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A monoclinic polymorph of (*R,R*)-4,4'-dibromo-2,2'-[cyclohexane-1,2-diylbis-(nitrilomethanylylidene)]diphenol

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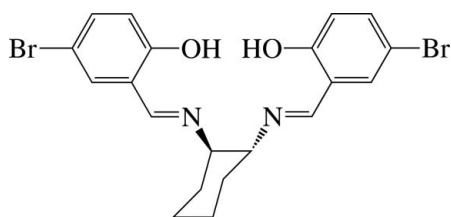
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 Key indicators: single-crystal X-ray study; $T = 200$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.039; wR factor = 0.108; data-to-parameter ratio = 16.5.

The title compound, $\text{C}_{20}\text{H}_{20}\text{Br}_2\text{N}_2\text{O}_2$, a tetradentate Schiff base, is the enantiomerically pure *R,R*-diastereomer of four possible stereoisomers. The molecular structure reveals two strong intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds between the hydroxy O atom and the imino N atom, which each generate $S(6)$ rings. In the crystal, molecules are stacked in columns along the a axis; when viewed down the b axis, successive columns are stacked in the opposite direction. The structure reported herein is the monoclinic polymorph of the previously reported orthorhombic form [Yi & Hu (2009). *Acta Cryst.* E65, o2643], in which the complete molecule is generated by a crystallographic twofold axis.

Related literature

For the orthorhombic polymorph, see: Yi & Hu (2009).



Experimental

Crystal data

 $\text{C}_{20}\text{H}_{20}\text{Br}_2\text{N}_2\text{O}_2$
 $M_r = 480.20$

 Monoclinic, $P2_1$
 $a = 5.9082$ (5) Å
 $b = 18.8626$ (15) Å
 $c = 9.0088$ (7) Å
 $\beta = 91.867$ (2)°
 $V = 1003.44$ (14) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 4.06$ mm⁻¹
 $T = 200$ K
 $0.31 \times 0.17 \times 0.16$ mm

Data collection

 Bruker SMART 1000 CCD diffractometer
 Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
 $T_{\min} = 0.786$, $T_{\max} = 1.000$

 7343 measured reflections
 3868 independent reflections
 2484 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.108$
 $S = 1.03$
 3868 reflections
 235 parameters
 1 restraint

 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.88$ e Å⁻³
 $\Delta\rho_{\min} = -0.47$ e Å⁻³
 Absolute structure: Flack (1983), 1331 Friedel pairs
 Flack parameter: -0.010 (16)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1O}\cdots\text{N1}$	0.84	1.82	2.581 (7)	150
$\text{O2}-\text{H2O}\cdots\text{N2}$	0.84	1.87	2.626 (7)	149

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Priority Research Centers Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (2011-0030747).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6734).

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supplementary materials

Acta Cryst. (2012). E68, o1449 [doi:10.1107/S1600536812016376]

A monoclinic polymorph of (*R,R*)-4,4'-dibromo-2,2'-[cyclohexane-1,2-diylbis(nitrilomethanylylidene)]diphenol

Kwang Ha

Comment

The crystal structure of the title compound, C₂₀H₂₀Br₂N₂O₂, was previously reported in the orthorhombic space group *P*2₁2₁2 (Yi & Hu, 2009). The structure presented herein is essentially the same as the published structure and represents a monoclinic polymorph.

The title compound is a tetradentate Schiff base (Fig. 1), which can act as a dibasic ligand, *i.e.* the N and O donor atoms can coordinate one metal ion. The compound has two chiral C centres and is one of four possible stereoisomers. Crystallographically, the absolute configuration has been established by anomalous dispersion effects, and the *R* configuration of the asymmetric C atoms (C1 and C6) could be assigned. The Schiff base reveals strong intramolecular O—H \cdots N hydrogen bonds between the hydroxy O atom and the imino N atom, with O \cdots N distances of 2.581 (7) and 2.626 (7) Å, forming nearly planar six-membered rings (Fig. 2, Table 1). In the crystal structure, the benzene rings are not parallel: the dihedral angle between the benzene rings is 67.20 (15)°. The N—C bond lengths and the C—N—C bond angles indicate that the imino N atoms are *sp*²-hybridized [N1=C7 = 1.274 (8) Å, N1—C1 = 1.461 (8) Å, <C7—N1—C1 = 118.7 (6)°; N2=C14 = 1.280 (8) Å, N2—C6 = 1.474 (8) Å, <C14—N2—C6 = 118.3 (6)°]. The molecules are stacked in columns along the *a* axis. When viewed down the *b* axis, the successive compounds are stacked in the opposite direction. In the columns, the shortest centroid-centroid distance between aromatic rings is 4.709 (3) Å.

