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Crystal structure of (*E*)-2-hydroxy-4′-methoxyazastilbene

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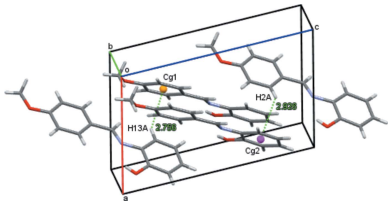
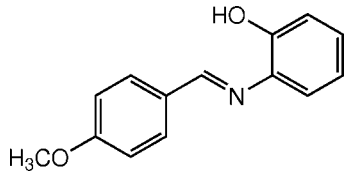
The title azastilbene derivative, $C_{14}H_{13}NO_2$ {systematic name: (*E*)-2-[(4-methoxybenzylidene)amino]phenol}, is a product of the condensation reaction between 4-methoxybenzaldehyde and 2-aminophenol. The molecule adopts an *E* conformation with respect to the azomethine C=N bond and is almost planar, the dihedral angle between the two substituted benzene rings being 3.29 (4)°. The methoxy group is coplanar with the benzene ring to which it is attached, the C_{methyl}—O—C—C torsion angle being −1.14 (12)°. There is an intramolecular O—H···N hydrogen bond generating an *S*(5) ring motif. In the crystal, molecules are linked *via* C—H···O hydrogen bonds, forming zigzag chains along [10$\bar{1}$]. The chains are linked *via* C—H···π interactions, forming a three-dimensional structure.

1. Chemical context

Azastilbenes have been reported to possess various biological activities such as antibacterial (Tamizh *et al.*, 2012), anti-oxidant (Cheng *et al.*, 2010; Lu *et al.*, 2012), antifungal (da Silva *et al.*, 2011) and antiproliferative (Fujita *et al.*, 2012) including lipoxygenase inhibitor (Aslam *et al.*, 2012*b*) activities. Pd^{II} and Ru^{III} complexes of azastilbenes have been synthesized and some have shown potent antibacterial activity (Briel *et al.*, 1998; Prabhakaran *et al.*, 2008; Puthilibai *et al.*, 2009). The interesting biological activities of azastilbenes have attracted us to synthesis a series of azastilbenes, including the title compound, and to study their antibacterial and anti-oxidant activities (Kaewmanee *et al.*, 2013, 2014). The anti-bacterial assay for the title compound indicated that it possesses moderate to weak antibacterial activity against *B. subtilis*, *S. aureus*, *P. aeruginosa*, *S. typhi* and *S. sonnei* with the MIC values in the range of 37.5 to 150 µg/ml. In addition, it also shows interesting antioxidant activity by DPPH assay with the IC_{50} value of 0.080±0.0004 µg/ml. Herein, we report on the synthesis, spectroscopic and crystallographic characterization of the title compound.





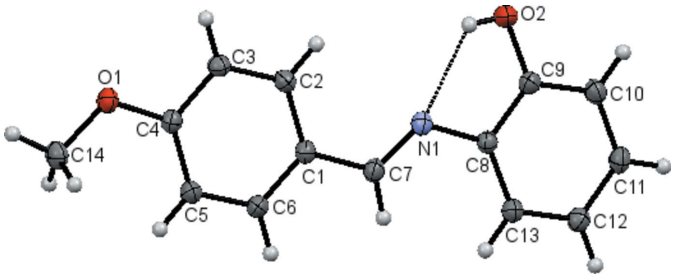


Figure 1
The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 60% probability level. The intramolecular O—H···N hydrogen bond is shown as a dashed line (see Table 1).

2. Structural commentary

The title azastilbene compound (Fig. 1) has an *E* conformation about the azomethine C7═N1 double bond [1.2825 (10) Å], the C8—N1—C7—C1 torsion angle being −178.67 (8)°. The molecule is almost planar with a dihedral angle of 3.29 (4)° between the two substituted benzene rings. The methoxy group is co-planar with the benzene ring to which it is attached, the C14—O1—C4—C5 torsion angle being −1.14 (12)°. There is an intramolecular O—H···N hydrogen bond (Fig. 1 and Table 1) that generates an *S*(5) ring motif. The bond lengths are comparable with those found for some closely related structures (Habibi *et al.*, 2013; Aslam *et al.*, 2012*a*; Kaewmanee *et al.*, 2013, 2014; Sun *et al.*, 2011).

