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(E)-3-[(3-Bromophenyl)iminomethyl]-benzene-1,2-diol: a combined X-ray and computational structural studyZeynep Keleşoğlu,^a Orhan Büyükgüngör,^{a*} Çiğdem Albayrak^b and Mustafa Odabaşoğlu^c

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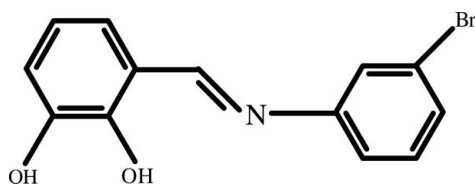
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.033; wR factor = 0.078; data-to-parameter ratio = 13.7.

The title compound, $\text{C}_{13}\text{H}_{10}\text{BrNO}_2$, exists as an enol-imine form in the crystal and adopts an *E* configuration with respect to the $\text{C}=\text{N}$ double bond. The molecule is close to planar, with a dihedral angle of 6.88 (14)° between the aromatic rings. Intramolecular $\text{O}-\text{H}\cdots\text{N}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds generate $S(6)$ and $S(5)$ ring motifs, respectively. The crystal structure is stabilized by intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen-bond interactions, forming $R_2^2(10)$ and $R_2^2(20)$ chains along $[100]$. *ab initio* Hartree-Fock (HF), density-functional theory (DFT) and semi-empirical (AM1 and PM3) calculations and full-geometry optimizations were also performed. Although there are some discrepancies between the experimental and calculated parameters, caused presumably by the $\text{O}-\text{H}\cdots\text{O}$ hydrogen-bond interactions, there is an acceptable general agreement between them.

Related literature

For general background to Schiff base compounds in coordination chemistry, see: Chen *et al.* (2008); May *et al.* (2004); Weber *et al.* (2007). For background to DFT calculations, see: Becke (1988, 1993); Lee *et al.* (1988); Schmidt & Polik *et al.* (2007); Friesner *et al.* (2005); Liu *et al.* (2004). For a related structure, see: Cao *et al.* (2009); Temel *et al.* (2007). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$\text{C}_{13}\text{H}_{10}\text{BrNO}_2$
 $M_r = 292.13$
 Orthorhombic, *Pbca*
 $a = 4.7411$ (2) Å
 $b = 18.9447$ (6) Å
 $c = 26.1417$ (10) Å
 $V = 2348.01$ (15) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 3.50$ mm⁻¹
 $T = 296$ K
 $0.66 \times 0.38 \times 0.10$ mm

Data collection

Stoe IPDS-II diffractometer
 Absorption correction: integration
 (*X-RED32*; Stoe & Cie, 2002)
 $T_{\min} = 0.229$, $T_{\max} = 0.735$
 7185 measured reflections
 2212 independent reflections
 1764 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.078$
 $S = 1.05$
 2212 reflections
 162 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.33$ e Å⁻³
 $\Delta\rho_{\min} = -0.42$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1}\cdots\text{N1}$	0.87 (4)	1.81 (4)	2.606 (3)	151 (3)
$\text{O2}-\text{H2}\cdots\text{O1}$	0.78 (4)	2.31 (5)	2.718 (3)	113 (4)
$\text{O2}-\text{H2}\cdots\text{O2}^{\text{i}}$	0.78 (4)	2.48 (5)	3.124 (3)	141 (5)
$\text{O2}-\text{H2}\cdots\text{O1}^{\text{ii}}$	0.78 (4)	2.46 (4)	2.986 (3)	126 (4)

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

Table 2

Selected geometric parameters (Å, °) from the X-ray structure and calculated by AM1, PM3, HF and DFT methods.

