Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

6,6′-[(1*E*,1′*E*)-Oxybis(4,1-phenylene)bis(azanylylidene)bis(methanylylidene)]bis(2-methylphenol): supramolecular assemblies in two dimensions mediated by weak C—H···N, C—H···O and C—H···π interactions

Received 12 March 2018
Accepted 17 April 2018

Edited by J. Jasinsk, Keene State College, USA

Keywords: crystal structure; oxybis Schiff base; T= 100 K; intermolecular interaction.

CCDC reference: 1435817

Supporting information: this article has supporting information at journals.iucr.org/e

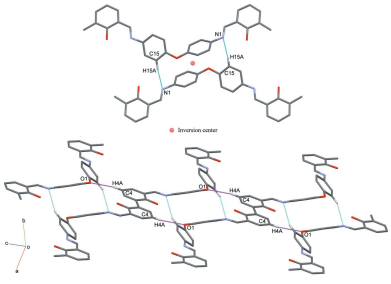
Md. Azharul Arafath,[a,b] Huey Chong Kwong,[a] Farook Adam[a]* and Mohd. R. Razali[a]

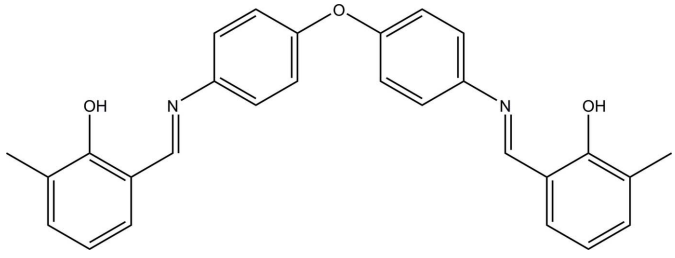
[a]School of Chemical Sciences, Universiti Sains Malaysia, Penang 11800 USM, Malaysia, and [b]Department of Chemistry, Shahjalal University of Science and Technology, Sylhet 3114, Bangladesh. *Correspondence e-mail: farook@usm.my

The title compound, $C_{28}H_{24}N_2O_3$, is a flexible Schiff base, having a dihedral angle of 59.53 (5)° between the mean planes of two phenyl rings bounded in the centre by a single O atom. The dihedral angles between the mean planes of the phenyl rings bonded to the central O atom and the mean planes of the terminal methylphenol rings are 31.47 (6) and 36.03 (5)°, respectively. The sp^2-hybridized character of the azanylylidene groups is confirmed by their bond lengths and bond angles. In the crystal, molecules are linked into centrosymmetric dimers by weak C—H···N interactions and connected into dimeric chains through weak C—H···O interactions. These chains are interconnected into a two-dimensional network parallel to (1$\bar{2}$1) *via* weak C—H···π interactions.

1. Chemical context

The oxybis Schiff base compound is an important group in chemistry. Bis-carbazones are formed by connecting *via* a ring or C—C bond to carbazone moieties having four coordinated sites. These tetradentate ligands can be used to entrap metal ions to form square-planer complexes (Alsop *et al.*, 2005; Blower *et al.*, 2003; Jasinski *et al.*, 2003). The length of the C—C bond in the backbone of the compounds affects the stability of the complexes. The higher the number of C—C bonds (obtained *via* alkylation or arylation) allows the cavity within the ligand to fit the metal ion with a proper orientation (Blower *et al.*, 2003). These tetradentate compounds and transition metal complexes have potential anticancer and antibacterial activity (Lobana *et al.*, 2009). The bis compounds chelate to transition metal ions *via* coordination sites to form complexes that may also exhibit fluorescent properties that could be used as biosensors and chemosensors (Liu *et al.*, 2011; Jiang & Guo, 2004).





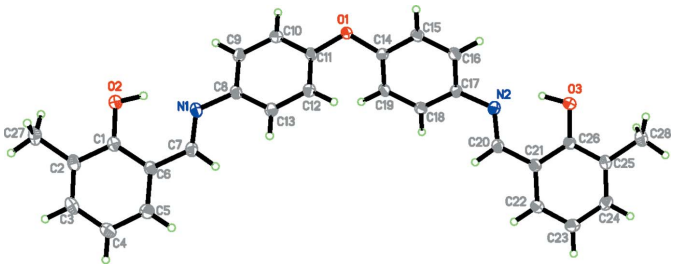


Figure 1
The title molecule with the atom-labelling scheme and 50% probability displacement ellipsoids.

In view of the above mentioned properties and of our research interest in the synthesis of oxybis Schiff base compounds, we present in this study the crystal structure and supramolecular features of the flexible Schiff base ligand 6,6′-{(1*E*,1′*E*)-[oxybis(4,1-phenylene)bis(azanylylidene)bis(methanylylidene)]bis(2-methylphenol}.

