

*N,N*-(2-benzothiazole)(2-pyridylmethyl)amine

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## Key indicators

Single-crystal X-ray study

*T* = 296 K

Mean  $\sigma$ (C–C) = 0.005 Å

*R* factor = 0.031

w*R* factor = 0.070

Data-to-parameter ratio = 8.5

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

The crystal structure of a new compound, *N,N*-(2-benzothiazole)(2-pyridylmethyl)amine C<sub>13</sub>H<sub>11</sub>N<sub>3</sub>S, has been determined by X-ray diffraction analysis. The amino group and the pyridine-N atom are involved in intermolecular hydrogen bonds, which link the molecules into one-dimensional chains.

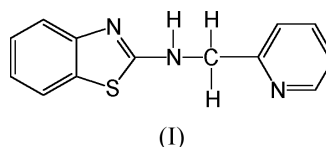
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## Comment

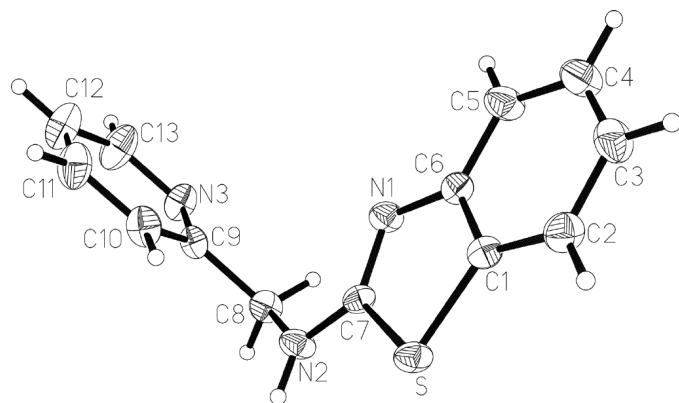
Schiff bases derived from aminobenzothiazole have been widely investigated because of their biological activity, such as antifungal (Dash *et al.*, 1984; Dash *et al.*, 1980) and anticancer (Armstrong *et al.*, 1992). Recently, reductive Schiff bases have aroused interest as they are more stable and more flexible (Chen *et al.*, 2000) than Schiff bases themselves. Here we report the synthesis and crystal structure of *N,N*-(2-benzothiazole)(2-pyridylmethyl)amine, (I).



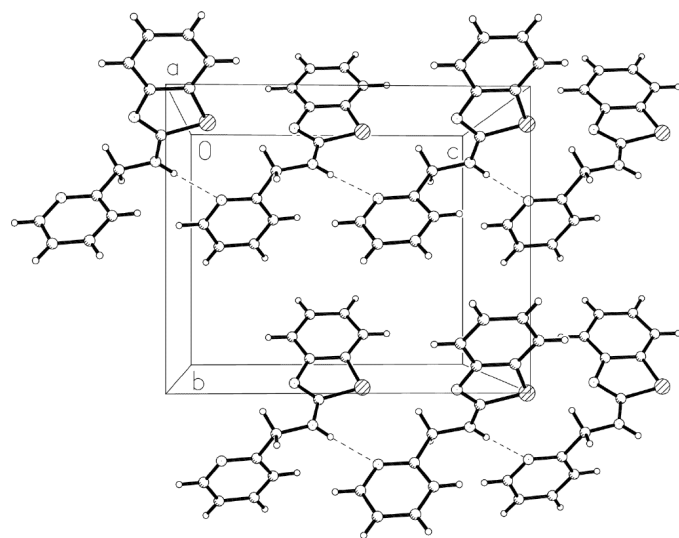
In the title compound, the N2–C8 bond distance [1.453 (4) Å] is equal to that found in the reductive Schiff base 4-[(3-pyridylamino)methyl]phenol (Chen *et al.*, 2001) and longer than that for C=N [1.285 (2) Å] in the Schiff base derived from picolinaldehyde *N*-oxide and 4-aminoanti-pyridine (Liang *et al.*, 2002). This bond length indicates that the C=N double bond of the Schiff base has been reduced by adding two H atoms from NaBH<sub>4</sub>. The N2–C8 bond is also longer than the other N–C bonds [N1–C6 1.391 (3), N1–C7 1.301 (3) and N3–C9 1.334 (4) Å]. The pyridyl ring and benzothiazole ring form a distorted V configuration, with a dihedral angle of 88.27 (6)°.