Parameters	X-ray	AM1	PM3	HF*	DFT/B3LYP*	
$\text{C1}-\text{C7}$	1.447 (4)	1.4659	1.4592	1.4655	1.4472	
$\text{C8}-\text{N1}$	1.416 (3)	1.4103	1.431	1.4082	1.4071	
$\text{C7}-\text{N1}$	1.278 (3)	1.2923	1.3028	1.2626	1.2947	
$\text{C2}-\text{O1}$	1.355 (3)	1.3711	1.3612	1.3414	1.35	
$\text{C3}-\text{O2}$	1.358 (3)	1.3749	1.3695	1.3472	1.3601	
$\text{C10}-\text{Br1}$	1.900 (2)	1.8743	1.8676	1.899	1.9138	
$\text{O1}-\text{C2}-\text{C1}$	122.8 (2)	126.384	124.0177	124.2818	123.5134	
$\text{N1}-\text{C7}-\text{C1}$	122.1 (2)	123.752	119.6344	123.297	121.9975	
$\text{O2}-\text{C3}-\text{C4}$	119.9 (2)	117.2553	115.9182	119.9887	120.7548	
$\text{O1}-\text{C2}-\text{C3}$	117.5 (2)	113.7932	116.4985	115.8053	116.4318	
$\text{O2}-\text{C3}-\text{C2}$	120.5 (2)	122.181	123.9237	119.978	119.4331	
$\text{C7}-\text{N1}-\text{C8}$	121.6 (2)	121.8246	122.1744	120.3634	121.3341	
$\text{C12}-\text{C13}-\text{H13}$		119.6	119.7856	119.8376	120.8687	121.0058
$\text{C8}-\text{C13}-\text{H13}$		119.6	120.1274	120.1469	119.0149	118.759
$\text{C1}-\text{C7}-\text{N1}-\text{C8}$	179.7 (2)	-179.2308	179.9974	-178.6515	-177.5099	
$\text{C9}-\text{C8}-\text{N1}-\text{C7}$	7.9 (4)	34.1092	0.0009	44.5418	35.1166	
$\text{C2}-\text{C1}-\text{C7}-\text{N1}$	-1.6 (4)	2.6542	0.0087	0.8066	0.3196	
$\text{N1}-\text{C8}-\text{C9}-\text{C10}$	-179.9 (2)	-177.3895	179.9976	179.3862	179.4699	
$\text{C8}-\text{C9}-\text{C10}-\text{Br1}$	-179.41 (19)	-179.8397	-180.0011	-179.9136	-179.7804	

*6-31G(d,p).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular

graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *GAUSSIAN* (Frisch *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2198).

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supporting information

Acta Cryst. (2009). E65, o2410–o2411 [doi:10.1107/S1600536809035053]

(*E*)-3-[(3-Bromophenyl)iminomethyl]benzene-1,2-diol: a combined X-ray and computational structural study

Zeynep Keleşoğlu, Orhan Büyükgüngör, Çiğdem Albayrak and Mustafa Odabaşoğlu

S1. Comment

Schiff base compounds have received considerable attention for many years, primarily due to their importance in the development of coordination chemistry related to magnetism (Weber *et al.*, 2007), catalysis (Chen *et al.*, 2008) and biological process (May *et al.*, 2004). In general, *O*-hydroxy Schiff bases exhibit two possible tautomeric forms, the enol-imine and keto-amine forms. Depending on the tautomers, two types of intra-molecular hydrogen bonds are possible: O—H \cdots N in enol-imine and N—H \cdots O in keto-amine form.

The molecule adopts an *E* configuration with respect to the C7=N1 double bond, with a C1—C7=N1—C8 torsion angle of 179.7 (2)° and a C7=N1—C8 angle of 121.6 (2)°. Similar results were observed for (*E*)-3-[(2-Bromophenyl) imino-methyl]-benzene-1,2-diol [178.4 (2) and 123.4 (2)°; Temel *et al.*, 2007]. The C7=N1 bond length is 1.278 (3) Å, and agree with the corresponding distance in (*E*)-3-Bromo-*N'*-(4-hydroxy-3-nitrobenzylidene) benzohydrazide [1.276 (4) Å; Cao *et al.*, 2009]. Intramolecular O—H \cdots N and O—H \cdots O hydrogen bonds generate S(6) and S(5) ring motifs (Bernstein *et al.*, 1995) (Fig. 1). The intermolecular O2—H2 \cdots O2 and O2—H2 \cdots O1 hydrogen bonds in the molecule at ($x + 1/2, y, -z + 1/2$) and ($x - 1/2, y, -z + 1/2$), forming $R_2^2(10)$ and $R_2^2(20)$ chains at [100] direction. (Table 1, Fig. 2). The dihedral angle between benzene rings A (C1—C6) and B (C8—C13) is 6.88 (15)°. The planar S(6) ring C(O1/H1/N1/C1/C2/C7) is oriented with respect to rings A and B at dihedral angles of 0.16 (44)° and 6.88 (41)°, respectively. These dihedral angles show that the molecule of (I) is almost planar. It is known that Schiff bases may exhibit thermochromism or photochromism, depending on the planarity or non-planarity of the molecule, respectively. Since the title molecule is planar, one can expect thermochromic properties in title compound.

