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Key indicators

Single-crystal X-ray study
T = 100 K
Mean $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$
R factor = 0.019
wR factor = 0.047
Data-to-parameter ratio = 20.5

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

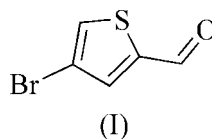
4-Bromothiophene-2-carboxaldehyde

The title compound, $\text{C}_4\text{H}_3\text{BrOS}$, (I), was recrystallized from ethanol at 273 K. The crystal structure of (I) has been determined at 100 K.

Received 2 October 2003
Accepted 16 October 2003
Online 23 October 2003

Comment

As part of with our structural studies on symmetric thenoins (Crundwell *et al.*, 2002*a,b*) and symmetric thenils (Crundwell *et al.*, 2003), we report the structure of 4-bromothiophene-2-carboxaldehyde, (I). This aldehyde crystallizes with one molecule in the asymmetric unit. An ORTEP-3 (Farrugia, 1997) view of (I) is shown in Fig. 1.



Experimental

Crystals of the title compound, (I), were obtained by recrystallizing 4-bromothiophene-2-carboxaldehyde as received from Aldrich. The aldehyde was dissolved in warm 95% ethanol and allowed to cool to room temperature. The colorless needles had a sharp melting point of 318 K, which, along with ¹H NMR data on (I), was in agreement with published values (Fournari *et al.*, 1967).

Crystal data

$\text{C}_4\text{H}_3\text{BrOS}$
 $M_r = 191.04$
Monoclinic, $P2_1/c$
 $a = 4.1169 (4) \text{ \AA}$
 $b = 8.4929 (8) \text{ \AA}$
 $c = 17.1626 (16) \text{ \AA}$
 $\beta = 90.788 (2)^\circ$
 $V = 600.02 (10) \text{ \AA}^3$
 $Z = 4$
 $D_x = 2.115 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation
Cell parameters from 5955 reflections
 $\theta = 2.4\text{--}28.3^\circ$
 $\mu = 7.08 \text{ mm}^{-1}$
 $T = 100 (2) \text{ K}$
Cube, colorless
 $0.26 \times 0.26 \times 0.26 \text{ mm}$

Data collection

Br-

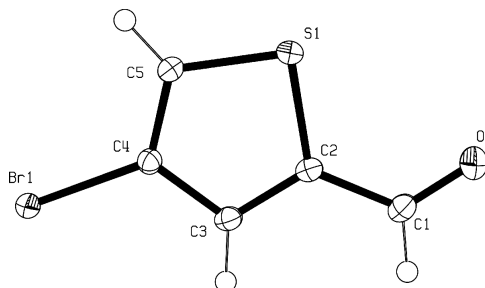


Figure 1

A view of (I) (Farrugia, 1997). Displacement ellipsoids are drawn at the 50% probability level.

uker SMART CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (Blessing, 1995)
 $T_{\min} = 0.141$, $T_{\max} = 0.159$
 5955 measured reflections

1499 independent reflections
 1408 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$
 $\theta_{\max} = 28.3^\circ$
 $h = -5 \rightarrow 5$
 $k = -11 \rightarrow 11$
 $l = -22 \rightarrow 22$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.019$
 $wR(F^2) = 0.047$
 $S = 1.05$
 1499 reflections
 73 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0039P)^2 + 0.449P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.004$
 $\Delta\rho_{\max} = 0.50 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.32 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Br1—C4	1.8804 (18)	C3—C2	1.374 (2)
C5—C4	1.371 (2)	C2—C1	1.457 (2)
C5—S1	1.7118 (19)	C2—S1	1.7218 (17)
C4—C3	1.414 (2)	O1—C1	1.213 (2)
C4—C5—S1	111.27 (14)	C3—C2—C1	125.71 (16)
C5—C4—C3	113.67 (16)	C3—C2—S1	112.23 (13)
C5—C4—Br1	123.40 (14)	C1—C2—S1	122.03 (14)
C3—C4—Br1	122.92 (13)	C5—S1—C2	91.61 (9)
C2—C3—C4	111.23 (16)	O1—C1—C2	124.39 (18)

All H atoms were placed in calculated positions, with C—H distances of 0.93 \AA , and were included in the refinement in riding-motion approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$ of the carrier atom.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINTE* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL*.

GC and VS acknowledge the Donors of the American Chemical Society Petroleum Research Fund for primary support of this research (#38867-B5m). MZ and JU were supported by NSF grant 0111511, and the diffractometer was funded by NSF grant 0087210, by Ohio Board of Regents grant CAP-491, and by YSU.

References

- Blessing, R. H. (1995). *Acta Cryst.* **A51**, 33–38.
 Bruker (1997). *SMART*, *SAINTE* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Crundwell, G., Meskill, T., Sayers, D. & Kantardjieff, K. (2002a). *Acta Cryst.* **E58**, o666–o667.
 Crundwell, G., Meskill, T., Sayers, D. & Kantardjieff, K. (2002b). *Acta Cryst.* **E58**, o668–o670.
 Crundwell, G., Sullivan, J., Pelto, R. & Kantardjieff, K. (2003). *J. Chem. Crystallogr.* **33**, 239–244.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Fournari, P., Guillard, R. & Person, M. (1967). *Bull. Soc. Chim. Fr.* pp. 4115–4120.
 Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.