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2,2′-[(1*E*,1′*E*)-1,2-Phenylenebis(azanylylidene)bis(methanylylidene)]bis(4-bromophenol)

Souad Dekar, Sabrina Bendia and Kamel Ouari*

Laboratoire d'Electrochimie, d'Ingénierie Moléculaire et de Catalyse Redox, Faculty of Technology, University of Ferhat Abbas Sétif-1, 19000-Sétif, Algeria. *Correspondence e-mail: k_ouari@yahoo.fr

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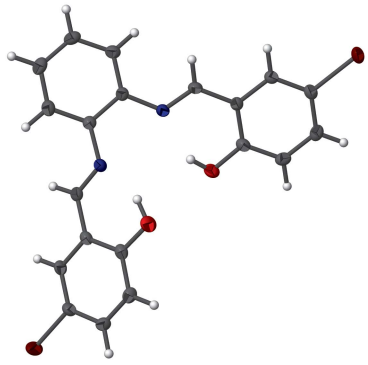
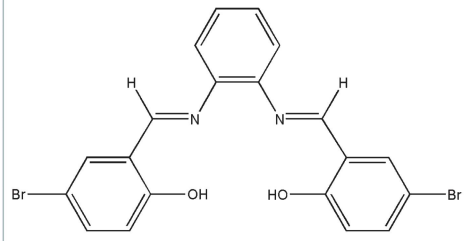
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{20}H_{14}Br_2N_2O_2$, there are two intramolecular O—H···N hydrogen bonds forming *S*(6) ring motifs. The outer benzene rings are inclined to the central benzene ring by 39.09 (11) and 24.31 (11)°, and to one another by 37.12 (11)°. In the crystal, molecules are linked by a short Br···O contact [3.1307 (19) Å], forming zigzag chains propagating along the *a*-axis direction. The chains are linked by weak offset π–π interactions [intercentroid distance = 3.716 (1) Å], forming layers parallel to the *ac* plane.

3D view



Chemical scheme



Structure description

Schiff base ligands are currently applied in coordination chemistry for the synthesis of transition metal complexes (Merzougui *et al.*, 2016; Ourari *et al.*, 2008; Ouari *et al.*, 2010, 2015; Majumder *et al.*, 2009; Salavati-Niasari *et al.*, 2008). A literature survey revealed that this kind of compound possesses diverse biological activities such as antianxiety, antidepressant (Jubie *et al.*, 2011) and anti-tumor, antibacterial, and fungicidal properties (Refat *et al.*, 2008; Kannan & Ramesh, 2006). We report herein on the synthesis, crystal structure and spectroscopic analysis of the title Schiff base compound.

The title compound, illustrated in Fig. 1, is photochromic and the molecule is not planar. The outer benzene rings (C8–C13 and C15–C20) are inclined to the central benzene ring (C1–C6) by 39.09 (11) and 24.31 (11)°, respectively, and to one another by 37.12 (11) °. There are two intramolecular O—H···N hydrogen bonds forming *S*(6) ring motifs (Fig. 1 and Table 1).

In the crystal, molecules are linked by a short Br2···O1($x + \frac{1}{2}$, y, $-z + \frac{1}{2}$) contact [3.1307 (19) Å], forming zigzag chains propagating along the *a*-axis direction (Fig. 2). Adjacent chains are linked by weak offset π–π interactions [$Cg1\cdots Cg2^{i,ii}$ = 3.716 (1) Å; *Cg*1 and *Cg*2 are the centroids of the C1–C6 and C8–C13 rings, respectively; symmetry

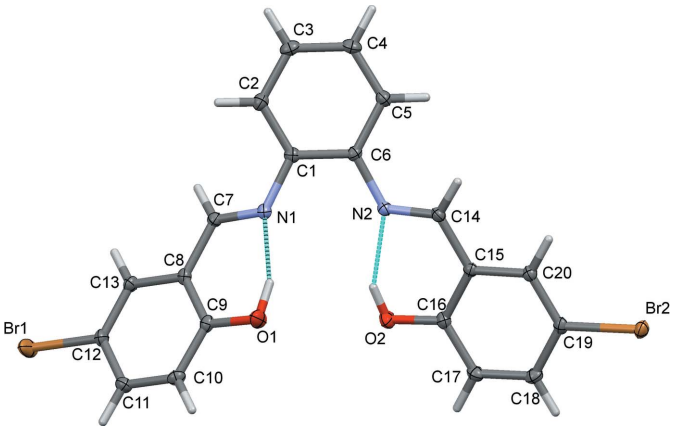


Figure 1
The molecular structure of the title compound, with the atom labelling and displacement ellipsoids drawn at the 50% probability level.

codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, -z$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, -z$], forming layers parallel to the *ac* plane (Fig. 3).

The spectroscopic analyses indicated: ^{1}H NMR spectra in $CDCl_3$ showed the aromatic protons as a multiplet in the range 6.80–8.00 p.p.m.. The azomethine proton resonance of the ligand appears as sets of sharp singlet at 8.54 p.p.m.. The hydroxy group (OH) is observed at 13.20 p.p.m.. In the ^{13}C NMR spectrum in $CDCl_3$ the aromatic carbon appears in the range 108–161 p.p.m.. The carbon of the hydroxy group appears at 160.32 p.p.m. and that of azomethine was observed at 162.40 p.p.m.. The DEPT-135 spectrum shows a disappearance of resonances at 110.53, 120.53, 142.17 and 160.32 p.p.m..

Synthesis and crystallization

The Schiff base ligand was prepared in 67% yield by condensation between 54 mg (0.5 mmol) of 1,2-diaminobenzene and 201 mg (1 mmol) of 5-bromosalicylaldehyde in methanol (15 ml). The mixture was refluxed and stirred under a nitrogen atmosphere for 3 h. The obtained orange-yellow precipitate was filtered, washed with methanol and diethylether and dried in vacuum over night. The isolated Schiff base ligand was recrystallized from dimethyl sulfoxide at room temperature, giving orange prismatic crystals.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*···N1	0.87 (4)	1.77 (4)	2.594 (3)	157 (3)
O2—H2*O*···N2	0.81 (4)	1.89 (4)	2.613 (3)	149 (3)

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{14}Br_2N_2O_2$
M_r	474.15
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	173
a, *b*, *c* (Å)	7.4379 (4), 18.7360 (11), 25.4469 (14)
V (Å^3)	3546.2 (3)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	4.59
Crystal size (mm)	0.25 × 0.22 × 0.20
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2010)
T_{min}, T_{max}	0.684, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24680, 4695, 3533
R_{int}	0.038
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.681
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.072, 1.04
No. of reflections	4695
No. of parameters	243
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.74, −0.82

Computer programs: *APEX2* and *SAINT* (Bruker, 2010), *SHELXS2013* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008, *SHELXL2013* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

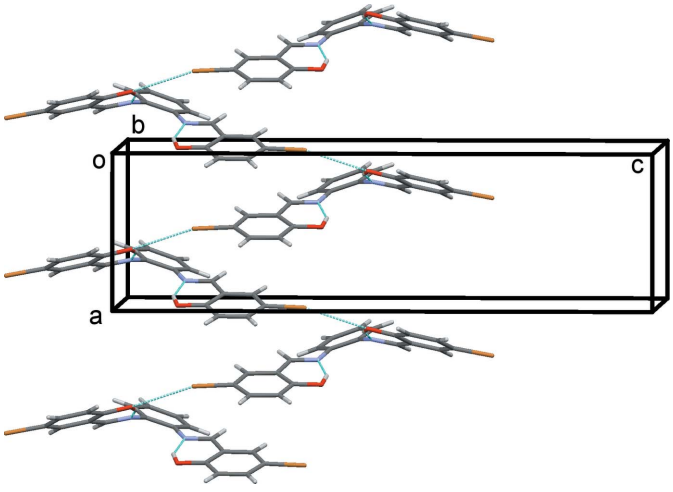


Figure 2
A partial view along the *b* axis of the crystal packing of the title compound. The intramolecular O—H···N hydrogen bonds (see Table 1) and the short Br···O interactions are shown as dashed lines.