The bond lengths in the 2-aminobenzothiazole ring system (Table 1) are normal, and agree with the corresponding values found in diacetatobis(2-aminobenzothiazole)zinc(II) (Usman *et al.*, 2003). In the pyridyl ring, there are no unusually long bonds and the long carbonyl bond [1.355 (6) Å *versus* 1.28 Å], while shorter than the normal single bond found in ethers and alcohols (>1.4 Å), is consistent with the corresponding values found in Schiff bases derived from picolinaldehyde *N*-oxide semicarbazone (Liang *et al.*, 2002). The bond angles in the aromatic ring system were found to be between 128.5 (2)° and 88.05 (12)°.

There is one intermolecular hydrogen bond involving the amino group, which acts as donor, and the pyridine N atom acting as acceptor, to form N2–H2N⋯N3<sup>1</sup> (symmetry code as



**Figure 1**  
ORTEP drawing (30% probability displacement ellipsoids) of the title compound.



**Figure 2**  
View of the packing of the title compound.

in Table 1). The molecules form hydrogen-bonded chains along the *c* direction.

## Experimental

The title compound was prepared according to the procedure of Chen *et al.* (2000). The two-step reaction gave an oil product that was recrystallized from  $\text{CHCl}_3$ . Pale yellowish prisms suitable for data collection were obtained in a yield of 62%. IR(KBr,  $\nu \text{ cm}^{-1}$ ): 3249(*s*), 3038(*s*) 1598(*s*), 1570(*s*), 1540(*m*), 1474(*m*), 1439(*s*), 1409(*m*), 1210(*m*), 757(*m*). Analysis, calculated for  $\text{C}_{13}\text{H}_{11}\text{N}_3\text{S}$ : C 64.72, H 4.59, N 17.41%; found: C 64.76, H 4.58, N 17.47%.

### Crystal data

$\text{C}_{13}\text{H}_{11}\text{N}_3\text{S}$   
 $M_r = 241.31$   
 Orthorhombic, *Iba*2  
 $a = 20.144$  (4) Å  
 $b = 9.774$  (2) Å  
 $c = 11.586$  (1) Å  
 $V = 2281.1$  (7) Å<sup>3</sup>  
 $Z = 8$   
 $D_x = 1.405 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation  
 Cell parameters from 36 reflections  
 $\theta = 4.0\text{--}15.3^\circ$   
 $\mu = 0.26 \text{ mm}^{-1}$   
 $T = 296$  (2) K  
 Prism, pale yellow  
 $0.52 \times 0.44 \times 0.44 \text{ mm}$

### Data collection

Siemens P4 diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.862$ ,  $T_{\max} = 0.887$   
 1561 measured reflections  
 1317 independent reflections  
 1107 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.011$   
 $\theta_{\text{max}} = 27.0^\circ$   
 $h = -1 \rightarrow 25$   
 $k = 0 \rightarrow 12$   
 $l = 0 \rightarrow 14$   
 3 standard reflections  
 every 97 reflections  
 intensity decay: 3.6%

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.070$   
 $S = 0.96$   
 1317 reflections  
 155 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0399P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.13 \text{ e \AA}^{-3}$   
 Extinction correction: SHELXL  
 Extinction coefficient: 0.0017 (4)

**Table 1**

Selected geometric parameters (Å, °).

S—C1	1.749 (3)	N2—C7	1.345 (3)
S—C7	1.766 (2)	N2—C8	1.453 (4)
N1—C7	1.301 (3)	C8—C9	1.507 (4)
N1—C6	1.391 (3)		
C1—S—C7	88.05 (12)	C7—N2—C8	120.9 (2)
C7—N1—C6	109.5 (2)		

**Table 2**

Hydrogen-bonding 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>
N2—H2N...N3 <sup>i</sup>	0.86	2.21	3.069 (3)	177

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

The H atoms were positioned geometrically and were treated as riding atoms and refined isotropically, with C—H distances of 0.93–0.96 Å, an N—H distance of 0.86 Å, and  $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5 U_{\text{eq}}(\text{C})$  and  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{N})$ .

Data collection: XSCANS (Siemens, 1994); cell refinement: XSCANS; data reduction: SHELXTL (Sheldrick, 1997a); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997b); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997b); molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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