

Christopher Glidewell,^{a*} John N. Low,^b Janet M. S. Skakle^b and James L. Wardell^c^aSchool of Chemistry, University of St Andrews, Fife KY16 9ST, Scotland, ^bDepartment of Chemistry, University of Aberdeen, Meston Walk, Old Aberdeen AB24 3UE, Scotland, and ^cInstituto de Química, Departamento de Química Inorgânica, Universidade Federal do Rio de Janeiro, 21945-970 Rio de Janeiro, RJ, Brazil

Correspondence e-mail: cg@st-andrews.ac.uk

Key indicators

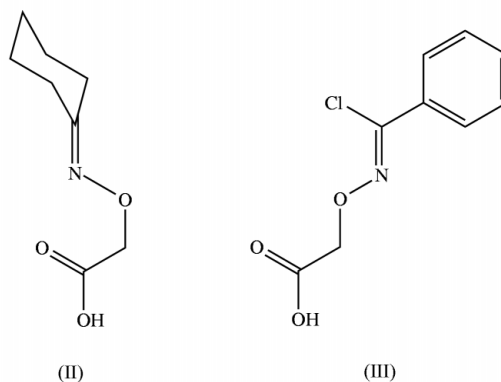
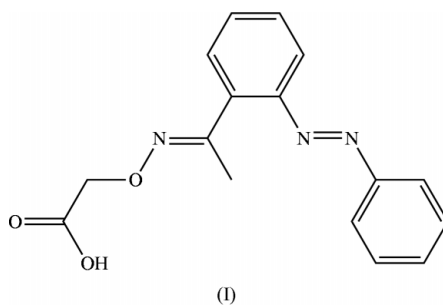
Single-crystal X-ray study
 $T = 120$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.069
 wR factor = 0.187
Data-to-parameter ratio = 16.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Hydrogen-bonded $R_2^2(8)$ dimers in (*E*)-[2-(phenyl-diazenyl)phenyl]ethylideneaminoxy}acetic acidMolecules of the title compound, $\text{C}_{16}\text{H}_{15}\text{N}_3\text{O}_3$, are linked by paired $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds [$\text{H}\cdots\text{O} = 1.84$ Å, $\text{O}\cdots\text{O} = 2.655(3)$ Å and $\text{O}-\text{H}\cdots\text{O} = 175^\circ$] into centrosymmetric $R_2^2(8)$ dimers.

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Comment

Persulfate oxidation of iminoxyacetic acids, $R(R')\text{C}=\text{N}-\text{OCH}_2\text{COOH}$, provides a useful route to iminyl radicals (Forrester *et al.*, 1979). The subsequent reactions of the iminyl radicals thus generated depend greatly on the substituents, and important species including nitrogen-containing heterocycles can result. We report here the crystal structure of the title compound, (I) (Fig. 1), and we compare (I) with the simpler analogues (II) and (III), whose structures we reported recently (Glidewell *et al.*, 2004).The C—O distances in the carboxyl group of (I) (Table 1) are consistent with the fully ordered location of the carboxyl H atom as deduced from a difference map. The distance O3—N4 corresponds exactly with the mean value for the —O—N= bond in oximes (Allen *et al.*, 1987). The other distances are all typical of their types. The interbond angle at O3 is less than the idealized tetrahedral value, and those at N4, N11 and N12

