Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-{(*Z*)-[(2,3-Dihydroxypropyl)amino]-methylidene}naphthalen-2(1*H*)-one

Mehmet Akkurt,[a]* Peter N. Horton,[b] Shaaban K. Mohamed,[c,d] Antar A. Abdelhamid[e] and Mahmoud A. A. El Remaily[e]

[a]Department of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Turkey, [b]School of Chemistry, University of Southampton, Highfield, Southampton SO17 1BJ, England, [c]Chemistry and Environmental Division, Manchester Metropolitan University, Manchester M1 5GD, England, [d]Chemistry Department, Faculty of Science, Minia University, El-Minia, Egypt, and [e]Department of Chemistry, Sohag University, 82524 Sohag, Egypt
Correspondence e-mail: akkurt@erciyes.edu.tr

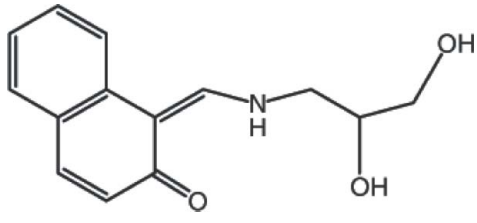
Received 12 December 2012; accepted 17 December 2012

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.058; wR factor = 0.156; data-to-parameter ratio = 14.4.

In the title molecule, $C_{14}H_{15}NO_3$, the ring system is essentially planar, with an r.m.s. deviation of 0.003 Å. The atoms of the ethane-1,2-diol group were refined as disordered over two sets of sites in a ratio of 0.815 (3):0.185 (3). The molecular conformation is stabilized in part by an intramolecular N—H···O hydrogen bond, which forms an S(6) ring. In the crystal, molecules are connected by N—H···O and O—H···O hydrogen bonds, forming a two-dimensional network parallel to (100). The network also features weak C—H···O hydrogen bonds. Weak C—H···π interactions also observed.

Related literature

For pharmaceutical and industrial applications of azomethines, see: Prakash & Adhikari (2011). For the effect of hydrophilicity on drug properties, see: Lin & Lu (1997). For standard bond lengths, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{14}H_{15}NO_3$
M_r = 245.27
Monoclinic, $P2_1/c$
a = 23.452 (16) Å
b = 5.809 (4) Å
c = 8.739 (6) Å
β = 96.445 (7)°
V = 1183.0 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 100 K
0.27 × 0.14 × 0.01 mm

Data collection

Rigaku AFC12 (Right) diffractometer
Absorption correction: multi-scan (*CrystalClear-SM Expert*; Rigaku, 2012)
T_{min} = 0.974, T_{max} = 0.999
8146 measured reflections
2650 independent reflections
2438 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.156
S = 1.11
2650 reflections
184 parameters
81 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C1–C5/C10 and C5–C10 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.88	1.87	2.560 (3)	135
N1—H1···O3A^{i}	0.88	2.56	3.166 (3)	127
O2A—H2A···O1^{ii}	0.84	1.83	2.663 (3)	175
O3A—H3A···O2A^{iii}	0.84	1.91	2.744 (3)	169
C12—H12B···O1^{iv}	0.99	2.60	3.174 (3)	117
C4—H4···*Cg*2^{v}	0.95	2.79	3.491 (3)	132
C9—H9···*Cg*1^{iv}	0.95	2.77	3.510 (3)	135

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$; (iii) $x, -y+\frac{5}{2}, z+\frac{1}{2}$; (iv) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (v) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *CrystalClear-SM Expert* (Rigaku, 2012); cell refinement: *CrystalClear-SM Expert*; data reduction: *CrystalClear-SM Expert*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON*.

