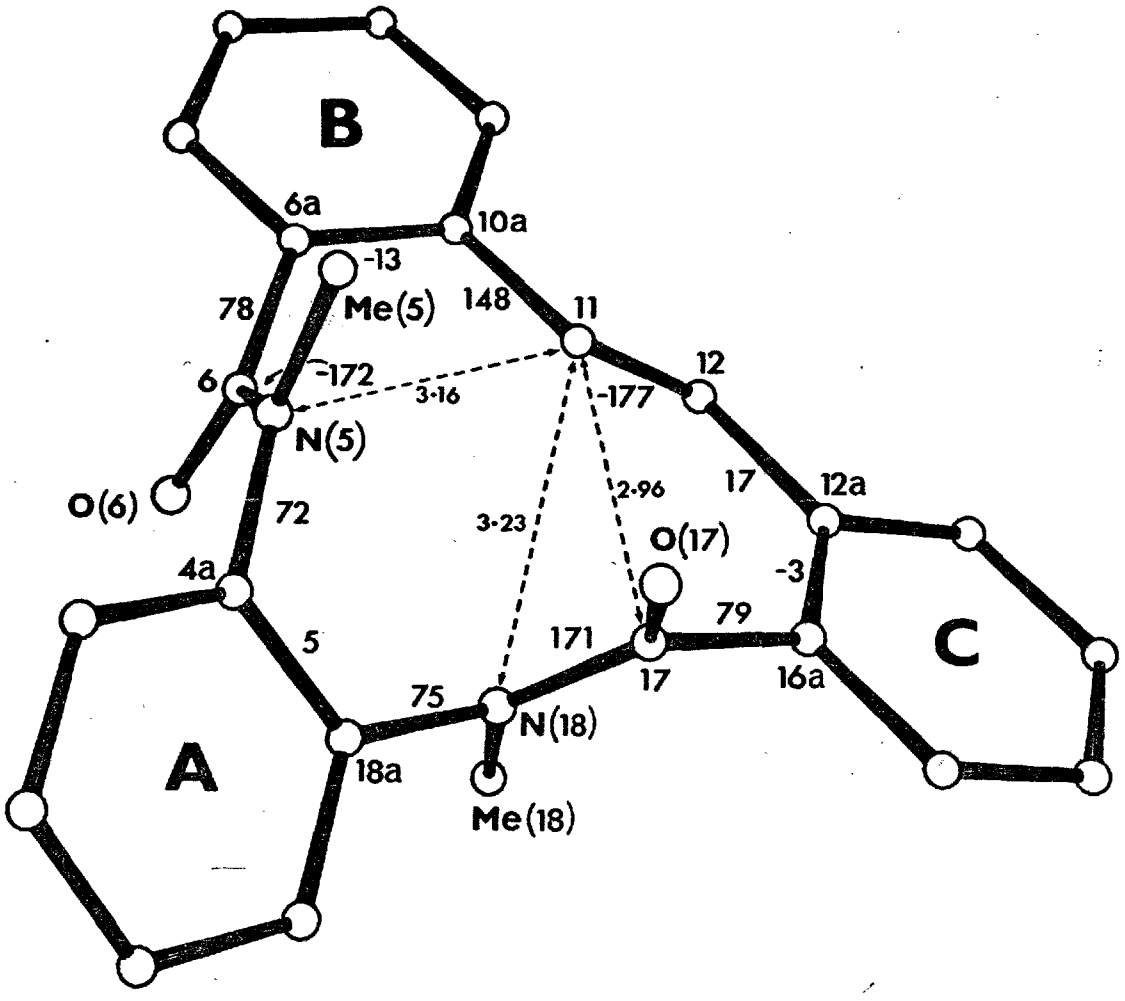


Figure 3. Torsion angles around the central 12-membered ring and trans-annular distances.

the rest of the molecule approximates well to C_2 symmetry. The C-C-C angles at C(11) (129°) and at C(12) (126°) are close to the average of 126.2° found in the recently redetermined structure of *trans*-stilbene.[17]

The bond lengths (Fig.2a) do not deviate significantly from expected values. The amide C-N bonds show a characteristic shortening reflecting their partial double-bond character and there is a small significant associated increase in the carbonyl C=O bond lengths, this being slightly more pronounced in the N(18)-C(17)=O(17) group. However, in neither case is the degree of bond modification as large as that normally associated with delocalisation effects in amides.[18]

The principal torsion angle about the C-N bond in each amide (-172° and 171°, Fig.3) shows that there are marked departures from planarity in each case. These values are very similar to those found for the substituted *trans* amides in the related structures of *N,N'*-dibenzyltrianthranilide (167° and 168°)[4] and *N,N'*-dimethyltrianthranilide (169° and 172°).[5] Also, as found in these related structures the distortions are not purely rotational; for example the amide group, linking rings A and C, shows significant out-of-plane bending at the nitrogen, (χ_N = 10°).[19-21] The values of the out-of-plane deformation parameters for both the present amides are given together with the Newman projections[16] (Fig.4). The large torsional twist (13°) about the aromatic C(6a)-C(10a) bond does not produce any significant buckling of ring B, the largest deviation from the mean plane from that ring being only 0.013Å, for C(10a) (Table 5). For ring A the deviations from planarity are larger, ranging up to 0.03Å (C(4a)), whilst ring C is appreciably flatter with a maximum deviation of only 0.009Å for C(15).

The structure is fairly loosely packed (Fig.4) with only four intermolecular contacts (Table 4) less than 3.5Å, the shortest being 3.26Å between C(8) and O(6).

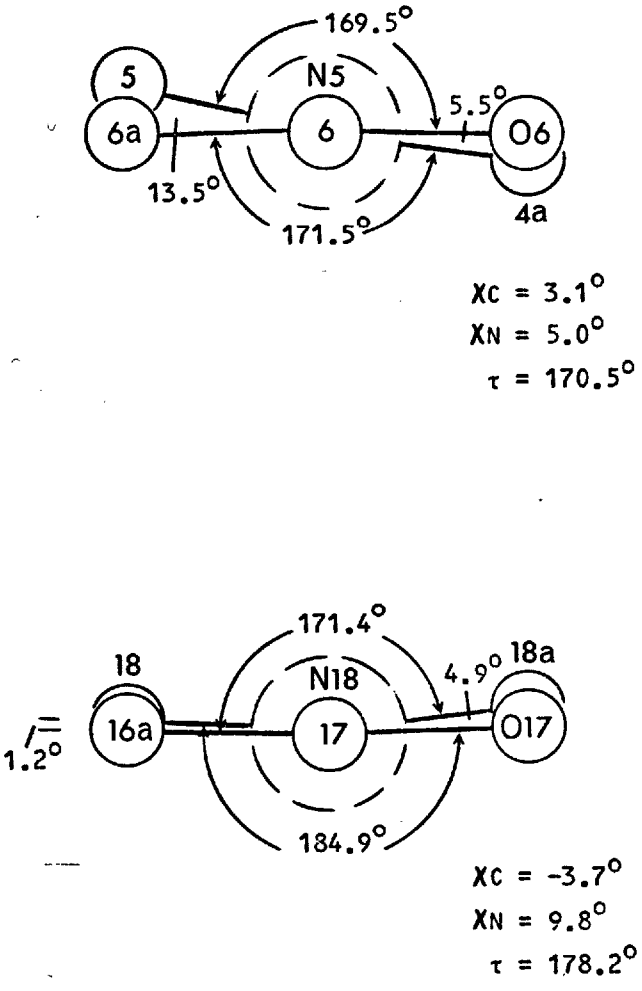


Figure 4. Newman projections and out-of-plane bending parameters for the *trans* amide groups.

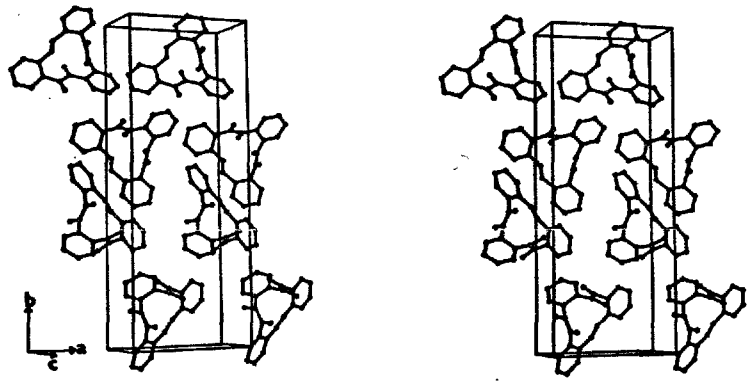


Figure 5. Stereo view of the packing of the molecules.

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Table 1

Fractional coordinates (X 10^4) for the non-hydrogen atoms with estimated standard deviations in parentheses

Atom	*x*	*y*	*z*
C(1)	68(4)	1626(1)	7165
C(2)	-274(4)	1998(1)	8534(10)
C(3)	652(5)	2242(1)	9642(8)
C(4)	1907(4)	2135(1)	9282(8)
C(4a)	2231(4)	1781(1)	7843(7)
N(5)	3532(3)	1688(1)	7412(6)
C(5)	4306(4)	1495(2)	9160(8)
C(6)	3980(4)	1819(1)	5444(7)
O(6)	3340(3)	2038(1)	4144(5)
C(6a)	5273(3)	1668(1)	4803(7)
C(7)	6217(4)	2006(1)	4527(8)
C(8)	7328(4)	1882(1)	3554(9)
C(9)	7506(4)	1425(1)	2794(9)
C(10)	6584(4)	1085(1)	3061(8)
C(10a)	5473(3)	1197(1)	4086(8)
C(11)	4464(4)	847(1)	4452(9)
C(12)	4158(5)	490(2)	3316(9)
C(12a)	3103(4)	162(1)	3732(8)
C(13)	3098(5)	-270(2)	2646(11)
C(14)	2142(4)	-594(1)	2912(9)
C(15)	1155(4)	-492(1)	4233(9)
C(16)	1145(4)	-65(1)	5345(8)
C(16a)	2100(4)	263(1)	5099(7)
C(17)	1976(4)	703(1)	6446(8)
O(17)	2167(3)	685(1)	8417(5)

Table 1 (contd.)

Atom	*x*	*y*	*z*
N(18)	1588(3)	1111(1)	5494(6)
C(18)	1254(5)	1141(2)	3195(8)
C(18a)	1306(4)	1510(1)	6842(7)

Table 2

Anisotropic thermal parameters* ($X10^3$ Å^2) for the non-hydrogen atoms with standard deviations in parentheses

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	35(2)	35(2)	47(3)	-0(2)	5(2)	-2(2)
C(2)	45(2)	35(2)	59(3)	9(2)	18(3)	-3(2)
C(3)	65(3)	28(2)	42(3)	7(2)	15(2)	-6(2)
C(4)	53(2)	26(2)	32(2)	-3(2)	5(2)	-3(2)
C(4a)	34(2)	28(2)	27(2)	-0(2)	5(2)	2(2)
N(5)	31(2)	34(2)	21(2)	-1(1)	-3(2)	2(1)
C(5)	45(2)	53(2)	28(2)	-0(2)	-11(2)	7(2)
C(6)	34(2)	26(2)	29(2)	-1(2)	0(2)	1(2)
O(6)	43(2)	49(2)	31(2)	11(1)	-0(1)	11(2)
C(6a)	30(2)	29(2)	26(2)	-1(1)	-2(2)	5(2)
C(7)	38(2)	33(2)	37(2)	-7(2)	-5(2)	0(2)
C(8)	37(2)	43(2)	43(2)	-12(2)	3(2)	5(2)
C(9)	31(2)	47(2)	47(3)	-2(2)	4(2)	6(2)
C(10)	29(2)	35(2)	43(3)	1(2)	3(2)	-0(2)
C(10a)	28(2)	28(2)	34(2)	-1(1)	-5(2)	3(2)
C(11)	29(2)	29(2)	49(3)	-1(2)	4(2)	-2(2)
C(12)	47(3)	43(2)	55(3)	-14(2)	21(3)	-15(3)
C(12a)	42(2)	31(2)	40(3)	-8(2)	8(2)	-7(2)
C(13)	52(3)	42(2)	69(4)	-11(2)	28(3)	-23(3)
C(14)	51(3)	36(2)	56(3)	-11(2)	10(3)	-17(2)
C(15)	40(2)	32(2)	44(3)	-8(2)	1(2)	-6(2)
C(16)	37(2)	31(2)	41(2)	-2(2)	6(2)	0(2)
C(16a)	34(2)	26(2)	29(2)	1(2)	-1(2)	-2(2)
C(17)	34(2)	28(2)	32(2)	-2(2)	1(2)	-4(2)
O(17)	71(2)	33(2)	28(2)	3(1)	-1(2)	2(1)

Table 2 (contd.)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(18)	32(2)	30(2)	25(2)	4(1)	-2(2)	-2(1)
C(18)	60(3)	46(3)	30(2)	13(2)	-11(2)	-4(2)
C(18a)	38(2)	25(2)	28(2)	4(2)	2(2)	0(2)

* In the form: $\exp[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^*+2U_{13}hla^*c^*+2U_{23}klb^*c^*)]$

Table 3

Fractional coordinates and isotropic thermal parameters (X 10^3) for the hydrogen atoms with estimated standard deviations (for those refined) in parentheses*

Atom	x	y	z	U(Å^2)
H(1)	-60	144	640	57
H(2)	-117	208	874	57
H(3)	42	249	1072	57
H(4)	257	231	1007	57
H(51)	519	145	864	63
H(52)	431	172	1041	63
H(53)	396	119	965	63
H(7)	608	234	504	57
H(8)	800	212	337	57
H(9)	831	134	206	57
H(10)	671	76	251	57
H(11)	373(4)	92(2)	544(9)	52(14)
H(12)	484(8)	36(3)	232(18)	176(36)
H(13)	381	-34	164	57
H(14)	217	-91	212	57
H(15)	45	-72	439	57
H(16)	44	1	636	57
H(181)	100	148	284	82
H(182)	199	105	229	82
H(183)	55	92	288	82

* The numbering of the hydrogen atoms is that of the atoms to which they are bonded.

Table 4

Selected intra- and intermolecular* contacts ≤ 3.5Å

C(11)...N(5)	3.16	C(17)...N(5)	3.29
O(17)...N(5)	3.25	N(18)...C(6)	3.25
N(18)...O(6)	3.33	C(18)...O(6)	3.43
C(5) ...O(17)	3.27	C(5) ...C(11)	3.45
C(17)...C(11)	2.96	N(18)...C(11)	3.23
O(17)...C(18^{i})	3.37	C(4) ...O(6^{i})	3.39
C(5) ...C(10a^{i})	3.40	C(8) ...O(6^{ii})	3.26

* Roman numeral superscripts denote the following equivalent positions relative to the reference molecule at x,y,z:

i $x,y,1+z$ ii $\frac{1}{2}+x,\frac{1}{2}-y,z$

Table 5

Equations of the least squares planes (in direct space) for the three aromatic rings in the structure together with their standard deviations and the largest displacements from them.

A $0.289x + 18.407y - 4.696z = -0.370$

$\sigma = 0.023$Å C(4a) 0.031Å

B $-4.192x + 7.020y - 5.490z = -3.684$

$\sigma = 0.009$Å C(10a) -0.013Å

C $-5.265x + 11.912y - 4.720z = -3.199$

$\sigma = 0.006$Å C(15) 0.009Å

Dihedral angles between the planes of the rings:

A,B = 35° A,C = 33° B,C = 14°

CHAPTER 11

In retrospect and the future ...

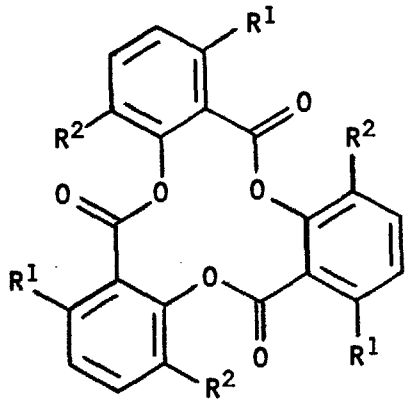
Looking back over these analyses, it is interesting to consider what, taking into account the original objectives, has been achieved, also what directions further studies should take. Many of the original objectives have been successfully fulfilled, but there are several instances where, not only are questions left unanswered, but more are posed after an analysis than were considered before.

In the case of tri-*o*-thymotide (TOT) (1), there were three main questions: (i) what are the dimensions of the channel and cavity, and the environments of the included molecule (ii) what is the solid-state conformation of TOT, and (iii) what is it about TOT that makes it form such a wide range of inclusion compounds? The first of these has been fully answered. To the second the simple answer is in each case 'propeller'. But, as has been seen, there is no unique propeller conformation, the molecule adopting significantly differing propeller conformations in different crystalline environments. There is thus an appreciable blurring of the conformational energy minimum. However, what has emerged is a consistent pattern of asymmetry of this conformation. Whilst it was reasonable to assume that structure analyses could provide the answers to the first two questions, it was perhaps a little naive to think that they could answer the third. It is fair to say that we are very little further towards understanding why TOT forms inclusion compounds now than we were to start with. No evidence has been found for example, of any keying together of the isopropyl groups of different molecules. A possible explanation however, is that the molecule has difficulty in packing by itself. This is evidenced by the structure of the unsolvated form which crystallises as a loosely packed racemic structure in which the TOT molecule is at its most distorted. There is a very significant asymmetry of the 12-membered ring and a

large rotation of one of the isopropyl groups. However, even if this explanation is correct, the question remains as to what is topologically so different between TOT and tri-*o*-carvacrotide (TOC) (2) that makes the one form inclusion compounds and the other not. The only chemical difference is that in TOC the methyl and isopropyl groups are interchanged which, from a study of models, does not appear to change the overall topology significantly. Preliminary crystallographic investigations have shown that TOC is monoclinic, $P2_1/c$ with $Z = 8$ mols/cell, *i.e.* two independent molecules in the asymmetric unit. Does this again represent a difficulty in packing of the molecules or could it be that there are two conformational species co-crystallising? An n.m.r. analysis of the relative populations of the different conformations in solution has shown that the ratio of 'helix' to 'propeller' is slightly greater for TOC than for TOT. To try to resolve these possibilities a full analysis of the structure of TOC is being carried out.

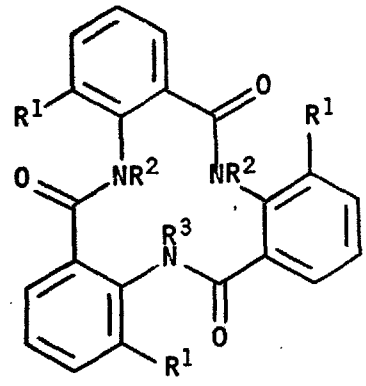
Returning to the cavity form of TOT, it was a surprise to find the structure does not just contain discrete cavities, but a continuous chain of linked large and small cavities; the structure though, is very different from the channel type. The existence of these small secondary cavities was totally unexpected and the fact that they are just large enough to contain either a hydrogen or helium molecule, is very interesting. We are currently trying to form the ethanol complex under a pressure of helium to see if any can be trapped in these cavities. Preliminary experiments, though encouraging, have been inconclusive.

Another topic yet to be investigated is whether TOT will resolve 2,3 dichlorobutane and if so, which 'hand' of one is associated with which 'hand' of the other. It should however, be said that this is largely of academic interest as large scale separation could only be carried out by means of seeded batch crystallisation and not as a



(1) $R^1=CH_3$, $R^2=CH(CH_3)_2$

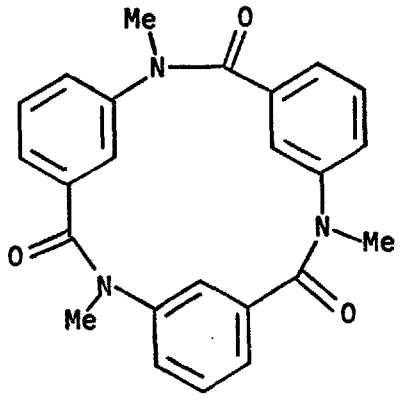
(2) $R^1=CH(CH_3)_2$, $R^2=CH_3$



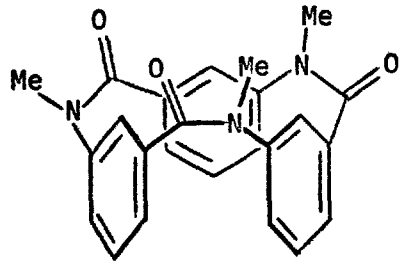
(3) $R^1=R^3=H$, $R^2=CH_2Ph$

(4) $R^1=R^2=CH_3$, $R^3=CH_3Ph$

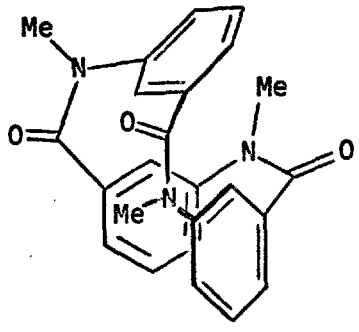
(9) $R^1=H$, $R^2=R^3=CH_3$



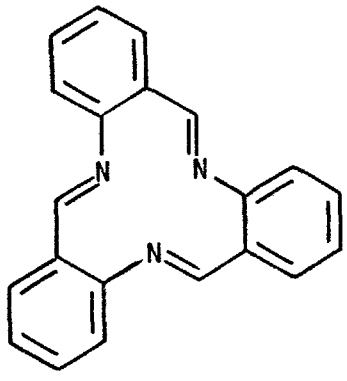
(5)



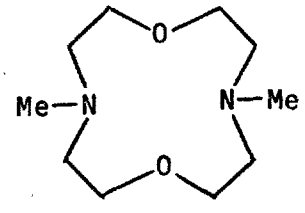
(6)



(7)



(8)



(10)

continuous process.

Among the other compounds studied, the trianthranilides and trithiosalicylides, unlike TOT, both adopt helical conformations in the solid-state. In the trianthranilides evidence has been found of transannular ring stabilisation by hydrogen bonding between opposite amide groups, in one case involving severe distortion of one of these groups. This hydrogen bonding must play an important role in determining the solid-state conformation. Also, one of these compounds (*N,N'*-dibenzyltrianthranilide (3)) forms inclusion compounds and may exhibit zeolitic properties - a point it is hoped to investigate further. Recent studies of the analogous monobenzyl compound (4) have shown that this also forms inclusion compounds and is of further interest as, unlike the dibenzyl compound, it is non-centrosymmetric and may thus be capable of resolving optical enantiomers.

The interesting thing to come out of the studies of the thiosalicylides is how a change in the position of the methyl group on the aromatic rings results in a large change in the conformation of the 12-membered ring. Also, how in one case the structure is centrosymmetric, whilst in the other there is spontaneous resolution on crystallisation. However, in this latter case, it offers an opportunity of trying to correlate optical rotation with absolute configuration.

Considering all the above structures, one point stands out, namely the power of n.m.r. studies in the elucidation of the most probable solid-state conformation. In all the above, the *X*-ray analyses have shown the n.m.r. proposals to be correct. In fact we were beginning to wonder if we were becoming redundant. We have fortunately been able recently to revise this view. Analysis of the 15-membered ring compound 1,9,17-trimethyl-1,9,17-triaza[2.2.2]metacyclophane-2,10,18-trione (5) has shown this molecule to adopt a 'crown' conformation (6) in the

solid-state, whereas the n.m.r. conclusion was that it was a 'saddle' (7).

One area of interest as yet barely touched upon is the potential of different forms of the above compounds to form complexes. The formation of a nickel(II) complex with tribenzo[*b*,*f*,*j*][1,5,9]triazacyclododecine (8) has been reported. Also the formation of the organic complex of benzylammoniumthiocyanate with *N*,*N*,*N*-trimethyltrianthranilide (9) has been achieved, though it has not been possible to produce crystals. These two results however, can only be considered as having merely scratched the surface of the problem and clearly there is very much more to be done. Still on this topic, the relationship of these compounds to crown ethers is apparent and, as a natural progression from the above, studies are currently being carried out on the structure of the 12-membered crown compound *N*,*N'*-dimethyl-1,7 diaza-4,10-dioxacyclododecane (10) which forms complexes with secondary alkyl ammonium salts.

In conclusion, it is worth mentioning again the *N*-acylurea compound which was initially discarded as it was assumed to be an adduct of *N*,*N'*-dimethyltrianthranilide and *N*,*N'*-dicyclohexylurea. Had it not been for the finding of an unusual hydrogen bond in the structure of *N*,*N'*-dimethyltrianthranilide, it would probably never have been investigated. The results of the analysis turned out to be a real bonus, giving considerable insight into the probable mechanisms involved in the cyclisation process. This can only be described as a very fortunate accident and demonstrates rather effectively the danger of having preconceived ideas.

APPENDIX I

Tables of observed and calculated structure factors for tri-*o*-thymotide - methylene iodide

Data Format:

	H	K
L	$10\times\|F_o\|$	$10\times\|F_c\|$

Reflections removed for extinction marked .... E

Reflections classed as unobserved marked ..... *

0,0,L

3	3186E	4827
6	2327	2584
9	2261	2205
12	423	328
15	175	167
18	314	314
21	616	587

0,1,L

-25	240	276
-24	430	336
-23	133	111
-22	148	169
-21	193	168
-20	235	149
-19	80	83
-18	149	175
-17	252	319
-16	950	875
-15	410	474
-14	703	734
-13	381	389
-12	440	416
-11	631	601
-10	588	525
-9	333	363
-8	1219	1215
-7	1730	1500
-6	443	405
-5	2083	2064
-4	2000	2125
-3	585	692
-2	681	661
-1	1322	1323
0	1322	1444
1	902	894
2	958	1110
3	494	676
4	140	166
5	1803	1696
6	644	582
7	1104	966
8	1213	1093
9	1003	964
10	488	393
11	161	257
12	777	803
13	424	423
14	346	369
15	809	881
16	484	496
17	505	494
18	491	503
19	231	171
20	428	399
21	63*	32
22	114	141

23	256	268
24	299	278
25	84	85

0,2,L

-24	368	392
-23	154	135
-22	297	320
-21	210	278
-20	557	524
-19	405	404
-18	382	432
-17	205	175
-16	623	631
-15	818	798
-14	191	253
-13	923	879
-12	855	900
-11	606	502
-10	168	217
-9	566	492
-8	526	478
-7	496	403
-6	400	302
-5	436	320
-4	230	150
-3	893	1094
-2	174	171
-1	651	759
0	1111	1081
1	1676	1682
2	1597	1630
3	1798	2038
4	969	940
5	251	279
6	359	202
7	253	122
8	2318	2262
9	1768	1643
10	249	276
11	1400	1416
12	502	578
13	138	151
14	800	833
15	154	207
16	112	161
17	581	591
18	290	358
19	117	87
20	221	263
21	435	478
22	166	120
23	87	143
24	180	141

0,3,L

-24	192	218
-23	198	227

-22	205	207
-21	64*	63
-20	524	506
-19	237	256
-18	228	146
-17	282	278
-16	448	534
-15	571	589
-14	926	881
-13	1248	1147
-12	1598	1503
-11	183	139
-10	536	593
-9	1349	1227
-8	247	169
-7	49*	162
-6	1849	1989
-5	61	49
-4	671	554
-3	1126	1160
-2	788	814
-1	847	928
0	688	700
1	1311	1298
2	1530	1496
3	515	606
4	916	970
5	253	150
6	444	368
7	474	565
8	1503	1386
9	579	568
10	981	966
11	382	452
12	518	514
13	861	894
14	183	211
15	66*	68
16	335	301
17	84	77
18	343	370
19	209	189
20	76	57
21	170	172
22	75	34
23	290	242
24	209	183

0,4,L

-23	62*	45
-22	62*	73
-21	230	266
-20	64*	24
-19	254	259
-18	130	141
-17	62*	60
-16	524	544
-15	64*	44
-14	67*	137

-13	700	713
-12	191	273
-11	309	218
-10	976	1026
-9	456	442
-8	449	463
-7	892	865
-6	63	85
-5	1487	1514
-4	1434	1420
-3	193	237
-2	507	560
-1	1427	1453
0	982	994
1	167	140
2	842	785
3	723	658
4	474	499
5	142	122
6	146	193
7	958	939
8	61	80
9	447	482
10	93	40
11	1239	1265
12	628	627
13	108	83
14	1053	1068
15	212	223
16	64*	72
17	649	657
18	230	297
19	305	301
20	315	330
21	267	288
22	171	207
23	66*	68

0,5,L

-21	65*	73
-20	158	162
-19	99	58
-18	76	14
-17	117	152
-16	64*	15
-15	74	35
-14	299	341
-13	64*	22
-12	143	151
-11	786	760
-10	204	140
-9	72	41
-8	198	196
-7	831	729
-6	201	255
-5	1228	1190
-4	532	548
-3	57	28
-2	480	537

-1	136	187
0	130	98
1	189	166
2	555	518
3	823	719
4	236	210
5	531	502
6	397	318
7	64	49
8	87	94
9	59*	45
10	644	669
11	257	308
12	191	208
13	115	99
14	327	301
15	232	266
16	295	250
17	69*	34
18	122	159
19	265	246
20	195	152
21	96	155

0,6,L

-20	78	103
-19	72*	68
-18	94	106
-17	158	194
-16	66*	51
-15	75	71
-14	74*	95
-13	66*	54
-12	208	252
-11	570	610
-10	447	412
-9	171	183
-8	87	90
-7	93	56
-6	545	558
-5	92	84
-4	170	156
-3	297	272
-2	596	638
-1	489	542
0	341	354
1	468	494
2	278	206
3	483	451
4	535	581
5	654	577
6	67*	102
7	408	364
8	173	159
9	155	158
10	492	419
11	656	621
12	257	188

0,6,L

13	70*	70
14	204	219
15	365	293
16	188	145
17	104	97
18	224	214
19	139	158
20	69*	3

0,7,L

-17	76*	48
-16	172	104
-15	233	214
-14	128	95
-13	141	167
-12	114	63
-11	66*	51
-10	352	344
-9	177	148
-8	383	383
-7	68*	31
-6	447	495
-5	344	241
-4	195	180
-3	665	734
-2	407	395
-1	266	285
0	646	665
1	86	82
2	329	298
3	649	624
4	290	281
5	244	190
6	695	613
7	199	129
8	243	202
9	146	101
10	272	198
11	174	173
12	95	34
13	111	140
14	104	118
15	85	85
16	73*	7
17	71*	5

0,8,L

-14	72*	41
-13	223	236
-12	235	181
-11	73*	31
-10	159	193
-9	262	257
-8	115	91
-7	296	287
-6	141	99

-5	132	162
-4	430	458
-3	414	360
-2	136	95
-1	241	209
0	114	141
1	67	49
2	337	293
3	188	168
4	76	49
5	416	395
6	67*	79
7	97	137
8	178	92
9	99	120
10	110	62
11	108	26
12	75*	71
13	572	558
14	182	195

0,9,L

-10	328	350
-9	139	108
-8	74*	136
-7	339	352
-6	77	79
-5	73*	156
-4	174	218
-3	67*	59
-2	263	268
-1	66*	19
0	184	235
1	266	263
2	105	53
3	174	212
4	97	111
5	64*	91
6	239	183
7	86	29
8	69*	45
9	270	294
10	71*	7

1,1,L

0	1630	1815
1	369	230
2	974	1066
3	1644	1740
4	505	571
5	1277	1221
6	1484	1326
7	1420	1304
8	1766	1706
9	663	543
10	210	217
11	1066	1027
12	240	266

13	422	431
14	787	776
15	183	163
16	272	259
17	834	818
18	60*	25
19	283	271
20	299	320
21	227	245
22	90	157
23	275	295
24	257	237

1,2,L

-24	92	115
-23	144	163
-22	150	120
-21	144	147
-20	291	355
-19	195	196
-18	186	199
-17	361	436
-16	214	190
-15	283	300
-14	531	588
-13	488	465
-12	713	659
-11	495	484
-10	450	452
-9	696	675
-8	1083	996
-7	1009	960
-6	911	866
-5	1128	1045
-4	1119	1099
-3	666	586
-2	784	816
-1	1471	1310
0	1025	821
1	1245	1220
2	292	211
3	2060	1983
4	990	1086
5	737	669
6	1447	1562
7	1012	1055
8	259	272
9	956	942
10	521	648
11	363	346
12	923	875
13	947	687
14	327	340
15	524	541
16	408	438
17	262	248
18	318	328
19	137	125
20	144	151

21	213	214
22	252	216
23	141	135
24	90	59

1,3,L

-23	67*	27
-22	107	130
-21	233	234
-20	101	130
-19	281	257
-18	206	218
-17	269	280
-16	555	523
-15	298	306
-14	539	570
-13	873	836
-12	183	223
-11	296	322
-10	848	740
-9	441	465
-8	579	591
-7	854	803
-6	112	171
-5	1312	1343
-4	1002	1054
-3	620	559
-2	1618	1606
-1	690	755
0	728	782
1	1158	1116
2	1514	1459
3	1332	1404
4	654	604
5	1021	997
6	1275	1203
7	482	440
8	967	979
9	684	682
10	96	112
11	661	706
12	647	599
13	62*	98
14	363	369
15	255	253
16	284	251
17	412	406
18	65	56
19	261	313
20	186	192
21	215	221
22	144	151
23	215	204

1,4,L

-22	123	126
-21	76	31
-20	136	165

-19	273	229
-18	106	96
-17	149	72
-16	124	113
-15	495	437
-14	159	184
-13	484	458
-12	599	582
-11	441	400
-10	797	742
-9	1238	1288
-8	272	262
-7	157	163
-6	1195	1167
-5	750	788
-4	542	596
-3	517	486
-2	473	531
-1	694	730
0	424	405
1	137	66
2	607	617
3	629	511
4	374	391
5	1022	992
6	187	198
7	579	615
8	268	275
9	249	251
10	131	75
11	714	680
12	507	480
13	417	368
14	221	237
15	686	649
16	146	127
17	76	70
18	450	491
19	159	187
20	247	274
21	378	366
22	140	122

1,5,L

-20	95	103
-19	137	171
-18	323	300
-17	164	114
-16	581	553
-15	97	65
-14	398	394
-13	552	524
-12	331	325
-11	314	263
-10	995	930
-9	354	291
-8	452	471
-7	919	929

1,5,L

-6	304	308
-5	493	475
-4	736	737
-3	269	250
-2	551	566
-1	825	804
0	400	451
1	588	610
2	449	483
3	455	422
4	713	679
5	339	282
6	453	438
7	663	667
8	705	615
9	330	330
10	613	601
11	572	581
12	302	283
13	89	122
14	375	346
15	182	150
16	272	263
17	357	364
18	101	120
19	232	253
20	220	196

1,6,L

-18	266	296
-17	152	133
-16	74*	53
-15	285	284
-14	70*	77
-13	278	270
-12	167	183
-11	227	258
-10	288	330
-9	212	279
-8	107	123
-7	400	410
-6	391	354
-5	308	300
-4	447	531
-3	454	525
-2	267	287
-1	541	592
0	466	470
1	151	168
2	563	595
3	625	586
4	347	369
5	666	625
6	691	693
7	156	128
8	643	647
9	247	222

10	276	230
11	422	377
12	235	224
13	70*	58
14	166	151
15	294	288
16	212	206
17	182	206
18	90	129

1,7,L

-16	109	118
-15	244	254
-14	77	83
-13	328	333
-12	381	377
-11	157	134
-10	408	427
-9	463	478
-8	329	335
-7	331	316
-6	85	81
-5	426	445
-4	212	195
-3	168	144
-2	523	553
-1	405	392
0	109	87
1	602	600
2	325	346
3	78	80
4	515	501
5	264	217
6	367	368
7	454	404
8	121	137
9	332	360
10	192	154
11	99	81
12	2,2	262
13	351	368
14	99	140
15	75*	31
16	105	119

1,8,L

-12	160	148
-11	217	195
-10	218	193
-9	157	226
-8	166	155
-7	218	166
-6	147	204
-5	386	414
-4	208	248
-3	129	133
-2	112	89
-1	64*	30

0	85	121
1	80	54
2	229	294
3	132	123
4	72	86
5	206	245
6	144	130
7	177	192
8	147	154
9	215	187
10	203	191
11	179	107
12	87	65

1,9,L

-6	216	226
-5	64*	36
-4	126	127
-3	64*	109
-2	101	160
-1	156	169
0	183	168
1	162	193
2	128	187
3	143	130
4	116	96
5	71	63
6	180	192

2,2,L

0	957	997
1	1936	1940
2	1330	1347
3	1320	1258
4	731	729
5	1417	1420
6	1069	1072
7	582	640
8	840	854
9	704	714
10	659	596
11	330	362
12	178	171
13	236	225
14	111	126
15	115	93
16	268	296
17	312	342
18	209	188
19	121	159
20	288	270
21	67*	55
22	155	145
23	213	181

2,3,L

-22	236	242

-21	230	192
-20	225	196
-19	205	222
-18	152	169
-17	154	94
-16	127	93
-15	164	143
-14	112	123
-13	309	291
-12	125	113
-11	258	204
-10	827	788
-9	357	375
-8	528	580
-7	424	463
-6	178	255
-5	598	670
-4	187	194
-3	544	616
-2	498	534
-1	301	239
0	946	1028
1	964	942
2	1169	1138
3	921	899
4	944	958
5	1063	993
6	621	561
7	398	421
8	448	417
9	521	495
10	697	638
11	263	282
12	235	206
13	284	254
14	246	260
15	125	155
16	172	103
17	68*	80
18	158	157
19	278	284
20	301	328
21	229	182
22	113	147

2,4,L

-21	223	246
-20	149	130
-19	73*	87
-18	293	244
-17	225	201
-16	258	227
-15	427	411
-14	70*	75
-13	131	166
-12	323	335
-11	254	222
-10	201	154
-9	270	287

-8	454	476
-7	197	226
-6	253	267
-5	841	830
-4	396	395
-3	521	520
-2	837	758
-1	470	484
0	379	406
1	989	984
2	570	524
3	698	655
4	182	175
5	506	491
6	268	296
7	664	719
8	946	867
9	378	362
10	139	161
11	213	198
12	427	414
13	189	160
14	317	258
15	282	274
16	266	330
17	376	351
18	321	293
19	251	251
20	249	258
21	72*	2

2,5,L

-19	295	300
-18	193	195
-17	175	186
-16	223	209
-15	265	275
-14	421	415
-13	330	324
-12	285	285
-11	165	162
-10	441	420
-9	270	283
-8	208	214
-7	323	298
-6	194	167
-5	76	98
-4	235	172
-3	126	179
-2	285	298
-1	70	59
0	263	250
1	972	995
2	229	236
3	132	178
4	613	609
5	429	417
6	262	264

2,5,L

7	358	358
8	337	353
9	123	91
10	174	214
11	523	516
12	240	268
13	253	253
14	343	330
15	351	340
16	121	143
17	73*	22
18	78*	68
19	224	226

2,6,L

-17	126	132
-16	179	163
-15	176	162
-14	76*	45
-13	114	107
-12	203	219
-11	256	229
-10	265	245
-9	174	126
-8	97	49
-7	285	318
-6	414	446
-5	242	201
-4	275	247
-3	488	493
-2	523	557
-1	267	248
0	321	305
1	478	495
2	190	144
3	241	295
4	377	406
5	175	135
6	261	286
7	389	362
8	414	383
9	227	279
10	441	398
11	256	244
12	264	261
13	465	467
14	187	214
15	99	114
16	345	333
17	75*	60

2,7,L

-14	143	136
-13	118	148
-12	137	142
-11	257	315

-10	264	232
-9	143	84
-8	217	227
-7	176	134
-6	361	353
-5	129	41
-4	239	286
-3	213	195
-2	371	367
-1	142	149
0	138	143
1	287	252
2	215	224
3	185	171
4	180	95
5	196	254
6	78	43
7	85	93
8	116	135
9	68*	91
10	138	146
11	237	266
12	238	289
13	289	298
14	157	136

2,8,L

-9	192	211
-8	69*	71
-7	242	259
-6	234	218
-5	197	250
-4	248	246
-3	157	100
-2	68*	73
-1	236	209
0	211	175
1	84	125
2	122	88
3	104	57
4	147	167
5	133	100
6	162	207
7	241	262
8	159	179
9	166	178

3,3,L

0	208	205
1	570	612
2	666	737
3	123	138
4	636	698
5	316	334
6	627	562
7	763	736
8	956	903
9	537	492

10	382	422
11	582	548
12	145	85
13	345	302
14	329	322
15	156	179
16	353	316
17	182	183
18	201	166
19	94	85
20	70*	3
21	145	157

3,4,L

-19	71*	24
-18	309	344
-17	456	442
-16	99	84
-15	309	300
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-8	186	84
-7	425	388
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-4	305	289
-3	239	194
-2	314	356
-1	366	381
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2	521	484
3	73	43
4	977	1053
5	220	186
6	488	515
7	756	733
8	423	385
9	475	483
10	504	455
11	244	233
12	425	418
13	388	340
14	132	149
15	201	179
16	212	197
17	198	178
18	234	183
19	147	130

3,5,L

-17	100	63
-16	72*	42
-15	279	259

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-9	425	439
-8	314	317
-7	204	245
-6	247	228
-5	348	314
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-1	68	94
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1	790	764
2	107	140
3	199	192
4	532	466
5	274	356
6	564	528
7	418	396
8	254	226
9	698	663
10	201	176
11	226	245
12	339	350
13	159	164
14	379	388
15	295	295
16	235	260
17	119	128

3,6,L

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-12	187	186
-11	215	237
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-7	218	198
-6	238	239
-5	70*	49
-4	162	139
-3	432	462
-2	242	273
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1	206	209
2	149	158
3	381	377
4	91	79
5	215	238
6	145	118
7	68*	104
8	189	209
9	236	234
10	67*	61

11	111	54
12	79	80
13	73*	77
14	68*	33

3,7,L

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1	213	197
2	164	121
3	256	234
4	154	130
5	159	105
6	198	146
7	136	90
8	75*	138
9	113	71
10	78	152

3,8,L

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1	163	189

4,4,L

0	766	715
1	487	454
2	107	94
3	571	567
4	136	113
5	442	448
6	221	231
7	248	308
8	366	421
9	179	97
10	247	308
11	239	225
12	68*	48
13	271	279
14	309	295
15	132	83
16	258	270
17	227	195

4,5,L

-15	67*	42

	4,5,L		5	320	332	-3	341	384	-2	226	280	10	252	249
			6	163	161	-2	349	340	-1	207	228	11	136	174
-14	75*	104	7	223	222	-1	68*	39	0	172	217	12	216	262
-13	105	80	8	304	313	0	107	125	1	82	65			
-12	99	146	9	89	104	1	206	174	2	177	156		5,6,L	
-11	72*	120	10	70*	54	2	135	146	3	175	242			
-10	383	385	11	302	254	3	84	65	4	248	200	-6	166	176
-9	117	106	12	71*	74	4	400	465	5	173	156	-5	145	196
-8	95	129	13	70*	45	5	147	161				-4	252	272
-7	541	582	14	69	130	6	67*	7		5,5,L		-3	81	185
-6	164	192				7	102	40				-2	148	206
-5	226	207		4,6,L		8	233	205	0	449	420	-1	248	292
-4	533	520				9	108	76	1	109	116	0	201	196
-3	209	198	-11	202	182	10	71*	126	2	221	250	1	162	198
-2	253	250	-10	275	265	11	139	132	3	542	571	2	155	145
-1	456	416	-9	124	109				4	180	143	3	305	326
0	66*	65	-8	315	297		4,7,L		5	72*	39	.4	72*	28
1	457	451	-7	158	207				6	265	226	5	77*	105
2	472	468	-6	381	435	-5	82	101	7	249	262	6	148	90
3	207	241	-5	326	376	-4	193	205	8	137	181			
4	333	259	-4	73*	49	-3	70*	20	9	205	223			

APPENDIX II

Tables of observed and calculated structure factors for tri-*o*-thymotide - ethanol

Data Format:

	H	K
L	$10\times\|F_o\|$	$10\times\|F_c\|$

Reflections removed for extinction marked .... E

Reflections classed as unobserved marked ..... *

	0,0,L		7	551	235	-9	748	750	-25	61	53	35	92	89
			8	496	446	-8	933	844	-24	152	146	36	12*	21
3	1746	1553	9	45	24	-7	436	576	-23	189	199			
6	713	416	10	218	112	-6	1121	1130	-22	49	41		4,0,L	
9	1302	1200	11	146	147	-5	1135	1266	-21	53	57			
12	243	253	12	93	122	-4	85	217	-20	188	193	-35	32	31
15	115	132	13	220	164	-3	956	998	-19	361	375	-34	34	45
18	406	377	14	162	141	-2	714	592	-18	111	94	-33	14*	8
21	244	246	15	41	45	-1	830	518	-17	218	212	-32	99	86
24	303	273	16	623	621	0	579	628	-16	28	47	-31	21	29
27	608	586	17	181	183	1	134	25	-15	254	266	-30	21	24
30	211	221	18	45	41	2	498	804	-14	304	253	-29	51	41
33	50	66	19	504	481	3	779	846	-13	141	114	-28	15*	19
36	178	197	20	51	55	4	356	337	-12	134	119	-27	16*	23
			21	39	31	5	135	143	-11	392	380	-26	141	131
	1,0,L		22	134	122	6	631	693	-10	19	59	-25	28	28
			23	17*	13	7	1056	1127	-9	300	260	-24	176	180
-36	16	9	24	576	567	8	618	439	-8	572	589	-23	202	206
-35	14*	1	25	152	137	9	162	106	-7	735	832	-22	370	368
-34	15*	10	26	18*	5	10	565	627	-6	419	357	-21	337	339
-33	142	142	27	288	301	11	322	343	-5	1177	1142	-20	73	74
-32	128	133	28	173	178	12	337	297	-4	352	447	-19	262	255
-31	171	161	29	146	137	13	34	66	-3	360	477	-18	114	111
-30	33	14	30	103	71	14	445	424	-2	722	753	-17	45	33
-29	45	46	31	44	51	15	488	468	-1	642	570	-16	25	24
-28	24	11	32	17	18	16	52	96	0	1078	986	-15	62	47
-27	20	9	33	73	57	17	64	60	1	249	286	-14	395	362
-26	121	107	34	43	49	18	45	53	2	418	378	-13	77	47
-25	103	111	35	97	89	19	14*	48	3	443	533	-12	418	358
-24	166	183	36	43	39	20	410	375	4	215	228	-11	815	771
-23	16*	34				21	34	39	5	62	45	-10	263	192
-22	146	165		2,0,L		22	103	102	6	1285	1351	-9	65	22
-21	53	42				23	88	71	7	107	144	-8	139	157
-20	40	25	-36	46	47	24	233	222	8	578	612	-7	440	446
-19	356	308	-35	99	96	25	128	127	9	635	654	-6	276	327
-18	265	263	-34	59	60	26	347	335	10	266	207	-5	389	323
-17	467	492	-33	148	152	27	213	209	11	563	573	-4	64	99
-16	101	100	-32	53	52	28	37	27	12	1108	1120	-3	210	190
-15	421	416	-31	76	70	29	56	64	13	795	782	-2	97	105
-14	422	371	-30	37	28	30	178	174	14	486	444	-1	326	251
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-11	389	502	-27	339	335	33	83	68	17	118	148	2	110	122
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-8	143	172	-24	193	202	36	25	35	20	245	242	5	1055	1077
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-6	203	274	-22	41	43		3,0,L		22	78	88	7	238	207
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6	80	72	-10	120	227	-26	104	121	34	14*	17			
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			5	108	125	-6	107	69	-15	49	45	-20	18	19
19	72	71	6	142	161	-5	359	235	-14	64	51	-19	90	84
20	122	134	7	607	591	-4	169	172	-13	172	187	-18	20	19
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22	25	17	9	171	166	-2	50	30	-11	227	222	-16	46	50
23	16*	14	10	167	121	-1	245	265	-10	148	135	-15	249	258
24	19	29	11	70	50	0	85	67	-9	243	217	-14	137	135
25	74	59	12	92	91	1	210	191	-8	276	261	-13	444	447
26	63	76	13	30	39	2	24	39	-7	137	161	-12	54	54
27	66	63	14	160	142	3	252	251	-6	168	139	-11	35	36
28	213	201	15	58	28	4	86	75	-5	213	203	-10	164	168
29	27	33	16	166	166	5	428	430	-4	137	125	-9	44	36
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32	68	60	19	70	81	8	49	63	-1	482	465	-6	59	49
33	91	86	20	96	103	9	328	320	0	91	65	-5	86	99
34	152	154	21	51	67	10	406	408	1	199	207	-4	250	247
35	30	33	22	154	149	11	667	651	2	47	45	-3	55	58
			23	28	21	12	163	152	3	91	70	-2	34	38
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9,0,L

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6	189	183
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9	22	34
10	216	221
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12	40	38
13	57	50
14	283	275
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16	152	153
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2,1,L

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-19	142	121
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9	44	28
10	475	445
11	117	127
12	532	555
13	357	335
14	376	364
15	236	215
16	141	153
17	107	123
18	207	204
19	123	109
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15	116	112
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21	29	28
22	19	16
23	50	57
24	93	90
25	31	39
26	12*	24

11,0,L

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25	218	218
26	64	78
27	100	97
28	169	163
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30	27	16
31	105	109
32	35	35
33	19	15
34	107	101
35	13	13
36	14	16

3,1,L

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-16	226	239
-15	122	108
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-13	291	283
-12	319	307
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-10	235	251
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6	367	404

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3	91	92
4	102	106
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6	25	33
7	37	38
8	261	268
9	23	7
10	27	22
11	34	36
12	40	38
13	20	21
14	40	31
15	63	56
16	45	41
17	37	42
18	87	98
19	66	69
20	53	62
21	109	112
22	59	57
23	18	14

12,0,L

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11	467	418
12	139	113
13	654	598
14	363	355
15	255	260
16	287	289
17	186	184
18	55	43
19	174	166
20	56	67
21	110	106
22	124	128
23	54	57
24	173	167
25	112	107
26	207	202
27	255	254
28	116	110
29	65	75
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4,1,L

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-25	185	181
-24	209	201
-23	98	99
-22	230	229
-21	128	133
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-19	188	186
-18	211	199
-17	116	102
-16	190	169
-15	364	339
-14	222	235
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-12	186	179
-11	525	511
-10	344	356
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6	16*	11
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9	48	51
10	102	93
11	68	67
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14	27	29
15	77	73
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13,0,L

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5	75	77
6	14*	21
7	36	22
8	80	81
9	17	8
10	29	34
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3	554	558
4	341	333
5	573	571
6	324	282
7	463	466
8	170	165
9	566	538
10	705	669
11	382	382
12	197	190
13	291	258
14	222	228
15	119	118
16	224	230
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18	109	110
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21	94	81
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23	86	89
24	145	136
25	188	178
26	144	153
27	71	65
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5,1,L

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-24	31	35
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14,0,L

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1,1,L

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6	678	429
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11	545	517
12	152	72
13	489	494
14	380	361
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16	320	311
17	453	405
18	103	92
19	108	111
20	164	151
21	176	157
22	218	217
23	207	202
24	318	310
25	107	114
26	197	194
27	239	242
28	80	76
29	31	31
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-14	151	147
-13	219	232
-12	89	97
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-9	237	224
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4	77	57
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6	304	301
7	426	407
8	372	333
9	383	380
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11	90	73
12	399	370
13	137	136
14	419	400
15	64	54
16	329	335
17	119	128
18	158	138
19	49	56
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22	75	67
23	68	70
24	138	133
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26	131	130
27	109	98
28	87	87
29	89	80
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6,1,L

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6,1,L

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-23	86	81
-22	113	127
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-19	259	255
-18	238	240
-17	151	152
-16	144	145
-15	245	263
-14	52	49
-13	188	174
-12	119	118
-11	168	160
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-9	120	127
-8	342	321
-7	111	115
-6	326	307
-5	40	36
-4	423	422
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-1	200	158
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3	182	180
4	181	173
5	137	146
6	111	133
7	286	293
8	234	232
9	46	52
10	241	220
11	208	211
12	104	93
13	241	236
14	75	90
15	133	127
16	257	234
17	220	227
18	135	147
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21	98	90
22	53	58
23	69	83
24	110	110
25	145	144
26	115	110

10,1,L

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11,1,L

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12,1,L

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7,1,L

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3	70	61
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5	141	131
6	209	199
7	101	101
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9	369	350
10	214	211
11	91	72
12	291	279
13	254	249
14	77	73
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9	53	50
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11	99	106
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13,1,L

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26	44	54
27	17	22
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8,1,L

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9	129	124
10	85	85
11	92	84
12	153	152
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15	131	132

2,2,L

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3	921	930
4	206	228
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6	755	803
7	270	311
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9	345	372
10	369	367
11	177	188
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13	230	237
14	127	145
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17	71	145
18	147	134
19	109	128
20	134	142
21	125	120
22	81	78
23	156	164
24	188	200
25	319	307
26	200	194
27	92	96
28	58	57
29	97	77
30	126	119
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35	76	70

3,2,L

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-23	83	92
-22	119	124
-21	237	233
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19	186	189
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28	16	11
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9,1,L

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5	25	15
6	209	203
7	148	157
8	47	49
9	301	301
10	246	238
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12	145	158
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15	85	79

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5	60	43
6	373	351
7	410	392
8	267	252
9	207	184
10	414	395
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12	157	164
13	105	129
14	74	56
15	148	152
16	213	195
17	221	208
18	127	137
19	199	183
20	53	53
21	101	115
22	203	202
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24	116	106
25	75	73
26	128	128
27	140	141
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30	180	180
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4,2,L

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22	48	51
23	31	36
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27	48	46

10,1,L

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-9	19	17
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3	110	111
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9	446	429
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14	257	254
15	115	94
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17	126	135
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24	76	74
25	83	82
26	57	58
27	158	164
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29	59	53

4,2,L

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5,2,L

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-13	140	138
-12	113	119
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-10	215	211
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3	140	132
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7	213	212
8	170	152
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10	235	222
11	176	174
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16	183	197

9,2,L

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10,2,L

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6	46	50
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11,2,L

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12	61	58
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17	50	47
18	40	38
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12	53	51
13	137	135
14	235	221
15	208	189
16	177	176
17	212	214
18	126	128
19	243	243
20	143	154
21	52	55
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25	33	38
26	130	133
27	38	45
28	63	59
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7,2,L

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-15	221	217
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12,2,L

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7	14*	8
8	89	88
9	47	46
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13,2,L

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3,3,L

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3	460	474
4	222	205
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6	535	542
7	459	435
8	443	407
9	381	370
10	133	139
11	164	156
12	69	58
13	221	185
14	145	133
15	174	153
16	47	50
17	211	198
18	130	121
19	306	296
20	139	134
21	107	106
22	73	79
23	246	252
24	193	198
25	99	104
26	73	70
27	66	63
28	152	149
29	93	96
30	61	61
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4,3,L

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-28	89	85
-27	29	27
-26	133	118
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-22	128	126
-21	266	269
-20	123	138
-19	133	134
-18	110	96
-17	287	275
-16	190	184
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-14	192	181
-13	24	26
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-11	156	168
-10	34	23
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3	165	178
4	263	228
5	422	404
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7	471	439
8	142	145
9	310	314
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12	76	69
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14	77	60
15	62	70
16	89	84
17	228	229
18	189	184
19	73	79
20	36	43
21	110	102
22	199	200
23	180	184
24	228	232
25	36	34
26	21	20
27	111	116
28	116	122
29	15*	11
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33	77	79

5,3,L

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-21	38	36
-20	230	226
-19	121	110
-18	125	122
-17	68	69
-16	176	183
-15	209	203
-14	258	263
-13	158	146
-12	66	70
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8,2,L

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-20	33	34
-19	117	130
-18	138	144
-17	42	40
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-9	77	64
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9,2,L

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-17	46	32
-16	82	86
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-14	79	86
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-9	114	119
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-7	170	174
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5,3,L

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9	179	155
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11	77	75
12	65	50
13	73	73
14	30	43
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16	90	92
17	125	126
18	54	46
19	162	161
20	141	125
21	93	96
22	118	117
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25	16*	22
26	130	123
27	74	79
28	85	76
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6,3,L

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-23	17	18
-22	93	93
-21	66	61
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-19	60	56
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10,3,L

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4	89	95
5	89	87
6	26	31
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8	76	78
9	81	74
10	89	82
11	47	43
12	35	34
13	104	111
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15	59	58
16	64	58
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18	61	63
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11,3,L

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-10	46	46
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3	24	27
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8	41	38
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11	36	37
12	39	36
13	59	50
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16	42	50

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-11	144	138
-10	176	163
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-7	186	173
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2	244	234
3	220	232
4	276	265
5	199	202
6	227	225
7	76	70
8	131	124
9	302	279
10	288	283
11	76	71
12	201	191
13	176	163
14	139	124
15	65	66
16	154	156
17	111	117
18	71	71
19	169	176
20	129	130
21	112	95
22	16*	11
23	63	56
24	99	95
25	77	82
26	56	51
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28	86	89
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7,3,L

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-20	112	110
-19	97	82

12,3,L

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6	25	26
7	39	32
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4,4,L

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6	236	217
7	197	190
8	42	40
9	194	178
10	72	56
11	218	210
12	33	26
13	112	101
14	105	105
15	212	200
16	144	143
17	131	138
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19	43	44
20	115	106
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22	70	68
23	115	105
24	154	151
25	71	66
26	65	61
27	145	146
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6	293	306
7	144	136
8	60	59
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25	40	45
26	62	59
27	13*	13
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8,3,L

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5,4,L

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-19	101	93
-18	93	101
-17	130	139
-16	222	203
-15	101	102
-14	97	81
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6	38	30
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10	249	244
11	86	84
12	223	216
13	125	127
14	127	135
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23	150	148
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27	42	48

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9,3,L

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6,4,L

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8	69	72
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10	176	171
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12	206	205
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7,4,L

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3	231	223
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7	106	105
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7,4,L

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10,3,L

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7,4,L

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8,4,L

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-13	63	60
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9,4,L

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19	79	86
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25	27	24

8,5,L

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6	156	153
7	228	232
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9	118	126
10	109	125
11	87	80
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10,4,L

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9,5,L

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3	99	90
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9	109	101
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16	48	46
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18	32	34

10,5,L

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5	41	40
6	21	21
7	36	38
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9	86	87
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12	14*	18
13	39	41
14	48	54
15	32	27
16	68	70
17	37	40

11,4,L

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3	37	38
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5	30	38
6	71	65
7	82	88
8	25	25
9	18	19
10	74	71
11	27	36
12	40	36

5,5,L

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2	173	174
3	163	171
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5	143	137
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7	149	133

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4	64	61
5	24	21
6	45	39
7	57	55
8	81	84
9	74	64
10	13*	4
11	82	89
12	35	35
13	26	25

11,5,L

-4	55	60
-3	116	110
-2	12*	3
-1	14	15
0	64	58
1	46	45
2	51	56
3	41	42
4	67	71

6,6,L

0	182	178
1	126	119
2	159	163
3	39	36
4	64	60
5	18	33
6	83	79
7	53	61
8	193	195
9	131	141
10	91	97
11	200	195
12	221	216
13	17*	21
14	65	60
15	61	59
16	109	92
17	156	165
18	100	102
19	80	78
20	37	39
21	42	43
22	40	38
23	32	17
24	24	16
25	12	10

7,6,L

-22	56	53

8	104	109
9	153	142
10	186	186
11	238	239
12	251	245
13	174	177
14	356	346
15	61	64
16	181	189
17	38	46
18	122	121
19	156	148
20	40	56
21	96	99
22	46	48
23	73	74
24	42	48
25	85	72
26	27	23
27	48	48
28	22	27
29	17	27

6,5,L

-27	62	66
-26	29	33
-25	53	53
-24	44	47
-23	72	72
-22	57	62
-21	16*	11
-20	43	42
-19	122	112
-18	64	66
-17	146	144
-16	92	89
-15	194	193
-14	116	104
-13	93	95
-12	78	78
-11	221	222
-10	198	212
-9	131	129
-8	177	179
-7	135	127
-6	124	120
-5	179	170
-4	16*	12
-3	154	164
-2	81	77
-1	110	109
0	247	247
1	102	96
2	221	210
3	114	115
4	149	156
5	171	173
6	126	124
7	48	45

-21	17	13
-20	30	24
-19	45	38
-18	39	32
-17	28	33
-16	15*	8
-15	17	11
-14	69	66
-13	57	57
-12	39	42
-11	67	65
-10	153	163
-9	48	45
-8	30	26
-7	72	71
-6	157	148
-5	109	107
-4	57	60
-3	67	58
-2	74	72
-1	23	25
0	149	142
1	22	18
2	85	72
3	141	130
4	54	50
5	151	143
6	97	89
7	192	196
8	113	104
9	136	138
10	62	64
11	76	71
12	33	28
13	29	19
14	86	79
15	55	60
16	75	71
17	53	55
18	49	54
19	32	34
20	13*	18
21	41	44
22	12*	12

8,6,L

-19	12*	15
-18	51	52
-17	51	61
-16	23	20
-15	23	22
-14	20	21
-13	30	28
-12	32	30
-11	15	16
-10	17	27
-9	76	70
-8	52	58
-7	42	39

8	69	72
9	118	113
10	250	255
11	237	231
12	164	156
13	217	216
14	82	88
15	207	202
16	91	96
17	93	96
18	65	58
19	110	113
20	38	31
21	109	104
22	38	38
23	14*	9
24	69	64
25	14*	14
26	41	40
27	38	39

7,5,L

-25	34	42
-24	39	36
-23	37	43
-22	57	61
-21	71	76
-20	61	63
-19	20	20
-18	48	50
-17	137	143
-16	122	113
-15	73	81
-14	127	136
-13	25	21
-12	114	124
-11	140	144
-10	136	145
-9	94	88
-8	44	34
-7	79	74
-6	63	64
-5	133	141
-4	128	124
-3	140	137
-2	135	130
-1	79	79
0	170	174
1	74	72
2	180	176
3	135	136
4	158	150
5	106	111
6	57	42
7	276	277
8	159	153
9	164	161
10	69	74

-6	25	24
-5	68	63
-4	86	85
-3	56	54
-2	38	48
-1	75	69
0	85	88
1	57	58
2	56	51
3	123	129
4	55	63
5	92	96
6	66	63
7	86	96
8	65	63
9	98	101
10	60	59
11	98	94
12	22	25
13	45	45
14	62	62
15	15	18
16	13*	21
17	21	20
18	66	66
19	21	19

9,6,L

-14	35	34
-13	29	24
-12	49	50
-11	13*	4
-10	32	39
-9	42	40
-8	62	70
-7	46	41
-6	52	59
-5	94	96
-4	38	42
-3	55	65
-2	28	25
-1	34	32
0	43	42
1	48	45
2	73	70
3	15*	19
4	39	49
5	25	26
6	73	75
7	89	85
8	22	19
9	62	62
10	18	19
11	35	32
12	19	25
13	34	36
14	57	58

10,6,L

-7	12*	8
-6	57	69
-5	70	77
-4	35	30
-3	31	35
-2	51	55
-1	37	39
0	15	18
1	72	70
2	29	33
3	20	28
4	32	31
5	18	13
6	88	92
7	64	71

7,7,L

0	159	165
1	35	34

2	92	97
3	105	100
4	28	24
5	76	77
6	51	50
7	55	60
8	15*	12
9	103	97
10	84	91
11	83	80
12	30	29
13	14*	14
14	37	39
15	45	45
16	37	39
17	45	45
18	38	33
19	17	15

8,7,L

-15	12*	18

-14	34	34
-13	53	50
-12	13*	10
-11	59	63
-10	48	52
-9	15	26
-8	63	59
-7	37	40
-6	39	40
-5	54	59
-4	31	27
-3	37	36
-2	24	35
-1	49	53
0	85	80
1	15*	10
2	35	32
3	48	44
4	42	42
5	26	28
6	39	46
7	51	47