Experimental

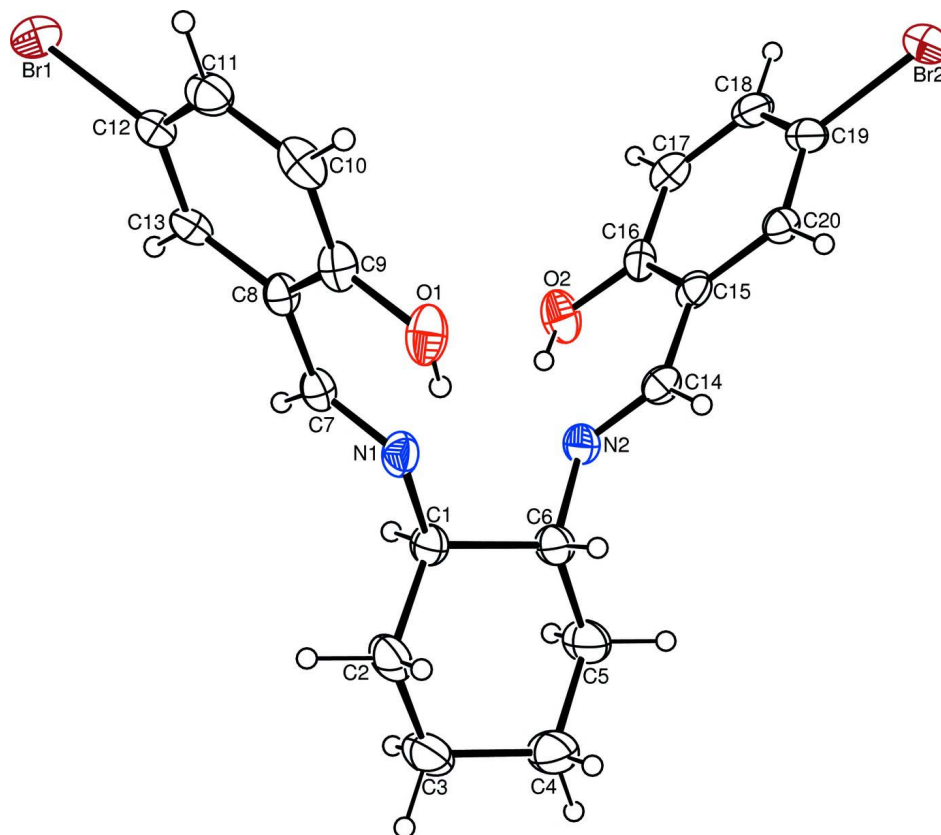
1,2-Diaminocyclohexane (0.8007 g, 7.012 mmol) and 5-bromosalicylaldehyde (2.8204 g, 14.031 mmol) in EtOH (20 ml) were stirred for 1 h at room temperature. After addition of pentane (30 ml) to the reaction mixture, the formed precipitate was separated by filtration, washed with ether, and dried at 323 K, to give a yellow powder (1.7660 g). Yellow blocks were obtained by slow evaporation from a CH₃CN solution at room temperature. The previous polymorph (Yi & Hu, 2009) was crystallised from methanol.

Refinement

Carbon-bound H atoms were positioned geometrically and allowed to ride on their respective parent atoms: C—H = 0.95–1.00 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The hydroxy H atoms were located from the difference Fourier map then allowed to ride on their parent atoms in the final cycles of refinement with O—H = 0.84 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The highest peak (0.88 e Å⁻³) and the deepest hole (-0.47 e Å⁻³) in the difference Fourier map are located 1.34 Å and 0.86 Å, respectively, from the atoms Br1 and Br2. The absolute configuration was established by anomalous dispersion effects *via* diffraction measurements on the crystal. The Flack parameter is -0.010 (16) in the final cycles of refinement.

Computing details

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

**Figure 1**

A structure detail of the title compound, with atom numbering. Displacement ellipsoids are drawn at the 30% probability level for non-H atoms.