3. Supramolecular features

In the crystal, molecules are linked *via* C—H···O hydrogen bonds, forming zigzag chains along [10$\bar{1}$] (Fig. 2 and Table 1). The chains are linked *via* C—H···π interactions (Fig. 3 and Table 1), forming a three-dimensional structure.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.36; Groom & Allen, 2014) for azastilbenes gave over 2800 hits. A search for 2-(benzylideneamino)phenols gave 78 hits, and for 2-[(4-methoxybenzylidene)amino]phenols there were five hits. In the compound that most closely resembles the title compound, namely 5-{[(2-hydroxyphenyl)imino]-methyl}-2-methoxyphenol (Habibi *et al.*, 2013), the two aromatic rings are inclined to one another by *ca* 16.9°.

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

*Cg*1 and *Cg*2 are the centroids of rings C1–C6 and C8–C13, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1*O2*···N1	0.774 (18)	2.078 (17)	2.6315 (11)	128.7 (17)
C14—H14*B*···O2^{i}	0.96	2.71	3.2876 (12)	119
C2—H2*A*···*Cg*2^{ii}	0.93	2.93	3.5662 (9)	127
C13—H13*A*···*Cg*1^{iii}	0.93	2.76	3.4671 (9)	134

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

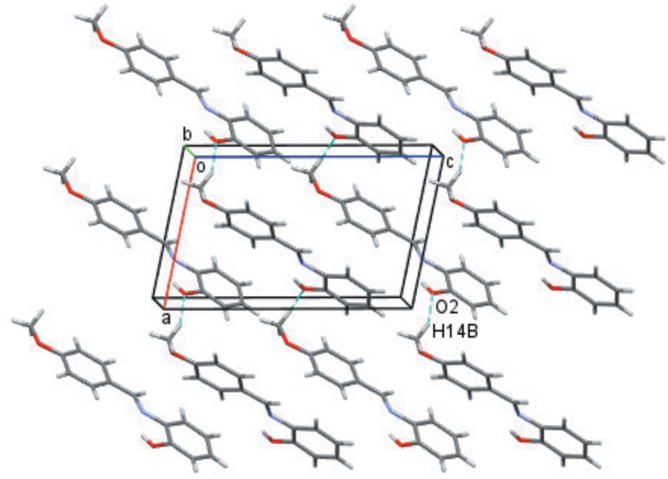


Figure 2
A view along the *b* axis of the crystal packing of the title compound. The C—H···O hydrogen bonds are shown as dashed lines (see Table 1 for details).

5. Synthesis and crystallization

A solution of 4-methoxybenzaldehyde (2.5 mmol, 0.37 g) in water (20 ml) and 2-aminophenol (2.5 mmol, 0.25 g) in water (20 ml) were mixed and stirred at room temperature for around 8 h until a white precipitate appeared. The resulting white solid was filtered, washed several times with cold ethanol and then dried *in vacuo* overnight to yield the desired azastilbene (430 mg, 76% yield). Colourless block-shaped crystals, suitable for X-ray structure analysis, were obtained by recrystallization from methanol by slow evaporation at room temperature after several days (m.p. 388–390 K).

UV–Vis (CH_3OH) λ_{max} (logε): 275 (1.93), 340 (0.61) nm; FT–IR (KBr) ν: 3337, 1595, 1510, 1248, 1027 cm^{-1}.; ^{1}H NMR (300 MHz, DMSO-d_6) δ, p.p.m.: 8.87 (*s*, 1H), 8.61 (*s*, 1H), 7.98 (*d*, *J* = 8.7 Hz, 2H), 7.18 (*dd*, *J* = 7.5, 1.2 Hz, 1H), 7.06 (*d*, *J* = 8.7 Hz, 2H), 7.03 (*td*, *J* = 7.5, 1.2 Hz, 1H), 6.83 (*td*, *J* = 7.5, 1.2 Hz, 1H), 6.09 (*dd*, *J* = 7.5, 1.2 Hz, 1H), 3.84 (*s*, –OCH_3). The UV–Vis spectroscopic data showed absorption bands of an azastilbene (275 and 340 nm) while the FT–IR spectrum