8	58	58
9	53	50
10	29	27
11	13*	14
12	50	44
13	63	67
14	12*	12
15	55	58

9,7,L

-8	30	28
-7	42	50
-6	21	29
-5	12*	2
-4	28	27
-3	69	68
-2	21	18
-1	46	47
0	18	12
1	16	11
2	63	62

3	37	39
4	62	57
5	19	25
6	16	23
7	33	37
8	23	14

8,8,L

0	60	62
1	73	62
2	62	55
3	18	21
4	52	50
5	46	39
6	59	58
7	28	29
8	31	36
9	34	36

APPENDIX III

Tables of observed and calculated structure factors for tri-*o*-thymotide - *n*-cetyl alcohol

Data Format:

	H	K
L	$10\times\lvert F_o\rvert$	$10\times\lvert F_c\rvert$

Reflections removed for extinction marked .... E

Reflections classed as unobserved marked ..... *

0,0,L

6	2171E	2533
12	410	383
18	202	223
24	172	172
30	32	31

1,0,L

1	817	615
2	1331	1358
3	1414	1474
4	948	939
5	307	281
6	253	231
7	613	636
8	199	209
9	1091	1094
10	174	188
11	282	277
12	177	188
13	791	785
14	456	442
15	81	81
16	360	345
17	219	225
18	176	182
19	179	170
20	228	220
21	164	168
22	193	199
23	58	63
24	77	81
25	132	132
26	58	59
27	22*	40
28	73	69
29	54	51
30	28	32
31	24	23
32	36	40
33	17*	12
34	27	20
35	15*	2
0	1194E	2985

1,1,L

0	23E	1298
1	689	989
2	357	319
3	1528	1601
4	183	174
5	375	390
6	779	773
7	277	282
8	457	439
9	499	490
10	395	374

1,7,L

27	36	44
28	39	38
29	50	48
30	38	40

1,8,L

0	48	35
1	85	90
2	147	134
3	43	44
4	70	67
5	259	258
6	31	39
7	72	69
8	45	35
9	84	87
10	101	116
11	126	113
12	142	141
13	74	75
14	21*	7
15	124	119
16	69	71
17	57	59
18	105	112
19	51	47
20	132	138
21	74	74
22	69	76
23	30	23
24	50	56
25	49	52
26	55	52
27	18*	14
28	64	70
29	22	21

1,9,L

0	75	62
1	54	56
2	167	160
3	93	114
4	184	193
5	239	237
6	120	135
7	136	152
8	137	132
9	191	196
10	68	73
11	67	61
12	172	175
13	78	74
14	113	102
15	87	90
16	164	165
17	95	92
11	548	545
12	388	386
13	632	609
14	388	374
15	389	395
16	146	134
17	153	147
18	304	310
19	55	60
20	108	116
21	87	98
22	147	155
23	39	31
24	105	113
25	201	208
26	132	136
27	47	41
28	62	56
29	89	84
30	79	85
31	49	50
32	37	39
33	18*	9
34	17*	22
35	15*	6

1,2,L

0	346	432
1	1234	1011
2	804	973
3	847	861
4	759	783
5	739	756
6	553	546
7	1322	1385
8	537	533
9	367	330
10	485	463
11	245	247
12	338	332
13	320	316
14	786	761
15	169	167
16	149	137
17	219	215
18	168	166
19	121	129
20	146	150
21	31	36
22	147	142
23	182	175
24	98	84
25	93	96
26	66	69
27	139	144
28	25	32
29	66	72
30	30	34
31	37	40
18	75	84
19	32	22
20	60	68
21	22	24
22	37	40
23	35	29
24	18*	26
25	47	53
26	16*	9
27	16*	7

1,10,L

0	22*	22
1	123	129
2	73	73
3	138	156
4	156	169
5	132	126
6	95	106
7	96	104
8	22	23
9	145	156
10	40	36
11	188	198
12	36	26
13	113	114
14	33	30
15	68	82
16	73	72
17	70	71
18	79	89
19	19*	16
20	28	29
21	64	54
22	38	50
23	17*	4
24	35	31
25	15*	11

1,11,L

0	225	228
1	44	39
2	48	53
3	115	121
4	55	49
5	117	122
6	96	99
7	126	135
8	121	117
9	31	31
10	112	108
11	28	26
12	49	56
13	92	88
14	40	44
15	30	39
16	20	30
17	39	33
32	59	62
33	28	23
34	48	52

1,3,L

0	131	233
1	943	829
2	762	709
3	175	144
4	745	757
5	343	364
6	378	370
7	556	553
8	342	336
9	270	272
10	238	243
11	580	563
12	292	286
13	139	171
14	210	222
15	217	212
16	174	163
17	131	118
18	44	43
19	175	164
20	77	89
21	143	138
22	23	17
23	43	26
24	133	138
25	21*	11
26	55	62
27	55	60
28	116	125
29	50	56
30	27	27
31	19	18
32	24	28
33	70	72
34	50	54

1,4,L

0	483	206
1	429	499
2	480	495
3	225	248
4	241	261
5	246	253
6	615	602
7	201	165
8	307	328
9	217	210
10	624	596
11	198	191
12	147	152
13	153	147
14	183	180
15	229	240
18	73	79
19	69	71
20	18*	15
21	17*	11
22	24	25

1,12,L

0	38	31
1	51	55
2	21	31
3	21*	11
4	72	69
5	20*	20
6	25	10
7	55	57
8	50	56
9	34	39
10	63	63
11	68	68
12	73	86
13	37	35
14	48	55
15	46	57
16	48	47
17	44	49
18	26	27
19	59	65

1,13,L

0	27	31
1	19*	17
2	80	86
3	59	72
4	80	78
5	37	40
6	80	88
7	18*	11
8	18*	12
9	32	28
10	17*	4
11	20	24
12	19	13
13	20	11
14	44	51
15	16	18

1,14,L

0	109	107
1	17*	22
2	73	74
3	22	20
4	17*	21
5	29	28
6	25	25
7	16*	16
8	39	32
9	25	29
16	130	122
17	72	78
18	88	84
19	58	61
20	197	198
21	99	103
22	32	40
23	46	50
24	161	145
25	91	95
26	96	102
27	94	98
28	77	80
29	38	37
30	46	49
31	30	29
32	21	21
33	47	51

1,5,L

0	485	466
1	111	91
2	439	398
3	203	221
4	79	105
5	429	453
6	111	124
7	563	552
8	108	111
9	324	317
10	244	263
11	260	230
12	122	112
13	154	144
14	246	253
15	206	199
16	60	48
17	70	69
18	106	113
19	54	52
20	88	79
21	209	215
22	158	154
23	165	173
24	78	74
25	119	112
26	85	86
27	48	53
28	28	32
29	40	44
30	57	57
31	17*	6
32	20	15

1,6,L

0	188	180
1	273	220
2	424	397

2,0,L

0	1288	360
1	372	278
2	954	1015
3	912	931
4	599	602
5	770	756
6	629	604
7	452	464
8	450	447
9	636	635
10	535	519
11	66	61
12	369	348
13	485	475
14	202	207
15	140	144
16	71	78
17	151	147
18	18*	17
19	269	275
20	106	101
21	110	108
22	115	123
23	156	150
24	142	135
25	104	106
26	31	37
27	59	54
28	51	58
29	38	46
30	65	68
31	19*	19
32	33	40
33	18*	16
34	29	35
35	19	24

2,1,L

0	1337	681
1	556	888
2	706	696
3	1073	1104
4	136	117
5	497	523
6	893	892
7	875	884
8	684	698
9	580	583
10	366	372
11	532	517
12	350	351
13	25	47
14	128	113
15	108	103
16	116	116
17	212	215
18	232	230
3	453	443
4	244	232
5	209	214
6	248	229
7	240	254
8	259	264
9	262	247
10	60	74
11	210	214
12	218	224
13	48	44
14	216	206
15	56	62
16	115	118
17	214	214
18	120	128
19	22*	21
20	51	40
21	113	110
22	40	36
23	135	137
24	63	64
25	35	26
26	78	93
27	58	63
28	54	63
29	39	37
30	71	73
31	16*	18

1,7,L

0	189	216
1	231	208
2	290	276
3	152	152
4	214	186
5	30	18
6	127	107
7	255	264
8	115	132
9	119	132
10	119	129
11	134	148
12	96	96
13	55	62
14	119	125
15	113	114
16	97	98
17	98	101
18	69	82
19	83	82
20	73	78
21	99	106
22	51	63
23	20*	17
24	52	46
25	48	45
26	94	100
19	125	128
20	26	28
21	106	110
22	45	58
23	190	196
24	63	58
25	117	115
26	142	146
27	82	89
28	67	58
29	71	70
30	49	46
31	67	65
32	46	49
33	29	22
34	16*	20

2,2,L

0	159	706
1	839	689
2	519	474
3	606	616
4	913	904
5	767	733
6	219	231
7	167	185
8	143	148
9	517	519
10	43	35
11	344	351
12	198	175
13	278	273
14	199	183
15	190	195
16	250	235
17	155	173
18	135	130
19	132	138
20	318	313
21	55	62
22	227	225
23	77	81
24	22*	20
25	147	148
26	53	53
27	27	28
28	52	53
29	103	103
30	23	19
31	43	47
32	63	72
33	34	30
34	16*	3

2,3,L

0	30	153

2.3.L

1	579	670
2	389	467
3	480	483
4	502	518
5	409	422
6	725	706
7	210	202
8	133	132
9	325	311
10	115	123
11	440	424
12	332	313
13	480	472
14	108	127
15	25	26
16	110	104
17	148	160
18	218	221
19	195	214
20	152	146
21	94	87
22	151	156
23	82	79
24	22*	17
25	69	68
26	44	38
27	46	46
28	48	45
29	29	30
30	42	38
31	18*	14
32	57	64
33	16*	17

2.4.L

0	167	235
1	417	330
2	312	352
3	230	264
4	250	220
5	679	688
6	36	44
7	282	289
8	151	154
9	144	134
10	279	277
11	81	88
12	264	245
13	222	207
14	156	149
15	55	49
16	145	128
17	43	39
18	146	145
19	164	170
20	118	113
21	72	75

22	102	102
23	142	142
24	21*	10
25	64	64
26	27	17
27	64	71
28	59	63
29	23	26
30	29	33
31	24	28
32	32	34
33	16	21

2.5.L

0	483	553
1	447	465
2	203	206
3	172	171
4	258	221
5	353	358
6	169	151
7	106	100
8	387	393
9	243	220
10	363	354
11	61	85
12	153	158
13	153	124
14	95	89
15	175	160
16	29	22
17	192	180
18	31	26
19	73	59
20	363	364
21	122	116
22	175	168
23	167	167
24	25	32
25	55	51
26	40	39
27	78	78
28	64	76
29	46	47
30	17*	7
31	17*	18
32	16*	24

2.6.L

0	79	39
1	180	206
2	38	36
3	248	234
4	39	35
5	112	123
6	235	221
7	55	56
8	90	98

9	235	260
10	117	124
11	90	78
12	91	82
13	115	117
14	256	263
15	51	47
16	81	82
17	134	140
18	88	93
19	22	21
20	79	74
21	21*	14
22	65	68
23	105	104
24	43	46
25	77	74
26	71	68
27	29	30
28	41	40
29	77	75
30	39	33
31	25	30

2.7.L

0	158	161
1	153	122
2	148	159
3	42	50
4	81	98
5	110	105
6	23	40
7	100	101
8	205	201
9	73	70
10	118	114
11	167	152
12	98	112
13	72	84
14	77	72
15	87	79
16	28	31
17	67	67
18	87	97
19	59	60
20	31	25
21	60	54
22	54	65
23	68	63
24	54	51
25	48	38
26	50	56
27	39	37
28	50	51
29	67	70

2.8.L

0	246	251

1	227	231
2	128	132
3	284	286
4	119	133
5	67	55
6	139	148
7	123	133
8	136	138
9	126	129
10	101	105
11	120	110
12	193	195
13	39	38
14	128	122
15	126	118
16	134	123
17	130	124
18	109	112
19	141	143
20	63	56
21	49	47
22	35	39
23	33	30
24	44	40
25	37	43
26	18	17
27	19	21
28	25	28

2.9.L

0	124	130
1	75	66
2	81	71
3	159	173
4	35	27
5	73	65
6	151	149
7	123	118
8	216	207
9	166	169
10	83	83
11	131	138
12	94	86
13	100	100
14	129	120
15	90	101
16	91	96
17	29	34
18	55	64
19	111	118
20	19*	5
21	35	37
22	19*	21
23	18*	3
24	17*	9
25	31	37
26	20	17

2.10.L

0	34	45
1	48	54
2	129	118
3	154	159
4	46	42
5	129	120
6	143	146
7	78	73
8	128	125
9	69	61
10	35	31
11	121	117
12	52	67
13	58	53
14	39	35
15	31	44
16	28	36
17	48	43
18	19*	3
19	45	53
20	18*	16
21	43	44
22	35	33
23	21	18

2.11.L

0	21*	1
1	79	99
2	75	65
3	84	94
4	45	51
5	52	64
6	90	85
7	96	87
8	67	71
9	78	81
10	88	91
11	76	81
12	63	72
13	77	70
14	21	12
15	47	53
16	18*	20
17	52	55
18	17*	21
19	17*	7
20	27	31
21	16*	9

2.12.L

0	64	61
1	60	64
2	77	81
3	48	45
4	89	83
5	34	36

2.12.L

6	42	46
7	22	17
8	71	75
9	23	25
10	19*	14
11	44	39
12	31	27
13	46	38
14	20	17
15	29	31
16	17*	7
17	27	25

2.13.L

0	54	56
1	21	13
2	79	84
3	35	27
4	18*	7
5	19	23
6	43	42
7	39	39
8	28	32
9	18*	16
10	23	22
11	16*	13
12	27	32

2.14.L

0	15*	10
1	23	32

3.0.L

0	2318	2088
1	313	650
2	788	806
3	663	629
4	405	432
5	1124	1100
6	717	715
7	502	497
8	433	415
9	150	134
10	192	190
11	74	91
12	230	232
13	193	187
14	142	148
15	122	132
16	86	81
17	252	238
18	83	68
19	93	96
20	71	66
21	169	162

22	60	54
23	131	131
24	138	140
25	65	58
26	103	101
27	101	110
28	44	53
29	63	67
30	27	37
31	55	48
32	18*	15
33	31	34
34	16*	3

3.1.L

0	189	280
1	1219	1087
2	121	56
3	671	653
4	624	621
5	903	935
6	698	707
7	284	277
8	723	710
9	255	251
10	298	285
11	229	229
12	68	74
13	182	182
14	171	174
15	190	177
16	71	63
17	78	85
18	148	141
19	50	52
20	104	104
21	118	114
22	182	184
23	66	67
24	82	80
25	136	146
26	158	160
27	67	73
28	128	133
29	68	71
30	24	21
31	59	59
32	80	85
33	17*	16
34	29	26

3.2.L

0	143	168
1	878	987
2	237	186
3	627	621
4	625	647
5	173	159

6	295	283
7	265	269
8	339	348
9	275	272
10	107	91
11	246	254
12	333	318
13	126	120
14	200	208
15	73	90
16	288	277
17	198	194
18	45	27
19	285	306
20	96	92
21	62	63
22	160	164
23	75	75
24	29	33
25	157	154
26	108	97
27	42	48
28	58	51
29	97	96
30	21	15
31	54	59
32	47	48
33	17*	10

3.3.L

0	720	627
1	168	209
2	457	539
3	181	163
4	116	118
5	324	317
6	540	521
7	603	571
8	67	64
9	557	557
10	257	258
11	165	152
12	392	370
13	24	37
14	189	180
15	196	197
16	341	346
17	168	168
18	50	48
19	108	117
20	151	153
21	115	111
22	80	80
23	265	256
24	95	97
25	78	74
26	38	50
27	49	55
28	20*	10

29	56	61
30	19*	12
31	35	42
32	64	62
33	15*	6

3.4.L

0	62	60
1	307	281
2	505	466
3	539	550
4	67	60
5	271	254
6	230	204
7	152	145
8	352	353
9	99	103
10	223	210
11	83	91
12	263	248
13	101	98
14	102	109
15	157	147
16	112	126
17	21*	18
18	181	177
19	170	173
20	195	191
21	123	126
22	168	179
23	33	41
24	135	146
25	120	127
26	45	48
27	35	32
28	20*	24
29	37	39
30	18*	19
31	17*	21
32	69	67

3.5.L

0	267	233
1	86	85
2	130	149
3	102	88
4	141	130
5	131	116
6	348	324
7	279	256
8	227	205
9	225	246
10	80	75
11	212	217
12	125	127
13	47	51
14	237	243
15	159	157

16	144	152
17	142	132
18	133	131
19	47	60
20	224	222
21	37	39
22	50	42
23	108	104
24	21*	32
25	66	69
26	20	18
27	27	22
28	37	42
29	18*	23
30	32	36
31	19	16

3.6.L

0	236	241
1	54	86
2	78	104
3	115	112
4	193	184
5	119	109
6	238	236
7	73	64
8	22	21
9	168	164
10	143	139
11	130	140
12	46	50
13	219	211
14	97	98
15	42	32
16	26	20
17	35	47
18	75	72
19	120	123
20	47	36
21	65	59
22	39	34
23	75	66
24	23	34
25	20	27
26	43	42
27	19	12
28	46	44
29	32	40
30	15*	10

3.7.L

0	46	58
1	245	256
2	83	81
3	166	163
4	62	45
5	240	246

3.7.L

6	160	151
7	94	97
8	165	162
9	26	28
10	21*	9
11	21*	27
12	150	153
13	53	63
14	97	111
15	79	73
16	163	153
17	152	142
18	100	104
19	21*	18
20	53	68
21	21*	23
22	51	59
23	33	36
24	38	40
25	31	29
26	37	35
27	36	38
28	16*	10

3.8.L

0	63	79
1	53	42
2	63	71
3	147	149
4	147	152
5	128	121
6	138	143
7	153	155
8	188	170
9	162	167
10	157	167
11	137	121
12	116	117
13	90	93
14	139	125
16	21*	6
17	132	128
18	36	32
19	25	22
20	20*	15
21	38	38
22	37	43
23	41	45
24	26	21
25	18	27
26	27	22

3.9.L

0	51	58
1	66	62
2	112	110

4.3.L

27	29	23
28	54	63
29	19*	18
30	27	27
31	46	56
32	41	39

4.4.L

0	123	87
1	244	261
2	289	317
3	287	293
4	162	164
5	184	180
6	197	180
7	101	99
8	152	154
9	112	105
10	193	191
11	80	95
12	112	101
13	208	215
14	170	181
15	138	128
16	95	99
17	240	238
18	102	102
19	142	154
20	134	143
21	68	66
22	57	52
23	43	46
24	82	75
25	26	27
26	28	25
27	58	60
28	65	73
29	26	30
30	30	26
31	16*	18

4.5.L

0	18*	10
1	300	267
2	136	145
3	362	347
4	96	93
5	193	207
6	56	25
7	194	186
8	19*	33
9	44	56
8	19*	33
9	44	56
10	39	42
11	112	119

3	33	25
4	122	123
5	45	42
6	118	117
7	121	123
8	93	96
9	74	63
10	88	88
11	62	58
12	39	44
13	26	17
14	22	20
15	64	79
16	43	46
17	21*	24
18	31	25
19	19*	3
20	34	31
21	18*	7
22	58	60
23	24	21
24	22	26

3.10.L

0	144	147
1	102	106
2	117	102
3	22*	19
4	32	41
5	30	29
6	80	82
7	21*	21
8	116	114
9	33	42
10	74	69
11	22	12
12	32	30
13	22	26
14	45	50
15	65	71
16	54	53
17	32	22
18	26	25
19	40	43
20	58	52
21	16*	9
22	15*	2

3.11.L

0	45	44
1	50	57
2	35	33
3	93	86
4	36	36
5	20*	15
6	80	83
7	26	34
8	19*	9

12	52	51
13	71	56
14	52	57
15	29	32
16	127	129
17	76	87
18	67	76
19	163	161
20	135	141
21	109	110
22	45	45
23	21*	18
24	20*	14
25	46	41
26	19*	14
27	29	36
28	26	28
29	18	18
30	38	37

4.6.L

0	50	36
1	91	82
2	145	122
3	134	113
4	82	84
5	199	198
6	58	68
7	116	107
8	229	233
9	141	131
10	181	167
11	39	22
12	100	102
13	41	44
14	32	39
15	113	113
16	156	148
17	169	168
18	57	62
20	72	71
21	47	47
22	28	25
23	40	39
24	39	47
25	21	28
26	28	20
27	20	16
28	19	20

4.7.L

0	20*	15
1	126	124
2	53	60
3	158	154
4	166	174
5	227	219
6	50	52

9	54	58
10	19*	14
11	22	26
12	37	34
13	51	48
14	19*	27
15	30	35
16	29	40
17	17*	21
18	27	28

3.12.L

0	51	41
1	31	31
2	34	33
3	19*	14
4	29	26
5	47	46
6	45	50
7	23	24
8	33	32
9	17*	4
10	48	47
11	17*	18
12	17*	15
13	16*	10
14	25	26

3.13.L

0	17*	18
1	22	24
2	25	31
3	16*	6
4	46	43
5	43	46
6	23	24
7	18	17

4.0.L

0	497	180
1	284	420
2	651	617
3	253	245
4	448	423
5	95	117
6	152	132
7	46	31
8	520	498
9	46	82
10	225	256
11	491	480
12	198	204
13	434	413
14	98	100
15	121	124
16	98	108
17	84	90

7	100	107
8	202	200
9	156	161
10	103	109
11	100	95
12	22*	11
13	186	184
14	81	78
15	36	36
16	49	46
17	21*	15
18	25	23
19	80	83
20	20*	23
21	76	71
22	62	63
23	39	46
24	37	31
25	18*	26
26	17*	25
27	25	33

4.8.L

0	25	13
1	129	130
2	160	164
3	47	40
4	48	41
5	152	139
6	141	136
7	65	79
8	77	81
9	152	159
10	44	45
11	60	65
12	72	78
13	111	115
14	41	32
15	44	46
16	61	61
17	40	46
18	20*	4
19	34	30
20	32	34
21	53	49
22	18*	6
23	17*	3
24	36	38
25	21	20

4.9.L

0	77	74
1	99	95
2	60	62
3	103	115
4	60	61
5	30	25
6	88	80

18	262	267
19	136	125
20	22	24
21	116	117
22	106	108
23	96	94
24	67	53
25	22*	19
26	224	228
27	36	31
28	132	141
29	72	76
30	93	94
31	29	29
32	19*	27
33	17*	9
34	15*	8

4.1.L

0	112	127
1	300	428
2	83	32
3	280	276
4	276	251
5	322	340
6	302	319
7	198	188
8	296	300
9	508	439
10	173	152
11	231	210
12	225	225
13	383	384
14	226	217
15	98	88
16	139	128
17	54	44
18	111	109
19	278	269
20	89	90
22	90	93
23	201	206
24	55	55
25	159	157
26	75	85
27	44	47
28	45	47
29	78	77
30	38	41
31	74	76
32	31	35
33	35	40

4.2.L

0	208	133
1	453	368
2	296	339
4	241	203

7	59	61
8	83	85
9	50	48
10	88	87
11	51	45
12	39	34
13	74	71
14	20*	23
15	31	29
16	23	25
17	26	22
18	19*	16
19	60	56
20	17*	3
21	47	49
22	16*	11

4.10.L

0	97	89
1	101	99
2	30	30
3	40	32
4	40	44
5	21*	26
6	58	58
7	54	49
8	60	55
9	58	59
10	19*	8
11	76	65
12	19*	16
13	20	23
14	27	31
15	29	26
16	34	35
17	55	58
18	30	33
19	50	48

4.11.L

0	35	40
1	40	40
2	29	26
3	44	42
4	22	18
5	32	31
6	59	59
7	19*	24
8	34	30
9	23	24
10	31	34
11	25	18
12	17*	13
13	20	19
14	16*	11
15	20	22
16	24	30

5	117	116
6	765	754
7	485	481
8	306	291
9	434	418
10	395	379
11	254	239
12	170	142
13	406	405
14	198	197
15	136	136
16	167	157
17	143	144
18	166	173
19	187	181
20	97	96
21	123	120
22	116	122
23	69	74
24	134	140
25	98	101
26	41	45
27	51	58
28	83	80
29	20*	27
30	24	20
31	45	52
32	44	44
33	21	19

4.3.L

0	56	122
1	532	490
2	616	568
3	157	139
4	131	116
5	167	149
6	263	264
7	295	268
8	254	255
9	210	201
10	161	155
11	42	53
12	114	103
13	80	74
14	158	168
15	140	142
16	229	226
17	206	195
18	162	170
19	112	122
20	71	74
21	60	61
22	246	247
23	179	177
24	21*	18
25	22	21
26	20*	21

4.12.L

0	17*	14
1	17*	17
2	33	28
3	46	48
4	36	45
5	17*	17
6	35	31
7	17*	24
8	23	21
9	22	29
10	15*	7

5.0.L

0	274	369
1	361	251
2	647	689
3	207	191
4	100	113
5	500	480
6	490	474
7	338	323
8	302	303
9	626	617
10	62	54
11	285	297
12	303	270
13	149	147
14	297	282
15	159	162
16	29	46
17	101	98
18	212	211
19	121	129
20	149	147
21	41	46
22	55	55
23	176	178
24	70	64
25	111	118
26	110	115
27	37	33
28	28	31
29	89	95
30	63	65
31	32	37
32	50	56
33	30	26

5.1.L

0	188	228
1	329	348
2	323	292
3	258	284
4	200	199
5	462	470

5,1,L

6	500	476
7	313	289
8	602	568
9	129	109
10	302	276
11	49	46
12	34	15
13	203	193
14	273	270
15	229	227
16	173	167
17	57	59
18	179	177
19	166	167
20	144	143
21	77	87
22	108	111
23	66	72
24	107	84
25	64	61
26	21*	19
27	53	50
28	68	79
29	29	21
30	46	44
31	25	19
32	44	44

5,2,L

0	172	203
1	408	361
2	227	182
3	718	736
4	190	202
5	174	170
6	356	339
7	356	348
8	253	254
9	147	144
10	162	164
11	275	271
12	108	107
13	69	76
14	62	65
15	202	205
16	88	94
17	129	138
18	116	124
19	142	148
20	121	118
21	81	86
22	160	168
23	116	129
24	85	84
25	89	101
26	25	35
27	65	73

5,11,L

0	28	31
1	31	40
2	31	29
3	55	58
4	48	51
5	65	61
6	36	29
7	35	41
8	32	31
9	19	16
10	16*	10
11	16*	9
12	24	20

6,0,L

0	275	278
1	121	141
2	225	186
3	332	337
4	96	74
5	296	265
6	356	338
7	62	52
8	199	223
9	250	225
10	271	250
11	56	70
12	123	136
13	90	78
14	104	98
15	85	102
16	180	159
17	44	35
18	106	97
19	81	92
20	157	156
21	201	202
22	82	95
23	49	55
24	94	84
25	86	81
26	81	78
27	26	25
28	48	47
29	19*	4
30	18*	17
31	29	29
32	68	68

6,1,L

0	610	575
1	193	184
2	411	424
3	34	51
4	40	34
5	306	291
28	42	40
29	19*	5
30	64	66
31	59	61
32	20	24

5,3,L

0	235	229
1	282	332
2	103	107
3	267	272
4	150	122
5	127	113
6	238	231
7	103	111
8	184	180
9	49	46
10	226	233
11	115	92
12	92	100
13	20*	15
14	73	71
15	183	178
16	112	103
17	136	133
18	283	301
19	67	84
20	93	93
21	34	40
22	149	135
23	65	73
24	77	64
25	66	74
26	29	30
27	49	55
28	19*	19
29	38	37
30	18	23
31	17	22

5,4,L

0	76	50
1	90	105
2	41	44
3	176	171
4	174	173
5	85	75
6	149	142
7	102	103
8	44	54
9	36	45
10	82	86
11	47	28
12	89	94
13	148	141
14	98	97
15	23	25
16	114	107
6	232	232
7	96	122
8	421	417
9	203	204
10	55	63
11	107	111
12	332	335
13	165	164
14	74	70
15	120	122
16	251	234
17	172	175
18	57	54
19	283	285
20	92	98
21	140	143
22	87	90
23	21*	22
24	92	91
25	37	31
26	20*	5
27	25	27
28	19*	8
29	26	25
30	23	22
31	95	100

6,2,L

0	307	328
1	255	218
2	287	265
3	349	373
4	169	158
5	139	161
6	145	135
7	91	92
8	84	68
9	212	211
10	103	103
11	247	237
12	75	74
13	124	128
14	198	194
15	188	180
16	240	231
17	67	62
18	123	117
19	94	100
20	29	30
21	162	166
22	143	146
23	61	65
24	59	56
25	20*	10
26	20*	24
27	34	36
28	19	28
29	17*	12
30	33	33
17	108	107
18	196	200
19	158	166
20	94	99
21	77	73
22	42	47
23	45	51
24	28	26
25	54	54
26	19*	21
27	18*	15
28	18*	22
29	16*	7
30	28	24

5,5,L

0	83	76
1	188	207
2	208	198
3	223	219
4	193	185
5	75	84
6	73	82
7	144	131
8	40	32
9	21	40
10	94	96
11	127	126
12	37	35
13	23	28
14	33	32
15	156	155
16	136	134
17	60	62
18	47	45
19	57	63
20	81	92
21	52	53
22	40	42
23	47	50
24	41	48
25	28	28
26	21	21
27	17*	6
28	18	23
29	17	19

5,6,L

0	172	153
1	105	114
2	84	92
3	56	63
4	167	182
5	41	35
6	176	179
7	28	23
8	148	139
9	29	29
31	31	31

6,3,L

0	62	76
1	248	251
2	123	150
3	383	371
4	180	190
5	187	197
6	161	142
7	204	210
8	63	60
9	95	112
10	184	183
11	58	61
12	76	78
13	134	136
14	194	185
15	125	112
16	177	183
17	94	90
18	201	207
19	33	42
20	101	108
21	45	50
22	55	69
23	34	43
24	24	25
25	25	29
26	30	31
27	30	30
28	37	37
29	17	17
30	20	16

6,4,L

0	36	25
1	208	214
2	48	38
3	105	119
4	140	147
5	236	236
6	72	61
7	109	94
8	49	54
9	128	117
10	134	141
11	52	57
12	66	58
13	77	78
14	102	98
15	61	60
16	111	107
17	79	81
18	47	58
19	119	114
20	129	127
21	28	34
10	102	100
11	192	192
12	108	112
13	152	149
14	63	58
15	104	107
16	85	73
17	64	66
18	37	31
19	74	80
20	73	71
21	53	48
22	72	67
23	19*	27
24	28	24
25	38	41
26	25	15
27	34	40

5,7,L

0	21*	17
1	148	142
2	81	70
3	84	100
4	201	211
5	172	187
6	136	134
7	107	114
8	196	197
9	28	33
10	50	46
11	132	138
12	62	48
13	101	100
14	84	87
15	23	31
16	125	118
17	82	85
18	20*	23
19	19*	20
20	47	48
21	19*	14
22	18*	12
23	24	28
24	32	34
25	15*	4

5,8,L

0	21*	13
1	44	60
2	50	41
3	169	164
4	109	113
5	92	94
6	84	85
7	121	113
8	64	75
9	46	43
22	70	72
23	44	46
24	60	70
25	32	43
26	18*	2
27	41	46
28	19	21

6,5,L

0	104	113
1	183	200
2	122	124
3	169	174
4	115	112
5	199	188
6	82	92
7	112	101
8	118	120
9	91	75
10	63	58
11	159	160
12	92	96
13	58	56
14	47	51
15	40	36
16	21*	17
17	58	54
18	98	97
19	21*	23
20	53	49
21	93	92
22	61	60
23	29	30
24	24	38
25	18*	16
26	26	28
27	18	6

6,6,L

0	50	44
1	179	187
2	130	123
3	174	170
4	284	275
5	145	161
6	194	192
7	37	35
8	79	69
9	63	68
10	154	148
11	156	149
12	45	55
13	40	35
14	80	85
15	47	53
16	83	79
17	65	60
18	81	79
10	95	87
11	30	26
12	70	66
13	21	34
14	116	116
15	46	50
16	44	49
17	48	46
18	18*	11
19	32	24
20	17*	8
21	17*	9
22	16*	3
23	27	31

5,9,L

0	102	84
1	155	156
2	48	50
3	65	50
4	91	94
5	47	37
6	21*	25
7	48	44
8	53	54
9	69	70
10	25	20
11	36	38
12	46	47
13	24	27
14	66	61
15	22	19
16	30	30
17	21	25
18	17*	11
19	43	43
20	21	28

5,10,L

0	20*	17
1	86	102
2	43	41
3	40	43
4	20*	27
5	102	101
6	33	39
7	33	30
8	24	24
9	30	34
10	18*	10
11	18*	20
12	18	13
13	17*	7
14	18	19
15	24	21
16	16*	7
17	34	40
19	27	25
20	23	17
21	46	45
22	18*	18
23	36	43
24	17*	10
25	25	23

6,7,L

0	71	79
1	118	118
2	195	198
3	192	203
4	22*	18
5	21*	14
6	51	49
7	22*	24
8	65	63
9	56	61
10	116	112
11	97	89
12	102	102
13	47	41
14	78	79
15	91	93
16	20*	19
17	19*	20
18	35	36
19	18*	17
20	31	35
21	29	38
22	17*	18
23	19	17

6,8,L

0	67	59
1	129	137
2	78	85
3	79	81
4	39	43
5	30	39
6	82	77
7	52	46
8	82	77
9	46	41
10	51	52
11	24	23
12	73	71
13	20*	18
14	29	30
15	33	35
16	18*	9
17	41	36
18	35	48
19	31	36
20	21	27

6,9,L

0	20*	15
1	79	83
2	20*	31
3	46	47
4	29	25
5	75	76
6	64	63
7	107	100
8	20*	19
9	26	26
10	19*	27
11	24	19
12	20	26
13	17*	7
14	20	15
15	33	29
16	18	25
17	32	32

6,10,L

0	28	26
1	60	55
2	18*	23
3	23	26
4	38	35
5	18*	20
6	64	66
7	53	48
8	17*	10
9	22	20
10	17*	19
11	19	17
12	21	20
13	15*	17

6,11,L

0	17	5
1	29	30
2	24	19
3	21	22
4	26	32
5	36	37

7,0,L

0	254	224
1	316	347
2	228	247
3	380	381
4	197	182
5	114	111
6	197	186
7	107	114
8	32	12
9	118	106
10	205	190

11	83	78
12	20*	18
13	26	24
14	116	120
15	63	68
16	145	143
17	221	229
18	133	133
19	163	160
20	47	49
21	101	102
22	82	84
23	69	69
24	124	117
25	36	37
26	22	24
27	41	35
28	48	50
29	72	73
30	17*	15
31	47	50

7,1,L

0	219	227
1	145	127
2	316	330
3	202	213
4	85	81
5	138	138
6	77	93
7	120	118
8	166	177
9	86	76
10	125	105
11	105	107
12	110	118
13	98	98
14	207	205
15	64	61
16	88	77
17	237	243
18	174	184
19	22*	22
20	164	163
21	129	124
22	36	31
23	64	68
24	29	28
25	39	36
26	41	48
27	73	68
28	27	31
29	43	34
30	55	49

7,2,L

0	137	155
1	30	48
2	85	76
3	149	134
4	89	101
5	104	81
6	95	108
7	272	256
8	41	35
9	139	151
10	118	124
11	59	57
12	109	100
13	110	121
14	135	129
15	135	142
16	66	64
17	152	163
18	109	110
19	153	150
20	62	63
21	126	144
22	56	60
23	20*	13
24	57	56
25	28	28
26	44	46
27	18*	13
28	17*	14
29	22	14

7,3,L

0	55	53
1	96	101
2	130	100
3	155	146
4	112	111
5	179	175
6	21	24
7	61	58
8	49	56
9	76	70
10	108	124
11	78	73
12	239	227
13	67	68
14	29	35
15	180	174
16	103	106
17	104	106
18	72	70
19	78	84
20	21*	13
21	63	58
22	39	40
23	21	24
24	75	79
25	36	34
26	18*	5
27	17*	14
28	20	21

7,4,L

0	73	51
1	47	41
2	55	54
3	100	114
4	97	85
5	96	107
6	52	62
7	154	143
8	57	51
9	30	27
10	198	209
11	87	90
12	97	93
13	99	113
14	47	50
15	77	78
16	43	41
17	75	74
18	56	51
19	99	100
20	96	105
21	20*	24
22	42	48
23	26	21
24	23	22
25	28	32
26	23	28
27	18	18

7,5,L

0	91	74
1	139	132
2	228	234
3	145	138
4	87	90
5	92	98
6	82	91
7	99	109
8	61	71
9	107	107
10	105	114
11	119	121
12	61	61
13	21*	17
14	36	24
15	33	27
16	21*	8
17	36	39
18	27	29
19	72	74
20	55	52
21	36	31
22	34	35
23	29	26
24	36	34
25	15*	10

7,6,L

0	106	96
1	30	27
2	208	208
3	94	103
4	22*	25
5	143	151
6	68	68
7	132	131
8	92	90
9	56	54
10	34	28
11	78	79
12	29	21
13	54	56
14	79	79
15	71	69
16	75	76
17	22	23
18	27	18
19	18*	19
20	30	28
21	19	22
22	38	36
23	16*	11

7,7,L

0	89	77
1	33	34
2	91	80
3	21*	6
4	84	81
5	61	66
6	164	169
7	88	83
8	22	22
9	36	44
10	65	63
11	50	43
12	20*	19
13	52	52
14	49	51
15	33	25
16	16*	23
17	45	50
18	28	33
19	54	52
20	16*	10
21	29	28

7,8,L

0	20*	6
1	28	37
2	78	69
3	90	75

7,8,L

4	45	42
5	98	99
6	65	63
7	65	67
8	32	32
9	25	26
10	23	27
11	34	34
12	19*	18
13	29	34
14	18*	21
15	29	30
16	17*	14
17	16*	11
18	35	37

7,9,L

0	71	72
1	27	31
2	46	47
3	19*	23
4	66	60
5	79	83
6	18*	8
7	34	37
8	18*	15
9	24	20
10	20	19
11	24	23
12	16*	10
13	20	21

7,10,L

0	30	21
1	26	21
2	23	22
3	67	68
4	72	73
5	72	71
6	16*	4
7	17	25

8,0,L

0	101	76
1	119	143
2	151	154
3	104	94
4	200	203
5	135	130
6	244	238
7	76	69
8	84	80
9	84	97
10	140	150
11	97	86

12	122	126
13	63	59
14	23	23
15	286	287
16	52	47
17	41	29
18	133	134
19	99	101
20	66	65
21	71	76
22	77	76
23	106	103
24	82	75
25	64	63
26	43	46
27	65	59
28	56	48
29	27	26
30	32	29

8,1,L

0	86	98
1	45	46
2	69	49
3	136	143
4	100	104
5	241	234
6	20*	19
7	88	104
8	190	192
9	89	74
10	194	193
11	78	88
12	143	145
13	85	94
14	22*	20
15	156	163
16	39	47
17	63	55
18	110	113
19	98	93
20	58	67
21	111	117
22	71	78
23	80	82
24	57	58
25	40	40
26	54	64
27	38	40
28	18	11
29	23	19

8,2,L

0	25	17
1	164	158
2	76	78
3	140	154
4	114	120
5	219	216
6	142	144
7	147	134
8	74	75
9	56	48
10	81	84
11	64	58
12	157	162
13	145	159
14	109	110
15	124	128
16	26	22
17	104	100
18	127	133
19	50	51
20	82	87
21	60	62
22	56	49
23	37	43
24	53	61
25	35	32
26	38	42
27	17	13
28	19	13

8,3,L

0	93	110
1	91	82
2	40	32
3	185	176
4	82	98
5	93	71
6	64	54
7	53	59
8	78	72
9	61	68
10	75	72
11	48	55
12	36	33
13	160	163
14	41	40
15	135	126
16	116	113
17	57	49
18	69	74
19	22*	34
20	94	98
21	41	39
22	87	93
23	71	83
24	37	43
25	38	42
26	18	13

8,4,L

0	23	15
1	113	121
2	141	136
3	137	129
4	36	38
5	43	47
6	87	98
7	31	31
8	86	100
9	77	79
10	133	130
11	67	64
12	87	82
13	217	220
14	37	37
15	34	32
16	65	67
17	75	73
18	38	37
19	20*	15
20	36	32
21	36	38
22	34	34
23	59	62
24	50	55
25	20	22

8,5,L

0	199	207
1	46	50
2	22	12
3	35	28
4	52	54
5	109	108
6	174	182
7	81	79
8	133	140
9	96	100
10	117	109
11	76	68
12	104	103
13	84	79
14	20*	10
15	29	36
16	28	32
17	20*	19
18	57	57
19	35	39
20	35	23
21	33	34
22	20	24
23	34	31

8,6,L

0	49	48
1	102	98
2	56	52
3	115	117
4	114	119
5	107	105
6	26	32
7	60	62
8	63	81
9	66	65
10	110	111
11	80	73
10	110	111
11	80	73
12	39	47
13	20*	16
14	74	70
15	53	64
16	36	35
17	37	34
18	27	35
19	37	37
20	16*	7
21	15	14

8,7,L

0	20*	14
1	54	59
2	43	55
3	113	113
4	108	102
5	89	80
6	61	58
7	19*	12
8	50	60
9	19*	14
10	19*	9
11	49	45
12	35	32
13	37	35
14	18*	13
15	30	27
16	17*	14
17	19	24
18	16*	18

8,8,L

0	57	47
1	19*	21
2	40	35
3	35	32
4	32	36
5	31	32
6	24	19
7	18*	12
8	18*	20
9	31	37
10	28	29
11	46	45
12	15*	8
13	20	21
14	23	24

8,8,L

0	17*	18
1	19	11
2	27	25
3	41	47
4	17*	11
5	29	25
6	15*	17
7	15*	16

9,0,L

0	53	40
1	107	80
2	80	78
3	218	209
4	188	190
5	100	86
6	60	43
7	77	78
8	42	53
9	123	112
10	200	196
11	191	178
12	189	183
13	81	84
14	28	31
15	119	112
16	40	46
17	102	109
18	38	42
19	68	62
20	59	52
21	64	66
22	26	32
23	44	47
24	22	26
25	19*	13
26	36	44
27	26	32
28	34	31

9,1,L

0	101	103
1	28	30
2	295	300
3	69	72
4	102	113
5	21*	12
6	105	88
7	21*	4
8	137	129
9	84	67
10	120	118
11	129	128
12	161	159
13	65	78
14	88	80

9,2,L

0	151	148
1	160	146
2	112	113
3	94	94
4	48	44
5	94	108
6	96	96
7	35	16
8	54	66
9	70	67
10	23	22
11	171	169
12	68	70
13	79	78
14	53	62
15	117	117
16	119	120
17	39	36
18	20*	9
19	36	43
20	70	72
21	42	37
22	19*	14
23	29	30
24	25	33
25	44	53
26	28	23

9,3,L

0	168	180
1	96	84
2	103	99
3	115	114
4	89	87
5	121	119
6	34	33
7	105	115
8	148	151
9	21*	21
10	102	109
11	151	158
12	115	115
13	71	71
14	51	54
15	86	99
16	22*	18
17	157	157
18	21*	20
19	54	53
20	33	31
21	45	44
22	25	20
23	19	12
24	18*	16
25	36	35
26	16*	17
27		

9,4,L

0	21*	3
1	41	54
2	32	20
3	59	63
4	73	70
5	47	45
6	185	186
7	71	56
8	171	168
9	91	93
10	66	64
11	104	110
12	21*	18
13	22	22
14	38	43
15	48	56
16	55	56
17	57	63
18	52	47
19	18*	17
20	38	36
21	17*	7
22	38	39

9,5,L

0	95	102
1	32	37
2	24	43
3	45	47
4	67	52
5	44	38
6	73	62
7	41	33
8	68	75
9	120	138
10	40	33
11	38	38
12	80	86
13	47	55
14	19*	5
15	55	63
16	72	67
17	23	28
18	18*	20
19	18	25
20	34	26

9,6,L

0	21*	17
1	95	92
2	70	58
3	48	54
4	71	68
5	20*	2
6	65	67
7	49	53
8	58	59
9	60	67
10	46	44
11	52	61
12	43	48
13	29	33
14	25	28
15	46	57
16	17*	12
17	49	53

9,7,L

0	26	27
1	28	18
2	49	47
3	32	34
4	25	25
5	43	42
6	18*	13
7	44	46
8	27	25
9	30	30
10	31	37
11	23	22
12	21	18
13	34	33

9,8,L

0	16*	0
1	22	28
2	17*	18
3	31	24
4	19	16
5	16*	6
6	16*	11
7	22	21

10,0,L

0	51	55
1	157	147
2	137	120
3	135	121
4	100	83
5	74	59
6	40	40
7	100	103
8	38	42
9	217	230
10	136	141
11	74	77
12	84	108
13	43	50
14	85	91
15	73	70
16	44	44
17	38	39
18	68	69
19	33	17
20	38	46
21	64	60
22	19*	3
23	18*	16
24	18*	8
25	52	44
26	16*	21

10,1,L

0	23	28
1	167	180
2	38	36
3	142	142
4	176	171
5	63	74
6	33	36
7	49	48
8	21*	15
9	44	39
10	71	94
11	87	83
12	56	45
13	104	90
14	82	80
15	88	87
16	44	38
17	79	75
18	22	14
19	20*	15
20	63	62
21	37	32
22	37	37
23	54	51
24	37	41
25	41	38

10,2,L

0	49	52
1	51	53
2	80	83
3	60	54
4	124	125
5	152	142
6	95	102

10,2,L

7	100	105
8	74	70
9	46	48
10	92	110
11	38	25
12	78	82
13	58	50
14	96	106
15	65	66
16	20*	7
17	20*	14
18	39	35
19	82	83
20	19*	16
21	20	29
22	28	29
23	45	46

10,3,L

0	37	50
1	59	61
2	21*	18
3	63	57
4	28	22
5	110	114
6	101	110
7	22*	21
8	109	107
9	27	30
10	62	61
11	41	44
12	39	37
13	41	44
14	68	70
15	72	72
16	67	67
17	19*	15
18	29	20
19	61	66
20	18*	17
21	52	54
22	37	34

10,4,L

0	21*	21
1	20*	13
2	28	28
3	47	48
4	38	46
5	64	56
6	22	12
7	44	44
8	24	9
9	98	92
12	30	24
10	37	38
13	28	24
14	60	67
11	58	57
15	50	42
16	39	39
17	18	18
18	20	23
19	29	28

10,5,L

0	61	68
1	31	33
2	49	46
3	39	40
4	28	28
5	63	61
6	39	34
7	25	16
8	31	43
9	19*	14
10	34	34
11	32	31
12	75	84
13	20	28
14	17*	13
15	20	23
16	26	30
17	43	45

10,6,L

0	46	53
1	38	38
2	33	30
3	35	34
4	18*	9
5	40	40
6	20	21
7	19	11
8	27	26
9	17*	11
10	27	26
11	38	32
12	16*	5
13	15*	3

10,7,L

0	16*	14
1	17*	16
2	17*	26
3	27	21
4	19	12
5	22	19
6	40	36
7	23	17

11,0,L

0	38	16
1	121	117
2	114	127
3	138	130
4	100	95
5	104	92
6	37	39
7	57	65
8	102	113
9	99	108
10	46	48
11	161	168
12	85	86
13	87	92
14	70	67
15	98	98
16	20*	22
17	90	86
18	30	33
19	53	59
20	52	54
21	18*	11
22	59	63
23	17*	11
24	27	27

11,1,L

0	107	101
1	62	64
2	50	54
3	68	72
4	80	94
5	120	129
6	83	87
7	40	42
8	89	96
9	47	39
10	25	32
11	53	59
12	74	79
13	45	57
14	73	79
15	54	54
16	40	30
17	20	15
18	47	53
19	67	70
20	63	67
21	83	86
22	50	54

11,2,L

0	58	51
1	62	65
2	64	63
3	20*	22
4	20*	7
5	21*	17
6	21*	21
7	65	61
8	88	85
9	24	20
10	32	37
11	47	45
12	67	69
13	80	80
14	79	80
15	37	39
16	79	69
17	40	36
18	22	25
19	56	59
20	30	26
21	42	43

11,3,L

0	20*	7
1	53	55
2	77	77
3	26	29
4	51	48
5	20*	23
6	54	53
7	20*	25
8	39	38
9	85	79
10	25	14
11	24	29
12	67	65
13	48	44
14	65	64
15	33	27
16	45	43
17	32	36
18	17*	20

11,4,L

0	19*	4
1	36	30
2	42	46
3	34	33
4	41	29
5	34	30
6	19*	13
7	62	58
8	23	23
9	19*	15
10	35	44
11	34	32
12	21	16
13	43	38
14	54	62
15	17	12
16	31	33

11,5,L

0	38	38
1	41	50
2	50	44
3	21	27
4	18*	13
5	54	47
6	18*	21
7	32	38
8	17*	13
9	40	35
10	17*	19
11	17*	14
12	21	19

11,6,L

0	16*	4
1	19	16
2	25	20
3	24	25
4	16*	14
5	37	34

12,0,L

0	146	148
1	42	39
2	82	101
3	78	80
4	82	78
5	146	137
6	47	53
7	87	84
8	32	35
9	21*	17
10	20*	20
11	38	46
12	57	70
13	46	43
14	29	30
15	29	29
16	79	84
17	65	63
18	44	41
19	24	28
20	21	19
21	23	18

12,1,L

0	42	35
1	36	28
4	37	48
5	48	40
6	40	43
7	21*	11
8	45	44
9	68	71

12,1,L

10	31	28
11	61	57
12	24	27
13	20*	18
14	20	29
15	30	36
16	56	56
17	20	31
18	79	73
19	25	16

12,2,L

0	20*	20
1	20	23
2	54	68
3	30	25
4	32	29
5	51	53
6	43	47
7	45	44
8	19*	6
9	34	25
10	19*	13
11	30	30
12	21	21
13	38	34
14	26	26
15	21	26
16	25	29
17	30	27

12,3,L

0	64	64
1	19*	11
2	41	48
3	31	23
4	19*	24
5	20	19
6	23	30
7	37	34
8	35	40
9	17*	15
11	30	40
12	17*	2
13	48	49
14	43	42

12,4,L

0	18*	8
1	38	36
2	43	46
3	19	18
4	62	67
6	27	31
7	23	32
8	45	45
9	35	40
10	39	50

13,0,L

0	20*	1
1	28	31
3	35	29
4	60	60
5	64	58
6	67	67
7	30	32
8	35	37
9	26	25
10	19*	15
11	19*	31
12	29	39
13	31	25
14	51	50
15	29	30
16	25	28
17	68	73
18	67	74

13,1,L

0	20	19
1	41	48
2	36	32
3	41	32
4	84	89
5	24	21
7	44	42
8	18*	7
9	26	26
10	22	16
12	18*	21
13	51	46
14	23	21
15	25	27

13,2,L

0	18*	21
1	36	37
2	22	27
3	23	15
4	46	57
5	18*	19
6	18*	12
7	20	16
8	17*	9
9	31	27
10	17*	14
11	29	28
12	44	43

13,3,L

0	17*	19
1	53	49
2	20	17
3	17	12
4	20	19
5	16*	16
7	16*	6

14,0,L

0	75	82
1	43	36
2	55	59
3	74	79
4	65	58
5	30	32
6	34	37
7	28	19
8	26	31
9	17*	11
10	17*	7
11	24	28
12	32	35
13	22	15

14,1,L

0	88	91
1	45	39
6	17*	14
7	30	25
8	23	29
9	20	25

14,2,L

0	42	43
1	16*	9

15,0,L

0	75	80
1	20	26
2	42	46
3	16*	22
4	30	30

APPENDIX IV

Tables of observed and calculated structure factors for unsolvated tri-*o*-thymotide

Data Format:

	K	L
H	$10\times\lvert F_o\rvert$	$10\times\lvert F_c\rvert$

Reflections removed for extinction marked .... E

Reflections classed as unobserved marked ..... *

H,0,0

2	595	619
4	1019	1020
6	190	172
8	975	977
10	483	471
12	80	82
14	71	71
16	28	35
18	17	20

H,0,1

2	1782	1817
4	1292	1312
6	416	389
8	207	207
10	474	446
12	81	59
14	174	175
16	20	19
18	44	48

H,0,2

0	1181	1257
2	1891	1971
4	1554	1604
6	363	348
8	581	566
10	325	306
12	234	240
14	89	92
16	117	119
18	32	32

H,0,3

2	392	385
4	841	817
6	220	228
8	602	580
10	163	155
12	169	171
14	167	165
16	54	57
18	16	18

H,0,4

0	339	319
2	1383	1398
4	307	288
6	963	946
8	340	318
10	228	220
12	134	128
14	68	77
16	143	139
18	83	85

H,0,5

2	136	85
4	497	477
6	432	410
8	164	160
10	218	212
12	141	152
14	116	108
16	137	139
18	71	75

H,0,6

0	518	480
2	370	338
4	627	586
6	365	347
8	222	223
10	98	98
12	118	113
14	54	45
16	88	91
18	67	70

H,0,7

2	717	708
4	141	135
6	179	173
8	210	198
10	197	199
12	12*	10
14	124	120
16	46	45

H,0,8

0	219	211
2	173	165
4	277	280
6	85	80
8	278	284
10	135	136
12	86	79
14	51	50
16	27	27

H,0,9

2	196	181
4	183	171
6	206	188
8	178	168
10	126	124
12	40	46
14	48	47
16	29	21

H,0,10

0	229	226
2	171	149
4	138	136
6	162	164
8	232	233
10	137	136
12	123	120
14	32	37
16	23	23

H,0,11

2	86	92
4	100	97
6	148	133
8	157	156
10	132	136
12	24	26
14	37	36

H,0,12

0	85	90
2	90	91
4	102	102
6	86	89
8	168	173
10	46	43
12	96	101
14	29	30

H,0,13

2	60	57
4	188	198
6	108	107
8	109	109
10	56	53
12	48	48

H,0,14

0	164	170
2	81	78
4	87	92
6	71	70
8	48	57
10	64	70

H,0,15

2	15	9
4	71	72
6	61	70
8	33	25

H,0,16

0	58	73
2	40	37
4	26	28
6	14	22

H,0,17

2	65	68

H,1,0

1	1413	1453
2	21	14
3	571	554
4	1100	1144
5	148	160
6	514	506
7	309	286
8	249	266
9	174	181
10	182	160
11	19	10
12	178	181
13	89	86
14	110	110
15	41	43
16	25	24
17	67	69
18	31	30
19	35	42

H,1,1

0	153	136
1	1114	1148
2	711	721
3	1305	1326
4	101	95
5	485	475
6	435	423
7	121	116
8	302	302
9	301	302
10	112	94
11	38	30
12	132	136
13	92	90
14	40	41
15	78	78
16	51	57
17	43	48
18	56	57
19	21	16

H,1,2

1	350	281
2	457	452
3	527	517
4	332	307
5	450	423
6	201	188
7	321	328
8	370	355
9	209	205
10	150	147
11	164	161
12	85	78
13	108	115
14	17	10
15	94	97
16	85	89
17	22	19
18	21	20
19	21	21

H,1,3

0	424	415
1	370	379
2	846	841
3	443	451
4	648	661
5	537	530
6	137	130
7	338	318
8	246	244
9	41	36
10	107	107
11	30	33
12	141	143
13	33	37
14	56	59
15	74	79
16	69	72
17	48	50
18	37	37
19	9*	8

H,1,4

1	441	427
2	621	611
3	396	372
4	561	543
5	46	29
6	420	403
7	212	194
8	108	115
9	163	151
10	30	26
11	132	133
12	202	204
13	78	76
14	120	124
15	65	68
16	30	25
17	70	76

H,1,4

18	37	37
19	20	20

H,1,5

0	285	274
1	539	541
2	314	308
3	371	376
4	304	283
5	211	209
6	700	704
7	92	82
8	239	234
9	61	65
10	156	161
11	90	93
12	186	181
13	131	129
14	152	162
15	40	33
16	81	83
17	47	51
18	48	49

H,1,6

1	145	132
2	254	253
3	171	165
4	672	632
5	194	185
6	263	254
7	182	188
8	136	125
9	70	65
10	141	141
11	81	75
12	135	136
13	96	100
14	73	74
15	114	117
16	88	94
17	36	38
18	38	38

H,1,7

0	490	480
1	185	188
2	486	475
3	184	181
4	152	140
5	162	160
6	219	222
7	24	15
8	86	75
9	63	72
10	55	58
11	178	175
12	164	172
13	61	57
14	148	150
15	84	84
16	43	45
17	26	28

H,1,8

1	229	213
2	209	193
3	177	166
4	60	57
5	204	193
6	212	205
7	155	153
8	117	130
9	42	37
10	144	144
11	51	50
12	93	97
13	112	105
14	55	58
15	11*	13
16	11*	16
17	22	21

H,1,9

0	295	275
1	218	222
2	188	192
3	120	111
4	143	137
5	142	136
6	156	148
7	42	49
8	191	201
9	124	122
10	79	88
11	57	56
12	105	111
13	13	9
14	30	28
15	11*	5
16	39	39

H,1,10

1	67	53
2	147	156
3	60	51
4	128	128
5	61	64
6	82	86
7	148	132
8	123	127
9	91	91
10	153	172
11	61	65
12	14	17
13	71	74
14	41	42
15	43	43

H,1,11

0	234	221
1	71	73
2	81	85
3	92	98
4	99	100
5	34	28
6	70	72
7	114	118
8	117	125
9	67	65
10	80	87
11	156	158
12	71	76
13	78	80
14	23	25
15	10	6

H,1,12

1	59	61
2	147	152
3	82	76
4	144	145
5	21	17
6	109	116
7	55	59
8	41	45
9	132	136
10	42	52
11	86	83
12	53	56
13	31	30
14	33	36

H,1,13

0	136	138
1	88	93
2	88	92
3	55	56
4	42	34
5	146	148
6	116	125
7	43	44
8	34	34
9	89	85
10	78	80
11	14	14
12	53	59

H,1,14

1	58	49
2	37	33
3	58	53
4	140	144
5	25	27
6	59	55
7	43	34
8	32	34
9	64	66
10	68	71
11	16	12

H,1,15

0	19	29
1	11*	9
2	44	50
3	37	35
4	57	63
5	51	59
6	61	57
7	25	34
8	12	12
9	40	36

H,1,16

1	25	22
2	22	21
3	23	25
4	14	9
5	31	30
6	22	27

H,1,17

0	49	57
1	14	16
2	36	42

H,2,0

0	970	1001
1	153	155
2	808	833
3	666	673
4	768	769
5	395	378
6	102	122
7	159	157
8	361	354
9	92	77
10	178	179
11	201	177
12	125	114
13	38	35
14	32	34
15	13	11
16	12*	13
17	20	20
18	36	32
19	35	34

H,2,1

1	364	381
2	546	536
3	730	746
4	667	654
5	98	95
6	469	451
7	98	97
8	96	109
9	253	253
10	54	44
11	119	117
12	112	118
13	56	55
14	144	154
15	28	31
16	40	38
17	18	15
18	49	51
19	27	31

H,2,2

0	916	937
1	213	210
2	1091	1079
3	460	452
4	801	818
5	635	646
6	212	211
7	145	155
8	429	403
9	144	165
10	119	117
11	104	105
12	114	107
13	142	140
14	34	35
15	67	64
16	21	19
17	33	33
18	23	24
19	17	16

H,2,3

1	511	505
2	583	567
3	378	391
4	646	634
5	69	57
6	36	32
7	222	230
8	348	335

H,2,3

8	72	70
10	150	148
11	110	120
12	92	90
13	105	107
14	63	64
15	25	19
16	112	116
17	60	57
18	32	32
19	37	37

H,2,4

0	1195	1212
1	282	288
2	629	617
3	421	429
4	706	698
5	59	44
6	148	155
7	315	304
8	245	237
9	86	97
10	222	228
11	158	158
12	123	124
13	52	53
14	120	122
15	126	130
16	11*	6
17	38	39
18	32	33
19	35	36

H,2,5

1	177	184
2	199	207
3	111	118
4	218	217
5	376	351
6	248	261
7	197	182
8	155	140
9	53	48
10	107	107
11	50	59
12	67	82
13	175	175
14	148	153
15	24	27
16	17	19
17	45	50
18	43	45

H,2,6

0	441	431
1	140	147
2	194	190
3	385	397
4	257	239
5	87	75
6	180	160
7	234	226
8	221	208
9	174	172
10	48	43
11	141	143
12	214	218
13	63	67
14	80	80
15	104	105
16	120	118
17	76	79
18	53	56

H,2,7

1	327	298
2	208	203
3	111	101
4	400	406
5	135	141
6	245	247
7	133	130
8	204	208
9	23	26
10	197	206
11	99	96
12	118	113
13	144	146
14	122	117
15	61	58
16	53	54
17	26	25

H,2,8

0	341	354
1	268	265
2	75	78
3	212	214
4	149	138
5	156	159
6	188	184
7	37	32
8	98	96
9	162	164
10	31	32
11	100	103
12	93	91
13	21	18
14	65	61
15	58	60
16	33	26
17	12	11

H,2,9

1	147	132
2	24	20
3	55	58
4	129	126
5	105	99
6	24	23
7	98	105
8	95	96
9	126	131
10	98	97
11	51	51
12	25	13
13	40	41
14	51	50
15	48	48
16	20	18

H,2,10

0	33	31
1	102	98
2	231	224
3	137	137
4	67	71
5	46	56
6	59	68
7	70	75
8	24	29
9	81	85
10	53	52
11	87	96
12	56	59
13	74	76
14	22	20
15	10*	4

H,2,11

1	205	208
2	174	174
3	43	46
4	108	100
5	92	97
6	64	71
7	58	61
8	43	42
9	43	49
10	92	93
11	88	96
12	20	18
13	11*	12
14	32	33

H,2,12

0	65	56
1	102	104
2	156	159
3	161	165
4	103	110
5	76	79
6	68	75
7	59	65
8	87	82
9	86	92
10	15	13
11	45	50
12	47	47
13	10*	13

H,2,13

1	95	92
2	58	46
3	107	105
4	45	45
5	68	72
6	96	102
7	91	97
8	25	24
9	72	75
10	35	34
11	51	56
12	18	25

H,2,14

0	109	113
1	50	51
2	20	22
3	76	78
4	87	94
5	77	74
6	60	62
7	41	43
8	33	34
9	59	63
10	42	38
11	60	63

H,2,15

1	48	47
2	28	20
3	51	50
4	85	88
5	24	23
6	33	33
7	40	39
8	10*	12
9	9*	7

H,2,16

0	43	42
1	25	25
2	20	13
3	13	19
4	23	21
5	33	31
6	36	38

H,3,0

1	404	416
2	38	16
3	354	346
4	413	378
5	167	164
6	215	198
7	11	9
8	216	201
9	13	18
10	65	61
11	71	67
12	59	44
13	67	72
14	42	38
15	97	102
16	29	28
17	11*	7
18	31	32
19	10	11

H,3,1

0	244	253
1	316	293
2	537	526
3	691	692
4	152	131
5	327	325
6	251	241
7	189	183
8	65	65
9	98	105
10	196	200
11	106	109
12	67	73
13	66	67
14	50	53
15	58	58
16	41	38
17	91	92
18	17	27
19	16	15

H,3,2

1	106	93
2	473	483
3	354	338
4	303	297
5	106	98
6	190	176
7	296	281

H,3,2

8	215	207
9	160	159
10	150	147
11	117	116
12	110	113
13	85	87
14	55	49
15	101	104
16	35	32
17	18	15
18	16	13
19	64	69

