

Crystal structure of 1,3-bis[(*E*)-4-methoxybenzylideneamino]propan-2-ol

Augusto Rivera,^{a*} Ingrid Miranda-Carvajal,^a Jaime Ríos-Motta^a and Michael Bolte^b

^aUniversidad Nacional de Colombia, Sede Bogotá, Facultad de Ciencias, Departamento de Química, Cra 30 No. 45-03, Bogotá, Código Postal 111321, Colombia, and ^bInstitut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von Laue-Strasse 7, 60438 Frankfurt/Main, Germany. *Correspondence e-mail: ariverau@unal.edu.co

Received 18 October 2016

Accepted 22 October 2016

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

Keywords: crystal structure; hydrogen bonding; C—H...O interactions; Schiff bases.

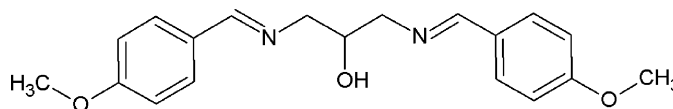
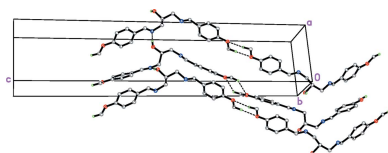
CCDC reference: 1511139

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

The title Schiff base, C₁₉H₂₂N₂O₃, was synthesized *via* the condensation reaction of 1,3-diaminopropan-2-ol with 4-methoxybenzaldehyde using water as solvent. The molecule exists in an *E,E* conformation with respect to the C=N imine bonds and the dihedral angle between the aromatic rings is 37.25 (15)°. In the crystal, O—H...N hydrogen bonds link the molecules into infinite *C*(5) chains propagating along the *a*-axis direction. The packing of these chains is consolidated by C—H...O interactions and C—H... π short contacts, forming a three-dimensional network.

1. Chemical context

Compounds containing the —C=N— (azomethine group) structure are known as Schiff bases, usually synthesized from the condensation of primary amines and active carbonyl groups (Bekdemir & Efil, 2014). Imines are one class of the most important and fundamental unsaturated organic compounds with a C=N double bond as their characteristic chemical bond and are extensively present in natural products and many drugs (Zhu *et al.*, 2010). The formation of imines underlies a discipline known as dynamic covalent chemistry (DCC), which is now used widely in the construction of exotic molecules and extended structures such as rotaxanes, catenanes, and so on (Patil & Adimurthy, 2013). Schiff base compounds derived from 1,*n*-diamines play an important role in coordination chemistry and have been studied extensively for their broad range of biological activities (Sahu *et al.* 2012; da Silva *et al.*, 2011; Przybylski *et al.* 2009; Dhar & Taploo, 1982). The common structural feature of these compounds is the presence of two azomethine groups linked by an *n*-methylene bridge, which can act as hydrogen-bond acceptors.



The title compound is interesting in that the presence of an OH group in the 1,3-diamine molecule is situated in a favorable position towards the azomethine groups to form an intramolecular hydrogen bond. Thus, one may expect that the charge distribution around the azomethine nitrogen atoms may be visibly perturbed by the presence of this type of interaction. Hence, 1,3-diaminepropan-2-ol was chosen with the expectation that the presence of an OH group would result

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 and Cg2 are the centroids of the C11–C16 and C21–C26 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–H1 \cdots N2 ⁱ	0.96 (5)	1.80 (5)	2.761 (4)	175 (4)
C17–H17B \cdots O3 ⁱⁱ	0.98	2.63	3.447 (5)	142
C27–H27B \cdots O2 ⁱⁱⁱ	0.98	2.65	3.415 (4)	135
C12–H12 \cdots Cg1 ^{iv}	0.95	2.99	3.658 (4)	129
C22–H22 \cdots Cg2 ^{iv}	0.95	2.92	3.628 (3)	132