This work was supported by the Ministry of Higher Education of Egypt under the collaporative PhD program 2012. The EPSRC National Crystallography Service is gratefully acknowledged for the X-ray diffraction measurementss. The authors are thankful to Manchester Metropolitan University, Sohag University and Erciyes Universitry for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5572).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Lin, J. H. & Lu, A. Y. H. (1997). *Pharmacol. Rev.* **49**, 403–449.
Prakash, A. & Adhikari, D. (2011). *Int. J. ChemTech Res.* **3**, 1891–1896.
Rigaku (2012). *CrystalClear-SM Expert*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supplementary materials

Acta Cryst. (2013). E**69**, o136–o137 [doi:10.1107/S1600536812051070]

1-{(*Z*)-[(2,3-Dihydroxypropyl)amino]methylidene}naphthalen-2(1*H*)-one

Mehmet Akkurt, Peter N. Horton, Shaaban K. Mohamed, Antar A. Abdelhamid and Mahmoud A. A. El Remaily

Comment

Azomethine compounds, which were named as Schiff's bases in 1864 are extensively incoporated in many pharmaceutical and food industry applications (Prakash & Adhikari, 2011). Elimination of excess drugs from the bloodstream or body is an essential process to protect against potential toxicity. In most cases the more hydrophilic drugs/pharmacophores are the more they are readily excreted by the kidneys in urine (Lin & Lu, 1997). The existance of conjugated double bonds and more hydroxylic groups in bioactive molecules increases not only their hydrophilicity but also the rate of their membrane absorption. Based on such facts we herein report the crystal structure of a potential bioactive hydrophilic azomethine derivative.

The molecluar structure of the title compound (I) is shown in Fig. 1. The naphthalene ring system (C1—C10) is essentially planar with an r.m.s. deviation of 0.003Å. The bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. In the crystal, molecules are connected by N—H···O and O—H···O hydrogen bonds to form a two-dimensional network parallel to (100). The network is further stabilized by weak C—H···O hydrogen bonds. Weak C—H···π interactions also observed. The O—H groups of the minor component of disorder are not considered in the description of the hydrogen bonding.

Experimental

A mixture of 1 mmol (172 mg) 2-hydroxynaphthalene-1-carbaldehyde and 1 mmol (91 mg) 3-aminopropane-1,2-diol in 40 ml ethanol was refluxed and monitored by TLC till completion after 12 h. On cooling of the reaction mixture at room temperature a quantitaive solid product was deposited, filtered and washed with cold ethanol. The crude product was crystallized from ethanol to afford x-ray quality yellow plates (m.p 505 K) in an excellent yield (90.6%) on a slow evaporation at room temperature for 24 h.

Refinement

All H-atoms were placed in calculated positions and refined by using a riding model with O—H = 0.84 Å, N—H = 0.88 Å, C—H = 0.95 Å (aromatic), 0.99 Å (methylene) and 1.00 Å (methine), and with U_{iso}(H) = 1.5U_{eq}(O) for hydroxyl and U_{iso}(H) = 1.2U_{eq}(C) for the other atoms. The atoms of the ethane-1,2-diol group are disordered over two sets of sites with occupancies 0.815 (3) and 0.185 (3).

Computing details

Data collection: *CrystalClear-SM Expert* (Rigaku, 2012); cell refinement: *CrystalClear-SM Expert* (Rigaku, 2012); data reduction: *CrystalClear-SM Expert* (Rigaku, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

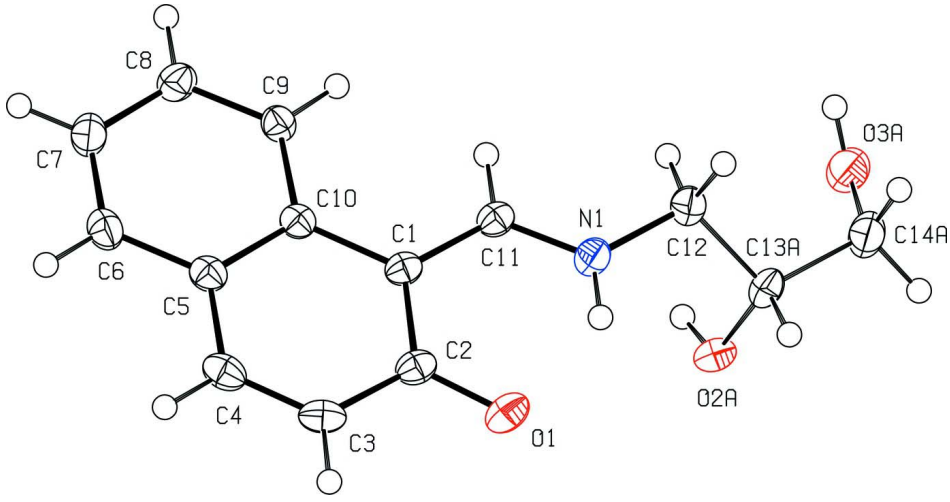


Figure 1

The molecular structure of the title compound with ellipsoids drawn at the 50% probability level. Only the major components of disorder are shown.