Ab-initio Hartree-Fock (HF), density-functional theory (DFT) (Schmidt & Polik, 2007) and semi-empirical (AM1 and PM3) calculations and full-geometry optimizations were performed by means of *GAUSSIAN* 03 W package (Frisch *et al.*, 2004). The selected bond lengths and angles together with the torsion angles are compared with the obtained ones from semi-empirical, *ab-initio* HF and DFT/B3-LYP (Becke 3 parameter Lee-Yang-Parr) (Becke, 1988, 1993; Lee *et al.*, 1988) (Table 2). We observe an acceptable general agreement between them. Although the DFT molecular orbital theory was considered as the most accurate method for geometry optimization for free and complex ligands (Friesner, 2005; Liu *et al.*, 2004), the HF method led to better results in regard to the bond lengths and angles.

S2. Experimental

For the preparation of compound (I) the mixture of 2,3-dihydroxybenzaldehyde (0.5 g, 3.6 mmol) in ethanol (20 ml) and 3-bromoaniline (0.62 g, 3.6 mmol) in ethanol (20 ml) was stirred for 1 h under reflux. The crystals suitable for X-ray analysis were obtained from ethanol by slow evaporation (yield; %88, m.p.; 402–403 K).

S3. Refinement

Due to their taking part in H-bonding interactions, the hydroxyl H atoms were preferred to locate in difference Fourier map and refined freely with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$. All other H-atoms were refined using a riding model with $d(\text{C}-\text{H}) = 0.93 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

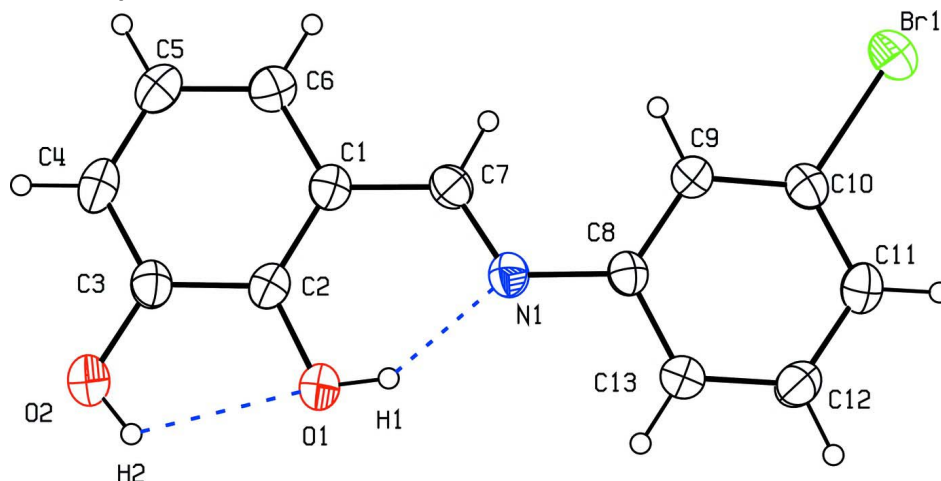


Figure 1

An ORTEP view of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids. Dashed lines indicate H-bonds.