H,3,3

0	848	844
1	655	638
2	402	398
3	177	165
4	112	96
5	186	187
6	172	165
7	383	372
8	156	151
9	126	116
10	53	56
11	40	39
12	28	26
13	37	42
14	62	55
15	44	43
16	24	18
17	75	77
18	38	40
19	9*	7

H,3,4

1	370	367
2	597	598
3	627	636
4	235	236
5	57	72
6	334	326
7	175	178
8	197	186
9	107	125
10	112	111
11	56	52
12	28	24
13	76	75
14	39	37
15	33	37
16	77	83
17	43	43
18	38	40

H,3,5

0	236	245
1	558	558
2	134	155
3	116	99
4	157	155
5	180	181
6	106	101
7	26	36
8	92	80
9	94	85
10	79	78
11	89	89
12	50	48
13	52	49
14	48	50
15	106	109
16	44	45
17	11*	10
18	13	18

H,3,6

1	153	154
2	75	63
3	396	390
4	232	217
5	326	319
6	139	139
7	151	142
8	212	215
9	109	111
10	225	225
11	23	29
12	14	19
13	187	189
14	20	15
15	61	56
16	21	24
17	43	39
18	68	73

H,3,7

0	219	226
1	152	155
2	92	93
3	71	66
4	78	84
5	21	23
6	105	101
7	165	156
8	182	177
9	45	45
10	73	73
11	242	240
12	38	29
13	27	28
14	112	112
15	36	36
16	21	25
17	40	36

H,3,8

1	186	180
2	138	133
3	268	273
4	126	116
5	94	97
6	128	137
7	20	15
8	142	139
9	171	177
10	20	16
11	24	21
12	124	124
13	112	112
14	42	38
15	44	45
16	32	35
17	9*	8

H,3,9

0	117	122
1	184	183
2	163	158
3	97	87
4	68	64
5	52	58
6	116	110
7	147	157
8	67	65
9	93	91
10	119	122
11	85	80
12	17	11
13	12*	5
14	23	24
15	42	41
16	30	34

H,3,10

1	124	122
2	50	54
3	97	89
4	100	107
5	92	93
6	56	56
7	65	64
8	112	112
9	64	70
10	26	26
11	19	15
12	59	57
13	34	36
14	18	18
15	12	13

H,3,11

0	163	170
1	119	117
2	79	81
3	141	148
4	75	71
5	51	54
6	61	67
7	12*	5
8	53	52
9	20	16
10	104	107
11	74	72
12	55	53
13	44	47
14	10*	4

H,3,12

1	123	120
2	81	86
3	84	82
4	45	37
5	79	82
6	67	64
7	24	23
8	46	46
9	22	20
10	78	84
11	31	35
12	48	47
13	20	25

H,3,13

0	116	108
1	48	49
2	80	80
3	85	90
4	25	23
5	28	22
6	28	31
7	52	58
8	58	53
9	69	66
10	21	23
11	39	44
12	17	17

H,3,14

1	88	87
2	45	48
3	12*	14
4	20	23
5	43	49
6	44	48
7	47	45
8	30	30
9	52	62
10	40	39

H,3,15

0	68	72
1	34	35
2	13	9
3	52	53
4	26	27
5	29	28
6	28	24
7	42	47
8	21	19

H,3,16

1	48	50
2	38	35
3	27	24
4	16	12
5	21	23
6	11	11

H,4,0

0	1441	1498
1	924	915
2	568	580
3	63	75
4	306	273
5	224	216
6	260	263
7	42	36
8	13	26
9	232	241
10	134	132
11	51	40
12	20	15
13	126	126
14	101	105
15	33	30
16	31	35
17	15	14
18	39	47
19	35	38

H,4,1

1	637	648
2	507	516
3	306	299
4	398	400
5	365	361
6	147	135
7	182	173
8	170	167
9	178	166

H,4,1

10	78	79
11	123	120
12	133	131
13	113	117
14	115	120
15	45	43
16	53	53
17	22	23
18	31	33
19	15	18

H,4,2

0	477	460
1	658	637
2	76	41
3	387	379
4	41	32
5	292	276
6	469	461
7	191	183
8	76	69
9	94	83
10	295	294
11	100	97
12	84	83
13	60	65
14	84	84
15	127	129
16	129	137
17	28	30
18	46	46

H,4,3

1	210	201
2	388	376
3	119	133
4	144	138
5	349	354
6	390	400
7	369	391
8	223	230
9	85	85
10	100	108
11	43	42
12	103	100
13	180	178
14	112	113
15	78	80
16	34	33
17	56	59
18	24	24

H,4,4

0	733	731
1	501	502
2	80	106
3	618	594
4	141	134
5	173	164
6	346	327
7	216	206
8	130	127
9	102	94
10	203	195
11	193	192
12	87	83
13	20	19
14	70	79
15	100	106
16	58	60
17	11*	10
18	54	57

H,4,5

1	52	65
2	430	415
3	78	75
4	200	204
5	223	219
6	68	73
7	306	311
8	127	129
9	48	44
10	110	111
11	73	73
12	46	50
13	113	115
14	54	55
15	54	59
16	51	52
17	60	60
18	18	18

H,4,6

0	267	260
1	50	27
2	40	39
3	154	149
4	126	112
5	165	148
6	28	29
7	74	67
8	214	210
9	125	124
10	147	146
11	73	69
12	118	118
13	128	128
14	15	21
15	56	51
16	65	62
17	74	79

H,4,7

1	70	76
2	256	261
3	104	107
4	151	149
5	83	82
6	179	170
7	129	125
8	209	203
9	90	100
10	184	189
11	202	205
12	21	22
13	66	66
14	63	58
15	40	38
16	47	48
17	14	13

H,4,8

0	170	159
1	224	218
2	213	207
3	199	200
4	99	82
5	209	209
6	225	227
7	155	166
8	308	312
9	191	193
10	61	62
11	134	134
12	95	100
13	12*	10
14	67	70
15	36	43
16	43	41

H,4,9

1	170	162
2	131	138
3	139	133
4	150	140
5	85	74
6	157	152
7	101	100
8	70	80
9	133	133
10	16	11
11	33	28
12	50	50
13	73	73
14	17	18
15	22	23
16	33	34

H,4,10

0	208	212
1	180	181
2	76	81
3	71	69
4	152	156
5	133	140
6	210	200
7	54	59
8	62	62
9	26	27
10	67	65
11	37	35
12	59	57
13	13	13
14	50	53
15	22	27

H,4,11

1	102	84
2	145	155
3	203	208
4	146	165
5	97	100
6	67	64
7	61	70
8	80	81
9	70	68
10	45	51
11	44	44
12	29	31
13	35	36
1	65	84

H,4,12

0	149	151
1	69	67
2	175	176
3	48	51
4	99	94
5	103	103
6	40	40
7	12*	9
8	57	54
9	54	56
10	24	27
11	42	49
12	15	11
13	16	21

H,4,13

1	59	63
2	106	115
3	45	43
4	97	107
5	34	36
6	72	71
7	20	21
8	22	14
9	11	6
10	24	27
11	36	38

H,4,14

0	201	201
1	104	107
2	73	75
3	58	58
4	53	52
5	35	43
6	42	39
7	57	58
8	23	22
9	15	14
10	48	49

H,4,15

1	67	68
2	68	73
3	41	44
4	17	18
5	63	61
6	29	24
7	14	22
8	42	51

H,4,16

0	81	80
1	77	76
2	21	26
3	54	53
4	17	15
5	22	22

H,5,0

1	178	169
2	25	18
3	444	438
4	720	709
5	213	202
6	53	56
7	268	249
8	99	95
9	180	164
10	161	158
11	12*	6
12	155	159
13	21	16
14	60	61
15	19	21
16	38	39
17	66	65

H,5,0

18	10*	1

H,5,1

0	385	393
1	408	408
2	278	269
3	151	144
4	311	290
5	260	257
6	420	401
7	208	208
8	210	200
9	125	126
10	27	31
11	119	112
12	88	85
13	83	84
14	188	183
15	36	35
16	66	66
17	21	20
18	43	45

H,5,2

1	75	67
2	335	329
3	298	280
4	488	459
5	366	354
6	292	276
7	104	83
8	209	199
9	246	239
10	58	66
11	20	22
12	186	196
13	96	97
14	117	119
15	78	74
16	71	73
17	11*	6
18	22	17

H,5,3

0	382	357
1	450	427
2	736	708
3	164	149
4	421	423
5	387	369
6	264	264
7	131	118
8	153	139
9	148	157
10	217	215
11	141	133
12	185	186
13	43	37
14	163	167
15	61	59
16	21	29
17	33	33
18	48	48

H,5,4

1	541	532
2	169	162
3	241	220
4	386	378
5	192	192
6	117	112
7	37	29
8	154	152
9	90	94
10	331	339
11	54	56
12	120	130
13	21	21
14	74	72
15	68	68
16	91	92
17	43	44
18	22	22

H,5,5

0	727	696
1	452	438
2	356	350
3	199	181
4	250	236
5	61	50
6	178	161
7	59	55
8	79	84
9	31	42
10	92	88
11	123	123
12	268	274
13	13*	6
14	73	69
15	65	62
16	28	34
17	14	14

H,5,6

1	179	170
2	39	42
3	281	270
4	140	149
5	112	108
6	78	74
7	122	124
8	109	112
9	77	80
10	141	147
11	126	125
12	47	48
13	68	74
14	81	79
15	69	69
16	43	43
17	20	20

H,5,7

0	115	99
1	170	170
2	77	67
3	78	83
4	93	89
5	109	129
6	22	121
7	340	350
8	171	172
9	139	138
10	114	116
11	97	100
12	113	117
13	91	95
14	78	75
15	36	43
16	25	26

H,5,8

1	173	175
2	65	69
3	265	259
4	310	306
5	176	172
6	69	71
7	214	213
8	163	167
9	84	94
10	155	158
11	157	168
12	115	114
13	55	57
14	47	48
15	27	31
16	60	60

H,5,9

0	198	198
1	285	286
2	300	303
3	197	205
4	92	92
5	165	170
6	122	121
7	100	103
8	175	185
9	90	94
10	55	55
11	76	77
12	29	28
13	43	42
14	26	21
15	10	11

H,5,10

1	209	210
2	161	149
3	248	251
4	77	90
5	212	221
6	279	288
7	100	107
8	25	23
9	76	82
10	47	51
11	56	57
12	20	25
13	38	41
14	36	43

H,5,11

0	147	148
1	275	286
2	95	99
3	165	169
4	112	119
5	55	57
6	86	82
7	103	112
8	52	50
9	53	58
10	16	15
11	47	48
12	26	26
13	51	54

H,5,12

1	84	94
2	79	82
3	155	159
4	66	73
5	152	155
6	25	24
7	68	70
8	45	42
9	82	85
10	41	41
11	41	42
12	55	50

H,5,13

0	63	61
1	78	74
2	102	105
3	51	51
4	74	80
5	88	92
6	35	33
7	75	80
8	43	48
9	50	47
10	48	44
11	22	19

H,5,14

1	43	48
2	59	57
3	61	61
4	22	23
5	11*	6
6	48	49
7	10*	7
8	53	52
9	36	38

H,5,15

0	76	76
1	16	15
2	36	41
3	36	36
4	35	31
5	45	48
6	91	91
7	57	56

H,5,16

1	23	24
2	49	50
3	44	39

H,6,0

0	194	194
1	368	374
2	165	164
3	112	106
4	565	530
5	402	383
6	354	331
7	74	63
8	86	93
9	230	227
10	138	142
11	12*	2
12	53	61
13	125	124
14	199	202

H,6,0

15	56	56
16	11*	5
17	13	14
18	23	21

H,6,1

1	94	91
2	442	443
3	447	450
4	48	47
5	294	297
6	297	281
7	209	203
8	236	241
9	130	136
10	147	153
11	116	120
12	82	77
13	84	88
14	100	94
15	35	33
16	80	84
17	25	27
18	25	26

H,6,2

0	463	448
1	377	360
2	579	559
3	347	339
4	215	191
5	343	317
6	230	219
7	220	208
8	163	158
9	99	99
10	72	66
11	147	148
12	252	252
13	113	117
14	87	89
15	94	99
16	62	70
17	36	37
18	19	19

H,6,3

1	394	381
2	367	345
3	500	453
4	296	292
5	287	292
6	75	80
7	94	107
8	161	158
9	117	113
10	290	302
11	15	16
12	41	42
13	135	141
14	82	78
15	12*	9
16	19	18
17	28	31
18	33	41

H,6,4

0	484	448
1	172	181
2	536	517
3	328	324
4	80	73
5	101	111
6	121	117
7	104	108
8	175	179
9	81	75
10	167	177
11	194	200
12	152	151
13	32	31
14	104	108
15	26	31
16	59	62
17	38	39

H,6,5

1	102	76
2	275	278
3	288	292
4	113	104
5	104	94
6	142	136
7	132	124
8	197	183
9	101	98
10	136	127
11	173	183
12	178	173
13	45	55
14	60	55
15	49	51
16	62	64
17	22	26

H,6,6

0	345	339
1	122	119
2	86	95
3	174	165
4	192	178
5	117	115
6	224	216
7	214	208
8	246	248
9	125	131
10	68	68
11	115	109
12	77	80
13	45	53
14	43	43
15	63	65
16	33	31
17	48	52

H,6,7

1	87	97
2	255	263
3	83	85
4	68	81
5	175	172
6	120	127
7	122	128
8	262	270
9	34	36
10	74	78
11	80	78
12	88	92
13	105	106
14	46	46
15	61	65
16	30	32

H,6,8

0	134	116
1	114	114
2	34	33
3	58	52
4	364	362
5	39	42
6	202	204
7	63	65
8	118	122
9	59	64
10	162	152
11	70	68
12	38	36
13	24	30
14	24	28
15	30	30

H,6,9

1	131	138
2	375	378
3	99	93
4	242	250
5	118	127
6	136	140
7	31	40
8	120	112
9	25	22
10	54	54
11	23	31
12	18	20
13	15	20
14	11	12
15	31	32

H,6,10

0	486	490
1	232	225
2	105	101
3	84	84
4	132	125
5	80	83
6	223	222
7	73	67
8	96	93
9	72	64
10	47	47
11	45	50
12	33	40
13	27	27
14	45	45

H,6,11

1	31	32
2	86	83
3	80	84
4	282	280
5	111	113
6	65	63
7	42	46
8	58	60
9	11*	8
10	76	67
11	30	27
12	25	24
13	19	18

H,6,12

0	97	102
1	143	144
2	224	212
3	137	135
4	120	118
5	34	38
6	65	62
7	69	74
8	51	48
9	62	63
10	15	14
11	42	39
12	47	48

H,6,13

1	20	19
2	46	50
3	61	65
4	81	83
5	100	99
6	48	50
7	53	57
8	50	56
9	34	37
10	9*	6

H,6,14

0	87	87
1	60	61
2	45	45
3	27	28
4	34	35
5	20	19
6	78	79
7	33	35
8	87	92

H,6,15

1	43	43
2	73	79
3	35	39
4	64	66
5	30	28
6	70	69

H,7,0

1	226	240
2	146	145
3	188	186
4	224	220
5	163	154
6	73	81
7	96	100
8	137	149
9	46	44
10	121	112
11	13*	3
12	98	101
13	71	65
14	13*	6
15	47	49
16	28	29
17	30	33

H,7,1

0	264	249
1	185	185
2	313	309
3	56	55
4	103	106
5	198	174
6	57	47
7	39	35
8	35	31
9	119	112
10	174	173
11	138	133
12	70	72
13	54	50
14	42	43
15	85	79
16	43	47
17	12	14

H,7,2

1	224	195
2	82	68
3	141	136
4	198	196
5	191	186
6	175	162
7	33	30
8	77	72
9	141	143
10	58	51
11	135	140
12	124	124
13	135	145
14	12*	11
15	51	57
16	47	48
17	13	12

H,7,3

0	145	134
1	64	68
2	185	175
3	118	117
4	185	174
5	132	135
6	48	44
7	144	135
8	33	33
9	187	191
10	59	55
11	135	137
12	39	40
13	45	45
14	34	29
15	56	58
16	29	27
17	34	43

H,7,4

1	109	92
2	159	151
3	225	217
4	151	145
5	69	68
6	169	159
7	81	80
8	64	59
9	138	143
10	70	76
11	222	223
12	98	95
13	71	78
14	28	32
15	69	76
17	33	42
16	50	56

H,7,5

0	344	338
1	93	96
2	55	55
3	113	105
4	143	132
5	101	96
6	53	43
7	104	110
8	84	94
9	132	125
10	36	38
11	69	68
12	19	17
13	53	54
14	91	95
15	41	45
16	24	20

H,7,6

1	180	168
2	104	104
3	93	96
4	100	90
5	59	64
6	100	100
7	264	257
8	114	120
9	187	187
10	72	83
11	49	51
12	63	71
13	97	96
14	90	94
15	43	43
16	39	42

H,7,7

0	58	58
1	223	211
2	100	104
3	60	62
4	123	109
5	136	139
6	71	76
7	146	144
8	89	81
9	143	149
10	90	86
11	66	66
12	62	63
13	72	79
14	22	23
15	45	43

H,7,8

1	132	136
2	49	42
3	164	166
4	190	181
5	200	200
6	68	62
7	226	236
8	152	154
9	39	36
10	98	99
11	38	34
12	14	10
13	40	38
14	66	64
15	33	36

H,7,9

0	146	144
1	129	124
2	151	156
3	277	275
4	66	72
5	189	195
6	172	163
7	101	97
8	145	149
9	35	28
10	30	35
11	41	48
12	51	53
13	21	21
14	9*	4

H,7,10

1	220	227
2	194	186
3	98	95
4	165	171
5	128	132
6	156	164
7	88	89
8	36	38
9	61	60
10	38	38
11	15	18
12	21	24
13	63	69

H,7,11

0	215	215
1	56	61
2	101	98
3	189	187
4	43	45
5	87	92
6	76	75
7	36	42
8	56	55
9	57	60
10	13	18
11	77	82
12	23	25

H,7,12

1	106	106
2	45	39
3	65	60
4	68	72
5	58	66
6	23	18
7	70	72
8	29	30
9	24	21
10	26	25
11	24	25

H,7,13

0	61	60
1	62	62
2	12*	14
3	38	38
4	50	50
5	75	72
6	41	44
7	31	30
8	44	44
9	47	52

H,7,14

1	28	29
2	15	21
3	69	67
4	19	17
5	15	22
6	26	25
7	9*	4

H,7,15

0	43	52
1	51	55
2	30	33
3	48	52
4	24	21

H,8,0

0	183	189
1	320	315
2	192	176
3	160	154
4	42	28
5	150	140
6	102	104
7	165	160
8	44	47
9	143	157
10	103	108
11	191	187
12	44	44
13	13*	10
14	44	53
15	67	70
16	39	46
17	41	47

H,8,1

1	191	191
2	97	103
3	160	154
4	64	58
5	185	193
6	103	106
7	161	161
8	70	66
9	68	64
10	74	80
11	52	51
12	57	54
13	97	98
14	92	89
15	25	25
16	23	21
17	45	50

H,8,2

0	116	110
1	208	205
2	31	20
3	199	202
4	56	50
5	175	174
6	128	114

H,8,2

7	73	69
8	113	117
9	83	85
10	75	70
11	87	88
12	15	19
13	19	15
14	31	30
15	58	60
16	77	79
17	14	15

H,8,3

1	221	231
2	56	53
3	282	289
4	137	128
5	130	133
6	206	203
7	100	92
8	72	78
9	156	163
10	105	110
11	133	133
12	37	35
13	30	36
14	48	51
15	53	63
16	44	44

H,8,4

0	443	436
1	127	122
2	85	87
3	71	72
4	46	33
5	93	89
6	188	189
7	45	51
8	71	71
9	167	165
10	32	26
11	68	70
12	41	43
13	42	41
14	26	23
15	30	30
16	73	82

H,8,5

1	110	104
2	188	187
3	41	35
4	101	102
5	201	208
6	39	38
7	92	97
8	81	80
9	106	105
10	56	50
11	48	43
12	33	36
13	83	89
14	28	24
15	31	40
16	18	18

H,8,6

0	76	69
1	131	123
2	174	177
3	68	68
4	83	81
5	107	116
6	108	100
7	95	95
8	98	101
9	75	77
10	69	74
11	64	64
12	78	82
13	43	45
14	27	29
15	82	90

H,8,7

1	86	84
2	70	72
3	94	93
4	55	59
5	92	90
6	48	48
7	71	69
8	111	114
9	23	26
10	21	19
11	37	37
12	19	16
13	58	57
14	52	48
15	31	32

H,8,8

0	178	188
1	76	74
2	79	76
3	27	35
4	58	58
5	84	81
6	38	36
7	39	43
8	66	67
9	91	81
10	36	36
11	75	70
12	55	59
13	43	42
14	27	27

H,8,9

1	102	97
2	99	99
3	150	151
4	93	92
5	62	65
6	14	14
7	127	129
8	73	75
9	97	102
10	24	27
11	88	89
12	74	72
13	10*	11

H,8,10

0	158	159
1	110	112
2	144	155
3	25	26
4	35	32
5	58	60
6	12*	7
7	107	108
8	23	22
9	75	81
10	22	26
11	21	18
12	10*	9

H,8,11

1	144	139
2	65	61
3	39	39
4	92	97
5	85	88
6	38	38
7	76	77
8	51	51
9	34	37
10	22	21
11	37	37

H,8,12

0	109	110
1	20	15
2	57	58
3	18	18
4	38	33
5	36	32
6	52	58
7	39	37
8	11*	6
9	43	48
10	13	15

H,8,13

1	20	16
2	59	59
3	15	15
4	53	56
5	52	54
6	28	29
7	21	21
8	17	13

H,8,14

0	89	87
1	14	7
2	37	41
3	43	42
4	27	22
5	12	14
6	9*	6

H,9,0

1	16	6
2	100	93
3	99	92
4	182	180
5	213	208
6	15	12
7	276	281
8	12*	11
9	13*	3
10	24	24
11	38	38
12	30	28
13	50	45
14	37	38
15	10*	3
16	16	15

H,9,1

0	282	288
1	72	67
2	223	214
3	151	153
4	145	144
5	187	195
6	118	119
7	138	148
8	24	27
9	30	27
10	102	107
11	42	39
12	30	29
13	32	32
14	12	15
15	23	24

H,10,2

0	261	264
1	148	143
2	126	129
3	186	183
4	80	75
5	173	163
6	203	205
7	34	29
8	147	141
9	125	129
10	128	128
11	86	87
12	101	107
13	48	48
14	67	67
15	22	21

H,10,3

1	101	99
2	255	243
3	58	59
4	136	133
5	134	132
6	40	29
7	117	118
8	160	158
9	55	56
10	130	132
11	89	94
12	74	79
13	75	76
14	24	21
15	71	69

H,10,4

0	229	221
1	223	219
2	151	153
3	94	97
4	219	220
5	29	38
6	82	84
7	103	97
8	97	95
9	181	191
10	36	31
11	89	87
12	83	86
13	51	50
14	66	65
15	32	37
16	23	24

H,9,2

1	79	61
2	113	117
3	28	21
4	176	181
5	265	269
6	218	222
7	105	92
8	86	88
9	206	206
10	34	31
11	26	24
12	59	58
13	46	42
14	28	29
15	49	52
16	22	25

H,9,3

0	31	33
1	15	16
2	111	113
3	95	97
4	24	17
5	82	80
6	103	92
7	61	64
8	162	155
9	86	82
10	86	90
11	127	135
12	29	36
13	98	103
14	36	38
15	32	32
16	51	55

H,9,4

1	196	186
2	60	61
3	43	33
4	59	62
5	43	43
6	107	109
7	108	111
8	83	84
9	30	32
10	112	116
11	61	63

H,9,4

12	72	72
13	66	72
14	38	39
15	17	22

H,9,5

0	117	121
1	52	46
2	110	116
3	196	203
4	114	113
5	41	32
6	118	120
7	40	39
8	86	78
9	27	23
10	94	94
11	45	48
12	24	26
13	24	23
14	54	62
15	19	26

H,9,6

1	42	41
2	141	139
3	115	113
4	82	82
5	72	71
6	31	27
7	70	65
8	122	128
9	82	87
10	64	71
11	66	70
12	37	40
13	27	29
14	44	46

H,9,7

0	91	95
1	28	32
2	98	96
3	58	63
4	49	53
5	54	45
6	82	80
7	138	139
8	29	28
9	54	57
10	66	63
11	69	74
12	34	32
13	10*	8
14	38	39

H,9,8

1	46	36
2	65	61
3	37	42
4	157	157
5	72	66
6	33	35
7	91	89
8	81	81
9	69	74
10	47	47
11	16	22
12	74	71
13	43	42

H,9,9

0	158	156
1	24	17
2	33	32
3	47	51
4	64	62
5	12*	8
6	92	86
7	113	116
8	83	87
9	15	18
10	11*	11
11	30	27
12	34	35

H,9,10

1	108	105
2	60	64
3	56	56
4	79	84
5	15	16
6	51	51
7	20	24
8	24	24
9	34	31
10	74	78
11	36	35

H,9,11

0	83	78
1	42	42
2	87	87
3	37	32
4	50	47
5	17	17
6	46	46
7	13	18
8	51	56
9	25	26
10	65	64

H,9,12

1	63	70
2	22	21
3	28	31
4	35	36
5	24	23
6	34	36
7	10*	5
8	35	35
9	19	24

H,9,13

0	79	78
1	53	55
2	55	58
3	33	29
4	43	45
5	26	25
6	38	40
7	20	19

H,9,14

1	39	36
2	22	24
3	11	18

H,10,0

0	183	195
1	538	540
2	120	121
3	144	142
4	117	118
5	188	184
6	210	208
7	150	158
8	12*	5
9	21	18
10	89	91
11	104	100
12	30	36
13	38	35
14	39	47
15	25	21

H,10,1

1	53	47
2	246	249
3	173	166
4	297	295
5	136	143
6	172	167
7	84	78
8	121	123
9	109	115
10	93	98
11	41	35
12	89	87
13	30	31
14	12*	16
15	37	43
16	23	24

H,9,5

1	129	132
2	147	147
3	103	100
4	226	230
5	78	89
6	85	83
7	78	80
8	46	61
9	52	55
10	44	50
11	67	68
12	64	67
13	42	45
14	9*	11

H,10,6

0	47	39
1	44	36
2	45	53
3	75	88
4	208	201
5	135	136
6	169	178
7	36	33
8	17	21
9	85	96
10	25	22
11	39	45
12	40	36
13	10*	11
14	19	23

H,10,7

1	147	156
2	75	80
3	77	78
4	110	122
5	66	64
6	109	114
7	145	150
8	105	107
9	25	29
10	69	67
11	11*	5
12	22	22
13	36	35

H,10,8

0	147	147
1	67	70
2	129	134
3	31	31

H,10,8

4	82	82
5	14	13
6	104	103
7	24	26
8	68	70
9	81	77
10	54	56
11	47	48
12	8*	1

H,10,9

1	13*	19
2	79	75
3	27	30
4	79	82
5	39	37
6	13	19
7	37	34
8	76	80
9	80	85
10	46	46
11	10	11

H,10,10

0	77	75
1	70	69
2	118	118
3	11*	9
4	54	50
5	11*	13
6	40	37
7	47	52
8	33	32
9	14	8
10	33	33

H,10,11

1	65	67
2	37	42
3	41	39
4	38	37
5	23	23
6	24	23
7	30	29
8	50	51
9	29	29

H,10,12

0	95	108
1	63	62
2	17	23
3	16	19
4	12	7
5	29	34
6	61	64
7	14	15

H,10,13

1	67	63
2	65	70
3	44	47
4	49	49

H,11,0

1	156	147
2	133	130
3	329	335
4	209	220
5	113	120
6	50	46
7	64	53
8	12*	8
9	12*	6
10	47	42
11	53	60
12	57	61
13	16	15
14	25	27

H,11,1

0	300	305
1	202	207
2	112	118
3	190	195
4	64	69
5	79	74
6	125	125
7	125	120
8	101	103
9	135	144
10	33	41
11	39	45
12	68	74
13	10*	12
14	12	13

H,11,2

1	256	263
2	248	255
3	87	79
4	184	188
5	174	175
6	118	123
7	184	192
8	68	67
9	99	97
10	35	35
11	93	94
12	44	37
13	33	34
14	40	41

H,11,3

0	141	135
1	206	208
2	228	233
3	179	181
4	102	108
5	102	108
6	57	59
7	110	108
8	18	18
9	166	162
10	52	52
11	68	70
12	20	16
13	26	28
14	34	37

H,11,4

1	124	132
2	59	57
3	182	188
4	164	167
5	75	76
6	91	92
7	52	53
8	57	53
9	51	52
10	51	50
11	68	74
12	11*	11
13	90	95

H,11,5

0	121	138
1	91	93
2	17	18
3	137	129
4	24	26
5	64	63
6	131	133
7	151	164
8	77	84
9	26	30
10	43	42
11	61	66
12	59	55
13	48	50

H,11,6

1	43	39
2	121	130
3	73	72
4	77	80
5	204	218
6	90	90
7	67	57
8	102	105
9	20	23
10	80	88
11	50	53
12	36	35

H,11,7

0	111	115
1	173	183
2	53	54
3	156	160
4	47	50
5	38	38
6	88	86
7	99	95
8	38	43
9	42	47
10	11*	4
11	42	41
12	58	59

H,11,8

1	55	51
2	78	80
3	138	150
4	51	52
5	82	82
6	74	76
7	53	60
8	67	75
9	87	89
10	51	54
11	23	21

H,11,9

0	17	23
1	119	122
2	60	57
3	47	55
4	12*	6
5	63	65
6	84	85
7	78	79
8	44	47
9	33	37
10	20	20

H,11,10

1	43	48
2	26	27
3	93	89
4	66	67
5	36	41
6	17	17
7	58	61
8	57	62
9	74	79

H,11,11

0	38	49
1	30	33
2	68	66
3	10*	13
4	19	25
5	61	59
6	56	55
7	46	50

H,11,12

1	60	55
2	28	33
3	13	17
4	80	83
5	78	81

H,12,0

0	335	340
1	250	248
2	66	64
3	50	45
4	13*	4
5	18	26
6	44	50
7	52	52
8	30	32
9	13	6
10	51	46
11	14	21
12	30	31
13	49	55

H,12,1

1	184	192
2	143	141
3	254	256
4	141	146
5	179	181
6	48	50
7	81	75
8	18	21
9	17	17
10	59	59
11	45	52
12	33	29
13	52	47

H,12,2

0	101	86

H,12,2

1	258	254
2	114	122
3	177	184
4	141	143
5	112	113
6	94	101
7	133	143
8	52	58
9	76	78
10	32	29
11	45	47
12	49	48
13	27	29

H,12,3

1	112	110
2	87	92
3	157	165
4	56	54
5	181	183
6	49	48
7	20	27
8	96	99
9	12	17
10	59	59
11	12	11
12	40	42
13	40	45

H,12,4

0	78	70
1	40	32
2	75	75
3	110	117
4	44	45
5	70	73
6	66	70
7	64	67
8	21	17
9	83	87
10	53	51
11	17	12
12	17	17

H,12,5

1	54	52
2	28	34
3	31	30
4	81	88
5	132	143
6	21	22
7	84	84
8	64	70
9	35	35
10	23	20
11	51	57
12	18	25

H,12,6

0	33	34
1	102	103
2	51	52
3	119	116
4	31	35
5	94	94
6	118	121
7	25	23
8	11*	6
9	58	56
10	42	41
11	56	56

H,12,7

1	76	76
2	27	32
3	25	25
4	78	82
5	37	44
6	43	45
7	89	93
8	40	44
9	33	35
10	32	30

H,12,8

0	95	96
1	12*	11
2	50	53
3	98	101
4	54	56
5	79	82
6	28	31
7	50	56
8	37	40
9	61	60

H,12,9

1	40	37
2	64	65
3	51	51
4	21	22
5	58	62
6	26	30
7	93	100
8	19	22

H,12,10

0	36	41
1	37	37
2	25	28
3	24	20
4	41	39
5	94	95
6	10*	6
7	20	23

H,12,11

1	12	16
2	32	31
3	54	57
4	59	57

H,13,0

1	332	324
2	35	35
3	59	55
4	62	59
5	43	42
6	12*	9
7	51	55
8	11*	9
9	11*	1
10	15	10
11	27	34
12	17	12

H,13,1

0	74	73
1	105	102
2	37	37
3	146	148
4	20	15
5	70	70
6	34	34
7	47	53
8	31	27
9	93	97
10	37	38
11	30	29
12	27	26

H,13,2

1	169	161
2	87	89
3	103	99
4	55	60
5	22	23
6	49	54
7	85	92
8	11*	9
9	35	39
10	10*	11
11	38	44

H,13,3

0	61	65
1	50	49
2	20	21
3	75	75
4	60	58
5	61	61
6	44	50
7	40	45
8	45	44
9	84	82
10	13	8
11	26	30

H,13,4

1	49	53
2	31	26
3	68	73
4	26	24
5	81	84
6	24	27
7	82	90
8	18	19
9	11	10
10	33	38
11	18	20

H,13,5

0	77	72
1	21	23
2	41	38
3	31	31
4	74	82
5	13	12
6	65	64
7	64	64
8	34	36
9	60	60
10	32	33

H,13,6

1	36	34
2	90	89
3	55	57
4	38	37
5	132	144
6	25	24
7	42	42
8	42	45
9	31	35

H,13,7

0	82	90
1	31	31
2	43	44
3	65	72
4	18	15
5	37	45
6	74	72
7	58	60
8	33	34
9	34	35

H,13,8

1	48	59
2	27	24
3	61	70
4	45	50
5	55	57
6	41	40
7	63	64

H,13,9

0	44	46
1	34	43
2	31	35
3	22	26
4	10*	7
5	18	15
6	55	61

H,13,10

1	41	43
2	44	46
3	10	6

H,14,0

0	16	24
1	13*	8
2	116	122
3	44	47
4	62	58
5	22	23
6	82	80
7	11*	4
8	11*	11
9	59	59
10	45	36

H,14,1

1	39	40
2	39	46
3	69	71
4	113	114
5	38	37
6	25	28
7	40	42
8	25	30
9	17	16
10	27	25

H,14,2

0	63	69
1	54	55
2	33	40
3	21	24
4	44	47
5	92	93
6	61	64
7	29	32
8	34	34
9	23	23
10	9*	9

H,14,3

1	23	24
2	48	52
3	50	53
4	52	56
5	32	35
6	30	33
7	33	39
8	23	20
9	33	35

H,14,4

0	71	67
1	20	18
2	59	61
3	11*	8
4	42	44
5	11*	8
6	15	10
7	57	56
8	40	43
9	63	63

H,14,5

1	37	37
2	35	36
3	42	46
4	22	20
5	34	37
6	17	17
7	57	57
8	21	21

H,14,6

0	40	38
1	69	65
2	11*	7
3	28	28
4	27	30
5	69	74
6	35	35
7	39	39

H,14,7

1	22	24
2	12	9
3	70	67
4	40	41
5	20	25
6	42	45

H,14,8

0	55	48
1	28	29
2	25	27
3	39	39
4	9*	10

H,14,9

1	9*	5

H,15,0

1	36	43
2	24	21
3	110	110
4	85	84
5	78	79
6	65	66
7	19	26
8	25	25

H,15,1

0	93	87
1	21	21
2	79	73
3	62	64
4	49	42
5	50	50
6	89	90
7	13	17
8	49	52

H,15,2

1	43	38
2	20	18
3	52	55
4	103	104
5	75	81
6	42	45
7	63	64

H,15,3

0	51	47
1	22	23
2	50	48
3	27	24
4	44	39
5	49	52
6	54	55
7	61	64

H,15,4

1	32	32
2	25	26
3	39	41
4	17	16
5	46	52
6	52	52

H,15,5

0	10*	18
1	41	41
2	14	13
3	10*	9
4	12	13
5	37	37

H,15,6

1	25	21
2	33	34
3	35	38
4	52	55

H,15,7

0	33	30
1	16	14

H,16,0

0	14	7
1	27	27
2	10*	4
3	9*	0
4	14	19

H,16,1

1	11	14
2	30	31
3	30	27
4	41	41

H,16,2

0	50	51
1	70	66
2	39	35
3	65	65
4	26	27

H,16,3

1	17	15
2	40	38
3	47	48

H,16,4

0	56	48
1	23	24

APPENDIX V

Tables of observed and calculated structure factors for 5,11-dibenzyltribenzo[*b*,*f*,*j*][1,5,9]triazacyclododecine-6(5*H*),12(11*H*),18(17*H*)-trione

Data Format:

	K	L
H	$10\times\lvert F_o\rvert$	$10\times\lvert F_c\rvert$

Reflections removed for extinction marked .... E

Reflections classed as unobserved marked ..... *

H,0,-17

2	84	82

H,0,-16

2	9*	0
4	62	62
6	15	30

H,0,-15

2	179	190
4	35	37
6	67	62
8	35	34

H,0,-14

2	376	379
4	116	111
6	9*	12
8	22	23
10	29	31

H,0,-13

2	11	17
4	31	43
6	333	330
8	150	139
10	64	74

H,0,-12

2	71	75
4	176	174
6	272	280
8	88	92
10	55	69
12	124	142

H,0,-11

2	10*	12
4	42	34
6	183	175
8	172	185
10	256	287
12	38	38

H,0,-10

2	212	219
4	490	496
6	227	206
8	69	67
10	98	101
12	9*	7
14	43	44

H,0,14

4	79	84
6	93	103

H,0,15

0	189	196
2	94	98
4	106	109
6	38	39

H,0,16

0	59	61
2	17	12
4	32	33

H,0,17

0	12	16

H,1,-17

1	20	27
2	20	19
3	62	62

H,1,-16

1	75	76
2	63	67
3	81	78
4	12	8
5	9*	18
6	8*	9
7	81	84

H,1,-15

1	35	45
2	50	56
3	34	39
4	27	29
5	53	54
6	28	33
7	9*	0
8	8*	4
9	60	59

H,1,-14

1	17	10
2	193	196
3	84	90
4	24	16
5	16	6
6	27	20
7	52	46
8	52	53

H,0,-9

2	226	227
4	84	77
6	128	131
8	90	88
10	15	14
12	125	128
14	71	64

H,0,-8

2	40	20
4	351	335
6	156	148
8	37	5
10	47	58
12	85	87
14	123	117

H,0,-7

2	326	303
4	111	119
6	88	78
8	18	22
10	31	19
12	110	119
14	37	29

H,0,-6

2	35	28
4	636	633
6	604	564
8	340	328
10	147	164
12	102	108
14	13	21

H,0,-5

2	783	868
4	747	730
6	434	416
8	82	66
10	161	168
12	86	86
14	18	27

H,0,-4

2	190	190
4	461	466
6	222	207
8	123	161
10	329	329
12	220	214
14	22	27

9	19	12
10	23	30

H,1,-13

1	272	278
2	291	288
3	229	232
4	254	254
5	10*	13
6	47	56
7	112	118
8	29	22
9	178	191
10	40	43
11	9*	2

H,1,-12

1	11	5
2	108	97
3	162	158
4	247	257
5	109	110
6	153	162
7	57	62
8	15	12
9	85	98
10	9*	0
11	54	47
12	19	7

H,1,-11

1	48	48
2	85	95
3	248	234
4	306	314
5	231	229
6	77	74
7	29	33
8	54	59
9	132	132
10	24	23
11	110	114
12	63	63
13	49	66

H,1,-10

1	32	17
2	19	18
3	91	84
4	93	81
5	322	313
6	150	157
7	98	94
8	102	92
9	165	159
10	32	36

H,0,-3

2	905	1024
4	298	301
6	595	600
8	172	168
10	52	49
12	185	177
14	57	62
16	93	115

H,0,-2

2	684	739
4	945	993
6	205	206
8	311	323
10	188	187
12	123	126
14	99	91
16	16	1

H,0,-1

2	1042E	1345
4	1198E	1339
6	179	170
8	616	581
10	230	203
12	31	40
14	164	167
16	29	18

H,0,0

2	950E	1103
4	1888E	2763
6	463	433
8	274	246
10	65	64
12	55	55
14	37	26

H,0,1

0	660E	1000
2	43	6
4	290	296
6	51	47
8	173	161
10	76	72
12	128	134
14	153	176

H,0,2

0	557	630
2	1251E	1630
4	578	515
6	267	253

11	85	84
12	52	45
13	82	71
14	12	18

H,1,-8

1	174	163
2	106	116
3	197	173
4	127	122
5	365	359
6	46	48
7	121	121
8	48	46
9	77	75
10	11	4
11	43	38
12	74	62
13	63	53
14	26	28

H,1,-6

1	182	161
2	177	166
3	125	132
4	21	7
5	110	100
6	14	13
7	113	103
8	18	12
9	152	157
10	52	54
11	111	110
12	71	77
13	41	36
14	48	49

H,1,-7

1	499	494
2	465	452
3	752	773
4	21	9
5	283	264
6	95	66
7	337	325
8	28	20
9	37	30
10	55	54
11	96	96
12	19	12
13	9*	11
14	39	40
15	58	69

H,1,-6

1	492	491

8	169	157
10	27	25
12	171	175
14	38	34

H,0,3

0	649	746
2	1073E	1283
4	136	127
6	463	442
8	208	190
10	23	34
12	100	105
14	10	1

H,0,4

0	13*	23
2	544	553
4	241	219
6	603	580
8	40	43
10	250	248
12	78	75
14	39	53

H,0,5

0	234	234
2	343	341
4	245	238
6	330	334
8	54	51
10	27	5
12	103	98
14	18	14

H,0,6

0	471	461
2	392	370
4	302	308
6	180	169
8	236	211
10	150	158
12	308	336
14	120	130

H,0,7

0	314	326
2	736	755
4	296	277
6	205	197
8	13	2
10	47	58
12	64	70

2	202	191
3	785	820
4	626	619
5	358	336
6	124	123
7	180	166
8	203	193
9	82	72
10	62	60
11	27	45
12	24	29
13	27	39
14	29	34
15	9*	6

H,1,-5

1	319	327
2	11	26
3	188	186
4	308	304
5	285	266
6	265	247
7	259	234
8	105	110
9	270	267
10	94	90
11	283	281
12	92	95
13	131	146
14	19	10
15	66	63

H,1,-4

1	737	823
2	47	18
3	772	814
4	130	120
5	384	372
6	82	91
7	11	1
8	161	151
9	415	380
10	285	286
11	203	221
12	96	96
13	31	24
14	34	30
15	50	54

H,1,-3

1	286	267
2	445	436
3	368	337
4	324	316
5	481	443
6	268	243
7	348	358

H,0,8

0	174	159
2	108	111
4	634	629
6	382	371
8	11*	9
10	38	40
12	23	22

H,0,9

0	104	101
2	187	175
4	74	82
6	38	37
8	139	141
10	12	12
12	34	43

H,0,10

0	255	257
2	55	52
4	118	103
6	83	78
8	139	136
10	47	43

H,0,11

0	157	158
2	33	20
4	18	16
6	24	20
8	40	35
10	61	59

H,0,12

0	104	103
2	120	113
4	12	6
6	44	35
8	25	33
10	8	5

H,0,13

0	162	163
2	45	46
4	9*	3
6	30	23
8	25	30

H,0,14

0	357	376
2	23	14

8	317	314
9	274	276
10	110	108
11	20	30
12	99	109
13	40	29
14	12	2
15	9*	7
16	20	26

H,1,-2

1	18	11
2	966E	1180
3	175	165
4	653	685
5	845	876
6	93	78
7	121	114
8	491	478
9	650	643
10	41	35
11	134	146
12	23	30
13	200	202
14	82	87
15	51	44
16	39	43

H,1,-1

1	895E	1211
2	423	424
3	992E	1131
4	251	247
5	702	721
6	147	146
7	44	33
8	235	230
9	378	381
10	32	22
11	16	10
12	118	124
13	39	31
14	84	97
15	97	110
16	15	11

H,1,0

1	452	454
2	450	468
3	1184E	1437
4	1306E	1601
5	112	71
6	237	249
7	100	114
8	395	384
9	214	198

H,1,0

10	133	122
11	51	37
12	99	111
13	98	116
14	64	69
15	94	110

H,1,1

0	141	149
1	948E	1221
2	41	31
3	1063	1196
4	816	836
5	669	673
6	491	458
7	35	14
8	217	193
9	59	55
10	12	6
11	63	71
12	118	120
13	62	50
14	23	21
15	30	29

H,1,2

0	327	338
1	197	198
2	919	1040
3	689	715
4	40	28
5	301	307
6	677	680
7	167	129
8	148	137
9	147	138
10	191	190
11	88	93
12	12	16
13	33	40
14	9*	2
15	46	43

H,1,3

0	183	174
1	851	962
2	969	1093
3	110	124
4	287	265
5	482	469
6	265	247
7	321	315
8	26	9
9	28	39
10	70	79
11	162	161
12	37	39
13	14	31
14	12	13
15	8*	11

H,1,4

0	416	415
1	82	69
2	687	726
3	289	285
4	112	100
5	581	580
6	374	358
7	16	19
8	65	66
9	35	24
10	93	93
11	159	143
12	34	38
13	14	24
14	63	69
15	94	117

H,1,5

0	401	409
1	250	260
2	130	123
3	18	2
4	72	74
5	201	197
6	21	35
7	126	107
8	209	201
9	72	64
10	86	76
11	242	255
12	55	59
13	106	105
14	17	16

H,1,6

0	218	217
1	399	394
2	102	88
3	122	135
4	8*	11
5	45	34
6	67	61
7	112	115
8	138	135
9	60	60
10	9*	11
11	82	74
12	61	65
13	15	21
14	10	6

H,1,7

0	28	28
1	435	404
2	466	456
3	53	61
4	64	60
5	160	150
6	159	155
7	221	222
8	53	45
9	50	60
10	76	75
11	88	108
12	35	32
13	48	54

H,1,8

0	243	227
1	117	111
2	65	57
3	127	98
4	65	61
5	146	138
6	57	46
7	174	174
8	12	10
9	19	6
10	44	53
11	15	10
12	17	14
13	30	32

H,1,9

0	150	148
1	113	106
2	176	167
3	337	314
4	137	123
5	121	109
6	106	111
7	37	30
8	110	110
9	140	145
10	89	99
11	84	92
12	9*	5

H,1,10

0	146	147
1	148	142
2	13	5
3	18	16
4	259	254
5	114	120
6	15	6
7	83	95
8	167	173
9	205	215
10	10*	16
11	51	51

H,1,11

0	87	88
1	123	112
2	28	29
3	30	31
4	52	56
5	158	145
6	85	91
7	10*	6
8	108	115
9	94	102
10	57	58
11	27	36

H,1,12

0	27	22
1	11*	0
2	51	53
3	74	74
4	12	10
5	9*	7
6	63	60
7	66	64
8	23	24
9	41	46
10	29	27

H,1,13

0	80	75
1	11	3
2	122	117
3	80	86
4	14	12
5	47	44
6	37	46
7	56	55
8	9*	3

H,1,14

0	75	78
1	180	181
2	99	100
3	153	155
4	9*	0
5	25	18
6	51	58
7	23	27

H,1,15

0	19	18
1	89	92
2	41	46
3	178	198
4	60	63
5	78	80
6	66	75

H,1,16

0	25	28
1	9*	1
2	96	98
3	85	98

H,2,-16

1	30	32
2	51	44
3	52	46
4	15	10
5	81	76
6	18	23
7	28	32

H,2,-15

1	19	10
2	62	61
3	15	6
4	12	7
5	11	4
6	33	24
7	28	23
8	42	47
9	35	28

H,2,-14

1	101	91
2	113	113
3	228	238
4	42	39
5	66	76
6	44	44
7	83	86
8	120	120
9	14	26
10	48	49

H,2,-13

1	293	304
2	147	150
3	342	349
4	157	158
5	145	146
6	60	50
7	11	8

H,2,-13

8	45	38
9	53	61
10	37	49
11	25	25

H,2,-12

1	63	55
2	197	207
3	137	137
4	160	164
5	148	151
6	205	198
7	193	205
8	13	8
9	10*	2
10	62	63
11	17	22
12	44	45

H,2,-11

1	129	114
2	179	172
3	316	311
4	12	19
5	32	28
6	278	276
7	53	44
8	178	176
9	135	142
10	42	34
11	60	69
12	78	86
13	15	7

H,2,-10

1	226	210
2	67	61
3	56	58
4	62	28
5	261	266
6	55	65
7	81	69
8	130	129
9	66	56
10	34	37
11	31	26
12	46	67
13	31	37

H,2,-9

1	43	55
2	215	205
3	122	116
4	256	245
5	134	131
6	116	133
7	33	35
8	71	76
9	11*	4
10	69	75
11	29	22
12	133	136
13	22	26
14	13	15

H,2,-8

1	405	383
2	148	135
3	122	119
4	358	338
5	33	31
6	124	116
7	29	29
8	45	49
9	11*	5
10	60	63
11	107	103
12	17	17
13	134	139
14	45	41

H,2,-7

1	128	104
2	257	254
3	424	401
4	43	35
5	372	345
6	53	52
7	209	191
8	91	95
9	147	134
10	17	33
11	160	159
12	119	127
13	130	140
14	72	69
15	63	64

H,2,-6

1	53	45
2	335	320
3	465	468
4	328	321
5	335	316
6	182	180
7	88	82
8	134	122
9	69	74
10	110	122
11	69	81
12	200	204
13	32	33
14	56	50
15	21	31

H,2,-5

1	383	388
2	836	905
3	28	28
4	351	330
5	359	359
6	204	177
7	10	12
8	87	87
9	126	110
10	40	24
11	168	169
12	124	121
13	78	70
14	32	32
15	68	79

H,2,-4

1	665	710
2	305	295
3	292	292
4	161	160
5	313	290
6	408	380
7	77	79
8	108	124
9	17	26
10	250	243
11	113	102
12	25	15
13	78	84
14	9*	3
15	47	53

H,2,-3

1	762	849
2	212	183
3	408	416
4	248	251
5	50	46
6	69	33
7	109	87
8	231	214
9	256	228
10	51	57
11	41	42
12	150	162
13	52	55
14	26	27
15	34	42

H,2,-2

1	231	224
2	354	341
3	273	248
4	331	312
5	36	15
6	37	37
7	63	48
8	110	105
9	221	207
10	47	36
11	82	90
12	82	83
13	126	134
14	51	42
15	44	54

H,2,-1

1	671	750
2	338	328
3	884	952
4	146	20
5	151	128
6	116	108
7	188	190
8	245	234
9	78	65
10	113	86
11	200	197
12	31	33
13	9*	5
14	62	54
15	143	172

H,2,0

0	925E	1537
1	582	617
2	145	73
3	721	727
4	538	496
5	413	386
6	342	315
7	266	255
8	560	537
9	62	66
10	125	135
11	188	190
12	61	52
13	56	63
14	90	107
15	115	140

H,2,1

0	280	243
1	69	58
2	596	618
3	1317E	1603
4	543	543
5	215	202
6	99	40
7	168	153
8	58	64
9	11	20
10	185	201
11	47	36
12	39	50
13	105	129
14	98	121
15	9	6

H,2,2

0	982E	1402
1	225	239
2	510	475
3	608	608
4	1070	1143
5	364	355
6	225	205
7	718	709
8	330	304
9	294	292
10	169	170
11	171	184
12	50	51
13	102	119
14	48	67
15	9*	4

H,2,3

0	187	159
1	578	593
2	360	340
3	690	668
4	563	546
5	65	40
6	195	159
7	374	356
8	81	84
9	205	202
10	74	83
11	82	85
12	17	2
13	53	63
14	39	50
15	63	63

H,2,4

0	204	190
1	705	727
2	610	610
3	361	343
4	227	229
5	753	738
6	326	303

H,2,4

7	16	12
8	72	77
9	87	91
10	35	27
11	53	49
12	63	70
13	52	50
14	9*	3

H,2,5

0	515	521
1	233	230
2	189	183
3	184	160
4	66	74
5	364	356
6	441	429
7	149	149
8	49	53
9	168	167
10	13	14
11	9*	4
12	67	60
13	9*	7
14	34	38

H,2,6

0	51	3
1	473	488
2	233	216
3	318	300
4	124	98
5	59	61
6	45	36
7	131	115
8	47	49
9	75	86
10	56	61
11	50	58
12	84	89
13	23	35
14	24	11

H,2,7

0	561	524
1	430	418
2	248	226
3	147	132
4	118	102
5	180	180
6	243	235
7	99	103
8	75	80
9	223	235
10	44	55

H,3,-8

9	166	162
10	15	10
11	52	59
12	98	89
13	13	7
14	99	96

H,3,-7

1	12	14
2	18	6
3	280	260
4	162	191
5	252	232
6	26	26
7	32	31
8	13	10
9	67	64
10	117	118
11	48	48
12	39	43
13	81	78
14	17	19
15	8*	6

H,3,-6

1	616	612
2	160	156
3	411	390
4	83	73
5	169	160
6	219	199
7	84	92
8	22	23
9	45	51
10	194	189
11	40	30
12	173	181
13	31	48
14	21	28
15	51	56

H,3,-5

1	187	184
2	641	659
3	73	48
4	70	78
5	25	4
6	243	235
7	179	164
8	103	95
9	67	67
10	202	206
11	29	36
12	182	196
13	68	82
11	47	41
12	9*	1
13	65	82

H,2,8

0	126	105
1	123	113
2	84	79
3	16	0
4	260	234
5	136	130
6	167	159
7	78	77
8	25	22
9	146	151
10	22	20
11	81	92
12	45	43
13	30	32

H,2,9

0	127	114
1	21	18
2	52	65
3	123	115
4	100	108
5	29	18
6	56	50
7	57	54
8	26	31
9	15	2
10	147	160
11	49	46
12	37	41

H,2,10

0	105	85
1	150	150
2	228	221
3	66	63
4	15	11
5	147	153
6	207	214
7	11	2
8	14	14
9	33	37
10	48	50
11	103	108

H,2,11

0	22	7
1	83	84
2	118	109
3	34	44
4	137	128
5	38	34
14	9*	1
15	20	18

H,3,-4

1	622	637
2	497	493
3	431	412
4	222	199
5	82	78
6	168	179
7	62	60
8	172	171
9	93	108
10	269	266
11	33	41
12	92	94
13	53	42
14	45	41
15	9*	2

H,3,-3

1	503	514
2	497	493
3	8*	6
4	294	275
5	445	428
6	15	8
7	195	204
8	173	160
9	16	23
10	68	65
11	24	9
12	113	136
13	35	43
14	45	55
15	136	146

H,3,-2

1	197	190
2	459	463
3	442	438
4	173	163
5	146	132
6	162	146
7	169	163
8	105	103
9	28	38
10	11	8
11	154	172
12	198	217
13	54	52
14	82	97
15	52	57

H,3,-1

1	506	525
6	31	40
7	16	17
8	81	83
9	12	9
10	11	8

H,2,12

0	238	235
1	136	141
2	85	83
3	67	63
4	24	23
5	91	92
6	103	104
7	115	118
8	9*	2
9	19	22

H,2,13

0	342	348
1	19	15
2	124	128
3	80	84
4	45	40
5	42	46
6	24	32
7	46	48
8	68	75

H,2,14

0	66	56
1	15	14
2	106	108
3	28	40
4	13	7
5	30	37
6	65	70
7	23	25

H,2,15

0	44	38
1	26	19
2	71	76
3	31	29
4	25	22
5	33	29

H,2,16

0	122	136
1	63	70
2	69	67
3	17	18

H,3,-16

2	268	271
3	798	815
4	7*	8
5	218	219
6	307	295
7	674	662
8	165	153
9	172	158
10	215	207
11	179	176
12	150	167
13	78	76
14	107	126
15	11	4

H,3,0

1	172	171
2	1545E	2128
3	105	93
4	325	324
5	182	162
6	143	137
7	389	378
8	297	284
9	186	167
10	75	82
11	71	80
12	225	242
13	23	14
14	44	55
15	34	36

H,3,1

0	219	198
1	57	61
2	702	701
3	1364E	1678
4	687	686
5	135	33
6	950	978
7	678	673
8	211	182
9	257	248
10	248	260
11	142	156
12	207	215
13	106	99
14	14	12
15	18	20

H,3,2

0	26	21
1	758	816
2	522	527
3	996	1073
4	314	300
5	266	241
1	12	15
2	32	32
3	9*	5
4	21	19
5	52	52
6	18	17

H,3,-15

1	178	180
2	12	4
3	22	24
4	84	87
5	92	93
6	72	76
7	9*	1
8	45	52

H,3,-14

1	99	95
2	145	142
3	9*	4
4	95	94
5	110	111
6	99	104
7	61	71
8	9*	2
9	18	30
10	32	37

H,3,-13

1	83	80
2	64	74
3	117	115
4	15	4
5	66	69
6	121	136
7	87	90
8	43	53
9	36	39
10	12	8
11	20	30

H,3,-12

1	35	34
2	71	72
3	239	241
4	346	354
5	24	11
6	153	160
7	158	172
8	73	68
9	198	189
10	53	51
11	37	43
12	78	83
6	371	364
7	619	612
8	340	311
9	82	77
10	119	114
11	89	81
12	19	25
13	75	83
14	19	28
15	8*	3

H,3,3

0	645	656
1	400	379
2	76	88
3	402	397
4	584	594
5	352	291
6	80	78
7	114	94
8	244	235
9	54	32
10	53	53
11	72	65
12	67	67
13	9*	6
14	41	39
15	8*	1

H,3,4

0	155	133
1	168	156
2	407	371
3	71	80
4	303	276
5	112	111
6	85	80
7	33	35
8	54	32
9	151	151
10	14	7
11	36	27
12	28	31
13	54	57
14	9*	8

H,3,5

0	89	83
1	126	113
2	210	201
3	198	188
4	135	109
5	313	287
6	48	24
7	17	15
8	280	280
9	209	209

H,3,-11

1	182	170
2	69	67
3	102	104
4	118	115
5	18	22
6	118	122
7	157	146
8	50	34
9	64	77
10	94	99
11	58	54
12	30	41
13	8*	4

H,3,-10

1	107	96
2	247	242
3	115	110
4	66	56
5	159	164
6	100	102
7	172	170
8	61	64
9	35	19
10	17	21
11	167	164
12	10*	17
13	120	117

H,3,-9

1	130	128
2	92	75
3	322	308
4	48	52
5	233	217
6	154	155
7	91	85
8	183	179
9	66	69
10	82	74
11	59	73
12	120	115
13	48	55
14	29	26

H,3,-8

1	198	202
2	240	218
3	36	17
4	28	50
5	147	148
6	77	68
7	31	25
8	10*	4
10	141	137
11	62	67
12	56	68
13	9*	8
14	41	43

H,3,6

0	180	170
1	53	43
2	400	377
3	186	163
4	133	122
5	207	199
6	58	48
7	22	21
8	312	309
9	162	156
10	140	138
11	41	51
12	54	69
13	67	70
14	63	80

H,3,7

0	575	566
1	153	150
2	229	216
3	86	94
4	347	321
5	19	13
6	111	113
7	61	60
8	105	104
9	140	147
10	63	62
11	108	119
12	32	41
13	44	49

H,3,8

0	271	246
1	219	209
2	161	147
3	64	50
4	142	137
5	71	67
6	240	229
7	30	12
8	184	182
9	111	122
10	41	41
11	63	62
12	9*	7

H,3,9

0	231	221
1	88	77
2	66	60
3	93	91
4	146	144
5	149	148
6	93	92
7	113	112
8	177	181
9	23	23
10	100	105
11	9*	1
12	85	95

H,3,10

0	30	44
1	23	22
2	61	66
3	125	120
4	18	17
5	209	210
6	126	119
7	69	74
8	83	89
9	203	224
10	52	51
11	17	16

H,3,11

0	80	73
1	174	172
2	80	74
3	43	47
4	26	32
5	119	114
6	203	205
7	85	92
8	59	62
9	114	125
10	122	129

H,3,12

0	43	18
1	36	36
2	66	72
3	82	82
4	20	21
5	38	46
6	58	53
7	22	22
8	36	35
9	27	30

H,3,13

H,4,-3

6	234	239
7	88	69
8	228	225
9	45	55
10	25	23
11	17	14
12	302	304
13	10*	3
14	140	156
15	64	71

H,4,-2

1	577	582
2	233	244
3	295	269
4	165	164
5	181	167
6	144	118
7	93	102
8	42	50
9	56	47
10	53	61
11	188	186
12	25	17
13	180	190
14	114	128
15	51	62

H,4,-1

1	681	698
2	486	465
3	264	245
4	112	90
5	625	601
6	468	448
7	109	119
8	123	112
9	28	31
10	41	36
11	210	216
12	16	13
13	89	81
14	61	64
15	10	14

H,4,0

0	106	88
1	323	294
2	397	391
3	557	543
4	95	74
5	311	293
6	289	292
7	76	83
8	72	57
0	20	14
1	18	20
2	18	28
3	171	178
4	60	59
5	145	150
6	11	8
7	59	54
8	66	66

H,3,14

0	225	236
1	51	51
2	42	43
3	20	13
4	34	38
5	43	41
6	68	72
7	8*	2

H,3,15

0	91	94
1	139	142
2	51	48
3	12	14
4	48	54
5	9*	5

H,3,16

0	23	22
1	22	22
2	78	82
3	57	69

H,4,-16

1	22	25
2	12	14
1	22	25
2	12	14
3	47	45
4	20	21
5	98	101

H,4,-15

1	9*	8
2	52	56
3	115	122
4	45	47
5	72	77
6	18	27
7	45	52
8	8*	3

H,4,-14

9	64	60
10	84	80
11	116	117
12	40	54
13	52	48
14	31	22
15	36	53

H,4,1

0	558	605
1	527	525
2	217	217
3	519	499
4	130	127
5	84	79
6	97	99
7	515	509
8	382	393
9	45	38
10	129	148
11	301	298
12	89	99
13	13	21
14	9*	16
15	8*	7

H,4,2

0	259	267
1	273	277
2	444	419
3	477	450
4	187	167
5	83	89
6	92	83
7	18	6
8	592	583
9	98	90
10	184	186
11	121	119
12	80	84
13	80	83
14	9	6
15	21	27

H,4,3

0	525	521
1	107	104
2	111	111
3	486	447
4	553	521
5	620	604
6	135	153
7	632	627
8	101	89
9	302	292
10	69	66
11	197	202
1	75	82
2	32	36
3	156	164
4	78	67
5	9*	14
6	37	42
7	108	119
8	9*	4
9	64	66

H,4,-13

1	86	89
2	69	68
3	184	180
4	23	21
5	32	26
6	53	49
7	28	21
8	34	29
9	57	48
10	65	66

H,4,-12

1	104	99
2	261	252
3	280	282
4	98	92
5	223	226
6	173	171
7	47	44
8	95	102
9	90	99
10	81	97
11	14	1

H,4,-11

1	122	111
2	173	188
3	121	119
4	208	205
5	111	103
6	185	198
7	31	42
8	125	141
9	150	163
10	177	185
11	37	46
12	11	7

H,4,-10

1	50	43
2	240	234
3	21	19
4	124	119
5	65	64
6	191	190
12	12	20
13	27	31
14	18	23

H,4,4

0	324	320
1	257	254
2	548	514
3	154	158
4	525	508
5	261	261
6	319	304
7	374	372
8	140	133
9	64	61
10	42	29
11	36	35
12	23	23
13	46	44
14	9*	5

H,4,5

0	206	183
1	339	317
2	132	138
3	450	435
4	115	106
5	20	11
6	24	5
7	71	71
8	134	123
9	19	13
10	78	83
11	40	42
12	70	76
13	29	34
14	11	16

H,4,6

0	292	281
1	108	79
2	228	196
3	247	237
4	169	152
5	194	168
6	141	136
7	39	39
8	268	271
9	235	234
10	113	116
11	47	57
12	77	79
13	21	24