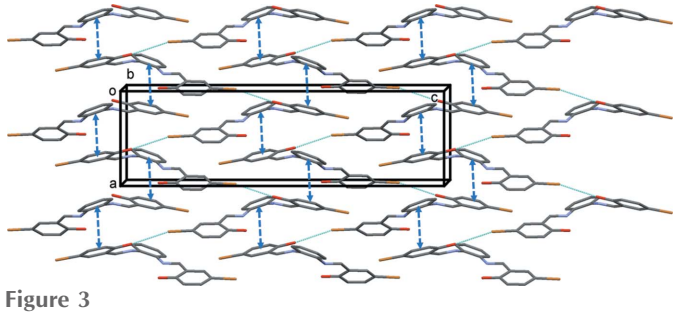


Figure 3
A view along the *b* axis of the crystal packing of the title compound. The short Br···O interactions are shown as dashed lines, and the offset π–π interactions as blue dashed double arrows. The H atoms have been omitted for clarity.

^{1}H NMR ($CDCl_3$, δ p.p.m.): 13.20 (s, C—OH), 8.54 (s, CH═N), 6.80–8.00 (m, ArH); ^{13}C NMR ($CDCl_3$, δ p.p.m.): 162.46 (CH═N), 108–161 (C—Ar).

The DEPT-135 spectrum shows a disappearance of resonances at 110.53, 120.53, 142.17 and 160.32 p.p.m..

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170077 [https://doi.org/10.1107/S2414314617000773]

2,2′-[(1*E*,1′*E*)-1,2-Phenylenebis(azanylylidene)bis(methanylylidene)]bis(4-bromophenol)

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2,2′-[(1*E*,1′*E*)-1,2-Phenylenebis(azanylylidene)bis(methanylylidene)]bis(4-bromophenol)

Crystal data

$C_{20}H_{14}Br_2N_2O_2$
M_r = 474.15
Orthorhombic, *Pbca*
a = 7.4379 (4) Å
b = 18.7360 (11) Å
c = 25.4469 (14) Å
V = 3546.2 (3) Å^3
Z = 8
F(000) = 1872
D_x = 1.776 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6049 reflections
θ = 2.2–29.0°
μ = 4.59 mm^{-1}
T = 173 K
Prism, orange
0.25 × 0.22 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine focus sealed tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2010)
T_{min} = 0.684, T_{max} = 0.746
24680 measured reflections
4695 independent reflections
3533 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 29.0°, θ_{min} = 2.2°
h = −10→10
k = −16→25
l = −34→34