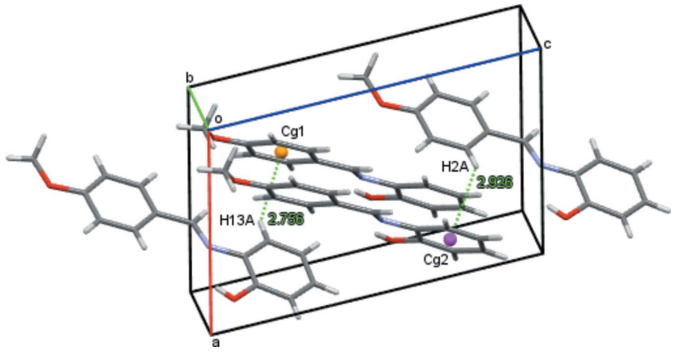


Figure 3
A view of the C—H···π interactions (dashed lines) in the crystal of the title compound (see Table 1 for details; ring centroids are shown as coloured spheres).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{13}NO_2$
M_r	227.25
Crystal system, space group	Monoclinic, *Pc*
Temperature (K)	100
a, *b*, *c* (Å)	8.0357 (3), 5.5554 (2), 12.8733 (5)
β (°)	101.312 (1)
V (Å^3)	563.52 (4)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.55 × 0.48 × 0.41
Data collection	
Diffractometer	Bruker APEXII D8 Venture
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.953, 0.964
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26314, 3449, 3414
R_{int}	0.023
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.715
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.100, 1.09
No. of reflections	3449
No. of parameters	160
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.28

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

exhibited the stretching vibrations of O—H (3337 cm^{-1}), C═N (1595 cm^{-1}), C═C (1510 cm^{-1}), C—N (1248 cm^{-1}1) and C—O (1027 cm^{-1}). The successful synthesis was also supported by the ^{1}H NMR spectroscopic data, which showed the characteristic signals of an olefinic proton at 8.61 (*s*, 1H) and *para*-substituted aromatic protons at 7.98 (*d*, *J* = 8.7 Hz, 2H) and 7.06 (*d*, *J* = 8.7 Hz, 2H), respectively. Moreover the ^{1}H NMR spectrum also showed typical signals of *ortho*-substituted aromatic protons at 7.18 (*dd*, *J* = 7.5, 1.2 Hz, 1H), 7.03 (*td*, *J* = 7.5, 1.2 Hz, 1H), 6.83 (*td*, *J* = 7.5, 1.2 Hz, 1H) and 6.09 (*dd*, *J* = 7.5, 1.2 Hz, 1H) and a methoxy proton at 3.84 (*s*, –OCH$_3$).

The antibacterial activity investigation of the title compound against Gram-positive bacteria, which are *B. subtilis*, *S. aureus*, MRSA and *E. faecalis*, and Gram-negative bacteria, which are *P. aeruginosa*, *S. sonnei* and *S. typhi*, showed moderate, mild or no inhibition. The most interesting antibacterial activity showed moderate activity against *P. aeruginosa* with an MIC value of 37.5 µg/ml.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The OH H atom was located in a difference Fourier map and freely refined. The C-bound H atoms were positioned geometrically and allowed to ride on their parent atoms: C—H = 0.93–0.96 Å with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for other H atoms.

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supporting information

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Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

(*E*)-2-[(4-Methoxybenzylidene)amino]phenol

Crystal data

$C_{14}H_{13}NO_2$
M_r = 227.25
Monoclinic, *Pc*
a = 8.0357 (3) Å
b = 5.5554 (2) Å
c = 12.8733 (5) Å
β = 101.312 (1)°
V = 563.52 (4) Å^3
Z = 2
F(000) = 240
D_x = 1.339 Mg m^{-3}
Melting point = 388–390 K
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 3449 reflections
θ = 2.6–30.5°
μ = 0.09 mm^{-1}
T = 100 K
Block, colorless
0.55 × 0.48 × 0.41 mm

Data collection

Bruker APEXII D8 Venture diffractometer
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.953, T_{max} = 0.964
26314 measured reflections
3449 independent reflections
3414 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 30.5°, θ_{min} = 2.6°
h = −11→11
k = −7→7
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.100
S = 1.09
3449 reflections
160 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0786P)^2 + 0.0298P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}

$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.054 (8)