H,4,7

0	229	204
7	210	214
8	15	11
9	109	122
10	46	48
11	111	100
12	58	72
13	14	1

H,4,-9

1	76	72
2	24	31
3	49	58
4	160	145
5	215	214
6	59	57
7	15	11
8	97	98
9	170	183
10	103	105
11	86	91
12	165	173
13	21	24

H,4,-8

1	371	344
2	211	213
3	182	174
4	216	203
5	273	270
6	23	12
7	92	90
8	12	8
9	218	229
10	23	20
11	77	75
12	155	163
13	66	61
14	84	81

H,4,-7

1	306	283
2	141	145
3	172	151
4	324	326
5	248	243
6	60	63
7	159	156
8	11*	21
9	125	127
10	59	55
11	158	159
12	18	14
13	23	23
14	20	15

H,4,-6

1	155	143
2	79	64
3	98	98
4	62	60
5	62	61
6	193	179
7	99	99
8	37	40
9	320	341
10	60	60
11	79	80
12	34	37
13	81	90

H,4,8

0	121	102
1	15	17
2	320	300
3	102	109
4	119	128
5	26	24
6	67	69
7	83	74
8	248	251
9	100	104
10	152	158
11	18	10
12	33	30

H,4,9

0	556	546
1	71	71
2	205	182
3	98	96
4	279	273
5	12	3
6	36	27
8	37	38
9	87	91
10	133	144
11	9*	3
12	29	30

H,4,10

0	285	286
1	13	3
2	120	108
3	52	47
4	208	218
5	30	25
6	49	44
7	101	100
8	38	36
9	47	37
10	88	93
11	48	50
1	219	209
2	778	779
3	143	129
4	180	178
5	19	16
6	122	104
7	108	113
8	102	82
9	231	240
10	76	74
11	53	62
12	100	101
13	107	116
14	29	31
15	24	35

H,4,-5

1	314	319
2	113	94
3	124	100
4	52	85
5	411	391
6	224	225
7	67	73
8	39	22
9	98	107
10	19	17
11	37	36
12	47	48
13	107	114
14	45	46
15	48	53

H,4,-4

1	61	63
2	701	717
3	77	61
4	258	258
5	155	152
6	72	59
7	25	21
8	238	235
9	120	116
10	96	99
11	67	75
12	251	269
13	20	5
14	159	161
15	52	49

H,4,-3

1	308	302
2	368	358
3	187	181
4	94	94
5	73	65

H,4,11

0	187	181
1	133	123
2	84	92
3	34	28
4	108	108
5	9*	2
6	69	73
7	24	30
8	43	44
9	9*	1
10	9*	6

H,4,12

0	218	213
1	154	152
2	69	67
3	23	20
4	32	32
5	191	197
6	98	107
7	41	41
8	42	42
9	21	27

H,4,13

0	132	132
1	40	37
2	40	46
3	106	99
4	13	15
5	54	52
6	13	10
7	51	52
8	14	11

H,4,14

0	47	48
1	114	114
2	210	218
3	18	13
4	111	117
5	54	55
6	47	47

H,4,15

0	54	54
1	17	15
2	84	90
3	9*	8
4	37	40

H,4,16

0	8*	13
1	9*	8
2	65	66

H,5,-16

1	15	12
2	44	47
3	24	24
4	11	13

H,5,-15

1	46	45
2	10	6
3	28	37
4	36	42
5	22	17
6	28	39
7	57	70

H,5,-14

1	9*	1
2	60	70
3	94	89
4	42	43
5	23	28
6	68	58
7	97	92
8	22	9
9	8*	1

H,5,-13

1	42	42
2	38	36
3	203	210
4	36	28
5	54	66
6	62	63
7	38	43
8	55	55
9	32	34
10	32	28

H,5,-12

1	133	132
2	60	56
3	51	50
4	128	122
5	129	115
6	9*	12
7	9*	3
8	28	27
9	126	124
10	22	21

H,5,2

11	168	170
12	126	134
13	25	12
14	74	94

H,5,3

0	511	499
1	185	168
2	173	147
3	638	632
4	198	193
5	236	204
6	497	459
7	110	88
8	398	399
9	198	190
10	57	48
11	48	52
12	55	41
13	13	15
14	9*	3

H,5,4

0	605	604
1	385	371
2	375	352
3	625	584
4	47	55
5	44	46
6	159	167
7	523	511
8	93	81
9	235	234
10	10*	15
11	20	24
12	14	20
13	27	26
14	9	16

H,5,5

0	299	258
1	95	83
2	69	64
3	164	151
4	48	41
5	214	197
6	15	11
7	238	233
8	74	73
9	129	129
10	81	89
11	70	64
12	45	52
13	9*	4

11	24	28

H,5,-11

1	208	205
2	44	37
3	30	21
4	48	47
5	300	305
6	240	250
7	62	45
8	153	167
9	93	109
10	95	95
11	43	39
12	12	19

H,5,-10

1	197	195
2	21	11
3	141	134
4	130	134
5	182	178
6	151	152
7	109	107
8	16	7
9	137	131
10	10*	13
11	75	85
12	69	74
13	36	40

H,5,-9

1	122	118
2	108	103
3	10*	18
4	42	40
5	35	20
6	12	21
7	75	66
8	97	105
9	47	51
10	65	73
11	92	92
12	48	59
13	89	86

H,5,-8

1	321	290
2	143	144
3	90	79
4	95	91
5	66	46
6	89	93
7	77	77
8	205	205
9	68	75

H,5,6

0	121	111
1	394	361
2	135	128
3	199	202
4	224	211
5	23	19
6	10*	2
7	178	172
8	197	201
9	63	63
10	116	114
11	31	34
12	36	45
13	26	36

H,5,7

0	219	216
1	32	23
2	454	433
3	169	172
4	102	94
5	71	59
6	77	70
7	50	52
8	141	134
9	184	182
10	63	60
11	25	35
12	152	172

H,5,8

0	76	58
1	183	157
2	55	53
3	85	85
4	194	189
5	42	39
6	76	67
7	180	183
8	117	114
9	42	48
10	115	123
11	13	16
12	82	97

H,5,9

0	302	286
1	50	47
2	72	71
3	126	123
4	19	8
5	120	115
6	51	50
7	137	137
8	139	141
10	33	40
11	168	166
12	103	116
13	21	24
14	34	25

H,5,-7

1	76	76
2	78	73
3	260	252
4	103	89
5	139	124
6	286	285
7	378	370
8	160	147
9	30	22
10	186	180
11	131	130
12	132	144
13	107	105
14	9*	10

H,5,-6

1	442	434
2	72	60
3	109	102
4	44	56
5	148	149
6	101	99
7	150	140
8	93	91
9	13	23
10	175	184
11	87	92
12	196	205
13	19	26
14	9	12

H,5,-5

1	267	244
2	156	146
3	13	9
4	118	106
5	56	58
6	43	38
7	29	33
8	71	70
9	60	65
10	117	105
11	111	107
12	65	58
13	56	56
14	20	23

H,5,-4

1	358	353
9	92	95
10	75	77
11	36	30

H,5,10

0	130	128
1	165	163
2	49	51
3	191	178
4	148	141
5	49	47
6	45	36
7	91	97
8	52	58
9	110	108
10	53	45

H,5,11

0	153	158
1	36	27
2	67	63
3	17	14
4	23	25
5	53	47
6	109	112
7	102	107
8	9*	1
9	10	12

H,5,12

0	48	49
1	12	16
2	70	56
3	44	36
4	116	114
5	10*	3
6	39	47
7	21	22
8	9*	1

H,5,13

0	54	56
1	85	83
2	65	73
3	23	25
4	182	190
5	114	116
6	111	115
7	33	36

H,5,14

0	16	10
1	61	57
2	39	33
3	92	95
2	20	32
3	603	573
4	321	283
5	295	283
6	21	21
7	260	262
8	56	38
9	130	123
10	115	121
11	360	366
12	147	157
13	137	143
14	28	9
15	21	22

H,5,-3

1	192	178
2	164	159
3	404	385
4	194	192
5	274	263
6	63	58
7	84	73
8	130	129
9	152	134
10	144	144
11	29	18
12	325	342
13	186	196
14	219	241
15	29	31

H,5,-2

1	530	515
2	663	652
3	238	224
4	247	244
5	184	167
6	94	91
7	65	52
8	45	46
9	54	42
10	40	36
11	212	224
12	101	118
13	72	59
14	41	55
15	15	5

H,5,-1

1	85	89
2	381	341
3	613	597
4	434	416
5	45	37
6	317	283
7	136	133
4	9*	6
5	83	86
6	116	123

H,5,15

0	22	24
1	78	84
2	39	37
3	73	83
4	40	37

H,5,16

0	68	77

H,6,-15

1	32	41
2	63	70
3	14	7
4	49	50
5	13	12
6	8	8

H,6,-14

1	37	33
2	124	122
3	94	91
4	111	113
5	9*	15
6	29	36
7	19	18
8	38	39

H,6,-13

1	133	137
2	15	27
3	15	1
4	67	75
5	55	60
6	11	5
7	22	26
8	29	41
9	52	57

H,6,-12

1	35	28
2	104	102
3	115	120
4	36	41
5	105	101
6	88	80
7	32	30
8	71	78
9	50	48
10	20	14
8	54	51
9	35	31
10	87	71
11	19	19
12	91	80
13	152	161
14	35	32
15	116	123

H,5,0

1	220	197
2	202	192
3	207	204
4	332	311
5	248	217
6	37	40
7	113	103
8	77	53
9	116	121
10	162	153
11	22	25
12	90	102
13	114	128
14	55	67
15	71	75

H,5,1

0	318	310
1	763	780
2	551	534
3	180	165
4	316	283
5	45	71
6	105	85
7	379	361
8	29	28
9	217	226
10	103	116
11	223	220
12	88	92
13	13	6
14	48	57
15	54	59

H,5,2

0	128	125
1	502	488
2	275	265
3	485	463
4	9*	2
5	272	252
6	181	165
7	411	391
8	111	83
9	41	41
10	147	148

H,6,-11

1	162	161
2	35	38
3	61	56
4	154	152
5	66	74
6	34	28
7	47	47
8	50	60
9	22	16
10	30	26
11	20	20

H,6,-10

1	89	86
2	75	61
3	74	75
4	109	115
5	44	38
6	198	189
7	245	262
8	11	17
9	208	226
10	111	124
11	33	33
12	12	4

H,6,-9

1	47	36
2	47	54
3	63	60
4	145	147
5	18	20
6	22	30
7	149	157
8	18	27
9	195	210
10	106	104
11	65	66
12	42	45
13	64	64

H,6,-8

1	276	267
2	106	108
3	26	28
4	45	42
5	283	280
6	300	305
7	36	19
8	105	96
9	238	246
10	73	77
11	39	32

H,6,-8

12	63	64
13	95	99

H,6,-7

1	291	285
2	283	278
3	178	172
4	158	156
5	214	200
6	186	193
7	59	70
8	177	174
9	263	274
10	123	128
11	107	108
12	86	93
13	33	41
14	32	30

H,6,-6

1	96	88
2	313	301
3	192	177
4	53	40
5	36	34
6	216	204
7	37	28
8	64	65
9	130	126
10	65	66
11	27	32
12	45	48
13	31	36
14	8*	2

H,6,-5

1	105	91
2	585	587
3	207	191
4	318	309
5	256	250
6	30	6
7	15	7
8	307	304
9	66	78
10	156	166
11	83	88
12	45	45
13	65	69
14	32	27

H,6,-4

1	93	105
2	812	834

H,6,10

4	251	258
5	12	10
6	62	59
7	195	214
8	82	95
9	156	169
10	30	31

H,6,11

0	87	85
1	16	25
2	154	163
3	223	225
4	101	89
5	13	7
6	59	57
7	128	137
8	101	108
9	95	102

H,6,12

0	56	54
1	20	28
2	163	164
3	189	201
4	10	10
5	105	103
6	70	68
7	9*	15
8	43	42

H,6,13

0	41	36
1	85	95
2	15	2
3	166	175
4	55	62
5	50	56
6	78	85
7	64	72

H,6,14

0	11	22
1	9*	9
2	53	56
3	36	47
4	57	53
5	47	53

H,6,15

0	51	61
1	83	80
2	37	39
3	400	379
4	345	342
5	359	341
6	155	153
7	15	14
8	270	284
9	327	329
10	86	91
11	269	284
12	141	147
13	24	10
14	19	16

H,6,-3

1	185	176
2	147	134
3	17	21
4	578	578
5	68	65
6	187	167
7	38	31
8	17	5
9	31	21
10	309	305
11	119	116
12	202	201
13	100	97
14	10	8

H,6,-2

1	35	28
2	284	267
3	265	264
4	196	183
5	155	141
6	60	63
7	27	34
8	117	106
9	62	33
10	34	34
11	123	125
12	11	6
13	183	203
14	34	38

H,6,-1

1	10	9
2	202	172
3	633	594
4	465	443
5	367	343
6	63	48
7	105	100
8	177	172
9	73	73
10	14	4
11	98	97

3	57	59

H,7,-15

1	15	14
2	82	84
3	65	68
4	12	4

H,7,-14

1	17	18
2	11	9
3	40	45
4	9*	7
5	84	92
6	43	38
7	11	16

H,7,-13

1	37	42
2	9*	0
3	78	82
4	145	141
5	52	49
6	48	59
7	22	27
8	60	70
9	8*	5

H,7,-12

1	11	3
2	38	43
3	40	38
4	67	60
5	23	26
6	113	114
7	9	6
8	51	59
9	28	20
10	58	56

H,7,-11

1	124	139
2	122	128
3	222	225
4	43	59
5	20	17
6	22	13
7	19	27
8	19	14
9	32	43
10	31	34
11	24	20

12	92	94
13	86	85
14	23	21

H,6,0

0	222	224
1	422	389
2	479	458
3	48	33
4	119	111
5	185	169
6	90	76
7	38	38
8	190	184
9	23	1
10	81	80
11	104	111
12	110	107
13	31	10
14	88	99

H,6,1

0	568	581
1	320	287
2	503	443
3	34	38
4	463	431
5	372	352
6	134	120
7	53	48
8	162	157
9	96	91
10	22	22
11	70	62
12	22	20
13	16	13
14	12	14

H,6,2

0	279	270
1	243	233
2	66	57
3	580	549
4	93	30
5	96	109
6	105	115
7	244	240
8	52	63
9	299	289
10	200	214
11	35	33
12	43	39
13	11	14
14	9*	16

H,6,3

H,7,-10

1	116	118
2	11*	13
3	204	200
4	128	131
5	31	27
6	93	104
7	9*	16
8	87	93
9	71	72
10	17	15
11	42	42

H,7,-9

1	25	21
2	166	164
3	176	169
4	34	20
5	151	149
6	150	148
7	65	56
8	77	87
9	22	21
10	137	137
11	9*	7
12	105	128

H,7,-8

1	81	76
2	51	46
3	212	209
4	29	29
5	133	125
6	164	167
7	102	98
8	9*	3
9	75	80
10	173	189
11	10	16
12	86	97
13	54	56

H,7,-7

1	108	108
2	35	39
3	183	178
4	12	5
5	63	60
6	83	75
7	309	309
8	36	36
9	139	137
10	10*	0
11	103	108
12	27	16
13	25	23

0	374	380
1	111	117
2	190	165
3	10*	5
4	35	25
5	152	136
6	164	153
7	30	48
8	71	68
9	136	141
10	238	244
11	10*	12
12	141	145
13	39	57
14	9	3

H,6,4

0	234	210
1	423	402
2	713	694
3	57	54
4	11	11
5	17	26
6	53	64
7	160	153
8	92	86
9	284	298
10	40	42
11	188	197
12	49	49
13	23	29

H,6,5

0	11	17
1	69	57
2	238	248
3	107	97
4	87	85
5	33	19
6	10*	6
7	105	107
8	165	165
9	143	148
10	260	284
11	68	70
12	103	111
13	76	93

H,6,6

0	74	61
1	89	69
2	21	4
3	211	205
4	34	22
5	26	29
6	204	194
7	202	210

H,7,-6

1	120	114
2	27	17
3	116	107
4	10	14
5	247	244
6	140	142
7	213	216
8	125	133
9	23	30
10	39	37
11	37	39
12	174	192
13	16	12

H,7,-5

1	124	109
2	9*	8
3	62	48
4	68	74
5	354	355
6	38	38
7	47	46
8	140	133
9	81	87
10	10*	6
11	72	70
12	169	177
13	52	53
14	79	94

H,7,-4

1	156	164
2	38	9
3	173	157
4	237	207
5	413	379
6	135	118
7	174	166
8	228	234
9	184	174
10	139	139
11	171	168
12	39	19
13	40	49
14	9	18

H,7,-3

1	113	104
2	106	80
3	68	72
4	404	377
5	32	46
6	75	56
7	101	89
8	46	52
8	145	146
9	97	103
10	74	84
11	21	22
12	51	50
13	66	81

H,6,7

0	61	59
1	79	72
2	17	13
3	142	137
4	17	3
5	61	58
6	88	83
7	67	71
8	228	223
9	303	319
10	82	83
11	111	122
12	34	38

H,6,8

0	166	159
1	104	100
2	88	92
3	61	66
4	120	125
5	35	31
6	87	82
7	10*	5
8	22	9
9	31	20
10	27	26
11	62	65

H,6,9

0	315	311
1	63	60
2	109	91
3	19	9
4	81	76
5	54	56
6	166	170
7	120	115
8	201	203
9	93	103
10	147	147
11	71	80

H,6,10

0	294	296
1	71	59
2	62	70
3	254	261

9	125	128
10	71	67
11	65	75
12	50	58
13	42	44
14	70	78

H,7,-2

1	82	71
2	143	134
3	282	261
4	25	25
5	127	124
6	14	19
7	81	80
8	47	39
9	103	97
10	269	272
11	21	20
12	112	128
13	51	71
14	43	49

H,7,-1

1	122	100
2	100	104
3	217	206
4	87	80
5	128	125
6	37	40
7	66	60
8	17	18
9	13	12
10	13	2
11	41	49
12	27	18
13	70	72
14	9*	5

H,7,0

1	194	189
2	133	120
3	136	130
4	224	201
5	59	45
6	247	234
7	52	43
8	36	31
9	192	190
10	65	69
11	19	17
12	81	74
13	92	106
14	18	26

H,7,1

0	280	293
1	266	261
2	581	556
3	200	187
4	40	50
5	255	255
6	112	102
7	38	30
8	30	27
9	87	88
10	85	97
11	119	117
12	17	36
13	85	81
14	29	35

H,7,2

0	327	301
1	475	442
2	185	190
3	298	277
4	499	477
5	114	109
6	26	4
7	69	51
8	85	80
9	46	39
10	219	216
11	116	129
12	90	86
13	100	111

H,7,3

0	587	584
1	399	376
2	60	47
3	168	164
4	15	8
5	58	42
6	32	35
7	186	181
8	190	184
9	55	49
10	80	66
11	62	57
12	34	42
13	10	7

H,7,4

0	433	419
1	134	125
2	57	58
3	25	21
4	242	229
5	17	12

H,8,-7

6	94	99
7	11	8
8	157	164
9	119	127
0	73	86
1	74	72
2	34	35

H,8,-6

1	81	74
2	88	88
3	182	181
4	220	214
5	262	259
6	39	38
7	91	91
8	62	62
9	260	273
10	17	33
11	116	127
12	44	41
13	22	14

H,8,-5

1	72	70
2	20	12
3	70	61
4	145	140
5	160	151
6	209	194
7	142	137
8	65	60
9	38	43
10	166	170
11	33	30
12	138	140
13	49	54

H,8,-4

1	89	91
2	66	68
3	222	208
4	271	254
5	12	10
6	89	92
7	78	78
8	76	76
9	125	119
10	122	133
11	104	110
12	32	35
13	46	48

6	145	139
7	34	34
8	13	5
9	203	200
10	125	135
11	174	181
12	123	135
13	44	41

H,7,5

0	197	193
1	289	282
2	25	27
3	339	320
4	110	93
5	19	6
6	147	148
7	11*	4
8	76	77
9	105	118
10	190	201
11	65	60
12	68	85
13	45	35

H,7,6

0	274	250
1	17	11
2	45	39
3	169	163
4	91	99
5	54	45
6	344	349
7	281	282
8	62	67
9	152	142
10	141	160
11	20	14
12	10	6

H,7,7

0	49	40
1	231	231
2	24	19
3	176	170
4	38	37
5	294	293
6	12*	10
7	283	283
8	56	62
9	22	24
10	40	46
11	17	18
12	25	18

H,7,8

H,8,-3

1	331	327
2	81	76
3	273	247
4	63	48
5	83	81
6	171	160
7	249	240
8	11*	12
9	293	290
10	22	15
11	151	152
12	9*	11
13	14	9

H,8,-2

1	41	29
2	161	160
3	35	29
4	100	96
5	67	67
6	394	381
7	223	221
8	30	19
9	227	236
10	85	94
11	47	40
12	41	41
13	49	56

H,8,-1

1	340	327
2	161	148
3	117	101
4	99	88
5	70	57
6	32	29
7	110	106
8	51	49
9	10*	13
10	88	96
11	126	121
12	90	93
13	70	67

H,8,0

0	28	35
1	95	101
2	71	60
3	11	10
4	11	3
5	29	16
6	100	92
7	12	9
8	46	48
9	77	91

0	200	198
1	107	98
2	70	57
3	119	118
4	37	30
5	202	200
6	251	254
7	75	75
8	10*	2
9	25	25
10	80	77
11	109	118

H,7,9

0	11	15
1	168	166
2	227	224
3	47	47
4	128	126
5	101	99
6	123	121
7	38	42
8	267	278
9	16	18
10	15	20

H,7,10

0	112	111
1	40	43
2	13	5
3	113	101
4	30	35
5	190	189
6	170	170
7	198	204
8	120	124
9	122	133

H,7,11

0	9*	7
1	55	52
2	62	65
3	10*	6
4	51	51
5	81	91
6	74	82
7	15	11
8	39	36

H,7,12

0	31	37
1	96	107
2	51	53
3	15	9
4	73	76
5	13	16

10	205	200
11	22	17
12	169	175
13	38	44

H,8,1

0	86	87
1	180	165
2	126	117
3	144	136
4	233	225
5	60	60
6	91	99
7	96	110
8	19	13
9	25	22
10	108	109
11	65	61
12	42	42
13	53	62

H,8,2

0	268	255
1	157	131
2	279	254
3	31	16
4	80	76
5	199	199
6	18	4
7	119	111
8	147	152
9	63	60
10	29	26
11	37	43
12	26	19
13	25	22

H,8,3

0	290	270
1	120	129
2	34	22
3	217	213
4	108	103
5	62	61
6	204	198
7	13	5
8	22	17
9	84	93
10	139	134
11	183	194
12	117	124
13	26	25

H,8,4

0	430	427
1	119	115

6	83	88
7	37	44

H,7,13

0	31	24
1	78	88
2	17	14
3	33	34
4	81	89
5	94	94
6	44	52

H,7,14

0	15	20
1	35	42
2	29	29
3	40	39
4	73	71

H,7,15

0	64	69
1	8*	14

H,8,-14

1	61	64
2	13	5
3	20	19
4	40	37
5	80	77

H,8,-13

1	80	85
2	32	31
3	15	5
4	9*	17
5	87	99
6	24	31
7	37	33

H,8,-12

1	24	26
2	172	189
3	77	77
4	64	73
5	20	8
6	29	22
7	117	116
8	77	80
9	15	18

H,8,-11

1	57	67
2	168	171
2	141	124
3	125	108
4	111	113
5	51	53
6	134	136
7	17	14
8	66	72
9	52	54
10	59	61
11	29	28
12	44	45

H,8,5

0	23	22
1	92	85
2	90	95
3	243	242
4	85	75
5	144	143
6	238	235
7	119	119
8	184	180
9	19	11
10	58	56
11	86	97
12	29	31

H,8,6

0	310	304
1	61	53
2	116	116
3	15	12
4	139	133
5	64	61
6	275	272
7	50	57
8	63	65
9	44	54
10	15	12
11	24	19

H,8,7

0	114	100
1	153	148
2	87	81
3	259	263
4	114	120
5	240	250
6	89	80
7	71	71
8	62	59
9	71	62
10	16	12
11	46	51

H,8,8

3	117	108
4	93	93
5	37	49
6	17	24
7	57	60
8	45	38
9	57	61
10	16	5

H,8,-10

1	88	86
2	122	121
3	261	267
4	54	62
5	157	154
6	136	147
7	164	160
8	57	70
9	30	26
10	9*	3
11	47	47

H,8,-9

1	111	118
2	30	45
3	260	253
4	179	181
5	10*	3
6	199	214
7	200	204
8	10*	7
9	149	161
10	42	49
11	10	7

H,8,-8

1	40	40
2	104	102
3	28	32
4	135	127
5	11*	7
6	169	174
7	139	153
8	11*	5
9	108	113
10	72	82
11	100	99
12	96	100

H,8,-7

1	42	42
2	102	106
3	36	26
4	31	29
5	59	62

0	12*	7
1	197	194
2	120	122
3	55	49
4	287	291
5	24	15
6	182	184
7	89	84
8	217	232
9	9*	3
10	71	71

H,8,9

0	56	55
1	53	55
2	119	114
3	190	182
4	77	78
5	191	208
6	54	53
7	75	76
8	106	114
9	48	60

H,8,10

0	26	24
1	125	125
2	74	77
3	54	40
4	25	30
5	49	52
6	9*	5
7	9*	6
8	24	18
9	11	6

H,8,11

0	194	193
1	60	55
2	61	62
3	61	65
4	21	20
5	9*	14
6	108	115
7	60	65
8	11	9

H,8,12

0	65	72
1	21	11
2	82	86
3	65	69
4	10	1
5	17	11
6	32	40

H,8,13

0	9*	0
1	12	7
2	9*	5
3	29	31
4	19	24
5	52	59

H,8,14

0	22	23
1	44	44
2	25	33

H,9,-14

1	71	82
2	40	40
3	21	24

H,9,-13

1	94	106
2	26	23
3	38	29
4	39	46
5	41	42
6	65	68

H,9,-12

1	15	5
2	68	63
3	57	56
4	123	121
5	10	2
6	39	50
7	37	38
8	28	23

H,9,-11

1	45	52
2	79	79
3	257	269
4	98	106
5	85	88
6	51	58
7	71	68
8	9*	7
9	17	11

H,9,-10

1	271	274
2	104	98
3	414	431
4	116	104
5	121	133

H,9,6

0	59	48
1	109	111
2	234	245
3	130	122
4	80	85
5	171	173
6	79	77
7	107	105
8	18	11
9	69	83
10	23	27
11	18	27

H,9,7

0	19	22
1	293	289
2	37	34
3	38	38
4	30	33
5	211	214
6	42	46
7	10*	9
8	9*	7
9	23	15
10	9*	1

H,9,8

0	137	138
1	213	226
2	23	27
3	135	134
4	72	68
5	97	105
6	95	102
7	168	172
8	90	93
9	66	78

H,9,9

0	179	179
1	186	192
2	86	80
3	189	190
4	40	40
5	53	52
6	65	66
7	152	164
8	22	26
9	20	26

H,9,10

0	145	120
1	66	64
2	106	119
6	81	85
7	154	148
8	65	72
9	9	4
10	35	44

H,9,-9

1	190	193
2	17	22
3	268	272
4	168	173
5	100	104
6	42	43
7	126	126
8	32	34
9	58	60
10	36	37
11	20	11

H,9,-8

1	28	23
2	101	104
3	120	113
4	121	124
5	72	76
6	54	52
7	105	107
8	17	23
9	38	36
10	30	37
11	11	10

H,9,-7

1	157	160
2	19	4
3	27	18
4	11	2
5	75	82
6	99	108
7	27	27
8	139	141
9	9*	2
10	18	18
11	15	23
12	18	8

H,9,-6

1	71	85
2	27	14
3	100	102
4	16	5
5	11*	4
6	69	78
7	107	110
8	10*	12
9	205	211

H,9,6

3	169	178
4	9*	16
5	34	37
6	57	65
7	10	12
8	68	73

H,9,11

0	103	99
1	119	124
2	39	41
3	59	61
4	37	39
5	9*	1
6	21	20
7	8*	2

H,9,12

0	161	162
1	26	27
2	28	32
3	37	44
4	65	66
5	23	28

H,9,13

0	34	32
1	13	18
2	8*	6
3	24	32

H,9,14

0	15	15

H,10,-13

1	12	4
2	108	112
3	8*	1

H,10,-12

1	40	46
2	13	3
3	48	47
4	33	30
5	48	60
6	24	24

H,10,-11

1	10*	4
2	187	197
3	138	137
4	41	47
5	9*	4
10	76	67
11	10	7
12	22	12

H,9,-5

1	186	188
2	44	35
3	97	96
4	48	50
5	209	209
6	177	173
7	58	65
8	95	110
9	108	109
10	10*	14
11	58	54
12	39	46

H,9,-4

1	137	116
2	72	60
3	15	16
4	292	284
5	30	30
6	63	62
7	231	240
8	38	45
9	129	124
10	115	114
11	21	11
12	22	22
13	107	119

H,9,-3

1	212	204
2	330	318
3	59	60
4	167	167
5	231	225
6	30	23
7	170	178
8	130	134
9	95	89
10	177	183
11	98	102
12	10	14
13	40	49

H,9,-2

1	93	82
2	212	206
3	75	65
4	126	119
5	200	200
6	49	56
7	58	49

H,10,-10

1	133	140
2	83	88
3	111	107
4	178	181
5	11	5
6	93	105
7	37	27
8	65	57
9	36	42

H,10,-9

1	23	6
2	36	25
3	42	59
4	184	188
5	89	82
6	15	6
7	13	6
8	79	72
9	91	90
10	34	36

H,10,-8

1	18	13
2	35	37
3	12	12
4	158	155
5	137	140
6	31	28
7	35	35
8	29	38
9	17	19
10	50	57

H,10,-7

1	19	12
2	75	70
3	180	187
4	133	131
5	154	156
6	104	113
7	44	46
8	21	31
9	30	26
10	49	50
11	48	43

H,10,-6

1	64	60
2	235	248
8	74	73
9	64	51
10	54	62
11	111	118
12	35	32
13	72	90

H,9,-1

1	85	80
2	284	264
3	102	104
4	160	153
5	45	47
6	119	106
7	133	135
8	122	118
9	34	31
10	71	75
11	168	176
12	56	60
13	97	116

H,9,0

1	159	159
2	53	43
3	309	300
4	23	16
5	120	104
6	143	125
7	69	70
8	40	45
9	104	99
10	32	31
11	85	90
12	34	38
13	54	69

H,9,1

0	239	231
1	152	134
2	128	120
3	10*	1
4	154	154
5	56	59
6	142	146
7	60	54
8	35	9
9	173	174
10	27	18
11	61	58
12	97	109
13	8*	6

H,9,2

0	307	301
1	181	166
3	79	79
4	78	75
5	137	134
6	94	87
7	13	20
8	113	120
9	58	55
10	15	20
11	26	22

H,10,-5

1	64	55
2	317	320
3	89	88
4	115	123
5	50	51
6	59	46
7	13	9
8	84	85
9	80	83
10	50	55
11	31	30
12	86	98

H,10,-4

1	48	52
2	47	48
3	157	155
4	31	28
5	143	143
6	42	47
7	36	27
8	84	83
9	30	33
10	44	25
11	16	17
12	86	88

H,10,-3

1	150	151
2	54	51
3	37	33
4	162	160
5	94	92
6	99	107
7	105	98
8	20	23
9	97	93
10	18	19
11	30	28
12	64	63

H,10,-2

1	297	298
2	140	140
3	81	73
2	176	171
3	204	191
4	131	128
5	13	6
6	33	20
7	22	18
8	14	6
9	197	198
10	13	22
11	21	12
12	49	57

H,9,3

0	114	117
1	22	14
2	48	47
3	202	187
4	37	34
5	14	19
6	97	97
7	26	32
8	58	62
9	10	9
10	35	39
11	15	26
12	109	121

H,9,4

0	125	109
1	108	92
2	62	65
3	331	317
4	187	171
5	63	63
6	85	83
7	71	74
8	16	16
9	111	120
10	113	118
11	9*	8
12	37	51

H,9,5

0	37	37
1	544	549
2	136	135
3	355	341
4	99	91
5	149	146
6	28	30
7	125	119
8	110	115
9	35	38
10	9*	8
11	21	18
4	56	55
5	88	92
6	91	91
7	102	111
8	20	26
9	171	183
10	61	69
11	18	14
12	22	16

H,10,-1

1	184	181
2	128	129
3	125	119
4	45	52
5	133	128
6	11*	14
7	106	106
8	29	19
9	206	210
10	9*	13
11	33	34
12	10	16

H,10,0

0	76	77
1	112	113
2	50	42
3	55	55
4	197	195
5	98	94
6	81	78
7	79	80
9	175	185
10	10*	11
11	21	17
12	86	91

H,10,1

0	235	238
1	117	118
2	311	310
3	39	41
4	366	345
5	234	244
6	108	100
7	140	150
8	54	48
9	212	222
10	126	127
11	57	55
12	36	46

H,10,2

0	53	41

H,10,2

1	352	344
2	50	36
3	14	23
4	47	42
5	58	58
6	40	33
7	17	9
8	26	15
9	86	93
10	29	32
11	20	18
12	28	28

H,10,3

0	64	56
1	81	82
2	153	153
3	215	219
4	43	44
5	172	181
6	206	209
7	124	127
8	24	13
9	19	14
10	40	47
11	9*	13

H,10,4

0	305	310
1	98	103
2	210	206
3	255	252
4	219	226
5	23	21
6	52	49
7	86	89
8	35	32
9	36	42
10	59	66
11	64	70

H,10,5

0	139	131
1	36	28
2	90	77
3	48	43
4	29	25
5	30	28
6	45	51
7	10	1
8	71	74
9	49	52
10	29	26

H,10,6

0	272	269
1	42	42
2	90	92
3	13	16
4	180	182
5	243	252
6	40	41
7	119	121
8	154	160
9	74	78
10	10	16

H,10,7

0	216	213
1	36	38
2	33	30
3	232	230
4	106	105
5	139	146
6	129	136
7	76	71
8	104	112
9	9	13

H,10,8

0	43	33
1	56	49
2	156	160
3	120	121
4	44	48
5	70	65
6	129	141
7	16	16
8	90	103
9	48	47

H,10,9

0	125	125
1	23	22
2	78	73
3	28	24
4	84	84
5	49	41
6	22	25
7	36	36
8	51	55

H,10,10

0	148	160
1	16	13
2	25	27
3	12	14
4	26	27
5	35	38
6	23	28
7	72	76

H,10,11

0	197	203
1	92	92
2	18	18
3	16	17
4	22	20
5	33	31

H,10,12

0	25	15
1	93	99
2	14	12
3	14	14
4	13	12

H,10,13

0	22	25
1	9	5

H,11,-12

1	13	13
2	37	37
3	41	63

H,11,-11

1	71	78
2	44	51
3	105	105
4	47	43
5	64	72
6	76	80

H,11,-10

1	55	51
2	58	64
3	23	32
4	25	26
5	29	27
6	60	64
7	39	44

H,11,-9

1	74	70
2	46	47
3	61	70
4	100	106
5	20	24
6	40	53
7	23	18
8	28	24

H,11,-8

1	163	165
2	178	179
3	52	56
4	268	276
5	22	24
6	128	136
7	30	26
8	67	70
9	12	12

H,11,-7

1	13	10
2	88	82
3	122	128
4	106	105
5	95	104
6	58	74
7	18	16
8	9*	10
9	13	14
10	75	85

H,11,-6

1	147	153
2	356	363
3	291	293
4	165	175
5	87	89
6	48	51
7	133	138
8	46	51
9	83	86
10	53	58

H,11,-5

1	76	69
2	13	1
3	19	25
4	104	108
5	23	25
6	18	18
7	123	127
8	76	86
9	33	26
10	25	19
11	45	39

H,11,-4

1	55	60
2	69	79
3	225	224
4	209	205
5	130	132
6	146	141
7	10	0
8	22	19
9	60	69
10	78	83
11	21	16

H,11,-3

1	170	179
2	191	196
3	334	336
4	146	143
5	30	37
6	28	17
7	12	17
8	48	54
9	23	23
10	87	87
11	29	36

H,11,-2

1	245	243
2	35	28
3	100	99
4	9*	4
5	124	115
6	28	11
7	28	18
8	32	20
9	9*	11
10	52	51
11	63	65

H,11,-1

1	32	37
2	28	31
3	11*	4
4	130	132
5	80	69
6	43	46
7	89	90
8	126	128
9	14	3
10	49	58
11	57	61

H,11,0

1	96	94
2	211	205
3	19	21
4	16	20
5	107	102
6	9*	8
7	39	46
8	207	222
9	40	40

H,11,0

9	55	55
10	12	8
10	53	63
11	68	84

H,11,1

0	112	118
1	144	146
2	166	170
3	47	45
4	72	83
5	33	40
6	13	18
7	15	16
8	122	131
9	135	155
10	84	90
11	27	17

H,11,2

0	211	218
1	70	63
2	185	179
3	189	194
4	45	53
5	74	73
6	58	73
7	18	1
8	152	159
9	77	84
10	66	72
11	37	32

H,11,3

0	484	494
1	335	339
2	201	207
3	176	171
4	82	76
5	109	109
6	13	17
7	37	25
8	66	71
9	51	43
10	66	70

H,11,4

0	64	65
1	142	146
2	61	68
3	41	43
4	51	58
5	111	116
6	115	125
7	65	68
8	10	10

H,11,5

0	105	102
1	32	30
2	14	18
3	46	43
4	51	46
5	75	78
6	119	129
7	24	25
8	10	8
9	16	23

H,11,6

0	188	196
1	30	34
2	237	247
3	176	176
4	129	131
5	74	79
6	72	71
7	55	61
8	55	57
9	20	25

H,11,7

0	162	161
1	68	77
2	58	65
3	35	43
4	138	143
5	17	16
6	90	102
7	59	69
8	31	32

H,11,8

0	108	107
1	119	119
2	86	96
3	22	18
4	74	81
5	52	54
6	9*	7
7	54	59

H,11,9

0	134	138
1	29	39
2	9*	11
3	33	39
4	46	46
5	58	56
6	23	28

H,11,10

0	25	26
1	36	37
2	55	56
3	9*	2
4	45	55
5	8*	2

H,11,11

0	91	93
1	78	86
2	47	48
3	73	80
4	15	11

H,11,12

0	66	68
1	123	131

H,12,-11

1	33	36
2	45	52
3	38	42

H,12,-10

1	97	103
2	39	35
3	26	29
4	25	29
5	73	79

H,12,-9

1	158	166
2	124	140
3	9*	2
4	72	77
5	13	1
6	9*	18
7	30	26

H,12,-8

1	24	26
2	84	85
3	53	57
4	9*	2
5	103	103
6	44	51
7	74	83
8	18	22

H,12,-7

1	246	253
2	115	130
3	279	283
4	19	12
5	160	170
6	72	78
7	19	14
8	8*	7

H,12,-6

1	128	131
2	52	53
3	157	163
4	75	74
5	19	18
6	38	33
7	34	34
8	25	28
9	17	23

H,12,-5

1	408	428
2	75	83
3	220	222
4	27	39
5	33	30
6	97	103
7	79	82
8	57	62
9	8*	3

H,12,-4

1	31	32
2	56	51
3	170	176
4	10*	10
5	42	47
6	117	124
7	129	130
8	105	111
9	47	53
10	20	11

H,12,-3

1	11	10
2	150	154
3	159	168
4	80	89
5	109	114
6	120	121
7	90	96
8	40	48
9	26	35
10	36	42

H,12,-2

1	403	412
2	58	49
3	72	70
4	99	97
5	63	61
6	89	97
7	64	65
8	38	39
9	12	19
10	8*	7

H,12,-1

1	189	193
2	9*	8
3	100	97
4	46	41
5	149	160
6	134	139
7	68	76
8	62	79
9	34	37
10	23	20

H,12,0

0	24	30
1	63	61
2	53	56
3	106	103
4	59	56
5	10*	6
6	158	174
7	53	55
8	20	21
9	66	84
10	32	28

H,12,1

0	109	116
1	173	180
2	177	176
3	65	57
4	127	131
5	117	123
6	166	172
7	173	194
8	54	56
9	145	163
10	15	8

H,12,2

0	312	327
1	152	152
2	120	126

H,12,2

3	196	202
4	191	195
5	26	19
6	39	35
7	59	62
8	15	13
9	20	24
10	16	24

H,12,3

0	207	214
1	136	136
2	76	68
3	83	99
4	180	182
5	36	40
6	37	51
7	94	108
8	66	74
9	63	76

H,12,4

0	44	35
1	128	126
2	47	44
3	40	41
4	33	36
5	44	36
6	43	53
7	11*	2
8	44	42
9	54	54

H,12,5

0	93	96
1	131	138
2	88	90
3	102	105
4	14	5
5	62	58
6	15	26
7	14	18
8	54	57

H,12,6

0	58	62
1	79	79
2	15	3
3	29	29
4	63	71
5	129	137
6	57	70
7	117	133
8	10*	1

H,12,7

0	11*	1
1	120	123
2	33	36
3	27	27
4	54	56
5	72	80
6	10*	16
7	63	72

H,12,8

0	45	39
1	34	40
2	11	4
3	43	39
4	45	47
5	36	36
6	15	17

H,12,9

0	11*	3
1	105	114
2	64	68
3	50	52
4	37	39
5	27	25

H,12,10

0	53	54
1	40	42
2	47	46
3	69	71

H,12,11

0	55	54

H,13,-9

1	40	40
2	57	51
3	11	10
4	22	31

H,13,-8

1	130	138
2	48	47
3	22	17
4	75	76
5	41	50
6	60	67

H,13,-7

1	14	6
2	82	84
3	9*	0
4	39	50
5	9	6
6	37	33
7	95	97

H,13,-6

1	96	103
2	170	181
3	117	125
4	158	172
5	9*	10
6	29	23
7	26	26

H,13,-5

1	114	127
2	10*	7
3	140	152
4	33	37
5	180	192
6	64	71
7	27	25
8	13	12

H,13,-4

1	63	64
2	145	159
3	24	25
4	33	36
5	29	28
6	42	36
7	45	54
8	98	99

H,13,-3

1	48	49
2	176	177
3	34	30
4	78	81
5	31	36
6	9*	2
7	70	81
8	8*	2
9	48	58

H,13,-2

1	86	87
2	252	255
3	196	206
4	24	26
5	164	168
6	94	96
7	51	46
8	33	30
9	27	26

H,13,-1

1	258	266
2	117	117
3	330	347
4	189	197
5	81	86
6	92	97
7	145	153
8	41	45
9	71	78

H,13,0

1	82	83
2	192	204
3	196	203
4	33	31
5	62	57
6	33	29
7	102	104
8	38	45
9	24	27

H,13,1

0	10*	14
1	14	5
2	294	302
3	90	89
4	22	12
5	37	37
6	115	119
7	9*	0
8	10	17

H,13,2

0	111	111
1	117	121
2	114	109
3	43	39
4	32	32
5	16	5
6	147	154
7	104	111
8	130	145

H,13,3

0	19	25
1	14	21
2	68	77
3	31	28
4	42	46
5	22	17
6	122	125
7	70	83
8	37	30

H,13,4

0	138	143
1	131	137
2	65	72
3	17	25
4	27	16
5	73	73
6	35	31
7	31	37

H,13,5

0	148	154
1	46	46
2	11	9
3	111	122
4	9*	18
5	30	29
6	131	141
7	21	17

H,13,6

0	21	19
1	65	72
2	13	3
3	30	24
4	118	119
5	42	41
6	65	66

H,13,7

0	40	38
1	9*	15
2	72	79
3	9*	10
4	9*	2
5	27	37

H,13,8

0	101	106
1	112	114
2	65	72
3	18	19
4	8*	8

H,13,9

0	20	21
1	49	59
2	54	50

H,14,-8

1	13	5

H,14,-7

1	18	10
2	39	48
3	66	74
4	18	9

H,14,-6

1	102	123
2	85	93
3	56	56
4	60	62
5	90	105

H,14,-5

1	79	80
2	52	57
3	66	76
4	45	56
5	9*	6
6	9	17

H,14,-4

1	14	15
2	112	118
3	100	100
4	72	78
5	45	51
6	58	53

H,14,-3

1	40	48
2	154	160
3	42	40
4	26	28
5	92	104
6	95	99
7	9*	4

H,14,-2

1	57	67
2	124	123
3	9*	3
4	58	62
5	9*	16
6	27	34
7	103	110

H,14,-1

1	15	25
2	148	159
3	99	99
4	91	97
5	80	77
6	74	88
7	8*	4

H,14,0

0	111	118
1	74	69
2	107	109
3	33	29
4	167	168
5	23	30
6	21	22
7	43	42

H,14,1

0	151	161
1	33	34
2	160	164
3	17	11
4	92	107
5	12	11
6	51	50
7	8*	15

H,14,2

0	10	2
1	52	47
2	41	44
3	95	99
4	51	52
5	110	115
6	35	42
7	8*	2

H,14,3

0	61	63
1	21	18
2	38	39
3	48	50
4	27	28
5	72	76
6	26	32

H,14,4

0	42	46
1	45	50
2	16	15
3	47	54
4	93	107
5	9*	9
6	62	63

H,14,5

0	76	83
1	47	53
2	49	56
3	57	62
4	59	63
5	12	10

H,14,6

0	147	152
1	14	17
2	63	62
3	26	31
4	13	8

H,14,7

0	155	169
1	66	77
2	99	106

H,15,-5

1	181	192
2	25	33

H,15,-4

1	37	38
2	46	48
3	17	12

H,15,-3

1	8*	0
2	39	43
3	8*	1
4	30	32

H,15,-2

1	51	50
2	76	78
3	34	37
4	22	24
5	29	25

H,15,-1

1	11	14
2	9*	12
3	36	33
4	23	21
5	37	39

H,15,0

1	21	26
2	69	74
3	112	122
4	95	103
5	52	49

H,15,1

0	107	112
1	55	60
2	39	45
3	38	48
4	70	82

H,15,2

0	25	25
1	77	81
2	9*	2
3	99	106
4	39	49

H,15,3

0	47	44
1	57	61
2	11	3
3	85	85

H,15,4

0	9*	0
1	143	146
2	8*	1
3	58	62

H,15,5

0	18	15
1	153	165

APPENDIX VI

Tables of observed and calculated structure factors for 5,11-dimethyltribenzo[*b*,*f*,*j*][1,5,9]triazacyclododecine-6(5*H*),12(11*H*),18(17*H*)-trione

Data Format:

	H	L
K	$10\times\lvert F_o\rvert$	$10\times\lvert F_c\rvert$

Reflections removed for extinction marked .... E

Reflections classed as unobserved marked ..... *

0,K,0

2	158	169
4	680	716
6	353	357
8	104	106
10	16	17
12	63	65
14	41	45

1,K,0

0	121	121
1	409	449
2	326	341
3	292	290
4	472	476
5	85	86
6	249	249
7	185	193
8	46	52
9	70	66
10	76	77
11	24	25
12	66	71
13	7*	6
14	6*	4
15	33	33

2,K,0

0	20	33
1	13	17
2	188	183
3	539	559
4	194	194
5	293	293
6	158	158
7	176	174
8	26	22
9	102	97
10	143	150
11	120	127
12	63	71
13	11	16
14	9	15
15	7	4

3,K,0

0	254	270
1	291	296
2	163	167
3	174	170
4	253	247
5	195	199
6	66	64
7	32	20
8	104	101
9	52	57
10	129	142
11	34	30
12	9	8
13	27	30
14	9	11
15	20	21

4,K,0

0	163	166
1	210	213
2	131	126
3	169	154
4	276	266
5	216	202
6	57	54
7	81	79
8	142	140
9	125	128
10	104	108
11	54	52
12	31	35
13	39	43
14	16	16

5,K,0

0	79	78
1	111	106
2	174	173
3	174	174
4	76	75
5	142	138
6	22	18
7	187	183
8	106	109
9	75	78
10	100	103
11	89	93
12	22	24
13	21	22
14	16	16

6,K,0

0	59	50
1	168	160
2	81	66
3	94	83
4	119	111
5	101	103
6	67	69
7	92	92
8	40	43
9	88	89
10	47	51
11	10	10
12	14	15
13	13	17

7,K,0

0	40	39
1	23	24
2	27	27
3	63	56
4	22	18
5	47	45
6	42	45
7	79	81
8	93	89
9	51	51
10	43	43
11	12	13
12	16	17
13	53	50

8,K,0

0	7*	1
1	22	25
2	24	30
3	90	87
4	35	33
5	39	41
6	45	50
7	76	79
8	46	49
9	58	61
10	15	15
11	6*	8
12	27	27

9,K,0

0	37	34
1	174	178
2	120	119
3	39	34
4	62	61
5	18	17
6	33	31
7	44	49
8	16	15
9	26	29
10	30	30
11	6*	3

10,K,0

0	48	41
1	89	84
2	46	45
3	65	60
4	83	80
5	68	74
6	14	17
7	35	39
8	37	38
9	43	43
10	29	32

11,K,0

0	26	20
1	32	35
2	66	64
3	19	20
4	53	56
5	42	44
6	21	22
7	28	27
8	34	30
9	28	28

12,K,0

0	7*	2
1	13	12
2	20	18
3	30	26
4	37	37
5	39	32
6	42	38
7	19	17

13,K,0

0	8	6
1	39	31
2	40	33
3	35	30
4	34	29
5	46	39

-13,K,1

0	11	6
1	32	30
2	18	19
3	28	24
4	28	24
5	38	35

-12,K,1

0	25	30
1	15	10
2	26	27
3	33	37
4	32	31
5	38	39
6	35	33
7	20	18

-11,K,1

0	61	58
1	68	70
2	180	175
3	62	58
4	66	67
5	19	14
6	58	57
7	12	12
8	15	17
9	29	24

-10,K,1

0	41	42
1	145	149
2	143	144
3	70	69
4	66	63
5	74	73
6	39	36
7	28	24
8	35	33
9	41	42
10	16	17

-9,K,1

0	72	67
1	89	85
2	62	64
3	100	103
4	85	86
5	54	51
6	75	79
7	30	33
8	41	38
9	31	30
10	14	14
11	15	17

-8,K,1

0	11	9
1	31	28
2	42	44
3	34	42
4	23	24
5	50	56
6	58	57
7	67	71
8	114	116
9	61	63
10	28	30
11	13	14
12	34	34

-7,K,1

0	100	89
1	173	172
2	88	90
3	9	14

-7,K,1

4	105	109
5	18	24
6	63	67
7	90	94
8	48	50
9	55	55
10	59	64
11	25	27
12	13	11
13	18	15

-6,K,1

0	70	64
1	139	137
2	34	36
3	202	200
4	59	63
5	148	150
6	50	50
7	133	140
8	100	108
9	68	70
10	87	98
11	47	50
12	10	13
13	32	33

-5,K,1

0	132	129
1	224	229
2	111	114
3	199	197
4	96	101
5	73	74
6	62	66
7	26	23
8	50	51
9	68	65
10	44	45
11	54	54
12	27	24
13	6*	9
14	21	21

-4,K,1

0	84	79
1	205	197
2	152	155
3	116	119
4	108	100
5	91	95
6	86	85
7	26	25
8	46	45
9	93	94
10	128	133
11	124	130
12	16	18
13	21	19
14	32	28

-3,K,1

0	601	624
1	477	486
2	290	289
3	163	170
4	68	64
5	226	217
6	118	113
7	73	75
8	63	60
9	49	49
10	91	94
11	50	49
12	16	18
13	16	18
14	18	19
15	14	13

-2,K,1

0	951E	1127
1	486	504
2	190	175
3	55	45
4	70	60
5	39	33
6	197	182
7	130	118
8	69	78
9	73	69
10	38	37
11	107	113
12	47	51
13	32	34
14	22	21
15	16	16

-1,K,1

0	23	14
1	704	750
2	235	237
3	215	206
4	303	297
5	197	183
6	144	144
7	58	63
8	56	54
9	46	42
10	48	50
11	27	25
12	16	23
13	10	13
14	28	27
15	40	38

0,K,1

0	506	505
1	284	286
2	588	599
3	281	274
4	191	187
5	278	266
6	367	342
7	26	35
8	177	174
9	87	90
10	80	83
11	38	44
12	26	29
13	28	25
14	29	35
15	32	31

1,K,1

0	374	418
1	129	126
2	94	93
3	78	77
4	267	266
5	109	112
6	160	146
7	137	130
8	99	100
9	81	85
10	144	144
11	47	44
12	55	57
13	51	55
14	31	36
15	14	18

2,K,1

0	422	458
1	369	380
2	187	192
3	378	372
4	318	302
5	316	303
6	89	85
7	131	129
8	158	157
9	15	12
10	153	157
11	79	81
12	38	41
13	18	18
14	8	9
15	21	23

3,K,1

0	123	132
1	305	318
2	199	197
3	448	442
4	299	298
5	282	272
6	84	73
7	184	176
8	90	89
9	202	201
10	121	125
11	78	81
12	50	55
13	11	7
14	22	24

4,K,1

0	276	279
1	196	196
2	161	155
3	361	354
4	339	329
5	81	78
6	64	63
7	166	167
8	177	174
9	56	56
10	61	61
11	65	71
12	18	16
13	35	36
14	6*	9

5,K,1

0	310	315
1	264	258
2	83	76
3	78	71
4	104	101
5	102	96
6	39	35
7	159	163
8	57	56
9	122	127
10	61	65
11	64	66
12	45	47
13	34	33
14	22	22

6,K,1

0	25	24
1	37	38
2	22	26
3	60	59
4	39	40
5	44	40
6	34	34
7	121	129
8	35	41
9	113	123
10	31	31
11	37	39
12	14	12
13	14	13

7,K,1

0	111	110
1	136	134
2	22	23
3	116	111
4	115	109
5	19	24
6	41	40
7	79	85
8	37	38
9	75	77
10	48	52
11	12	15
12	34	36

8,K,1

0	146	146
1	89	90
2	94	97
3	98	102
4	37	33
5	24	26
6	38	39
7	14	21
8	15	18
9	45	54
10	15	13
11	7	7
12	15	18

9,K,1

0	76	72
1	90	90
2	20	17
3	111	113
4	55	56
5	92	98
6	42	50
7	54	55
8	16	19
9	38	41
10	6*	3
11	19	18

10,K,1

1	126	121
2	110	111
3	40	41
4	84	86
5	29	31
6	47	51
7	9	7
8	27	28
9	7	6
10	21	21

11,K,1

0	7*	6
1	19	22
2	32	32
3	7*	6
4	24	22
5	10	11
6	21	20
7	16	14
8	30	27

12,K,1

0	19	13
1	19	19
2	10	10
3	19	17
4	8	6
5	14	14
6	41	38

13,K,1

0	20	17
1	6	7
2	6	3
3	5*	3

-14,K,2

0	5*	5

-13,K,2

0	18	20
1	32	32
2	30	29
3	6*	4
4	40	42
5	19	18

-12,K,2

0	7*	7
1	32	33
2	58	60
3	48	50
4	18	20
5	20	19
6	12	12
7	5*	2

-11,K,2

0	72	71
1	54	51
2	124	122
3	85	78
4	67	66
5	25	24
6	32	29
7	31	28
8	19	22
9	11	8

-10,K,2

0	12	17
1	29	30
2	46	43
3	41	41
4	31	30
5	40	44
6	34	33
7	25	27
8	69	68
9	23	25
10	15	16

-9,K,2

0	46	40
1	86	86
2	46	46
3	63	65
4	39	33
5	58	61
6	63	60
7	21	19
8	35	39
9	48	48
10	6*	8
11	6	6

-8,K,2

0	136	126
1	112	115
2	95	101
3	138	142
4	86	86
5	71	73
6	136	138
7	103	106
8	63	67
9	30	31

10	11	15
11	34	33
12	9	6

-7,K,2

0	30	24
1	75	70
2	245	246
3	66	66
4	28	29
5	81	86
6	190	197
7	42	38
8	70	72
9	58	62
10	66	65
11	48	54
12	29	29
13	15	17

-6,K,2

0	171	168
1	132	128
2	183	186
3	204	203
4	80	77
5	122	125
6	119	117
7	51	52
8	47	46
9	172	172
10	43	37
11	51	52
12	41	42
13	29	25

-5,K,2

0	50	54
1	103	99
2	26	32
3	82	78
4	64	59
5	77	73
6	53	57
7	47	42
8	73	73
9	98	94
10	50	52
11	70	69
12	40	39
13	29	28
14	24	26

-4,K,2

0	86	96
1	120	108
2	114	113
3	44	48
4	99	96
5	87	79
6	130	128
7	103	97
8	32	31
9	80	79
10	67	68
11	123	123
12	22	21
13	9	7
14	27	28

-3,K,2

0	172	169
1	295	279
2	188	181
3	166	164
4	142	135
5	73	76
6	74	72
7	150	140
8	96	91
9	41	37
10	61	62
11	65	66
12	43	43
13	31	35
14	23	22

-2,K,2

0	616	583
1	699	697
2	114	118
3	124	125
4	77	68
5	245	236
6	118	114
7	47	47
8	107	105
9	60	60
10	44	44
11	39	37
12	29	27
13	53	55
14	6*	3

-1,K,2

0	888	855
1	630E	640
2	455	465
3	154	151
4	267	256
5	126	128
6	154	146
7	238	226
8	71	66
9	93	90
10	58	57
11	13	15
12	47	52
13	50	53
14	15	12

0,K,2

0	145	147
1	271	265
2	264	258
3	99	95
4	33	39
5	127	121
6	215	206
7	36	38
8	64	60
9	119	119
10	86	85
11	23	21
12	53	53
13	8	8
14	27	30

1,K,2

0	146	151
1	117	116
2	255	253
3	28	22
4	255	250
5	91	78
6	41	32
7	46	48
8	110	113
9	38	37
10	158	157
11	66	63
12	76	79
13	26	27
14	38	39

2,K,2

0	260	262
1	91	91
2	153	146
3	121	123
4	268	257
5	42	36
6	68	63
7	102	108
8	124	117
9	121	124
10	152	148
11	41	40
12	42	44

2,K,2

13	33	35
14	15	16

3,K,2

0	103	103
1	240	232
2	174	158
3	84	83
4	39	40
5	110	111
6	104	99
7	94	95
8	120	120
9	54	58
10	134	135
11	89	91
12	23	25
13	37	38
14	24	23

4,K,2

0	82	86
1	46	43
2	154	135
3	64	60
4	97	91
5	24	18
6	45	44
7	143	145
8	81	83
9	120	120
10	99	102
11	37	35
12	28	33
13	10	9
14	35	36

5,K,2

0	105	103
1	82	76
2	101	101
3	74	67
4	141	143
5	25	27
6	18	20
7	169	169
8	77	73
9	38	35
10	29	27
11	16	18
12	40	38
13	46	49

6,K,2

0	246	250
1	67	69
2	23	18
3	132	134
4	75	66
5	50	47
6	40	39
7	79	82
8	9	2
9	32	36
10	18	21
11	33	35
12	15	18

7,K,2

0	70	71
1	208	214
2	103	103
3	154	156
4	9	4
5	25	24
6	54	59
7	81	85
8	15	15
9	53	54
10	34	35
11	18	17
12	20	23

8,K,2

0	125	126
1	57	56
2	90	87
3	75	76
4	43	47
5	58	60
6	97	101
7	27	31
8	70	73
9	29	29
10	13	8
11	9	10

9,K,2

0	64	67
1	84	78
2	57	56
3	45	41
4	21	16
5	54	58
6	32	36
7	9	10
8	16	13
9	22	24
10	19	20

10,K,2

0	40	43
1	7*	5
2	40	42
3	40	40
4	14	17
5	34	30
6	10	10
7	14	17
8	24	17

11,K,2

0	24	24
1	23	24
2	11	13
3	28	23
4	19	21
5	23	19
6	10	7
7	23	22

12,K,2

0	7	4
1	29	24
2	22	17
3	11	9
4	44	41

-13,K,3

0	13	11
1	9	10
2	50	52
3	58	54
4	16	21

-12,K,3

0	6*	6
1	35	35
2	40	38
3	18	16
4	55	57
5	20	23
6	20	17
7	14	13

-11,K,3

0	37	35
1	27	29
2	44	44
3	39	35
4	52	52
5	15	15
6	12	12
7	30	30
8	30	27

-10,K,3

0	70	66
1	28	28
2	64	61
3	52	49
4	37	34
5	11	14
6	43	44
7	25	28
8	64	65
9	22	18
10	18	19

-9,K,3

0	73	78
1	30	27
2	51	51
3	38	37
4	20	26
5	67	66
6	82	86
7	31	34
8	68	66
9	18	18
10	6*	1
11	8	4

-8,K,3

0	84	84
1	56	53
2	88	85
3	47	46
4	65	67
5	47	55
6	33	32
7	37	38
8	113	116
9	64	67
10	35	36
11	9	9
12	33	29

-7,K,3

0	111	108
1	92	94
2	32	30
3	69	75
4	77	75
5	52	43
6	41	45
7	26	22
8	46	47
9	28	24
10	25	23
11	22	26
12	49	49

-6,K,3

0	77	69
1	39	45
2	73	71
3	25	25
4	42	39
5	62	56
6	66	69
7	13	11
8	27	22
9	86	81
10	64	59
11	121	118
12	48	44
13	26	25

-5,K,3

0	57	50
1	36	21
2	124	119
3	64	51
4	14	6
5	93	92
6	35	34
7	48	46
8	44	45
9	75	71
10	61	57
11	58	59
12	24	22
13	23	24

-4,K,3

0	23	13
1	646	626
2	168	170
3	272	266
4	63	60
5	121	114
6	58	54
7	123	116
8	47	38
9	60	60
10	37	37
11	42	39
12	36	35
13	16	17

-3,K,3

0	112	95
1	99	100
2	187	183
3	219	214

-3,K,3

4	108	100
5	66	56
6	91	84
7	125	118
8	41	41
9	56	53
10	23	20
11	46	47
12	34	35
13	6*	9
14	27	30

-2,K,3

0	36	23
1	147	151
2	96	104
3	175	167
4	99	97
5	166	151
6	172	165
7	77	71
8	38	37
9	31	31
10	72	69
11	42	42
12	29	30
13	40	41
14	17	20

-1,K,3

0	406	390
1	262	273
2	50	51
3	84	87
4	109	102
5	78	78
6	101	101
7	91	89
8	31	31
9	91	83
10	46	46
11	67	68
12	50	48
13	9	10
14	14	15

0,K,3

0	135	130
1	190	185
2	74	74
3	107	103
4	65	60
5	25	25
6	109	106
7	50	46
8	33	26
9	123	123
10	83	81
11	77	77
12	32	34
13	32	31
14	33	34

1,K,3

0	24	19
1	146	132
2	118	109
3	116	118
4	79	74
5	123	121
6	61	58
7	36	38
8	54	57
9	109	107
10	169	166
11	54	53
12	48	46
13	33	34
14	32	31

2,K,3

0	99	99
1	226	214
2	331	315
3	102	93
4	219	212
5	109	106
6	75	70
7	160	158
8	91	87
9	49	45
10	61	62
11	78	75
12	20	23
13	27	29

3,K,3

0	65	67
1	178	179
2	110	102
3	120	114
4	257	246
5	145	136
6	43	40
7	127	118
8	182	179
9	52	47
10	85	83
11	28	20
12	23	23
13	28	29

4,K,3

0	67	72
1	109	109
2	184	179
3	42	45
4	103	97
5	116	117
6	45	42
7	92	94
8	187	187
9	78	76
10	40	38
11	15	16
12	21	24
13	28	28