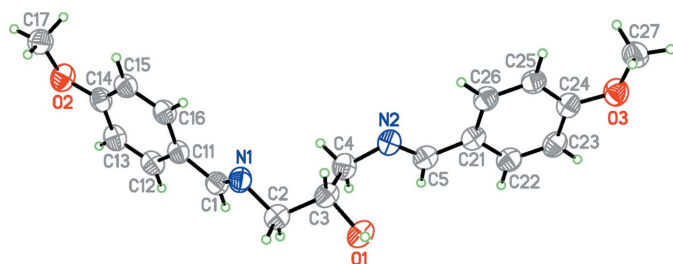
 Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, z$; (ii) $-x, -y + 1, z - \frac{1}{2}$; (iii) $-x, -y + 1, z + \frac{1}{2}$; (iv) $-x + \frac{1}{2}, y + \frac{3}{2}, z + \frac{1}{2}$.

in an intramolecular hydrogen bond. The title compound was synthesized quickly and efficiently by condensation of 1,3-diamine-2-propanol and *p*-methoxybenzaldehyde using a simple water-mediated procedure that requires neither a catalyst nor any additive (Rivera, *et al.*, 2016). To the best of our knowledge, no X-ray crystal structure of either the uncoordinated or the coordinated title compound has been reported previously.

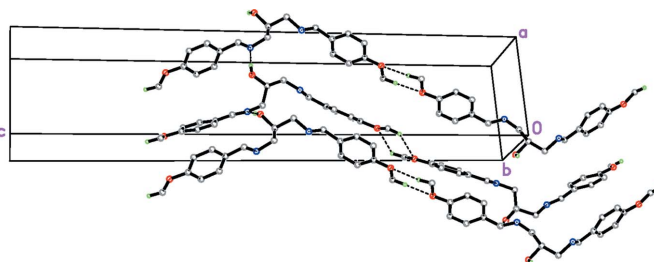
2. Structural commentary

The molecular structure of the title compound is illustrated in Fig. 1. The title compound exists in an *E,E* conformation with respect to the N1=C1 and N2=C5 azomethine bonds and the C2–N1=C1–C11 and C4–N2=C5–C21 torsion angles are 175.6 (3) and -178.3 (3)° respectively. The N1=C1 and N2=C5 distances of 1.265 (4) and 1.271 (4) Å, respectively, are consistent with C=N double bonding. The bond angles of 117.0 (3) and 117.7 (3)° around the N1 and N2 atoms confirm their *sp*² character. The slight differences between N=C distances and C–N=C angles are due to the significant effect of the hydrogen bond on the geometric parameters of the nitrogen atom (N2) involved in the intermolecular hydrogen bond (see below).

The N1–C2–C3–C4 torsion angle is -64.4 (4)° and the C2–C3–C4–N2 torsion angle is 175.0 (3)°. The O1–C3–C4–N2 torsion angle is -65.3 (3)°, which has a significant role to play in the hydrogen-bonding pattern in the crystal of the title compound (see below). The two methoxy substituents are essentially coplanar with their bound benzene rings with


Figure 1

The molecular structure of the title compound, Displacement ellipsoids are drawn at the 50% probability level.


Figure 2

Partial packing diagram of the title compound, showing an extended hydrogen-bonded network. H atoms not involved in hydrogen bonds have been omitted for clarity.

torsion angles C17–O2–C14–C13 = 169.3 (3)° and C27–O3–C24–C23 = -172.2 (3)°.

3. Supramolecular features

Rather than the proposed intramolecular O–H \cdots N hydrogen bond, adjacent molecules in the crystal of the title compound are linked by intermolecular O–H \cdots N hydrogen bonds (Table 1, Fig. 2), forming an infinite zigzag *C*(5) chains extending along the *a*-axis direction. The chains are further linked to neighbouring chains through a pair of weak C–H \cdots O hydrogen bonds (Table 1). Furthermore, C12–H12 and C22–H22 form weaker C–H \cdots Cg (π -ring) interactions (Table 1), which connect the chains of consecutive layers, thus forming a three-dimensional supramolecular network (Fig. 2).

Table 2

Experimental details.