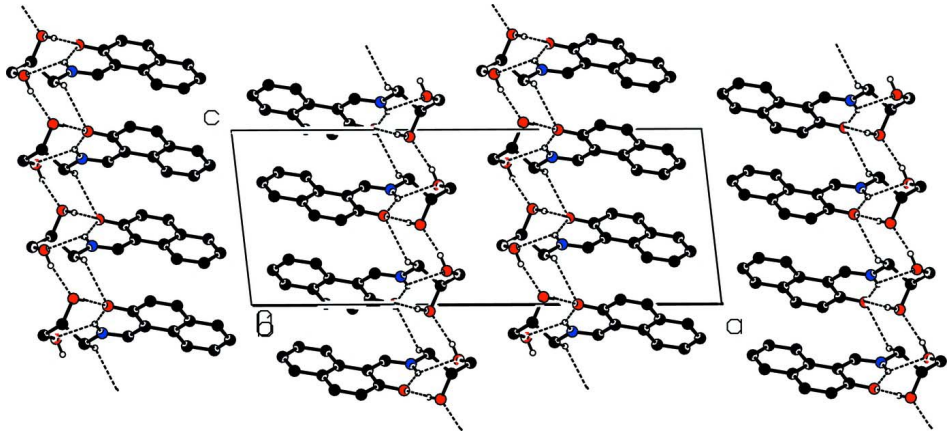


Figure 2

Crystal packing of (I) viewed along the *b* axis. Only the major component of disorder is shown. The hydrogen atoms not involved in the hydrogen bonds have been omitted for clarity.

1-{(*Z*)-[(2,3-Dihydroxypropyl)amino]methylidene}naphthalen- 2(1*H*)-one

Crystal data

$C_{14}H_{15}NO_3$
$M_r = 245.27$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 23.452$ (16) Å
$b = 5.809$ (4) Å
$c = 8.739$ (6) Å
$\beta = 96.445$ (7)°
$V = 1183.0$ (14) Å^3
$Z = 4$

$F(000) = 520$
$D_x = 1.377$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Cell parameters from 2698 reflections
$\theta = 2.4$–27.6°
$\mu = 0.10$ mm^{-1}
$T = 100$ K
Sheet, yellow
0.27 × 0.14 × 0.01 mm

Data collection

Rigaku AFC12 (Right) diffractometer
Radiation source: Rotating Anode
Detector resolution: 28.5714 pixels mm^{-1}
profile data from ω–scans
Absorption correction: multi-scan (*CrystalClear-SM Expert*; Rigaku, 2012)
T_{min} = 0.974, T_{max} = 0.999

8146 measured reflections
2650 independent reflections
2438 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 27.5°, θ_{min} = 3.5°
h = −30→30
k = −7→7
l = −11→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.156
S = 1.11
2650 reflections
184 parameters
81 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
$w = 1/[\sigma^2(F_o^2) + (0.0733P)^2 + 0.7284P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.30508 (5)	0.3921 (2)	0.50408 (16)	0.0291 (4)	
O2A	0.37874 (6)	1.0576 (3)	0.45655 (17)	0.0239 (5)	0.815 (3)
O3A	0.42610 (7)	1.3999 (3)	0.6847 (2)	0.0333 (5)	0.815 (3)
N1	0.32519 (6)	0.7647 (3)	0.65713 (18)	0.0236 (4)	
C1	0.23196 (7)	0.5877 (3)	0.62006 (19)	0.0194 (5)	
C2	0.25288 (7)	0.4010 (3)	0.5343 (2)	0.0222 (5)	
C3	0.21329 (8)	0.2228 (3)	0.4789 (2)	0.0252 (5)	
C4	0.15774 (8)	0.2281 (3)	0.5059 (2)	0.0249 (5)	
C5	0.13503 (7)	0.4101 (3)	0.59118 (19)	0.0211 (5)	
C6	0.07683 (7)	0.4098 (3)	0.6178 (2)	0.0255 (5)	
C7	0.05463 (7)	0.5851 (3)	0.6992 (2)	0.0277 (5)	
C8	0.09095 (7)	0.7645 (3)	0.7572 (2)	0.0257 (5)	
C9	0.14798 (7)	0.7680 (3)	0.7335 (2)	0.0211 (5)	
C10	0.17201 (7)	0.5925 (3)	0.64858 (19)	0.0191 (5)	
C11	0.27077 (7)	0.7636 (3)	0.67604 (19)	0.0205 (5)	
C12	0.36595 (7)	0.9416 (3)	0.7169 (2)	0.0252 (5)	
C13A	0.40851 (18)	0.9966 (7)	0.6026 (5)	0.0238 (8)	0.815 (3)