2. Structural commentary

In the title oxybisbenzenyl compound (Fig. 1), the mean planes of the phenyl rings bonded to the central oxygen atom form a dihedral angle of 59.53 (5)°, and the mean planes of the C1–C6 and C21–C26 methylphenol rings are twisted similarly by 31.47 (6) and 36.03 (5)°, respectively, from the adjacent phenyl rings. The terminal methylphenol rings are almost parallel to each other, forming a dihedral angle of 2.46 (6)° between their mean planes. The C7═N1 and C20═N2 bond lengths of 1.2880 (14) Å and 1.2834 (13) Å, confirm the presence of the double bonds while the C8—N1 and C17—N2 bond lengths, 1.4156 (12) and 1.4154 (12) Å, respectively, confirm their single-bond character. The C7—N1—C8, C17—N2—C20, N1—C7—C6 and N2—C20—C21 angles are 121.11 (9), 119.51 (9), 121.63 (9) and 122.42 (9)°, respectively. These values are consistent with a sp^2-hybridized character for atoms C7, C20, N1 and N2 (Khalaji *et al.*, 2012). Two intramolecular N—H···O hydrogen bonds occur (Table 1).

3. Supramolecular features

In the crystal, molecules are linked into centrosymmetric dimers by weak C15—H15*A*···N1 interactions forming an $R_2^2(18)$ ring motif (Fig. 2*a*, Table 1). These dimers are linked into chains propagating along [111] by weak C4—H4*A*···O1 interactions (Fig. 2*b*). At the same time, these dimeric chains are further connected into a two-dimensional network parallel to (121) *via* C—H···π interactions (Fig. 3, Table 1).

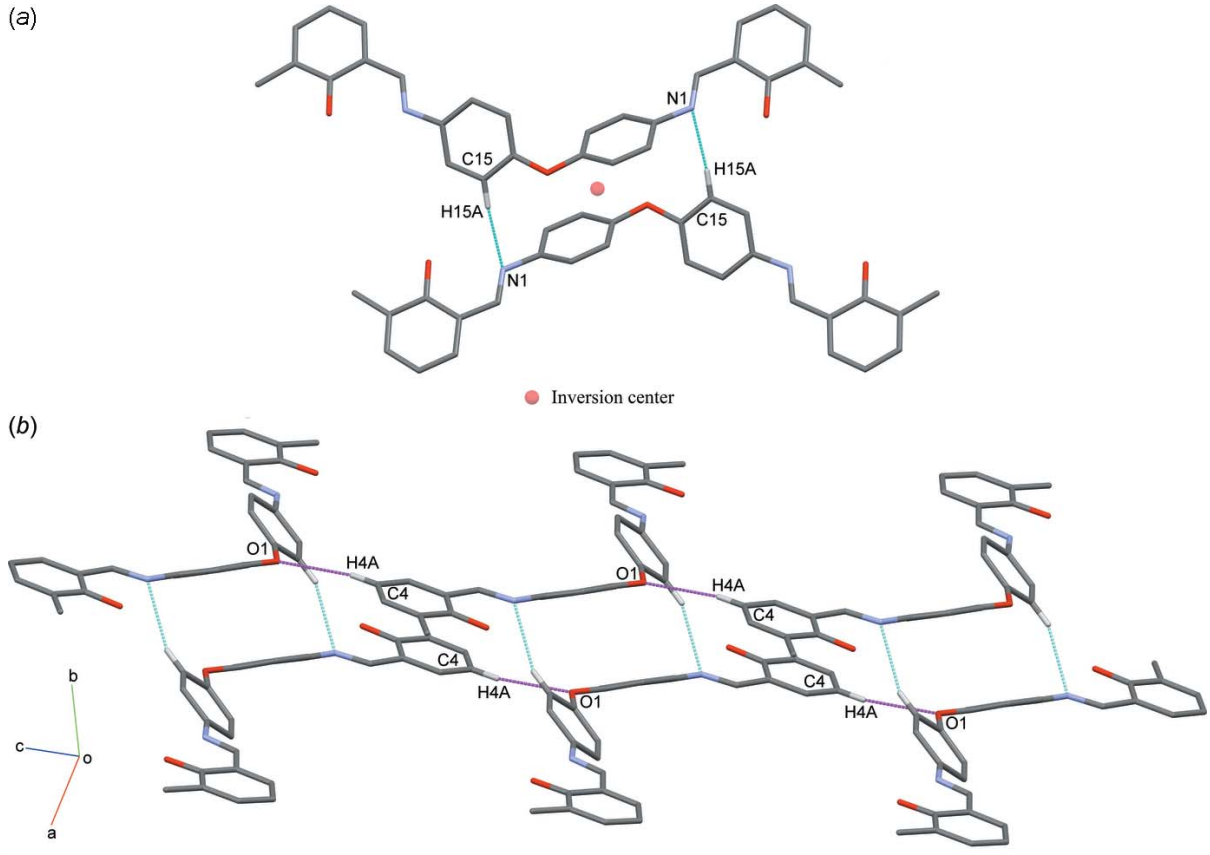


Figure 2
(*a*) A view of a centrosymmetric dimer of $C_{28}H_{24}N_2O_3$ with weak intermolecular C15—H15*A*···N1 interactions shown as cyan dotted lines. (*b*) A view of a dimeric chain with weak intermolecular C4—H4*A*···O1 shown as megenta lines. Hydrogen atoms not involved in with these interactions are omitted for clarity.