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.072
S = 1.04
4695 reflections
243 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0242P)^2 + 4.011P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.82 e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.7048 (3)	0.33306 (14)	0.05240 (8)	0.0191 (5)
C2	0.6445 (3)	0.39534 (15)	0.02823 (9)	0.0249 (6)
H2	0.6014	0.3937	−0.0069	0.030*
C3	0.6469 (3)	0.45938 (15)	0.05489 (10)	0.0270 (6)
H3	0.6052	0.5015	0.0381	0.032*
C4	0.7100 (3)	0.46261 (15)	0.10622 (10)	0.0266 (6)
H4	0.7125	0.5070	0.1243	0.032*
C5	0.7689 (3)	0.40151 (14)	0.13089 (9)	0.0239 (6)
H5	0.8123	0.4040	0.1659	0.029*
C6	0.7654 (3)	0.33587 (14)	0.10490 (8)	0.0192 (5)
C7	0.7319 (3)	0.25946 (14)	−0.02176 (9)	0.0207 (5)
H7	0.7665	0.3004	−0.0413	0.025*
C8	0.7172 (3)	0.19090 (14)	−0.04795 (8)	0.0198 (5)
C9	0.6626 (3)	0.12922 (14)	−0.02093 (9)	0.0213 (5)
C10	0.6488 (3)	0.06442 (15)	−0.04746 (9)	0.0234 (5)
H10	0.6120	0.0228	−0.0290	0.028*
C11	0.6882 (3)	0.06019 (15)	−0.10042 (9)	0.0242 (5)
H11	0.6788	0.0160	−0.1185	0.029*
C12	0.7417 (4)	0.12132 (15)	−0.12683 (9)	0.0267 (6)
C13	0.7571 (3)	0.18612 (15)	−0.10195 (9)	0.0233 (5)
H13	0.7943	0.2272	−0.1209	0.028*
C14	0.8331 (3)	0.26220 (14)	0.17711 (9)	0.0216 (5)
H14	0.7835	0.2979	0.1993	0.026*
C15	0.9085 (3)	0.19823 (13)	0.20043 (9)	0.0193 (5)
C16	0.9742 (3)	0.14191 (14)	0.16938 (9)	0.0218 (5)
C17	1.0386 (3)	0.08025 (15)	0.19341 (9)	0.0246 (6)
H17	1.0811	0.0418	0.1725	0.029*
C18	1.0408 (3)	0.07479 (15)	0.24765 (10)	0.0254 (6)
H18	1.0851	0.0327	0.2639	0.030*
C19	0.9781 (3)	0.13082 (14)	0.27826 (9)	0.0216 (5)
C20	0.9118 (3)	0.19168 (14)	0.25534 (9)	0.0206 (5)
H20	0.8681	0.2295	0.2767	0.025*
N1	0.6987 (3)	0.26546 (11)	0.02769 (7)	0.0204 (4)
N2	0.8315 (3)	0.27181 (11)	0.12698 (7)	0.0195 (4)
O1	0.6211 (3)	0.13052 (12)	0.03072 (7)	0.0320 (5)
O2	0.9777 (3)	0.14578 (12)	0.11642 (7)	0.0290 (4)
Br1	0.78824 (7)	0.11466 (2)	−0.20013 (2)	0.05940 (13)
Br2	0.98786 (3)	0.12364 (2)	0.35269 (2)	0.02677 (8)
H1O	0.644 (5)	0.175 (2)	0.0388 (14)	0.064 (13)*
H2O	0.925 (5)	0.182 (2)	0.1081 (14)	0.056 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0168 (11)	0.0203 (14)	0.0203 (10)	−0.0007 (10)	0.0021 (9)	0.0003 (9)

C2	0.0250 (12)	0.0270 (16)	0.0228 (11)	0.0021 (11)	−0.0015 (9)	0.0032 (11)
C3	0.0235 (13)	0.0231 (16)	0.0345 (13)	0.0039 (12)	0.0022 (10)	0.0050 (11)
C4	0.0275 (13)	0.0198 (15)	0.0324 (13)	0.0022 (12)	0.0035 (11)	−0.0047 (11)
C5	0.0260 (13)	0.0231 (15)	0.0227 (11)	−0.0018 (11)	−0.0006 (9)	−0.0036 (10)
C6	0.0187 (11)	0.0199 (14)	0.0190 (10)	0.0001 (10)	0.0018 (9)	0.0013 (10)
C7	0.0214 (12)	0.0211 (14)	0.0198 (10)	0.0007 (11)	−0.0016 (9)	0.0022 (10)
C8	0.0192 (11)	0.0238 (15)	0.0163 (10)	−0.0003 (11)	−0.0009 (8)	0.0008 (10)
C9	0.0181 (11)	0.0267 (15)	0.0192 (10)	0.0001 (11)	−0.0006 (8)	0.0028 (10)
C10	0.0221 (12)	0.0203 (15)	0.0279 (12)	−0.0029 (11)	0.0023 (10)	0.0039 (11)
C11	0.0274 (13)	0.0200 (14)	0.0252 (11)	−0.0014 (11)	−0.0021 (10)	−0.0029 (10)
C12	0.0380 (14)	0.0258 (16)	0.0163 (10)	0.0008 (13)	0.0006 (10)	−0.0011 (10)
C13	0.0295 (13)	0.0229 (15)	0.0174 (10)	−0.0026 (12)	0.0020 (9)	0.0041 (10)
C14	0.0258 (13)	0.0198 (14)	0.0191 (10)	−0.0007 (11)	0.0003 (9)	−0.0038 (10)
C15	0.0196 (12)	0.0186 (14)	0.0196 (10)	−0.0030 (10)	−0.0014 (9)	0.0011 (10)
C16	0.0210 (12)	0.0255 (15)	0.0188 (10)	−0.0015 (11)	−0.0011 (9)	−0.0024 (10)
C17	0.0232 (13)	0.0225 (15)	0.0281 (12)	0.0024 (11)	−0.0002 (9)	−0.0054 (11)
C18	0.0224 (12)	0.0225 (15)	0.0312 (12)	0.0021 (11)	−0.0033 (10)	0.0037 (11)
C19	0.0208 (11)	0.0245 (14)	0.0194 (10)	−0.0061 (11)	−0.0021 (9)	0.0024 (10)
C20	0.0207 (12)	0.0221 (15)	0.0191 (10)	0.0003 (11)	−0.0001 (9)	−0.0019 (10)
N1	0.0237 (10)	0.0203 (12)	0.0172 (8)	0.0009 (9)	−0.0019 (8)	−0.0005 (8)
N2	0.0216 (10)	0.0191 (12)	0.0179 (8)	−0.0012 (9)	−0.0014 (7)	−0.0014 (8)
O1	0.0480 (12)	0.0282 (13)	0.0198 (8)	−0.0048 (10)	0.0085 (8)	0.0033 (8)
O2	0.0356 (11)	0.0320 (12)	0.0196 (8)	0.0078 (10)	0.0022 (7)	−0.0041 (8)
Br1	0.1315 (4)	0.02926 (18)	0.01740 (12)	0.0059 (2)	0.01253 (16)	−0.00138 (12)
Br2	0.03229 (13)	0.02816 (15)	0.01988 (11)	−0.00264 (12)	−0.00415 (10)	0.00563 (10)