C14A	0.4511 (3)	1.1822 (11)	0.6651 (7)	0.0321 (10)	0.815 (3)
O2B	0.4314 (4)	0.8181 (15)	0.5357 (10)	0.043 (2)*	0.185 (3)
O3B	0.4728 (6)	1.153 (3)	0.8021 (16)	0.082 (4)*	0.185 (3)
C13B	0.4028 (10)	1.008 (3)	0.591 (2)	0.028 (3)*	0.185 (3)
C14B	0.4461 (17)	1.192 (5)	0.653 (3)	0.032 (3)*	0.185 (3)
H4	0.13300	0.10710	0.46700	0.0300*	
H6	0.05260	0.28710	0.57900	0.0310*	
H7	0.01530	0.58460	0.71590	0.0330*	
H8	0.07590	0.88560	0.81380	0.0310*	
H9	0.17170	0.89070	0.77500	0.0250*	
H11	0.25630	0.88810	0.73060	0.0250*	
H12A	0.38710	0.88780	0.81480	0.0300*	0.815 (3)
H12B	0.34480	1.08320	0.73870	0.0300*	0.815 (3)
H13A	0.43090	0.85330	0.58790	0.0290*	0.815 (3)
H14A	0.47050	1.13040	0.76570	0.0380*	0.815 (3)
H14B	0.48070	1.19870	0.59380	0.0380*	0.815 (3)
H1	0.33820	0.65070	0.60460	0.0280*	
H2A	0.35380	1.15760	0.46900	0.0360*	0.815 (3)
H3	0.22650	0.09830	0.42190	0.0300*	
H3A	0.41610	1.40930	0.77390	0.0500*	0.815 (3)
H2B	0.45860	0.77900	0.60140	0.0640*	0.185 (3)
H3B	0.50210	1.07090	0.79770	0.1230*	0.185 (3)
H12C	0.39200	0.87960	0.80430	0.0300*	0.185 (3)
H12D	0.34520	1.07520	0.75410	0.0300*	0.185 (3)
H13B	0.37720	1.07550	0.50300	0.0330*	0.185 (3)
H14C	0.47610	1.20420	0.58210	0.0390*	0.185 (3)
H14D	0.42600	1.34240	0.65150	0.0390*	0.185 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0279 (7)	0.0284 (7)	0.0328 (8)	0.0057 (5)	0.0117 (5)	−0.0005 (5)
O2A	0.0279 (8)	0.0233 (8)	0.0218 (8)	0.0035 (6)	0.0084 (6)	−0.0008 (6)
O3A	0.0305 (9)	0.0319 (9)	0.0388 (10)	−0.0010 (7)	0.0096 (7)	−0.0029 (7)
N1	0.0210 (7)	0.0253 (7)	0.0253 (8)	−0.0004 (6)	0.0056 (6)	0.0002 (6)
C1	0.0219 (8)	0.0192 (8)	0.0174 (8)	0.0022 (6)	0.0038 (6)	0.0024 (6)
C2	0.0258 (8)	0.0234 (8)	0.0182 (8)	0.0032 (6)	0.0054 (6)	0.0038 (6)
C3	0.0363 (10)	0.0202 (8)	0.0193 (9)	0.0047 (7)	0.0044 (7)	−0.0015 (6)
C4	0.0339 (9)	0.0191 (8)	0.0209 (9)	−0.0028 (7)	−0.0003 (7)	−0.0004 (6)
C5	0.0246 (8)	0.0212 (8)	0.0172 (8)	−0.0013 (6)	0.0008 (6)	0.0025 (6)
C6	0.0240 (8)	0.0267 (9)	0.0252 (9)	−0.0056 (7)	−0.0002 (7)	0.0005 (7)
C7	0.0208 (8)	0.0346 (10)	0.0274 (10)	−0.0030 (7)	0.0021 (6)	0.0023 (8)
C8	0.0233 (8)	0.0271 (9)	0.0272 (9)	0.0042 (7)	0.0046 (7)	−0.0018 (7)
C9	0.0206 (8)	0.0201 (8)	0.0222 (8)	−0.0007 (6)	0.0009 (6)	−0.0013 (6)
C10	0.0212 (8)	0.0194 (8)	0.0163 (8)	0.0006 (6)	0.0006 (6)	0.0029 (6)
C11	0.0219 (8)	0.0215 (8)	0.0186 (8)	0.0022 (6)	0.0040 (6)	0.0033 (6)
C12	0.0212 (8)	0.0295 (9)	0.0251 (9)	−0.0027 (7)	0.0032 (6)	−0.0002 (7)
C13A	0.0181 (13)	0.0256 (12)	0.0287 (14)	0.0030 (9)	0.0065 (12)	0.0002 (9)
C14A	0.0221 (19)	0.0333 (15)	0.0417 (19)	−0.0031 (13)	0.0076 (12)	−0.0039 (13)