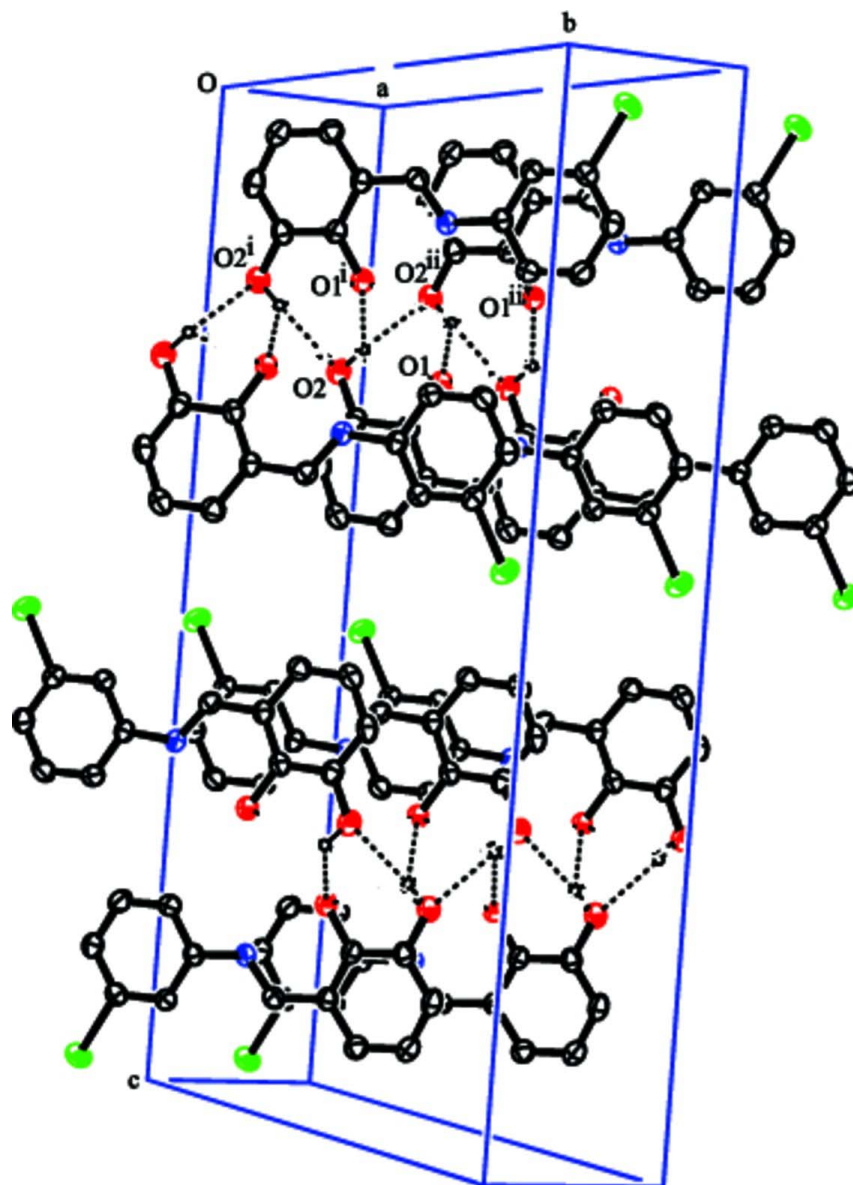


Figure 2

A packing diagram for (I), showing the O—H···O hydrogen bonds, forming $R_2^2(10)$ and $R_2^2(20)$ chains at [100]. [Symmetry codes; (i): $x + 1/2, y, -z + 1/2$; (ii): $x - 1/2, y, -z + 1/2$]. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

(E)-3-[(3-Bromophenyl)iminomethyl]benzene-1,2-diol

Crystal data

$C_{13}H_{10}BrNO_2$

$M_r = 292.13$

Orthorhombic, $Pbca$

Hall symbol: $-P\ 2ac\ 2ab$

$a = 4.7411(2)\ \text{\AA}$

$b = 18.9447(6)\ \text{\AA}$

$c = 26.1417(10)\ \text{\AA}$

$V = 2348.01(15)\ \text{\AA}^3$

$Z = 8$

$F(000) = 1168$

$D_x = 1.653\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 7185 reflections

$\theta = 1.3\text{--}26.2^\circ$

$\mu = 3.50 \text{ mm}^{-1}$
 $T = 296 \text{ K}$

Plate, red
 $0.66 \times 0.38 \times 0.10 \text{ mm}$

Data collection

Stoe IPDS-II
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 Detector resolution: $6.67 \text{ pixels mm}^{-1}$
 rotation method scans
 Absorption correction: integration
 (*X-RED32*; Stoe & Cie, 2002)
 $T_{\min} = 0.229$, $T_{\max} = 0.735$

7185 measured reflections
 2212 independent reflections
 1764 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$
 $\theta_{\max} = 25.6^\circ$, $\theta_{\min} = 1.6^\circ$
 $h = -5 \rightarrow 5$
 $k = -22 \rightarrow 22$
 $l = -31 \rightarrow 31$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.078$
 $S = 1.05$
 2212 reflections
 162 parameters
 0 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
 $w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 0.8167P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.33 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.42 \text{ e } \text{\AA}^{-3}$
 Extinction correction: *SHELXL97* (Sheldrick,
 2008)
 Extinction coefficient: 0

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.