Geometric parameters (Å, º)

C1—C2	1.393 (4)	C11—C12	1.386 (4)
C1—C6	1.411 (3)	C11—H11	0.9500
C1—N1	1.415 (3)	C12—C13	1.374 (4)
C2—C3	1.379 (4)	C12—Br1	1.901 (2)
C2—H2	0.9500	C13—H13	0.9500
C3—C4	1.389 (4)	C14—N2	1.288 (3)
C3—H3	0.9500	C14—C15	1.450 (3)
C4—C5	1.377 (4)	C14—H14	0.9500
C4—H4	0.9500	C15—C20	1.403 (3)
C5—C6	1.397 (4)	C15—C16	1.406 (3)
C5—H5	0.9500	C16—O2	1.350 (3)
C6—N2	1.414 (3)	C16—C17	1.392 (4)
C7—N1	1.287 (3)	C17—C18	1.384 (3)
C7—C8	1.451 (4)	C17—H17	0.9500
C7—H7	0.9500	C18—C19	1.388 (4)
C8—C9	1.405 (3)	C18—H18	0.9500
C8—C13	1.409 (3)	C19—C20	1.372 (3)
C9—O1	1.350 (3)	C19—Br2	1.900 (2)
C9—C10	1.393 (4)	C20—H20	0.9500
C10—C11	1.382 (3)	O1—H1O	0.87 (4)

