Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Amino-4-[4-(benzyloxy)phenyl]-5-methylthiazol-3-ium bromide monohydrate

Dao-Hang He, Gao Cao and Ai-Xi Hu*

The School of Chemical and Energy Engineering, South China University of Technology, Guangzhou 510640, People's Republic of China

Correspondence e-mail: axhu0731@yahoo.com.cn

Received 4 November 2006
Accepted 8 November 2006

The crystal packing of the hydrated title salt, $C_{17}H_{17}N_2OS^+\cdot Br^-\cdot H_2O$, dominated by an extensive N—H···O_{water}, N—H···Br and O_{water}—H···Br hydrogen-bonding network between organic molecules, bromine anions and water molecules. The anions are located on crystallograpic twofold axes.

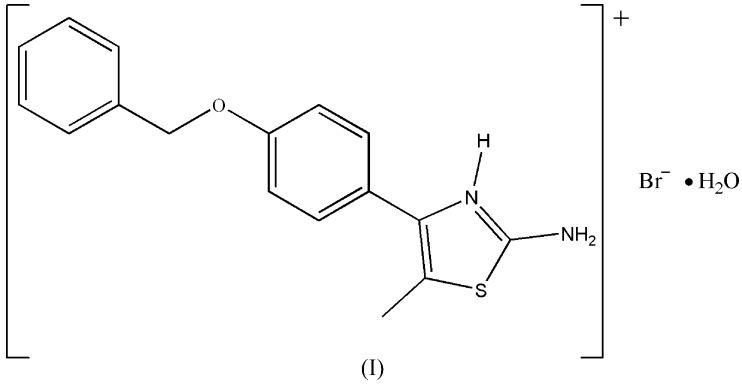
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.034
wR factor = 0.086
Data-to-parameter ratio = 17.8

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

Comment

2-Amino-4-arylthiazoles are an important class of heterocyclic compounds in the field of organic pharmaceutical chemistry (Marcantonio *et al.*, 2002). Heterocyclic compounds containing a thiazole ring generally exhibit broad-spectrum biological activity and some thiazole derivatives have been used as local anaesthetics, as anticonvulsant, antivirus, and antimicrobial agents, insecticides and so on (Narayana *et al.*, 2004). We report here the synthesis and structure of the title 2-amino-4-arylthiazole derivative, (I).



(I)

Fig. 1 shows the molecular structure of (I), with the atomic numbering scheme. The molecule of (I) contains a planar thiazole ring and two benzene rings, with dihedral angles of 42.7 (2) and 10.6 (2)°, respectively, between the least-squares planes of the two benzene rings (C5–C10 and C12–C17) and the thiazole ring. The dihedral angle between the two benzene rings is 51.3 (2)°.

The anions lie on twofold axes. The cations, anions and water molecules in (I) associate *via* N—H···O hydrogen bonds between the amino H atoms and water O atoms, with the hydrogen-bonding array additionally involving O—H···Br and N—H···Br hydrogen bonds (Table 1). The crystal structure is further stabilized by van der Waals forces.

Experimental

1-[4-(Benzyloxy)phenyl]propan-1-one (0.005 mol) was dissolved in 100 ml ethanol and the mixture was stirred and heated to reflux.

© 2006 International Union of Crystallography
All rights reserved

Cupric bromide (0.01 mol) was added to the reaction mixture in batches and the course of the reaction was followed by thin-layer chromatography. After the reaction had finished, the mixture was filtered, 0.05 mol thiurea was added to the filtrate, and the mixture was heated at reflux for 3 h. The mixture was then cooled in a refrigerator, giving a yellow precipitate, which was filtered off and dried to obtain the title compound (I). MS (m/z): 296 (base, M^+), 205 (M^+–$PhCH_2$), 91 (100%, $PhCH_2^+$), 80, 65, 51. Crystals suitable for X-ray crystallographic analysis were obtained by slow evaporation of an ethanol solution at room temperature.