Crystal data	
Chemical formula	C ₁₉ H ₂₂ N ₂ O ₃
M_r	326.38
Crystal system, space group	Orthorhombic, <i>Pna</i> 2 ₁
Temperature (K)	173
a, b, c (Å)	7.9081 (3), 5.8434 (3), 37.4435 (16)
V (Å ³)	1730.27 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.09
Crystal size (mm)	0.28 × 0.19 × 0.08
Data collection	
Diffractometer	Stoe <i>IPDS</i> II two-circle
Absorption correction	Multi-scan (<i>X-AREA</i> ; Stoe & Cie, 2001)
T_{\min}, T_{\max}	0.625, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12316, 3084, 2786
R_{int}	0.038
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.608
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.046, 0.123, 1.01
No. of reflections	3084
No. of parameters	224
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.15, -0.16

Computer programs: *X-AREA* (Stoe & Cie, 2001), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *XP* in *SHELXTL-Plus* (Sheldrick, 2008).

4. Database survey

No comparable structure of either the uncoordinated or the coordinated title compound has been found in the Cambridge Crystallographic Database.

5. Synthesis and crystallization

The title compound was prepared according to our published method (Rivera *et al.*, 2016). The crude product was dissolved in benzene and acetonitrile was added to the solution: upon slow evaporation of the solvent, colorless plates of the title compound arose. M.p. 403 K, yield 88%.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The hydroxyl H atom was refined freely; however, the remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with $d(\text{C}-\text{H}) = 0.95 \text{ \AA}$ for aromatic and azomethine atoms, $d(\text{C}-\text{H}) = 0.99 \text{ \AA}$ for methylene, $d(\text{C}-\text{H}) = 1.00 \text{ \AA}$ for C3-H3 and 0.98 \AA for CH₃ atoms. The U_{iso} values were constrained to be $1.5U_{\text{eq}}$ of the carrier atom for methyl H atoms and $1.2U_{\text{eq}}$ for the remaining H atoms. A rotating group model was used for the methyl groups. The absolute structure of the crystal chosen for data collection was indeterminate in the present refinement.

Acknowledgements

We acknowledge the Dirección de Investigaciones, Sede Bogotá (DIB) de la Universidad Nacional de Colombia for financial support of this work (research project No. 28427). IMC is also grateful to COLCIENCIAS for her doctoral scholarship

References

- Bekdemir, Y. & Efil, K. (2014). *Org. Chem. Int.* article ID 816487.
- Dhar, D. N. & Taploo, C. L. (1982). *J. Sci. Ind. Res.* **41**, 501–506.
- Patil, R. D. & Adimurthy, S. (2013). *Asia. J. Org. Chem.* **2**, 726–744.
- Przybylski, P., Huczynski, A., Pyta, K., Brzezinski, B. & Bartl, F. (2009). *Curr. Org. Chem.* **13**, 124–148.
- Rivera, A., Miranda-Carvajal, I. & Ríos-Motta, J. (2016). *Int. J. Chem.* **8**, 62–68.
- Sahu, R., Thakur, D. S. & Kashyap, P. (2012). *Int. J. Pharm. Sci. Nanotech.* **5**, 1757–1764.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Silva, C. M. da, da Silva, D. L., Modolo, L. V., Alves, R. B., de Resende, M. A., Martins, C. V. B., de Fátima, Á. & Ângelo, (2011). *J. Adv. Res.* **2**, 1–8.
- Stoe & Cie (2001). *X-Area* and *X-RED32*. Stoe & Cie, Darmstadt, Germany.
- Zhu, X.-Q., Liu, Q.-Y., Chen, Q. & Mei, L.-R. (2010). *J. Org. Chem.* **75**, 789–808.

supporting information

Acta Cryst. (2016). E72, 1731-1733 [https://doi.org/10.1107/S2056989016016947]

Crystal structure of 1,3-bis[(*E*)-4-methoxybenzylideneamino]propan-2-ol

Augusto Rivera, Ingrid Miranda-Carvajal, Jaime Ríos-Motta and Michael Bolte

Computing details

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA* (Stoe & Cie, 2001); data reduction: *X-AREA* (Stoe & Cie, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015).