5,K,3

0	54	56
1	52	48
2	85	81
3	47	46
4	56	57
5	26	25
6	87	89
7	65	66
8	104	111
9	46	48
10	19	19
11	19	18
12	36	39

6,K,3

0	9	11
1	108	114
2	91	95
3	139	142
4	60	59
5	59	61
6	63	64
7	47	48
8	64	71
9	23	26
10	23	21
11	21	23

7,K,3

0	121	120
1	100	96
2	71	67
3	100	102
4	62	62
5	62	66
6	22	20
7	64	65
8	12	15
9	49	56
10	15	16
11	17	14

8,K,3

0	89	85
1	83	85
2	83	79
3	106	107
4	28	26
5	12	17
6	12	12
7	6*	8
8	14	11
9	27	25
10	18	19

9,K,3

0	52	50
1	25	22
2	8	14
3	67	64
4	55	53
5	15	14
6	18	21
7	21	22
8	18	16

10,K,3

0	7*	4
1	37	36
2	34	31
3	22	24
4	15	12
5	18	20
6	15	12
7	24	21

11,K,3

0	12	11
1	31	28
2	12	13
3	40	35
4	28	24

-13,K,4

0	5*	1
1	18	16
2	10	10

-12,K,4

0	10	7
1	15	10
2	56	57
3	41	41
4	7	9
5	13	12
6	8	10

-11,K,4

0	7*	8
1	30	32
2	18	23
3	26	24
4	15	15
5	14	12
6	15	15
7	27	27

-10,K,4

0	58	62
1	18	22
2	42	41
3	35	37
4	41	44
5	16	13
6	30	32
7	38	38
8	47	49
9	21	22

-9,K,4

0	42	48
1	54	58
2	47	47
3	44	42
4	34	40
5	18	18
6	34	36
7	50	51
8	52	55
9	25	26
10	26	28

-8,K,4

0	69	69
1	59	50
2	108	114
3	46	50
4	36	39
5	29	32
6	72	74
7	51	57
8	23	21
9	33	36
10	27	26
11	55	57

-7,K,4

1	71	77
2	19	20
3	115	124
4	83	84
5	48	46
6	83	84
7	93	86
8	8	11
9	50	55
10	50	50
11	44	41

-6,K,4

0	28	24
1	42	36
2	11	10
3	23	19
4	34	31
5	48	54
6	63	58
7	45	50
8	43	38
9	93	92
10	65	61
11	30	30
12	37	35

-5,K,4

0	26	21
1	41	44
2	61	56
3	29	30
4	29	35
5	74	79
6	79	81
7	55	56
8	13	14
9	46	44
10	65	58
11	10	10
12	20	20

-4,K,4

0	167	155
1	190	192
2	51	44
3	144	148
4	99	99
5	114	117
6	82	82
7	67	63
8	48	44
9	38	40
10	15	18
11	26	27
12	17	20
13	9	12

-3,K,4

0	165	118
1	343	337
2	124	132
3	70	70
4	41	45
5	50	52
6	34	33
7	102	98
8	38	36
9	51	50
10	41	38
11	8	8
12	39	36
13	14	14

-2,K,4

0	68	66
1	119	123
2	92	103
3	26	20
4	20	19
5	45	45
6	64	65
7	93	94
8	18	18
9	90	85
10	15	13
11	70	69
12	6*	8
13	27	26

-1,K,4

0	101	101
1	55	56
2	114	115
3	15	18
4	21	20
5	88	86
6	63	61
7	88	82
8	55	54
9	96	90
10	49	48
11	72	68
12	57	55
13	18	16

0,K,4

0	124	131
1	128	115
2	117	115
3	130	128
4	110	107
5	68	65
6	34	34
7	30	29
8	8*	4
9	144	143
10	47	48
11	43	37
12	35	33
13	6*	3

1,K,4

0	28	25
1	26	20
2	72	63
3	202	189
4	108	114
5	71	72
6	112	108
7	42	41
8	131	130
9	43	42
10	40	42
11	36	39
12	34	34
13	5*	4

2,K,4

0	42	45
1	8	9
2	186	179
3	111	118
4	44	41
5	49	51
6	95	88
7	114	115
8	140	140
9	83	80
10	65	61
11	13	12
12	46	47

3,K,4

0	51	54
1	57	61
2	42	32
3	60	56
4	88	88
5	14	20
6	130	128
7	67	68
8	136	132
9	32	30
10	15	20
11	9	8
12	23	26

4,K,4

0	70	70
1	48	57
2	55	62
3	53	55
4	87	88
5	75	74
6	49	48
7	74	76
8	33	36
9	20	21
10	34	34
11	16	17

5,K,4

0	15	19
1	114	115
2	190	196
3	71	73
4	97	100
5	61	64
6	75	73
7	30	29
8	10	15
9	45	48
10	8	6
11	41	44

6,K,4

0	14	15
1	175	179
2	190	188
3	177	181
4	33	33
5	60	65
6	67	66
7	41	38
8	23	25
9	7	5
10	29	26

7,K,4

0	121	116
1	127	125
2	44	46
3	57	53
4	61	59
5	49	43
6	11	10
7	51	52
8	36	37
9	17	17

8,K,4

0	45	46
1	53	48
2	28	28
3	9	13
4	49	47
5	43	47
6	13	13
7	15	8
8	33	30

9,K,4

0	6*	4
1	16	13
2	39	36
3	15	7
4	26	23
5	14	11
6	9	6

10,K,4

0	33	29
1	15	13
2	45	38
3	29	25
4	44	39

-12,K,5

0	12	9
1	8	8
2	22	26
3	11	13

-11,K,5

0	6*	8
1	34	30
2	19	18
3	19	20
4	9	9
5	29	30
6	10	10

-10,K,5

0	36	40
1	10	16
2	52	53
3	10	11
4	21	25
5	49	54
6	10	10
7	24	23

-9,K,5

0	8	5
1	53	52

-9,K,5

2	51	51
3	7*	12
4	50	56
5	47	47
6	14	14
7	37	38
8	14	14

-8,K,5

0	38	40
1	20	21
2	63	61
3	24	25
4	33	30
5	55	57
6	56	56
7	13	14
8	24	25
9	27	28

-7,K,5

0	36	42
1	33	31
2	65	63
3	36	31
4	23	25
5	31	38
6	82	86
7	28	31
8	15	12
9	19	20
10	73	72

-6,K,5

0	81	85
1	64	68
2	81	85
3	40	35
4	83	86
5	53	52
6	17	20
7	49	50
8	33	35
9	38	36
10	14	9
11	17	21

-5,K,5

0	198	194
1	204	212
2	135	139
4	81	86
5	85	88
6	36	37

-6,K,6

0	58	58
1	46	42
2	86	87
3	47	53
4	20	20
5	23	32
6	16	16
7	8	9
8	28	28
9	9	11

-5,K,6

0	183	175
1	118	129
2	73	80
3	63	63
4	67	76
5	40	41
6	34	33
7	25	27
8	12	13
9	29	25

-4,K,6

0	16	9
1	14	10
2	26	21
3	22	23
4	55	59
5	48	46
6	53	50
7	20	23
8	8	10
9	32	34
10	54	55

-3,K,6

0	11	9
1	13	20
2	71	69
3	67	67
4	8*	6
5	43	45
6	58	53
7	42	41
8	52	54
9	45	45
10	11	12

-2,K,6

0	85	91
1	102	103
2	102	103
3	25	25

7	84	82
8	43	42
9	44	45
10	13	15
11	25	26

-4,K,5

0	7*	8
1	31	30
2	219	220
3	83	86
4	64	64
5	34	31
6	56	59
7	55	52
8	32	28
9	7*	8
10	35	33
11	31	32

-3,K,5

0	66	50
1	122	124
2	82	84
3	67	74
4	48	48
5	78	81
6	72	68
7	18	17
8	42	41
9	20	22
10	57	55
11	73	68
12	16	15

-2,K,5

0	32	24
1	25	28
2	38	40
3	40	41
4	23	20
5	43	35
6	44	38
7	39	42
8	24	23
9	89	88
10	45	42
11	12	16
12	6	7

-1,K,5

0	43	44
1	22	21
2	49	51
3	105	105
4	12	15

-1,K,6

0	141	153
1	19	17
2	58	58
3	103	111
4	52	49
5	119	120
6	22	23
7	82	84
8	28	24
9	61	66
10	22	25

0,K,6

0	13	13
1	54	54
2	57	55
3	54	53
4	26	24
5	26	25
6	65	64
7	119	117
8	19	23
9	31	33
10	41	41

1,K,6

0	48	53
1	62	63
2	60	60
3	29	28
4	25	23
5	7*	3
6	36	33
7	43	48
8	46	46
9	53	53

2,K,6

0	23	27
1	43	45
2	20	18
3	58	61
4	26	29
5	36	39
6	6*	3
7	7	8
8	48	47

-3,K,8

1	25	30

5	23	22
6	88	88
7	25	29
8	33	36
9	68	68
10	12	8
11	57	58
12	23	22

0,K,5

0	20	17
1	84	82
2	68	72
3	73	76
4	35	38
5	40	35
6	58	56
7	43	40
8	73	73
9	31	33
10	46	41
11	6*	4

1,K,5

0	77	71
1	64	62
2	26	21
3	45	41
4	106	113
5	41	38
6	111	108
7	14	12
8	70	70
9	80	78
10	40	39
11	24	22

2,K,5

0	106	117
1	30	34
2	55	57
3	38	33
4	41	37
5	23	20
6	40	41
7	53	51
8	73	68
9	32	29
10	23	29
11	12	11

3,K,5

0	80	85
1	55	59
2	108	112
3	44	45

9	23	26

3,K,6

0	30	41
1	50	51
2	55	56
3	32	35
4	24	26
5	25	24
6	26	28
7	14	17
8	23	27

4,K,6

0	61	61
1	35	44
2	106	112
3	62	60
4	29	32
5	62	65
6	8	6
7	13	10

5,K,6

0	49	44
1	28	26
2	33	37
3	63	66
4	71	69
5	10	10
6	34	39

6,K,6

0	26	26
1	35	33
2	9	13
3	21	22
4	13	18

7,K,6

0	5*	7
1	8	9

-9,K,7

0	6	8
1	15	18

-8,K,7

0	45	52
1	41	44
2	13	21
3	8	8
4	5*	9

4	45	44
5	19	21
6	52	51
7	17	19
8	78	81
9	23	24
10	52	50

4,K,5

0	15	10
1	74	74
2	83	83
3	136	141
4	49	51
5	33	33
6	24	25
7	17	17
8	35	33
9	13	12
10	18	17

5,K,5

0	178	189
1	75	73
2	58	58
3	91	95
4	16	18
5	18	16
6	27	30
7	38	43
8	29	32
9	12	10

6,K,5

0	48	50
1	55	56
2	114	114
3	72	77
4	66	68
5	38	38
6	29	32
7	36	39
8	18	17

7,K,5

0	33	29
1	12	12
2	38	35
3	24	27
4	23	20
5	16	17
6	22	27
7	30	33

8,K,5

0	38	39
1	24	20
2	25	23
3	58	55
4	30	30
5	36	35

9,K,5

0	11	9
1	61	57

-11,K,6

0	8	13
1	31	36
2	11	12

-10,K,6

0	9	9
1	9	11
2	16	19
3	7	8
4	12	11
5	8	10

-9,K,6

0	19	18
1	17	15
2	10	10
3	20	22
4	6*	9
5	13	14
6	31	34

-8,K,6

0	78	89
1	32	31
2	20	19
3	12	14
4	40	43
5	39	40
6	23	30
7	5*	3

-7,K,6

0	28	35
1	23	21
2	22	21
3	8	13
4	12	14
5	26	29
6	27	28
7	19	18
8	18	19

-7,K,7

0	83	89
1	14	22
2	27	36
3	50	56
4	6*	4
5	15	15

-6,K,7

0	48	52
1	9	11
2	26	28
3	25	27
4	18	16
5	27	31
6	29	28

-5,K,7

0	9	13
1	48	46
2	20	18
3	32	33
4	13	10
5	42	40
6	34	32

-4,K,7

0	41	34
1	19	15
2	25	24
3	30	32
4	29	30
5	20	23
6	27	29
7	18	21

-3,K,7

0	26	25
1	25	27
2	51	52
3	20	27
4	32	36
5	38	40
6	21	26
7	18	14

-2,K,7

0	25	21
1	53	63
2	10	8
3	10	12
4	52	52
5	29	32
6	57	60

7	41	47

-1,K,7

0	15	14
1	12	19
2	21	23
3	54	55
4	22	28
5	21	20
6	30	30
7	28	31

0,K,7

0	7*	10
1	41	38
2	7*	5
3	43	44
4	25	29
5	21	21
6	18	18
7	32	31

1,K,7

0	38	43
1	25	28
2	35	35
3	27	30
4	17	19
5	39	40
6	12	13

2,K,7

0	56	55
1	32	30
2	76	84
3	56	61
4	49	50
5	12	10

3,K,7

0	17	24
1	60	63
2	21	22
3	13	18
4	74	80

4,K,7

0	25	27
1	38	41
2	30	32

-2,K,8

0	25	28

APPENDIX VII

Tables of observed and calculated structure factors for 4,10,16-trimethyltribenzo[*b*,*f*,*j*][1,5,9]trithiacyclododecine-6,12,18-trione

Data Format:

	K	L
H	$10\times\|F_o\|$	$10\times\|F_c\|$

Reflections removed for extinction marked .... E

Reflections classed as unobserved marked ..... *

H,0,-18

1	14*	21
2	200	200
3	19	13
4	119	115
5	53	55
6	178	185
7	182	185
8	35	35
9	280	272
10	57	60
11	132	129
12	15	7
13	73	71
14	82	85
15	60	58
16	57	63

H,0,-16

1	93	90
2	43	47
3	25	24
4	58	59
5	60	61
6	50	48
7	328	326
8	187	187
9	466	463
10	59	71
11	129	128
12	15*	7
13	270	268
14	132	141
15	150	146
16	239	247
17	234	240
18	112	110

H,0,-14

1	394	394
2	48	45
3	41	40
4	58	57
5	169	164
6	183	176
7	384	386
8	92	95
9	473	469
10	58	45
11	15*	3
12	88	87
13	310	306
14	419	423
15	33	18
16	247	246
17	425	423
18	241	246
19	144	141
20	37	27

H,0,-12

1	82	74
2	220	215
3	177	182
4	271	257
5	32	47
6	334	316
7	94	117
8	49	49
9	244	239
10	22	9
11	31	37
12	93	84
13	68	76
14	121	117
15	178	174
16	277	263
17	306	307
18	183	182
19	41	36
20	13*	7
21	236	237

H,0,-10

1	111	120
2	160	152
3	220	211
4	471	485
5	523	530
6	509	518
7	211	229
8	246	244
9	42	46
10	115	112
11	57	72
12	110	110
13	35	34
14	186	213
15	311	346
16	311	343
17	123	136
18	133	149
19	39	51
20	67	72
21	28	31
22	77	75

H,0,-8

1	112	99
2	187	215
3	821	818
4	667	690
5	533E	1399
6	416	461
7	177	183
8	149	164
9	131	75
10	467	469
11	208	175
12	16*	2
13	233	233
14	16*	16
15	224	235
16	192	197
17	119	117
18	96	95
19	65	70
20	208	214
21	140	163
22	93	110

H,0,-6

1	125	126
2	1050	1090
3	909	925
4	333	388
5	216	241
6	466	455
7	258	227
8	449	447
9	187	154
10	208	211
11	663	663
12	396	362
13	601	613
14	63	60
15	350	362
16	181	176
17	105	118
18	204	212
19	50	48
20	59	55
21	137	143
22	126	123

H,0,-4

1	805	794
2	627E	796
3	1420E	1603
4	873	850
5	870	872
6	679	659
7	515	508
8	186	194
9	43	44
10	165	148
11	658	670
12	88	92
13	905	945
14	345	360
15	72	71
16	439	448
17	209	221
18	222	237
19	32	8
20	83	88
21	17	13
22	189	194

H,0,-2

1	173	209
2	1234E	1429
3	458	452
4	690	661
5	365	353
6	444	426
7	281	269
8	265	265
9	424	431
10	86	73
11	467	498
12	17	10
13	532	545
14	171	178
15	212	224
16	245	253
17	160	156
18	162	172
19	82	89
20	213	215
21	53	58
22	221	229

H,0,0

1	121	163
2	956E	1066
3	988	1065
4	321	318
5	580	554
6	553	537
7	541	513
8	187	159
9	370	382
10	508	501
11	211	235
12	133	140
13	284	282
14	320	324
15	177	181
16	410	422
17	21*	8
18	86	83
19	130	137
20	213	213
21	65	66

H,0,2

0	1602E	2047
1	256	252
2	181	167
3	38	43
4	1185E	1312
5	532	545
6	297	254
7	1438	1487
8	242	266
9	588	596
10	575	575

H,0,2

11	320	325
12	138	132
13	24	23
14	34	35
15	37	49
16	17	28
17	169	170
18	189	191
19	123	123
20	264	265

H,0,4

0	64	96
1	711	716
2	446	470
3	865	900
4	132	104
5	75	70
6	564	569
7	667	671
8	525	545
9	710	740
10	126	120
11	157	158
12	134	147
13	19	16
14	55	61
15	180	199
16	137	141
17	126	121
18	123	121
19	148	151

H,0,6

0	280	308
1	199	172
2	241	228
3	283	262
4	1001	1002
5	180	210
6	268	297
7	373	434
8	386	377
9	288	297
10	151	157
11	230	234
12	26	29
13	113	119
14	62	72
15	244	261
16	148	151
17	256	268
18	86	94

H,0,8

0	204	232
1	73	81
2	130	155
3	97	73
4	418	435
5	387	385
6	201	219
7	376	378
8	294	307
9	48	13
10	42	46
11	455	506
12	40	39
13	106	106
14	80	97
15	161	181
16	32	25

H,0,10

0	380	385
1	17	3
2	411	481
3	147	170
4	670E	811
5	160	184
6	311	357
7	197	232
8	150	168
9	46	47
10	77	91
11	46	56
12	44	59
13	133	154
14	12*	15

H,0,12

0	279	283
1	122	117
2	256	272
3	222	225
4	392	413
5	190	186
6	404	416
7	66	76
8	43	53
9	81	85
10	38	40
11	148	155
12	50	50

H,0,14

0	368	369
1	131	131
2	140	134
3	194	202
4	273	289
5	82	83
6	193	198
7	102	88
8	86	75
9	97	89

H,0,16

0	117	113
1	46	50
2	287	289
3	50	53
4	210	211
5	24	21
6	138	127

H,0,18

0	238	236
1	41	38
2	169	164

H,1,-19

2	99	97
3	38	44
4	29	33
5	56	54
6	14	11
7	80	85
8	13*	7
9	19	19
10	49	52
11	35	35
12	71	74
13	101	108

H,1,-18

1	94	97
2	15	7
3	94	90
4	231	227
5	105	105
6	172	168
7	47	48
8	30	38
9	91	88
10	21	26
11	75	74
12	85	85
13	89	88
14	180	167
15	55	42

H,1,-17

1	26	31
2	85	88
3	39	36
4	24	22
5	32	38
6	22	27
7	121	126
8	40	30
9	26	20
10	75	78
11	21	22
12	58	59
13	19	21
14	82	81
15	31	29
16	71	80
17	35	36

H,1,-16

1	61	63
2	62	60
3	294	298
4	193	192
5	176	179
6	138	134
7	135	130
8	39	30
9	73	70
10	69	72
11	125	121
12	156	144
13	53	50
14	77	60
15	160	151
16	49	54
17	103	105
18	50	48

H,1,-15

1	48	48
2	172	175
3	64	65
4	115	115
5	35	32
6	15*	18
7	71	67
8	185	184
9	15*	8
10	70	70
11	100	101
12	27	27
13	50	41
14	146	147
15	79	77
16	134	133
17	52	52
18	42	44
19	12*	14

H,1,-14

1	393	400
2	94	91
3	531	534
4	168	164
5	119	127
6	27	23
7	98	97
8	81	76
9	43	43
10	294	284

H,1,-14

11	62	63
12	244	231
13	94	82
14	213	209
15	119	114
16	75	74
17	91	93
18	88	76
19	32	26
20	12	12

H,1,-13

1	115	117
2	155	154
3	40	31
4	17	24
5	17	15
6	87	85
7	20	16
8	116	116
9	138	142
10	58	56
11	190	195
12	158	159
13	83	79
14	141	140
15	54	49
16	108	107
17	67	69
18	92	99
19	13*	15
20	12*	5
21	30	32

H,1,-12

1	571	586
2	187	186
3	406	412
4	161	158
5	124	112
6	233	229
7	331	325
8	118	110
9	32	37
10	581	574
11	146	144
12	513	502
13	62	53
14	228	226
15	19	15
16	97	88
17	61	54
18	32	30
19	21	23
20	58	55
21	240	241

H,1,-11

1	323	321
2	177	164
3	193	192
4	20	16
5	51	53
6	22	16
7	174	170
8	129	132
9	305	289
10	36	44
11	15*	7
12	39	55
13	99	107
14	14*	9
15	23	20
16	106	125
17	101	123
18	78	96
19	49	55
20	74	83
21	137	144
22	15	12

H,1,-10

1	686	691
2	208	199
3	21	43
4	116	116
5	662	632
6	216	219
7	39	38
8	401	394
9	22	11
10	440	499
11	53	49
12	477	546
13	178	202
14	14	10
15	80	86
16	38	40
17	17	29
18	14	13
19	191	217
20	44	45
21	236	263
22	30	30

H,1,-9

1	26	46
2	186	173
3	308	287
4	188	154
5	328	314
6	95	77
7	128	123
8	121	134
9	43	24
10	128	133
11	163	179
12	28	7
13	87	84
14	134	125
15	88	94
16	15*	6
17	76	79
18	15*	12
19	149	171
20	79	89
21	120	141
22	66	88

H,1,-8

1	489	502
2	82	62
3	188	190
4	146	136
5	466	456
6	349	380
7	498	547
8	644E	758
9	26	20
10	594	602
11	118	123
12	416	396
13	74	60
14	127	122
15	77	85
16	133	134
17	68	69
18	199	199
19	331	329
20	40	46
21	114	118
22	31	36

H,1,-7

1	126	116
2	25	26
3	515	496
4	547	517
5	25	5
6	250	268
7	253	171
8	234	218
9	240	224
10	250	245
11	412	399
12	186	182
13	57	58
14	15*	4
15	29	13
16	37	33
17	65	60
18	56	70
19	127	125
20	48	47
21	12*	3
22	22	17

H,1,-6

1	185	183
2	193	188
3	203	201
4	247	271
5	187	211
6	273	304
7	431	425
8	768	770
9	266	267
10	814	799
11	197	186
12	248	229
13	44	43
14	152	159
15	148	147
16	29	31
17	182	185
18	201	195
19	283	278
20	61	55
21	13*	5
22	12*	12

H,1,-5

1	930	922
2	293	269
3	76	80
4	84	84
5	513	496
6	802	780
7	191	175
8	215	229
9	250	232
10	46	31
11	42	23
12	159	168
13	117	106
14	224	241
15	90	89
16	124	136
17	67	66
18	131	134
19	244	254
20	129	134
21	16	17
22	105	104

H,1,-4

1	184	164
2	1196	1232
3	593	582
4	165	160
5	1178	1184
6	790	776
7	701	708
8	716	734
9	554	516
10	119	109
11	21	14

H,1,-4

12	175	166
13	38	28
14	82	75
15	30	33
16	487	495
17	439	441
18	332	329
19	40	30
20	33	26
21	50	52
22	18	16

H,1,-3

1	1260	1324
2	45	35
4	1573E	1695
5	354	345
6	295	300
7	236	221
8	164	132
9	383	355
10	127	110
11	89	90
12	161	171
13	147	142
14	142	138
15	129	126
16	33	25
17	70	80
18	64	56
19	107	106
20	139	139
21	27	22
22	11*	15

H,1,-2

1	143	160
2	1254	1342
3	289	277
4	257	255
5	441	429
6	928	931
7	932	910
8	395	391
9	127	102
10	335	331
11	145	140
12	28	13
13	113	107
14	376	383
15	244	249
16	806	815
17	256	244
18	156	149
19	72	72
20	46	50
21	17	6
22	10*	9

H,1,-1

1	898	918
2	931	935
3	444	411
4	115	104
5	784	735
6	282	255
7	333	335
8	108	95
9	439	418
10	332	309
11	73	56
12	257	256
13	149	147
14	160	157
15	154	150
16	73	75
17	58	65
18	93	88
19	62	65
20	13*	1
21	64	66

H,1,0

1	33	19
2	545	539
3	214	190
4	559	545
5	860	861
6	767	775
7	118	127
8	174	162
9	124	112
10	290	284
11	79	87
12	16	10
13	90	87
14	577	574
15	161	156
16	341	339
17	283	283
18	19	26
19	22	19
20	18	16
21	24	32

H,1,1

0	413	397
1	71	77
2	101	100
3	413	418
4	202	187
5	976	961
6	425	396
7	132	138
8	32	9
9	134	121
10	393	360
11	45	33
12	50	46
13	115	108
14	16*	9
15	155	157
16	22	4
17	75	72
18	58	59
19	13*	7
20	47	41
21	53	53

H,1,2

0	1128	1223
1	148	137
2	33	25
3	1272E	1443
4	464	486
5	746	775
6	985	963
7	247	225
8	31	25
9	82	59
10	243	233
11	14	8
12	178	187
13	123	123
14	330	318
15	189	179
16	145	141
17	87	85
18	42	47
19	36	31
20	41	33

H,1,3

0	277	269
1	108	113
2	819	826
3	209	204
4	596	592
5	151	126
6	396	372
7	454	424
8	61	22
9	160	157
10	18	27
11	24	26
12	62	72
13	52	44
14	171	171
15	29	20
16	13*	13
17	40	44
18	60	59
19	12*	1
20	14	17

H,1,4

0	253	248
1	678	702
2	65	88
3	937	1004
4	793	806
5	690	680
6	485	462
7	99	75
8	335	310
9	54	16
10	161	149
11	90	88
12	329	318
13	108	129
14	371	366
15	107	101
16	14*	4
17	14*	12
18	33	29
19	11*	9

H,1,5

0	186	225
1	162	151
2	555	563
3	616	586
4	176	189
5	245	235
6	585	555
7	103	114
8	180	169
9	123	116
10	21	10
11	74	71
12	212	218
13	79	60
14	91	95
15	126	131
16	19	12
17	25	23
18	16	15

H,1,6

0	13	26
1	800	848
2	519	488
3	599	636
4	110	92
5	288	276
6	54	54
7	195	194
8	119	129
9	111	111
10	308	300
11	205	214
12	375	351
13	80	95
14	198	194
15	34	38
16	61	64
17	49	45

H,1,6

18	39	37

H,1,7

0	160	182
1	117	139
2	20	16
3	157	162
4	218	214
5	170	179
6	14*	11
7	35	44
8	67	63
9	16*	11
10	83	74
11	38	27
12	155	152
13	82	92
14	56	59
15	13*	8
16	33	36
17	23	33

H,1,8

0	114	129
1	693E	824
2	98	111
3	364	367
4	30	15
5	131	126
6	124	123
7	23	3
8	179	174
9	125	119
10	329	308
11	124	129
12	316	306
13	18	23
14	144	166
15	52	55
16	10*	10

H,1,9

0	235	227
1	157	169
2	15	28
3	47	48
4	108	130
5	34	35
6	116	127
7	92	91
8	35	26
9	71	77
10	159	157
11	63	65
12	80	84
13	79	81
14	22	12
15	22	26

H,1,10

0	56	62
1	455	475
2	275	297
3	228	255
4	251	282
5	123	146
6	47	46
7	25	24
8	213	220
9	58	52
10	305	318
11	18	18
12	183	205
13	28	24
14	20	19

H,1,11

0	251	250
1	148	148
2	122	133
3	242	236
4	142	159
5	112	128
6	161	176
7	96	116
8	42	46
9	128	139
10	119	140
11	85	77
12	40	38
13	106	100

H,1,12

0	200	195
1	383	385
2	482	488
3	41	43
4	163	155
5	33	30
6	25	22
7	212	204
8	277	258
9	80	68
10	233	215
11	135	123
12	43	39

H,1,13

0	39	36
1	68	63
2	39	36
3	59	61
4	69	67
5	198	192
6	71	61
7	41	30
8	77	73
9	14*	11
10	23	11
11	46	38

H,1,14

0	167	171
1	114	116
2	68	62
3	15*	3
4	56	58
5	100	100
6	89	76
7	191	180
8	228	208
9	173	163

H,1,15

0	210	208
1	99	95
2	15*	6
3	26	20
4	30	30
5	67	65
6	69	67
7	44	42
8	70	72

H,1,16

0	42	39
1	49	50
2	18	15
3	70	66
4	37	39
5	132	128
6	110	102

H,1,17

0	68	70
1	75	79
2	14*	2
3	34	35
4	12*	6

H,1,18

0	107	109
1	23	18

H,2,-19

4	25	26
5	53	54
6	50	55
7	66	66
8	40	40
9	184	186
10	18	13
11	117	119

H,2,-18

1	43	41
2	14*	15
3	26	27
4	37	42
5	90	92
6	14*	4
7	27	8
8	14*	7
9	193	188
10	16	13
11	188	185
12	114	110
13	39	40
14	13*	3

H,2,-17

1	51	48
2	132	135
3	68	65
4	312	309
5	59	59
6	99	99
7	150	146
8	15*	7
9	122	122
10	41	39
11	37	35
12	77	75
13	18	12
14	24	26
15	64	62
16	97	107

H,2,-16

1	114	109
2	142	143
3	249	246
4	107	110
5	206	206
6	64	54
7	235	236
8	94	91
9	115	100
10	22	28
11	125	130
12	138	138
13	62	61
14	123	131
15	49	50
16	47	53
17	110	106
18	161	162

H,2,-15

1	81	75

H,2,-15

2	267	259
3	49	53
4	243	231
5	78	77
6	51	49
7	139	133
8	133	130
9	16*	9
10	117	113
11	244	237
12	132	125
13	16*	4
14	59	61
15	29	28
16	64	60
17	14*	6
18	128	128
19	49	48

H,2,-14

1	58	56
2	100	101
3	150	150
4	194	188
5	233	241
6	247	251
7	203	197
8	277	277
9	171	163
10	128	123
11	118	114
12	152	148
13	23	24
14	96	96
15	191	193
16	86	82
17	146	137
18	200	194
19	36	33

H,2,-13

1	75	78
2	136	130
3	123	125
4	38	46
5	311	308
6	146	145
7	246	241
8	159	154
9	97	84
10	71	73
11	138	132
12	48	51
13	200	199
14	70	74
15	125	121
16	67	58
17	19	4
18	66	60
19	76	80
20	65	68

H,2,-12

1	154	156
2	170	153
3	72	66
4	295	287
5	391	378
6	219	224
7	359	343
8	401	397
9	309	297
10	365	355
11	410	402
12	339	330
13	92	80
14	249	243
15	223	206
16	204	202
17	97	88
18	117	110
19	14*	18
20	63	53
21	55	60

H,2,-11

1	15*	4
2	172	165
3	72	84
4	132	140
5	340	343
6	157	165
7	334	322
8	94	80
9	131	127
10	32	22
11	17*	17
12	154	161
13	14*	15
14	120	131
15	141	154
16	95	109
17	46	49
18	13*	7
19	35	44
20	15	21
21	19	21

H,2,-10

1	33	26
2	115	108
3	17	15
4	297	294
5	501	499
6	317	313
7	637	625
8	89	64
9	43	47
10	118	146
11	175	191
12	15*	3
13	224	257
14	17	10
15	302	331
16	67	71
17	36	28
18	32	30
19	47	54
20	43	46
21	53	60

H,2,-9

1	14	10
2	37	24
3	41	50
4	297	277
5	221	199
6	270	266
7	279	268
8	37	34
9	197	233
10	26	21
11	287	327
12	237	230
13	202	205
14	255	254
15	168	175
16	86	81
17	131	138
18	50	51
19	28	31
20	65	67
21	82	85
22	61	66

H,2,-8

1	105	94
2	344	347
3	536	504
4	196	206
5	136	88
6	338	377
7	366	387
8	47	42
9	323	301
10	199	187
11	15*	9
12	162	171
13	599	596
14	68	56
15	323	322
16	178	183
17	15*	8
18	97	102
19	85	81
20	133	141
21	14	14
22	45	44

H,2,-7

1	523	499
2	574	539
3	287	312
4	602	595
5	56	41
6	404	425
7	56	44
8	145	112
9	152	154
10	231	218
11	220	198
12	41	34
13	323	320
14	99	95
15	253	253
16	36	31
17	172	176
18	177	182
19	56	57
20	100	102
21	153	155
22	185	188

H,2,-6

1	256	225
2	294	332
3	576	541
4	175	216
5	533	603
6	93	101
7	420	396
8	186	184
9	185	181
10	210	206
11	289	294
12	37	32
13	507	507
14	323	326
15	192	182
16	152	164
17	22	16
18	123	126
19	36	37
20	94	100
21	149	144
22	174	171

H,2,-5

1	485	469
2	818	812
3	281	301
4	283	284
5	61	67
6	278	264
7	87	89
8	143	140
9	340	324

H,2,-5

10	75	48
11	118	126
12	89	76
13	148	154
14	54	44
15	186	184
16	44	39
17	46	49
18	95	94
19	31	30
20	139	142
21	12*	3
22	85	84

H,2,-4

1	254	233
2	1093	1124
3	741	735
4	875	849
5	195	176
6	584	555
7	435	390
8	448	416
9	173	176
10	298	270
11	416	422
12	38	29
13	440	444
14	202	207
15	94	97
16	52	50
17	158	163
18	17	19
19	56	53
20	32	38
21	122	123
22	259	259

H,2,-3

1	31	31
2	663	653
3	619	587
4	1272	1316
5	204	206
6	785	733
7	157	136
8	301	271
9	158	156
10	35	34
11	468	482
12	126	122
13	161	155
14	84	84
15	114	121
16	122	120
17	36	32
18	76	76
19	44	51
20	13*	7
21	40	45

H,2,-2

1	853	827
2	1802E	2000
3	257	189
4	828	791
5	544	509
6	500	472
7	623	593
8	72	70
9	214	231
10	75	81
11	778	783
12	85	82
13	190	183
14	186	191
15	117	122
16	62	70
17	37	34
18	14*	5
19	24	23
20	151	143
21	55	59

H,2,-1

1	452	424
2	874	833
3	106	98
4	705	651
5	351	343
6	385	357
7	168	163
8	393	387
9	441	436
10	394	381
11	498	498
12	58	51
13	214	205
14	69	80
15	297	308
16	71	66
17	15	6
18	29	26
19	66	77
20	79	80
21	24	25

H,2,0

0	637	647
1	600	582
2	113	69
3	149	131
4	447	416
5	498	489
6	58	48
7	305	278
8	69	85
9	827	831
10	276	272
11	1029	1039
12	114	121
13	88	92
14	230	226
15	15*	12
16	71	79
17	95	99
18	29	23
19	163	167
20	180	173
21	37	40

H,2,1

0	237	194
1	196	187
2	251	235
3	489	491
4	86	71
5	278	267
6	364	349
7	327	296
8	20	6
9	321	330
10	242	224
11	504	496
12	373	366
13	230	235
14	53	50
15	278	280
16	156	155
17	55	58
18	90	89
19	60	65
20	82	82

H,2,2

0	900	912
1	452	450
2	490	481
3	389	373
4	124	108
5	148	153
6	263	275
7	252	248
8	224	217
9	467	455
10	101	81
11	697	694
12	85	81
13	28	29
14	328	313
15	37	39
16	21	15
17	172	172
18	139	126
19	131	136
20	177	175

H,2,3

0	121	104
1	236	212
2	335	335
3	164	160
4	277	281
5	46	42
6	38	29
7	81	97
8	276	263
9	229	232
10	530	512
11	313	317
12	84	74
13	195	191
14	37	23
15	14*	8
16	59	49
17	63	64
18	165	163
19	76	76

H,2,4

0	579	583
1	523	499
2	388	370
3	230	205
4	169	157
5	208	197
6	347	362
7	62	59
8	227	232
9	385	384
10	111	101
11	56	50
12	166	166
13	72	61
14	26	15
15	50	43
16	107	105
17	215	209
18	239	231
19	151	154

H,2,5

0	43	21
1	557	538
2	310	305
3	246	236
4	134	124
5	265	268
6	180	184
7	184	189
8	253	246
9	120	121
10	60	47
11	132	129
12	56	58
13	65	66
14	41	36

H,2,5

15	77	85
16	80	74
17	60	53
18	111	108

H,2,6

0	382	417
1	19	9
2	236	242
3	155	154
4	307	290
5	92	97
6	579	587
7	375	368
8	205	204
9	297	277
10	122	118
11	47	54
12	69	67
13	54	58
14	35	42
15	109	92
16	124	123
17	127	144

H,2,7

0	115	122
1	357	408
2	91	87
3	52	45
4	226	214
5	494	493
6	220	226
7	117	110
8	512	491
9	121	113
10	33	40
11	34	30
12	24	26
13	57	59
14	45	44
15	55	48
16	32	33

H,2,8

0	15	4
1	201	223
2	359	375
3	139	150
4	768	771
5	254	265
6	624	634
7	147	139
8	109	104
9	121	113
10	69	72
11	71	62
12	27	18
13	77	71
14	19	17
15	162	167
16	35	30

H,2,9

0	17	19
1	122	103
2	318	324
3	239	247
4	37	32
5	313	318
6	276	275
7	118	118
8	185	166
9	19	14
10	28	40
11	13*	6
12	62	62
13	28	30
14	11	9
15	148	139

H,2,10

0	35	25
1	90	86
2	55	50
3	51	52
4	375	383
5	352	353
6	144	152
7	92	79
8	184	182
9	110	110
10	48	38
11	18	8
12	73	69
13	157	142
14	11*	14

H,2,11

0	50	43
1	163	155
2	153	152
3	113	105
4	16*	12
5	221	224
6	37	41
7	91	87
8	39	37
9	157	146
10	37	34
11	64	59
12	25	22
13	61	59

H,2,12

0	23	16
1	164	161
2	152	150
3	22	4
4	36	14
5	165	166
6	154	148
7	23	16
8	26	26
9	14*	3
10	149	143
11	68	66

H,2,13

0	162	158
1	45	40
2	274	272
3	45	49
4	39	36
5	42	35
6	115	111
7	58	51
8	45	50
9	21	23
10	12*	8

H,2,14

0	29	24
1	198	199
2	428	426
3	111	108
4	179	170
5	30	28
6	49	45
7	41	45
8	78	71
9	31	35

H,2,15

0	138	138
1	121	117
2	204	201
3	35	33
4	174	165
5	14*	18
6	13*	5
7	12*	3

H,2,16

0	133	127
1	24	21
2	272	275
3	14*	3
4	75	70
5	12*	6

H,2,17

0	208	212
1	26	23
2	154	147
3	82	77

H,2,18

0	237	236

H,3,-18

2	18	10
3	13*	4
4	105	101
5	13*	8
6	85	79
7	35	39
8	63	61
9	45	41
10	13*	13
11	12*	1
12	17	14

H,3,-17

1	41	37
2	155	157
3	90	90
4	51	52
5	150	151
6	63	54
7	71	75
8	87	84
9	28	24
10	16	20
11	71	68
12	97	93
13	77	69
14	195	196
15	128	134

H,3,-16

1	25	29
2	91	86
3	89	86
4	97	86
5	15*	4
6	150	153
7	26	25
8	15*	8
9	60	64
10	17	14
11	41	44
12	94	89
13	55	64
14	257	258
15	187	180
16	22	23

H,3,-15

1	72	69

H,3,-15

2	231	234
3	168	162
4	126	137
5	221	219
6	14*	4
7	15*	19
8	25	28
9	119	118
10	67	61
11	95	92
12	206	200
13	138	141
14	191	192
15	44	43
16	13*	5
17	50	51
18	71	72

H,3,-14

1	205	212
2	93	80
3	105	104
4	241	239
5	19	13
6	208	204
7	66	56
8	52	53
9	100	98
10	15*	6
11	79	73
12	191	174
13	77	73
14	114	108
15	126	121
16	14*	1
17	31	26
18	44	45

H,3,-13

1	270	268
2	204	208
3	235	234
4	32	28
5	25	29
6	182	175
7	247	237
8	145	138
9	277	271
10	88	92
11	124	114
12	184	175
13	32	31
14	88	89
15	21	15
16	68	66
17	14*	19
18	21	23
19	60	67

H,3,-12

1	387	390
2	216	218
3	258	263
4	201	192
5	35	30
6	126	121
7	14*	2
8	52	40
9	71	72
10	21	14
11	92	79
12	277	260
13	153	151
14	119	117
15	120	118
16	15*	3
17	88	91
18	64	65
19	30	22
20	55	53

H,3,-11

1	198	199
2	227	222
3	79	82
4	141	140
5	190	189
6	149	149
7	366	361
8	15*	5
9	59	59
10	333	321
11	260	256
12	164	157
13	218	210
14	83	78
15	68	70
16	39	40
17	86	90
18	64	72
19	136	140
20	18	23

H,3,-10

1	432	434
2	144	148
3	96	89
4	100	95
5	49	51
6	14*	14
7	96	103
8	107	109
9	80	75
10	573	564
11	93	87
12	447	445
13	189	187
14	115	119
15	97	99
16	50	49
17	80	80
18	69	63
19	139	139
20	53	47
21	134	132

H,3,-9

1	318	315
2	200	179
3	88	80
4	153	145
5	29	17
6	43	50
7	194	190
8	477	483
9	105	94
10	537	540
11	257	248
12	99	97
13	103	97
14	167	164
15	25	19
16	142	149
17	125	123
18	80	86
19	84	80
20	63	75
21	31	19

H,3,-8

1	46	51
2	51	31
3	13*	9
4	44	33
5	193	184
6	116	115
7	61	76
8	354	348
9	76	77
10	378	376
11	103	105
12	138	124
13	166	163
14	72	65
15	40	36
16	20	26
17	15*	12
18	111	102
19	263	266
20	42	40
21	180	181

H,3,-7

1	89	93
2	236	252
3	243	237
4	24	17
5	202	188
6	382	365
7	59	60
8	664	653
9	118	106
10	209	204
11	21	12
12	91	88
13	31	11
14	284	298
15	83	84
16	51	56
17	161	162
18	127	130
19	107	108
20	66	64
21	148	158

H,3,-6

1	148	139
2	177	169
3	162	171
4	264	236
5	198	184
6	255	254
7	652	639
8	119	121
9	45	46
10	100	102
11	56	45
12	77	74
13	17	14
14	26	24
15	112	113
16	210	213
17	43	49
18	207	207
19	265	258
20	79	76
21	96	94

H,3,-5

1	36	34
2	448	415
3	547E	768
4	306	294
5	573	552
7	288	282
8	683	674
9	284	271
10	100	103
11	171	166
12	126	125
13	30	30
14	96	91
15	124	118
16	105	108
17	128	118
18	146	145
19	175	174

H,3,-5

20	106	100
21	88	95

H,3,-4

1	417	396
2	445	429
3	19	18
4	85	76
5	729	720
6	224	226
7	219	213
8	623	628
9	192	185
10	169	170
11	184	175
12	59	62
13	129	130
14	172	174
15	50	50
16	244	238
17	63	64
18	183	187
19	153	149
20	27	30
21	50	48

H,3,-3

1	286	290
2	287	265
3	447	418
4	73	72
5	269	260
6	342	331
7	383	369
8	306	288
9	213	228
10	172	166
11	15*	8
12	220	231
13	129	123
14	14*	3
15	167	159
16	105	106
17	59	54
18	209	212
19	56	51
20	12*	6
21	19	15

H,3,-2

1	38	16
2	392	370
3	471	461
4	200	177
5	1089	1030
6	743	713
7	276	256
8	328	357
9	281	287
10	236	241
11	194	183
12	15*	7
13	15*	6
14	117	114
15	18	11
16	164	147
17	139	138
18	76	78
19	108	109
20	63	67
21	45	42

H,3,-1

1	158	156
2	79	70
3	358	334
4	111	71
5	622	581
6	336	353
7	215	210
8	52	32
9	53	37
10	238	239
11	154	152
12	23	16
13	43	40
14	49	43
15	41	33
16	132	135
17	43	36
18	152	149
19	26	19
20	13	20

H,3,0

1	255	232
2	113	91
3	353	377
4	120	120
5	813E	1156
6	405	393
7	190	165
8	230	237
9	54	57
10	64	68
11	243	230
12	261	268
13	138	133
14	265	261
15	50	55
16	234	226
17	226	223
18	13*	5
19	48	57
20	19	17

H,3,1

0	233	221
1	183	162
2	224	240
3	312	330
4	209	229
5	376	370
6	482	468
7	249	258
8	45	28
9	35	42
10	90	75
11	29	6
12	364	359
13	104	98
14	140	141
15	27	26
16	272	270
17	49	45
18	15	17
19	86	84

H,3,2

0	22	8
1	265	244
2	421	405
3	385	404
4	307	317
5	54	52
6	47	53
7	31	26
8	55	55
9	36	39
10	64	58
11	231	221
12	428	422
13	45	40
14	232	224
15	73	67
16	66	62
17	121	122
18	40	41
19	92	98

H,3,3

0	547	536
1	338	326
2	366	351
3	640	663
4	17	6
5	439	453
6	90	80
7	256	247
8	142	145
9	65	57
10	16*	5
11	198	188
12	143	138
13	367	357
14	274	274
15	48	46
16	149	149
17	125	125
18	85	89

H,3,4

0	304	300
1	56	83
2	406	382
3	706	735
4	612	618
5	205	215
6	163	160
7	240	235
8	83	77
9	506	490
10	272	266
11	170	163
12	45	50
13	114	115
14	206	197
15	94	86
16	47	49
17	43	46
18	59	59

H,3,5

0	144	161
1	355	359
2	37	39
3	494	509
4	13*	7
5	80	87
6	19	12
7	145	144
8	199	200
9	98	96
10	24	17
11	231	222
12	151	150
13	53	45
14	215	209
15	54	52
16	78	70
17	62	55

H,3,6

0	295	307
1	647	660
2	470	459
3	483	479
4	350	355
5	139	142
6	354	353
7	110	119
8	106	104
9	449	437
10	340	325
11	70	64
12	212	201

H,3,6

13	15*	6
14	88	87
15	52	47
16	99	94

H,3,7

0	372	377
1	544	563
2	107	106
3	269	275
4	100	96
5	247	252
6	214	209
7	17*	4
8	294	281
9	16*	14
10	135	131
11	32	35
12	234	227
13	105	100
14	172	167
15	67	56
16	101	93

H,3,8

0	137	141
1	400	415
2	174	175
3	237	247
4	119	122
5	74	69
6	436	440
7	126	118
8	136	132
9	48	28
10	274	254
11	67	76
12	248	240
13	118	109
14	36	38
15	18	23

H,3,9

0	27	6
1	306	318
2	73	80
3	148	163
4	44	43
5	106	102
6	367	372
7	154	157
8	86	81
9	45	45
10	186	181
11	79	78
12	139	142
13	64	53
14	100	95

H,3,10

0	141	142
1	186	190
2	68	62
3	174	180
4	41	42
5	203	209
6	295	287
7	298	283
8	235	219
9	159	156
10	159	149
11	18	18
12	130	128
13	124	108

H,3,11

0	286	284
1	226	240
2	26	20
3	69	70
4	23	27
5	104	104
6	83	77
7	16*	5
8	259	248
9	48	51
10	178	175
11	40	41
12	63	60

H,3,12

0	26	25
1	217	215
2	135	132
3	52	51
4	16*	10
5	16*	9
6	26	24
7	102	90
8	113	105
9	70	66
10	146	139
11	47	47

H,3,13

0	213	207
1	199	201
2	53	48
3	172	173
4	36	28
5	148	146
6	137	130
7	20	11
8	138	135
9	53	52

H,3,14

0	18	24
1	171	173
2	68	70
3	23	20
4	161	154
5	92	85
6	51	51
7	92	85
8	120	109

H,3,15

0	112	104
1	76	75
2	31	26
3	177	169
4	23	13
5	13*	9
6	64	54

H,3,16

0	46	48
1	38	44
2	13*	4
3	71	68
4	12*	2

H,3,17

0	165	155
1	136	132
2	40	41

H,4,-17

1	12*	1
2	28	29
3	83	82
4	67	74
5	66	68
6	164	170
7	190	198
8	34	36
9	209	210
10	68	68
11	25	24
12	31	37

H,4,-16

1	171	170
2	33	39
3	19	12
4	14*	1
5	130	136
6	105	102
7	57	61
8	61	63
9	112	103
10	61	52
11	84	75
12	137	137
13	64	65
14	84	81

H,4,-15

1	54	53
2	64	61
3	49	51
4	137	137
5	86	88
6	88	93
7	213	211
8	44	40
9	156	153
10	135	135
11	59	59
12	15*	3
13	184	180
14	14*	5
15	41	45
16	151	158

H,4,-14

1	138	132
2	61	61
3	110	116
4	51	52
5	14*	8
6	149	152
7	113	105
8	64	61
9	205	198
10	188	184
11	24	10
12	44	51
13	48	48
14	15*	2
15	38	32
16	46	52
17	104	99

H,4,-13

1	15*	11
2	110	101
3	15*	11
4	38	54
5	76	55
6	109	108
7	116	113
8	190	185
9	187	182
10	89	93
11	18	15
12	79	75
13	72	73
14	122	125
15	43	42

H,4,-13

16	212	216
17	141	145
18	98	99

H,4,-12

1	285	292
2	25	15
3	19	36
4	209	213
5	97	103
6	51	46
7	157	152
8	98	99
9	135	126
10	196	191
11	52	53
12	125	120
13	126	127
14	118	117
15	171	168
16	66	65
17	125	118
18	100	92

H,4,-11

1	184	193
2	102	107
3	223	215
4	247	246
5	265	258
6	154	142
7	98	94
8	22	21
9	178	173
10	246	242
11	16*	7
12	143	147
13	19	16
14	134	135
15	126	125
16	170	159
17	177	194
18	19	17
19	68	73

H,4,-10

1	53	35
2	116	116
3	325	321
4	273	272
5	31	16
6	133	137
7	86	77
8	322	318
9	22	7
10	130	122
11	62	55
12	168	163
13	99	96
14	20	12
15	151	141
16	117	114
17	14*	3
18	130	121
19	74	78

H,4,-9

1	193	190
2	216	229
3	543	543
4	264	263
5	240	237
6	132	128
7	111	109
8	502	499
9	31	25
10	306	302
11	16*	3
12	16*	5
13	112	106
14	74	68
15	209	210
16	110	105
17	75	71
18	13*	9
19	79	83
20	21	12

H,4,-8

1	374	366
2	365	358
3	74	59
4	287	293
5	259	254
6	150	150
7	752	749
8	178	175
9	375	377
10	261	259
11	24	11
12	247	245
13	174	173
14	76	80
15	69	61
16	163	159
17	14*	18
18	71	70
19	12*	8
20	40	40

H,4,-7

1	103	111
2	218	234
3	289	297
4	408	415
5	38	45
6	368	363
7	73	79
8	89	88
9	352	354
10	136	138
11	115	110
12	132	132
13	260	250
14	75	74
15	127	123
16	28	24
17	16	17
18	32	33
19	60	66
20	11*	0

H,4,-6

1	226	224
2	471	480
3	137	137
4	78	88
5	643	644
6	120	129
7	408	398
8	101	95
9	68	66
10	205	209
11	107	108
12	200	194
13	95	91
14	177	192
15	70	64
16	209	220
17	55	68
18	14*	10
19	95	100
20	12	11

H,4,-5

1	36	49
2	347	352
3	21	30
4	359	355
5	319	302
6	607	600
7	175	168
8	50	44
9	166	148
10	117	117
11	301	296
12	101	106
13	379	397
14	172	182
15	152	160
16	136	144
17	15*	5
18	30	24
19	95	98
20	11*	10

H,4,-4

1	242	232
2	402	394
3	293	284
4	174	161
5	131	134
6	62	45
7	37	16
8	63	50
9	189	176
10	327	316
11	123	130
12	56	64
13	196	186
14	287	304
15	38	35
16	34	36
17	64	63
18	44	48
19	89	86
20	40	37

H,4,-3

1	41	41
2	390	398
3	119	117
4	160	153
5	214	198
6	62	50
7	305	301
8	28	15
9	75	36
10	41	36
11	274	274
12	132	143
13	413	424
14	39	39
15	154	151
16	97	88
17	48	47
18	95	102
19	12*	1
20	37	36

H,4,-2

1	222	221
2	221	224
3	307	317
4	52	32
5	540	510
6	92	93
7	170	157
8	306	308
9	178	182
10	98	98
11	351	353
10	98	98
11	351	353
12	85	94
13	229	224

H,4,-2

14	214	216
15	124	120
16	93	92
17	98	100
18	20	19
19	191	187
20	70	66

H,4,-1

1	74	85
2	297	292
3	82	69
4	83	72
5	161	138
6	98	95
7	35	31
8	14*	2
9	172	176
10	141	147
11	369	370
12	135	135
13	104	91
14	139	132
15	48	40
16	16	16
17	89	90
18	79	77
19	103	102

H,4,0

0	612	628
1	365	335
2	157	115
3	107	104
4	303	278
5	33	10
6	58	55
7	123	119
8	327	337
9	163	161
10	218	215
11	244	237
12	330	323
13	41	39
14	122	124
15	49	49
16	36	30
17	127	125
18	108	112
19	118	118

H,4,1

0	757	781
1	357	363
2	366	376
3	98	124
4	462	448
5	38	13
6	192	196
7	493	468
8	99	39
9	365	361
10	113	105
11	118	112
12	90	97
13	78	73
14	20	9
15	53	50
16	22	25
17	13*	2
18	47	32

H,4,2

0	371	386
1	361	359
2	122	105
3	188	160
4	69	30
5	144	141
6	313	312
7	84	65
8	340	330
9	223	207
10	149	149
11	448	444
12	249	248
13	74	64
14	15*	10
15	99	96
16	44	43
17	130	124
18	44	36

H,4,3

0	724	731
1	530	520
2	21	6
3	450	441
4	443	439
5	90	93
6	89	83
7	312	309
8	439	433
9	506	498
10	317	315
11	211	205
12	135	117
13	80	84
14	127	125
15	14*	6
16	28	18
17	12*	5

H,4,4

0	95	116
1	81	89
2	237	224
3	60	57
4	148	159
5	48	35
6	217	226
7	244	237
8	181	175
9	472	464
10	40	41
11	156	160
12	206	201
13	26	25
14	20	12
15	112	107
16	51	54
17	127	121

H,4,5

0	287	287
1	104	98
2	405	403
3	307	302
4	110	108
5	15*	6
6	85	82
7	539	533
8	599	595
9	375	369
10	501	489
11	97	92
12	15*	17
13	14*	3
14	50	51
15	72	71
16	159	144

H,4,6

0	38	52
1	15	28
2	144	145
3	72	77
4	195	200
5	63	56
6	260	256
7	22	7
8	327	324
9	114	105
10	225	213
11	99	90
12	82	85
13	70	71
14	93	89
15	148	140

H,4,7

0	144	138
1	65	63
2	120	112
3	48	50
4	35	39
5	136	138
6	272	275
7	419	420
8	110	105
9	16*	16
10	101	89
11	22	19
12	40	43
13	27	25
14	80	73
15	77	73

H,4,8

0	15*	6
1	98	85
2	104	98
3	89	85
4	195	198
5	68	58
6	134	129
7	127	125
8	105	104
9	168	169
10	36	33
11	35	32
12	108	104
13	173	161
14	81	73

H,4,9

0	114	114
1	14*	2
2	58	58
3	253	248
4	261	265
5	111	108
6	110	111
7	16*	4
8	69	67
9	45	41
10	25	29
11	139	140
12	18	12
13	56	52

H,4,10

0	178	176
1	188	179
2	174	176
3	128	123
4	171	172
5	54	49
6	46	44
7	130	124
8	47	42
9	109	113
10	15	9
11	94	93
12	58	53

H,4,11

0	187	195
1	80	80
2	15*	9
3	53	52
4	361	364
5	63	59
6	74	67
7	87	85
8	93	88
9	52	48
10	38	34
11	36	30

H,4,12

0	91	86
1	178	166
2	299	298
3	149	149
4	75	75
5	43	36
6	80	80
7	87	84
8	57	58
9	13	9

H,4,13

0	141	149
1	16	17
2	180	179
3	19	20
4	295	294
5	86	87
6	129	125
7	85	79
8	16	12

H,4,14

0	110	106
1	127	125
2	172	171
3	121	124
4	90	87
5	74	66
6	40	36

H,4,15

0	23	11
1	14*	14
2	255	254
3	54	60
4	137	137

H,4,16

0	109	105
1	61	59
2	13	6

H,5,-16

2	67	62
3	59	66
4	90	92
5	41	37
6	146	145
7	106	103
8	71	67
9	78	75
10	13*	7
11	107	106

H,5,-15

1	117	123
2	80	80
3	146	149
4	115	127
5	35	35
6	18	24
7	13*	11
8	98	90
9	77	73
10	14*	7
11	149	145
12	140	133
13	132	131

H,5,-14

1	24	34
2	48	48
3	20	31
4	187	189
5	14*	2
6	74	67
7	14*	8
8	27	29
9	211	208
10	61	64
11	134	130
12	31	22
13	26	30
14	117	121
15	206	217

H,5,-13

1	38	26
2	103	112
3	161	165
4	227	234
5	17	4
6	46	47
7	15	13
8	49	49
9	23	23
10	208	202
11	100	101
12	177	163
13	99	98
14	89	87
15	75	78
16	54	54

H,5,-12

1	35	41
2	179	182
3	84	80
4	235	227
5	24	29
6	33	21
7	84	80
8	23	28
9	153	152
10	46	46
11	41	44
12	115	113
13	82	71
14	95	97
15	193	194
16	13*	6
17	57	51

H,5,-11

1	230	236
2	55	46
3	91	88
4	24	20
5	89	90
6	72	64
7	24	4
8	105	104
9	23	25
10	166	157
11	179	180
12	178	171
13	66	63
14	15*	3
15	34	37
16	74	72
17	12*	9

H,5,-10

1	247	258
2	296	292
3	138	141
4	393	382
5	44	42
6	22	25
7	148	143
8	56	52
9	93	100
10	30	35
11	62	58
12	70	64
13	172	170
14	29	34
15	33	28
16	79	82
17	64	64
18	157	158

H,5,-9

1	347	352
2	73	64
3	105	115
4	34	36
5	134	133
6	108	103
7	18	15
8	250	247
9	100	94
10	271	264
11	133	132
12	103	94
13	16*	3
14	45	45
15	57	60
16	47	46
17	38	36
18	42	39

H,5,-8

1	128	131
2	363	365
3	89	84
4	161	158
5	81	78
6	108	106
7	70	63
8	354	359
9	52	48
10	37	37
11	27	12
12	61	50
13	147	143
14	15*	3
15	30	30
16	37	28
17	95	96
18	251	255

H,5,-7

1	70	63
2	42	34
3	155	163
4	108	110
5	336	330
6	345	346
7	248	240
8	688	691
9	305	291
10	354	346
11	34	32
12	67	65
13	37	34
14	49	55

H,5,-7

15	63	68
16	13*	1
17	115	114
18	96	104
19	163	154

H,5,-6

1	52	49
2	166	166
3	69	67
4	321	320
5	300	299
6	106	100
7	238	231
8	93	97
9	48	38
10	202	198
11	263	264
12	69	65
13	55	57
14	27	12
15	39	51
16	108	98
17	83	88
18	186	185
19	100	101

H,5,-5

1	76	73
2	21	17
3	185	182
4	32	33
5	129	128
6	199	195
7	194	193
8	286	285
9	24	10
10	195	184
11	76	85
12	145	156
13	105	106
14	134	137
15	94	103
16	119	111
17	177	172
18	50	45
19	88	89

H,5,-4

1	145	135
2	44	51
3	121	111
4	290	289
5	608	605
6	150	148
7	117	116
8	105	101
9	80	84
10	114	113
11	174	173
12	165	171
13	33	30
14	57	53
15	210	217
16	196	194
17	65	58
18	12*	11
19	110	116

H,5,-3

1	53	52
2	163	148
3	189	181
4	16	13
5	115	124
6	254	253
7	186	179
8	265	250
9	36	32
10	61	55
11	25	26
12	22	12
13	32	38
14	78	78
15	15*	11
16	157	153
17	170	165
18	65	61

H,5,-2

1	40	28
2	256	259
3	216	212
4	148	157
5	158	147
6	174	164
7	31	10
8	193	195
9	213	222
10	53	59
11	56	54
12	238	261
13	96	85
14	50	55
15	176	180
16	160	162
17	133	129
18	54	54

H,5,-1

1	133	124
2	152	143
3	26	23
4	191	180
5	344	340
6	151	158
7	208	210
8	73	71
9	16*	18
10	32	17
11	37	43
12	34	39
13	128	132
14	235	231
15	83	76
16	188	190
17	105	104
18	40	37

H,5,0

1	227	214
2	422	420
3	476	472
4	232	223
5	30	29
6	306	314
7	238	231
8	269	267
9	89	85
10	128	137
11	32	29
12	75	73
13	158	149
14	39	26
15	22	22
16	71	73
17	62	58
18	19	19

H,5,1

0	38	32
1	133	129
2	62	67
3	643	649
4	56	32
5	498	490
6	66	73
7	114	103
8	16*	18
9	91	93
10	65	65
11	77	74
12	104	96
13	45	39
14	208	209
15	30	25
16	172	173
17	39	42

H,5,2

0	158	157
1	440	452
2	422	431
3	348	361
4	54	46
5	186	174
6	423	420
7	155	152
8	179	170
9	38	34
10	219	220
11	210	195
12	30	26
13	175	172
14	34	22
15	150	144
16	12*	14
17	28	25

H,5,3

0	124	125
1	222	220
2	160	166
3	434	446
4	282	288
5	325	331
6	186	182
7	120	120
8	44	49
9	291	288
10	197	189
11	56	52
12	233	224
13	78	82
14	188	186
15	14	17
16	94	97

H,5,4

0	260	268
1	90	99
2	279	292
3	15	5
4	143	145
5	180	188
6	133	133
7	18*	21
8	108	105
9	376	362
10	118	112
11	229	220
12	85	83
13	48	43
14	145	151
15	168	164

H,5,5

0	54	61
1	193	198
2	248	245
3	303	326
4	23	14
5	163	173
6	92	79
7	123	124

H,5,5

8	113	103
9	44	38
10	42	45
11	17	8
12	178	172
13	18	17
14	186	186
15	51	56

H,5,6

0	240	240
1	59	75
2	26	23
3	62	58
4	146	142
5	65	62
6	215	224
7	382	370
8	106	102
9	338	331
10	18	7
11	14	6
12	176	169
13	130	128
14	44	49

H,5,7

0	35	15
1	340	345
2	37	40
3	345	356
4	35	39
5	184	187
6	162	156
7	161	150
8	227	229
9	28	27
10	51	45
11	36	38
12	165	163
13	54	58

H,5,8

0	75	87
1	223	242
2	181	178
3	71	79
4	338	340
5	17*	17
6	94	103
7	198	187
8	85	84
9	100	92
10	53	43
11	15	13
12	12*	12

H,5,9

0	61	69
1	326	342
2	72	82
3	246	256
4	15*	7
5	37	35
6	15*	3
7	79	74
8	135	130
9	60	67
10	200	191
11	74	74

H,5,10

0	55	52
1	94	94
2	236	230
3	19	11
4	159	166
5	16*	5
6	61	59
7	102	93
8	65	62
9	79	78
10	26	17

H,5,11

0	55	63
1	178	179
2	45	47
3	16*	2
4	66	67
5	14*	2
6	69	65
7	49	51
8	83	77
9	71	73

