

2-Bromo-*N'*-[(*E*)-(4-fluorophenyl)-methylene]-5-methoxybenzohydrazide monohydrate

B. Narayana,^a K. Sunil,^a H. S. Yathirajan,^b B. K. Sarojini^c and Michael Bolte^{d*}

^aDepartment of Studies in Chemistry, Mangalore University, Mangalagangotri 574 199, India, ^bDepartment of Studies in Chemistry, University of Mysore, Manasa-gangotri, Mysore 570 006, India, ^cDepartment of Chemistry, P. A. College of Engineering, Nadupadavu, Mangalore 574 153, India, and ^dInstitut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438

Frankfurt/Main, Germany

Correspondence e-mail: bolte@chemie.uni-frankfurt.de

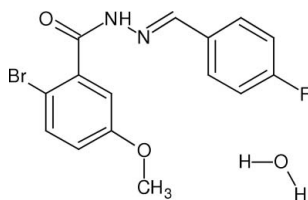
Received 16 May 2007; accepted 17 May 2007

Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.013$ Å; R factor = 0.080; wR factor = 0.202; data-to-parameter ratio = 13.7.

The crystal packing of the title compound, $\text{C}_{15}\text{H}_{12}\text{BrFN}_2\text{O}_2 \cdot \text{H}_2\text{O}$, is stabilized by $\text{N}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds. There are two molecules in the asymmetric unit, differing in the dihedral angle between the two aromatic rings, which are 62.3 (2) and 49.9 (2)°.

Related literature

For related structures, see: Bruno *et al.* (1998); Harrison *et al.* (2005); Yathirajan, Sarojini *et al.* (2007); Yathirajan, Narayana, *et al.* (2007). For related literature, see: Varma *et al.* (1986); Misra *et al.* (1981); Agarwal *et al.* (1983); Singh *et al.* (1988); Hodnett *et al.* (1970).



Experimental

Crystal data

$\text{C}_{15}\text{H}_{12}\text{BrFN}_2\text{O}_2 \cdot \text{H}_2\text{O}$
 $M_r = 369.19$

Monoclinic, Cc
 $a = 30.1171$ (18) Å
 $b = 8.0187$ (7) Å
 $c = 13.4661$ (8) Å
 $\beta = 111.902$ (4)°

$V = 3017.3$ (4) Å³
 $Z = 8$

Mo $K\alpha$ radiation
 $\mu = 2.75$ mm⁻¹
 $T = 173$ (2) K
 $0.37 \times 0.35 \times 0.33$ mm

Data collection

Stoe IPDS II two-circle diffractometer

Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)

$T_{\min} = 0.379$, $T_{\max} = 0.394$

16531 measured reflections
5477 independent reflections
4843 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.059$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.080$

$wR(F^2) = 0.202$

$S = 1.02$

5477 reflections

400 parameters

2 restraints

H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.56$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.76$ e Å⁻³
Absolute structure: Flack (1983),
2642 Friedel pairs
Flack parameter: 0.018 (17)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{N1}-\text{H1} \cdots \text{O1W}$	0.88	2.03	2.901 (9)	172
$\text{N1A}-\text{H1A} \cdots \text{O1WA}$	0.88	2.01	2.860 (9)	163
$\text{O1W}-\text{H1W1} \cdots \text{O1}^{\text{i}}$	0.84	1.99	2.832 (8)	180
$\text{O1W}-\text{H1W2} \cdots \text{O1A}^{\text{ii}}$	0.84	2.01	2.856 (8)	180
$\text{O1WA}-\text{H1W3} \cdots \text{O1}^{\text{iii}}$	0.84	2.06	2.897 (8)	180
$\text{O1WA}-\text{H1W4} \cdots \text{O1A}^{\text{iv}}$	0.84	1.96	2.802 (7)	180

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

Data collection: *X-Area* (Stoe & Cie, 2001); cell refinement: *X-Area*; data reduction: *X-Area*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

KS thanks the Department of Chemistry, Mangalore University for research facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2297).

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