1,3-Bis[(*E*)-4-methoxybenzylideneamino]propan-2-ol

Crystal data

C₁₉H₂₂N₂O₃

M_r = 326.38

Orthorhombic, *Pna*2₁

a = 7.9081 (3) Å

b = 5.8434 (3) Å

c = 37.4435 (16) Å

V = 1730.27 (13) Å³

Z = 4

F(000) = 696

D_x = 1.253 Mg m⁻³

Mo *Kα* radiation, λ = 0.71073 Å

Cell parameters from 12316 reflections

θ = 2.2–26.0°

μ = 0.09 mm⁻¹

T = 173 K

Plate, colourless

0.28 × 0.19 × 0.08 mm

Data collection

Stoe IPDS II two-circle
diffractometer

Radiation source: Genix 3D IμS microfocus X-
ray source

ω scans

Absorption correction: multi-scan
(*X-AREA*; Stoe & Cie, 2001)

T_{min} = 0.625, *T_{max}* = 1.000

12316 measured reflections

3084 independent reflections

2786 reflections with *I* > 2σ(*I*)

R_{int} = 0.038

θ_{max} = 25.6°, θ_{min} = 2.2°

h = -9→9

k = -7→7

l = -41→45

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.046

wR(*F*²) = 0.123

S = 1.01

3084 reflections

224 parameters

1 restraint

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

w = 1/[σ²(*F_o*²) + (0.0961*P*)²]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} < 0.001

Δρ_{max} = 0.15 e Å⁻³

Δρ_{min} = -0.16 e Å⁻³

Extinction correction: *SHELXL2014*
(Sheldrick, 2015),

*F_c** = *kF_c*[1 + 0.001*xF_c*²λ³/sin(2θ)]^{-1/4}

Extinction coefficient: 0.046 (8)

Special details

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.5510 (4)	0.4188 (4)	0.44173 (8)	0.0467 (6)
N2	0.3474 (4)	0.4764 (4)	0.54792 (8)	0.0453 (6)
O1	0.7066 (3)	0.4483 (4)	0.53519 (7)	0.0513 (6)
H1	0.754 (7)	0.302 (9)	0.5410 (13)	0.073 (13)*
O2	0.1888 (4)	0.4687 (4)	0.28786 (6)	0.0547 (6)
O3	0.0967 (3)	0.4509 (4)	0.71286 (7)	0.0542 (6)
C1	0.5258 (4)	0.5772 (6)	0.41931 (9)	0.0463 (7)
H1A	0.5738	0.7234	0.4238	0.056*
C2	0.6638 (5)	0.4706 (6)	0.47176 (9)	0.0518 (8)
H2A	0.6906	0.6361	0.4716	0.062*
H2B	0.7711	0.3856	0.4687	0.062*
C3	0.5858 (4)	0.4072 (5)	0.50766 (9)	0.0461 (7)
H3	0.5540	0.2416	0.5076	0.055*
C4	0.4306 (4)	0.5507 (5)	0.51505 (9)	0.0491 (8)
H4A	0.4637	0.7134	0.5173	0.059*
H4B	0.3507	0.5371	0.4948	0.059*
C5	0.3529 (4)	0.6102 (5)	0.57466 (9)	0.0448 (7)
H5	0.4082	0.7533	0.5717	0.054*
C11	0.4253 (4)	0.5452 (5)	0.38653 (9)	0.0414 (7)
C12	0.4251 (5)	0.7189 (5)	0.36069 (10)	0.0477 (7)
H12	0.4806	0.8597	0.3655	0.057*
C13	0.3447 (4)	0.6874 (6)	0.32820 (9)	0.0484 (8)
H13	0.3464	0.8057	0.3108	0.058*
C14	0.2617 (4)	0.4832 (5)	0.32098 (9)	0.0442 (7)
C15	0.2578 (4)	0.3105 (5)	0.34676 (9)	0.0436 (7)
H15	0.1994	0.1716	0.3421	0.052*
C16	0.3392 (4)	0.3430 (5)	0.37899 (8)	0.0437 (7)
H16	0.3365	0.2247	0.3964	0.052*
C17	0.1278 (5)	0.2506 (6)	0.27655 (10)	0.0553 (8)
H17A	0.2219	0.1415	0.2758	0.083*
H17B	0.0778	0.2645	0.2527	0.083*
H17C	0.0420	0.1961	0.2934	0.083*
C21	0.2798 (4)	0.5588 (5)	0.60975 (9)	0.0435 (7)
C22	0.3029 (4)	0.7163 (5)	0.63743 (9)	0.0472 (7)
H22	0.3628	0.8540	0.6328	0.057*
C23	0.2409 (5)	0.6766 (5)	0.67121 (9)	0.0499 (8)
H23	0.2581	0.7865	0.6896	0.060*
C24	0.1526 (4)	0.4751 (5)	0.67851 (9)	0.0445 (7)
C25	0.1277 (4)	0.3152 (5)	0.65135 (9)	0.0445 (7)