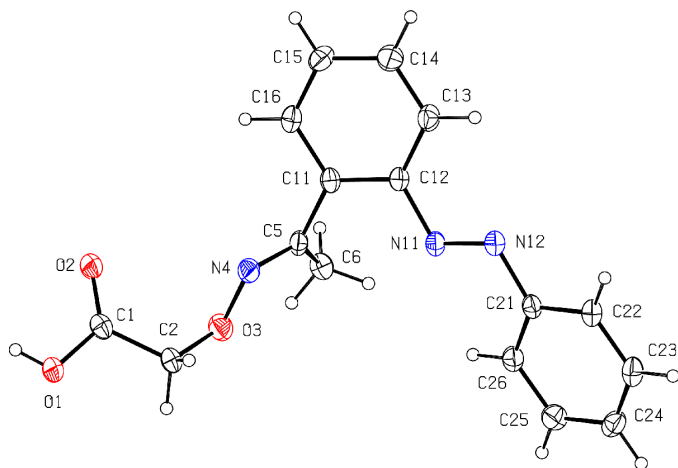


Figure 1
View of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

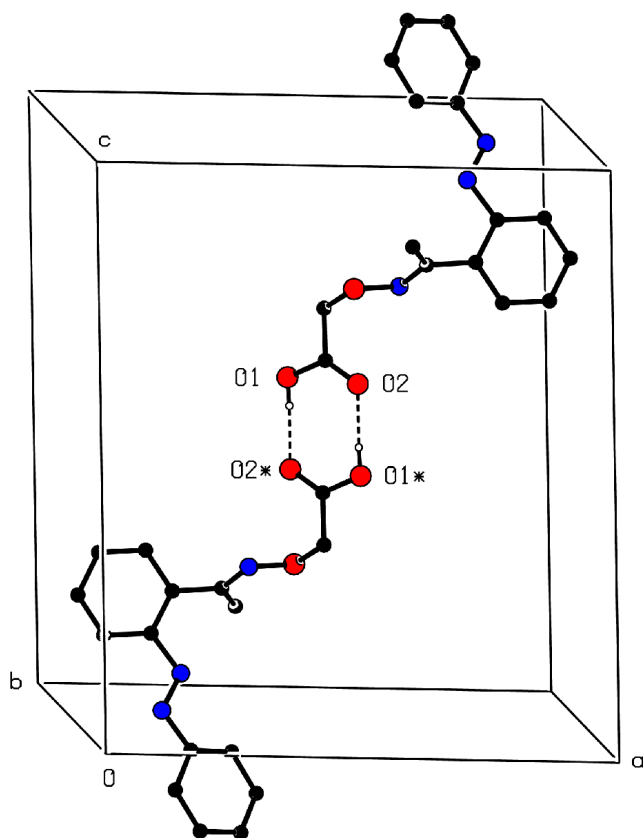


Figure 2
Part of the crystal structure of (I), showing the formation of an $R_2^2(8)$ dimer centred at (0.5, 0.5, 0.5). For the sake of clarity, H atoms bonded to C atoms have been omitted. Atoms marked with an asterisk (*) are at the symmetry position (1 - x, 1 - y, 1 - z).

are all significantly less than 120° , pointing in every case to the stereochemical influence of the unshared pairs of electrons. The angles at C5 indicate planarity at this atom. While the azobenzene fragment is effectively planar, as indicated by the key torsion angles (Table 1), the conformation of the side chain between O1 and C11 (Fig. 1) is not amenable to simple explanation. Compounds (I) and (III) have configurations at the C=N double bond [*viz.* (*E*) in (I) and (*Z*) in (III)] such

that the sterically smaller substituent at C5 is on the same side as the OCH_2COOH substituent.

The molecules of (I) are linked by paired, and nearly linear, $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2) into a centrosymmetric $R_2^2(8)$ (Bernstein *et al.*, 1995) dimer, selected for the sake of convenience to lie across the inversion centre at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ (Fig. 2). In this respect, the primary aggregation in (I) is the same as that in (II) and (III). The structure of (I) differs from that of (III), however, in that there are no direction-specific interactions between the dimers in (I), whereas those in (III) are linked into chains by a single aromatic $\pi-\pi$ stacking interaction.

Experimental

The title compound was prepared by reaction of $\text{ClCH}_2\text{CO}_2\text{H}$ with the oxime derived from 2-(PhN=N) $\text{C}_6\text{H}_4\text{COCH}_3$ (Forrester *et al.*, 1979), following the general procedure described recently (Glidewell *et al.*, 2004). Crystals suitable for single-crystal X-ray diffraction were grown by slow evaporation of a solution in ethanol (m.p. 420–421 K).