H,5,12

0	142	150
1	55	59
2	114	110
3	93	94
4	31	34
5	120	109
6	128	124
7	186	183

H,5,13

0	83	88
1	15	10
2	86	81
3	42	43
4	25	24
5	18	16
6	24	22

H,5,14

0	62	62
1	14*	17
2	33	30
3	95	95
4	21	18

H,5,15

0	64	62
1	50	48

H,6,-14

1	113	102
2	91	94
3	13*	16
4	108	115
5	92	89
6	66	62
7	40	41
8	31	29
9	92	94
10	146	145
11	80	73

H,6,-13

1	59	64
2	49	49
3	60	59
4	56	62
5	153	159
6	94	99
7	187	192
8	19	16
9	118	116
10	50	49
11	28	27
12	90	92
13	12*	8

H,6,-12

1	74	74
2	143	152
3	91	90
4	129	132
5	175	175
6	15*	8
7	54	52
8	144	145
9	104	95
10	219	218
11	132	130
12	92	96
13	107	103
14	117	124

H,6,-11

1	16	14
2	16	23
3	16	15
4	96	94
5	149	152
6	128	131
7	155	154
8	106	103
9	34	48
10	94	103
11	58	60
12	190	204
13	195	204
14	15	2
15	199	208

H,6,-10

1	35	37
2	132	138
3	85	82
4	46	40
5	14*	4
6	80	83
7	75	72
8	242	251
9	254	254
10	31	33
11	166	166
12	262	271
13	48	45
14	145	152
15	87	85

H,6,-9

1	87	98
2	40	37
3	17	14
4	116	113
5	146	144
6	17	9
7	101	97
8	16*	16
9	120	119
10	56	57
11	50	49
12	110	114
13	186	188
14	75	77
15	153	156
16	55	51

H,6,-8

1	263	269
2	54	56
3	140	139
4	131	132
5	19	19
6	98	96
7	97	93

H,6,-8

8	171	168
9	95	89
10	56	47
11	61	48
12	167	161
13	60	58
14	78	79
15	45	49
16	108	108

H,6,-7

1	49	55
2	217	222
3	88	81
4	105	105
5	154	152
6	184	188
7	45	47
8	68	76
9	23	20
10	39	33
11	34	31
12	15*	0
13	142	145
14	25	17
15	114	116
16	116	124
17	12*	12

H,6,-6

1	345	351
2	144	146
3	35	33
4	34	30
5	300	301
6	91	88
7	321	319
8	49	47
9	21	12
10	121	115
11	73	69
12	72	60
13	55	43
14	109	115
15	51	50
16	80	75
17	35	34

H,6,-5

1	248	251
2	452	455
3	474	479
4	268	261
5	31	27
6	129	123
7	156	152
8	32	27
9	43	41
10	92	95
11	144	137
12	27	33
13	178	176
14	52	51
15	153	162
16	128	141
17	11	17

H,6,-4

1	358	364
2	23	20
3	415	417
4	260	257
5	504	501
6	188	196
7	204	200
8	169	172
9	83	82
10	156	157
11	17*	16
12	43	55
13	86	93
14	128	146
15	13*	13
16	16	8
17	11*	2

H,6,-3

1	240	244
2	471	472
3	410	402
4	119	112
5	115	117
6	41	39
7	84	89
8	88	85
9	98	98
10	16*	9
11	234	241
12	15*	9
13	260	268
14	71	71
15	13*	11
16	71	80
17	22	26

H,6,-2

1	54	57
2	167	157
3	351	359
4	29	25
5	210	206
6	116	113
7	258	254
8	298	306
9	171	181
10	127	126
11	79	87
12	128	135
13	67	72
14	133	135
15	72	74
16	29	25

H,6,-1

1	231	228
2	172	172
3	189	183
4	39	34
5	50	45
6	17*	8
7	42	28
8	26	9
9	175	171
10	16*	4
11	211	205
12	53	61
13	114	114
14	110	125
15	28	26
16	44	52
15	28	26
16	44	52

H,6,0

0	129	136
1	342	346
2	232	224
3	178	185
4	85	86
5	107	113
6	204	202
7	41	36
8	289	292
9	16*	7
10	58	61
11	152	151
12	215	214
13	65	67
14	53	50
15	50	51
16	28	30

H,6,1

0	378	383
1	395	410
2	35	34
3	118	120
4	20	10
5	176	172
6	21	20
7	46	45
8	69	66
9	91	88
10	107	112
11	199	194
12	27	33
13	77	79
14	12*	3
15	17	22

H,6,2

0	58	57
1	235	247
2	106	106
3	119	129
4	82	83
5	46	39
6	337	340
7	110	115
8	87	83
9	134	127
10	49	39
11	82	85
12	187	187
13	85	83
14	79	83
15	68	67

H,6,3

0	109	107
1	57	55
2	107	90
3	32	31
4	24	9
5	20	20
6	185	195
7	63	63
8	52	45
9	211	201
10	41	44
11	222	236
12	151	147
13	121	119
14	87	84

H,6,4

0	114	118
1	175	181
2	122	121
3	19	7
4	213	213
5	151	153
6	156	159
7	18	12
8	68	70
9	93	89
10	37	31
11	127	124
12	149	150
13	17	19
14	59	52

H,6,5

0	107	112

H,6,5

1	26	23
2	39	46
3	44	44
4	220	227
5	192	201
6	226	222
7	218	206
8	136	135
9	140	139
10	24	22
11	16	19
12	21	15
13	83	82

H,6,6

0	25	27
1	306	325
2	49	45
3	137	141
4	175	182
5	132	128
6	50	55
7	66	60
8	28	17
9	102	102
10	76	70
11	97	97
12	68	64

H,6,7

0	15*	1
1	43	55
2	31	41
3	26	24
4	139	138
5	216	214
6	246	244
7	113	104
8	77	78
9	81	79
10	96	96
11	15	22

H,6,8

0	87	97
1	17	23
2	169	165
3	199	206
4	173	175
5	104	101
6	25	16
7	35	37
8	146	138
9	122	119
10	61	56

H,6,9

0	59	63
1	163	178
2	49	48
3	202	213
4	130	123
5	26	32
6	78	84
7	104	106
8	35	32
9	114	123

H,6,10

0	74	66
1	172	181
2	178	172
3	80	79
4	201	208
5	61	62
6	99	95
7	36	33
8	126	125

H,6,11

0	15*	17
1	154	171
2	164	166
3	124	131
4	132	131
5	14*	18
6	144	143

H,6,12

0	83	82
1	133	135
2	160	162
3	60	61
4	13*	8
5	15	13

H,6,13

0	44	45
1	16	10
2	143	140
3	11*	6

H,6,14

0	61	62

H,7,-12

1	41	44
2	24	24
3	19	18
4	184	185
5	13*	9
6	125	134
7	130	129
8	84	87
9	145	149

H,7,-11

1	90	98
2	89	92
3	75	79
4	72	68
5	37	33
6	14*	2
7	110	117
8	69	67
9	82	77
10	119	118
11	83	88

H,7,-10

1	43	44
2	101	97
3	54	54
4	131	128
5	23	18
6	19	16
7	154	157
8	68	61
9	155	159
10	26	34
11	14*	12
12	12*	2

H,7,-9

1	140	139
2	72	72
3	20	14
4	89	85
5	26	20
6	45	45
7	179	183
8	156	159
9	48	40
10	198	212
11	15*	10
12	97	110
13	70	69

H,7,-8

1	15*	15
2	219	220
3	97	104
4	238	241
5	103	108
6	127	127
7	247	250
8	56	49
9	33	30
10	15*	11
11	152	154
12	43	41
13	80	84

H,7,-7

1	75	68
2	173	176
3	101	117
4	38	33
5	28	29
6	15*	4
7	168	166
8	93	89
9	26	24
10	175	175
11	42	37
12	48	60
13	13*	11
14	12*	9

H,7,-6

1	35	34
2	218	225
3	42	42
4	44	41
5	66	73
6	111	106
7	116	119
8	18	4
9	32	28
10	60	62
11	151	156
12	18	15
13	23	22
14	126	126

H,7,-5

1	23	18
2	224	230
3	200	200
4	50	44
5	148	150
6	58	58
7	79	74
8	183	183
9	23	29
10	167	171
11	19	11
12	25	22
13	31	35
14	81	83

H,7,-4

1	129	134
2	16*	16
3	114	125
4	219	224
5	153	150
6	122	123
7	86	90

H,7,-4

8	39	36
9	110	110
10	118	128
11	92	95
12	59	60
13	50	47
14	101	99

H,7,-3

1	90	83
2	64	69
3	159	168
4	133	130
5	121	117
6	40	40
7	118	110
8	200	202
9	63	60
10	29	23
11	60	65
12	36	30
13	12*	1
14	63	60

H,7,-2

1	258	257
2	91	86
3	252	248
4	283	281
5	307	306
6	129	132
7	110	113
8	185	192
9	285	294
10	134	139
11	14*	6
12	98	100
13	100	101
14	71	69

H,7,-1

1	202	195
2	244	240
3	179	177
4	28	30
5	232	243
6	146	148
7	17*	15
8	105	106
9	87	84
10	63	69
11	16	12
12	29	35
13	13*	4
14	133	133

H,7,0

1	198	202
2	80	85
3	126	129
4	149	154
5	18*	2
6	17*	12
7	288	288
8	118	122
9	251	264
10	96	96
11	145	141
12	148	160
13	268	274

H,7,1

0	91	92
1	199	204
2	19	11
3	97	99
4	68	64
5	143	148
6	222	226
7	119	124
8	137	146
9	15*	2
10	14*	4
11	55	52
12	143	138
13	110	117

H,7,2

0	44	47
1	18	7
2	173	177
3	24	23
4	36	41
5	72	60
6	55	59
7	190	192
8	65	68
9	19	7
10	106	110
11	267	267
12	57	56

H,7,3

0	107	112
1	145	150
2	73	72
3	152	156
4	133	133
5	21	27
6	115	117
7	25	29
8	15*	16
9	14*	6
10	16	6
11	110	117
12	96	96

H,7,4

0	79	81
1	20	11
2	115	123
3	20	13
4	112	105
5	17*	8
6	175	175
7	90	97
8	56	58
9	165	162
10	36	37
11	51	48

H,7,5

0	161	161
1	73	67
2	53	63
3	178	181
4	158	164
5	73	71
6	117	113
7	40	38
8	49	55
9	88	79
10	12*	7

H,7,6

0	252	253
1	15*	2
2	59	59
3	16*	18
4	104	97
5	35	26
6	105	105
7	20	24
8	13	13
9	126	123

H,7,7

0	118	124
1	208	213
2	53	50
3	205	224
4	84	82
5	100	106
6	42	44
7	13*	2
8	34	32

H,7,8

0	36	34
1	20	16
2	103	96
3	15*	5
4	211	214
5	71	69
6	12*	4
7	201	201

H,7,9

0	48	53
1	152	161
2	51	52
3	134	140
4	14*	3
5	59	56
6	24	26

H,7,10

0	81	77
1	155	165
2	205	209
3	38	44
4	140	149

H,7,11

0	13	16
1	21	12
2	24	24

H,8,-9

1	82	88
2	94	104
3	67	71
4	26	27
5	21	19
6	16	19

H,8,-8

1	108	116
2	45	43
3	67	69
4	75	80
5	77	85
6	51	47
7	131	135
8	36	38

H,8,-7

1	117	117
2	80	75
3	13*	9
4	56	58
5	111	116
6	24	23
7	108	104
8	23	22
9	69	70

H,8,-6

1	77	76
2	120	136
3	64	67
4	63	61
5	38	51
6	103	106
7	132	139
8	24	29
9	14*	11
10	166	180

H,8,-5

1	104	105
2	79	82
3	45	50
4	40	41
5	204	210
6	55	56
7	147	155
8	15*	9
9	33	36
10	210	225

H,8,-4

1	21	14
2	15*	5
3	104	106
4	36	33
5	115	123
6	27	28
7	41	40
8	115	119
9	46	52
10	120	127

H,8,-3

1	118	124
2	200	208
3	202	207
4	22	28
5	130	136
6	71	73
7	85	93
8	97	95
9	49	57
10	191	204

H,8,-2

1	173	184
2	46	43
3	235	247
4	37	40
5	78	77
6	27	25
7	28	30
8	121	124
9	14*	8
10	52	56

H,8,-1

1	163	162
2	106	109
3	129	125
4	75	78
5	96	104
6	22	20
7	70	69
8	146	139
9	65	64
10	113	116

H,8,0

0	47	46
1	153	154
2	41	35
3	156	159
4	23	22
5	15*	9
6	118	119
7	74	75
8	92	94
9	60	63
10	32	34

H,8,1

0	133	135
1	85	98
2	45	51
3	96	99
4	29	22
5	17	21
6	105	96
7	15*	12
8	173	176
9	82	82

H,8,2

0	126	130
1	190	195
2	92	94
3	143	152
4	17	21
5	31	26
6	144	140
7	58	53
8	26	23
9	46	43

H,8,3

0	171	177
1	94	99
2	82	84
3	78	83
4	66	57
5	79	81
6	183	169
7	44	33
8	155	164

H,8,4

0	39	39
1	146	149
2	18	14
3	47	49
4	98	101
5	14*	6
6	144	143
7	22	20

H,8,5

0	126	135
1	141	150
2	14*	3
3	47	56
4	89	82
5	22	15
6	163	165

H,8,6

0	57	57
1	40	41
2	71	71
3	63	66
4	114	118
5	13*	6

H,8,7

0	23	22
1	14*	24
2	90	93
3	93	93
4	131	135

H,8,8

0	32	32
1	92	97
2	13*	4

H,9,-3

1	13*	7

H,9,-2

1	52	61
2	85	94
3	35	36

H,9,-1

1	220	237
2	132	137
3	153	165

H,9,0

1	124	138
2	156	173
3	15	13

H,9,1

0	111	119
1	92	91
2	143	150

H,9,2

0	31	26
1	89	97

APPENDIX VIII

Tables of observed and calculated structure factors for 1,7,13-trimethyltribenzo[*b*,*f*,*j*][1,5,9]trithiacyclododecine-6,12,18-trione

Data Format:

	H	K
L	$10\times\lvert F_o\rvert$	$10\times\lvert F_c\rvert$

Reflections removed for extinction marked .... E

Reflections classed as unobserved marked ..... *

0,0,L

2	1355E	1686
4	123	96
6	69	66
8	258	224
10	300	295
12	17*	7
14	60	53
16	143	142
18	58	56
20	16	17

0,1,L

1	339	335
2	741	748
3	641	639
4	42	31
5	535	540
6	399	412
7	144	132
8	1006	1019
9	25	19
10	359	350
11	214	206
12	44	41
13	160	154
14	189	195
15	23	23
16	189	190
17	33	31
18	21	14
19	52	51
20	66	70

0,2,L

0	1098E	1331
1	454	453
2	1124	1162
3	819	841
4	129	126
5	314	302
6	148	147
7	285	283
8	432	436
9	486	489
10	31	38
11	185	187
12	196	193
13	59	50
14	25	21
15	74	70
16	32	28
17	36	37
18	90	92
19	40	36

0,3,L

1	812	811
2	765	776
3	172	152
4	1163	1138
5	849	849
6	301	290
7	856	853
8	345	336
9	26	35
10	245	258
11	380	391
12	21	18
13	178	176
14	126	129
15	103	101
16	276	276
17	124	119
18	177	171
19	98	101

0,4,L

0	474	484
1	178	177
2	1000	990
3	292	309
4	401	397
5	586	573
6	409	393
7	225	225
8	51	46
9	124	125
10	375	373
11	44	51
12	236	233
13	67	70
14	16*	8
15	20	17
16	32	35
17	87	83
18	39	42
19	24	24

0,5,L

1	62	65
2	376	378
3	310	311
4	886	899
5	79	72
6	146	148
7	56	55
8	175	152
9	154	154
10	40	36
11	95	94
12	130	137
13	220	221
14	151	149
15	247	237
16	35	25
17	29	30
18	89	90
19	172	166

0,6,L

0	252	256
1	130	123
2	211	211
3	307	293
4	235	232
5	68	79
6	333	338
7	526	519
8	24	38
9	88	73
10	162	159
11	169	168
12	287	278
13	351	352
14	261	252
15	158	153
16	90	87
17	37	38
18	13*	5
19	58	61

0,7,L

1	108	101
2	138	136
3	34	27
4	55	26
5	139	142
6	109	116
7	321	307
8	88	98
9	154	152
10	33	36
11	16*	21
12	222	221
13	122	117
14	164	165
15	287	287
16	156	152
17	14*	19
18	52	42

0,8,L

0	328	336
1	260	254
2	203	188
3	29	42
4	98	93
5	105	98
6	15*	24
7	475	462
8	48	52
9	139	127
10	186	183
11	148	154
12	188	194
13	72	71
14	270	273
15	116	110
16	104	106
17	140	134
18	44	43

0,9,L

1	351	370
2	28	27
3	392	402
4	240	252
5	61	56
6	67	60
7	240	232
8	110	108
9	329	341
10	88	88
11	202	197
12	16*	12
13	15*	5
14	79	73
15	88	91
16	105	102
17	13	9

0,10,L

0	433	419
1	15*	18
2	276	257
3	71	70
4	129	126
5	115	109
6	155	151
7	205	201
8	244	241
9	150	140
10	20	14
11	206	195
12	68	65
13	50	49
14	15*	3
15	84	74
16	73	81
17	124	124

0,11,L

1	31	21
2	103	107
3	302	303
4	213	214
5	147	147
6	114	110
7	540	544
8	368	379
9	353	355
10	172	164
11	40	40
12	113	116
13	25	23
14	92	93
15	71	73
16	21	22

0,12,L

0	342	340
1	63	57
2	17	7
3	58	60
4	95	106
5	73	72
6	203	208
7	289	289
8	164	164
9	203	206
10	16*	5
11	52	49
12	17	21
13	115	115
14	106	111
15	119	122

0,13,L

1	166	176
2	15*	6
3	68	66
4	191	204
5	309	313
6	298	307
7	183	183
8	38	34
9	16*	9
10	15*	6
11	15*	15
12	42	42
13	14*	3
14	17	16

0,14,L

0	251	250
1	32	26
2	52	55
3	101	98
4	80	74
5	183	183
6	155	155
7	161	159
8	82	82

0,14,L

9	133	126
10	111	105
11	19	17
12	132	134
13	81	85

0,15,L

1	116	120
2	338	340
3	84	84
4	180	179
5	56	57
6	49	52
7	58	64
8	14*	10
9	17	19
10	105	107
11	15	16
12	35	35

0,16,L

0	94	93
1	112	108
2	85	83
3	157	159
4	110	110
5	29	27
6	94	96
7	17	10
8	75	71
9	70	72
10	152	147
11	57	59

0,17,L

1	86	91
2	76	67
3	144	139
4	124	125
5	144	146
6	121	112
7	156	155
8	14	7
9	13	10

0,18,L

0	200	196
1	76	71
2	92	87
3	93	85
4	28	28
5	97	100
6	62	64
7	139	145

0,19,L

1	62	70
2	57	60
3	23	17
4	11*	2

1,0,L

1	589	576
2	854	848
3	260	256
4	523	526
5	83	80
6	477	488
7	17	22
8	66	88
9	257	262
10	297	290
11	313	309
12	279	281
13	126	125
14	123	121
15	53	52
16	16*	7
17	99	96
18	21	25
19	36	36

1,1,L

0	109	109
1	405	389
2	879	886
3	633	636
4	78	64
5	505	488
6	264	248
7	273	264
8	198	183
9	279	278
10	157	147
11	228	230
12	258	260
13	170	172
14	286	288
15	31	27
16	151	150
17	94	90
18	18	20
19	31	26

1,2,L

0	529	531
1	556	548
2	714	710
3	1202	1204
4	617	610
5	607	601
6	333	331
7	213	193
8	259	261
9	371	367
10	192	187
11	16	11
12	122	111
13	103	96
14	130	122
15	177	179
16	29	32
17	139	141
18	79	82
19	109	110

1,3,L

0	77	76
1	217	214
2	542	539
3	523	519
4	416	415
5	238	234
6	362	368
7	248	237
8	169	152
9	151	155
10	205	213
11	227	219
12	332	342
13	188	180
14	82	87
15	158	156
16	79	78
17	113	113
18	24	22
19	89	86

1,4,L

0	407	401
1	973	1000
2	1153	1175
3	338	331
4	272	266
5	815	804
6	408	403
7	444	445
8	91	89
9	154	166
10	62	56
11	99	96
12	243	239
13	198	198
14	65	57
15	104	104
16	164	168
17	154	149
18	139	133
19	95	95

1,5,L

0	533	542
1	581	578
2	554	539
3	870	872
4	400	397
5	181	184
6	342	335
7	409	410
8	250	245
9	372	364
10	271	268
11	144	147
12	77	74
13	288	283
14	35	34
15	133	128
16	54	52
17	51	51
18	55	57
19	18	22

1,6,L

0	226	226
1	708	712
2	370	357
3	543	535
4	335	326
5	631	628
6	260	257
7	285	285
8	200	203
9	157	148
10	347	335
11	239	234
12	82	85
13	116	116
14	175	173
15	134	129
16	172	172
17	110	112
18	43	42

1,7,L

0	652	667
1	113	114
2	660	644
3	100	88
4	392	381
5	194	196
6	520	507
7	410	412
8	214	211
9	464	463
10	309	304
11	159	153
12	132	129
13	183	184
14	109	112
15	97	98
16	81	75
17	79	81
18	97	92

1,8,L

0	55	57
1	171	159
2	284	301
3	263	268
4	291	286
5	153	148
6	170	171
7	265	259
8	564	570
9	117	111
10	314	318
11	225	223
12	150	155
13	109	107
14	90	88
15	83	84
16	86	85
17	44	45
18	48	51

1,9,L

0	700	703
1	362	369
2	104	107
3	526	537
4	167	156
5	304	309
6	221	223
7	132	140
8	176	172
9	37	35
10	71	59
11	214	218
12	116	116
13	43	45
14	56	52
15	80	73
16	88	91
17	60	62

1,10,L

0	340	347
1	349	351
2	229	236
3	260	262
4	79	79

1,10,L

5	292	305
6	79	82
7	329	326
8	155	158
9	44	52
10	236	238
11	192	197
12	102	107
13	186	186
14	73	73
15	38	35
16	89	88
17	47	48

1,11,L

0	222	232
1	377	378
2	97	95
3	438	448
4	180	181
5	159	164
6	189	188
7	166	174
8	139	142
9	67	77
10	199	202
11	145	148
12	50	49
13	76	75
14	90	93
15	93	90
16	54	52

1,12,L

0	33	37
1	65	60
2	264	272
3	48	48
4	213	216
5	116	113
6	127	129
7	109	105
8	164	161
9	205	205
10	147	149
11	101	105
12	80	83
13	139	139
14	103	102
15	132	128

1,13,L

0	191	197
1	53	51
2	83	79

2,6,L

8	206	215
9	122	123
10	156	156
11	244	251
12	133	129
13	181	186
14	124	129
15	21	18
16	125	123
17	98	93
18	88	89

2,7,L

0	145	140
1	398	393
2	412	419
3	168	164
4	586	586
5	275	268
6	548	537
7	111	103
8	114	110
9	262	265
10	183	187
11	93	89
12	113	111
13	70	74
14	97	91
15	141	141
16	78	76
17	101	101
18	60	55

2,8,L

0	132	119
1	307	314
2	154	152
3	256	254
4	155	160
5	119	114
6	83	81
7	165	162
8	223	226
9	184	184
10	109	106
11	64	58
12	86	89
13	68	68
14	102	97
15	54	50
16	52	48
17	73	72

2,9,L

0	37	26
3	52	50
4	217	217
5	72	74
6	305	306
7	195	189
8	162	157
9	144	147
10	71	69
11	53	53
12	56	55
13	83	84
14	33	34

1,14,L

0	102	94
1	127	128
2	95	94
3	95	93
4	88	92
5	243	244
6	116	117
7	50	50
8	88	93
9	22	15
10	73	72
11	14*	8
12	58	57
13	76	76

1,15,L

0	24	23
1	39	35
2	69	64
3	49	54
4	52	53
5	81	81
6	71	74
7	120	118
8	123	126
9	39	35
10	76	74
11	70	66
12	27	25

1,16,L

0	29	29
1	79	78
2	61	61
3	120	120
4	137	135
5	99	104
6	25	24
7	74	76
8	15	9
9	90	88
10	68	63
11	52	56

1	300	290
2	80	84
3	113	107
4	141	123
5	113	112
6	115	115
7	93	97
8	93	97
9	307	305
10	194	191
11	105	101
12	112	105
13	106	110
14	130	131
15	76	72
16	104	108
17	54	53

2,10,L

0	205	201
1	229	225
2	248	254
3	70	66
4	222	227
5	130	126
6	360	367
7	80	82
8	39	40
9	130	136
10	92	97
11	123	122
12	109	115
13	35	35
14	49	50
15	80	84
16	65	69

2,11,L

0	36	29
1	157	148
2	198	200
3	82	80
4	207	201
5	73	64
6	220	221
7	68	73
8	220	222
9	79	73
10	110	108
11	36	32
12	137	137
13	70	70
14	92	86
15	61	62
16	35	31

1,17,L

0	30	29
1	86	88
2	71	73
3	97	98
4	68	67
5	33	34
6	83	86
7	49	50
8	51	47
9	53	53

1,18,L

0	15	13
1	38	37
2	87	86
3	98	99
4	14	12
5	74	75
6	81	81
7	33	29

1,19,L

0	115	119
1	25	25
2	31	30
3	89	90

2,0,L

0	472	478
1	452	446
2	350	345
3	564	546
4	823	828
5	182	186
6	498	515
7	32	14
8	238	238
9	253	260
10	273	280
11	332	342
12	200	201
13	269	263
14	29	15
15	63	54
16	151	146
17	52	58
18	100	97
19	33	34

2,1,L

0	174	176
1	691	686
2	413	409
3	947	959

2,12,L

0	105	100
1	123	124
2	314	313
3	167	170
4	240	247
5	80	80
6	155	155
7	134	131
8	87	90
9	210	208
10	99	100
11	54	53
12	44	46
13	73	69
14	47	43
15	53	53

2,13,L

0	100	101
1	208	208
2	215	216
3	56	60
4	204	201
5	220	231
6	196	203
7	159	159
8	72	70
9	28	29
10	152	152
11	81	82
12	99	92
13	42	43
14	83	80

2,14,L

0	47	39
1	155	151
2	72	67
3	133	130
4	113	107
5	95	91
6	188	186
7	58	59
8	82	82
9	98	103
10	65	66
11	16	17
12	82	82
13	113	111

2,15,L

0	15*	6
1	18	19
2	175	174
3	57	58
4	282	288
5	561	568
6	395	395
7	306	306
8	471	464
9	161	151
10	300	309
11	150	159
12	124	124
13	105	111
14	211	209
15	110	108
16	192	192
17	126	126
18	31	29
19	71	69

2,2,L

0	762	765
1	1074	1087
2	854	871
3	869	890
4	418	412
5	725	712
6	151	150
7	315	315
8	206	210
9	268	271
10	144	148
11	190	190
12	80	73
13	250	254
14	58	58
15	80	81
16	61	63
17	62	65
18	92	91
19	71	70

2,3,L

0	200	184
1	748	749
2	460	448
3	423	415
4	206	213
5	360	361
6	397	389
7	211	214
8	272	262
9	383	381
10	65	62
11	259	258
12	171	169
13	251	253
14	160	155
15	111	112
16	139	140
17	104	102

4	212	211
5	59	58
6	157	160
7	44	39
8	111	106
9	92	95
10	98	95
11	54	52
12	83	85

2,16,L

0	84	80
1	143	141
2	32	29
3	133	128
4	95	89
5	14*	4
6	188	187
7	98	100
8	97	96
9	59	59
10	111	110

2,17,L

0	51	49
1	157	157
2	81	76
3	18	16
4	77	79
5	147	144
6	105	107
7	94	95
8	24	21

2,18,L

0	48	50
1	101	100
2	34	35
3	176	175
4	62	63
5	37	36
6	62	62

2,19,L

0	30	30
1	81	81

3,0,L

1	368	349
2	417	418
3	556	537
4	518	505
5	117	121
6	139	130
7	95	102
18	44	45
19	44	39

2,4,L

0	216	203
1	872	872
2	408	403
3	517	513
4	425	417
5	473	455
6	435	426
7	191	180
8	265	259
9	206	214
10	310	312
11	307	314
12	197	197
13	308	304
14	112	112
15	16*	17
16	126	122
17	76	78
18	128	133
19	25	26

2,5,L

0	56	32
1	440	435
2	319	330
3	223	208
4	353	359
5	353	339
6	273	262
7	41	32
8	260	273
9	195	184
10	156	152
11	122	109
12	183	189
13	337	343
14	150	149
15	188	194
16	84	83
17	101	100
18	30	27

2,6,L

0	348	346
1	303	314
2	419	405
3	594	590
4	228	227
5	165	164
6	291	288
7	137	143

8	149	141
9	447	465
10	378	386
11	267	271
12	199	205
13	98	97
14	27	29
15	257	257
16	197	199
17	182	176
18	84	79
19	115	113

3,1,L

0	307	303
1	553	543
2	159	157
3	251	238
4	289	288
5	134	144
6	354	329
7	452	452
8	179	180
9	296	292
10	168	156
11	274	274
12	91	89
13	82	76
14	57	54
15	84	89
16	52	53
17	96	94
18	72	66
19	88	85

3,2,L

0	200	196
1	441	428
2	331	313
3	213	192
4	252	250
5	540	532
6	45	33
7	294	293
8	341	339
9	288	296
10	261	258
11	150	151
12	252	256
13	114	113
14	120	116
15	188	191
16	22	21
17	194	197
18	75	80
19	72	66

3,3,L

0	883	884
1	381	381
2	693	698
3	325	330
4	768	765
5	337	325
6	259	257
7	265	262
8	138	144
9	76	75
10	163	162
11	199	201
12	80	78
13	209	209
14	182	183
15	114	121
16	118	119
17	81	80
18	18	14

3,4,L

0	266	269
1	339	345
2	409	415
3	670	657
4	370	363
5	300	291
6	213	216
7	73	62
8	214	220
9	211	223
10	328	325
11	291	295
12	311	309
13	124	119
14	111	109
15	59	61
16	25	25
17	36	35
18	88	90

3,5,L

0	68	66
1	430	434
2	415	410
3	471	479
4	643	638
5	488	475
6	330	335
7	197	200
8	238	240
9	282	281
10	77	80
11	177	173
12	102	107
13	156	157

4,0,L

10	350	357
11	297	301
12	61	53
13	39	39
14	111	104
15	18	10
16	14*	2
17	50	49
18	84	79

4,1,L

0	235	220
1	42	37
2	534	530
3	335	342
4	500	480
5	443	460
6	224	224
7	80	89
8	243	242
9	269	275
10	83	81
11	123	131
12	125	127
13	261	265
14	74	72
15	116	117
16	92	91
17	63	62
18	108	108

4,2,L

0	72	68
1	376	364
2	284	293
3	193	184
4	116	123
5	235	222
6	105	100
7	558	558
8	291	303
9	328	338
10	153	153
11	63	59
12	221	222
13	143	147
14	164	167
15	55	51
16	68	67
17	48	48
18	12*	13

4,3,L

0	555	568
1	255	254
2	224	237
3	104	94
4	63	68
5	231	237
6	191	211
7	169	163
8	253	260
9	105	105
10	58	50
11	167	167
12	331	336
13	28	34
14	148	150
15	150	147
16	85	84
17	85	86
18	78	82

4,4,L

0	686	690
1	135	142
2	197	201
3	296	286
4	242	239
5	104	103
6	180	179
7	113	118
8	266	268
9	142	145
10	260	267
11	114	119
12	143	146
13	55	54
14	210	214
15	56	54
16	113	112
17	42	38

4,5,L

0	188	189
1	165	154
2	197	191
3	295	287
4	97	92
5	80	94
6	85	95
7	178	175
8	261	269
9	290	291
10	197	200
11	241	237
12	131	135
13	100	101
14	120	122
15	65	62
16	47	45
17	55	54
18	198	198
19	97	101
16	64	67
17	55	49
18	25	24

3,6,L

0	109	104
1	172	156
2	391	389
3	265	279
4	631	632
5	177	178
6	137	136
7	216	211
8	134	131
9	193	190
10	269	271
11	368	368
12	284	288
13	139	139
14	88	88
15	122	128
16	37	42
17	41	42
18	51	54

3,7,L

0	277	264
1	78	76
2	250	244
3	189	199
4	655	655
5	289	300
6	422	420
7	171	175
8	108	108
9	105	106
10	46	39
11	75	71
12	101	99
13	181	186
14	74	73
15	42	44
16	52	55
17	56	51

3,8,L

0	293	289
1	168	156
2	540	542
3	324	334
4	506	505
5	211	209
6	96	95
7	152	147
8	119	121
9	54	47
10	174	177
11	142	149
12	84	85
13	23	25
14	163	162
15	78	80
16	74	75
17	14	16

3,9,L

0	88	97
1	187	194
2	108	106
3	241	244
4	241	246
5	177	174
6	285	287
7	150	157
8	268	264
9	154	153
10	156	148
11	24	21
12	52	48
13	154	157
14	140	138
15	127	130
16	94	92

3,10,L

0	177	182
1	253	250
2	309	310
3	33	29
4	74	75
5	228	232
6	129	133
7	53	52
8	134	134
9	77	78
10	26	20
11	105	105
12	101	102
13	67	63
14	50	52
15	49	47
16	23	24

3,11,L

0	278	282
1	114	115
2	139	142
3	134	127
4	293	296
5	81	80
6	241	248
7	232	234
8	172	164
9	104	103
10	146	141
11	74	80
12	32	37
13	76	73
14	80	83
15	75	73

3,12,L

0	209	210
1	158	158
2	318	322
3	242	246
4	214	219
5	118	126
6	126	124
7	39	41
8	161	160
9	34	32
10	37	32
11	40	39
12	56	60
13	26	26
14	69	72

3,13,L

0	80	82
1	73	71
2	82	84
3	141	143
4	229	230
5	164	165
6	70	63
7	116	118
8	108	109
9	48	52
10	118	124
11	82	75
12	59	56
13	77	78

3,14,L

0	106	109
1	53	51
2	126	121
3	159	160
4	59	54
5	145	147
6	85	82
7	48	45
8	80	82
9	152	153
10	125	128
11	165	165
12	70	70

4,6,L

0	303	289
1	335	345
2	143	144
3	265	276
4	31	27
5	101	103
6	113	125
7	192	196
8	81	86
9	128	132
10	133	141
11	66	68
12	83	89
13	105	103
14	67	69
15	21	20
16	87	80
17	130	131

4,7,L

0	189	191
1	123	124
2	211	209
3	141	147
4	185	180
5	182	183
6	101	104
7	167	175
8	27	26
9	187	189
10	133	139
11	187	189
12	101	100
13	99	96
14	76	77
15	124	126
16	60	61

4,8,L

0	38	53
1	276	273
2	267	261
3	193	194
4	201	208
5	260	271
6	237	250
7	413	421
8	20	15
9	186	185
10	35	31
11	54	52
12	76	80
13	56	55
14	44	45
15	66	68
16	62	59

4,9,L

0	36	42
1	463	469
2	60	54
3	163	168
4	181	181
5	141	141
6	157	158
7	136	143
8	113	112
9	130	128
10	78	80
11	25	21
12	141	144
13	61	67
14	117	117
15	137	134

4,10,L

0	33	30
1	196	198
2	215	220
3	18	16
4	114	107
5	247	253
6	85	86
7	244	247
8	83	84
9	121	120
10	81	75
11	53	56
12	59	54
13	65	62
14	31	35
15	41	44

4,11,L

0	141	138
1	346	344
2	256	255
3	162	158
4	92	102
5	129	135
6	93	95
7	132	133
8	18	20
9	62	57
10	81	87
11	99	97
12	158	155
13	112	116
14	112	110

4,12,L

0	96	95
1	106	105
2	200	196
3	129	125
4	148	147
5	125	129
6	81	84
7	87	89
8	39	39
9	56	57
10	84	86
11	28	30
12	75	81
13	50	56

4,13,L

0	60	59
1	52	56
2	80	76
3	176	172
4	46	43
5	106	107
6	67	67
7	34	35
8	90	97
9	86	86
10	76	78
11	148	150
12	54	57

4,14,L

0	153	152
1	100	101
2	90	84
3	164	165
4	161	161
5	162	159
6	101	101
7	106	103
8	26	26
9	42	41
10	13*	4
11	93	94

4,15,L

0	14*	12
1	103	99
2	104	103
3	82	74
4	146	147
5	90	92
6	22	19
7	66	62
8	115	118
9	89	89
10	17	19

3,15,L

0	49	48
1	89	90
2	109	109
3	137	140
4	15*	8
5	102	109
6	84	81
7	58	53
8	34	27
9	51	48
10	101	101
11	148	153

3,16,L

0	31	31
1	92	92
2	39	41
3	136	134
4	93	97
5	33	30
6	102	107
7	77	74
8	85	84
9	46	39

3,17,L

0	33	35
1	13*	15
2	75	74
3	30	29
4	81	81
5	64	60
6	82	84
7	100	96

3,18,L

0	64	63
1	19	16
2	72	74
3	56	56
4	49	52

4,0,L

0	132	122
1	79	85
2	213	198
3	88	96
4	379	373
5	666	678
6	370	385
7	288	290
8	473	450
9	15*	19

4,16,L

0	67	67
1	96	92
2	68	70
3	47	51
4	45	46
5	58	58
6	110	109
7	119	117
8	60	64

4,17,L

0	161	161
1	55	52
2	86	87
3	89	92
4	41	42
5	89	86

5,0,L

1	321	310
2	190	186
3	29	43
4	354	354
5	53	62
6	76	70
7	65	63
8	117	124
9	185	188
10	137	138
11	80	85
12	151	152
13	17	14
14	56	57
15	111	116
16	42	46
17	93	94

5,1,L

0	374	375
1	203	201
2	332	322
3	228	240
4	354	363
5	231	228
6	168	170
7	95	100
8	69	62
9	174	180
10	108	115
11	43	43
12	254	262
13	195	197
14	120	128
15	151	154
16	107	106

5,15,L

0	126	124
1	115	119
2	52	50
3	111	112
4	20	18
5	76	74
6	96	94
7	109	109
8	41	42

5,16,L

0	23	21
1	97	93
2	55	58
3	66	66
4	16	15
5	55	57

6,0,L

0	18	20
1	523	513
2	20	19
3	106	105
4	91	97
5	80	75
6	43	50
7	153	156
8	215	219
9	113	108
10	153	154
11	17	5
12	77	84
13	17	18
14	17	20
15	29	29
16	35	41

6,1,L

0	42	39
1	266	272
2	69	66
3	151	148
4	171	180
5	95	99
6	128	129
7	130	138
8	105	110
9	163	167
10	111	108
11	51	52
12	74	74
13	104	100
14	50	48
15	121	120
16	105	106
17	67	65

6,2,L

0	77	85
1	372	371
2	218	219
3	222	225
4	229	244
5	279	264
6	229	222
7	210	213
8	226	234
9	171	175
10	298	303
11	158	172
12	117	117
13	95	94
14	86	89
15	95	96
16	13*	10
17	31	29

6,3,L

0	192	201
1	217	203
2	283	281
3	179	177
4	129	125
5	139	148
6	110	109
7	227	222
8	62	50
9	138	145
10	134	133
11	16*	11
12	63	67
13	81	80
14	155	157
15	36	38
16	147	141
17	27	28

6,4,L

0	328	323
1	193	187
2	332	334
3	131	131
4	128	131
5	57	50
6	244	244
7	41	44
8	439	442
9	88	84
10	103	104
11	133	130
12	135	136
13	30	28

6,5,L

0	445	438
1	262	262
2	320	312
3	294	298
4	197	201
5	223	226
6	46	45
7	121	121
8	184	184
9	79	76
10	24	15
11	122	126
12	76	79
13	49	46
14	105	103
15	48	46
16	84	78

6,6,L

0	455	453
1	262	260
2	96	92
3	206	202
4	214	212
5	165	170
6	264	264
7	83	86
8	67	61
9	235	232
10	94	87
11	190	186
12	15*	18
13	26	25
14	16	18
15	31	30
16	22	26

6,7,L

0	16*	23
1	258	258
2	154	152
3	129	125
4	194	194
5	278	277
6	85	88
7	234	233
8	140	150
9	72	73
10	178	172
11	40	38
12	126	127
13	42	37

13	77	80
14	92	93
15	39	36

6,5,L

0	319	320
1	35	32
2	53	50
3	213	214
4	66	65
5	291	287
6	252	257
7	122	120
8	234	237
9	70	68
10	45	43
11	95	93
12	109	108
13	74	73
14	127	124
15	24	22

6,6,L

0	67	67
1	268	269
2	168	167
3	207	210
4	74	72
5	288	291
6	169	164
7	35	33
8	192	193
9	66	72
10	48	43
11	46	42
12	112	108
13	142	139
14	49	55

6,7,L

0	91	89
1	275	278
2	252	255
3	201	196
4	196	195
5	155	155
6	61	59
7	36	42
8	133	131
9	75	72
10	50	50
11	174	179
12	82	81
13	37	36
14	66	66

14	54	56
15	91	90

5,8,L

0	150	157
1	156	160
2	182	176
3	139	129
4	119	115
5	140	135
6	73	72
7	144	140
8	73	76
9	201	200
10	62	69
11	84	81
12	52	51
13	109	112
14	67	65
15	91	93

5,9,L

0	118	107
1	283	280
2	151	152
3	244	247
4	152	152
5	276	273
6	105	104
7	238	240
8	68	66
9	22	18
10	124	125
11	86	87
12	91	90
13	87	87
14	26	23

5,10,L

0	103	92
1	228	227
2	212	215
3	72	73
4	68	63
5	172	172
6	128	125
7	95	92
8	124	125
9	61	57
10	97	95
11	83	86
12	90	90
13	60	57
14	11*	4

6,8,L

0	140	141
1	194	194
2	85	93
3	108	105
4	172	171
5	58	59
6	212	202
7	173	181
8	41	39
9	56	55
10	138	136
11	58	56
12	93	92
13	162	162

6,9,L

0	151	153
1	259	259
2	132	131
3	16	18
4	103	105
5	177	175
6	63	63
7	57	58
8	181	184
9	33	33
10	172	177
11	51	51
12	62	71
13	62	63

6,10,L

0	110	105
1	34	14
2	85	86
3	126	127
4	36	38
5	119	117
6	18	14
7	173	180
8	114	119
9	149	154
10	97	94
11	31	33
12	71	69

6,11,L

0	107	102
1	159	153
2	168	166
3	49	46
4	46	46
5	67	66
6	146	148
7	21	17

5,11,L

0	87	84
1	104	97
2	126	122
3	79	79
4	127	124
5	136	141
6	20	20
7	162	160
8	67	67
9	111	109
10	71	61
11	54	55
12	83	86
13	12*	7

5,12,L

0	165	154
1	67	63
2	17	18
3	30	24
4	91	91
5	51	46
6	61	59
7	113	115
8	123	126
9	145	139
10	35	33
11	110	109
12	92	93

5,13,L

0	26	24
1	105	104
2	48	47
3	153	153
4	43	40
5	152	151
6	73	70
7	40	39
8	13*	3
9	97	101
10	71	71
11	88	89

5,14,L

0	63	59
1	52	50
2	14*	10
3	117	116
4	13*	2
5	108	106
6	92	92
7	62	63
8	74	72
9	117	117

8	125	126
9	35	39
10	79	77
11	64	61

6,12,L

0	77	73
1	16	20
2	14*	7
3	69	69
4	27	23
5	42	39
6	109	105
7	77	80
8	165	163
9	100	100
10	118	114

6,13,L

0	178	177
1	67	68
2	95	92
3	81	81
4	92	91
5	60	57
6	75	73
7	59	64
8	19	13
9	58	52

6,14,L

0	80	78
1	115	113
2	36	33
3	27	27
4	37	32
5	46	43
6	118	117
7	28	31

6,15,L

0	63	61
1	78	78
2	41	39
3	127	122
4	19	18

7,0,L

1	25	23
2	278	283
3	101	98
4	186	182
5	316	316
6	89	95

7,0,L

7	52	51
8	78	79
9	61	68
10	81	77
11	83	86
12	44	45
13	101	101
14	33	33

7,1,L

0	195	195
1	136	139
2	115	118
3	203	206
4	98	95
5	127	134
6	94	96
7	97	92
8	62	63
9	32	36
10	88	83
11	71	67
12	65	63
13	164	166
14	32	35

7,2,L

0	46	50
1	75	70
2	137	140
3	320	315
4	46	43
5	265	264
6	115	116
7	98	96
8	122	125
9	101	102
10	85	86
11	112	106
12	40	39
13	55	58
14	56	61

7,3,L

0	203	205
1	183	181
2	175	174
3	268	267
4	77	87
5	219	228
6	63	65
7	36	39
8	95	95
9	131	133
10	79	82
11	111	112
12	47	50
13	134	138
14	73	75

7,4,L

0	156	155
1	124	121
2	195	190
3	150	144
4	147	154
5	156	157
6	119	114
7	82	81
8	194	191
9	122	125
10	66	70
11	104	105
12	51	52
13	24	21

7,5,L

0	123	115
1	92	92
2	177	172
3	178	178
4	74	74
5	125	124
6	194	197
7	133	135
8	27	24
9	108	106
10	102	105
11	64	64
12	81	84
13	48	50

7,6,L

0	114	108
1	50	48
2	231	233
3	83	84
4	109	104
5	25	19
6	36	29
7	135	139
8	85	85
9	185	192
10	67	68
11	60	58
12	77	74
13	21	22

7,7,L

0	152	156
1	196	186
2	33	31
3	72	74
4	107	108
5	96	96
6	142	136
7	101	103
8	85	84
9	25	27
10	55	57
11	30	31
12	39	41

7,8,L

0	35	27
1	98	100
2	67	70
3	91	90
4	68	72
5	57	60
6	50	50
7	119	116
8	21	20
9	148	155
10	109	114
11	59	59
12	110	106

7,9,L

0	54	50
1	104	95
2	116	112
3	33	29
4	131	130
5	63	59
6	111	111
7	100	103
8	49	45
9	50	48
10	17	14
11	44	45

7,10,L

0	66	66
1	15	9
2	29	29
3	47	44
4	55	50
5	62	64
6	93	91
7	22	26
8	51	53
9	36	34
10	105	100

7,11,L

0	90	89
1	45	47
2	130	125
3	62	63
4	155	148
5	92	88
6	109	105
7	14	14
8	16	18
9	48	52

7,12,L

0	34	38
1	13*	7
2	96	96
3	89	84
4	62	63
5	53	54
6	38	36
7	51	45

7,13,L

0	38	44
1	92	90
2	54	51
3	131	127
4	75	69
5	70	68

7,14,L

0	90	86
1	68	69
2	103	101

8,0,L

0	70	75
1	153	146
2	40	43
3	103	105
4	21	18
5	16*	6
6	125	126
7	144	145
8	43	39
9	27	33
10	16	12
11	12*	5
12	12*	14

8,1,L

0	57	54
1	42	40
2	72	72
3	63	62
4	141	140
5	63	63
6	119	119
7	56	52
8	69	67
9	118	122
10	22	19
11	46	46
12	44	42

8,2,L

0	33	31
1	121	121
2	140	139
3	88	93
4	183	186
5	75	79
6	31	26
7	52	57
8	47	47
9	80	79
10	46	46
11	65	62
12	67	66

8,3,L

0	55	52
1	102	96
2	112	112
3	136	136
4	175	182
5	23	18
6	62	60
7	35	32
8	24	28
9	67	71
10	61	52
11	12*	3
12	75	70

8,4,L

0	39	37
1	51	55
2	134	135
3	104	103
4	97	91
5	156	157
6	116	118
7	60	66
8	66	65
9	110	109
10	66	63
11	109	108

8,5,L

0	129	124
1	88	85

8,6,L

0	191	193
1	81	77
2	74	73
3	135	129
4	36	33
5	122	123
6	72	69
7	74	69
8	55	45
9	128	128
10	60	55

8,7,L

0	99	89
1	72	67
2	152	150
3	15*	7
4	69	68
5	136	136
6	25	26
7	108	104
8	132	129
9	12*	1
10	72	69

8,8,L

0	179	176
1	61	59
2	106	104
3	76	80
4	75	75
5	50	46
6	136	134
7	30	22
8	52	50
9	77	78

8,9,L

0	68	66
1	65	62
2	113	109
3	61	66
4	99	92
5	153	153
6	85	83
7	110	111
8	62	59

8,10,L

0	17	19
1	88	86
2	40	36
3	164	160
4	60	53
5	60	56
6	88	87

8,11,L

0	77	76
1	49	51
2	56	59
3	20	18
4	48	52
5	73	71

8,12,L

0	23	24
1	49	51

9,0,L

1	15*	5
2	98	98
3	80	90
4	28	22
5	16	8
6	116	109
7	100	99
8	153	154
9	12*	3

9,1,L

0	149	149
1	53	51
2	78	75
3	183	181
4	57	50
5	109	118
6	134	134
7	56	57
8	121	123
9	26	30

9,2,L

0	16	6
1	176	174
2	42	44
3	61	56
4	130	133
5	91	94
6	93	95
7	52	54
8	73	72
9	15	13

9,3,L

0	64	64
1	88	83
2	49	42
3	156	155
4	44	42
5	142	143
6	44	44
7	39	40
8	30	28

9,4,L

0	15*	17
1	26	17
2	102	101
3	92	92
4	102	104
5	48	48
6	19	17
7	34	28
8	21	18

9,5,L

0	14*	4
1	42	43
2	55	51
3	36	32
4	104	106
5	84	83
6	104	105
7	57	63

9,6,L

0	84	79
1	100	99
2	48	47
3	42	43
4	113	108
5	29	31
6	25	17
7	26	25

9,7,L

0	59	63
1	47	45
2	18	16
3	37	36
4	39	39
5	92	94
6	13	16

9,8,L

0	54	56
1	44	41
2	32	32
3	135	133
4	13	14

9,9,L

0	12*	4
1	25	22

10,0,L

0	86	85
1	20	22
2	19	9
3	32	30

10,1,L

0	27	22
1	24	26
2	42	44
3	20	16

10,2,L

0	59	60
1	65	65
2	49	50
3	12	10

10,3,L

0	38	37
1	65	65
2	93	89

APPENDIX IX

Tables of observed and calculated structure factors for 1,3-dicyclohexyl-1-[*N*-methyl-*N*-(*N*-anthraniloyl-*N*-methylanthraniloyl)anthraniloyl] urea

Data Format:

	H	K
L	$10\times\lvert F_o\rvert$	$10\times\lvert F_c\rvert$

Reflections removed for extinction marked .... E

Reflections classed as unobserved marked ..... *

0,0,L

2	1644E	1765
4	430	415
6	196	196
8	128	135
10	166	160
12	418	410
14	136	140
16	152	162
18	135	147
20	61	70

0,1,L

1	926	989
2	102	89
3	1650E	1775
4	985	999
5	152	148
6	402	400
7	513	515
8	45	39
9	246	245
10	20	12
11	218	203
12	73	73
13	24	23
14	64	64
15	125	126
16	153	162
17	231	234
18	36	32
19	32	35
20	30	31
21	16*	5

0,2,L

0	1257E	1363
1	347	353
2	940	972
3	237	234
4	166	169
5	588	582
6	390	382
7	720	727
8	40	40
9	680	666
10	894	883
11	281	276
12	363	361
13	63	62
14	88	93
15	18*	4
16	169	172
17	190	202
18	107	111
19	83	78
20	52	54

0,14,L

5	223	232
6	18*	1
7	85	92
8	93	93
9	158	166
10	17*	0
11	17*	1

0,15,L

1	100	103
2	122	132
3	143	146
4	221	232
5	125	128
6	17*	16
7	16*	10
8	85	90
9	56	53

0,16,L

0	207	221
1	21	28
2	115	122
3	30	28
4	26	19
5	119	128
6	58	54

1,0,L

-21	71	79
-19	149	153
-17	186	187
-15	85	92
-13	156	155
-11	286	274
-9	345	316
-7	187	196
-5	588	593
-3	1202	1246
-1	575	593
1	296	313
3	281	299
5	394	391
7	97	83
9	148	134
11	60	47
13	238	243
15	92	91
17	197	195
19	38	44

1,1,L

-21	41	41
-20	17*	5

0,3,L

1	807	821
2	408	416
3	713	692
4	340	333
5	636	650
6	811	818
7	452	439
8	280	283
9	545	519
10	274	278
11	60	61
12	223	229
13	52	49
14	288	295
15	92	95
16	19*	12
17	23	16
18	216	216
19	22	26
20	17*	8

0,4,L

0	178	174
1	881	903
2	42	28
3	1335	1334
4	342	344
5	1079	1051
6	31	17
7	246	237
8	734	708
9	93	86
10	125	90
11	31	33
12	65	63
13	174	172
14	251	260
15	30	23
16	220	223
17	94	103
18	21*	28
19	63	63
20	34	37

0,5,L

1	193	181
2	71	54
3	241	241
4	146	149
5	250	240
6	53	47
7	94	92
8	113	113
9	44	30
10	233	227
11	84	72

1,2,L

-21	36	36
-20	25	26
-19	100	93
-18	55	48
-17	240	246
-16	41	48
-15	114	125
-14	121	121
-13	33	28
-12	382	384
-11	509	498
-10	105	126
-9	494	470
-8	225	215
-7	220	226
-6	533	519
-5	539	554
-4	356	341
-3	304	305
-2	253	246
-1	68	72
0	345	337
1	1182	1237
2	221	207
3	1190	1206
4	207	206
5	285	276
6	565	555
7	52	31
8	215	210
9	449	447
10	470	459
11	17*	17
12	166	154
13	62	57
14	61	60
15	21	19
16	63	60
17	115	119
18	33	36
19	115	122
20	65	71

1,3,L

-20	91	99
-19	30	27
-18	103	109
-17	34	24
-16	23	40
-15	137	137
-14	148	156
-13	88	80
-12	16*	6
-11	234	232
-10	42	30
-9	52	52
-8	364	359
-7	283	283
-6	121	106
-5	484	498
-4	24	24
-3	70	54
-2	856	874
-1	85	79
0	415	419
1	400	418
2	126	131
3	335	322
4	547	542
5	346	330
6	196	198
7	363	352
8	123	118
9	247	246
10	16*	10
11	57	38
12	157	161
13	446	448
14	284	283
15	130	124
16	32	25
17	48	38
18	224	233
19	106	111
20	20	26

0,6,L

0	1327	1340
1	386	357
2	635	616
3	101	94
4	148	137
5	230	240
6	173	140
7	167	149
8	96	104
9	145	148
10	418	414
11	161	172
12	245	236
13	182	185
14	94	103
15	109	104
16	358	370
17	120	117
18	139	149
19	142	149

0,7,L

1	391	386
2	15*	8
3	444	422
4	526	506
5	43	47
6	78	83
7	18*	24
8	101	108
9	174	176
10	108	101
11	32	25
12	219	219
13	294	301
14	180	182
15	103	112
16	132	139
17	141	160
18	165	170
19	83	92

0,8,L

0	1168	1146
1	176	173
2	517	520

3	86	73
4	20	14
5	129	117
6	71	78
7	16*	15
8	188	181
9	206	201
10	251	252
11	24	5
12	138	143
13	101	107
14	227	237
15	275	277
16	21*	16
17	65	58
18	48	53

0,9,L

1	29	24
2	235	215
3	138	137
4	197	209
5	219	206
6	58	52
7	90	99
8	175	172
9	193	202
10	98	100
11	230	226
12	325	330
13	140	147
14	117	119
15	106	112
16	21	19
17	108	110

0,10,L

0	52	53
1	181	171
2	77	67
3	400	406
4	146	135
5	18*	15
6	222	212
7	82	91
8	165	167
9	276	280
10	248	255
11	30	31
12	89	84
13	92	97
14	41	42
15	112	112
16	21	21
17	110	115

1,4,L

-20	17	19
-19	33	32
-18	19*	13
-17	84	79
-16	115	120
-15	118	124
-14	73	81
-13	193	191
-12	252	256
-11	302	290
-10	274	266
-9	82	79
-8	106	109
-7	160	159
-6	67	56
-5	59	71
-4	125	134
-3	195	125
-2	787	804
-1	324	325
0	710	713
1	320	302
2	50	51
3	642	646
4	846	850
5	352	344
6	14*	1
7	363	336
8	482	480
9	543	519
10	211	191
11	130	141
12	320	319
13	122	117
14	141	150
15	104	108
16	224	225
17	127	126
18	19*	8
19	100	101
20	17*	1

1,5,L

-20	17*	4
-19	91	100
-18	19*	26
-17	118	108
-16	18*	13
-15	18*	8
-14	185	196
-13	212	214
-12	45	45
-11	52	48
-10	619	615
-9	142	138
-8	781	755
-7	109	109
-6	746	736
-5	104	109
-4	208	217
-3	29	21
-2	103	98
-1	87	82
0	779	791
1	344	355
2	396	387
3	61	56
4	698	707
5	446	437
6	183	181
7	330	320
8	360	352
9	26	5
10	25	22
11	167	163
12	146	149
13	218	233
14	198	207
15	256	251
16	55	59
17	19*	29
18	106	113
19	17*	7

1,6,L

-19	18*	7
-18	19	8
-17	49	41
-16	56	61
-15	52	48
-14	19*	9
-13	156	157
-12	122	121
-11	93	100
-10	282	276
-9	16*	3
-8	63	50
-7	180	160
-6	94	89
-5	468	482
-4	14*	10
-3	162	164
-2	425	411
-1	40	38
0	368	376

0,11,L

1	138	139
2	80	88
3	365	360
4	18*	17
5	281	273
6	80	85
7	238	243
8	188	190
9	90	98
10	62	59
11	26	38
12	50	59
13	21	16
14	18*	13
15	62	64
16	110	116

0,12,L

0	27	32
1	81	85
2	19*	19
3	35	42
4	76	73
5	126	131
6	136	134
7	20*	7
8	350	360
9	55	67
10	202	209
11	23	26
12	19*	12
13	72	80
14	30	38

0,13,L

1	94	89
2	100	107
3	33	33
4	191	195
5	20*	17
6	19*	3
7	26	31
8	76	66
9	198	200
10	207	203
11	64	62
12	146	157
13	53	55

0,14,L

0	171	180
1	142	136
2	164	172
3	22	25
4	59	65

1,6,L

1	230	224
2	142	145
3	627	610
4	480	494
5	228	205
6	498	485
7	106	96
8	74	54
9	56	66
10	176	172
11	262	246
12	271	279
13	145	149
14	163	166
15	137	134
16	71	74
17	107	110
18	82	87
19	17*	10

1,7,L

-19	175	173
-18	18*	3
-17	167	175
-16	42	44
-15	18*	8
-14	243	251
-13	18*	2
-12	124	128
-11	57	63
-10	196	197
-9	101	96
-8	27	19
-7	277	277
-6	48	29
-5	148	148
-4	124	106
-3	308	307
-2	58	57
-1	257	366
0	129	123
1	330	321
2	283	281
3	403	379
4	325	333
5	410	411
6	147	132
7	82	83
8	247	238
9	85	90
10	283	278
11	142	145
12	74	65
13	117	122
14	31	44
15	20*	17
16	18*	5

1,8,L

-18	129	131
-17	68	70
-16	62	70
-15	130	126
-14	229	234
-13	172	171
-12	68	74
-11	126	130
-10	17*	12
-9	249	251
-8	123	124
-7	74	65
-6	63	48
-5	96	89
-4	26	2
-3	48	27
-2	245	222
-1	20	1
0	317	322
1	16*	9
2	58	73
3	28	23
4	281	270
5	145	146
6	103	115
7	71	55
8	52	61
9	82	85
10	89	88
11	167	168
12	334	330
13	133	132
14	93	82
15	19*	6
16	48	36
17	18*	11
18	60	55

1,9,L

-18	47	48
-17	123	131
-16	22	16
-15	37	38
-14	49	53
-13	97	95
-12	181	188
-11	71	70
-10	126	132
-9	36	22
-8	40	37
-7	187	192
-6	116	116
-5	283	280
-4	89	88

1,10,L

-17	17*	8
-16	72	71
-15	18*	11
-14	35	39
-13	216	216
-12	44	40
-11	30	18
-10	92	90
-9	127	130
-8	141	125
-7	342	349
-6	91	98
-5	174	174
-4	196	196
-3	239	227
-2	115	118
-1	211	231
0	87	87
1	139	138
2	198	185
3	65	72
4	17*	10
5	244	252
6	24	12
7	37	36
8	207	211
9	28	24
10	78	76
11	135	139
12	19*	20
13	71	70
14	41	38
15	18*	13
16	42	46

1,11,L

-16	89	85
-15	25	24
-14	43	41
-13	50	50
-12	18*	3
-11	103	96
-10	131	134
-9	305	309
-8	556	561
-7	184	172
-6	328	332
-5	43	45
-4	101	86
-3	18*	4
-2	220	214
-1	98	85
0	20	15
1	169	172
2	176	189
3	117	115
4	214	220
5	40	40
6	33	33
7	83	85
8	19*	13
9	134	141
10	42	42
11	153	151
12	40	53
13	62	63
14	17*	7
15	64	55

1,12,L

-15	69	63
-14	24	18
-13	56	59
-12	37	46
-11	96	93
-10	131	126
-9	173	180
-8	76	87
-7	20*	16
-6	191	199
-5	190	186
-4	19*	1
-3	206	210
-2	207	203
-1	73	83
0	30	26
1	202	204
2	19*	18
3	150	151
4	130	121
5	233	247
6	133	135
7	115	120

1,13,L

-13	17*	14
-12	17*	6
-11	18*	16
-10	49	42
-9	32	26
-8	151	148
-7	216	214
-6	251	257
-5	64	73
-4	182	186
-3	146	150
-2	26	24
-1	38	40
0	59	53
1	97	106
2	25	15
3	116	119
4	192	195
5	21	35
6	18*	12
7	85	84
8	19*	21
9	17*	7
10	53	50
11	102	100
12	17*	2
13	41	39

1,14,L

-12	42	32
-11	16*	2
-10	17*	19
-9	101	101
-8	90	87
-7	72	66
-6	89	97
-5	252	253
-4	97	97
-3	31	33
-2	85	96
-1	142	147
0	22	38
1	24	30
2	91	98
3	114	125
4	56	59
5	44	40
6	38	42
7	50	53

1,14,L

8	157	154
9	24	25
10	71	81
11	44	47

1,15,L

-9	29	29
-8	91	94
-7	26	35
-6	42	37
-5	18*	12
-4	85	92
-3	19*	12
-2	63	70
-1	57	64
0	74	63
1	42	50
2	87	92
3	232	245
4	106	108
5	100	109
6	72	73
7	29	22
8	146	150
9	46	44

1,16,L

-6	33	39
-5	56	48
-4	18*	21
-3	50	51
-2	92	92
-1	76	83
0	88	99
1	80	84
2	131	137
3	18*	25
4	17*	7
5	17*	3
6	176	183

2,0,L

-20	140	151
-18	25	30
-16	251	242
-14	652	660
-12	213	201
-10	201	192
-8	16	16
-6	585	589
-4	47	54
-2	129	126
0	204	219
2	79	88
4	391	381

2,1,L

-21	31	32
-20	23	25
-19	184	191
-18	137	148
-17	19*	28
-16	143	149
-15	29	26
-14	48	42
-13	242	232
-12	66	68
-11	27	32
-10	46	34
-9	491	471
-8	356	342
-7	428	402
-6	114	125
-5	87	74
-4	1150	1203
-3	32	38
-2	856	901
-1	1699E	2014
0	288	278
1	1386	1465
2	1407	1457
3	174	157
4	596	599
5	649	653
6	236	238
7	191	187
8	387	392
9	216	214
10	24	17
11	88	103
12	28	35
13	140	136
14	61	67
15	263	272
16	141	144
17	243	248
18	92	102
19	184	186
20	16*	2