H25	0.0677	0.1776	0.6561	0.053*
C26	0.1910 (4)	0.3579 (5)	0.61733 (9)	0.0455 (7)
H26	0.1734	0.2485	0.5989	0.055*
C27	0.0252 (5)	0.2384 (6)	0.72315 (10)	0.0582 (9)
H27A	-0.0747	0.2069	0.7085	0.087*
H27B	-0.0079	0.2450	0.7484	0.087*
H27C	0.1086	0.1163	0.7197	0.087*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0514 (14)	0.0482 (13)	0.0404 (13)	-0.0007 (12)	0.0008 (12)	-0.0031 (12)
N2	0.0506 (15)	0.0425 (13)	0.0429 (14)	0.0044 (11)	-0.0030 (12)	-0.0012 (11)
O1	0.0585 (14)	0.0457 (12)	0.0498 (13)	0.0004 (11)	-0.0133 (11)	-0.0031 (10)
O2	0.0675 (16)	0.0507 (13)	0.0459 (14)	0.0031 (11)	-0.0074 (11)	0.0050 (10)
O3	0.0623 (15)	0.0522 (13)	0.0479 (13)	-0.0001 (11)	0.0034 (12)	-0.0082 (10)
C1	0.0470 (17)	0.0461 (16)	0.0459 (18)	-0.0049 (14)	0.0055 (14)	-0.0027 (13)
C2	0.0499 (18)	0.056 (2)	0.049 (2)	-0.0019 (14)	-0.0035 (15)	-0.0018 (14)
C3	0.0507 (17)	0.0425 (15)	0.0451 (17)	-0.0028 (13)	-0.0076 (14)	-0.0013 (13)
C4	0.0588 (18)	0.0434 (16)	0.0451 (18)	0.0032 (14)	-0.0021 (14)	0.0040 (14)
C5	0.0472 (17)	0.0373 (15)	0.0501 (18)	0.0021 (12)	-0.0068 (14)	0.0020 (13)
C11	0.0440 (16)	0.0396 (16)	0.0405 (16)	0.0009 (12)	0.0048 (13)	-0.0003 (12)
C12	0.0526 (18)	0.0377 (15)	0.0529 (18)	0.0008 (14)	0.0095 (14)	0.0011 (13)
C13	0.0595 (19)	0.0396 (16)	0.0462 (19)	0.0048 (13)	0.0062 (14)	0.0082 (13)
C14	0.0446 (16)	0.0453 (16)	0.0428 (17)	0.0074 (12)	0.0050 (14)	0.0021 (13)
C15	0.0464 (16)	0.0381 (16)	0.0464 (17)	-0.0004 (13)	0.0050 (13)	0.0016 (12)
C16	0.0482 (17)	0.0396 (15)	0.0432 (17)	0.0010 (13)	0.0043 (13)	0.0059 (13)
C17	0.0550 (19)	0.061 (2)	0.0503 (19)	-0.0044 (16)	-0.0028 (15)	0.0035 (15)
C21	0.0439 (16)	0.0383 (15)	0.0482 (18)	0.0037 (12)	-0.0056 (13)	-0.0018 (12)
C22	0.0511 (18)	0.0375 (16)	0.0530 (18)	-0.0005 (13)	-0.0054 (15)	-0.0027 (13)
C23	0.0587 (19)	0.0419 (15)	0.0491 (19)	0.0014 (15)	-0.0078 (15)	-0.0095 (13)
C24	0.0453 (16)	0.0438 (16)	0.0444 (17)	0.0066 (13)	-0.0016 (13)	-0.0049 (13)
C25	0.0459 (16)	0.0398 (16)	0.0478 (17)	-0.0018 (13)	-0.0018 (14)	-0.0040 (13)
C26	0.0486 (17)	0.0400 (15)	0.0478 (17)	0.0019 (13)	-0.0026 (14)	-0.0082 (13)
C27	0.060 (2)	0.062 (2)	0.0529 (19)	-0.0114 (17)	0.0086 (17)	-0.0079 (15)