Crystal data

$\text{C}_{16}\text{H}_{15}\text{N}_3\text{O}_3$
 $M_r = 297.31$
Monoclinic, $P2_1/c$
 $a = 16.927(2) \text{ \AA}$
 $b = 4.5244(5) \text{ \AA}$
 $c = 19.673(2) \text{ \AA}$
 $\beta = 105.828(5)^\circ$
 $V = 1449.5(3) \text{ \AA}^3$
 $Z = 4$

$D_x = 1.362 \text{ Mg m}^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 3256 reflections
 $\theta = 3.7\text{--}27.6^\circ$
 $\mu = 0.10 \text{ mm}^{-1}$
 $T = 120(2) \text{ K}$
Block, colourless
 $0.24 \times 0.18 \times 0.10 \text{ mm}$

Data collection

Nonius KappaCCD diffractometer
 φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (SORTAV; Blessing, 1995, 1997)
 $T_{\text{min}} = 0.967$, $T_{\text{max}} = 0.990$
13 640 measured reflections
3256 independent reflections

1443 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.114$
 $\theta_{\text{max}} = 27.6^\circ$
 $h = -21 \rightarrow 21$
 $k = -5 \rightarrow 5$
 $l = -25 \rightarrow 23$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.069$
 $wR(F^2) = 0.187$
 $S = 0.95$
3256 reflections
201 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0887P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.33 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.30 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

C1—O1	1.306 (4)	C2—O3	1.419 (4)
C1—O2	1.216 (4)	O3—N4	1.416 (3)
C1—C2	1.497 (5)	N4—C5	1.321 (4)
C2—O3—N4	107.6 (2)	N4—C5—C6	126.8 (3)
O3—N4—C5	107.8 (2)	N4—C5—C11	114.1 (3)
N12—N11—C12	114.1 (2)	C6—C5—C11	119.0 (3)
N11—N12—C21	113.9 (3)	O1—C1—C2—O3	157.5 (3)
O1—C1—C2—O3	157.5 (3)	N4—C5—C11—C12	114.9 (3)
C1—C2—O3—N4	83.0 (3)	C11—C12—N11—N12	−171.6 (3)
C2—O3—N4—C5	174.9 (3)	C12—N11—N12—C21	−177.0 (2)
O3—N4—C5—C11	176.4 (2)	N11—N12—C21—C22	−169.2 (3)

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1-H1 \cdots O2^i$	0.82	1.84	2.655 (3)	175

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

All H atoms were located in difference maps and then treated as riding atoms in idealized positions, with distances $C-H = 0.95$ (aromatic), 0.98 (CH_3) or 0.99 Å (CH_2), and $O-H = 0.82$ Å, and with $U_{iso}(H) = 1.2U_{eq}(C,O)$ or $1.5U_{eq}(C_{methyl})$. The low proportion (ca 44%) of the reflections labelled observed, even at 120 (2) K, together with the rather high merging index (0.11), are suggestive of poorly diffracting crystals, which may in turn be associated with the very limited intermolecular aggregation.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England. The

authors thank the staff for all their help and advice. JNL thanks NCR Self-Service, Dundee, for grants which have provided computing facilities for this work. JLW thanks CNPq and FAPERJ for financial support.

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supporting information

Acta Cryst. (2004). E60, o1560–o1562 [https://doi.org/10.1107/S1600536804019877]

Hydrogen-bonded $R_2^2(8)$ dimers in (*E*)-{[2-(phenyldiazenyl)phenyl]ethylideneaminoxy}acetic acid

Christopher Glidewell, John N. Low, Janet M. S. Skakle and James L. Wardell

(*E*)-{[2-(phenyldiazenyl)phenyl]ethylideneaminoxy}acetic acid

Crystal data

$C_{16}H_{15}N_3O_3$

$M_r = 297.31$

Monoclinic, *P2/c*

Hall symbol: -P 2yc

$a = 16.927$ (2) Å

$b = 4.5244$ (5) Å

$c = 19.673$ (2) Å

$\beta = 105.828$ (5)°

$V = 1449.5$ (3) Å³

$Z = 4$

$F(000) = 624$

$D_x = 1.362$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3256 reflections

