

2-(Pyrimidin-2-ylsulfanyl)acetic acid

Jian Xin Pan and Qian Wang Chen*

Hefei National Laboratory for Physical Sciences at the Microscale and Department of Materials Science & Engineering, University of Science and Technology of China, Hefei 230026, People's Republic of China
Correspondence e-mail: cqw@ustc.edu.cn

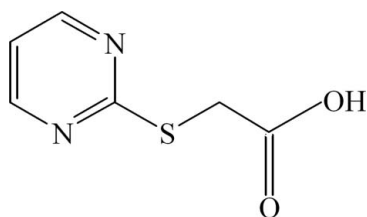
Received 24 January 2009; accepted 21 February 2009

Key indicators: single-crystal X-ray study; $T = 153$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.032; wR factor = 0.086; data-to-parameter ratio = 13.0.

The molecule of the title compound, $\text{C}_6\text{H}_6\text{N}_2\text{O}_2\text{S}$, lies on a crystallographic mirror plane with the methylene H atoms related by mirror symmetry. In the crystal packing, molecules are linked into layers by intermolecular $\text{O}-\text{H}\cdots\text{N}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For the coordination chemistry of thioether ligands, see: Li & Bu (2008); Bu *et al.* (2003); Chen *et al.* (2003); Demadis & Coucouvanis (1995); Peng *et al.* (2006). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

 $\text{C}_6\text{H}_6\text{N}_2\text{O}_2\text{S}$
 $M_r = 170.19$

 Orthorhombic, $Pnma$
 $a = 14.660$ (6) Å

 $b = 6.579$ (2) Å

 $c = 7.664$ (3) Å

 $V = 739.2$ (5) Å³
 $Z = 4$

 Mo $K\alpha$ radiation

 $\mu = 0.38$ mm⁻¹
 $T = 153$ K

 $0.22 \times 0.20 \times 0.07$ mm

Data collection

Bruker P4 diffractometer
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.920$, $T_{\max} = 0.974$

5392 measured reflections
911 independent reflections
828 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.086$
 $S = 1.07$

911 reflections

70 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.22$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.20$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O}2-\text{H}1\cdots\text{N}2^{\text{i}}$	0.89 (3)	1.78 (3)	2.663 (2)	178 (3)
$\text{C}6-\text{H}6\cdots\text{O}1^{\text{ii}}$	0.93	2.44	3.266 (3)	148
$\text{C}5-\text{H}5\cdots\text{O}2^{\text{iii}}$	0.93	2.47	3.403 (3)	178

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

We gratefully acknowledge the financial support of the National Natural Science Foundation of China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2292).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Bu, X.-H., Xie, Y.-B., Li, J.-R. & Zhang, R.-H. (2003). *Inorg. Chem.* **42**, 7422–7430.
- Chen, C.-L., Su, C.-Y., Cai, Y.-P., Zhang, H.-X., Xu, A.-W., Kang, B.-S. & zur Loye, H.-C. (2003). *Inorg. Chem.* **42**, 3738–3750.
- Demadis, K. D. & Coucouvanis, D. (1995). *Inorg. Chem.* **34**, 3658–3666.
- Li, J.-R. & Bu, X.-H. (2008). *Eur. J. Inorg. Chem.* pp. 27–40.
- Peng, R., Li, D., Wu, T., Zhou, X.-P. & Ng, S. W. (2006). *Inorg. Chem.* **45**, 4035–4046.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Siemens (1994). *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Siemens (1996). *SMART*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

supplementary materials

Acta Cryst. (2009). E65, o652 [doi:10.1107/S1600536809006400]

2-(Pyrimidin-2-ylsulfanyl)acetic acid

J. X. Pan and Q. W. Chen

Comment

Great efforts have been focused on the rational design and synthesis of metal-organic coordination architectures by using flexible bridging ligands due to their flexibility and conformational freedoms, which offer the possibility for the construction of unprecedented frameworks (Li & Bu, 2008). Recently, flexible thioethers have been well established ligands in coordination and metallocsupramolecular chemistry because of their rich structural information (Bu *et al.*, 2003; Chen *et al.*, 2003; Demadis & Coucouvanis, 1995; Peng *et al.*, 2006). In the process of preparing metal-organic coordination architectures, single-crystals of the title compound were obtained unexpectedly.

The molecular structure and the atom-numbering scheme of the title compound are shown in Fig. 1. The molecule lies on a mirror plane, with the methylene H atoms related by mirror symmetry. All bond lengths (Allen *et al.*, 1987) and angles show normal value. In the crystal packing, molecules are linked into layers perpendicular to the *b* axis by intermolecular O—H...N and C—H...O hydrogen bonds (Table 1).