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the C14–C19 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H1*O*3···N2	0.99 (2)	1.73 (2)	2.6441 (13)	151.0 (17)
O2—H1*O*2···N1	0.91 (2)	1.76 (2)	2.6011 (13)	151.4 (18)
C15—H15*A*···N1^{i}	0.95	2.53	3.4211 (15)	156
C4—H4*A*···O1^{ii}	0.95	2.72	3.6626 (14)	171
C27—H27*A*···*Cg*1^{iii}	0.98	2.98	3.9242 (14)	162

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x+1, y+1, z+1$; (iii) $x+1, y+1, z$.

4. Synthesis and crystallization

To a sample of 2-hydroxy-3-methylbenzaldehyde (0.68 g, 5.00 mmol) dissolved in 20.0 ml methanol was added 0.20 ml glacial acetic acid and the mixture was refluxed for 30 min. A solution of 4,4′-oxydianiline (0.50 g, 2.50 mmol) in 20.0 ml methanol was then added dropwise with stirring to the aldehyde solution. The resulting yellow solution was refluxed for 4 h (Fig. 4). A yellow-coloured precipitate formed. The precipitate was filtered and washed with 5.0 ml ethanol and 5.0 ml *n*-hexane. The recovered product was dissolved in acetone for recrystallization. Yellow single crystals suitable for X-ray diffraction were obtained by slow evaporation of acetone.

6,6′-{(1*E*,1′*E*)-[Oxybis(4,1-phenylene)bis(azanylylidene)-bis(methanylylidene)]bis(2-methylphenol}: m.p. 398–399 K; yield 96%. IR (KBr pellets υ_{max}/cm^{-1}): 3430 υ(OH), 2884 υ(CH$_3$), 1612 υ(C═N), 1496 υ(C═C, aromatic), 1272 υ(C–H, aromatic), 1239 υ(C—O, ether), 1195 υ(C—O, phenol), 1081 υ(C—N). ^{1}H NMR (500 MHz, DMSO-d_6, Me$_4$Si ppm): δ 13.581 [*s* (1.97 H), OH], δ 8.952 [*s* (2.00 H), HC═N], δ 7.504–6.888 [multiplet (13.86 H), aromatic], δ 2.221 [*s* (6.11 H), Ph—CH$_3$H ppm. The ^{13}C NMR (DMSO-d_6, Me4Si ppm): δ 163.21 (C═N), δ 158.60–118.32 (C-aromatic), δ 15.13 (CH$_3$) ppm. Analysis calculated for $C_{28}H_{24}N_2O_3$ (FW: 436.51 g mol^{-1}) C, 77.00; H, 5.50; N, 6.42; found: C, 77.05; H, 5.48; N, 6.40%.

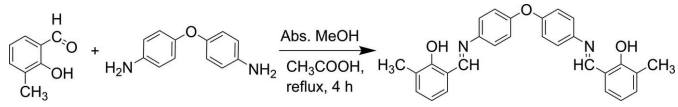


Figure 4
Reaction scheme for the synthesis of the title compound.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{28}H_{24}N_2O_3$
M_r	436.49
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, *b*, *c* (Å)	10.2293 (4), 10.9623 (4), 11.3087 (4)
α, β, γ (°)	108.5568 (10), 96.7616 (10), 110.4087 (10)
V (Å^3)	1088.76 (7)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.35 × 0.31 × 0.13
Data collection	
Diffractometer	Bruker APEXII DUO CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.903, 0.960
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	42726, 6513, 5433
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.711
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.045, 0.131, 1.03
No. of reflections	6513
No. of parameters	308
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.32

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS97* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2006) and *PLATON* (Spek, 2009).