$\theta = 3.7$ – 27.6 °

$\mu = 0.10$ mm⁻¹

$T = 120$ K

Block, colourless

$0.24 \times 0.18 \times 0.10$ mm

Data collection

Nonius KappaCCD

diffractometer

Radiation source: rotating anode

Graphite monochromator

φ scans, and ω scans with κ offsets

Absorption correction: multi-scan

(SORTAV; Blessing, 1995, 1997)

$T_{\min} = 0.967$, $T_{\max} = 0.990$

13640 measured reflections

3256 independent reflections

1443 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.114$

$\theta_{\max} = 27.6$ °, $\theta_{\min} = 3.7$ °

$h = -21 \rightarrow 21$

$k = -5 \rightarrow 5$

$l = -25 \rightarrow 23$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.069$

$wR(F^2) = 0.187$

$S = 0.95$

3256 reflections

201 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0887P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.33$ e Å⁻³

$\Delta\rho_{\min} = -0.30$ e Å⁻³

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.46906 (14)	0.7971 (5)	0.54731 (11)	0.0437 (6)

O2	0.55689 (14)	0.4231 (6)	0.58201 (11)	0.0434 (6)
O3	0.57470 (13)	0.5937 (6)	0.72230 (11)	0.0446 (6)
N4	0.66025 (15)	0.5730 (7)	0.73040 (13)	0.0393 (7)
N11	0.80586 (15)	0.6485 (6)	0.90340 (12)	0.0324 (7)
N12	0.85988 (16)	0.7732 (6)	0.95175 (13)	0.0344 (7)
C1	0.52388 (19)	0.6478 (8)	0.59434 (16)	0.0356 (8)
C2	0.5416 (2)	0.7907 (8)	0.66556 (16)	0.0454 (9)
C5	0.69242 (19)	0.4093 (7)	0.78678 (15)	0.0334 (8)
C6	0.6478 (2)	0.2676 (8)	0.83366 (17)	0.0444 (9)
C11	0.78107 (19)	0.3522 (7)	0.79952 (15)	0.0319 (8)
C12	0.83809 (18)	0.4609 (7)	0.85880 (14)	0.0299 (7)
C13	0.9206 (2)	0.3874 (8)	0.87194 (17)	0.0396 (9)
C14	0.9458 (2)	0.2030 (8)	0.82658 (17)	0.0443 (9)
C15	0.8899 (2)	0.0953 (8)	0.76677 (17)	0.0430 (9)
C16	0.8080 (2)	0.1681 (8)	0.75322 (16)	0.0382 (8)
C21	0.82756 (19)	0.9473 (7)	0.99800 (14)	0.0322 (8)
C22	0.8830 (2)	1.1286 (7)	1.04418 (15)	0.0373 (8)
C23	0.8578 (2)	1.2983 (8)	1.09284 (16)	0.0415 (9)
C24	0.7775 (2)	1.2874 (8)	1.09551 (16)	0.0437 (9)
C25	0.7221 (2)	1.1054 (8)	1.04992 (17)	0.0439 (9)
C26	0.7466 (2)	0.9344 (7)	1.00096 (16)	0.0374 (8)
H1	0.4617	0.7184	0.5085	0.052*
H2A	0.5801	0.9515	0.6676	0.054*
H2B	0.4912	0.8748	0.6715	0.054*
H6A	0.5898	0.2978	0.8145	0.067*
H6B	0.6653	0.3540	0.8799	0.067*
H6C	0.6593	0.0595	0.8368	0.067*
H13	0.9587	0.4631	0.9115	0.048*
H14	1.0009	0.1502	0.8362	0.053*
H15	0.9076	-0.0262	0.7357	0.052*
H16	0.7705	0.0944	0.7131	0.046*
H22	0.9373	1.1364	1.0425	0.045*
H23	0.8952	1.4201	1.1238	0.050*
H24	0.7605	1.4027	1.1281	0.052*
H25	0.6679	1.0976	1.0521	0.053*
H26	0.7091	0.8118	0.9703	0.045*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0491 (14)	0.0479 (16)	0.0282 (12)	0.0134 (12)	0.0006 (11)	0.0019 (11)
O2	0.0488 (15)	0.0421 (16)	0.0332 (12)	0.0099 (12)	0.0011 (11)	0.0013 (11)
O3	0.0356 (14)	0.0591 (17)	0.0381 (13)	0.0006 (12)	0.0087 (10)	0.0011 (11)
N4	0.0253 (15)	0.0535 (19)	0.0371 (15)	-0.0034 (13)	0.0053 (12)	-0.0110 (14)
N11	0.0368 (16)	0.0308 (16)	0.0259 (13)	-0.0019 (13)	0.0020 (12)	-0.0003 (12)
N12	0.0359 (15)	0.0373 (17)	0.0276 (13)	-0.0019 (13)	0.0046 (12)	-0.0003 (12)
C1	0.0306 (19)	0.041 (2)	0.0333 (18)	-0.0016 (17)	0.0063 (15)	0.0072 (16)
C2	0.049 (2)	0.052 (2)	0.0281 (17)	0.0165 (18)	-0.0006 (15)	0.0035 (16)