C10—H10	0.9500	O2—H2O	0.81 (4)
C2—C1—C6	119.3 (2)	C12—C11—H11	120.4
C2—C1—N1	122.9 (2)	C13—C12—C11	122.0 (2)
C6—C1—N1	117.7 (2)	C13—C12—Br1	119.66 (19)
C3—C2—C1	120.5 (2)	C11—C12—Br1	118.27 (19)
C3—C2—H2	119.8	C12—C13—C8	119.2 (2)
C1—C2—H2	119.8	C12—C13—H13	120.4
C2—C3—C4	120.3 (3)	C8—C13—H13	120.4
C2—C3—H3	119.8	N2—C14—C15	121.6 (2)
C4—C3—H3	119.8	N2—C14—H14	119.2
C5—C4—C3	120.0 (2)	C15—C14—H14	119.2
C5—C4—H4	120.0	C20—C15—C16	119.2 (2)
C3—C4—H4	120.0	C20—C15—C14	119.1 (2)
C4—C5—C6	120.7 (2)	C16—C15—C14	121.6 (2)
C4—C5—H5	119.7	O2—C16—C17	118.5 (2)
C6—C5—H5	119.7	O2—C16—C15	121.8 (2)
C5—C6—C1	119.2 (2)	C17—C16—C15	119.7 (2)
C5—C6—N2	123.6 (2)	C18—C17—C16	120.2 (2)
C1—C6—N2	117.1 (2)	C18—C17—H17	119.9
N1—C7—C8	120.8 (2)	C16—C17—H17	119.9
N1—C7—H7	119.6	C17—C18—C19	120.0 (2)
C8—C7—H7	119.6	C17—C18—H18	120.0
C9—C8—C13	119.1 (2)	C19—C18—H18	120.0
C9—C8—C7	121.7 (2)	C20—C19—C18	120.7 (2)
C13—C8—C7	119.2 (2)	C20—C19—Br2	119.76 (19)
O1—C9—C10	118.1 (2)	C18—C19—Br2	119.54 (19)
O1—C9—C8	121.8 (2)	C19—C20—C15	120.2 (2)
C10—C9—C8	120.1 (2)	C19—C20—H20	119.9
C11—C10—C9	120.5 (2)	C15—C20—H20	119.9
C11—C10—H10	119.8	C7—N1—C1	120.4 (2)
C9—C10—H10	119.8	C14—N2—C6	121.0 (2)
C10—C11—C12	119.1 (2)	C9—O1—H1O	102 (2)
C10—C11—H11	120.4	C16—O2—H2O	107 (3)
C6—C1—C2—C3	1.2 (4)	C9—C8—C13—C12	0.0 (4)
N1—C1—C2—C3	177.4 (2)	C7—C8—C13—C12	−179.5 (2)
C1—C2—C3—C4	0.1 (4)	N2—C14—C15—C20	177.9 (2)
C2—C3—C4—C5	−0.6 (4)	N2—C14—C15—C16	−3.7 (4)
C3—C4—C5—C6	−0.2 (4)	C20—C15—C16—O2	−178.7 (2)
C4—C5—C6—C1	1.6 (4)	C14—C15—C16—O2	2.9 (4)
C4—C5—C6—N2	176.9 (2)	C20—C15—C16—C17	1.1 (4)
C2—C1—C6—C5	−2.0 (3)	C14—C15—C16—C17	−177.3 (2)
N1—C1—C6—C5	−178.4 (2)	O2—C16—C17—C18	178.7 (2)
C2—C1—C6—N2	−177.7 (2)	C15—C16—C17—C18	−1.1 (4)
N1—C1—C6—N2	5.9 (3)	C16—C17—C18—C19	0.2 (4)
N1—C7—C8—C9	1.5 (4)	C17—C18—C19—C20	0.7 (4)
N1—C7—C8—C13	−179.1 (2)	C17—C18—C19—Br2	−178.33 (19)

C13—C8—C9—O1	−179.5 (2)	C18—C19—C20—C15	−0.7 (4)
C7—C8—C9—O1	0.0 (4)	Br2—C19—C20—C15	178.32 (18)
C13—C8—C9—C10	0.1 (4)	C16—C15—C20—C19	−0.2 (4)
C7—C8—C9—C10	179.6 (2)	C14—C15—C20—C19	178.2 (2)
O1—C9—C10—C11	179.5 (2)	C8—C7—N1—C1	−176.9 (2)
C8—C9—C10—C11	−0.1 (4)	C2—C1—N1—C7	37.9 (3)
C9—C10—C11—C12	0.0 (4)	C6—C1—N1—C7	−145.9 (2)
C10—C11—C12—C13	0.1 (4)	C15—C14—N2—C6	−177.0 (2)
C10—C11—C12—Br1	−178.15 (19)	C5—C6—N2—C14	27.9 (4)
C11—C12—C13—C8	−0.1 (4)	C1—C6—N2—C14	−156.6 (2)
Br1—C12—C13—C8	178.13 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···N1	0.87 (4)	1.77 (4)	2.594 (3)	157 (3)
O2—H2*O*···N2	0.81 (4)	1.89 (4)	2.613 (3)	149 (3)