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(*E*)-*N*′-(5-Bromo-2-hydroxybenzylidene)-furan-2-carbohydrazide monohydrate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.029
wR factor = 0.069
Data-to-parameter ratio = 12.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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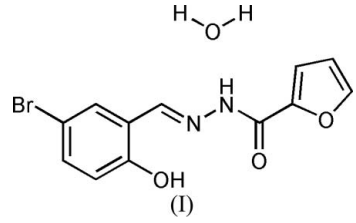
In the title molecule, $C_{12}H_9BrN_2O_3\cdot H_2O$, the dihedral angle between the benzene and furan rings is 10.0 (2)°. In the crystal structure, (*E*)-*N*′-(5-bromo-2-hydroxybenzylidene)furan-2-carbohydrazide molecules and water molecules, are linked by O—H···O and N—H···O hydrogen bonds into a two-dimensional network perpendicular to the *c* axis.

Comment

Schiff base complexes are widely used in the fields of biology, catalysis and materials science.



(I)

The asymmetric unit of the title compound, (I), is shown in Fig. 1. The dihedral angle between the benzene ring and the furan ring is 10.0 (2)°. Some key torsion are listed in Table 1. In the crystal structure, (*E*)-*N*′-(5-bromo-2-hydroxybenzylidene)furan-2-carbohydrazide molecules and water molecules are linked by O—H···O and N—H···O hydrogen bonds into a two-dimensional network perpendicular to the *c* axis (Fig. 2 and Table 2). There are also two weak C—H···O hydrogen bonds present in the crystal structure.

Experimental

A mixture of 5-bromo-2-hydroxybenzaldehyde (0.01 mol) and furan-2-carbohydrazide (0.01 mol) in ethanol (10 ml) was refluxed for 90 min. After cooling, filtration and drying, (*E*)-*N*′-(5-bromo-2-hydroxybenzylidene)furan-2-carbohydrazide was obtained. 10 mg of this compound was dissolved in 15 ml ethanol solution (95%) and the solution was allowed to evaporate at room temperature, whereupon

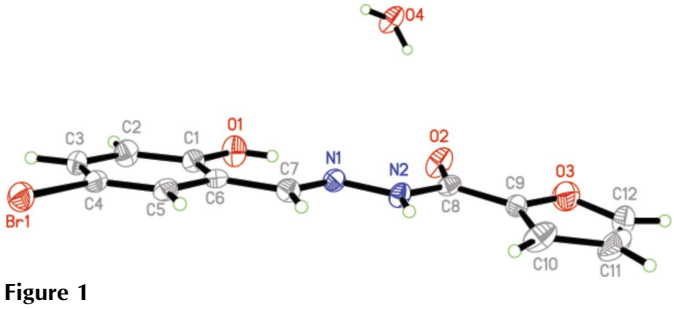


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

light-yellow single crystals of the title compound were formed after 12 d.

Crystal data

$C_{12}H_9BrN_2O_3\cdot H_2O$
$M_r = 327.13$
Orthorhombic, $P2_12_12_1$
$a = 4.8880$ (8) Å
$b = 12.495$ (2) Å
$c = 20.889$ (4) Å
$V = 1275.8$ (4) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 3.23$ mm^{-1}
$T = 294$ (2) K
0.20 × 0.18 × 0.14 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min} = 0.541$, $T_{max} = 0.634$
6358 measured reflections
2238 independent reflections
1954 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.070$
$S = 1.02$
2238 reflections
174 parameters
15 restraints
H-atom parameters constrained
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Absolute structure: Flack (1983), 795 Friedel pairs
Flack parameter: 0.007 (11)

Table 1
Selected torsion angles (°).

C7—N1—N2—C8	−178.7 (3)	N1—N2—C8—C9	−177.3 (3)
Br1—C4—C5—C6	−179.3 (2)	C12—O3—C9—C10	−0.1 (4)
O1—C1—C6—C7	−2.5 (5)	C12—O3—C9—C8	−178.6 (3)
N2—N1—C7—C6	−179.1 (3)	O2—C8—C9—C10	−176.6 (4)
C1—C6—C7—N1	5.0 (5)	N2—C8—C9—C10	2.9 (6)
C5—C6—C7—N1	−178.2 (3)	O2—C8—C9—O3	1.7 (5)
N1—N2—C8—O2	2.2 (5)	N2—C8—C9—O3	−178.8 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O4^{i}	0.86	1.95	2.792 (3)	166
O1—H1···N1	0.82	2.03	2.738 (4)	145
O4—H4A···O2^{ii}	0.86	1.99	2.847 (3)	174
O4—H4B···O2^{iii}	0.85	1.96	2.787 (3)	163
C7—H7···O4^{i}	0.93	2.47	3.257 (4)	142
C10—H10···O4^{i}	0.93	2.30	3.152 (5)	152

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

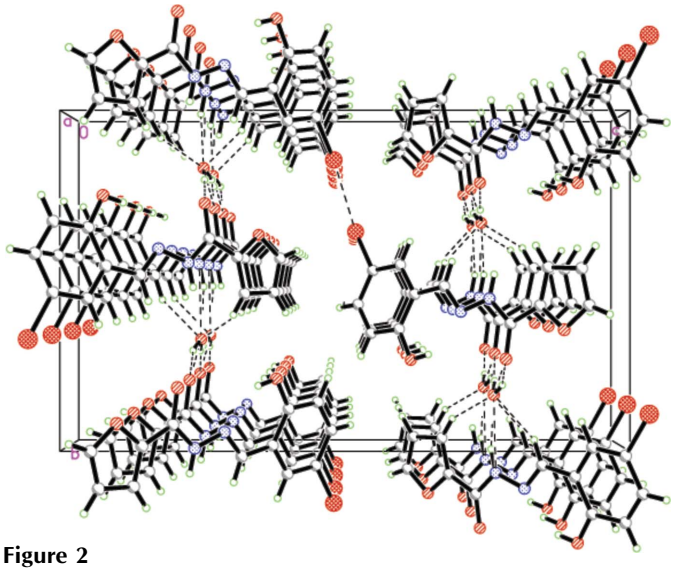


Figure 2
The crystal packing of (I), viewed along the *a* axis. Dashed lines indicate hydrogen bonds.

Water H atoms were located in a difference map and refined as riding in their as-found relative positions, with $U_{iso}(H) = 1.2U_{eq}(O)$. All other H atoms were positioned geometrically, with C—H = 0.93 Å, N—H = 0.86 Å and hydroxyl O—H = 0.82 Å, and refined in a riding model, with $U_{iso}(H) = 1.2$ or $1.5U_{eq}$(carrier).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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