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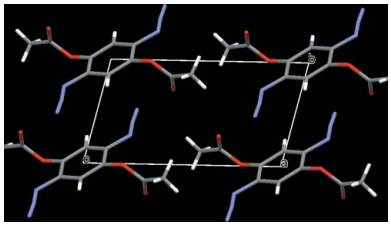
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Crystal structures of 2,5-diazido-1,4-phenylene diacetate and 2,5-diazido-1,4-phenylene dibutyrate

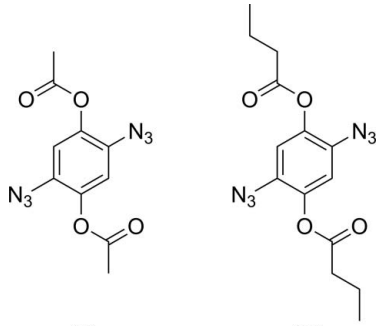
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The asymmetric units of the title compounds, $C_{10}H_8N_6O_4$, (I), and $C_{14}H_{16}N_6O_4$, (II), each contain half of the respective molecule which is completed by inversion symmetry. The two molecules differ in the ester moiety (acetate *versus* butyrate) and the crystal symmetry is different, *i.e.* triclinic for (I) and monoclinic for (II). The diazidophenylene moieties are essentially planar [maximum deviation of 0.0216 (7) Å for (I) and 0.0330 (14) Å for (II)], and the ester functionalities are almost perpendicular to these planes, making dihedral angles of 79.93 (3)° for (I) and 79.42 (6)° for (II). In the crystals of both (I) and (II), there are no significant intermolecular interactions present.

1. Chemical context

In recent years, copper(I)-catalysed cycloaddition of organic azides and alkynes towards 1,4-disubstituted triazoles attained immense interest in various fields of organic chemistry and became famous as the 'cream of the crop' of click chemistry (Moses & Moorhouse, 2007). In materials chemistry, this kind of reaction is often applied for the synthesis of functional polymers (Qin *et al.*, 2010).



(I) (II)

The title compounds, (I) and (II), were synthesized to investigate their applicability in such polymerizations, *viz.* *AA*–*BB* polymerizations with dialkynes. The synthetic accessibility of the two compounds from inexpensive starting materials is remarkable, making them suitable for large scale preparation. However, their electron-deficient character represents a challenge to the polymerization parameters. The crystal structures of (I) and (II) are reported herein.

2. Structural commentary

The molecular structures of (I) and (II) are displayed in Figs. 1 and 2, respectively. Both molecules possess inversion symmetry. Although the two molecules differ only in the ester moiety (acetate *versus* butyrate), the crystal symmetry is

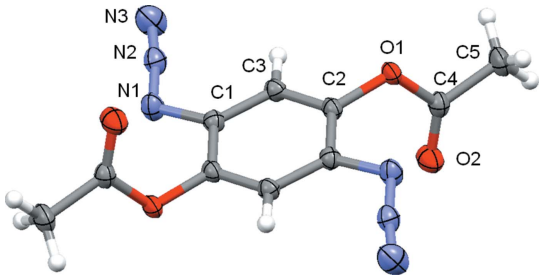


Figure 1
The molecular structure of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 80% probability level. Unlabelled atoms are generated by the symmetry code $(-x+1, -y, -z)$.

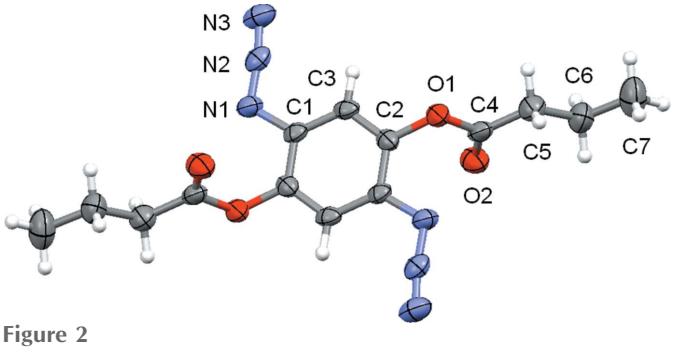


Figure 2
The molecular structure of compound (II), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 80% probability level. Unlabelled atoms are generated by the symmetry code $(-x+1, -y, -z)$.

different, *i.e.* triclinic for (I), with $Z = 1$, and monoclinic for (II), with $Z = 2$. The diazidophenylene moieties do not differ significantly from planarity, with a maximum deviation of 0.0216 (7) Å in (I) and 0.0330 (14) Å in (II), for the unsubstituted atom C3 in both cases. The azide groups, both in *trans* positions to each other, deviate slightly from a linear arrangement, with an N—N—N angle of 173.01 (9)° for (I) and 172.59 (16)° for (II). The mean planes of the acetate [C—C(=O)—O)] and butyrate [C—C—C—C(=O)—O] groups are almost normal to the mean planes of the diazidophenylene moieties, with a dihedral angle of 79.93 (3)° for (I) and 79.42 (6)° for (II).