Special details

Experimental. The data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness 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 threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) 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}
O1	0.29289 (8)	0.08802 (12)	0.07528 (5)	0.01815 (14)
O2	0.92146 (10)	0.70962 (12)	0.58775 (6)	0.02323 (15)
H1O2	0.859 (2)	0.653 (3)	0.5407 (15)	0.028 (3)*
N1	0.72131 (9)	0.33548 (14)	0.53665 (5)	0.01630 (16)
C1	0.54115 (10)	0.13926 (16)	0.38967 (6)	0.01455 (16)
C2	0.55623 (10)	0.31817 (15)	0.31478 (7)	0.01598 (16)
H2A	0.6239	0.4524	0.3353	0.019*
C3	0.47132 (10)	0.29620 (15)	0.21094 (7)	0.01586 (16)
H3A	0.4826	0.4149	0.1618	0.019*
C4	0.36790 (10)	0.09459 (15)	0.17945 (6)	0.01416 (16)
C5	0.35026 (11)	−0.08418 (16)	0.25290 (6)	0.01607 (17)
H5A	0.2812	−0.2171	0.2326	0.019*
C6	0.43785 (11)	−0.05985 (16)	0.35704 (6)	0.01649 (16)
H6A	0.4273	−0.1791	0.4061	0.020*
C7	0.63122 (10)	0.15284 (17)	0.49969 (6)	0.01611 (17)
H7A	0.6229	0.0242	0.5446	0.019*
C8	0.81013 (9)	0.34278 (15)	0.64262 (6)	0.01427 (16)
C9	0.91560 (10)	0.54613 (15)	0.66557 (6)	0.01633 (16)
C10	1.01507 (11)	0.57944 (17)	0.76609 (7)	0.01860 (17)
H10A	1.0854	0.7133	0.7803	0.022*
C11	1.00837 (11)	0.41075 (16)	0.84506 (7)	0.01799 (17)
H11A	1.0752	0.4309	0.9122	0.022*
C12	0.90092 (10)	0.21016 (17)	0.82364 (6)	0.01711 (16)
H12A	0.8951	0.0994	0.8770	0.021*
C13	0.80332 (10)	0.17641 (15)	0.72308 (6)	0.01595 (16)
H13A	0.7331	0.0424	0.7092	0.019*
C14	0.19195 (12)	−0.11830 (17)	0.03898 (7)	0.02058 (18)
H14A	0.1551	−0.1096	−0.0365	0.031*
H14B	0.0948	−0.1225	0.0720	0.031*
H14C	0.2582	−0.2615	0.0570	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0188 (3)	0.0212 (3)	0.0130 (3)	−0.0025 (2)	−0.0003 (2)	−0.0004 (2)
O2	0.0342 (3)	0.0193 (3)	0.0161 (3)	−0.0091 (3)	0.0045 (2)	0.0009 (2)
N1	0.0173 (3)	0.0180 (4)	0.0132 (3)	−0.0009 (2)	0.0019 (3)	−0.0010 (2)
C1	0.0157 (4)	0.0152 (3)	0.0125 (3)	−0.0003 (3)	0.0023 (3)	−0.0016 (3)
C2	0.0172 (4)	0.0142 (3)	0.0162 (4)	−0.0019 (3)	0.0024 (3)	−0.0010 (3)
C3	0.0170 (3)	0.0146 (3)	0.0155 (3)	−0.0005 (3)	0.0021 (3)	0.0013 (3)
C4	0.0133 (3)	0.0159 (4)	0.0132 (4)	0.0003 (3)	0.0026 (3)	−0.0010 (2)
C5	0.0177 (3)	0.0163 (4)	0.0142 (4)	−0.0031 (3)	0.0030 (3)	−0.0013 (3)
C6	0.0208 (4)	0.0158 (3)	0.0131 (3)	−0.0027 (3)	0.0039 (3)	−0.0002 (3)
C7	0.0176 (4)	0.0178 (4)	0.0131 (3)	−0.0008 (3)	0.0032 (3)	−0.0013 (3)
C8	0.0148 (3)	0.0150 (3)	0.0131 (3)	−0.0002 (3)	0.0029 (3)	−0.0014 (3)
C9	0.0183 (4)	0.0166 (3)	0.0148 (3)	−0.0022 (3)	0.0050 (3)	−0.0013 (3)
C10	0.0188 (4)	0.0196 (4)	0.0174 (3)	−0.0040 (3)	0.0036 (3)	−0.0042 (3)
C11	0.0172 (3)	0.0220 (4)	0.0141 (3)	−0.0008 (3)	0.0013 (3)	−0.0030 (3)
C12	0.0179 (4)	0.0184 (4)	0.0147 (4)	−0.0001 (3)	0.0025 (3)	0.0006 (3)
C13	0.0172 (3)	0.0162 (4)	0.0141 (4)	−0.0016 (3)	0.0023 (3)	−0.0005 (3)
C14	0.0194 (4)	0.0224 (4)	0.0178 (4)	−0.0031 (3)	−0.0015 (3)	−0.0028 (3)

Geometric parameters (Å, º)