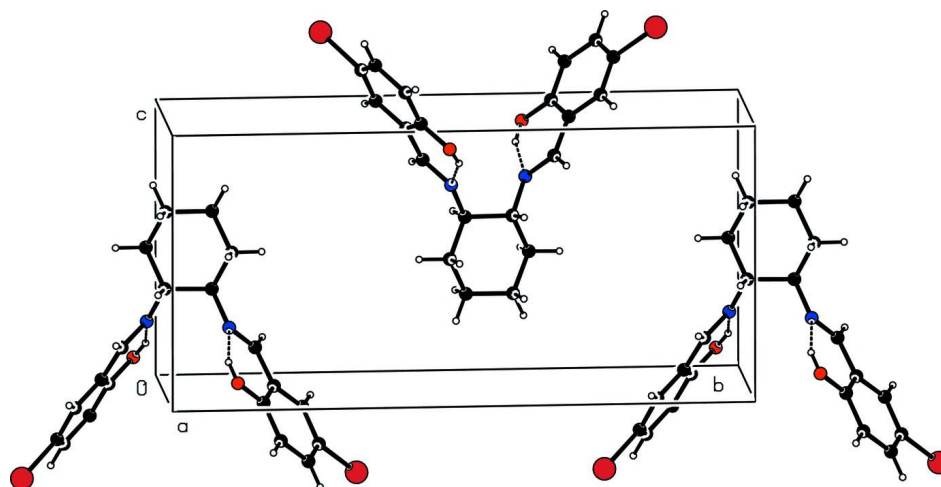


Figure 2

A view of the unit-cell contents of the title compound. Intramolecular O—H...N hydrogen-bond interactions are drawn with dashed lines.

(*R,R*)-4,4'-dibromo-2,2'-[cyclohexane-1,2-diylbis(nitrilomethanylidene)]diphenol

Crystal data

$C_{20}H_{20}Br_2N_2O_2$
 $M_r = 480.20$
 Monoclinic, $P2_1$
 Hall symbol: $P\ 2yb$
 $a = 5.9082\ (5)\ \text{\AA}$
 $b = 18.8626\ (15)\ \text{\AA}$
 $c = 9.0088\ (7)\ \text{\AA}$
 $\beta = 91.867\ (2)^\circ$
 $V = 1003.44\ (14)\ \text{\AA}^3$
 $Z = 2$

$F(000) = 480$
 $D_x = 1.589\ \text{Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$
 Cell parameters from 2758 reflections
 $\theta = 2.5\text{--}25.8^\circ$
 $\mu = 4.06\ \text{mm}^{-1}$
 $T = 200\ \text{K}$
 Block, yellow
 $0.31 \times 0.17 \times 0.16\ \text{mm}$

Data collection

Bruker SMART 1000 CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (*SADABS*; Bruker, 2000)
 $T_{\min} = 0.786$, $T_{\max} = 1.000$

7343 measured reflections
 3868 independent reflections
 2484 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$
 $\theta_{\max} = 28.3^\circ$, $\theta_{\min} = 2.2^\circ$
 $h = -7 \rightarrow 7$
 $k = -20 \rightarrow 25$
 $l = -11 \rightarrow 11$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.108$
 $S = 1.03$
 3868 reflections
 235 parameters
 1 restraint

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
 $w = 1/[\sigma^2(F_o^2) + (0.0434P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.88 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.47 \text{ e } \text{\AA}^{-3}$