3. Supramolecular features

There are no notable features in terms of π–π stacking interactions or hydrogen bonding in either structure. The crystal packing of (I) and (II) seems to be dominated mainly by van der Waals forces (Figs. 3 and 4, respectively).

4. Database survey

In the Cambridge Structural Database (Version 5.35, last update February 2014; Allen, 2002) no structures of compounds containing a *trans*-diazidophenylene entity are listed, making the two examples presented herein the only ones reported so far.

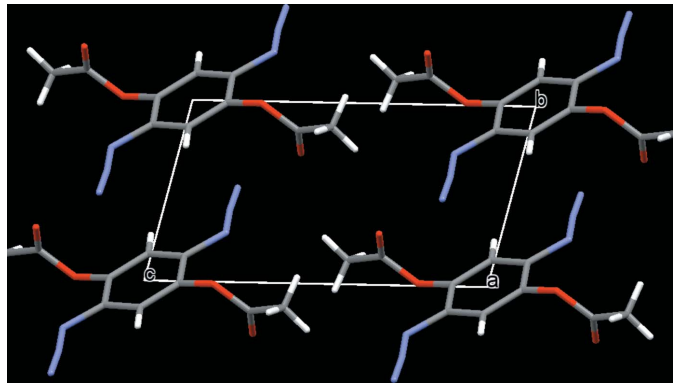


Figure 3
A view along [100] of the crystal packing of compound (I). Colour code: O red, C grey, N light-blue and H white.

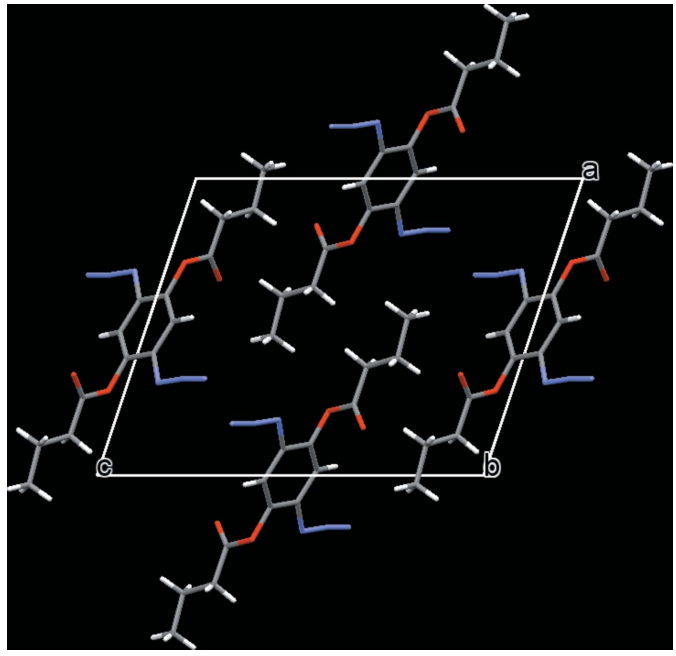


Figure 4
A view along [010] of the crystal packing of compound (II). Colour code: O red, C grey, N light-blue and H white.

5. Synthesis and crystallization

Both target compounds were synthesized following a two-step protocol (Fig. 5), previously published for 2,5-diazido-1,4-phenylene diacetate by Moore *et al.* (1969). In view of the light sensitivity of the intermediate compound 2,5-diazidobenzene-1,4-diol, all reactions were carried out under light protection.