O1—C4	1.3586 (9)	C6—H6A	0.9300
O1—C14	1.4287 (10)	C7—H7A	0.9300
O2—C9	1.3599 (11)	C8—C13	1.3973 (11)
O2—H1O2	0.772 (19)	C8—C9	1.4084 (11)
N1—C7	1.2825 (10)	C9—C10	1.3935 (11)
N1—C8	1.4107 (10)	C10—C11	1.3915 (13)
C1—C6	1.3972 (11)	C10—H10A	0.9300
C1—C2	1.4065 (11)	C11—C12	1.4035 (12)
C1—C7	1.4605 (10)	C11—H11A	0.9300
C2—C3	1.3818 (11)	C12—C13	1.3884 (11)
C2—H2A	0.9300	C12—H12A	0.9300
C3—C4	1.4062 (11)	C13—H13A	0.9300
C3—H3A	0.9300	C14—H14A	0.9600
C4—C5	1.3975 (11)	C14—H14B	0.9600
C5—C6	1.3932 (11)	C14—H14C	0.9600
C5—H5A	0.9300		
C4—O1—C14	117.25 (7)	C13—C8—C9	118.98 (7)
C9—O2—H1O2	101.3 (12)	C13—C8—N1	127.73 (7)
C7—N1—C8	121.55 (7)	C9—C8—N1	113.29 (7)
C6—C1—C2	118.64 (7)	O2—C9—C10	119.93 (8)
C6—C1—C7	118.99 (7)	O2—C9—C8	119.18 (7)
C2—C1—C7	122.36 (7)	C10—C9—C8	120.88 (7)
C3—C2—C1	120.54 (7)	C11—C10—C9	119.45 (8)
C3—C2—H2A	119.7	C11—C10—H10A	120.3

C1—C2—H2A	119.7	C9—C10—H10A	120.3
C2—C3—C4	120.07 (8)	C10—C11—C12	120.11 (8)
C2—C3—H3A	120.0	C10—C11—H11A	119.9
C4—C3—H3A	120.0	C12—C11—H11A	119.9
O1—C4—C5	124.37 (7)	C13—C12—C11	120.24 (8)
O1—C4—C3	115.38 (7)	C13—C12—H12A	119.9
C5—C4—C3	120.24 (7)	C11—C12—H12A	119.9
C6—C5—C4	118.88 (7)	C12—C13—C8	120.31 (8)
C6—C5—H5A	120.6	C12—C13—H13A	119.8
C4—C5—H5A	120.6	C8—C13—H13A	119.8
C5—C6—C1	121.63 (8)	O1—C14—H14A	109.5
C5—C6—H6A	119.2	O1—C14—H14B	109.5
C1—C6—H6A	119.2	H14A—C14—H14B	109.5
N1—C7—C1	122.48 (7)	O1—C14—H14C	109.5
N1—C7—H7A	118.8	H14A—C14—H14C	109.5
C1—C7—H7A	118.8	H14B—C14—H14C	109.5

C6—C1—C2—C3	−0.41 (12)	C2—C1—C7—N1	4.45 (12)
C7—C1—C2—C3	178.77 (7)	C7—N1—C8—C13	−6.46 (13)
C1—C2—C3—C4	0.40 (12)	C7—N1—C8—C9	173.81 (7)
C14—O1—C4—C5	−1.14 (12)	C13—C8—C9—O2	−179.42 (8)
C14—O1—C4—C3	177.64 (7)	N1—C8—C9—O2	0.34 (11)
C2—C3—C4—O1	−178.73 (7)	C13—C8—C9—C10	1.49 (12)
C2—C3—C4—C5	0.10 (12)	N1—C8—C9—C10	−178.75 (7)
O1—C4—C5—C6	178.14 (7)	O2—C9—C10—C11	−179.85 (8)
C3—C4—C5—C6	−0.58 (12)	C8—C9—C10—C11	−0.77 (13)
C4—C5—C6—C1	0.57 (13)	C9—C10—C11—C12	−0.61 (14)
C2—C1—C6—C5	−0.09 (13)	C10—C11—C12—C13	1.27 (13)
C7—C1—C6—C5	−179.29 (7)	C11—C12—C13—C8	−0.54 (13)
C8—N1—C7—C1	−178.67 (8)	C9—C8—C13—C12	−0.82 (12)
C6—C1—C7—N1	−176.38 (8)	N1—C8—C13—C12	179.45 (7)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of rings C1–C6 and C8–C13, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1*O*2···N1	0.774 (18)	2.078 (17)	2.6315 (11)	128.7 (17)
C14—H14*B*···O2^{i}	0.96	2.71	3.2876 (12)	119
C2—H2*A*···*Cg*2^{ii}	0.93	2.93	3.5662 (9)	127
C13—H13*A*···*Cg*1^{iii}	0.93	2.76	3.4671 (9)	134

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