Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(Methylsulfanyl)-1*H*-benzimidazole

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Received 21 October 2005
Accepted 15 November 2005
Online 23 November 2005

Key indicators

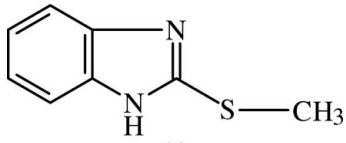
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.002 Å
R factor = 0.033
wR factor = 0.090
Data-to-parameter ratio = 13.4

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

The benzimidazole ring system in the title molecule, $C_8H_8N_2S$, is planar The imidazole ring does not exhibit a delocalized aromatic bond system. Molecules are linked by N—H···N hydrogen bonds along the c axis. The crystal structure is further stabilized by C—H···π interactions.

Comment

2-Mercaptobenzimidazole (MBI), a widely used antioxidant for rubbers and plastics, has a potent thyrotoxic effect in rats (Kawasaki *et al.*, 1998). Human exposure to MBI occurs through the use of rubber products processed with this antioxidant for vulcanization (Airaudo *et al.*, 1990). MBI is rather stable and might act as an environmental endocrine disrupter. Methylated derivatives of MBI for industrial supply are much less toxic (Paynter *et al.*, 1988). Further, they are known to be efficient corrosion inhibitors for metals and alloys in various aggressive media (Donnelly *et al.*, 1978). Keeping in view the importance of such compounds, we report here the crystal structure of the title compound, (I).



(I)

The fused ring system in (I) is planar with a maximum deviation of 0.011 (1) Å for the atom C3; atoms S1 and C8 are also coplanar with it. The geometrical parameters of the imidazole ring system are consistent with those in the literature (Ravishankar *et al.*, 2005). In the imidazole ring, there is significant shortening of the N1—C3 bond and lengthening of the N1—C4 bond (Table 1) compared with the values for

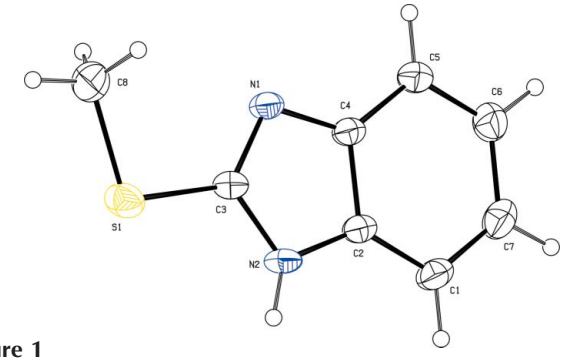


Figure 1
A view of (I) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

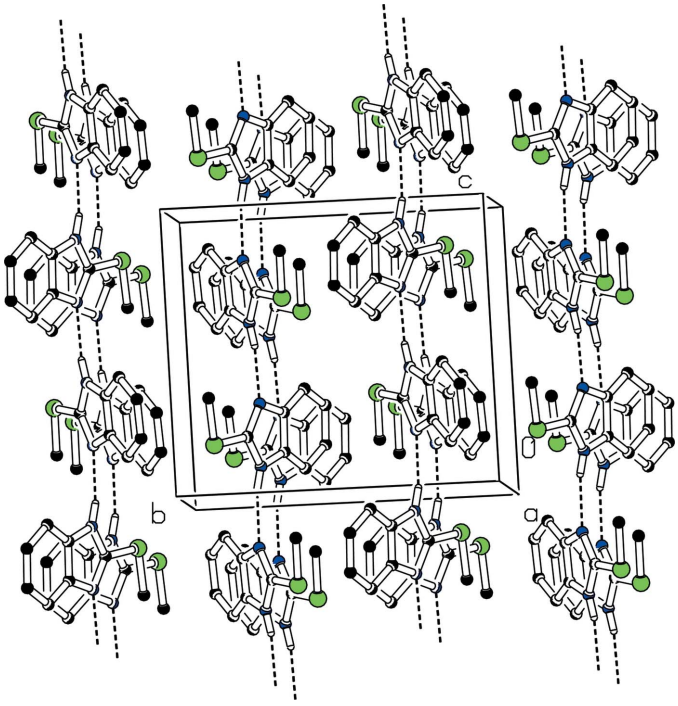


Figure 2
A packing diagram of (I), showing the N—H···N interactions along the *c* axis. H atoms not involved in hydrogen bonding have been omitted for clarity.

2-mercaptobenzimidazole (Form *et al.*, 1976); this indicates a failure to form the delocalized aromatic system which might be expected for this molecule. The C3—S1 and C8—S1 bond lengths [1.7374 (16) and 1.783 (2) Å] possess 36% and 19% SCF-π bond character, respectively (Trinajstic, 1968). The methyl substituent at atom S1 has an impact on the bond lengths and angles of the five-membered heterocycle. This can be seen clearly by comparing S1—C3—N2 and S1—C3—N1 (Table 1) with the corresponding angles in structures with no substitution at the S atom (Kitano *et al.*, 1991; Ravikumar *et al.*, 1995).

The molecules are linked by N—H···N hydrogen bonds, forming chains along the *c* axis (Fig. 2). The structure is further stabilized by a C—H···π interaction involving the methyl H8*A* atom and the nine-membered benzimidazole ring system (Table 2).

Experimental

The title compound was obtained from Sigma–Aldrich and recrystallized from methanol.

Crystal data

$C_8H_8N_2S$
M_r = 164.22
Monoclinic, $P2_1/c$
a = 6.9279 (4) Å
b = 11.4613 (7) Å
c = 10.1980 (7) Å
β = 99.052 (1)°
V = 799.66 (9) Å^3
Z = 4
D_x = 1.364 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2320 reflections
θ = 2.7–27.8°
μ = 0.33 mm^{-1}
T = 273 (2) K
Block, colourless
0.22 × 0.18 × 0.16 mm

Data collection

Bruker Smart APEX CCD area-detector diffractometer
ω scans
Absorption correction: none
7479 measured reflections
1405 independent reflections
1298 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 25.0°
$h = -8 \rightarrow 8$
$k = -13 \rightarrow 13$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.090
S = 1.03
1405 reflections
105 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.2519P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C2—N2	1.378 (2)	C3—N2	1.3584 (19)
C3—N1	1.3160 (19)	C4—N1	1.3931 (19)
N1—C3—S1	126.90 (11)	N2—C3—S1	119.56 (11)
C1—C2—C4—N1	178.88 (14)	N2—C3—S1—C8	176.47 (13)
S1—C3—N2—C2	176.79 (10)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*N*···N1^{i}	0.84 (2)	2.07 (2)	2.8769 (17)	160 (2)
C8—H8*A*···*Cg*1^{ii}	0.96	2.71	3.58	150

Symmetry codes: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $-x+2, y+\frac{1}{2}, -z+\frac{1}{2}$. *Cg*1 is the centroid of the benzimidazole ring system.

The H atom attached to the N atom was located in a difference density map and refined freely. All other H atoms were placed in geometrically idealized positions and allowed to ride with C—H distances in the range 0.93–0.97 Å, and with U_{iso}(H)=1.2–1.5U_{eq}(C)..

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

The authors thank Dr J. S. Yadav, Director, IICT, Hyderabad, for his kind encouragement.

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