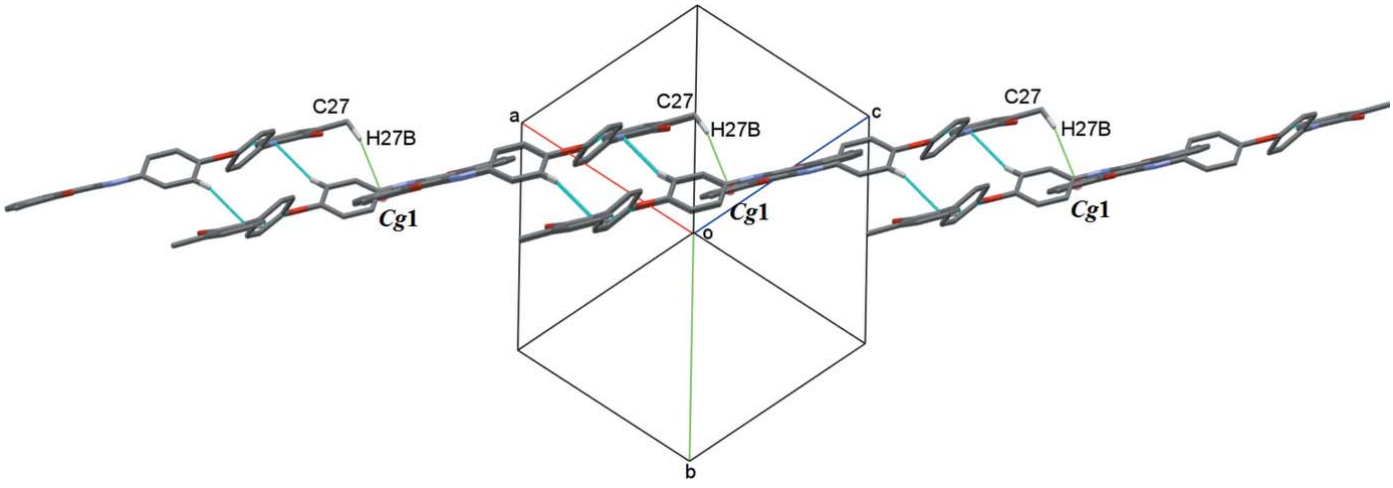


Figure 3
A view along (111) showing weak C—H···π (green dotted lines) supramolecular interactions in the title compound.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The phenolic hydrogen atoms were located in difference-Fourier maps and refined freely. All other H atoms attached calculated geometrically and refined using a riding model with C—H = 0.95–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C-methyl).

Funding information

The research was supported financially by the RU grant 1001/PKIMIA/811269 from Universiti Sains Malaysia. Universiti Sains Malaysia and The World Academy of Science are thanked for a USM–TWAS fellowship to MdAA. HCK thanks the Malaysian Government for a MyBrain15 scholarship.

References

Alsop, L., Cowley, A. R., Dilworth, J. R., Donnelly, P. S., Peach, J. M. & Rider, J. T. (2005). *Inorg. Chim. Acta*, **358**, 2770–2780.

Blower, P. J., Castle, T. C., Cowley, A. R., Dilworth, J. R., Donnelly, P. S., Labisbal, E., Sowrey, F. E., Teat, S. J. & Went, M. J. (2003). *Dalton Trans.* pp. 4416–4425.

Bruker (2012). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison. Wisconsin, USA.

Jasinski, J. P., Bianchani, J. R., Cueva, J., El-Saied, F. A., El-Asmy, A. A. & West, D. X. (2003). *Z. Anorg. Allg. Chem.* **629**, 202–206.

Jiang, P. & Guo, Z. (2004). *Coord. Chem. Rev.* **248**, 205–229.

Khalaji, A. D., Fejfarova, K. & Dusek, M. (2012). *J. Chem. Crystallogr.* **42**, 263–266.

Liu, K., Shi, W. & Cheng, P. (2011). *Dalton Trans.* **40**, 8475–8490.

Lobana, T. S., Sharma, R., Bawa, G. & Khanna, S. (2009). *Coord. Chem. Rev.* **253**, 977–1055.

Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2018). E**74**, 687-690 [https://doi.org/10.1107/S2056989018005959]

6,6′-[(1*E*,1′*E*)-Oxybis(4,1-phenylene)bis(azanylylidene)bis(methanylylidene)]bis-(2-methylphenol): supramolecular assemblies in two dimensions mediated by weak C—H···N, C—H···O and C—H···π interactions

Md. Azharul Arafath, Huey Chong Kwong, Farook Adam and Mohd. R. Razali

Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *SHELXL2013* (Sheldrick, 2015) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL2013* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

6,6′-[(1*E*,1′*E*)-Oxybis(4,1-phenylene)bis(azanylylidene)bis(methanylylidene)]bis(2-methylphenol)

Crystal data

$C_{28}H_{24}N_2O_3$
M_r = 436.49
Triclinic, $P\overline{1}$
a = 10.2293 (4) Å
b = 10.9623 (4) Å
c = 11.3087 (4) Å
α = 108.5568 (10)°
β = 96.7616 (10)°
γ = 110.4087 (10)°
V = 1088.76 (7) Å^3
Z = 2
$F(000)$ = 460
D_x = 1.331 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9984 reflections
θ = 2.2–30.2°
μ = 0.09 mm^{-1}
T = 100 K
Block, yellow
0.35 × 0.31 × 0.13 mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2012)
T_{min} = 0.903, T_{max} = 0.960
42726 measured reflections
6513 independent reflections
5433 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 30.4°, θ_{min} = 2.0°
h = −14→14
k = −15→15
l = −16→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.131
S = 1.03
6513 reflections
308 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0747P)^2 + 0.3053P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