Geometric parameters (Å, °)

N1—C1	1.265 (4)	C12—H12	0.9500
N1—C2	1.467 (5)	C13—C14	1.388 (5)
N2—C5	1.271 (4)	C13—H13	0.9500
N2—C4	1.461 (4)	C14—C15	1.397 (5)
O1—C3	1.426 (4)	C15—C16	1.381 (5)
O1—H1	0.96 (5)	C15—H15	0.9500
O2—C14	1.370 (4)	C16—H16	0.9500
O2—C17	1.427 (4)	C17—H17A	0.9800
O3—C24	1.367 (4)	C17—H17B	0.9800
O3—C27	1.418 (4)	C17—H17C	0.9800

C1—C11	1.474 (5)	C21—C26	1.397 (5)
C1—H1A	0.9500	C21—C22	1.398 (5)
C2—C3	1.525 (5)	C22—C23	1.376 (5)
C2—H2A	0.9900	C22—H22	0.9500
C2—H2B	0.9900	C23—C24	1.396 (5)
C3—C4	1.511 (5)	C23—H23	0.9500
C3—H3	1.0000	C24—C25	1.395 (4)
C4—H4A	0.9900	C25—C26	1.391 (5)
C4—H4B	0.9900	C25—H25	0.9500
C5—C21	1.466 (5)	C26—H26	0.9500
C5—H5	0.9500	C27—H27A	0.9800
C11—C16	1.393 (4)	C27—H27B	0.9800
C11—C12	1.402 (5)	C27—H27C	0.9800
C12—C13	1.385 (5)		
C1—N1—C2	117.0 (3)	O2—C14—C15	124.8 (3)
C5—N2—C4	117.7 (3)	C13—C14—C15	119.8 (3)
C3—O1—H1	106 (3)	C16—C15—C14	119.6 (3)
C14—O2—C17	117.8 (3)	C16—C15—H15	120.2
C24—O3—C27	118.4 (3)	C14—C15—H15	120.2
N1—C1—C11	123.0 (3)	C15—C16—C11	121.4 (3)
N1—C1—H1A	118.5	C15—C16—H16	119.3
C11—C1—H1A	118.5	C11—C16—H16	119.3
N1—C2—C3	112.3 (3)	O2—C17—H17A	109.5
N1—C2—H2A	109.1	O2—C17—H17B	109.5
C3—C2—H2A	109.1	H17A—C17—H17B	109.5
N1—C2—H2B	109.1	O2—C17—H17C	109.5
C3—C2—H2B	109.1	H17A—C17—H17C	109.5
H2A—C2—H2B	107.9	H17B—C17—H17C	109.5
O1—C3—C4	108.6 (3)	C26—C21—C22	117.9 (3)
O1—C3—C2	109.0 (3)	C26—C21—C5	123.5 (3)
C4—C3—C2	110.8 (3)	C22—C21—C5	118.5 (3)
O1—C3—H3	109.5	C23—C22—C21	121.6 (3)
C4—C3—H3	109.5	C23—C22—H22	119.2
C2—C3—H3	109.5	C21—C22—H22	119.2
N2—C4—C3	110.8 (3)	C22—C23—C24	120.0 (3)
N2—C4—H4A	109.5	C22—C23—H23	120.0
C3—C4—H4A	109.5	C24—C23—H23	120.0
N2—C4—H4B	109.5	O3—C24—C25	124.8 (3)
C3—C4—H4B	109.5	O3—C24—C23	115.7 (3)
H4A—C4—H4B	108.1	C25—C24—C23	119.5 (3)
N2—C5—C21	124.5 (3)	C26—C25—C24	119.8 (3)
N2—C5—H5	117.8	C26—C25—H25	120.1
C21—C5—H5	117.8	C24—C25—H25	120.1
C16—C11—C12	118.3 (3)	C25—C26—C21	121.2 (3)
C16—C11—C1	122.7 (3)	C25—C26—H26	119.4
C12—C11—C1	118.9 (3)	C21—C26—H26	119.4
C13—C12—C11	120.7 (3)	O3—C27—H27A	109.5