Geometric parameters (Å, º)

O1—C2	1.282 (2)	C9—C10	1.415 (3)
O2A—C13A	1.429 (5)	C12—C13B	1.52 (2)
O2B—C13B	1.41 (2)	C12—C13A	1.523 (5)
O3A—C14A	1.412 (7)	C13A—C14A	1.528 (8)
O3B—C14B	1.40 (3)	C13B—C14B	1.53 (4)
O2A—H2A	0.8400	C3—H3	0.9500
O2B—H2B	0.8400	C4—H4	0.9500
O3A—H3A	0.8400	C6—H6	0.9500
O3B—H3B	0.8400	C7—H7	0.9500
N1—C12	1.460 (3)	C8—H8	0.9500
N1—C11	1.305 (2)	C9—H9	0.9500
N1—H1	0.8800	C11—H11	0.9500
C1—C11	1.418 (3)	C12—H12C	0.9900
C1—C2	1.436 (3)	C12—H12D	0.9900
C1—C10	1.455 (3)	C12—H12A	0.9900
C2—C3	1.438 (3)	C12—H12B	0.9900
C3—C4	1.350 (3)	C13A—H13A	1.0000
C4—C5	1.430 (3)	C13B—H13B	1.0000
C5—C10	1.424 (3)	C14A—H14A	0.9900
C5—C6	1.410 (3)	C14A—H14B	0.9900
C6—C7	1.377 (3)	C14B—H14C	0.9900
C7—C8	1.404 (3)	C14B—H14D	0.9900
C8—C9	1.376 (3)		

C13A—O2A—H2A	109.00	C3—C4—H4	119.00
C13B—O2B—H2B	109.00	C5—C4—H4	119.00
C14A—O3A—H3A	109.00	C7—C6—H6	120.00
C14B—O3B—H3B	109.00	C5—C6—H6	120.00
C11—N1—C12	124.65 (16)	C6—C7—H7	120.00
C12—N1—H1	118.00	C8—C7—H7	120.00
C11—N1—H1	118.00	C9—C8—H8	119.00
C2—C1—C10	119.81 (15)	C7—C8—H8	119.00
C10—C1—C11	121.46 (15)	C10—C9—H9	119.00
C2—C1—C11	118.72 (15)	C8—C9—H9	119.00
C1—C2—C3	118.30 (15)	C1—C11—H11	118.00
O1—C2—C1	121.88 (15)	N1—C11—H11	118.00
O1—C2—C3	119.81 (16)	N1—C12—H12C	110.00
C2—C3—C4	121.61 (16)	N1—C12—H12A	109.00
C3—C4—C5	122.07 (16)	N1—C12—H12B	109.00
C6—C5—C10	120.34 (15)	C13A—C12—H12B	109.00
C4—C5—C6	120.60 (16)	H12A—C12—H12B	108.00
C4—C5—C10	119.06 (15)	C13B—C12—H12C	107.00
C5—C6—C7	120.88 (16)	C13B—C12—H12D	112.00
C6—C7—C8	119.08 (15)	H12C—C12—H12D	108.00
C7—C8—C9	121.13 (16)	N1—C12—H12D	110.00
C8—C9—C10	121.29 (16)	C13A—C12—H12A	109.00
C5—C10—C9	117.27 (15)	O2A—C13A—H13A	108.00
C1—C10—C9	123.57 (15)	C14A—C13A—H13A	108.00