Preparation of 2,5-diazidobenzene-1,4-diol: 1,4-benzoquinone (10.81 g, 100.0 mmol, 1.0 equivalent) was dissolved in glacial acetic acid (100 ml, 1.0 *M*) and cooled to 288 K using an ice-water bath. NaN_3 (14.3 g, 220 mol, 2.2 equivalents) was dissolved in water (44 ml, 5.0 *M*) and added to the cooled and stirred solution of 1,4-benzoquinone in one portion. Stirring was stopped after 15 min and the flask was sealed and stored at 278 K overnight for crystallization. Vacuum filtration afforded a light-yellow solid, which was washed three times with water and dried *in vacuo* overnight to afford 2,5-di-

Table 1
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{10}H_8N_6O_4$	$C_{14}H_{16}N_6O_4$
M_r	276.2	332.3
Crystal system, space group	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/n$
Temperature (K)	100	100
a, b, c (Å)	5.4293 (6), 5.5678 (6), 10.4945 (12)	11.5875 (19), 5.1485 (8), 14.327 (2)
α, β, γ (°)	101.508 (3), 104.544 (3), 97.057 (3)	90, 108.496 (5), 90
V (Å^3)	295.86 (6)	810.6 (2)
Z	1	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.12	0.10
Crystal size (mm)	0.65 × 0.55 × 0.25	0.65 × 0.25 × 0.08
Data collection		
Diffractometer	Bruker Kappa APEXII CCD	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.92, 0.97	0.97, 0.99
No. of measured, independent and observed [$I > 3\sigma(I)$] reflections	15989, 2182, 1983	17268, 1781, 1211
R_{int}	0.037	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.764	0.662
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.056, 3.22	0.042, 0.048, 2.15
No. of reflections	2182	1781
No. of parameters	91	109
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.46, −0.23	0.26, −0.23

Computer programs: *APEX2* and *SAINT-Plus* (Bruker, 2013), *SUPERFLIP* (Palatinus & Chapuis, 2007), *JANA2006* (Petříček, *et al.*, 2014), *Mercury* (Macrae *et al.*, 2008) and *publCIF* (Westrip, 2010).

azidobenzene-1,4-diol (yield: 6.60 g, 34.4 mmol, 69%). 1,4-Benzoquinone serves as starting material and as oxidation reagent in this reaction, resulting in a theoretical molar yield of only half of the applied starting material (50 mmol).

Preparation of 2,5-diazido-1,4-phenylene diacetate, (I): 2,5-diazidobenzene-1,4-diol (1.92 g, 10.0 mmol) was added to preheated (313 K) acetic anhydride (100 ml, 0.1 *M*) in one portion and the reaction stirred until complete dissolution of the starting material. The reaction mixture was then allowed to cool to room temperature and stored overnight to allow 2,5-diazido-1,4-phenylene diacetate to crystallize. Vacuum filtration afforded light-orange crystals of compound (I), which were washed with water three time (yield: 1.73 g, 6.26 mmol, 63%). ^{1}H NMR ($CDCl_3$, 200 MHz): δ 6.89 (*s*, 2H), 2.33 (*s*, 6H); ^{13}C NMR ($CDCl_3$, 50 MHz): δ 168.3 (*s*), 140.0 (*s*), 129.3 (*s*), 115.3 (*d*), 20.4 (*q*).

Preparation of 2,5-diazido-1,4-phenylene dibutyrate, (II): 2,5-diazidobenzene-1,4-diol (1.34 g, 7.0 mmol) was added to preheated (333 K) butyric anhydride (20 ml, 0.35 *M*) in one portion and the resulting suspension stirred for 45 min at this temperature. The reaction mixture was then allowed to cool to room temperature and stored for 5 days to allow 2,5-diazido-1,4-phenylene dibutyrate to crystallize. Vacuum filtration afforded yellow crystals of compound (II), which were washed with water three times and with ethanol twice (yield: 814 mg, 2.45 mmol, 35%). ^{1}H NMR ($CDCl_3$, 200 MHz): δ 6.88 (*s*, 2H), 2.57 (*t*, J = 7.4 Hz, 4H), 1.80 (*sext*, J = 7.4 Hz, 4H), 1.05 (*t*, J = 7.4 Hz, 6H); ^{13}C NMR ($CDCl_3$, 50 MHz): δ 171.1 (*s*), 140.0 (*s*), 129.3 (*s*), 115.3 (*d*), 35.6 (*t*), 18.3 (*t*), 13.6 (*q*).

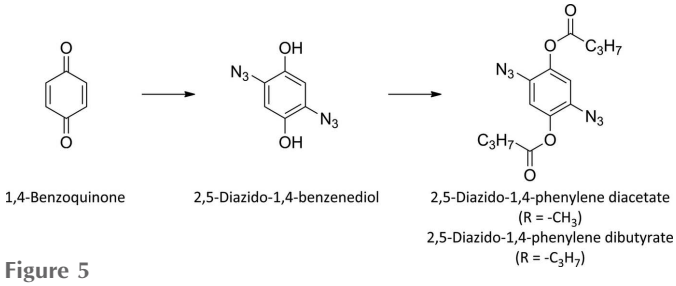


Figure 5
Reaction scheme for the synthesis of the title compounds.