Special details

Experimental. The following wavelength and cell were deduced by SADABS from the direction cosines etc. They are given here for emergency use only: CELL 0.71062 10.322 11.055 11.397 108.521 96.732 110.436

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.76527 (8)	0.48598 (7)	0.45322 (7)	0.01951 (16)
O2	1.54997 (8)	1.09474 (8)	0.70552 (7)	0.02197 (16)
O3	0.06378 (8)	0.07922 (8)	0.64561 (7)	0.02142 (16)
N1	1.29823 (9)	0.93739 (9)	0.71785 (9)	0.01841 (17)
N2	0.32630 (9)	0.26192 (9)	0.67203 (8)	0.01845 (17)
C1	1.57792 (11)	1.16561 (10)	0.83396 (10)	0.01812 (19)
C2	1.70943 (11)	1.28524 (11)	0.89546 (11)	0.0208 (2)
C3	1.73960 (11)	1.35727 (11)	1.02776 (11)	0.0237 (2)
H3A	1.8280	1.4382	1.0703	0.028*
C4	1.64482 (12)	1.31511 (11)	1.10050 (11)	0.0237 (2)
H4A	1.6693	1.3654	1.1912	0.028*
C5	1.51434 (11)	1.19879 (11)	1.03847 (10)	0.0218 (2)
H5A	1.4485	1.1701	1.0870	0.026*
C6	1.47866 (11)	1.12316 (10)	0.90474 (10)	0.01809 (19)
C7	1.33802 (11)	1.00598 (11)	0.84107 (10)	0.01925 (19)
H7A	1.2739	0.9794	0.8916	0.023*
C8	1.16198 (10)	0.82216 (10)	0.65723 (10)	0.01726 (19)
C9	1.09958 (11)	0.79317 (10)	0.52934 (10)	0.01908 (19)
H9A	1.1491	0.8497	0.4867	0.023*
C10	0.96575 (11)	0.68236 (10)	0.46405 (10)	0.01876 (19)
H10A	0.9225	0.6645	0.3778	0.023*
C11	0.89561 (10)	0.59785 (10)	0.52567 (9)	0.01665 (18)
C12	0.95985 (10)	0.62060 (10)	0.65062 (10)	0.01793 (19)
H12A	0.9136	0.5592	0.6905	0.022*
C13	1.09192 (10)	0.73371 (10)	0.71658 (10)	0.01777 (19)
H13A	1.1350	0.7511	0.8028	0.021*
C14	0.66246 (10)	0.43684 (10)	0.51590 (9)	0.01645 (18)
C15	0.57873 (10)	0.29247 (10)	0.46457 (10)	0.01831 (19)
H15A	0.5973	0.2321	0.3937	0.022*
C16	0.46798 (11)	0.23692 (10)	0.51734 (10)	0.01851 (19)
H16A	0.4099	0.1383	0.4817	0.022*
C17	0.44103 (10)	0.32475 (10)	0.62243 (9)	0.01667 (18)
C18	0.52465 (10)	0.47018 (10)	0.67105 (9)	0.01735 (19)
H18A	0.5059	0.5310	0.7414	0.021*