C13—C12—H12	119.7	O3—C27—H27B	109.5
C11—C12—H12	119.7	H27A—C27—H27B	109.5
C12—C13—C14	120.2 (3)	O3—C27—H27C	109.5
C12—C13—H13	119.9	H27A—C27—H27C	109.5
C14—C13—H13	119.9	H27B—C27—H27C	109.5
O2—C14—C13	115.4 (3)		
C2—N1—C1—C11	175.6 (3)	C13—C14—C15—C16	-1.2 (4)
C1—N1—C2—C3	129.7 (3)	C14—C15—C16—C11	0.2 (5)
N1—C2—C3—O1	176.2 (3)	C12—C11—C16—C15	1.1 (5)
N1—C2—C3—C4	-64.4 (4)	C1—C11—C16—C15	-174.5 (3)
C5—N2—C4—C3	110.7 (3)	N2—C5—C21—C26	-2.0 (5)
O1—C3—C4—N2	-65.3 (3)	N2—C5—C21—C22	176.6 (3)
C2—C3—C4—N2	175.0 (3)	C26—C21—C22—C23	0.1 (5)
C4—N2—C5—C21	-178.3 (3)	C5—C21—C22—C23	-178.6 (3)
N1—C1—C11—C16	5.1 (5)	C21—C22—C23—C24	0.1 (5)
N1—C1—C11—C12	-170.5 (3)	C27—O3—C24—C25	7.6 (5)
C16—C11—C12—C13	-1.6 (5)	C27—O3—C24—C23	-172.2 (3)
C1—C11—C12—C13	174.3 (3)	C22—C23—C24—O3	179.7 (3)
C11—C12—C13—C14	0.6 (5)	C22—C23—C24—C25	-0.1 (5)
C17—O2—C14—C13	169.3 (3)	O3—C24—C25—C26	-179.8 (3)
C17—O2—C14—C15	-10.5 (5)	C23—C24—C25—C26	0.1 (5)
C12—C13—C14—O2	-179.0 (3)	C24—C25—C26—C21	0.1 (5)
C12—C13—C14—C15	0.8 (5)	C22—C21—C26—C25	-0.2 (5)
O2—C14—C15—C16	178.6 (3)	C5—C21—C26—C25	178.4 (3)

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

Cg1 and Cg2 are the centroids of the C11—C16 and C21—C26 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots N2 ⁱ	0.96 (5)	1.80 (5)	2.761 (4)	175 (4)
C17—H17B \cdots O3 ⁱⁱ	0.98	2.63	3.447 (5)	142
C27—H27B \cdots O2 ⁱⁱⁱ	0.98	2.65	3.415 (4)	135
C12—H12 \cdots Cg1 ^{iv}	0.95	2.99	3.658 (4)	129
C22—H22 \cdots Cg2 ^{iv}	0.95	2.92	3.628 (3)	132

Symmetry codes: (i) $x+1/2, -y+1/2, z$; (ii) $-x, -y+1, z-1/2$; (iii) $-x, -y+1, z+1/2$; (iv) $-x+1/2, y+3/2, z+1/2$.