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 $F^2 > 2\sigma(F^2)$ 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>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2287 (5)	0.59650 (12)	0.38493 (9)	0.0430 (5)
C2	0.1687 (5)	0.56587 (13)	0.33762 (9)	0.0441 (5)
C3	-0.0340 (6)	0.51215 (13)	0.33440 (10)	0.0480 (6)
C4	-0.1727 (6)	0.49065 (14)	0.37771 (11)	0.0543 (7)
H4	-0.3082	0.4553	0.3753	0.065*
C5	-0.1148 (6)	0.52049 (15)	0.42490 (11)	0.0556 (7)
H5	-0.2106	0.5052	0.4539	0.067*
C6	0.0848 (6)	0.57283 (14)	0.42865 (10)	0.0524 (6)
H6	0.1248	0.5927	0.4603	0.063*
C7	0.4352 (5)	0.65240 (13)	0.38933 (9)	0.0451 (6)
H7	0.4674	0.6726	0.4212	0.054*
C8	0.7753 (5)	0.72987 (12)	0.35557 (9)	0.0409 (5)

C9	0.8643 (5)	0.75859 (13)	0.40177 (9)	0.0461 (6)
H9	0.7918	0.7419	0.4325	0.055*
C10	1.0603 (6)	0.81192 (13)	0.40147 (9)	0.0475 (6)
C11	1.1712 (6)	0.83889 (14)	0.35705 (10)	0.0520 (6)
H11	1.3031	0.8752	0.3578	0.062*
C12	1.0810 (6)	0.81048 (15)	0.31139 (10)	0.0572 (7)
H12	1.1510	0.8283	0.2808	0.069*
C13	0.8888 (6)	0.75614 (15)	0.31054 (10)	0.0513 (6)
H13	0.8342	0.7368	0.2794	0.062*
N1	0.5747 (4)	0.67489 (11)	0.35080 (8)	0.0442 (5)
O1	0.2990 (5)	0.58565 (11)	0.29377 (7)	0.0583 (5)
O2	-0.0900 (5)	0.48050 (12)	0.28892 (8)	0.0684 (6)
Br1	1.18395 (9)	0.85040 (2)	0.464746 (12)	0.08086 (16)
H1	0.415 (8)	0.619 (2)	0.3026 (13)	0.088 (12)*
H2	-0.007 (10)	0.499 (2)	0.2666 (14)	0.113 (16)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0352 (13)	0.0422 (12)	0.0517 (13)	0.0035 (10)	-0.0009 (10)	0.0026 (10)
C2	0.0396 (13)	0.0415 (13)	0.0513 (13)	-0.0004 (11)	0.0019 (11)	0.0055 (11)
C3	0.0454 (14)	0.0416 (13)	0.0570 (14)	-0.0023 (11)	-0.0068 (12)	0.0033 (11)
C4	0.0431 (15)	0.0433 (14)	0.0764 (18)	-0.0048 (12)	0.0014 (13)	0.0124 (13)
C5	0.0503 (16)	0.0549 (16)	0.0616 (16)	-0.0008 (13)	0.0088 (13)	0.0107 (13)
C6	0.0495 (15)	0.0553 (15)	0.0525 (14)	0.0032 (13)	0.0019 (12)	0.0019 (12)
C7	0.0432 (13)	0.0457 (13)	0.0465 (12)	0.0027 (11)	-0.0039 (11)	-0.0036 (10)
C8	0.0359 (12)	0.0393 (12)	0.0476 (12)	0.0023 (10)	-0.0044 (10)	0.0006 (9)
C9	0.0475 (15)	0.0472 (14)	0.0436 (12)	-0.0054 (12)	-0.0012 (11)	0.0028 (10)
C10	0.0485 (15)	0.0441 (14)	0.0498 (13)	-0.0009 (12)	-0.0058 (12)	-0.0038 (11)
C11	0.0490 (15)	0.0440 (14)	0.0630 (15)	-0.0050 (12)	0.0027 (13)	-0.0010 (11)
C12	0.0615 (18)	0.0578 (16)	0.0524 (14)	-0.0089 (14)	0.0103 (13)	0.0035 (12)
C13	0.0551 (16)	0.0548 (16)	0.0441 (13)	-0.0062 (13)	-0.0012 (12)	-0.0012 (11)
N1	0.0396 (11)	0.0440 (11)	0.0490 (11)	-0.0024 (9)	-0.0028 (9)	0.0001 (9)
O1	0.0626 (12)	0.0612 (12)	0.0512 (10)	-0.0231 (10)	0.0022 (9)	-0.0014 (9)
O2	0.0769 (15)	0.0665 (14)	0.0618 (12)	-0.0291 (12)	-0.0049 (11)	-0.0011 (10)
Br1	0.1009 (3)	0.0846 (2)	0.05706 (19)	-0.0355 (2)	-0.01118 (17)	-0.01177 (16)

Geometric parameters (Å, °)