C19	0.63458 (10)	0.52671 (10)	0.61781 (9)	0.01706 (19)
H19A	0.6902	0.6257	0.6506	0.020*
C20	0.33650 (11)	0.31399 (11)	0.79342 (10)	0.01902 (19)
H20A	0.4225	0.3926	0.8481	0.023*
C21	0.22143 (10)	0.25721 (10)	0.85028 (9)	0.01744 (19)
C22	0.24188 (11)	0.31750 (11)	0.98398 (10)	0.0217 (2)
H22A	0.3289	0.3969	1.0353	0.026*
C23	0.13736 (12)	0.26316 (12)	1.04218 (11)	0.0247 (2)
H23A	0.1518	0.3047	1.1329	0.030*
C24	0.01010 (12)	0.14628 (12)	0.96590 (11)	0.0237 (2)
H24A	−0.0613	0.1085	1.0064	0.028*
C25	−0.01556 (11)	0.08364 (11)	0.83349 (10)	0.0201 (2)
C26	0.09098 (11)	0.14035 (10)	0.77475 (9)	0.01703 (18)
C27	1.81029 (12)	1.33195 (13)	0.81651 (12)	0.0279 (2)
H27A	1.7559	1.3335	0.7401	0.042*
H27B	1.8558	1.2660	0.7894	0.042*
H27C	1.8849	1.4267	0.8686	0.042*
C28	−0.15322 (12)	−0.04094 (12)	0.75086 (12)	0.0289 (2)
H28A	−0.1306	−0.1120	0.6897	0.043*
H28B	−0.2132	−0.0103	0.7032	0.043*
H28C	−0.2056	−0.0817	0.8058	0.043*
H1O3	0.153 (2)	0.131 (2)	0.6250 (18)	0.052 (5)*
H1O2	1.458 (2)	1.027 (2)	0.6813 (19)	0.056 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0152 (3)	0.0190 (3)	0.0165 (3)	0.0016 (3)	0.0049 (3)	0.0028 (3)
O2	0.0198 (4)	0.0216 (4)	0.0199 (4)	0.0045 (3)	0.0050 (3)	0.0068 (3)
O3	0.0221 (4)	0.0196 (3)	0.0162 (3)	0.0042 (3)	0.0033 (3)	0.0043 (3)
N1	0.0148 (4)	0.0158 (4)	0.0220 (4)	0.0048 (3)	0.0036 (3)	0.0060 (3)
N2	0.0165 (4)	0.0193 (4)	0.0205 (4)	0.0071 (3)	0.0064 (3)	0.0086 (3)
C1	0.0165 (4)	0.0169 (4)	0.0213 (5)	0.0074 (4)	0.0037 (4)	0.0075 (4)
C2	0.0165 (4)	0.0184 (4)	0.0269 (5)	0.0066 (4)	0.0030 (4)	0.0097 (4)
C3	0.0169 (4)	0.0191 (5)	0.0290 (5)	0.0056 (4)	−0.0009 (4)	0.0060 (4)
C4	0.0219 (5)	0.0230 (5)	0.0216 (5)	0.0105 (4)	0.0006 (4)	0.0032 (4)
C5	0.0197 (5)	0.0234 (5)	0.0217 (5)	0.0104 (4)	0.0045 (4)	0.0066 (4)
C6	0.0162 (4)	0.0169 (4)	0.0203 (5)	0.0069 (3)	0.0039 (4)	0.0062 (4)
C7	0.0153 (4)	0.0178 (4)	0.0239 (5)	0.0061 (4)	0.0059 (4)	0.0075 (4)
C8	0.0139 (4)	0.0155 (4)	0.0208 (5)	0.0056 (3)	0.0048 (3)	0.0053 (4)
C9	0.0192 (4)	0.0176 (4)	0.0200 (5)	0.0062 (4)	0.0068 (4)	0.0076 (4)
C10	0.0192 (4)	0.0191 (4)	0.0169 (4)	0.0075 (4)	0.0047 (4)	0.0060 (4)
C11	0.0137 (4)	0.0152 (4)	0.0180 (4)	0.0052 (3)	0.0043 (3)	0.0032 (3)
C12	0.0165 (4)	0.0178 (4)	0.0199 (5)	0.0067 (4)	0.0057 (4)	0.0077 (4)
C13	0.0163 (4)	0.0190 (4)	0.0183 (4)	0.0076 (4)	0.0042 (3)	0.0071 (4)
C14	0.0135 (4)	0.0183 (4)	0.0158 (4)	0.0053 (3)	0.0038 (3)	0.0057 (3)
C15	0.0175 (4)	0.0171 (4)	0.0171 (4)	0.0067 (4)	0.0042 (3)	0.0032 (4)
C16	0.0171 (4)	0.0156 (4)	0.0192 (4)	0.0046 (3)	0.0035 (3)	0.0048 (4)

C17	0.0136 (4)	0.0185 (4)	0.0165 (4)	0.0056 (3)	0.0031 (3)	0.0064 (3)
C18	0.0165 (4)	0.0175 (4)	0.0166 (4)	0.0069 (3)	0.0037 (3)	0.0049 (3)
C19	0.0151 (4)	0.0150 (4)	0.0172 (4)	0.0045 (3)	0.0027 (3)	0.0039 (3)
C20	0.0154 (4)	0.0183 (4)	0.0207 (5)	0.0052 (3)	0.0035 (3)	0.0066 (4)
C21	0.0166 (4)	0.0173 (4)	0.0173 (4)	0.0064 (3)	0.0039 (3)	0.0060 (4)
C22	0.0203 (5)	0.0204 (5)	0.0190 (5)	0.0053 (4)	0.0030 (4)	0.0048 (4)
C23	0.0264 (5)	0.0266 (5)	0.0183 (5)	0.0094 (4)	0.0069 (4)	0.0064 (4)
C24	0.0226 (5)	0.0252 (5)	0.0245 (5)	0.0083 (4)	0.0104 (4)	0.0113 (4)
C25	0.0177 (4)	0.0179 (4)	0.0228 (5)	0.0054 (4)	0.0046 (4)	0.0078 (4)
C26	0.0174 (4)	0.0156 (4)	0.0176 (4)	0.0071 (3)	0.0035 (3)	0.0058 (3)
C27	0.0200 (5)	0.0257 (5)	0.0348 (6)	0.0039 (4)	0.0055 (4)	0.0142 (5)
C28	0.0216 (5)	0.0248 (5)	0.0303 (6)	0.0009 (4)	0.0042 (4)	0.0089 (5)