C5	0.039 (2)	0.0326 (19)	0.0235 (15)	-0.0021 (15)	0.0005 (14)	-0.0035 (14)
C6	0.0361 (19)	0.051 (2)	0.0418 (19)	-0.0008 (17)	0.0028 (16)	-0.0037 (17)
C11	0.0352 (19)	0.0347 (19)	0.0239 (15)	-0.0021 (15)	0.0048 (14)	0.0045 (14)
C12	0.0324 (19)	0.0313 (18)	0.0248 (15)	-0.0037 (14)	0.0058 (14)	0.0009 (14)
C13	0.036 (2)	0.047 (2)	0.0341 (17)	-0.0071 (16)	0.0064 (15)	-0.0066 (16)
C14	0.038 (2)	0.052 (2)	0.045 (2)	-0.0031 (17)	0.0136 (17)	-0.0035 (18)
C15	0.047 (2)	0.046 (2)	0.0396 (19)	-0.0021 (18)	0.0177 (17)	-0.0096 (16)
C16	0.045 (2)	0.042 (2)	0.0256 (16)	-0.0035 (17)	0.0061 (15)	-0.0013 (15)
C21	0.0335 (19)	0.0349 (19)	0.0246 (15)	0.0007 (15)	0.0020 (14)	0.0025 (14)
C22	0.040 (2)	0.040 (2)	0.0279 (16)	-0.0051 (16)	0.0037 (15)	-0.0004 (15)
C23	0.049 (2)	0.039 (2)	0.0313 (17)	-0.0086 (17)	0.0019 (16)	-0.0012 (16)
C24	0.063 (3)	0.038 (2)	0.0303 (18)	0.0054 (18)	0.0146 (18)	-0.0007 (15)
C25	0.041 (2)	0.047 (2)	0.043 (2)	0.0021 (18)	0.0108 (17)	0.0007 (17)
C26	0.041 (2)	0.037 (2)	0.0297 (17)	-0.0004 (16)	0.0039 (15)	0.0002 (15)

Geometric parameters (Å, °)

C1—O1	1.306 (4)	C13—H13	0.93
C1—O2	1.216 (4)	C14—C15	1.382 (5)
C1—C2	1.497 (5)	C14—H14	0.93
O1—H1	0.82	C15—C16	1.378 (5)
C2—O3	1.419 (4)	C15—H15	0.93
C2—H2A	0.97	C16—H16	0.93
C2—H2B	0.97	N11—N12	1.259 (3)
O3—N4	1.416 (3)	N12—C21	1.421 (4)
N4—C5	1.321 (4)	C21—C22	1.383 (4)
C5—C11	1.475 (4)	C21—C26	1.389 (4)
C5—C6	1.488 (5)	C22—C23	1.382 (4)
C6—H6A	0.96	C22—H22	0.93
C6—H6B	0.96	C23—C24	1.376 (5)
C6—H6C	0.96	C23—H23	0.93
C11—C12	1.385 (4)	C24—C25	1.380 (5)
C11—C16	1.400 (4)	C24—H24	0.93
C12—C13	1.389 (4)	C25—C26	1.384 (4)
C12—N11	1.431 (4)	C25—H25	0.93
C13—C14	1.372 (5)	C26—H26	0.93
O2—C1—O1	124.6 (3)	C14—C13—H13	120.0
O2—C1—C2	124.2 (3)	C12—C13—H13	120.0
O1—C1—C2	111.2 (3)	C13—C14—C15	120.4 (3)
C1—O1—H1	109.5	C13—C14—H14	119.8
O3—C2—C1	113.6 (3)	C15—C14—H14	119.8
O3—C2—H2A	108.8	C16—C15—C14	119.9 (3)
C1—C2—H2A	108.8	C16—C15—H15	120.0
O3—C2—H2B	108.8	C14—C15—H15	120.0
C1—C2—H2B	108.8	C15—C16—C11	120.4 (3)
H2A—C2—H2B	107.7	C15—C16—H16	119.8
C2—O3—N4	107.6 (2)	C11—C16—H16	119.8