Absolute structure: Flack (1983), 1331 Friedel
 pairs
 Flack parameter: -0.010 (16)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.25215 (12)	0.33723 (3)	-0.33161 (7)	0.0600 (3)
Br2	0.27364 (11)	-0.23777 (3)	-0.33104 (7)	0.0551 (2)
O1	0.7141 (7)	0.1204 (3)	0.0604 (6)	0.0539 (13)
H1O	0.6245	0.1070	0.1252	0.081*
O2	-0.2482 (8)	-0.0312 (3)	0.0322 (6)	0.0587 (14)
H2O	-0.1588	-0.0127	0.0955	0.088*
N1	0.3538 (9)	0.1159 (3)	0.2147 (5)	0.0428 (12)
N2	0.1109 (9)	-0.0185 (2)	0.2097 (5)	0.0427 (12)
C1	0.2247 (11)	0.0899 (5)	0.3390 (7)	0.0414 (18)
H1	0.0634	0.1054	0.3257	0.050*
C2	0.3242 (15)	0.1210 (4)	0.4830 (7)	0.0601 (19)
H2A	0.4888	0.1111	0.4893	0.072*
H2B	0.3038	0.1731	0.4816	0.072*
C3	0.2143 (15)	0.0908 (5)	0.6200 (10)	0.068 (2)
H3A	0.2893	0.1107	0.7106	0.081*
H3B	0.0525	0.1045	0.6194	0.081*
C4	0.2344 (16)	0.0103 (5)	0.6219 (10)	0.071 (3)
H4A	0.1588	-0.0089	0.7097	0.086*
H4B	0.3961	-0.0035	0.6288	0.086*
C5	0.1241 (15)	-0.0204 (4)	0.4802 (7)	0.061 (2)
H5A	0.1385	-0.0727	0.4818	0.073*
H5B	-0.0392	-0.0085	0.4763	0.073*
C6	0.2343 (11)	0.0086 (5)	0.3428 (8)	0.0452 (19)
H6	0.3957	-0.0073	0.3416	0.054*
C7	0.2650 (10)	0.1629 (4)	0.1295 (7)	0.0373 (15)
H7	0.1164	0.1795	0.1471	0.045*
C8	0.3885 (9)	0.1916 (3)	0.0051 (6)	0.0344 (12)
C9	0.6051 (10)	0.1676 (3)	-0.0268 (7)	0.0439 (14)
C10	0.7125 (11)	0.1940 (5)	-0.1518 (7)	0.0477 (19)
H10	0.8586	0.1771	-0.1751	0.057*
C11	0.6082 (11)	0.2443 (3)	-0.2412 (6)	0.0459 (15)
H11	0.6819	0.2623	-0.3255	0.055*
C12	0.3947 (9)	0.2685 (3)	-0.2071 (5)	0.0406 (12)

C13	0.2877 (10)	0.2432 (3)	-0.0852 (7)	0.0381 (16)
H13	0.1428	0.2612	-0.0622	0.046*
C14	0.2091 (10)	-0.0645 (4)	0.1293 (7)	0.0378 (15)
H14	0.3597	-0.0784	0.1555	0.045*
C15	0.0974 (10)	-0.0959 (3)	-0.0004 (6)	0.0366 (13)
C16	-0.1247 (10)	-0.0773 (3)	-0.0454 (6)	0.0387 (13)
C17	-0.2241 (12)	-0.1068 (4)	-0.1734 (7)	0.0443 (18)
H17	-0.3742	-0.0939	-0.2032	0.053*
C18	-0.1054 (10)	-0.1550 (3)	-0.2579 (6)	0.0443 (14)
H18	-0.1728	-0.1752	-0.3452	0.053*
C19	0.1098 (10)	-0.1725 (3)	-0.2129 (5)	0.0416 (13)
C20	0.2136 (9)	-0.1450 (3)	-0.0861 (6)	0.0333 (14)
H20	0.3628	-0.1592	-0.0572	0.040*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0820 (6)	0.0589 (6)	0.0384 (4)	0.0047 (4)	-0.0070 (3)	0.0073 (4)
Br2	0.0668 (5)	0.0587 (6)	0.0400 (4)	0.0071 (4)	0.0051 (3)	-0.0076 (4)
O1	0.042 (3)	0.041 (3)	0.080 (4)	0.010 (2)	0.004 (2)	0.005 (3)
O2	0.044 (3)	0.050 (3)	0.082 (4)	0.010 (2)	0.003 (3)	-0.012 (3)
N1	0.049 (3)	0.030 (3)	0.049 (3)	-0.004 (2)	0.000 (2)	0.002 (2)
N2	0.056 (3)	0.031 (3)	0.042 (3)	-0.007 (2)	0.003 (2)	0.000 (2)
C1	0.049 (4)	0.033 (4)	0.042 (5)	-0.007 (3)	0.004 (3)	0.000 (3)
C2	0.089 (6)	0.039 (4)	0.053 (4)	-0.013 (4)	0.007 (4)	-0.013 (3)
C3	0.100 (7)	0.058 (6)	0.046 (5)	-0.023 (5)	0.006 (4)	-0.014 (5)
C4	0.111 (7)	0.056 (6)	0.046 (5)	-0.022 (5)	-0.001 (4)	0.003 (5)
C5	0.086 (6)	0.047 (4)	0.049 (4)	-0.026 (4)	0.003 (4)	-0.004 (3)
C6	0.060 (5)	0.035 (5)	0.041 (5)	-0.012 (3)	-0.001 (4)	-0.002 (3)
C7	0.036 (3)	0.030 (4)	0.045 (4)	-0.001 (3)	-0.002 (3)	-0.007 (3)
C8	0.031 (3)	0.030 (3)	0.041 (3)	0.000 (2)	-0.002 (2)	-0.003 (2)
C9	0.041 (3)	0.035 (3)	0.056 (4)	0.004 (3)	0.000 (3)	-0.004 (3)
C10	0.038 (3)	0.048 (5)	0.058 (4)	-0.008 (3)	0.011 (3)	-0.018 (3)
C11	0.051 (4)	0.047 (4)	0.040 (3)	-0.011 (3)	0.007 (3)	-0.007 (3)
C12	0.054 (3)	0.036 (3)	0.031 (3)	0.000 (3)	-0.001 (2)	-0.006 (3)
C13	0.040 (3)	0.043 (4)	0.031 (3)	0.000 (3)	-0.001 (2)	-0.012 (3)
C14	0.038 (3)	0.038 (4)	0.038 (3)	-0.003 (3)	0.003 (3)	0.007 (3)
C15	0.042 (3)	0.029 (3)	0.038 (3)	-0.006 (2)	0.001 (2)	0.009 (2)
C16	0.039 (3)	0.029 (3)	0.049 (3)	0.004 (2)	0.006 (3)	0.004 (3)
C17	0.044 (4)	0.044 (4)	0.044 (4)	-0.003 (3)	-0.003 (3)	0.012 (3)
C18	0.056 (4)	0.044 (4)	0.032 (3)	-0.007 (3)	-0.005 (2)	0.007 (3)
C19	0.047 (3)	0.047 (4)	0.031 (3)	-0.002 (3)	0.002 (2)	0.000 (3)
C20	0.029 (3)	0.037 (4)	0.033 (3)	0.002 (2)	0.001 (2)	0.003 (3)