Geometric parameters (Å, º)

O1—C11	1.3841 (11)	C12—H12A	0.9500
O1—C14	1.3864 (11)	C13—H13A	0.9500
O2—C1	1.3506 (13)	C14—C15	1.3885 (13)
O2—H1O2	0.91 (2)	C14—C19	1.3895 (13)
O3—C26	1.3456 (12)	C15—C16	1.3855 (14)
O3—H1O3	0.988 (19)	C15—H15A	0.9500
N1—C7	1.2880 (14)	C16—C17	1.3962 (14)
N1—C8	1.4156 (12)	C16—H16A	0.9500
N2—C20	1.2834 (13)	C17—C18	1.3985 (13)
N2—C17	1.4154 (12)	C18—C19	1.3864 (13)
C1—C2	1.4078 (14)	C18—H18A	0.9500
C1—C6	1.4097 (14)	C19—H19A	0.9500
C2—C3	1.3880 (16)	C20—C21	1.4521 (14)
C2—C27	1.5045 (15)	C20—H20A	0.9500
C3—C4	1.3956 (16)	C21—C22	1.3998 (14)
C3—H3A	0.9500	C21—C26	1.4122 (13)
C4—C5	1.3866 (15)	C22—C23	1.3792 (15)
C4—H4A	0.9500	C22—H22A	0.9500
C5—C6	1.4030 (14)	C23—C24	1.3962 (15)
C5—H5A	0.9500	C23—H23A	0.9500
C6—C7	1.4549 (14)	C24—C25	1.3819 (15)
C7—H7A	0.9500	C24—H24A	0.9500
C8—C13	1.3954 (14)	C25—C26	1.4058 (14)
C8—C9	1.3960 (14)	C25—C28	1.5027 (15)
C9—C10	1.3879 (14)	C27—H27A	0.9800
C9—H9A	0.9500	C27—H27B	0.9800
C10—C11	1.3870 (14)	C27—H27C	0.9800
C10—H10A	0.9500	C28—H28A	0.9800
C11—C12	1.3905 (14)	C28—H28B	0.9800
C12—C13	1.3874 (13)	C28—H28C	0.9800
C11—O1—C14	118.92 (7)	C16—C15—H15A	120.2
C1—O2—H1O2	105.6 (12)	C14—C15—H15A	120.2

C26—O3—H1O3	104.7 (11)	C15—C16—C17	120.52 (9)
C7—N1—C8	121.11 (9)	C15—C16—H16A	119.7
C20—N2—C17	119.51 (9)	C17—C16—H16A	119.7
O2—C1—C2	117.80 (9)	C16—C17—C18	118.95 (9)
O2—C1—C6	121.55 (9)	C16—C17—N2	117.94 (9)
C2—C1—C6	120.64 (9)	C18—C17—N2	123.08 (9)
C3—C2—C1	118.03 (10)	C19—C18—C17	120.84 (9)
C3—C2—C27	122.46 (10)	C19—C18—H18A	119.6
C1—C2—C27	119.49 (10)	C17—C18—H18A	119.6
C2—C3—C4	122.38 (10)	C18—C19—C14	119.21 (9)
C2—C3—H3A	118.8	C18—C19—H19A	120.4
C4—C3—H3A	118.8	C14—C19—H19A	120.4
C5—C4—C3	119.06 (10)	N2—C20—C21	122.42 (9)
C5—C4—H4A	120.5	N2—C20—H20A	118.8
C3—C4—H4A	120.5	C21—C20—H20A	118.8
C4—C5—C6	120.60 (10)	C22—C21—C26	119.10 (9)
C4—C5—H5A	119.7	C22—C21—C20	119.12 (9)
C6—C5—H5A	119.7	C26—C21—C20	121.75 (9)
C5—C6—C1	119.24 (9)	C23—C22—C21	120.85 (10)
C5—C6—C7	119.47 (9)	C23—C22—H22A	119.6
C1—C6—C7	121.25 (9)	C21—C22—H22A	119.6
N1—C7—C6	121.63 (9)	C22—C23—C24	119.09 (10)
N1—C7—H7A	119.2	C22—C23—H23A	120.5
C6—C7—H7A	119.2	C24—C23—H23A	120.5
C13—C8—C9	119.20 (9)	C25—C24—C23	122.23 (10)
C13—C8—N1	123.39 (9)	C25—C24—H24A	118.9
C9—C8—N1	117.33 (9)	C23—C24—H24A	118.9
C10—C9—C8	120.50 (9)	C24—C25—C26	118.34 (9)
C10—C9—H9A	119.7	C24—C25—C28	122.39 (10)
C8—C9—H9A	119.7	C26—C25—C28	119.27 (9)
C11—C10—C9	119.52 (9)	O3—C26—C25	117.66 (9)
C11—C10—H10A	120.2	O3—C26—C21	121.97 (9)
C9—C10—H10A	120.2	C25—C26—C21	120.37 (9)
O1—C11—C10	116.44 (9)	C2—C27—H27A	109.5
O1—C11—C12	122.74 (9)	C2—C27—H27B	109.5
C10—C11—C12	120.67 (9)	H27A—C27—H27B	109.5
C13—C12—C11	119.50 (9)	C2—C27—H27C	109.5
C13—C12—H12A	120.2	H27A—C27—H27C	109.5
C11—C12—H12A	120.2	H27B—C27—H27C	109.5
C12—C13—C8	120.47 (9)	C25—C28—H28A	109.5
C12—C13—H13A	119.8	C25—C28—H28B	109.5
C8—C13—H13A	119.8	H28A—C28—H28B	109.5
O1—C14—C15	116.46 (8)	C25—C28—H28C	109.5
O1—C14—C19	122.52 (9)	H28A—C28—H28C	109.5
C15—C14—C19	120.80 (9)	H28B—C28—H28C	109.5
C16—C15—C14	119.63 (9)		