6. Refinement

For both structures, (I) and (II), the H atoms were included in calculated positions and treated as riding atoms, with C—H = 0.96 Å and U_{iso}(H) = 1.2U_{eq}(C).

Acknowledgements

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supporting information

Acta Cryst. (2014). E**70**, 39-42 [doi:10.1107/S1600536814013762]

Crystal structures of 2,5-diazido-1,4-phenylene diacetate and 2,5-diazido-1,4-phenylene dibutyrate

Florian Glöcklhofer, Johannes Fröhlich, Berthold Stöger and Matthias Weil

Computing details

For both compounds, data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT-Plus* (Bruker, 2013); data reduction: *SAINT-Plus* (Bruker, 2013); program(s) used to solve structure: SUPERFLIP (Palatinus & Chapuis, 2007); program(s) used to refine structure: JANA2006 (Petříček, *et al.*, 2014); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

(I) 2,5-Diazido-1,4-phenylene diacetate

Crystal data

$C_{10}H_8N_6O_4$
M_r = 276.2
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 5.4293 (6) Å
b = 5.5678 (6) Å
c = 10.4945 (12) Å
α = 101.508 (3)°
β = 104.544 (3)°
γ = 97.057 (3)°
V = 295.86 (6) Å^3
Z = 1
$F(000)$ = 142
D_x = 1.550 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
θ = 3.8–32.8°
μ = 0.12 mm^{-1}
T = 100 K
Irregular, light-orange
0.65 × 0.55 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: X-ray tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
T_{min} = 0.92, T_{max} = 0.97
15989 measured reflections
2182 independent reflections
1983 reflections with $I > 3\sigma(I)$
R_{int} = 0.037
θ_{max} = 32.9°, θ_{min} = 2.1°
h = −8→8
k = −8→8
l = −15→16

Refinement

Refinement on F
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.056
S = 3.22
2182 reflections
91 parameters
0 restraints
16 constraints
H-atom parameters constrained
Weighting scheme based on measured s.u.'s $w = 1/(\sigma^2(F) + 0.0001F^2)$
$(\Delta/\sigma)_{max}$ = 0.011
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.25671 (10)	0.01146 (10)	0.20279 (5)	0.01189 (16)
O2	0.59540 (11)	0.28134 (10)	0.35546 (6)	0.01772 (18)
N1	0.36886 (13)	0.27117 (12)	−0.19926 (6)	0.0141 (2)
N2	0.19623 (12)	0.39755 (11)	−0.19328 (6)	0.01377 (19)
N3	0.04446 (14)	0.51922 (13)	−0.19896 (8)	0.0208 (2)
C1	0.42743 (13)	0.13837 (12)	−0.09681 (7)	0.0106 (2)
C2	0.38596 (13)	0.01109 (13)	0.10373 (7)	0.01038 (19)
C3	0.31388 (13)	0.14839 (12)	0.00901 (7)	0.0108 (2)
C4	0.38466 (14)	0.15794 (13)	0.33011 (7)	0.0119 (2)
C5	0.22479 (16)	0.13357 (15)	0.42495 (7)	0.0174 (2)
H1c3	0.185611	0.250721	0.016023	0.013*
H1c5	0.054271	0.162226	0.38606	0.0208*
H2c5	0.213484	−0.031171	0.440361	0.0208*
H3c5	0.303627	0.253962	0.509525	0.0208*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0113 (3)	0.0152 (2)	0.0096 (2)	0.00109 (19)	0.00522 (18)	0.00195 (18)
O2	0.0164 (3)	0.0197 (3)	0.0148 (3)	−0.0021 (2)	0.0057 (2)	0.0004 (2)
N1	0.0169 (3)	0.0155 (3)	0.0139 (3)	0.0069 (2)	0.0072 (2)	0.0064 (2)
N2	0.0161 (3)	0.0132 (3)	0.0137 (3)	0.0024 (2)	0.0056 (2)	0.0056 (2)
N3	0.0214 (4)	0.0201 (3)	0.0276 (4)	0.0089 (3)	0.0118 (3)	0.0119 (3)
C1	0.0113 (3)	0.0107 (3)	0.0096 (3)	0.0016 (2)	0.0032 (2)	0.0021 (2)
C2	0.0105 (3)	0.0116 (3)	0.0091 (3)	0.0012 (2)	0.0042 (2)	0.0011 (2)
C3	0.0106 (3)	0.0115 (3)	0.0107 (3)	0.0027 (2)	0.0040 (2)	0.0018 (2)
C4	0.0144 (3)	0.0124 (3)	0.0102 (3)	0.0039 (2)	0.0049 (2)	0.0028 (2)
C5	0.0186 (4)	0.0228 (4)	0.0129 (3)	0.0030 (3)	0.0091 (3)	0.0037 (3)