O3—N4—C5	107.8 (2)	C22—C21—C26	119.8 (3)
N12—N11—C12	114.1 (2)	C22—C21—N12	116.1 (3)
N11—N12—C21	113.9 (3)	C26—C21—N12	124.1 (3)
N4—C5—C6	126.8 (3)	C23—C22—C21	120.2 (3)
N4—C5—C11	114.1 (3)	C23—C22—H22	119.9
C6—C5—C11	119.0 (3)	C21—C22—H22	119.9
C5—C6—H6A	109.5	C24—C23—C22	120.0 (3)
C5—C6—H6B	109.5	C24—C23—H23	120.0
H6A—C6—H6B	109.5	C22—C23—H23	120.0
C5—C6—H6C	109.5	C23—C24—C25	120.0 (3)
H6A—C6—H6C	109.5	C23—C24—H24	120.0
H6B—C6—H6C	109.5	C25—C24—H24	120.0
C12—C11—C16	118.9 (3)	C24—C25—C26	120.4 (3)
C12—C11—C5	121.6 (3)	C24—C25—H25	119.8
C16—C11—C5	119.4 (3)	C26—C25—H25	119.8
C11—C12—C13	120.4 (3)	C25—C26—C21	119.5 (3)
C11—C12—N11	115.6 (3)	C25—C26—H26	120.3
C13—C12—N11	124.0 (3)	C21—C26—H26	120.3
C14—C13—C12	120.0 (3)		
O2—C1—C2—O3	-23.1 (5)	C13—C14—C15—C16	-1.4 (5)
O1—C1—C2—O3	157.5 (3)	C14—C15—C16—C11	0.4 (5)
C1—C2—O3—N4	83.0 (3)	C12—C11—C16—C15	0.4 (5)
C2—O3—N4—C5	174.9 (3)	C5—C11—C16—C15	-175.5 (3)
O3—N4—C5—C11	176.4 (2)	C11—C12—N11—N12	-171.6 (3)
O3—N4—C5—C6	0.6 (4)	C13—C12—N11—N12	8.3 (4)
N4—C5—C11—C12	114.9 (3)	C12—N11—N12—C21	-177.0 (2)
C6—C5—C11—C12	-68.9 (4)	N11—N12—C21—C22	-169.2 (3)
N4—C5—C11—C16	-69.4 (4)	N11—N12—C21—C26	13.7 (4)
C6—C5—C11—C16	106.8 (3)	C26—C21—C22—C23	-0.5 (5)
C16—C11—C12—C13	-0.1 (4)	N12—C21—C22—C23	-177.7 (3)
C5—C11—C12—C13	175.6 (3)	C21—C22—C23—C24	0.0 (5)
C16—C11—C12—N11	179.8 (3)	C22—C23—C24—C25	0.4 (5)
C5—C11—C12—N11	-4.5 (4)	C23—C24—C25—C26	-0.4 (5)
C11—C12—C13—C14	-0.9 (5)	C24—C25—C26—C21	0.0 (5)
N11—C12—C13—C14	179.3 (3)	C22—C21—C26—C25	0.5 (5)
C12—C13—C14—C15	1.6 (5)	N12—C21—C26—C25	177.5 (3)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots O2 ⁱ	0.82	1.84	2.655 (3)	175

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