2,2,L

-21	46	51
-20	78	82
-19	41	42
-18	145	146
-17	104	112
-16	37	38
-15	115	120
-14	258	257
-13	105	98
-12	16*	6
-11	67	69
-10	291	289
-9	364	351
-8	32	23
-7	111	104
-6	242	254
-5	139	137
-4	663	673
-3	158	179
-2	1813E	2078
-1	1567E	1735
0	1023	1056
1	1082	1105
2	787	803
3	364	369
4	617	586
5	718	704
6	380	373
7	190	177
8	454	440
9	169	167
10	290	289
11	125	125
12	306	305
13	99	100
14	239	241
15	375	384
16	170	170
17	206	213
18	24	24
19	18*	13
20	157	170

2,3,L

-21	19	9
-20	45	50
-19	95	103
-18	160	164
-17	103	106
-16	145	156
-15	325	332
-14	83	83
-13	87	85
-12	42	42
-11	16*	5
-10	172	153
-9	342	333
-8	272	273
-7	239	227
-6	122	121
-5	695	725
-4	690	711
-3	672	688

-2	134	131
-1	391	396
0	727	749
1	450	454
2	415	386
3	37	32
4	198	200
5	157	149
6	91	101
7	67	54
8	258	241
9	314	302
10	234	233
11	244	235
12	95	91
13	146	153
14	455	456
15	71	79
16	133	131
17	162	163
18	80	86
19	211	217
20	17*	2

2,4,L

-20	24	21
-19	18*	13
-18	62	66
-17	134	131
-16	72	79
-15	206	209
-14	75	74
-13	19	14
-12	133	128
-11	317	310
-10	334	331
-9	506	497
-8	329	319
-7	388	377
-6	431	430
-5	62	61
-4	616	624
-3	688	696
-2	666	679
-1	284	241
0	677	683
1	1267	1285
2	475	461
3	450	432
4	755	740
5	822	811
6	323	310
7	307	270
8	95	98
9	16*	22
10	17*	3
11	227	220
12	17*	4
13	103	109

8	91	89
9	57	40
10	44	48
11	81	94
12	79	88
13	66	66
14	91	88

2,5,L

-20	69	69
-19	18*	6
-18	131	137
-17	65	69
-16	192	204
-15	19*	12
-14	53	52
-13	158	161
-12	48	41
-11	197	195
-10	88	86
-9	155	135
-8	171	159
-7	521	499
-6	142	143
-5	115	110
-4	124	117
-3	387	389
-2	546	563
-1	318	314
0	279	283
1	349	334
2	37	12
3	233	248
4	917	904
5	569	542
6	278	258
7	523	517
8	160	142
9	41	45
10	23	19
11	68	68
12	71	59
13	61	60
14	112	116
15	25	25
16	90	89
17	90	103
18	83	85
19	17*	14

2,6,L

-19	17*	4
-18	126	139
-17	46	48
-16	78	76
-15	68	71
-14	33	27
-13	163	162

2,6,L

-12	45	40
-11	17*	17
-10	73	72
-9	185	174
-8	67	78
-7	34	6
-6	104	104
-5	194	180
-4	82	101
-3	46	51
-2	480	478
-1	278	271
0	56	77
1	495	501
2	182	149
3	309	311
4	437	446
5	1079	1055
6	342	329
7	180	172
8	138	141
9	79	81
10	184	170
11	67	70
12	48	38
13	186	194
14	195	203
15	89	98
16	153	153
17	18*	19
18	99	107
19	16*	19

2,7,L

-19	36	42
-18	103	115
-17	52	57
-16	19*	20
-15	38	32
-14	194	206
-13	18*	2
-12	60	60
-11	76	78
-10	87	88
-9	17*	11
-8	192	192
-7	16*	6
-6	93	91
-5	116	117
-4	146	151
-3	319	321
-2	149	156
-1	600	567
0	45	28
1	964	971
2	55	27
3	261	265

2,14,L

-2	25	31
-1	190	190
0	72	75
1	197	207
2	19*	11
3	135	142
4	111	103
5	48	56
6	38	46
7	18*	5
8	27	33
9	18*	18
10	112	121

2,15,L

-8	34	33
-8	41	42
-7	79	77
-6	18*	5
-5	88	87
-4	18*	10
-3	122	124
-2	35	32
-1	34	34
0	127	132
1	105	113
2	90	90
3	76	75
4	116	119
5	70	71
6	38	45
7	18*	16
8	22	20

2,16,L

-6	18*	18
-5	16*	2
-4	25	28
-3	25	19
-2	17*	5
-1	37	29
0	33	31
1	17*	2
2	86	84
3	52	49
4	18*	22
5	35	34

3,0,L

-21	194	196
-19	109	116
-17	161	174
-15	323	336
-13	27	37
-11	377	351
4	253	235
5	15*	24
6	99	91
7	189	203
8	48	28
9	222	222
10	247	253
11	31	27
12	116	123
13	194	198
14	44	44
15	82	85
16	90	91
17	75	87
18	95	106

2,8,L

-18	32	35
-17	55	50
-16	88	98
-15	106	110
-14	78	84
-13	42	36
-12	234	241
-11	213	220
-10	101	97
-9	60	57
-8	108	106
-7	152	152
-6	37	44
-5	65	84
-4	231	240
-3	15*	7
-2	93	102
-1	361	354
0	216	217
1	218	213
2	145	130
3	219	209
4	41	40
5	25	33
6	61	57
7	24	22
8	106	100
9	196	201
10	182	180
11	41	39
12	158	161
13	38	42
14	208	215
15	57	58
16	67	72
17	85	96

2,9,L

-18	91	80
-17	31	33
-16	117	114
-9	148	153
-7	205	205
-5	48	27
-3	992	999
-1	1435E	1529
1	406	443
3	1552	1602
5	858	836
7	139	133
9	497	486
11	23	5
13	309	307
15	21*	21
17	28	20
19	25	21

3,1,L

-21	34	38
-20	19*	15
-19	39	38
-18	139	146
-17	146	151
-16	21	27
-15	51	43
-14	18*	13
-13	99	98
-12	61	61
-11	16*	2
-10	167	166
-9	344	341
-8	97	96
-7	153	142
-6	405	392
-5	361	357
-4	339	336
-3	28	54
-2	765	791
-1	196	206
0	283	266
1	592	594
2	2074E	2218
3	837	848
4	535	536
5	53	48
6	584	564
7	159	166
8	37	34
9	92	96
10	125	122
11	73	76
12	48	57
13	204	203
14	204	209
15	90	92
16	142	148
17	21	11
18	56	60
19	52	46

-15	26	20
-14	101	95
-13	136	143
-12	116	123
-11	98	106
-10	18*	16
-9	40	35
-8	74	77
-7	232	246
-6	150	148
-5	72	81
-4	267	268
-3	53	49
-2	216	199
-1	82	96
0	43	46
1	246	248
2	242	224
3	253	235
4	59	54
5	186	186
6	17*	0
7	56	54
8	116	111
9	101	101
10	18*	0
11	52	47
12	142	152
13	83	90
14	44	50
15	45	41
16	69	62
17	23	26

2,10,L

-17	53	63
-16	18*	3
-15	23	13
-14	187	189
-13	18*	10
-12	91	94
-11	179	178
-10	57	62
-9	19*	6
-8	19*	7
-7	47	39
-6	73	73
-5	211	212
-4	98	105
-3	39	36
-2	155	93
-1	100	96
0	314	327
1	286	289
2	320	303
3	98	102
4	313	315
5	20	1
6	76	76

3,2,L

-21	91	92
-20	45	43
-19	50	49
-18	71	76
-17	112	117
-16	229	236
-15	33	24
-14	307	312
-13	121	133
-12	191	192
-11	302	287
-10	467	440
-9	404	382
-8	422	412
-7	110	98
-6	249	225
-5	55	54
-4	191	201
-3	219	219
-2	194	191
-1	734	765
0	504	486
1	967	982
2	587	584
3	416	395
4	240	252
5	586	566
6	318	299
7	105	99
8	231	230
9	27	23
10	366	372
11	104	111
12	27	21
13	96	96
14	65	61
15	54	52
16	143	151
17	129	136
18	46	43
19	137	133

3,3,L

-20	32	28
-19	137	141
-18	94	86
-17	41	43
-16	103	107
-15	124	121
-14	104	103
-13	37	30
-12	167	172
-11	131	133
-10	86	96
-9	482	475
-8	325	319
-7	823	802
7	18*	20
8	50	46
9	104	105
10	319	338
11	53	52
12	226	236
13	66	66
14	89	98
15	18*	15
16	17	7

2,11,L

-16	30	29
-15	28	30
-14	18*	12
-13	222	230
-12	72	77
-11	44	49
-10	58	60
-9	104	104
-8	102	96
-7	328	328
-6	139	141
-5	19*	12
-4	229	231
-3	193	196
-2	219	213
-1	43	43
0	151	151
1	22	25
2	100	90
3	98	100
4	160	166
5	171	174
6	110	122
7	162	167
8	64	60
9	73	58
10	89	92
11	151	165
12	93	99
13	33	36
14	17*	6
15	16*	3

2,12,L

-15	33	30
-14	76	83
-13	22	27
-12	92	95
-11	74	70
-10	86	90
-9	238	234
-8	20*	14
-7	21*	22
-6	35	35
-5	101	96
-4	293	297
-6	46	46
-5	103	97
-4	174	170
-3	26*	27
-2	336	345
-1	98	86
0	411	408
1	502	498
2	361	364
3	75	76
4	599	578
5	452	455
6	528	506
7	192	201
8	103	91
9	82	76
10	275	256
11	74	90
12	191	195
13	36	31
14	94	98
15	123	114
16	114	110
17	168	164
18	37	33
19	18*	22

3,4,L

-20	58	56
-19	30	30
-18	18*	2
-17	23	15
-16	100	101
-15	25	17
-14	232	232
-13	32	30
-12	100	109
-11	60	62
-10	115	116
-9	186	167
-8	231	236
-7	851	842
-6	40	22
-5	207	206
-4	129	118
-3	316	320
-2	363	367
-1	187	179
0	173	156
1	504	506
2	91	91
3	319	302
4	216	211
5	40	32
6	378	363
7	240	236
8	227	209
9	209	208
10	93	80
-3	120	118
-2	19*	2
-1	86	78
0	69	85
1	37	25
2	132	130
3	59	65
4	77	62
5	149	136
6	84	85
7	44	33
8	193	200
9	127	120
10	231	234
11	166	176
12	18	18
13	70	76
14	21	30

2,13,L

-13	38	42
-12	17*	2
-11	35	37
-10	18*	5
-9	45	48
-8	164	164
-7	148	141
-6	20*	24
-5	19*	2
-4	31	37
-3	114	121
-2	61	57
-1	145	145
0	119	121
1	57	52
2	210	229
3	73	67
4	133	138
5	22	22
6	160	163
7	44	49
8	20	24
9	69	69
10	56	60
11	18*	13
12	58	63

2,14,L

-11	48	52
-10	116	119
-9	115	119
-8	30	20
-7	29	26
-6	36	39
-5	80	77
-4	86	88
-3	19	14
11	49	35
12	94	93
13	49	58
14	209	204
15	108	113
16	45	49
17	19*	19
18	47	45
19	17*	11

3,5,L

-20	21	20
-19	44	38
-18	19*	16
-17	59	53
-16	68	65
-15	21*	14
-14	265	264
-13	107	109
-12	74	72
-11	104	100
-10	154	160
-9	55	40
-8	83	74
-7	16*	26
-6	191	202
-5	32	42
-4	397	386
-3	477	462
-2	389	385
-1	15	7
0	169	170
1	195	208
2	44	39
3	342	338
4	264	243
5	155	163
6	449	439
7	368	344
8	115	102
9	70	82
10	241	236
11	18*	19
12	199	200
13	147	151
14	53	55
15	99	102
16	59	59
17	109	114
18	135	137

3,6,L

-19	124	125
-18	19*	3
-17	81	88
-16	158	161
-15	70	76

3,6,L

-14	314	311
-13	133	133
-12	53	50
-11	340	333
-10	38	44
-9	155	161
-8	47	43
-7	25	30
-6	315	307
-5	208	215
-4	838	824
-3	422	404
-2	15*	10
-1	272	277
0	119	132
1	295	288
2	785	777
3	101	97
4	62	64
5	121	119
6	72	74
7	94	95
8	25	29
9	205	204
10	25	20
11	381	381
12	19*	3
13	19*	21
14	56	57
15	92	78
16	31	25
17	18*	16
18	25	24

3,7,L

-19	76	78
-18	148	155
-17	126	131
-16	83	79
-15	238	238
-14	32	37
-13	415	418
-12	99	99
-11	91	86
-10	84	76
-9	219	211
-8	253	250
-7	319	313
-6	28	31
-5	248	252
-4	96	97
-3	126	133
-2	276	265
-1	88	71
0	88	85
1	107	102
2	423	410

3,14,L

6	131	139
7	41	46
8	110	111
9	168	168
10	17*	3

3,15,L

-9	31	28
-8	51	42
-7	68	76
-6	69	74
-5	38	37
-4	108	105
-3	163	164
-2	79	81
-1	18*	0
0	135	140
1	18*	5
2	76	79
3	147	154
4	62	57
5	90	91
6	73	81
7	56	56

3,16,L

-5	83	82
-4	19	18
-3	17*	1
-2	71	69
-1	51	51
0	54	57
1	74	79
2	55	58
3	78	87
4	30	34

4,0,L

-20	37	31
-18	93	89
-16	214	208
-14	21	27
-12	240	231
-10	455	442
-8	206	188
-6	14*	6
-4	683	663
-2	890	895
0	1558	1587
2	847	855
4	86	94
6	59	57
8	408	406
10	149	143
12	122	117

3	250	247
4	180	182
5	171	160
6	82	88
7	323	323
8	82	81
9	259	264
10	39	43
11	90	92
12	19*	7
13	19*	11
14	44	45
15	85	87
16	40	36
17	76	74

3,8,L

-18	18*	16
-17	82	83
-16	181	177
-15	242	260
-14	99	99
-13	145	141
-12	112	111
-11	209	194
-10	362	358
-9	288	292
-8	36	34
-7	26	25
-6	48	45
-5	175	175
-4	48	42
-3	113	112
-2	69	64
-1	240	228
0	231	226
1	36	46
2	211	223
3	153	146
4	93	97
5	19	18
6	69	67
7	195	187
8	18*	15
9	71	71
10	119	116
12	54	50
13	19*	4
14	18*	2
15	48	50
16	44	45
17	18*	11

3,9,L

-17	65	68
-16	53	44
-15	77	76
-14	31	31
14	98	106
16	26	34
18	18*	4

4,1,L

-21	16*	7
-20	38	29
-19	32	27
-18	24	34
-17	63	57
-16	20*	15
-15	337	342
-14	77	79
-13	223	227
-12	20	27
-11	163	153
-10	164	172
-9	211	190
-8	51	57
-7	86	88
-6	57	55
-5	293	289
-4	505	516
-3	769	778
-2	79	93
-1	197	187
0	51	54
1	663	666
2	216	214
3	224	211
4	467	451
5	393	385
6	145	128
7	67	54
8	145	143
9	101	102
10	76	67
11	89	89
12	107	107
13	235	229
14	206	208
15	398	412
16	147	153
17	111	112
18	34	43
19	97	101

4,2,L

-20	17*	5
-19	93	95
-18	19*	17
-17	222	232
-16	19*	1
-15	125	120
-14	19	15
-13	129	126
-12	98	90
-11	17*	5

-13	266	266
-12	112	112
-11	94	105
-10	477	462
-9	454	455
-8	29	27
-7	463	472
-6	47	56
-5	89	83
-4	159	152
-3	209	223
-2	51	55
-1	36	41
0	238	222
1	150	144
2	199	196
3	28	21
4	187	179
5	135	135
6	22	9
7	119	120
8	152	150
9	239	236
10	94	86
11	191	197
12	135	135
13	20*	13
14	149	153
15	19*	15
16	35	40

3,10,L

-17	88	84
-16	64	74
-15	42	37
-14	18*	1
-13	25	26
-12	118	115
-11	105	101
-10	157	146
-9	19*	2
-8	19*	10
-7	63	60
-6	467	472
-5	108	105
-4	111	119
-3	135	149
-2	61	56
-1	143	132
0	154	157
1	346	336
2	21	3
3	56	56
4	138	136
5	22	13
6	18*	10
7	205	216
8	100	113
9	156	161

-10	467	449
-9	376	367
-8	144	150
-7	75	81
-6	310	313
-5	69	68
-4	486	495
-3	89	101
-2	260	254
-1	66	56
0	743	750
1	621	617
2	323	294
3	224	210
4	46	38
5	344	337
6	442	443
7	84	104
8	109	97
9	302	290
10	16*	5
11	59	53
12	32	21
13	18*	7
14	20*	23
15	145	151
16	49	47
17	168	176
18	17*	12
19	45	44

4,3,L

-20	50	51
-19	39	41
-18	39	39
-17	37	38
-16	28	31
-15	39	37
-14	85	94
-13	190	185
-12	89	89
-11	151	156
-10	294	295
-9	114	111
-8	128	126
-7	76	66
-6	372	397
-5	573	584
-4	385	391
-3	305	311
-2	719	723
-1	304	326
0	271	284
1	46	7
2	284	279
3	213	193
4	73	67
5	275	279
6	324	324

10	24	29
11	77	90
12	35	33
13	68	63
14	81	83
15	31	41

3,11,L

-16	47	48
-15	18*	11
-14	83	89
-13	21	13
-12	96	95
-11	54	53
-10	193	187
-9	20*	1
-8	87	87
-7	132	126
-6	19*	15
-5	132	132
-4	45	33
-3	260	263
-2	94	92
-1	32	14
0	235	247
1	87	91
2	86	83
3	120	119
4	140	141
5	37	30
6	87	93
7	64	67
8	200	202
9	79	88
10	219	214
11	41	37
12	43	44
13	19	17
14	33	38

3,12,L

-14	18*	10
-13	18*	11
-12	19*	10
-11	32	28
-10	91	92
-9	102	95
-8	42	42
-7	484	486
-6	239	240
-5	183	192
-4	201	201
-3	107	114
-2	153	148
-1	73	70
0	57	43
1	105	93
2	46	48

7	36	37
8	83	75
9	55	52
10	128	114
11	123	125
12	44	47
13	127	120
14	367	369
15	39	41
16	73	71
17	49	56
18	108	116

4,4,L

-20	56	58
-19	103	106
-18	17*	4
-17	199	210
-16	89	92
-15	19*	26
-14	119	117
-13	68	64
-12	39	38
-11	39	43
-10	295	288
-9	343	347
-8	485	475
-7	464	464
-6	138	150
-5	567	555
-4	463	462
-3	294	283
-2	113	110
-1	209	209
0	678	667
1	720	739
2	354	348
3	168	170
4	146	119
5	18	8
6	57	64
7	127	130
8	78	72
9	16*	2
10	141	149
11	110	112
12	135	139
13	235	248
14	71	70
15	140	141
16	19*	5
17	133	131
18	69	71

4,5,L

-20	51	54
-19	59	63
-18	92	92

3	53	65
4	18*	17
5	128	131
6	108	124
7	167	164
8	46	44
9	137	140
10	23	26
11	32	29
12	22	27
13	20	24

3,13,L

-13	18*	14
-12	54	59
-11	47	43
-10	18*	5
-9	86	86
-8	95	96
-7	216	228
-6	37	34
-5	19*	17
-4	84	81
-3	178	171
-2	131	126
-1	123	129
0	26	28
1	138	145
2	94	95
3	41	37
4	214	219
5	73	69
6	29	30
7	24	25
8	19*	17
9	110	110
10	113	118
11	38	35

3,14,L

-11	66	68
-10	68	71
-9	18*	11
-8	20	17
-7	18*	1
-6	95	92
-5	25	23
-4	102	101
-3	22	13
-2	137	137
-1	46	43
0	98	96
1	45	48
2	19*	5
3	234	245
4	55	56
5	61	60

-17	152	150
-16	203	196
-15	67	62
-14	319	316
-13	158	157
-12	126	132
-11	49	57
-10	19	11
-9	54	46
-8	16*	13
-7	478	484
-6	25	17
-5	28	19
-4	306	302
-3	69	60
-2	310	274
-1	408	413
0	695	691
1	645	652
2	546	528
3	359	347
4	444	424
5	472	469
6	334	324
7	17*	11
8	214	205
9	66	68
10	37	36
11	85	80
12	319	325
13	127	127
14	111	117
15	139	149
16	85	81
17	118	127
18	47	46

4,6,L

-19	27	35
-18	25	27
-17	47	38
-16	37	37
-15	241	240
-14	65	75
-13	19*	5
-12	67	62
-11	62	66
-10	32	34
-9	149	163
-8	34	24
-7	23	31
-6	120	113
-5	136	131
-4	68	62
-3	102	91
-2	34	20
-1	214	206
0	417	418

4,6,L

1	186	188
2	493	488
3	292	297
4	128	134
5	225	207
6	299	290
7	289	280
8	311	315
9	36	32
10	50	47
11	75	76
12	44	52
13	18*	3
14	100	108
15	38	38
16	114	128
17	55	51

4,7,L

-19	108	98
-18	114	120
-17	19*	13
-16	53	59
-15	131	135
-14	255	250
-13	73	80
-12	275	278
-11	61	53
-10	170	173
-9	23	19
-8	203	209
-7	326	327
-6	124	119
-5	258	258
-4	33	22
-3	243	227
-2	89	90
-1	53	45
0	17*	26
1	110	106
2	142	140
3	119	101
4	71	61
5	50	51
6	243	249
7	103	95
8	239	229
9	176	184
10	244	248
11	111	116
12	99	90
13	25	26
14	18*	20
15	106	110
16	55	52
17	61	66

4,8,L

-18	17*	5
-17	236	238
-16	32	28
-15	166	169
-14	70	67
-13	63	65
-12	55	54
-11	18*	17
-10	356	353
-9	119	117
-8	81	79
-7	17*	22
-6	122	130
-5	188	203
-4	243	248
-3	26	30
-2	292	287
-1	71	73
0	169	155
1	481	485
2	261	254
3	288	281
4	121	115
5	116	107
6	126	131
7	126	117
8	30	30
9	132	124
10	97	90
11	198	205
12	19*	9
13	121	124
14	18*	7
15	109	107
16	75	80

4,9,L

-17	34	36
-16	28	22
-15	31	26
-14	25	39
-13	62	64
-12	19*	1
-11	29	20
-10	27	21
-9	363	370
-8	131	136
-7	168	171
-6	18*	15
-5	82	77
-4	172	164
-3	123	119
-2	17*	18
-1	85	80
0	171	167
1	223	209
2	329	332
3	200	208
4	212	207
5	18*	7
6	75	72
7	119	121
8	206	205
9	181	180
10	61	61
11	249	259
12	63	63
13	22	32
14	40	38
15	34	36

4,10,L

-16	31	23
-15	18*	13
-14	61	60
-13	56	58
-12	186	196
-11	33	31
-10	270	269
-9	64	52
-8	118	113
-7	41	37
-6	101	98
-5	139	143
-4	19*	19
-3	79	76
-2	35	20
-1	142	145
0	350	348
1	225	228
2	356	354
3	85	86
4	93	104
5	175	176
6	140	140
7	61	47
8	18*	3
9	75	78
10	19*	1
11	40	46
12	90	102
13	45	49
14	56	57

4,11,L

-15	39	38
-14	48	44
-13	86	88
-12	101	101
-11	122	123
-10	19*	4
-9	52	45
-8	24	27
-7	213	218
-6	55	53
-5	151	149
-4	209	199
-3	30	17
-2	248	250
-1	290	291
0	259	271
1	59	71
2	20	0
3	161	169
4	146	146
5	18*	5
6	75	73
7	66	64
8	25	20
9	77	88
10	84	90
11	20	22
12	50	50
13	126	138

4,12,L

-14	17*	0
-13	18*	12
-12	21*	14
-11	18*	5
-10	144	134
-9	64	64
-8	249	242
-7	223	221
-6	170	175
-5	265	271
-4	25	31
-3	258	256
-2	64	65
-1	146	154
0	281	287
1	123	126
2	219	217
3	53	58
4	101	107
5	18*	3
6	23	26
7	59	58
8	70	81
9	19*	2
10	75	90
11	18*	9
12	51	48

4,13,L

-12	36	35
-11	50	48
-10	20	19
-9	73	68
-8	60	59
-7	145	144
-6	54	55
-5	29	17
-4	121	120
-3	116	114
-2	232	234
-1	97	100
0	58	72
1	101	101
2	37	36
3	71	72
4	133	135
5	37	39
6	97	91
7	136	148
8	26	30
9	107	108
10	27	33

4,14,L

-10	18*	12
-9	53	50
-8	38	35
-7	18*	14
-6	18*	1
-5	104	105
-4	33	39
-3	40	46
-2	162	172
-1	89	89
0	55	48
1	56	67
2	40	38
3	169	172
4	18*	4
5	104	108
6	21	29
7	146	151
8	17*	12
9	30	36

4,15,L

-8	58	57
-7	135	131
-6	18*	13
-5	95	103
-4	36	29
-3	92	89
-2	54	59
-1	19*	17
0	62	63
1	18*	20
2	81	88
3	117	122
4	37	42
5	89	89
6	58	67

4,16,L

-3	16*	5
-2	25	19
-1	92	96
0	37	39
1	133	135

5,0,L

-19	57	61
-17	18*	0
-15	111	116
-13	19*	17
-11	227	244
-9	487	475
-7	197	192
-5	715	705
-3	388	391
-1	62	76
1	124	86
3	210	206
5	636	613
7	697	705
9	377	365
11	304	316
13	48	46
15	33	43
17	18*	8

5,1,L

-20	73	74
-19	50	52
-18	113	123
-17	96	104
-16	136	140
-15	71	75
-14	97	91
-13	201	198
-12	294	284
-11	103	93
-10	85	82
-9	250	252
-8	39	49
-7	97	97
-6	315	309
-5	63	51
-4	90	73
-3	52	51
-2	83	81
-1	104	92
0	23	37
1	77	76
2	292	281
3	16	33
4	373	375
5	447	425
6	243	227
7	206	201
8	28	33
9	89	87
10	215	203
11	20	18
12	300	301
13	30	29
14	174	180
15	118	114
16	72	74
17	18*	17
18	20	12

5,2,L

-20	71	70
-19	18*	18
-18	40	30
-17	211	224
-16	240	246
-15	60	66
-14	372	391
-13	116	116
-12	17*	0
-11	265	261
-10	233	231
-9	394	389
-8	402	372
-7	294	274
-6	15*	3
-5	186	181
-4	483	491
-3	442	433
-2	240	225
-1	335	316
0	304	303
1	660	648
2	353	342
3	345	339
4	465	437
5	258	254
6	274	253
7	263	264
8	48	35
9	36	31
10	79	84
11	193	190
12	148	160
13	54	57
14	20*	28
15	65	69
16	33	32
17	73	77
18	17*	4

5,3,L

-20	17*	16
-19	29	38
-18	80	91
-17	196	208
-16	159	150
-15	74	79
-14	174	175
-13	94	91
-12	19	12
-11	17*	16
-10	155	161
-9	247	253
-8	203	184
-7	371	359
-6	169	141
-5	433	410
-4	755	746
-3	73	72
-2	363	335
-1	180	192
0	389	388
1	475	470
2	794	779
3	574	555
4	370	368
5	16*	33
6	123	123
7	394	378
8	195	188
9	236	226
10	137	125
11	110	120
12	159	164
13	146	144
14	20*	11
15	91	98
16	67	66
17	179	179
18	58	55

5,4,L

-20	118	116
-19	39	42
-18	66	63
-17	19*	5
-16	214	217
-15	19*	14
-14	266	283
-13	24	25
-12	17*	17
-11	79	75
-10	199	195
-9	188	184
-8	117	133
-7	281	279
-6	104	107
-5	646	612
-4	642	627
-3	237	224
-2	323	322
-1	546	512
0	15*	18
1	286	280
2	24	28
3	342	331
4	508	488
5	153	140
6	526	513
7	133	119
8	230	229
9	358	352
10	130	127
11	226	223
12	148	140
13	96	106
14	85	85
15	51	51
16	78	81
17	39	33

5,5,L

-19	54	51
-18	55	65
-17	225	226
-16	118	122
-15	69	62
-14	307	301
-13	219	221
-12	107	98
-11	34	26
-10	143	142
-9	125	108
-8	43	34
-7	53	54
-6	182	172
-5	396	380
-4	16*	29
-3	66	47
-2	561	552
-1	152	131
0	46	39
1	82	87
2	47	49
3	499	500
4	158	153
5	459	438
6	151	132
7	389	388
8	119	121
9	147	135
10	185	174
11	150	148
12	109	100
13	87	89
14	25	25
15	163	165
16	18	19
17	74	74

5,6,L

-19	24	17
-18	27	27
-17	118	120
-16	195	197
-15	136	133
-14	78	87
-13	104	96
-12	48	51
-11	166	160
-10	67	74
-9	234	228
-8	111	101
-7	119	121
-6	484	483
-5	238	238
-4	65	69
-3	168	169
-2	134	112
-1	109	108
0	133	122
1	152	157
2	132	136
3	62	63
4	58	52
5	323	331
6	367	361
7	330	333
8	189	190
9	75	86
10	162	154
11	50	60
12	18*	14
13	18*	5
14	35	23
15	41	36
16	53	52

5,7,L

-18	46	50
-17	19	10
-16	18*	24
-15	84	93
-14	52	53
-13	128	136
-12	137	131
-11	77	76
-10	21	11
-9	67	67
-8	140	150
-7	210	194
-6	232	234
-5	76	89
-4	67	63
-3	218	210
-2	84	67
-1	251	241
0	168	170
1	62	61
2	17*	28

5,7,L

3	43	48
4	29	34
5	323	325
6	311	319
7	18*	7
8	141	144
9	261	262
10	223	222
11	38	14
12	23	19
13	193	200
14	136	146
15	102	108
16	59	55

5,8,L

-18	21	20
-17	116	121
-16	20	16
-15	141	147
-14	218	222
-13	37	32
-12	19*	11
-11	281	290
-10	224	231
-9	177	185
-8	82	84
-7	171	169
-6	237	239
-5	43	39
-4	205	208
-3	73	61
-2	301	313
-1	122	130
0	87	88
1	93	103
2	163	160
3	319	311
4	217	224
5	190	191
6	63	57
7	24	15
8	28	26
9	146	152
10	146	142
11	145	157
12	19*	4
13	126	129
14	48	54
15	17*	4

5,9,L

-17	43	49
-16	49	45
-15	40	51
-14	168	171

6,2,L

-11	24	23
-10	85	86
-9	333	321
-8	157	154
-7	203	202
-6	79	79
-5	157	146
-4	94	79
-3	348	333
-2	213	200
-1	33	37
0	218	213
1	74	81
2	300	313
3	161	155
4	571	550
5	342	342
6	240	234
7	101	98
8	87	85
9	113	104
10	173	170
11	53	61
12	149	148
13	243	254
14	39	49
15	69	78
16	80	84
17	50	51

6,3,L

-19	42	40
-18	149	157
-17	82	86
-16	178	175
-15	111	111
-14	19*	11
-13	151	152
-12	19*	11
-11	32	28
-10	253	256
-9	66	62
-8	116	121
-7	163	148
-6	83	69
-5	36	26
-4	127	119
-3	32	44
-2	283	283
-1	240	228
0	427	408
1	144	153
2	395	379

6,1,L

-14	37	35
-13	80	86
-12	177	187
-11	228	234
-10	90	93
-9	19*	16
-8	165	166
-7	55	51
-6	190	197
-5	40	39
-4	160	157
-3	56	59
-2	18*	14
-1	18*	1
0	18*	11
1	117	118
2	405	410
3	124	130
4	18*	5
5	198	207
6	270	275
7	74	80
8	280	280
9	114	113
10	63	64
11	45	51
12	98	99
13	78	86
14	39	50

5,10,L

-16	18	24
-15	68	73
-14	18*	9
-13	157	160
-12	19*	16
-11	210	216
-10	269	282
-9	238	249
-8	345	350
-7	245	248
-6	147	138
-5	291	289
-4	188	187
-3	232	232
-2	103	98
-1	162	166
0	110	100
1	298	303
2	69	65
3	19*	7
4	72	65
5	236	245
6	18*	17
7	240	248
8	149	145
9	23	29
10	60	59
11	113	126
12	24	28

-13	18*	8
-12	43	48
-11	202	196
-10	320	315
-9	250	247
-8	108	115
-7	162	161
-6	47	42
-5	244	235
-4	15*	5
-3	136	136
-2	91	97
-1	358	350
0	406	396

6,3,L

3	59	73
4	166	160
5	33	43
6	209	202
7	239	220
8	18*	13
9	69	67
10	143	152
11	110	111
12	83	92
13	54	58
14	184	186
15	62	60
16	55	64
17	98	95

6,4,L

-19	121	116
-18	36	24
-17	20*	4
-16	104	96
-15	143	143
-14	182	180
-13	69	63
-12	18*	17
-11	127	130
-10	110	114
-9	16*	7
-8	35	50
-7	82	78
-6	152	148
-5	82	89
-4	124	101
-3	465	462
-2	67	68
-1	469	447
0	313	291
1	302	281
2	51	44
3	181	191
4	229	212
5	149	150
6	323	324
7	355	355
8	84	83
9	41	32
10	142	143
11	250	256
12	19*	3
13	178	182
14	25	32
15	168	178
16	23	19

6,5,L

-19	30	19
-18	106	113
-17	77	71
-16	131	148
-15	109	97
-14	183	185
-13	185	192
-12	256	265
-11	38	25
-10	86	94
-9	18*	8
-8	47	51
-7	173	171
-6	193	199
-5	50	51
-4	79	74
-3	266	265
-2	228	220
-1	257	247
0	206	197
1	196	189
2	298	302
3	155	154
4	299	296
5	374	365
6	28	16
7	45	43
8	19*	6
9	64	56
10	27	33
11	38	36
12	110	118
13	111	106
14	18*	14
15	81	91
16	24	27

6,6,L

-18	34	32
-17	19*	16
-16	71	76
-15	84	82
-14	17*	6
-13	109	100
-12	110	107
-11	90	95
-10	76	75
-9	178	175
-8	190	184
-7	52	47
-6	329	332
-5	136	142
-4	88	84
-3	136	129
-2	43	34
-1	89	73
0	101	105
1	78	96
2	131	126
3	36	17
4	214	215
5	576	583
6	35	28
7	187	181
8	114	115
9	37	46
10	237	236
11	38	42
12	105	96
13	106	109
14	38	28
15	100	108

6,7,L

-18	37	39
-17	56	51
-16	35	37
-15	51	63
-14	94	97
-13	21	24
-12	130	121
-11	19*	6
-10	120	122
-9	164	166
-8	127	124
-7	18*	14
-6	235	234
-5	42	41
-4	126	119
-3	37	37
-2	329	338
-1	23	12
0	119	122
1	32	32
2	155	163
3	126	114
4	131	130
5	23	9
6	19*	1
7	25	28
8	399	408
9	20*	26
10	272	276
11	121	124

5,11,L

-15	42	46
-14	17*	14
-13	39	46
-12	44	45
-11	54	56
-10	71	75
-9	80	81
-8	193	201
-7	145	152
-6	190	189
-5	27	24
-4	280	299
-3	233	241
-2	320	329
-1	146	156
0	133	136
1	73	78
2	121	118
3	114	110
4	210	214
5	71	65
6	135	128
7	18*	1
8	19*	6
9	43	49
10	52	46
11	17*	9
12	76	77

5,12,L

-13	97	95
-12	95	100
-11	77	83
-10	49	50
-9	117	120
-8	68	68
-7	57	61
-6	173	176
-5	182	184
-4	170	173
-3	19*	9
-2	82	81
-1	263	270
0	308	314
1	287	288
2	223	231
3	61	57
4	64	67
5	34	47
6	46	51
7	136	136
8	33	24
9	53	51
10	35	32
11	66	76

5,13,L

-12	178	180
-11	28	30
-10	119	112
-9	71	78
-8	18*	6
-7	59	58
-6	18*	4
-5	149	151
-4	62	67
-3	221	219
-2	77	88
-1	61	64
0	59	45
1	128	135
2	78	84
3	113	111
4	22	21
5	67	63
6	36	32
7	22	18
8	18*	13
9	61	64

5,14,L

-9	133	136
-8	31	18
-7	163	165
-6	99	93
-5	83	80
-4	18*	20
-3	19*	13
-2	63	67
-1	20	9
0	17*	6
1	19*	13
2	39	36
3	75	83
4	47	48
5	18*	11
6	87	88
7	107	113

5,15,L

-6	18*	21
-5	150	149
-4	18*	16
-3	19*	23
-2	35	48
-1	17*	1
0	30	34
1	33	34
2	72	79
3	32	25
4	71	78

6,0,L

-20	45	47
-18	59	47
-18	196	200
-14	376	370
-12	489	498
-10	66	63
-8	144	134
-6	339	336
-4	88	93
-2	409	397
0	248	255
2	68	55
4	15*	12
6	309	300
8	213	212
10	42	19
12	196	210
14	183	199
16	98	98

6,1,L

-20	57	64
-19	18*	24
-18	83	85
-17	120	132
-16	158	167
-15	148	155
1	15*	30
2	262	254
3	41	38
4	79	77
5	16*	8
6	95	105
7	24	37
8	117	111
9	28	25
10	191	191
11	22	22
12	19*	22
13	18*	3
14	142	144
15	24	16
16	50	47
17	118	125

6,2,L

-20	86	84
-19	17*	12
-18	18*	8
-17	18*	8
-16	84	90
-15	19*	3
-14	56	56
-13	182	188
-12	141	145
12	45	48
13	39	44
14	177	188
15	18	20

6,8,L

-17	17*	14
-16	25	25
-15	20	18
-14	139	142
-13	130	135
-12	156	168
-11	78	80
-10	51	56
-9	28	27
-8	196	197
-7	155	155
-6	92	101
-5	89	87
-4	86	95
-3	98	104
-2	137	135
-1	227	227
0	333	331
1	73	75
2	173	172
3	175	173
4	237	243
5	94	98
6	19*	6
7	229	233
8	110	111
9	18*	1
10	194	204
11	59	65
12	188	201
13	154	159
14	132	143

6,9,L

-16	47	47
-15	63	61
-14	37	30
-13	94	93
-12	251	257
-11	21	14
-10	149	152
-9	81	83
-8	52	48
-7	148	149
-6	35	36
-5	52	39
-4	208	215
-3	19*	3
-2	51	48
-1	99	104
0	149	149

6,9,L

1	205	203
2	179	183
3	339	340
4	172	179
5	131	133
6	20	9
7	95	104
8	33	32
9	72	77
10	194	202
11	87	90
12	26	29
13	17*	15

6,10,L

-15	91	90
-14	104	103
-13	20	30
-12	127	119
-11	222	223
-10	29	24
-9	178	187
-8	90	98
-7	65	60
-6	19*	3
-5	53	47
-4	30	25
-3	233	234
-2	288	290
-1	37	45
0	313	320
1	118	123
2	203	202
3	130	124
4	176	174
5	36	34
6	65	58
7	44	44
8	25	22
9	20	6
10	147	152
11	18	2
12	156	166

6,11,L

-14	28	32
-13	113	110
-12	71	72
-11	64	69
-10	18*	10
-9	83	85
-8	103	102
-7	61	62
-6	58	58
-5	29	27
-4	132	125

7,4,L

-5	327	324
-4	69	56
-3	118	120
-2	142	138
-1	37	31
0	213	224
1	149	158
2	205	190
3	95	92
4	304	280
5	53	60
6	110	107
7	86	87
8	303	312
9	139	138
10	94	98
11	34	31
12	91	93
13	68	77
14	88	90
15	58	57

7,5,L

-18	17*	9
-17	56	59
-16	49	46
-15	39	49
-14	33	28
-13	207	215
-12	24	29
-11	155	164
-10	161	165
-9	93	94
-8	104	109
-7	114	113
-6	62	68
-5	23	14
-4	17	19
-3	16*	16
-2	236	226
-1	214	228
0	27	15
1	72	69
2	87	86
3	162	161
4	17*	10
5	102	103
6	23	19
7	107	102
8	18*	8
9	138	142
10	144	152
11	19*	7
12	137	143
13	49	40
14	26	22
15	105	110

-3	199	198
-2	37	35
-1	86	84
0	58	64
1	105	100
2	53	47
3	18*	11
4	18*	10
5	38	32
6	19*	8
7	149	154
8	18*	6
9	18*	14
10	17*	11
11	67	68

6,12,L

-12	30	28
-11	32	36
-10	96	102
-9	54	51
-8	151	148
-7	28	18
-6	69	64
-5	92	86
-4	213	224
-3	86	98
-2	90	87
-1	48	56
0	65	55
1	89	91
2	62	67
3	44	47
4	77	77
5	121	123
6	168	172
7	85	89
8	64	64
9	24	35

6,13,L

-10	68	72
-9	18*	19
-8	117	108
-7	74	73
-6	96	95
-5	214	221
-4	51	51
-3	173	188
-2	113	118
-1	18*	11
0	105	109
1	58	58
2	18*	5
3	84	87
4	22	22
5	100	103
6	62	64

7,6,L

-17	76	70
-16	68	69
-15	141	148
-14	174	181
-13	172	177
-12	19*	3
-11	74	75
-10	46	49
-9	71	62
-8	25	26
-7	18*	1
-6	23	14
-5	119	113
-4	136	144
-3	17*	25
-2	85	89
-1	77	78
0	24	5
1	291	293
2	176	176
3	135	133
4	282	284
5	189	192
6	93	100
7	147	146
8	154	157
9	112	116
10	54	56
11	66	70
12	41	33
13	18*	16
14	42	47

7,7,L

-17	68	68
-16	32	25
-15	18*	18
-14	29	31
-13	88	85
-12	66	70
-11	29	39
-10	19*	6
-9	129	136
-8	43	36
-7	30	34
-6	144	134
-5	89	98
-4	62	65
-3	41	31
-2	81	84
-1	18*	2
0	70	58
1	64	64
2	19*	10
3	122	122
4	304	311
5	283	293

6	68	73
7	71	73
8	155	157
9	18*	16
10	32	34
11	18*	2
12	78	75
13	35	36

7,8,L

-16	72	71
-15	85	83
-14	98	106
-13	20*	20
-12	21	25
-11	44	52
-10	47	45
-9	85	97
-8	41	37
-7	19*	9
-6	240	237
-5	33	34
-4	150	146
-3	149	153
-2	58	62
-1	41	40
0	306	311
1	20*	19
2	223	228
3	38	27
4	116	122
5	136	138
6	476	481
7	20*	15
8	67	61
9	64	63
10	46	49
11	74	75
12	17*	13
13	16*	15

7,9,L

-15	44	50
-14	136	146
-13	20	19
-12	19*	11
-11	160	170
-10	73	74
-9	79	71
-8	53	56
-7	191	182
-6	20*	38
-5	75	80
-4	167	174
-3	50	54
-2	147	151
-1	200	198
0	50	64

7	17*	2
8	79	65

6,14,L

-8	173	172
-7	74	76
-6	207	214
-5	124	120
-4	88	91
-3	123	127
-2	131	138
-1	78	79
0	73	77
1	84	85
2	19	9
3	82	82
4	16*	10
5	49	46

6,15,L

-3	59	65
-2	44	45
-1	33	40
0	40	41

7,0,L

-19	121	122
-17	18*	6
-15	177	174
-13	92	93
-11	55	52
-9	246	250
-7	177	183
-5	94	88
-3	468	454
-1	87	79
1	161	143
3	83	109
5	227	228
7	44	42
9	64	74
11	192	203
13	128	123
15	53	53

7,1,L

-19	19	9
-18	27	29
-17	29	27
-16	74	74
-15	141	147
-14	180	187
-13	63	61
-12	312	313
-11	333	347
-10	142	140

-9	93	90
-8	73	78
-7	16*	10
-6	109	100
-5	88	99
-4	316	303
-3	100	105
-2	492	491
-1	244	219
0	159	148
1	53	63
2	177	170
3	24	6
4	241	239
5	187	196
6	32	6
7	38	32
8	87	81
9	58	68
10	178	179
11	130	129
12	43	42
13	40	38
14	130	134
15	45	44
16	43	52

7,2,L

-19	16*	0
-18	105	98
-17	18*	9
-16	59	63
-15	159	161
-14	286	299
-13	153	161
-12	98	99
-11	35	30
-10	165	166
-9	61	63
-8	16*	6
-7	38	55
-6	183	186
-5	39	35
-4	31	10
-3	133	137
-2	40	30
-1	16*	5
0	260	248
1	141	132
2	231	218
3	362	337
4	54	47
5	30	28
6	28	19
7	67	66
8	69	70
9	25	19
10	98	92
11	77	68

7,10,L

-14	16*	10
-13	18*	6
-12	31	23
-11	48	44
-10	41	44
-9	19*	4
-8	38	42
-7	18*	8
-6	55	64
-5	76	80
-4	90	94
-3	57	57
-2	86	80
-1	90	92
0	169	167
1	25	22
2	258	267
3	144	143
4	20	10
5	76	78
6	93	103
7	26	23
8	122	130
9	19	20
10	65	61
11	17*	18

7,11,L

-13	17*	18
-12	38	38
-11	17*	11
-10	72	71
-9	18*	6
-8	37	28
-7	22	8
-6	137	139
-5	46	49
-4	76	68
-3	84	80
-2	55	55
-1	99	103
0	25	20
1	23	13
2	98	106

12	161	165
13	77	85
14	116	120
15	18*	17
16	17*	14

7,3,L

-19	36	44
-18	44	37
-17	77	83
-16	59	47
-15	80	77
-14	141	133
-13	76	72
-12	297	300
-11	291	305
-10	100	98
-9	185	168
-8	111	109
-7	205	199
-6	394	375
-5	49	56
-4	109	110
-3	208	196
-2	65	73
-1	245	235
0	22	23
1	46	34
2	61	54
3	35	40
4	197	189
5	72	69
6	166	155
7	299	286
8	259	261
9	81	90
10	65	62
11	173	179
12	33	31
13	18*	5
14	72	77
15	18*	24

7,4,L

-18	17*	14
-17	133	145
-16	133	130
-15	52	54
-14	204	205
-13	19*	1
-12	36	34
-11	106	96
-10	83	80
-9	86	88
-8	292	302
-7	92	91
-6	178	185

3	96	98
4	26	22
5	127	129
6	61	66
7	133	136
8	21	24
9	84	83

7,12,L

-11	20	26
-10	18*	16
-9	50	54
-8	18*	14
-7	18*	9
-6	18*	11
-5	115	123
-4	58	56
-3	30	35
-2	34	48
-1	18*	2
0	48	44
1	18	12
2	31	29
3	33	30
4	18*	4
5	64	66
6	45	40
7	18*	22
8	17*	12

7,13,L

-9	49	43
-8	33	31
-7	18*	22
-6	48	45
-5	18*	12
-4	42	44
-3	28	23
-2	36	26
-1	23	21
0	24	20
1	26	16
2	65	65
3	32	28
4	126	127
5	75	81

7,14,L

-5	18	11
-4	81	81
-3	43	41
-2	17*	1
-1	17*	20
0	40	40
1	63	64

H,2,3

8	72	70
10	150	148
11	110	120
12	92	90
13	105	107
14	63	64
15	25	19
16	112	116
17	60	57
18	32	32
19	37	37

H,2,4

0	1195	1212
1	282	288
2	629	617
3	421	429
4	706	698
5	59	44
6	148	155
7	315	304
8	245	237
9	86	97
10	222	228
11	158	158
12	123	124
13	52	53
14	120	122
15	126	130
16	11*	6
17	38	39
18	32	33
19	35	36

H,2,5

1	177	184
2	199	207
3	111	118
4	218	217
5	376	351
6	248	261
7	197	182
8	155	140
9	53	48
10	107	107
11	50	59
12	67	82
13	175	175
14	148	153
15	24	27
16	17	19
17	45	50
18	43	45

H,2,6

0	441	431
1	140	147
2	194	190
3	385	397
4	257	239
5	87	75
6	180	160
7	234	226
8	221	208
9	174	172
10	48	43
11	141	143
12	214	218
13	63	67
14	80	80
15	104	105
16	120	118
17	76	79
18	53	56

H,2,7

1	327	298
2	208	203
3	111	101
4	400	406
5	135	141
6	245	247
7	133	130
8	204	208
9	23	26
10	197	206
11	99	96
12	118	113
13	144	146
14	122	117
15	61	58
16	53	54
17	26	25

H,2,8

0	341	354
1	268	265
2	75	78
3	212	214
4	149	138
5	156	159
6	188	184
7	37	32
8	98	96
9	162	164
10	31	32
11	100	103
12	93	91
13	21	18
14	65	61
15	58	60
16	33	26
17	12	11

H,2,9

1	147	132
2	24	20
3	55	58
4	129	126
5	105	99
6	24	23
7	98	105
8	95	96
9	126	131
10	98	97
11	51	51
12	25	13
13	40	41
14	51	50
15	48	48
16	20	18

H,2,10

0	33	31
1	102	98
2	231	224
3	137	137
4	67	71
5	46	56
6	59	68
7	70	75
8	24	29
9	81	85
10	53	52
11	87	96
12	56	59
13	74	76
14	22	20
15	10*	4

H,2,11

1	205	208
2	174	174
3	43	46
4	108	100
5	92	97
6	64	71
7	58	61
8	43	42
9	43	49
10	92	93
11	88	96
12	20	18
13	11*	12
14	32	33

H,2,12

0	65	56
1	102	104
2	156	159
3	161	165
4	103	110
5	76	79
6	68	75
7	59	65
8	87	82
9	86	92
10	15	13
11	45	50
12	47	47
13	10*	13

H,2,13

1	95	92
2	58	46
3	107	105
4	45	45
5	68	72
6	96	102
7	91	97
8	25	24
9	72	75
10	35	34
11	51	56
12	18	25

H,2,14

0	109	113
1	50	51
2	20	22
3	76	78
4	87	94
5	77	74
6	60	62
7	41	43
8	33	34
9	59	63
10	42	38
11	60	63

H,2,15

1	48	47
2	28	20
3	51	50
4	85	88
5	24	23
6	33	33
7	40	39
8	10*	12
9	9*	7

H,2,16

0	43	42
1	25	25
2	20	13
3	13	19
4	23	21
5	33	31
6	36	38

H,3,0

1	404	416
2	38	16
3	354	346
4	413	378
5	167	164
6	215	198
7	11	9
8	216	201
9	13	18
10	65	61
11	71	67
12	59	44
13	67	72
14	42	38
15	97	102
16	29	28
17	11*	7
18	31	32
19	10	11

H,3,1

0	244	253
1	316	293
2	537	526
3	691	692
4	152	131
5	327	325
6	251	241
7	189	183
8	65	65
9	98	105
10	196	200
11	106	109
12	67	73
13	66	67
14	50	53
15	58	58
16	41	38
17	91	92
18	17	27
19	16	15

H,3,2

1	106	93
2	473	483
3	354	338
4	303	297
5	106	98
6	190	176
7	296	281

H,3,2

8	215	207
9	160	159
10	150	147
11	117	116
12	110	113
13	85	87
14	55	49
15	101	104
16	35	32
17	18	15
18	16	13
19	64	69

H,3,3

0	848	844
1	655	638
2	402	398
3	177	165
4	112	96
5	186	187
6	172	165
7	383	372
8	156	151
9	126	116
10	53	56
11	40	39
12	28	26
13	37	42
14	62	55
15	44	43
16	24	18
17	75	77
18	38	40
19	9*	7

H,3,4

1	370	367
2	597	598
3	627	636
4	235	236
5	57	72
6	334	326
7	175	178
8	197	186
9	107	125
10	112	111
11	56	52
12	28	24
13	76	75
14	39	37
15	33	37
16	77	83
17	43	43
18	38	40

H,3,5

0	236	245
1	558	558
2	134	155
3	116	99
4	157	155
5	180	181
6	106	101
7	26	36
8	92	80
9	94	85
10	79	78
11	89	89
12	50	48
13	52	49
14	48	50
15	106	109
16	44	45
17	11*	10
18	13	18

H,3,6

1	153	154
2	75	63
3	396	390
4	232	217
5	326	319
6	139	139
7	151	142
8	212	215
9	109	111
10	225	225
11	23	29
12	14	19
13	187	189
14	20	15
15	61	56
16	21	24
17	43	39
18	68	73

H,3,7

0	219	226
1	152	155
2	92	93
3	71	66
4	78	84
5	21	23
6	105	101
7	165	156
8	182	177
9	45	45
10	73	73
11	242	240
12	38	29
13	27	28
14	112	112
15	36	36
16	21	25
17	40	36

H,3,8

1	186	180
2	138	133
3	268	273
4	126	116
5	94	97
6	128	137
7	20	15
8	142	139
9	171	177
10	20	16
11	24	21
12	124	124
13	112	112
14	42	38
15	44	45
16	32	35
17	9*	8

H,3,9

0	117	122
1	184	183
2	163	158
3	97	87
4	68	64
5	52	58
6	116	110
7	147	157
8	67	65
9	93	91
10	119	122
11	85	80
12	17	11
13	12*	5
14	23	24
15	42	41
16	30	34

H,3,10

1	124	122
2	50	54
3	97	89
4	100	107
5	92	93
6	56	56
7	65	64
8	112	112
9	64	70
10	26	26
11	19	15
12	59	57
13	34	36
14	18	18
15	12	13

H,3,11

0	163	170
1	119	117
2	79	81
3	141	148
4	75	71
5	51	54
6	61	67
7	12*	5
8	53	52
9	20	16
10	104	107
11	74	72
12	55	53
13	44	47
14	10*	4

H,3,12

1	123	120
2	81	86
3	84	82
4	45	37
5	79	82
6	67	64
7	24	23
8	46	46
9	22	20
10	78	84
11	31	35
12	48	47
13	20	25

H,3,13

0	116	108
1	48	49
2	80	80
3	85	90
4	25	23
5	28	22
6	28	31
7	52	58
8	58	53
9	69	66
10	21	23
11	39	44
12	17	17

H,3,14

1	88	87
2	45	48
3	12*	14
4	20	23
5	43	49
6	44	48
7	47	45
8	30	30
9	52	62
10	40	39

H,3,15

0	68	72
1	34	35
2	13	9
3	52	53
4	26	27
5	29	28
6	28	24
7	42	47
8	21	19

H,3,16

1	48	50
2	38	35
3	27	24
4	16	12
5	21	23
6	11	11

H,4,0

0	1441	1498
1	924	915
2	568	580
3	63	75
4	306	273
5	224	216
6	260	263
7	42	36
8	13	26
9	232	241
10	134	132
11	51	40
12	20	15
13	126	126
14	101	105
15	33	30
16	31	35
17	15	14
18	39	47
19	35	38

H,4,1

1	637	648
2	507	516
3	306	299
4	398	400
5	365	361
6	147	135
7	182	173
8	170	167
9	178	166

H,4,1

10	78	79
11	123	120
12	133	131
13	113	117
14	115	120
15	45	43
16	53	53
17	22	23
18	31	33
19	15	18

H,4,2

0	477	460
1	658	637
2	76	41
3	387	379
4	41	32
5	292	276
6	469	461
7	191	183
8	76	69
9	94	83
10	295	294
11	100	97
12	84	83
13	60	65
14	84	84
15	127	129
16	129	137
17	28	30
18	46	46

H,4,3

1	210	201
2	388	376
3	119	133
4	144	138
5	349	354
6	390	400
7	369	391
8	223	230
9	85	85
10	100	108
11	43	42
12	103	100
13	180	178
14	112	113
15	78	80
16	34	33
17	56	59
18	24	24

H,4,4

0	733	731
1	501	502
2	80	106
3	618	594
4	141	134
5	173	164
6	346	327
7	216	206
8	130	127
9	102	94
10	203	195
11	193	192
12	87	83
13	20	19
14	70	79
15	100	106
16	58	60
17	11*	10
18	54	57

H,4,5

1	52	65
2	430	415
3	78	75
4	200	204
5	223	219
6	68	73
7	306	311
8	127	129
9	48	44
10	110	111
11	73	73
12	46	50
13	113	115
14	54	55
15	54	59
16	51	52
17	60	60
18	18	18

H,4,6

0	267	260
1	50	27
2	40	39
3	154	149
4	126	112
5	165	148
6	28	29
7	74	67
8	214	210
9	125	124
10	147	146
11	73	69
12	118	118
13	128	128
14	15	21
15	56	51
16	65	62
17	74	79

H,4,7

1	70	76
2	256	261
3	104	107
4	151	149
5	83	82
6	179	170
7	129	125
8	209	203
9	90	100
10	184	189
11	202	205
12	21	22
13	66	66
14	63	58
15	40	38
16	47	48
17	14	13

H,4,8

0	170	159
1	224	218
2	213	207
3	199	200
4	99	82
5	209	209
6	225	227
7	155	166
8	308	312
9	191	193
10	61	62
11	134	134
12	95	100
13	12*	10
14	67	70
15	36	43
16	43	41

H,4,9

1	170	162
2	131	138
3	139	133
4	150	140
5	85	74
6	157	152
7	101	100
8	70	80
9	133	133
10	16	11
11	33	28
12	50	50
13	73	73
14	17	18
15	22	23
16	33	34

H,4,10

0	208	212
1	180	181
2	76	81
3	71	69
4	152	156
5	133	140
6	210	200
7	54	59
8	62	62
9	26	27
10	67	65
11	37	35
12	59	57
13	13	13
14	50	53
15	22	27

H,4,11

1	102	84
2	145	155
3	203	208
4	146	165
5	97	100
6	67	64
7	61	70
8	80	81
9	70	68
10	45	51
11	44	44
12	29	31
13	35	36
1	65	84

H,4,12

0	149	151
1	69	67
2	175	176
3	48	51
4	99	94
5	103	103
6	40	40
7	12*	9
8	57	54
9	54	56
10	24	27
11	42	49
12	15	11
13	16	21

H,4,13

1	59	63
2	106	115
3	45	43
4	97	107
5	34	36
6	72	71
7	20	21
8	22	14
9	11	6
10	24	27
11	36	38

H,4,14

0	201	201
1	104	107
2	73	75
3	58	58
4	53	52
5	35	43
6	42	39
7	57	58
8	23	22
9	15	14
10	48	49

H,4,15

1	67	68
2	68	73
3	41	44
4	17	18
5	63	61
6	29	24
7	14	22
8	42	51

H,4,16

0	81	80
1	77	76
2	21	26
3	54	53
4	17	15
5	22	22

H,5,0

1	178	169
2	25	18
3	444	438
4	720	709
5	213	202
6	53	56
7	268	249
8	99	95
9	180	164
10	161	158
11	12*	6
12	155	159
13	21	16
14	60	61
15	19	21
16	38	39
17	66	65

H,5,0

18	10*	1

H,5,1

0	385	393
1	408	408
2	278	269
3	151	144
4	311	290
5	260	257
6	420	401
7	208	208
8	210	200
9	125	126
10	27	31
11	119	112
12	88	85
13	83	84
14	188	183
15	36	35
16	66	66
17	21	20
18	43	45

H,5,2

1	75	67
2	335	329
3	298	280
4	488	459
5	366	354
6	292	276
7	104	83
8	209	199
9	246	239
10	58	66
11	20	22
12	186	196
13	96	97
14	117	119
15	78	74
16	71	73
17	11*	6
18	22	17

H,5,3

0	382	357
1	450	427
2	736	708
3	164	149
4	421	423
5	387	369
6	264	264
7	131	118
8	153	139
9	148	157
10	217	215
11	141	133
12	185	186
13	43	37
14	163	167
15	61	59
16	21	29
17	33	33
18	48	48

H,5,4

1	541	532
2	169	162
3	241	220
4	386	378
5	192	192
6	117	112
7	37	29
8	154	152
9	90	94
10	331	339
11	54	56
12	120	130
13	21	21
14	74	72
15	68	68
16	91	92
17	43	44
18	22	22

H,5,5

0	727	696
1	452	438
2	356	350
3	199	181
4	250	236
5	61	50
6	178	161
7	59	55
8	79	84
9	31	42
10	92	88
11	123	123
12	268	274
13	13*	6
14	73	69
15	65	62
16	28	34
17	14	14

H,5,6

1	179	170
2	39	42
3	281	270
4	140	149
5	112	108
6	78	74
7	122	124
8	109	112
9	77	80
10	141	147
11	126	125
12	47	48
13	68	74
14	81	79
15	69	69
16	43	43
17	20	20

H,5,7

0	115	99
1	170	170
2	77	67
3	78	83
4	93	89
5	109	129
6	22	121
7	340	350
8	171	172
9	139	138
10	114	116
11	97	100
12	113	117
13	91	95
14	78	75
15	36	43
16	25	26

H,5,8

1	173	175
2	65	69
3	265	259
4	310	306
5	176	172
6	69	71
7	214	213
8	163	167
9	84	94
10	155	158
11	157	168
12	115	114
13	55	57
14	47	48
15	27	31
16	60	60

H,5,9

0	198	198
1	285	286
2	300	303
3	197	205
4	92	92
5	165	170
6	122	121
7	100	103
8	175	185
9	90	94
10	55	55
11	76	77
12	29	28
13	43	42
14	26	21
15	10	11

H,5,10

1	209	210
2	161	149
3	248	251
4	77	90
5	212	221
6	279	288
7	100	107
8	25	23
9	76	82
10	47	51
11	56	57
12	20	25
13	38	41
14	36	43

H,5,11

0	147	148
1	275	286
2	95	99
3	165	169
4	112	119
5	55	57
6	86	82
7	103	112
8	52	50
9	53	58
10	16	15
11	47	48
12	26	26
13	51	54

H,5,12

1	84	94
2	79	82
3	155	159
4	66	73
5	152	155
6	25	24
7	68	70
8	45	42
9	82	85
10	41	41
11	41	42
12	55	50

H,5,13

0	63	61
1	78	74
2	102	105
3	51	51
4	74	80
5	88	92
6	35	33
7	75	80
8	43	48
9	50	47
10	48	44
11	22	19

H,5,14

1	43	48
2	59	57
3	61	61
4	22	23
5	11*	6
6	48	49
7	10*	7
8	53	52
9	36	38

H,5,15

0	76	76
1	16	15
2	36	41
3	36	36
4	35	31
5	45	48
6	91	91
7	57	56

H,5,16

1	23	24
2	49	50
3	44	39

H,6,0

0	194	194
1	368	374
2	165	164
3	112	106
4	565	530
5	402	383
6	354	331
7	74	63
8	86	93
9	230	227
10	138	142
11	12*	2
12	53	61
13	125	124
14	199	202

H,6,0

15	56	56
16	11*	5
17	13	14
18	23	21

H,6,1

1	94	91
2	442	443
3	447	450
4	48	47
5	294	297
6	297	281
7	209	203
8	236	241
9	130	136
10	147	153
11	116	120
12	82	77
13	84	88
14	100	94
15	35	33
16	80	84
17	25	27
18	25	26

H,6,2

0	463	448
1	377	360
2	579	559
3	347	339
4	215	191
5	343	317
6	230	219
7	220	208
8	163	158
9	99	99
10	72	66
11	147	148
12	252	252
13	113	117
14	87	89
15	94	99
16	62	70
17	36	37
18	19	19

H,6,3

1	394	381
2	367	345
3	500	453
4	296	292
5	287	292
6	75	80
7	94	107
8	161	158
9	117	113
10	290	302
11	15	16
12	41	42
13	135	141
14	82	78
15	12*	9
16	19	18
17	28	31
18	33	41