Geometric parameters (Å, º)

O1—C2	1.3924 (10)	C1—C3	1.3943 (11)
O1—C4	1.3758 (8)	C2—C3	1.3810 (11)
O2—C4	1.1971 (9)	C3—H1c3	0.96
N1—N2	1.2456 (10)	C4—C5	1.4904 (12)
N1—C1	1.4167 (10)	C5—H1c5	0.96
N2—N3	1.1269 (10)	C5—H2c5	0.96
C1—C2^{i}	1.3944 (11)	C5—H3c5	0.96
C2—O1—C4	116.60 (5)	C2—C3—H1c3	120
N2—N1—C1	115.40 (7)	O1—C4—O2	122.32 (7)
N1—N2—N3	173.01 (9)	O1—C4—C5	110.16 (6)
N1—C1—C2^{i}	116.58 (7)	O2—C4—C5	127.51 (6)
N1—C1—C3	124.83 (7)	C4—C5—H1c5	109.47
C2^{i}—C1—C3	118.59 (7)	C4—C5—H2c5	109.47

O1—C2—C1^{i}	119.80 (7)	C4—C5—H3c5	109.47
O1—C2—C3	118.66 (7)	H1c5—C5—H2c5	109.47
C1^{i}—C2—C3	121.42 (7)	H1c5—C5—H3c5	109.47
C1—C3—C2	120.00 (7)	H2c5—C5—H3c5	109.47
C1—C3—H1c3	120		

Symmetry code: (i) −*x*+1, −*y*, −*z*.

(II) 2,5-Diazido-1,4-phenylene dibutyrate

Crystal data

$C_{14}H_{16}N_6O_4$
M_r = 332.3
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 11.5875 (19) Å
b = 5.1485 (8) Å
c = 14.327 (2) Å
β = 108.496 (5)°
V = 810.6 (2) Å^3
Z = 2
$F(000)$ = 348
D_x = 1.361 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7352 reflections
θ = 2.7–27.0°
μ = 0.10 mm^{-1}
T = 100 K
Rod, light-yellow
0.65 × 0.25 × 0.08 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: X-ray tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
T_{min} = 0.97, T_{max} = 0.99
17268 measured reflections
1781 independent reflections
1211 reflections with $I > 3\sigma(I)$
R_{int} = 0.043
θ_{max} = 28.1°, θ_{min} = 2.0°
h = −13→14
k = −6→6
l = −17→18

Refinement

Refinement on F
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.048
S = 2.15
1781 reflections
109 parameters
0 restraints
32 constraints
H-atom parameters constrained
Weighting scheme based on measured s.u.'s $w = 1/(\sigma^2(F) + 0.0001F^2)$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.28390 (9)	0.01294 (17)	0.04347 (7)	0.0217 (4)
O2	0.33949 (10)	−0.32997 (19)	0.14715 (7)	0.0269 (4)
N1	0.68785 (12)	0.3626 (2)	0.07891 (8)	0.0224 (5)
N2	0.67449 (11)	0.5255 (2)	0.13953 (9)	0.0225 (5)
N3	0.67447 (13)	0.6825 (2)	0.19484 (9)	0.0296 (5)
C1	0.58925 (14)	0.1863 (2)	0.04072 (10)	0.0177 (5)
C2	0.39470 (14)	0.0013 (3)	0.02402 (10)	0.0181 (5)
C3	0.48219 (14)	0.1877 (3)	0.06446 (10)	0.0190 (5)
C4	0.26254 (15)	−0.1781 (3)	0.10334 (10)	0.0214 (6)