O2—C1—C2—C3	−179.09 (9)	C11—O1—C14—C15	−144.71 (9)

C6—C1—C2—C3	1.68 (14)	C11—O1—C14—C19	40.71 (13)
O2—C1—C2—C27	2.00 (14)	O1—C14—C15—C16	−176.07 (8)
C6—C1—C2—C27	−177.23 (9)	C19—C14—C15—C16	−1.39 (15)
C1—C2—C3—C4	0.05 (16)	C14—C15—C16—C17	−0.68 (15)
C27—C2—C3—C4	178.92 (10)	C15—C16—C17—C18	1.97 (15)
C2—C3—C4—C5	−1.33 (16)	C15—C16—C17—N2	179.91 (9)
C3—C4—C5—C6	0.88 (16)	C20—N2—C17—C16	146.74 (10)
C4—C5—C6—C1	0.80 (15)	C20—N2—C17—C18	−35.40 (14)
C4—C5—C6—C7	−176.86 (9)	C16—C17—C18—C19	−1.23 (14)
O2—C1—C6—C5	178.69 (9)	N2—C17—C18—C19	−179.06 (9)
C2—C1—C6—C5	−2.11 (14)	C17—C18—C19—C14	−0.79 (14)
O2—C1—C6—C7	−3.69 (15)	O1—C14—C19—C18	176.47 (9)
C2—C1—C6—C7	175.51 (9)	C15—C14—C19—C18	2.12 (15)
C8—N1—C7—C6	179.01 (9)	C17—N2—C20—C21	178.32 (9)
C5—C6—C7—N1	177.01 (9)	N2—C20—C21—C22	178.44 (10)
C1—C6—C7—N1	−0.61 (15)	N2—C20—C21—C26	0.19 (15)
C7—N1—C8—C13	−30.61 (15)	C26—C21—C22—C23	0.78 (16)
C7—N1—C8—C9	152.59 (10)	C20—C21—C22—C23	−177.52 (10)
C13—C8—C9—C10	3.47 (15)	C21—C22—C23—C24	0.16 (17)
N1—C8—C9—C10	−179.59 (9)	C22—C23—C24—C25	−0.62 (17)
C8—C9—C10—C11	−1.67 (15)	C23—C24—C25—C26	0.10 (16)
C14—O1—C11—C10	−152.24 (9)	C23—C24—C25—C28	−179.15 (11)
C14—O1—C11—C12	32.17 (13)	C24—C25—C26—O3	−179.28 (9)
C9—C10—C11—O1	−177.53 (8)	C28—C25—C26—O3	0.00 (14)
C9—C10—C11—C12	−1.84 (15)	C24—C25—C26—C21	0.87 (15)
O1—C11—C12—C13	178.90 (9)	C28—C25—C26—C21	−179.86 (9)
C10—C11—C12—C13	3.49 (15)	C22—C21—C26—O3	178.85 (9)
C11—C12—C13—C8	−1.64 (15)	C20—C21—C26—O3	−2.90 (15)
C9—C8—C13—C12	−1.80 (15)	C22—C21—C26—C25	−1.30 (15)
N1—C8—C13—C12	−178.55 (9)	C20—C21—C26—C25	176.95 (9)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C14–C19 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H1*O3*···N2	0.99 (2)	1.73 (2)	2.6441 (13)	151.0 (17)
O2—H1*O2*···N1	0.91 (2)	1.76 (2)	2.6011 (13)	151.4 (18)
C15—H15*A*···N1^{i}	0.95	2.53	3.4211 (15)	156
C4—H4*A*···O1^{ii}	0.95	2.72	3.6626 (14)	171
C27—H27*A*···*Cg*1^{iii}	0.98	2.98	3.9242 (14)	162

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) *x*+1, *y*+1, *z*+1; (iii) *x*+1, *y*+1, *z*.