H,6,4

0	484	448
1	172	181
2	536	517
3	328	324
4	80	73
5	101	111
6	121	117
7	104	108
8	175	179
9	81	75
10	167	177
11	194	200
12	152	151
13	32	31
14	104	108
15	26	31
16	59	62
17	38	39

H,6,5

1	102	76
2	275	278
3	288	292
4	113	104
5	104	94
6	142	136
7	132	124
8	197	183
9	101	98
10	136	127
11	173	183
12	178	173
13	45	55
14	60	55
15	49	51
16	62	64
17	22	26

H,6,6

0	345	339
1	122	119
2	86	95
3	174	165
4	192	178
5	117	115
6	224	216
7	214	208
8	246	248
9	125	131
10	68	68
11	115	109
12	77	80
13	45	53
14	43	43
15	63	65
16	33	31
17	48	52

H,6,7

1	87	97
2	255	263
3	83	85
4	68	81
5	175	172
6	120	127
7	122	128
8	262	270
9	34	36
10	74	78
11	80	78
12	88	92
13	105	106
14	46	46
15	61	65
16	30	32

H,6,8

0	134	116
1	114	114
2	34	33
3	58	52
4	364	362
5	39	42
6	202	204
7	63	65
8	118	122
9	59	64
10	162	152
11	70	68
12	38	36
13	24	30
14	24	28
15	30	30

H,6,9

1	131	138
2	375	378
3	99	93
4	242	250
5	118	127
6	136	140
7	31	40
8	120	112
9	25	22
10	54	54
11	23	31
12	18	20
13	15	20
14	11	12
15	31	32

H,6,10

0	486	490
1	232	225
2	105	101
3	84	84
4	132	125
5	80	83
6	223	222
7	73	67
8	96	93
9	72	64
10	47	47
11	45	50
12	33	40
13	27	27
14	45	45

H,6,11

1	31	32
2	86	83
3	80	84
4	282	280
5	111	113
6	65	63
7	42	46
8	58	60
9	11*	8
10	76	67
11	30	27
12	25	24
13	19	18

H,6,12

0	97	102
1	143	144
2	224	212
3	137	135
4	120	118
5	34	38
6	65	62
7	69	74
8	51	48
9	62	63
10	15	14
11	42	39
12	47	48

H,6,13

1	20	19
2	46	50
3	61	65
4	81	83
5	100	99
6	48	50
7	53	57
8	50	56
9	34	37
10	9*	6

H,6,14

0	87	87
1	60	61
2	45	45
3	27	28
4	34	35
5	20	19
6	78	79
7	33	35
8	87	92

H,6,15

1	43	43
2	73	79
3	35	39
4	64	66
5	30	28
6	70	69

H,7,0

1	226	240
2	146	145
3	188	186
4	224	220
5	163	154
6	73	81
7	96	100
8	137	149
9	46	44
10	121	112
11	13*	3
12	98	101
13	71	65
14	13*	6
15	47	49
16	28	29
17	30	33

H,7,1

0	264	249
1	185	185
2	313	309
3	56	55
4	103	106
5	198	174
6	57	47
7	39	35
8	35	31
9	119	112
10	174	173
11	138	133
12	70	72
13	54	50
14	42	43
15	85	79
16	43	47
17	12	14

H,7,2

1	224	195
2	82	68
3	141	136
4	198	196
5	191	186
6	175	162
7	33	30
8	77	72
9	141	143
10	58	51
11	135	140
12	124	124
13	135	145
14	12*	11
15	51	57
16	47	48
17	13	12

H,7,3

0	145	134
1	64	68
2	185	175
3	118	117
4	185	174
5	132	135
6	48	44
7	144	135
8	33	33
9	187	191
10	59	55
11	135	137
12	39	40
13	45	45
14	34	29
15	56	58
16	29	27
17	34	43

H,7,4

1	109	92
2	159	151
3	225	217
4	151	145
5	69	68
6	169	159
7	81	80
8	64	59
9	138	143
10	70	76
11	222	223
12	98	95
13	71	78
14	28	32
15	69	76
17	33	42
16	50	56

H,7,5

0	344	338
1	93	96
2	55	55
3	113	105
4	143	132
5	101	96
6	53	43
7	104	110
8	84	94
9	132	125
10	36	38
11	69	68
12	19	17
13	53	54
14	91	95
15	41	45
16	24	20

H,7,6

1	180	168
2	104	104
3	93	96
4	100	90
5	59	64
6	100	100
7	264	257
8	114	120
9	187	187
10	72	83
11	49	51
12	63	71
13	97	96
14	90	94
15	43	43
16	39	42

H,7,7

0	58	58
1	223	211
2	100	104
3	60	62
4	123	109
5	136	139
6	71	76
7	146	144
8	89	81
9	143	149
10	90	86
11	66	66
12	62	63
13	72	79
14	22	23
15	45	43

H,7,8

1	132	136
2	49	42
3	164	166
4	190	181
5	200	200
6	68	62
7	226	236
8	152	154
9	39	36
10	98	99
11	38	34
12	14	10
13	40	38
14	66	64
15	33	36

H,7,9

0	146	144
1	129	124
2	151	156
3	277	275
4	66	72
5	189	195
6	172	163
7	101	97
8	145	149
9	35	28
10	30	35
11	41	48
12	51	53
13	21	21
14	9*	4

H,7,10

1	220	227
2	194	186
3	98	95
4	165	171
5	128	132
6	156	164
7	88	89
8	36	38
9	61	60
10	38	38
11	15	18
12	21	24
13	63	69

H,7,11

0	215	215
1	56	61
2	101	98
3	189	187
4	43	45
5	87	92
6	76	75
7	36	42
8	56	55
9	57	60
10	13	18
11	77	82
12	23	25

H,7,12

1	106	106
2	45	39
3	65	60
4	68	72
5	58	66
6	23	18
7	70	72
8	29	30
9	24	21
10	26	25
11	24	25

H,7,13

0	61	60
1	62	62
2	12*	14
3	38	38
4	50	50
5	75	72
6	41	44
7	31	30
8	44	44
9	47	52

H,7,14

1	28	29
2	15	21
3	69	67
4	19	17
5	15	22
6	26	25
7	9*	4

H,7,15

0	43	52
1	51	55
2	30	33
3	48	52
4	24	21

H,8,0

0	183	189
1	320	315
2	192	176
3	160	154
4	42	28
5	150	140
6	102	104
7	165	160
8	44	47
9	143	157
10	103	108
11	191	187
12	44	44
13	13*	10
14	44	53
15	67	70
16	39	46
17	41	47

H,8,1

1	191	191
2	97	103
3	160	154
4	64	58
5	185	193
6	103	106
7	161	161
8	70	66
9	68	64
10	74	80
11	52	51
12	57	54
13	97	98
14	92	89
15	25	25
16	23	21
17	45	50

H,8,2

0	116	110
1	208	205
2	31	20
3	199	202
4	56	50
5	175	174
6	128	114

H,8,2

7	73	69
8	113	117
9	83	85
10	75	70
11	87	88
12	15	19
13	19	15
14	31	30
15	58	60
16	77	79
17	14	15

H,8,3

1	221	231
2	56	53
3	282	289
4	137	128
5	130	133
6	206	203
7	100	92
8	72	78
9	156	163
10	105	110
11	133	133
12	37	35
13	30	36
14	48	51
15	53	63
16	44	44

H,8,4

0	443	436
1	127	122
2	85	87
3	71	72
4	46	33
5	93	89
6	188	189
7	45	51
8	71	71
9	167	165
10	32	26
11	68	70
12	41	43
13	42	41
14	26	23
15	30	30
16	73	82

H,8,5

1	110	104
2	188	187
3	41	35
4	101	102
5	201	208
6	39	38
7	92	97
8	81	80
9	106	105
10	56	50
11	48	43
12	33	36
13	83	89
14	28	24
15	31	40
16	18	18

H,8,6

0	76	69
1	131	123
2	174	177
3	68	68
4	83	81
5	107	116
6	108	100
7	95	95
8	98	101
9	75	77
10	69	74
11	64	64
12	78	82
13	43	45
14	27	29
15	82	90

H,8,7

1	86	84
2	70	72
3	94	93
4	55	59
5	92	90
6	48	48
7	71	69
8	111	114
9	23	26
10	21	19
11	37	37
12	19	16
13	58	57
14	52	48
15	31	32

H,8,8

0	178	188
1	76	74
2	79	76
3	27	35
4	58	58
5	84	81
6	38	36
7	39	43
8	66	67
9	91	81
10	36	36
11	75	70
12	55	59
13	43	42
14	27	27

H,8,9

1	102	97
2	99	99
3	150	151
4	93	92
5	62	65
6	14	14
7	127	129
8	73	75
9	97	102
10	24	27
11	88	89
12	74	72
13	10*	11

H,8,10

0	158	159
1	110	112
2	144	155
3	25	26
4	35	32
5	58	60
6	12*	7
7	107	108
8	23	22
9	75	81
10	22	26
11	21	18
12	10*	9

H,8,11

1	144	139
2	65	61
3	39	39
4	92	97
5	85	88
6	38	38
7	76	77
8	51	51
9	34	37
10	22	21
11	37	37

H,8,12

0	109	110
1	20	15
2	57	58
3	18	18
4	38	33
5	36	32
6	52	58
7	39	37
8	11*	6
9	43	48
10	13	15

H,8,13

1	20	16
2	59	59
3	15	15
4	53	56
5	52	54
6	28	29
7	21	21
8	17	13

H,8,14

0	89	87
1	14	7
2	37	41
3	43	42
4	27	22
5	12	14
6	9*	6

H,9,0

1	16	6
2	100	93
3	99	92
4	182	180
5	213	208
6	15	12
7	276	281
8	12*	11
9	13*	3
10	24	24
11	38	38
12	30	28
13	50	45
14	37	38
15	10*	3
16	16	15

H,9,1

0	282	288
1	72	67
2	223	214
3	151	153
4	145	144
5	187	195
6	118	119
7	138	148
8	24	27
9	30	27
10	102	107
11	42	39
12	30	29
13	32	32
14	12	15
15	23	24

H,10,2

0	261	264
1	148	143
2	126	129
3	186	183
4	80	75
5	173	163
6	203	205
7	34	29
8	147	141
9	125	129
10	128	128
11	86	87
12	101	107
13	48	48
14	67	67
15	22	21

H,10,3

1	101	99
2	255	243
3	58	59
4	136	133
5	134	132
6	40	29
7	117	118
8	160	158
9	55	56
10	130	132
11	89	94
12	74	79
13	75	76
14	24	21
15	71	69

H,10,4

0	229	221
1	223	219
2	151	153
3	94	97
4	219	220
5	29	38
6	82	84
7	103	97
8	97	95
9	181	191
10	36	31
11	89	87
12	83	86
13	51	50
14	66	65
15	32	37
16	23	24

H,9,2

1	79	61
2	113	117
3	28	21
4	176	181
5	265	269
6	218	222
7	105	92
8	86	88
9	206	206
10	34	31
11	26	24
12	59	58
13	46	42
14	28	29
15	49	52
16	22	25

H,9,3

0	31	33
1	15	16
2	111	113
3	95	97
4	24	17
5	82	80
6	103	92
7	61	64
8	162	155
9	86	82
10	86	90
11	127	135
12	29	36
13	98	103
14	36	38
15	32	32
16	51	55

H,9,4

1	196	186
2	60	61
3	43	33
4	59	62
5	43	43
6	107	109
7	108	111
8	83	84
9	30	32
10	112	116
11	61	63

H,9,4

12	72	72
13	66	72
14	38	39
15	17	22

H,9,5

0	117	121
1	52	46
2	110	116
3	196	203
4	114	113
5	41	32
6	118	120
7	40	39
8	86	78
9	27	23
10	94	94
11	45	48
12	24	26
13	24	23
14	54	62
15	19	26

H,9,6

1	42	41
2	141	139
3	115	113
4	82	82
5	72	71
6	31	27
7	70	65
8	122	128
9	82	87
10	64	71
11	66	70
12	37	40
13	27	29
14	44	46

H,9,7

0	91	95
1	28	32
2	98	96
3	58	63
4	49	53
5	54	45
6	82	80
7	138	139
8	29	28
9	54	57
10	66	63
11	69	74
12	34	32
13	10*	8
14	38	39

H,9,8

1	46	36
2	65	61
3	37	42
4	157	157
5	72	66
6	33	35
7	91	89
8	81	81
9	69	74
10	47	47
11	16	22
12	74	71
13	43	42

H,9,9

0	158	156
1	24	17
2	33	32
3	47	51
4	64	62
5	12*	8
6	92	86
7	113	116
8	83	87
9	15	18
10	11*	11
11	30	27
12	34	35

H,9,10

1	108	105
2	60	64
3	56	56
4	79	84
5	15	16
6	51	51
7	20	24
8	24	24
9	34	31
10	74	78
11	36	35

H,9,11

0	83	78
1	42	42
2	87	87
3	37	32
4	50	47
5	17	17
6	46	46
7	13	18
8	51	56
9	25	26
10	65	64

H,9,12

1	63	70
2	22	21
3	28	31
4	35	36
5	24	23
6	34	36
7	10*	5
8	35	35
9	19	24

H,9,13

0	79	78
1	53	55
2	55	58
3	33	29
4	43	45
5	26	25
6	38	40
7	20	19

H,9,14

1	39	36
2	22	24
3	11	18

H,10,0

0	183	195
1	538	540
2	120	121
3	144	142
4	117	118
5	188	184
6	210	208
7	150	158
8	12*	5
9	21	18
10	89	91
11	104	100
12	30	36
13	38	35
14	39	47
15	25	21

H,10,1

1	53	47
2	246	249
3	173	166
4	297	295
5	136	143
6	172	167
7	84	78
8	121	123
9	109	115
10	93	98
11	41	35
12	89	87
13	30	31
14	12*	16
15	37	43
16	23	24

H,9,5

1	129	132
2	147	147
3	103	100
4	226	230
5	78	89
6	85	83
7	78	80
8	46	61
9	52	55
10	44	50
11	67	68
12	64	67
13	42	45
14	9*	11

H,10,6

0	47	39
1	44	36
2	45	53
3	75	88
4	208	201
5	135	136
6	169	178
7	36	33
8	17	21
9	85	96
10	25	22
11	39	45
12	40	36
13	10*	11
14	19	23

H,10,7

1	147	156
2	75	80
3	77	78
4	110	122
5	66	64
6	109	114
7	145	150
8	105	107
9	25	29
10	69	67
11	11*	5
12	22	22
13	36	35

H,10,8

0	147	147
1	67	70
2	129	134
3	31	31

7,14,L

2	63	62

8,0,L

-18	43	46
-16	32	21
-14	180	179
-12	213	213
-10	212	212
-8	144	152
-6	209	207
-4	394	385
-2	153	147
0	205	186
2	185	183
4	127	126
6	33	36
8	138	141
10	125	128
12	33	41
14	37	47

8,1,L

-18	22	20
-17	33	28
-16	31	31
-15	24	16
-14	109	107
-13	167	173
-12	39	30
-11	331	336
-10	31	24
-9	324	324
-8	51	50
-7	361	363
-6	122	122
-5	101	90
-4	86	90
-3	68	58
-2	174	159
-1	178	175
0	129	123
1	40	40
2	20	22
3	116	107
4	50	53
5	175	174
6	177	188
7	206	206
8	116	113
9	101	99
10	23	11
11	63	62
12	87	94
13	23	27
14	31	37

8,2,L

-18	17*	9
-17	55	50
-16	113	107
-15	144	141
-14	29	21
-13	64	68
-12	48	49
-11	156	163
-10	239	247
-9	19*	13
-8	22	17
-7	23	21
-6	47	46
-5	16*	7
-4	94	112
-3	194	190
-2	309	309
-1	77	82
0	178	163
1	67	53
2	274	272
3	29	40
4	53	59
5	44	46
6	75	77
7	20*	3
8	94	92
9	27	23
10	50	57
11	17*	9
12	54	44
13	101	104
14	61	59

8,3,L

-18	17*	23
-17	16*	0
-16	18*	19
-15	20*	13
-14	280	292
-13	81	81
-12	418	428
-11	64	57
-10	198	207
-9	19*	11
-8	18*	12
-7	74	71
-6	108	103
-5	224	228
-4	187	180
-3	29	26
-2	627	615
-1	28	30
0	261	253
1	132	118
2	237	223
3	150	159

8,4,L

-17	42	52
-16	28	30
-15	181	191
-14	47	48
-13	65	70
-12	39	31
-11	317	322
-10	119	121
-9	115	114
-8	102	114
-7	57	58
-6	26	28
-5	40	28
-4	39	59
-3	129	130
-2	81	68
-1	18*	11
0	231	234
1	36	25
2	164	166
3	330	335
4	81	79
5	39	44
6	62	62
7	101	109
8	38	42
9	25	22
10	68	62
11	101	102
12	52	60
13	17*	5
14	26	24

8,5,L

-17	63	66
-16	19	19
-15	44	40
-14	185	188
-13	71	72
-12	284	292
-11	19*	14
-10	19*	23
-9	81	76
-8	25	11
-7	93	91

8,6,L

-16	38	37
-15	19	15
-14	124	117
-13	67	66
-12	19*	15
-11	63	67
-10	33	31
-9	73	69
-8	23	15
-7	168	182
-6	46	40
-5	89	96
-4	74	77
-3	57	59
-2	121	120
-1	103	119
0	81	75
1	506	514
2	286	293
3	237	232
4	94	96
5	213	225
6	58	55
7	174	179
8	55	58
9	105	104
10	74	80
11	83	90
12	162	178
13	46	49

8,7,L

-16	60	52
-15	28	28
-14	31	29
-13	100	94

8,8,L

-15	16*	5
-14	20	30
-13	29	28
-12	95	88
-11	24	30
-10	36	40
-9	116	120
-8	31	32
-7	206	200
-6	26	24
-5	96	93
-4	81	78
-3	178	183
-2	57	59
-1	87	90
0	152	152
1	187	195
2	223	223
3	280	283
4	26	23
5	18*	2
6	25	22
7	155	161
8	166	176
9	18*	10
10	17*	9
11	22	32

8,9,L

-14	17*	13

8,9,L

-13	88	79
-12	43	38
-11	57	68
-10	19*	22
-9	79	93
-8	96	112
-7	76	84
-6	200	217
-5	63	77
-4	64	68
-3	202	213
-2	24	1
-1	68	69
0	47	49
1	45	52
2	41	41
3	93	101
4	138	136
5	43	39
6	172	178
7	19*	17
8	103	108
9	30	31
10	17*	14

8,10,L

-13	42	45
-12	25	30
-11	46	49
-10	129	126
-9	100	107
-8	99	113
-7	47	46
-6	34	39
-5	138	149
-4	46	50
-3	45	40
-2	283	290
-1	72	70
0	156	158
1	141	140
2	174	175
3	53	52
4	93	98
5	69	65
6	55	63
7	46	47
8	106	109
9	46	46

8,11,L

-11	101	104
-10	26	19
-9	23	19
-8	34	45
-7	124	140

8,12,L

-8	47	40
-8	159	163
-7	54	49
-6	48	47
-5	18*	7
-4	136	131
-3	146	148
-2	107	112
-1	70	79
0	53	48
1	19	18
2	30	33
3	98	94
4	70	80
5	71	76

8,13,L

-6	16*	17
-5	16*	3
-4	65	67
-3	50	54
-2	35	41
-1	101	96
0	17*	17
1	40	45
2	94	91

9,0,L

-17	60	67
-15	57	44
-13	190	201
-11	57	61
-9	511	521
-7	88	80
-5	166	172
-3	129	120
-1	17*	7
1	376	374
3	364	365
5	204	209
7	145	149

9,1,L

-17	17*	5
-16	62	58
-15	40	40
-14	28	20
-13	133	140
-12	216	212
-11	78	79
-10	282	285
-9	202	201
-8	190	195
-7	167	166
-6	96	98
-5	109	111
-4	120	123
-3	140	143
-2	84	72
-1	40	43
0	290	288
1	19*	3
2	45	49
3	41	40
4	221	218
5	19*	9
6	64	65
7	115	112
8	116	112
9	123	127
10	34	25
11	23	22
12	20	13
13	24	19

9,2,L

-17	73	77
-16	17*	2
-15	67	64
-14	76	73
-13	209	204
-12	252	256
-11	28	27
-10	337	342
-9	114	112
-8	121	121
-7	36	36
-6	59	68
-5	168	175
-4	118	124
-3	86	72
-2	142	144
-1	147	142
0	160	147
1	352	358
2	18*	8
3	176	182
4	34	32
5	73	70
6	189	190
7	80	85
8	23	19
9	18*	4
10	18*	5
11	66	68
12	43	44
13	62	68

9,3,L

-17	38	40
-16	24	22
-15	34	32
-14	24	24
-13	20*	13
-12	25	23
-11	116	124
-10	19*	12
-9	54	48
-8	21	11
-7	76	85
-6	18*	0
-5	109	106
-4	17*	3
-3	178	165
-2	55	52
-1	168	167
0	18*	11
1	32	34
2	232	225
3	180	174
4	161	167
5	158	175
6	31	28
7	140	144
8	46	34
9	196	203
10	101	97
11	17*	5
12	16*	5

9,4,L

-16	33	39
-15	88	92
-14	141	143
-13	97	96
-12	40	48
-11	136	130
-10	51	50
-9	60	63
-8	18*	12
-7	18*	2
-6	116	134
-5	85	84
-4	46	52

-3	29	25
-2	81	84
-1	59	74
0	107	106
1	156	153
2	167	153
3	52	45
4	129	135
5	32	27
6	396	408
7	70	74
8	180	186
9	66	64
10	39	47
11	30	20
12	16*	15

9,5,L

-16	96	96
-15	74	74
-14	54	51
-13	18*	2
-12	124	127
-11	66	69
-10	139	138
-9	111	116
-8	121	123
-7	45	43
-6	121	116
-5	20*	19
-4	209	204
-3	24	16
-2	131	133
-1	86	93
0	164	171
1	175	168
2	44	51
3	66	58
4	258	261
5	27	33
6	205	208
7	18*	3
8	104	110
9	175	182
10	151	164
11	65	70
12	90	101

9,6,L

-15	128	126
-14	65	73
-13	110	113
-12	17*	7
-11	68	70
-10	91	92
-9	19*	4
-8	118	125

9,6,L

-7	138	140
-6	87	99
-5	35	36
-4	113	117
-3	123	120
-2	82	86
-1	172	179
0	65	73
1	198	208
2	140	131
3	351	347
4	39	34
5	77	75
6	118	126
7	272	281
8	27	32
9	19*	24
10	91	90
11	36	42

9,7,L

-14	23	17
-13	70	67
-12	92	103
-11	18*	12
-10	52	53
-9	71	65
-8	54	63
-7	68	81
-6	104	85
-5	67	64
-4	31	37
-3	41	40
-2	18*	12
-1	154	154
0	92	91
1	161	162
2	62	72
3	39	41
4	319	323
5	171	173
6	43	36
7	54	60
8	42	43
9	62	64
10	38	50

9,8,L

-13	78	75
-12	90	92
-11	116	124
-10	242	246
-9	133	143
-8	211	217
-7	44	49
-6	18*	1

10,5,L

-3	106	104
-2	258	272
-1	69	71
0	139	142
1	26	31
2	97	94
3	197	199
4	55	55
5	208	202
6	104	106
7	77	81
8	160	169
9	19*	28

10,6,L

-13	79	83
-12	46	49
-11	61	58
-10	96	112
-9	18*	7
-8	70	84
-7	45	48
-6	19*	27
-5	53	56
-4	45	61
-3	120	129
-2	124	126
-1	84	86
0	49	52
1	100	102
2	177	177
3	53	45
4	19*	11
5	130	131
6	18*	2
7	52	51
8	46	49
9	114	123

10,7,L

-13	44	52
-12	68	67
-11	75	76
-10	19	14
-9	63	66
-8	54	54
-7	160	174
-6	18*	4
-5	52	54
-4	19	12
-3	90	106
-2	18*	7
-1	39	38
0	38	45
1	103	106
2	74	81

-5	55	41
-4	19*	14
-3	19*	9
-2	105	101
-1	19*	2
0	19*	8
1	128	134
2	63	55
3	62	62
4	106	104
5	96	91
6	43	47
7	19*	15
8	46	42
9	92	95

9,9,L

-12	17*	19
-11	24	18
-10	77	75
-8	84	86
-8	58	61
-7	154	163
-6	126	136
-5	113	108
-4	49	44
-3	26	16
-2	95	97
-1	87	74
0	41	42
1	80	81
2	208	205
3	86	88
4	18*	13
5	129	134
6	135	138
7	18*	12
8	35	28

9,10,L

-11	17*	6
-10	105	110
-9	95	97
-8	42	34
-7	61	62
-6	18*	6
-5	25	22
-4	34	27
-3	19*	16
-2	100	97
-1	23	10
0	19*	3
1	40	41
2	32	41
3	147	147
4	41	42
5	91	88
6	17*	7

3	193	183
4	56	62
5	70	66
6	53	51
7	19	18
8	105	112

10,8,L

-11	58	56
-10	18*	3
-9	79	84
-8	18*	0
-7	155	157
-6	137	148
-5	68	66
-4	47	49
-3	162	171
-2	69	67
-1	79	79
0	80	85
1	19*	20
2	70	67
3	18*	2
4	81	78
5	54	50
6	18	11
7	120	125

10,9,L

-10	27	31
-9	17*	5
-8	97	87
-7	47	49
-6	65	56
-5	80	75
-4	56	62
-3	19	3
-2	84	95
-1	67	68
0	80	84
1	108	112
2	71	63
3	155	155
4	70	76
5	85	89

10,10,L

-8	68	72
-7	16*	7
-6	36	35
-5	21	20
-4	116	116
-3	32	21
-2	71	73
-1	18*	5
0	25	23
1	66	70

7	17*	9

9,11,L

-9	33	29
-8	64	64
-7	68	70
-6	17*	12
-5	63	68
-4	33	39
-3	17*	14
-2	73	70
-1	29	37
0	127	126
1	101	98
2	113	110
3	19	20
4	32	38

9,12,L

-6	16*	3
-5	16*	1
-4	22	18
-3	17*	6
-2	57	60
-1	18	20
0	50	53
1	16*	15

10,0,L

-16	24	18
-14	17*	7
-12	46	50
-10	257	259
-8	96	102
-6	230	236
-4	318	320
-2	41	43
0	313	321
2	268	265
4	215	218
6	149	160
8	57	57
10	137	137

10,1,L

-16	24	19
-15	122	122
-14	17*	8
-13	138	140
-12	175	175
-11	154	146
-10	28	24
-9	176	178
-8	39	33
-7	366	373
-6	19*	10

2	38	47
3	69	72

10,11,L

-3	16*	14
-2	17*	14
-1	26	28

11,0,L

-13	18*	6
-11	144	143
-9	69	64
-7	49	59
-5	24	36
-3	185	195
-1	161	154
1	88	86
3	35	44
5	157	156
7	42	32
9	16*	3

11,1,L

-14	49	44
-13	114	114
-12	170	176
-11	65	73
-10	70	62
-9	103	99
-8	78	81
-7	39	34
-6	51	54
-5	84	84
-4	37	41
-3	159	157
-2	64	60
-1	46	57
0	20*	19
1	102	99
2	48	46
3	18*	13
4	30	33
5	47	53
6	53	53
7	172	176
8	122	124
9	50	51

11,2,L

-14	35	36
-13	130	124
-12	46	37
-11	18*	6
-10	19*	15
-9	199	196
-8	19*	0

-5	21	31
-4	75	82
-3	184	183
-2	276	282
-1	204	199
0	230	219
1	81	80
2	124	119
3	226	217
4	46	44
5	132	133
6	179	184
7	19*	7
8	43	44
9	21	26
10	51	51
11	28	32

10,2,L

-15	16*	3
-14	93	88
-13	89	91
-12	18*	2
-11	93	91
-10	220	222
-9	142	145
-8	175	183
-7	171	172
-6	87	94
-5	234	250
-4	43	40
-3	32	36
-2	39	35
-1	116	112
0	133	132
1	25	30
2	124	121
3	26	18
4	50	54
5	166	180
6	137	142
7	125	128
8	109	115
9	41	43
10	17*	3
11	57	57

10,3,L

-15	19	14
-14	32	36
-13	151	154
-12	103	101
-11	83	83
-10	161	166
-9	18*	9
-8	49	47
-7	61	73
-6	19	17

-7	68	70
-6	219	214
-5	53	53
-4	139	140
-3	113	113
-2	67	64
-1	38	37
0	111	108
1	103	98
2	108	120
3	145	154
4	173	172
5	39	53
6	18*	19
7	53	60
8	123	122

11,3,L

-13	17*	14
-12	135	133
-11	18*	10
-10	239	245
-9	169	168
-8	79	84
-7	72	68
-6	20*	17
-5	50	48
-4	105	98
-3	127	134
-2	19*	8
-1	106	98
0	66	70
1	18*	10
2	33	34
3	81	81
4	59	56
5	195	192
6	18*	11
7	66	73
8	73	81

11,4,L

-13	97	95
-12	43	45
-11	112	106
-10	46	47
-9	17*	15
-8	135	146
-7	18*	9
-6	29	31
-5	42	40
-4	113	113
-3	25	21
-2	19*	15
-1	18*	2
0	53	52
1	36	33
2	80	87

-5	65	67
-4	236	254
-3	186	184
-2	89	100
-1	35	42
0	104	89
1	115	107
2	57	54
3	76	74
4	18*	3
5	157	160
6	22	18
7	118	114
8	178	181
9	48	49
10	97	111

10,4,L

-15	55	54
-14	77	78
-13	92	99
-12	99	104
-11	175	176
-10	52	51
-9	18*	10
-8	49	53
-7	154	145
-6	40	37
-5	114	120
-4	48	50
-3	112	114
-2	66	64
-1	212	215
0	189	195
1	34	32
2	91	92
3	118	116
4	64	69
5	175	184
6	117	121
7	190	191
8	119	126
9	17*	15
10	95	96

10,5,L

-14	43	34
-13	100	108
-12	114	120
-11	32	30
-10	41	48
-9	71	69
-8	26	27
-7	52	55
-6	25	22
-5	166	178
-4	39	47

3	30	30
4	18*	6
5	166	176
6	213	222
7	84	83

11,5,L

-12	17*	4
-11	51	54
-10	57	54
-9	85	86
-8	59	58
-7	18*	3
-6	36	45
-5	112	112
-4	40	32
-3	18*	3
-2	134	136
-1	94	94
0	252	258
1	89	90
2	95	97
3	40	51
4	115	125
5	164	171
6	84	86
7	25	31

11,6,L

-11	18*	24
-10	44	43
-9	103	106
-8	22	18
-7	17*	0
-6	41	39
-5	71	73
-4	162	171
-3	60	65
-2	103	110
-1	41	45
0	68	66
1	18*	3
2	65	65
3	137	138
4	24	10
5	175	181
6	154	160

11,7,L

-10	34	30
-9	17*	7
-8	50	54
-7	23	30
-6	39	46
-5	143	141
-4	21	21

11,7,L

-3	90	91
-2	35	25
-1	33	34
0	63	67
1	18*	7
2	54	56
3	92	92
4	18*	24
5	82	88

11,8,L

-8	80	83
-7	32	33
-6	16*	2
-5	61	65
-4	142	146
-3	50	58
-2	117	128
-1	17*	10
0	52	52
1	17*	7
2	18	19
3	17*	15

11,9,L

-5	89	93
-4	17*	15
-3	114	111
-2	62	68
-1	17*	9
0	131	130

12,0,L

-10	147	169
-8	269	300
-6	53	70
-4	98	96
-2	133	132
0	20*	21
2	55	52
4	195	201

12,1,L

-11	17*	13
-10	18*	11
-9	54	48
-8	19*	27
-7	161	171
-6	172	174
-5	173	180
-4	22	11
-3	115	119
-2	19	22
-1	59	56
0	89	88
1	31	37
2	18*	15
3	19	15
4	48	55
5	54	51

12,2,L

-11	17*	6
-10	61	66
-9	154	157
-8	153	155
-7	171	173
-6	95	96
-5	33	27
-4	18*	11
-3	29	25
-2	19*	12
-1	151	150
0	18*	1
1	44	49
2	190	191
3	63	73
4	38	45
5	78	81

12,3,L

-10	92	96
-9	18*	8
-8	18*	5
-7	18*	10
-6	141	150
-5	17*	3
-4	198	205
-3	18*	11
-2	38	34
-1	30	31
0	61	53
1	17*	2
2	22	27
3	76	78
4	82	79
5	17*	11

12,4,L

-10	90	94
-9	19	12
-8	20	12
-7	105	109
-6	63	73
-5	41	49
-4	18*	18
-3	46	44
-2	18*	5
-1	72	70
0	23	22
1	196	202
2	32	30
3	103	109
4	18*	17

12,5,L

-9	22	21
-8	49	58
-7	17*	6
-6	110	121
-5	64	69
-4	18*	12
-3	140	149
-2	17*	5
-1	81	77
0	17*	6
1	18*	7
2	75	67
3	44	35

12,6,L

-7	46	47
-6	103	102
-5	69	73
-4	109	112
-3	54	54
-2	21	19
-1	110	112
0	89	93
1	139	146

12,7,L

-4	16*	0
-3	111	119
-2	57	52

13,0,L

-5	17*	14
-3	56	57
-1	73	70

13,1,L

-6	66	79
-5	38	46
-4	17*	3
-3	60	56
-2	32	38
-1	18	29
0	89	85

13,2,L

-5	88	86
-4	16*	1
-3	20	16
-2	78	81
-1	19	19

13,3,L

-3	64	70

APPENDIX X

Tables of observed and calculated structure factors for 5,18-dimethyl-5,18-dihydrotribenzo[*b*,*f*,*j*][1,4] diazacyclododecine-6,17-dione

Data Format:

	H	L
K	$10\times\|F_o\|$	$10\times\|F_c\|$

Reflections removed for extinction marked .... E

Reflections classed as unobserved marked ..... *

0,K,0

2	56	60
4	577	649
6	740	815
8	786	852
10	278	266
12	155	144
14	68	82
16	53	43
18	288	276
20	41	34
22	379	378
24	70	82
26	54	51
28	46	52
30	72	82
32	104	102
34	82	79

1,K,0

1	142	133
2	713E	872
3	386	396
4	214	204
5	51	36
6	308	283
7	114	117
8	177	185
9	359	337
10	249	240
11	289	271
12	12	6
13	279	263
14	352	319
15	174	147
16	13	10
17	81	79
18	160	165
19	204	193
20	293	284
21	16	18
22	233	225
23	103	98
24	74	75
25	49	46
26	133	137
27	125	128
28	11	2
29	10	9
30	101	97
31	79	84
32	73	69
33	22	20
34	41	50

2,K,0

0	610E	724

9,K,0

1	341	344
2	174	178
3	29	21
4	39	41
5	55	48
6	171	171
7	53	56
8	8*	13
9	97	95
10	9	17
11	14	9
12	8*	2
13	86	88
14	74	83
15	11	10
16	113	114
17	8*	8
18	44	51
19	70	73
20	11	4
21	76	78
22	57	50
23	7*	5
24	18	22
25	62	58

10,K,0

0	25	20
1	151	158
2	159	161
3	14	8
4	274	275
5	153	153
6	55	53
7	148	161
8	146	142
9	8*	11
10	62	70
11	52	55
12	24	15
13	56	59
14	39	42
15	28	28
16	29	31
17	38	41
18	16	16
19	48	48
20	32	32
21	12	10
22	16	15

11,K,0

1	50	48
2	28	28
3	99	101
4	59	62
5	52	60
6	102	110
7	25	21
8	33	31
9	29	38
10	11	2
11	44	40
12	15	10
13	31	32
14	27	27
15	21	19
15	22	28
17	6*	7
18	88	96

12,K,0

0	88	90
1	26	20
2	87	87
3	18	15
4	54	59
5	7*	6
6	11	13
7	6*	0
8	38	47
9	9	14
10	10	14
11	128	137
12	13	17
13	17	13
14	38	37

13,K,0

1	17	23
2	88	81
3	25	21
4	10	2
5	18	16

0,K,1

1	784E	904
3	594	648
5	547	559
7	852E	948
9	316	312
11	967	1039
13	504	498
15	290	280
17	183	156
19	251	231
21	51	57
23	247	250
25	109	107
27	174	180
29	100	103
31	17	20
33	151	155
1	314	324
2	532	572
3	250	243
4	348	336
5	176	156
6	161	168
7	891	944
8	355	337
9	146	146
10	166	171
11	427	398
12	192	182
13	6*	2
14	111	90
15	12	7
16	243	232
17	110	109
18	183	167
19	191	181
20	185	177
21	59	59
22	176	176
23	251	252
24	331	333
25	420	424
26	148	145
27	123	126
28	222	227
29	16	11
30	18	11
31	21	30
32	9	20
33	12	15
34	32	32

3,K,0

1	457	463
2	420	433
3	254	235
4	278	288
5	891	950
6	419	421
7	32	49
8	189	158
9	128	116
10	91	91
11	320	305
12	238	218
13	253	234
14	141	137
15	74	79
16	145	140
17	258	266
18	216	192
19	44	34
20	234	234
21	85	88
22	107	112
23	48	46
24	106	108
25	52	48
26	118	122
27	187	192
28	149	152
29	22	23
30	78	85
31	74	73
32	96	98
33	138	145

4,K,0

0	215	221
1	316	299
2	63	52
3	690	709
4	10	7
5	295	266
6	35	20
7	164	157
8	311	298
9	193	180
10	295	276
11	25	16
12	273	256
13	75	60
14	156	154
15	9	6
16	27	20
17	99	102
18	229	233
19	137	123
20	287	277
21	47	41
22	36	38
23	39	32
24	53	52
25	214	213
26	99	95
27	102	111
28	30	27
29	151	153
30	108	104
31	38	37
32	96	96
33	16	20

5,K,0

1	223	224
2	382	373
3	339	319
4	542	542
5	54	68
6	293	272
7	510	509
8	94	83
9	422	406
10	33	42

1,K,1

1	646E	763
2	743E	884
3	1050E	1367
4	301	284
5	78	66
6	917E	1013
7	278	259
8	410	416
9	327	327
10	93	81
11	322	308
12	196	180
13	375	361
14	208	199
15	78	79
16	55	49
17	164	151
18	144	129
19	74	75
20	117	116
21	73	63
22	110	108
23	71	68
24	156	151
25	52	56
26	212	219
27	212	215
28	46	54
29	138	138
30	22	19
31	68	66
32	27	29
33	6*	4
34	47	48

2,K,1

0	476	526
1	205	197
2	540	569
3	594	626
4	688	729
5	710	747
6	217	203
7	148	134
8	440	435
9	267	256
10	158	147
11	492	480
12	86	80
13	16	6
14	365	352
15	213	195
16	201	176
17	128	121
18	236	231
19	315	308
20	194	192
11	10	11
12	125	125
13	36	32
14	192	196
15	143	128
16	7*	5
17	43	46
18	7*	7
19	46	44
20	179	179
21	139	139
22	20	14
23	19	21
24	114	110
25	57	63
26	45	48
27	7*	2
28	33	41
29	110	111
30	23	21
31	17	14
32	22	23

6,K,0

0	121	100
1	217	201
2	82	80
3	48	19
4	70	57
5	127	137
6	53	40
7	380	348
8	91	88
9	27	11
10	292	275
11	109	113
12	54	48
13	130	131
14	102	95
15	111	102
16	158	160
17	8*	0
18	136	138
19	327	333
20	11	4
21	205	206
22	363	368
23	54	50
24	121	120
25	68	54
26	36	39
27	128	134
28	29	31
29	12	15
30	112	115

7,K,0

1	19	7
21	163	157
22	184	180
23	110	117
24	55	54
25	165	163
26	158	150
27	133	126
28	35	32
29	25	18
30	48	57
31	34	46
32	60	66
33	15	10

3,K,1

1	368	368
2	215	203
3	182	177
4	474	477
5	77	68
6	580	588
7	461	459
8	357	337
9	274	257
10	74	78
11	333	301
12	168	168
13	135	116
14	267	246
15	225	219
16	292	289
17	126	113
18	84	81
19	96	93
20	87	78
21	219	218
22	257	257
23	157	150
24	148	154
25	23	21
26	157	160
27	89	91
28	56	58
29	55	53
30	92	97
31	108	117
32	40	41
33	54	54

4,K,1

0	461	470
1	316	311
2	248	234
3	226	204
4	128	122
5	347	314
6	432	404
7	197	184
2	32	28
3	20	14
4	27	24
5	154	139
6	239	232
7	350	355
8	127	122
9	79	79
10	76	68
11	34	39
12	68	75
13	71	66
14	28	30
15	45	43
16	256	264
17	74	82
18	65	64
19	67	65
20	28	29
21	171	173
22	61	62
23	32	29
24	65	69
25	127	133
26	61	62
27	32	34
28	24	29
29	194	189

8,K,0

0	26	20
1	31	38
2	185	175
3	228	227
4	146	146
5	112	110
6	275	272
7	203	190
8	49	49
9	218	218
10	71	77
11	9	12
12	88	92
13	18	17
14	80	72
15	170	187
16	83	90
17	197	201
18	82	76
19	91	86
20	170	174
21	85	85
22	61	67
23	73	74
24	14	17
25	11	11
26	16	22
27	70	78
8	14	27
9	459	432
10	147	128
11	217	200
12	139	129
13	161	158
14	279	267
15	148	125
16	43	33
17	48	45
18	190	185
19	174	171
20	181	174
21	170	168
22	227	223
23	111	107
24	145	145
25	110	105
26	67	73
27	68	70
28	76	76
29	64	62
30	31	33
31	64	61
32	24	24

5,K,1

1	307	295
2	440	439
3	388	375
4	263	248
5	154	149
6	225	203
7	215	195
8	144	137
9	104	99
10	311	283
11	145	135
12	96	85
13	48	48
14	14	13
15	132	132
16	112	110
17	191	185
18	217	208
19	190	184
20	228	227
21	75	78
22	8*	5
23	54	48
24	63	61
25	46	49
26	49	48
27	87	91
28	57	59
29	32	34
30	37	38

5,K,1

31	29	21

6,K,1

0	335	327
1	216	219
2	139	126
3	85	86
4	176	161
5	123	122
6	176	175
7	207	185
8	144	130
9	135	124
10	144	131
11	136	133
12	114	112
13	11	12
14	192	196
15	72	72
16	51	42
17	115	114
18	80	75
19	124	126
20	253	262
21	150	145
22	81	84
23	61	60
24	48	46
25	51	49
26	67	65
27	36	37
28	72	76
29	32	33
30	63	65

7,K,1

1	35	27
2	158	148
3	69	66
4	171	168
5	275	274
6	202	203
7	178	177
8	149	144
9	89	88
10	192	188
11	114	107
12	38	38
13	44	45
14	86	90
15	137	142
16	131	131
17	259	271
18	249	246
19	165	166
20	8	7

3,K,2

9	285	279
10	284	259
11	228	209
12	131	120
13	167	146
14	109	102
15	419	395
16	61	56
17	184	174
18	139	130
19	82	78
20	149	157
21	207	205
22	106	99
23	201	206
24	53	52
25	72	72
26	115	117
27	63	60
28	90	91
29	43	46
30	29	27
31	13	6
32	28	21

4,K,2

0	399	394
1	87	56
2	98	86
3	203	165
4	192	172
5	93	94
6	203	185
7	84	79
8	194	181
9	76	74
10	148	138
11	188	181
12	223	199
13	100	96
14	155	153
15	42	51
16	229	221
17	104	98
18	96	90
19	188	193
20	134	129
21	64	63
22	84	92
23	28	29
24	116	116
25	51	50
26	34	36
27	20	15
28	71	72
29	45	45
30	20	15

21	110	109
22	82	79
23	142	149
24	93	99
25	58	61
26	33	35
27	40	46
28	106	110

8,K,1

0	169	166
1	116	117
2	79	87
3	211	211
4	217	216
5	183	183
6	17	7
7	74	71
8	42	41
9	27	29
10	7*	9
11	77	79
12	56	56
13	111	112
14	154	153
15	30	27
16	86	83
17	134	132
18	156	160
19	41	44
20	101	106
21	23	27
22	37	41
23	32	33
24	28	26
25	115	117
26	32	34
27	100	108

9,K,1

1	158	167
2	67	70
3	69	69
4	67	66
5	76	74
6	130	138
7	186	186
8	193	200
9	134	135
10	207	216
11	75	76
12	119	123
13	52	59
14	94	92
15	111	117
16	54	53
17	46	49
18	42	41

31	59	57

5,K,2

1	122	102
2	127	104
3	68	39
4	293	286
5	25	18
6	153	131
7	153	128
8	153	150
9	266	250
10	111	108
11	121	115
12	258	256
13	246	247
14	220	207
15	141	142
16	193	191
17	258	261
18	101	95
19	190	185
20	120	111
21	57	57
22	61	55
23	128	128
24	54	50
25	47	43
26	86	86
27	76	79
28	52	55
29	42	42
30	71	67

6,K,2

0	168	164
1	74	54
2	104	102
3	36	36
4	209	214
5	71	60
6	109	109
7	55	17
8	49	47
9	212	206
10	260	248
11	128	130
12	180	172
13	144	136
14	65	66
15	79	80
16	98	90
17	157	155
18	62	64
19	75	72
20	75	70
21	95	92
22	75	65

19	96	100
20	10	11
21	44	46
22	107	107
23	10	11
24	41	43

10,K,1

0	259	258
1	127	117
2	28	31
3	132	132
4	154	160
5	44	36
6	98	103
7	122	130
8	97	101
9	38	41
10	100	101
11	59	59
12	136	141
13	64	69
14	35	34
15	29	29
16	48	42
17	60	66
18	16	17
19	10	8
20	50	53
21	36	35
22	29	27

11,K,1

1	102	99
2	75	75
3	92	92
4	29	31
5	60	60
6	34	38
7	98	101
8	42	47
9	46	47
10	62	62
11	37	41
12	30	33
13	64	71
14	39	44
15	38	44
16	30	26
17	35	36
18	39	42

12,K,1

0	70	76
1	58	56
2	42	40
3	47	48
23	49	48
24	48	45
25	12	5
26	83	89
27	21	18
28	42	43
29	41	48

7,K,2

1	84	90
2	58	63
3	106	109
4	227	220
5	205	210
6	257	263
7	83	68
8	161	159
9	102	101
10	169	173
11	157	157
12	103	97
13	52	52
14	66	67
15	37	35
16	152	148
17	191	198
18	122	121
19	78	79
20	106	110
21	60	63
22	70	70
23	49	49
24	104	116
25	57	55
26	38	36
27	34	35

8,K,2

0	193	201
1	169	175
2	153	147
3	136	141
4	193	194
5	211	216
6	110	95
7	121	117
8	116	120
9	208	207
10	79	78
11	101	99
12	61	55
13	135	138
14	74	77
15	113	119
16	173	174
17	98	92
18	25	26
19	127	126

4	36	31
5	39	41
6	46	47
7	49	51
8	38	42
9	36	30
10	22	24
11	40	39
12	47	51
13	69	74

13,K,1

1	15	17
2	71	67

0,K,2

0	1113E	1570
2	345	356
4	615	627
6	252	220
8	513	512
10	635	642
12	593	602
14	138	168
16	138	125
18	57	45
20	108	101
22	142	126
24	126	138
26	60	64
28	109	105
30	78	86
32	69	74

1,K,2

1	431	444
2	308	280
3	727	780
4	197	188
5	172	173
6	270	252
7	413	402
8	221	211
9	319	296
10	547	535
11	221	212
12	153	138
13	148	131
14	156	131
15	68	66
16	246	240
17	150	147
18	121	114
19	98	87
20	130	126
21	41	38
22	92	81
20	48	48
21	54	59
22	17	20
23	10	6
24	22	23
25	35	39

9,K,2

1	184	187
2	186	191
3	215	221
4	162	167
5	116	121
6	92	102
7	59	53
8	149	146
9	66	68
10	60	66
11	36	37
12	41	43
13	97	98
14	102	105
15	82	83
16	57	55
17	123	129
18	67	75
19	43	45
20	70	77
21	73	74
22	106	108
23	40	43

10,K,2

0	108	106
1	76	74
2	71	71
3	26	26
4	97	91
5	37	29
6	132	136
7	55	53
8	29	22
9	50	56
10	42	42
11	42	41
12	40	39
13	44	37
14	20	18
15	53	49
16	42	40
17	64	68
18	43	43
19	53	50
20	56	54

11,K,2

1	66	62

23	84	76
24	107	110
25	158	159
26	191	193
27	71	71
28	53	50
29	37	42
30	71	73
31	34	36
32	92	94
33	45	49

2,K,2

0	654	709
1	83	46
2	125	69
3	397	396
4	418	407
5	240	242
6	213	210
7	316	272
8	324	294
9	124	120
10	190	176
11	177	148
12	286	249
13	168	174
14	67	53
15	172	159
16	177	175
17	158	152
18	48	46
19	219	213
20	139	136
21	136	134
22	117	114
23	101	101
24	123	123
25	92	77
26	108	109
27	71	76
28	87	88
29	136	143
30	17	20
31	39	43
32	33	37
33	57	59

3,K,2

1	430	412
2	226	196
3	56	32
4	178	163
5	305	269
6	141	116
7	368	350
8	359	347
2	144	149
3	80	80
4	54	53
5	46	43
6	133	140
7	40	45
8	47	48
10	63	66
9	57	59
10	63	66
11	32	30
12	84	89
13	32	30
14	36	35
15	39	37
16	54	57

12,K,2

0	73	66
1	15	20
2	31	32
3	8	9
4	30	30
5	37	34
6	53	52
7	39	43
8	13	17
9	42	46
10	33	33

0,K,3

1	149	141
3	182	187
5	192	179
7	497	482
9	342	342
11	65	50
13	336	320
15	96	84
17	191	195
19	77	72
21	111	115
23	215	221
25	173	187
27	174	184
29	216	229
31	33	28

1,K,3

1	171	167
2	358	341
3	184	177
4	276	258
5	119	119
6	255	237
7	150	136

1,K,3

8	320	303
9	228	211
10	210	194
11	239	236
12	172	162
13	146	129
14	274	268
15	58	56
16	13	4
17	90	86
18	38	16
19	127	130
20	65	68
21	69	86
22	147	151
23	89	97
24	50	52
25	77	78
26	108	111
27	122	130
28	49	48
29	56	58
30	8	13
31	62	65

2,K,3

0	246	236
1	121	114
2	272	253
3	303	297
4	315	300
5	292	280
6	215	206
7	367	350
8	103	93
9	158	143
10	321	306
11	104	107
12	79	79
13	82	74
14	104	93
15	69	71
16	82	76
17	109	105
18	156	162
19	129	132
20	66	61
21	25	32
22	87	92
23	134	146
24	107	105
25	52	54
26	84	87
27	79	75
28	78	77
29	41	43
30	87	89

11,K,3

7	32	36
8	8	8
9	9	8
10	73	70
11	46	45
12	44	43
13	23	26

12,K,3

0	75	73
1	68	69
2	22	21
3	64	59

0,K,4

0	119	113
2	363	343
4	89	88
6	315	297
8	120	114
10	167	160
12	216	216
14	399	403
16	382	385
18	161	161
20	160	158
22	95	86
24	208	214
26	115	113
28	158	161

1,K,4

1	116	102
2	47	41
3	154	142
4	333	322
5	108	94
6	87	84
7	126	117
8	64	60
9	263	253
10	100	93
11	182	183
12	242	247
13	59	53
14	116	113
15	127	128
16	315	319
17	43	45
18	160	165
19	28	28
20	97	106
21	78	85
22	105	106
23	56	54
31	44	49

3,K,3

1	213	209
2	328	304
3	432	414
4	235	228
5	175	173
6	265	257
7	301	298
8	118	114
9	193	188
10	107	123
11	117	116
12	138	123
13	71	70
14	145	140
15	59	60
16	172	166
17	94	90
18	143	143
19	44	37
20	179	188
21	38	43
22	44	50
23	67	70
24	76	77
25	31	30
26	46	45
27	79	79
28	104	105
29	19	18
30	48	52

4,K,3

0	528	516
1	109	102
2	118	115
3	358	336
4	212	194
5	77	71
6	76	64
7	72	59
8	65	63
9	85	85
10	147	146
11	85	80
12	148	148
13	120	110
14	69	65
15	248	255
16	94	93
17	119	119
18	177	184
19	146	145
20	148	150
21	111	110
22	183	194
24	39	37
25	124	130
26	1[illegible]	15
27	69	71
28	21	19
29	75	84

2,K,4

0	384	364
1	52	48
2	113	105
3	281	269
4	253	242
5	97	93
6	71	66
7	226	215
8	184	177
9	103	100
10	141	137
11	229	232
12	209	219
13	75	79
14	127	132
15	139	130
16	54	49
17	87	81
18	100	96
19	115	113
20	106	115
21	60	52
22	42	42
23	78	81
24	65	69
25	53	52
26	47	52
27	23	26
28	14	8
29	39	40

3,K,4

1	20	28
2	121	127
3	76	71
4	114	119
5	182	181
6	62	65
7	67	54
8	74	73
9	156	156
10	39	44
11	105	98
12	148	153
13	120	126
14	278	273
15	75	75
16	129	134
17	102	104
18	58	58
23	58	60
24	65	68
25	27	31
26	20	21
27	19	25
28	17	22
29	40	45
30	41	39

5,K,3

1	89	76
2	195	191
3	155	149
4	73	69
5	134	131
6	141	135
7	59	57
8	43	48
9	151	141
10	164	161
11	80	79
12	217	210
13	46	47
14	58	60
15	87	88
16	215	219
17	128	125
18	133	136
19	172	174
20	37	41
21	71	74
22	124	127
23	39	41
24	38	43
25	24	21
26	114	114
27	57	60
28	30	34

6,K,3

0	62	73
1	144	148
2	88	89
3	95	90
4	194	188
5	121	111
6	241	237
7	254	255
8	201	201
9	143	147
10	137	134
11	144	141
12	94	94
13	77	72
14	206	215
15	116	121
16	114	107
17	64	63
19	38	33
20	54	57
21	94	94
22	25	32
23	58	54
24	16	19
25	23	23
26	35	38
27	68	70
28	15	19

4,K,4

0	76	77
1	204	196
2	116	115
3	19	13
4	101	96
5	51	42
6	69	69
7	40	43
8	233	230
9	136	134
10	210	215
11	356	359
12	65	69
13	181	177
14	191	188
15	201	197
16	131	132
17	96	95
18	158	162
19	95	96
20	86	87
21	12	10
22	8	14
23	17	22
24	46	49
25	42	54
26	71	68
27	17	13

5,K,4

1	74	67
2	31	37
3	62	64
4	72	61
5	93	91
6	127	123
7	123	123
8	173	175
9	198	193
10	103	108
11	50	61
12	144	142
13	155	154
14	78	76
15	75	75
16	91	96
18	64	69
19	74	70
20	129	131
21	25	20
22	82	75
23	43	42
24	67	68
25	39	40
26	39	43
27	46	41

7,K,3

1	76	73
2	148	149
3	26	24
4	142	153
5	276	281
6	110	121
7	84	79
8	228	233
9	116	116
10	112	109
11	251	247
12	15	17
13	55	58
14	102	105
15	88	91
16	78	81
17	45	44
18	47	48
19	85	85
20	38	34
21	66	67
22	53	54
23	53	57
24	36	38
25	48	47

8,K,3

0	199	189
1	66	58
2	135	135
3	148	155
4	65	66
5	145	148
6	57	63
7	24	27
8	86	83
9	111	104
10	105	93
11	90	96
12	51	47
13	47	46
14	104	111
15	79	80
16	28	30
17	75	74
18	47	48
17	108	104
18	46	43
19	45	49
20	83	81
21	76	73
22	55	58
23	24	21
24	31	35
25	81	82
26	11	8

6,K,4

0	107	105
1	69	71
2	109	110
3	73	75
4	146	148
5	118	118
6	157	161
7	233	238
8	210	206
9	155	150
10	106	107
11	120	117
12	84	78
13	235	242
14	156	156
15	124	126
16	67	63
17	130	146
18	78	83
19	136	135
20	20	20
21	44	50
22	51	45
23	61	61
24	52	54

7,K,4

1	90	102
2	87	89
3	83	85
4	22	24
5	151	157
6	270	271
7	100	99
8	131	133
9	163	163
10	84	82
11	9	4
12	57	58
13	129	133
14	93	91
15	89	93
16	12	15
17	33	36
18	77	75
19	21	24
19	70	68
20	39	40
21	37	37
22	33	40
23	29	31

9,K,3

1	90	88
2	157	157
3	133	135
4	82	91
5	78	79
6	124	130
7	63	61
8	32	35
9	108	108
10	58	57
11	68	74
12	88	88
13	79	81
14	47	48
15	36	38
16	67	73
17	67	67
18	87	88
19	22	21
20	83	88
21	32	41

10,K,3

0	144	153
1	65	66
2	86	90
3	40	40
4	31	27
5	52	49
6	17	13
7	51	50
8	82	90
9	109	114
10	81	79
11	39	39
12	84	89
13	16	16
14	33	32
15	58	55
16	28	21
17	15	14

11,K,3

1	75	75
2	74	71
3	126	131
4	37	39
5	88	89
6	84	85
20	16	13
21	17	17
22	28	29

8,K,4

0	162	162
1	62	63
2	31	29
3	58	57
4	57	66
5	64	67
6	83	89
7	66	65
8	57	64
9	120	120
10	98	106
11	90	96
12	62	67
13	57	60
14	90	94
15	38	40
16	50	48
17	43	48
18	28	33
19	16	16
20	73	72

9,K,4

1	34	29
2	63	63
3	97	100
4	43	44
5	61	66
6	64	69
7	50	53
8	69	74
9	75	72
10	49	47
11	66	67
12	31	25
13	37	38
14	31	35
15	56	61
16	31	27
17	31	38

10,K,4

0	29	23
1	63	65
2	19	16
3	33	31
4	61	59
5	82	82
6	52	52
7	33	33
8	36	40

10,K,4

9	28	25
10	25	26
11	35	38
12	58	60
13	27	30

11,K,4

1	102	97
2	81	79
3	36	35
4	47	44
5	12	8

0,K,5

1	159	165
3	106	113
5	206	203
7	128	117
9	245	240
11	193	193
13	208	213
15	219	213
17	290	297
19	128	138
21	96	97
23	113	121
25	38	37

1,K,5

1	41	45
2	57	55
3	181	174
4	31	29
5	153	143
6	46	42
7	207	212
8	168	165
9	147	151
10	141	136
11	110	103
12	56	54
13	90	85
14	65	62
15	134	134
16	64	64
17	48	50
18	67	64
19	64	67
20	40	41
21	47	50
22	68	74
23	73	77
24	71	74
25	21	18

2,K,6

14	27	22
15	24	27
16	70	70
17	60	58
18	47	48
19	43	48
20	60	61

3,K,6

1	81	86
2	50	50
3	63	65
4	155	153
5	111	116
6	40	42
7	37	35
8	68	69
9	169	177
10	133	140
11	87	86
12	87	87
13	93	93
14	119	121
15	15	17
16	107	110
17	27	31
18	29	30
19	52	48

4,K,6

0	93	100
1	41	41
2	17	17

2,K,5

0	150	149
1	125	119
2	22	23
3	72	70
4	50	48
5	91	87
6	119	121
7	195	196
8	259	252
9	107	103
10	263	266
11	261	256
12	93	93
13	166	164
14	37	38
15	52	51
16	70	67
17	12	6
18	28	26
19	35	36
20	44	54
21	41	41
22	112	113
23	23	25
24	20	18
25	82	82

3,K,5

1	176	180
2	83	75
3	185	185
4	98	90
5	118	119
6	113	117
7	182	183
8	179	184
9	41	44
10	202	209
11	64	62
12	66	70
13	57	57
14	205	205
15	75	71
16	114	115
17	126	126
18	170	173
19	8	10
20	7	8
21	44	40
22	51	47
23	60	63
24	22	22

4,K,5

0	193	198
1	94	99
2	84	83
3	195	200
4	28	26
5	22	27
6	118	117
7	67	68
8	95	95
9	28	28
10	59	54
11	91	90
12	209	215
13	43	40
14	151	152
15	175	174
16	33	37
17	58	58
18	27	25
19	87	86
20	67	68
21	34	30
22	73	70
23	49	51

5,K,5

1	58	65
2	20	18
3	49	49
4	162	171
5	70	68
6	118	117
7	64	65
8	94	95
9	97	95
10	117	117
11	151	164
12	49	53
13	96	103
14	62	72
15	66	63
16	131	136
17	58	64
18	69	69
19	38	43
20	9	6
21	32	31
22	23	30

6,K,5

0	80	86
1	50	47
2	180	191
3	74	81
4	140	142
5	59	61
6	96	103
7	93	96
8	148	153
9	79	76

6,K,6

0	83	89
1	57	57
2	36	39
3	35	34
4	75	81
5	70	67
6	15	17
7	35	33
8	63	67
9	58	62
10	63	64
11	83	81
12	26	34
13	16	20
14	29	30

7,K,6

1	97	107
2	78	84
3	108	113
4	70	74
5	86	95
6	45	48
7	10	10
8	59	63
9	12	12
10	37	38

8,K,6

0	63	68
1	20	19
2	46	48
10	63	65
11	36	36
12	50	51
13	86	92
14	64	65
15	64	68
16	93	98
17	68	69
18	84	87
19	120	123
20	32	26

7,K,5

1	36	39
2	104	103
3	42	39
4	109	114
5	34	34
6	32	38
7	26	21
8	30	29
9	7*	6
10	69	72
11	99	102
12	101	106
13	30	29
14	85	95
15	61	61
16	31	28
17	20	26
18	30	31

8,K,5

0	118	112
1	85	91
2	91	95
3	81	84
4	52	57
5	41	42
6	113	115
7	31	33
8	76	75
9	103	107
10	26	24
11	88	93
12	64	70
13	35	41
14	46	47
15	95	91

9,K,5

1	48	52
2	47	46
3	42	47
4	20	21
5	42	36
6	57	57

0,K,7

1	19	25
3	15	12
5	86	95
7	130	140
9	55	60
11	44	45
13	69	73

1,K,7

1	82	85
2	70	68
3	15	17
4	45	51
5	70	71
6	42	40
7	61	65
8	74	81
9	55	61
10	42	40
11	32	26
12	76	78
13	25	23

2,K,7

0	48	54
1	53	50
2	79	81
3	60	57
4	59	63
5	40	40
6	28	30
7	75	79
8	78	82
9	40	38
10	109	115
11	75	74
12	57	59

3,K,7

1	50	48
2	88	92
3	42	40
4	90	96
5	94	93
6	108	118
7	16	17
8	18	18
9	25	21
10	52	54
11	33	31

4,K,7

0	70	71
1	59	65
2	46	49
3	52	52
4	35	41
5	52	54
6	48	53
7	44	46
8	57	62

5,K,7

1	65	74
2	30	32
3	52	50

0,K,6

0	22	18
2	153	156
4	37	30
6	180	178
8	93	88
10	68	68
12	80	83
14	66	68
16	72	73
18	30	28
20	59	53

1,K,6

1	93	95
2	88	93
3	109	110
4	259	261
5	20	19
6	32	33
7	62	62
8	109	111
9	60	61
10	71	70
11	52	52
12	87	85
13	35	38
14	9	10
15	61	65
16	37	32
17	76	84
18	77	74
19	84	86
20	34	43
21	42	42

2,K,6

0	57	53
1	173	177
2	122	123
3	105	108
4	72	75
5	61	59
6	89	86
7	121	122
8	51	51
9	54	53
10	66	70
11	113	114
12	34	43
13	61	61