C1—C10—C5	119.15 (15)	C12—C13A—H13A	108.00
N1—C11—C1	123.96 (16)	O2B—C13B—H13B	108.00
N1—C12—C13B	108.8 (7)	C12—C13B—H13B	108.00
N1—C12—C13A	111.4 (2)	C14B—C13B—H13B	108.00
O2A—C13A—C14A	112.2 (4)	H14A—C14A—H14B	108.00
O2A—C13A—C12	110.3 (3)	C13A—C14A—H14B	109.00
C12—C13A—C14A	111.3 (4)	O3A—C14A—H14A	109.00
C12—C13B—C14B	109.2 (15)	O3A—C14A—H14B	109.00
O2B—C13B—C14B	110 (2)	C13A—C14A—H14A	109.00
O2B—C13B—C12	112.4 (12)	O3B—C14B—H14C	109.00
O3A—C14A—C13A	114.3 (5)	O3B—C14B—H14D	108.00
O3B—C14B—C13B	115 (2)	C13B—C14B—H14C	109.00
C2—C3—H3	119.00	C13B—C14B—H14D	108.00
C4—C3—H3	119.00	H14C—C14B—H14D	107.00

C12—N1—C11—C1	−178.57 (16)	C3—C4—C5—C6	−179.74 (17)
C11—N1—C12—C13A	−141.4 (2)	C4—C5—C6—C7	−179.69 (16)
C10—C1—C2—O1	178.69 (16)	C4—C5—C10—C9	−179.45 (16)
C11—C1—C2—C3	179.61 (16)	C10—C5—C6—C7	0.1 (3)
C10—C1—C2—C3	0.0 (2)	C4—C5—C10—C1	−0.5 (2)
C11—C1—C2—O1	−1.7 (3)	C6—C5—C10—C9	0.8 (2)
C11—C1—C10—C5	−179.31 (16)	C6—C5—C10—C1	179.68 (16)
C11—C1—C10—C9	−0.5 (3)	C5—C6—C7—C8	−0.6 (3)
C2—C1—C11—N1	−1.4 (3)	C6—C7—C8—C9	0.2 (3)
C10—C1—C11—N1	178.20 (16)	C7—C8—C9—C10	0.7 (3)
C2—C1—C10—C5	0.3 (2)	C8—C9—C10—C5	−1.1 (3)
C2—C1—C10—C9	179.17 (16)	C8—C9—C10—C1	180.00 (16)
O1—C2—C3—C4	−178.79 (17)	N1—C12—C13A—O2A	54.6 (3)
C1—C2—C3—C4	−0.1 (3)	N1—C12—C13A—C14A	179.9 (3)
C2—C3—C4—C5	−0.2 (3)	O2A—C13A—C14A—O3A	58.8 (5)
C3—C4—C5—C10	0.5 (3)	C12—C13A—C14A—O3A	−65.4 (5)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the C1–C5/C10 and C5–C10 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.88	1.87	2.560 (3)	135
N1—H1···O3*A*^{i}	0.88	2.56	3.166 (3)	127
O2*A*—H2*A*···O1^{ii}	0.84	1.83	2.663 (3)	175
O3*A*—H3*A*···O2*A*^{iii}	0.84	1.91	2.744 (3)	169
C12—H12*B*···O1^{iv}	0.99	2.60	3.174 (3)	117
C4—H4···*Cg*2^{v}	0.95	2.79	3.491 (3)	132
C9—H9···*Cg*1^{iv}	0.95	2.77	3.510 (3)	135

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*, *y*+1, *z*; (iii) *x*, −*y*+5/2, *z*+1/2; (iv) *x*, −*y*+3/2, *z*+1/2; (v) *x*, −*y*+1/2, *z*−1/2.