Geometric parameters (\AA , $^\circ$)

Br1—C12	1.894 (6)	C5—H5B	0.9900
Br2—C19	1.912 (6)	C6—H6	1.0000
O1—C9	1.337 (7)	C7—C8	1.461 (8)
O1—H1O	0.8400	C7—H7	0.9500

O2—C16	1.345 (7)	C8—C13	1.391 (8)
O2—H2O	0.8400	C8—C9	1.396 (8)
N1—C7	1.274 (8)	C9—C10	1.403 (9)
N1—C1	1.461 (8)	C10—C11	1.377 (10)
N2—C14	1.280 (8)	C10—H10	0.9500
N2—C6	1.474 (8)	C11—C12	1.385 (8)
C1—C2	1.524 (10)	C11—H11	0.9500
C1—C6	1.534 (7)	C12—C13	1.370 (8)
C1—H1	1.0000	C13—H13	0.9500
C2—C3	1.523 (10)	C14—C15	1.451 (9)
C2—H2A	0.9900	C14—H14	0.9500
C2—H2B	0.9900	C15—C20	1.398 (8)
C3—C4	1.522 (8)	C15—C16	1.405 (8)
C3—H3A	0.9900	C16—C17	1.393 (9)
C3—H3B	0.9900	C17—C18	1.390 (9)
C4—C5	1.528 (11)	C17—H17	0.9500
C4—H4A	0.9900	C18—C19	1.363 (8)
C4—H4B	0.9900	C18—H18	0.9500
C5—C6	1.520 (10)	C19—C20	1.380 (8)
C5—H5A	0.9900	C20—H20	0.9500
C9—O1—H1O	107.9	N1—C7—H7	119.6
C16—O2—H2O	106.3	C8—C7—H7	119.6
C7—N1—C1	118.7 (6)	C13—C8—C9	119.0 (5)
C14—N2—C6	118.3 (6)	C13—C8—C7	119.6 (5)
N1—C1—C2	109.1 (6)	C9—C8—C7	121.5 (5)
N1—C1—C6	109.5 (7)	O1—C9—C8	121.4 (5)
C2—C1—C6	110.6 (7)	O1—C9—C10	119.1 (6)
N1—C1—H1	109.2	C8—C9—C10	119.4 (6)
C2—C1—H1	109.2	C11—C10—C9	120.6 (6)
C6—C1—H1	109.2	C11—C10—H10	119.7
C3—C2—C1	112.5 (7)	C9—C10—H10	119.7
C3—C2—H2A	109.1	C10—C11—C12	119.4 (6)
C1—C2—H2A	109.1	C10—C11—H11	120.3
C3—C2—H2B	109.1	C12—C11—H11	120.3
C1—C2—H2B	109.1	C13—C12—C11	120.7 (5)
H2A—C2—H2B	107.8	C13—C12—Br1	120.3 (4)
C4—C3—C2	110.3 (8)	C11—C12—Br1	119.0 (4)
C4—C3—H3A	109.6	C12—C13—C8	120.9 (5)
C2—C3—H3A	109.6	C12—C13—H13	119.6
C4—C3—H3B	109.6	C8—C13—H13	119.6
C2—C3—H3B	109.6	N2—C14—C15	122.0 (6)
H3A—C3—H3B	108.1	N2—C14—H14	119.0
C3—C4—C5	109.8 (9)	C15—C14—H14	119.0
C3—C4—H4A	109.7	C20—C15—C16	118.5 (5)
C5—C4—H4A	109.7	C20—C15—C14	119.8 (5)
C3—C4—H4B	109.7	C16—C15—C14	121.7 (5)
C5—C4—H4B	109.7	O2—C16—C17	117.8 (6)
H4A—C4—H4B	108.2	O2—C16—C15	122.0 (5)