C1—C2	1.395 (3)	C8—C13	1.387 (3)
C1—C6	1.405 (4)	C8—C9	1.390 (3)
C1—C7	1.447 (4)	C8—N1	1.416 (3)
C2—O1	1.355 (3)	C9—C10	1.373 (4)
C2—C3	1.402 (3)	C9—H9	0.9300
C3—O2	1.358 (3)	C10—C11	1.373 (4)
C3—C4	1.371 (4)	C10—Br1	1.900 (2)
C4—C5	1.384 (4)	C11—C12	1.377 (4)
C4—H4	0.9300	C11—H11	0.9300

C5—C6	1.374 (4)	C12—C13	1.375 (4)
C5—H5	0.9300	C12—H12	0.9300
C6—H6	0.9300	C13—H13	0.9300
C7—N1	1.278 (3)	O1—H1	0.87 (4)
C7—H7	0.9300	O2—H2	0.78 (4)
C2—C1—C6	119.3 (2)	C13—C8—C9	118.6 (2)
C2—C1—C7	120.9 (2)	C13—C8—N1	116.7 (2)
C6—C1—C7	119.8 (2)	C9—C8—N1	124.6 (2)
O1—C2—C1	122.8 (2)	C10—C9—C8	119.2 (2)
O1—C2—C3	117.5 (2)	C10—C9—H9	120.4
C1—C2—C3	119.7 (2)	C8—C9—H9	120.4
O2—C3—C4	119.9 (2)	C9—C10—C11	122.5 (2)
O2—C3—C2	120.5 (2)	C9—C10—Br1	119.09 (19)
C4—C3—C2	119.7 (2)	C11—C10—Br1	118.4 (2)
C3—C4—C5	121.3 (3)	C10—C11—C12	117.9 (2)
C3—C4—H4	119.4	C10—C11—H11	121.0
C5—C4—H4	119.3	C12—C11—H11	121.0
C6—C5—C4	119.6 (3)	C13—C12—C11	120.8 (3)
C6—C5—H5	120.2	C13—C12—H12	119.6
C4—C5—H5	120.2	C11—C12—H12	119.6
C5—C6—C1	120.5 (3)	C12—C13—C8	120.8 (2)
C5—C6—H6	119.8	C12—C13—H13	119.6
C1—C6—H6	119.8	C8—C13—H13	119.6
N1—C7—C1	122.1 (2)	C7—N1—C8	121.6 (2)
N1—C7—H7	118.9	C2—O1—H1	105 (2)
C1—C7—H7	118.9	C3—O2—H2	111 (3)
C6—C1—C2—O1	-179.8 (2)	C6—C1—C7—N1	178.8 (2)
C7—C1—C2—O1	0.6 (4)	C13—C8—C9—C10	0.1 (4)
C6—C1—C2—C3	0.1 (4)	N1—C8—C9—C10	-179.9 (2)
C7—C1—C2—C3	-179.5 (2)	C8—C9—C10—C11	0.7 (4)
O1—C2—C3—O2	1.6 (4)	C8—C9—C10—Br1	-179.41 (19)
C1—C2—C3—O2	-178.3 (2)	C9—C10—C11—C12	-0.4 (4)
O1—C2—C3—C4	-179.6 (2)	Br1—C10—C11—C12	179.8 (2)
C1—C2—C3—C4	0.5 (4)	C10—C11—C12—C13	-0.9 (4)
O2—C3—C4—C5	178.2 (3)	C11—C12—C13—C8	1.7 (4)
C2—C3—C4—C5	-0.6 (4)	C9—C8—C13—C12	-1.3 (4)
C3—C4—C5—C6	0.2 (4)	N1—C8—C13—C12	178.7 (2)
C4—C5—C6—C1	0.4 (4)	C1—C7—N1—C8	179.7 (2)
C2—C1—C6—C5	-0.5 (4)	C13—C8—N1—C7	-172.2 (2)
C7—C1—C6—C5	179.0 (2)	C9—C8—N1—C7	7.9 (4)
C2—C1—C7—N1	-1.6 (4)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots N1	0.87 (4)	1.81 (4)	2.606 (3)	151 (3)

O2—H2···O1	0.78 (4)	2.31 (5)	2.718 (3)	113 (4)
O2—H2···O2 ⁱ	0.78 (4)	2.48 (5)	3.124 (3)	141 (5)
O2—H2···O1 ⁱⁱ	0.78 (4)	2.46 (4)	2.986 (3)	126 (4)

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