C5	0.13432 (15)	−0.1622 (3)	0.10373 (11)	0.0265 (6)
C6	0.10348 (15)	−0.3423 (3)	0.17548 (11)	0.0303 (6)
C7	−0.02989 (17)	−0.3320 (4)	0.16734 (13)	0.0411 (7)
H1c3	0.468982	0.31648	0.108459	0.0228*
H1c5	0.080047	−0.194143	0.038568	0.0318*
H2c5	0.116086	0.013496	0.116656	0.0318*
H1c6	0.152049	−0.298391	0.241353	0.0364*
H2c6	0.125093	−0.51698	0.164467	0.0364*
H1c7	−0.045158	−0.450116	0.21394	0.0493*
H2c7	−0.050726	−0.158801	0.180958	0.0493*
H3c7	−0.078376	−0.380637	0.101973	0.0493*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0263 (7)	0.0157 (5)	0.0273 (6)	0.0017 (5)	0.0143 (5)	0.0033 (4)
O2	0.0324 (7)	0.0217 (6)	0.0303 (6)	0.0055 (5)	0.0150 (5)	0.0053 (5)
N1	0.0290 (9)	0.0153 (6)	0.0251 (7)	−0.0013 (6)	0.0114 (6)	−0.0036 (6)
N2	0.0264 (9)	0.0159 (6)	0.0247 (7)	−0.0015 (6)	0.0072 (6)	0.0037 (6)
N3	0.0397 (10)	0.0189 (7)	0.0297 (7)	−0.0022 (6)	0.0101 (7)	−0.0052 (6)
C1	0.0231 (10)	0.0108 (7)	0.0194 (7)	−0.0002 (6)	0.0069 (7)	0.0020 (6)
C2	0.0218 (10)	0.0148 (7)	0.0208 (8)	0.0040 (7)	0.0109 (7)	0.0048 (6)
C3	0.0283 (10)	0.0112 (7)	0.0189 (8)	0.0023 (6)	0.0095 (7)	0.0016 (6)
C4	0.0309 (11)	0.0135 (7)	0.0225 (8)	−0.0025 (7)	0.0124 (7)	−0.0029 (6)
C5	0.0286 (11)	0.0212 (8)	0.0320 (9)	0.0005 (7)	0.0131 (7)	0.0019 (7)
C6	0.0338 (11)	0.0259 (9)	0.0356 (9)	−0.0051 (8)	0.0173 (8)	0.0004 (7)
C7	0.0376 (12)	0.0516 (12)	0.0386 (11)	−0.0118 (9)	0.0184 (9)	0.0030 (9)

Geometric parameters (Å, º)

O1—C2	1.399 (2)	C4—C5	1.490 (3)
O1—C4	1.3780 (19)	C5—C6	1.509 (2)
O2—C4	1.2023 (17)	C5—H1c5	0.96
N1—N2	1.2518 (18)	C5—H2c5	0.96
N1—C1	1.4257 (18)	C6—C7	1.513 (3)
N2—N3	1.1318 (18)	C6—H1c6	0.96
C1—C2^{i}	1.392 (2)	C6—H2c6	0.96
C1—C3	1.387 (2)	C7—H1c7	0.96
C2—C3	1.3825 (19)	C7—H2c7	0.96
C3—H1c3	0.96	C7—H3c7	0.96
C2—O1—C4	116.81 (11)	C4—C5—H2c5	109.47
N2—N1—C1	115.62 (14)	C6—C5—H1c5	109.47
N1—N2—N3	172.59 (16)	C6—C5—H2c5	109.47
N1—C1—C2^{i}	115.94 (15)	H1c5—C5—H2c5	103.47
N1—C1—C3	124.96 (13)	C5—C6—C7	112.50 (13)
C2^{i}—C1—C3	119.09 (13)	C5—C6—H1c6	109.47
O1—C2—C1^{i}	119.18 (12)	C5—C6—H2c6	109.47

O1—C2—C3	118.96 (13)	C7—C6—H1c6	109.47
C1^{i}—C2—C3	121.71 (15)	C7—C6—H2c6	109.47
C1—C3—C2	119.20 (14)	H1c6—C6—H2c6	106.26
C1—C3—H1c3	120.4	C6—C7—H1c7	109.47
C2—C3—H1c3	120.4	C6—C7—H2c7	109.47
O1—C4—O2	122.63 (16)	C6—C7—H3c7	109.47
O1—C4—C5	109.84 (12)	H1c7—C7—H2c7	109.47
O2—C4—C5	127.53 (15)	H1c7—C7—H3c7	109.47
C4—C5—C6	114.88 (12)	H2c7—C7—H3c7	109.47
C4—C5—H1c5	109.47		

Symmetry code: (i) $-x+1, -y, -z$.