Crystal data

$C_{17}H_{17}N_2OS^+\cdot Br^-\cdot H_2O$
M_r = 395.31
Monoclinic, $C2/c$
a = 10.0462 (7) Å
b = 16.2513 (11) Å
c = 21.7802 (15) Å
β = 95.1720 (10)°
V = 3541.4 (4) Å^3
Z = 8
D_x = 1.483 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.45 mm^{-1}
T = 294 (2) K
Block, yellow
0.48 × 0.45 × 0.40 mm

Data collection

Bruker AXS SMART 1000 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.328, T_{max} = 0.375
8967 measured reflections
3841 independent reflections
2494 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.086
S = 1.02
3841 reflections
216 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0329P)^2 + 2.5508P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2W	0.86	1.88	2.724 (3)	166
N2—H2A···Br2	0.86	2.68	3.483 (2)	155
N2—H2B···Br1^{i}	0.86	2.59	3.362 (2)	149
O2W—H2C···Br1	0.78 (3)	2.52 (4)	3.290 (2)	171 (4)
O2W—H2D···Br2	0.79 (3)	2.50 (4)	3.259 (2)	161 (4)

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

All H atoms except for the water H atoms were refined in the riding-model approximation, with N—H distances of 0.86 Å and C—H distances of 0.93 (aromatic), 0.96 (methyl) and 0.97 Å (methylene), and with $U_{iso}(H) = 1.2U_{eq}(C,N)$ or $1.5U_{eq}$(methyl C). The water H atoms were located in Fourier syntheses and $U_{iso}(H)$ values were set equal to $1.2U_{eq}(O)$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; 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*.

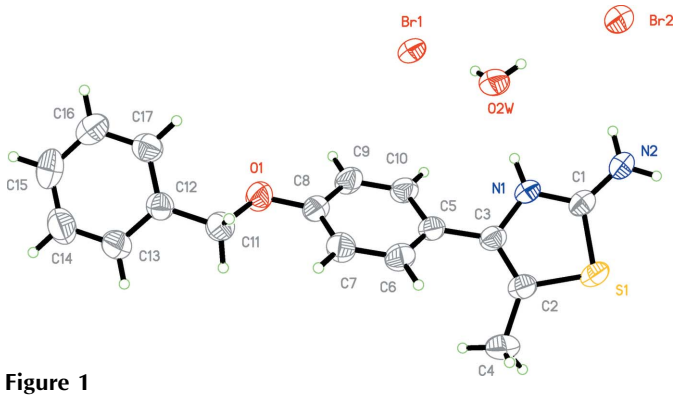


Figure 1
The molecular structure of (I), showing the atom-labelling scheme and 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

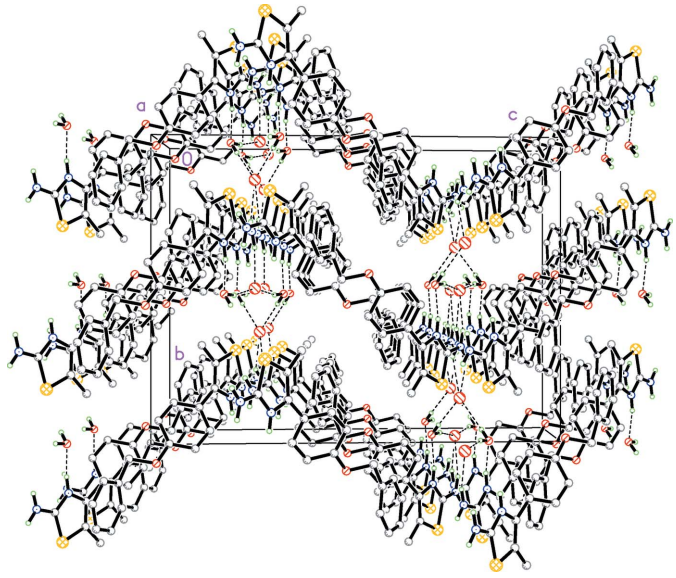


Figure 2
A packing diagram for (I). Dashed lines indicate hydrogen bonds.

This work was supported by the Natural Science Foundation of Guangdong Province (No. 04300531).

References

Bruker (1997). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
Marcantonio, K. M., Frey, L. F., Murry, J. A. & Chen, C. Y. (2002). *Tetrahedron Lett.* **43**, 8845–8848.
Narayana, B., Vijaya Raj, K. K., Ashalatha, B. V., Suchetha Kumari, N. & Sarojini, B. K. (2004). *Eur. J. Med. Chem.* **39**, 867–872.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.