C6—C5—C4	111.2 (6)	C17—C16—C15	120.2 (6)
C6—C5—H5A	109.4	C18—C17—C16	120.5 (6)
C4—C5—H5A	109.4	C18—C17—H17	119.7
C6—C5—H5B	109.4	C16—C17—H17	119.7
C4—C5—H5B	109.4	C19—C18—C17	118.5 (6)
H5A—C5—H5B	108.0	C19—C18—H18	120.7
N2—C6—C5	108.9 (6)	C17—C18—H18	120.7
N2—C6—C1	108.2 (7)	C18—C19—C20	122.7 (5)
C5—C6—C1	111.2 (7)	C18—C19—Br2	118.3 (4)
N2—C6—H6	109.5	C20—C19—Br2	119.0 (4)
C5—C6—H6	109.5	C19—C20—C15	119.5 (5)
C1—C6—H6	109.5	C19—C20—H20	120.2
N1—C7—C8	120.9 (6)	C15—C20—H20	120.2
C7—N1—C1—C2	-106.0 (7)	C9—C10—C11—C12	-0.3 (10)
C7—N1—C1—C6	132.8 (6)	C10—C11—C12—C13	0.4 (9)
N1—C1—C2—C3	-174.3 (7)	C10—C11—C12—Br1	-179.6 (5)
C6—C1—C2—C3	-53.9 (9)	C11—C12—C13—C8	-1.4 (9)
C1—C2—C3—C4	56.4 (11)	Br1—C12—C13—C8	178.5 (4)
C2—C3—C4—C5	-57.8 (10)	C9—C8—C13—C12	2.4 (9)
C3—C4—C5—C6	58.7 (10)	C7—C8—C13—C12	-176.7 (5)
C14—N2—C6—C5	-109.5 (7)	C6—N2—C14—C15	177.7 (6)
C14—N2—C6—C1	129.6 (7)	N2—C14—C15—C20	178.8 (6)
C4—C5—C6—N2	-175.8 (7)	N2—C14—C15—C16	0.4 (9)
C4—C5—C6—C1	-56.7 (9)	C20—C15—C16—O2	179.1 (5)
N1—C1—C6—N2	-66.8 (7)	C14—C15—C16—O2	-2.4 (8)
C2—C1—C6—N2	173.0 (5)	C20—C15—C16—C17	-0.6 (9)
N1—C1—C6—C5	173.7 (5)	C14—C15—C16—C17	177.9 (6)
C2—C1—C6—C5	53.5 (8)	O2—C16—C17—C18	-179.7 (6)
C1—N1—C7—C8	178.9 (6)	C15—C16—C17—C18	0.1 (10)
N1—C7—C8—C13	-179.5 (6)	C16—C17—C18—C19	-0.1 (10)
N1—C7—C8—C9	1.5 (9)	C17—C18—C19—C20	0.7 (9)
C13—C8—C9—O1	176.9 (5)	C17—C18—C19—Br2	-179.2 (5)
C7—C8—C9—O1	-4.1 (9)	C18—C19—C20—C15	-1.3 (9)
C13—C8—C9—C10	-2.3 (9)	Br2—C19—C20—C15	178.6 (4)
C7—C8—C9—C10	176.7 (5)	C16—C15—C20—C19	1.2 (8)
O1—C9—C10—C11	-177.9 (6)	C14—C15—C20—C19	-177.3 (5)
C8—C9—C10—C11	1.3 (10)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1 <i>O</i> ...N1	0.84	1.82	2.581 (7)	150
O2—H2 <i>O</i> ...N2	0.84	1.87	2.626 (7)	149