Experimental

A mixture of Co(Ac)₂·6H₂O (0.142 g, 0.50 mmol), (2-Pyrimidylthio)acetic acid (0.035 g, 0.20 mmol) and sodium azide (0.032 g, 0.50 mmol) in H₂O (10 ml) was stirred for 1 h, then filtered, and the filtrate was kept at room temperature. Single crystals of the title compound were obtained by slow evaporation of the solvent after a few days.

Refinement

Hydrogen atoms bound to C atoms were positioned geometrically with C—H = 0.93–0.97 Å, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The H atom bound to O was freely refined.

Figures

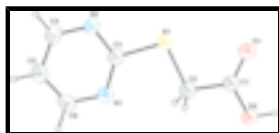


Fig. 1. The molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

2-(Pyrimidin-2-ylsulfanyl)acetic acid

Crystal data

C₆H₆N₂O₂S

$M_r = 170.19$

$F_{000} = 352$

$D_x = 1.529 \text{ Mg m}^{-3}$

supplementary materials

Orthorhombic, $Pnma$

Hall symbol: -P 2ac 2n

$a = 14.660$ (6) Å

$b = 6.579$ (2) Å

$c = 7.664$ (3) Å

$V = 739.2$ (5) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 2019 reflections

$\theta = 4.3$ – 27.5°

$\mu = 0.38$ mm⁻¹

$T = 153$ K

Prism, colorless

$0.22 \times 0.20 \times 0.07$ mm

Data collection

Bruker P4
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 153$ K

ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)

$T_{\min} = 0.920$, $T_{\max} = 0.974$

5392 measured reflections

911 independent reflections

828 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\max} = 27.5^\circ$

$\theta_{\min} = 4.3^\circ$

$h = -18 \rightarrow 18$

$k = -8 \rightarrow 7$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.086$

$S = 1.07$

911 reflections

70 parameters

Primary atom site location: structure-invariant direct
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring
sites

H atoms treated by a mixture of
independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 0.2357P]$$

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

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
S1	0.36018 (3)	0.2500	0.16539 (6)	0.0429 (2)	
O2	0.09853 (9)	0.2500	0.24621 (18)	0.0421 (4)	
H1	0.067 (2)	0.2500	0.345 (4)	0.088 (10)*	
O1	0.21943 (9)	0.2500	0.42130 (18)	0.0516 (4)	
N2	0.50091 (10)	0.2500	-0.0392 (2)	0.0373 (4)	
C2	0.24089 (12)	0.2500	0.1111 (3)	0.0415 (5)	
H2A	0.2262	0.3696	0.0426	0.050*	0.50
H2B	0.2262	0.1304	0.0426	0.050*	0.50
C3	0.40934 (12)	0.2500	-0.0428 (2)	0.0334 (4)	
C4	0.54355 (13)	0.2500	-0.1933 (3)	0.0408 (5)	
H4	0.6070	0.2500	-0.1960	0.049*	
C1	0.18678 (12)	0.2500	0.2774 (2)	0.0349 (4)	
N1	0.35745 (10)	0.2500	-0.1845 (2)	0.0395 (4)	
C6	0.40261 (14)	0.2500	-0.3361 (2)	0.0437 (5)	
H6	0.3690	0.2500	-0.4390	0.052*	
C5	0.49614 (14)	0.2500	-0.3477 (3)	0.0446 (5)	
H5	0.5259	0.2500	-0.4549	0.054*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0244 (3)	0.0774 (4)	0.0270 (3)	0.000	-0.00018 (16)	0.000
O2	0.0221 (6)	0.0738 (10)	0.0304 (7)	0.000	-0.0008 (5)	0.000
O1	0.0293 (7)	0.0959 (12)	0.0298 (7)	0.000	-0.0031 (5)	0.000
N2	0.0246 (7)	0.0571 (10)	0.0304 (8)	0.000	0.0002 (6)	0.000
C2	0.0251 (8)	0.0698 (14)	0.0298 (9)	0.000	-0.0004 (7)	0.000
C3	0.0262 (8)	0.0448 (10)	0.0292 (8)	0.000	-0.0004 (7)	0.000
C4	0.0284 (9)	0.0549 (12)	0.0391 (10)	0.000	0.0054 (7)	0.000
C1	0.0254 (8)	0.0481 (11)	0.0311 (9)	0.000	-0.0012 (7)	0.000
N1	0.0293 (8)	0.0593 (11)	0.0299 (8)	0.000	-0.0015 (6)	0.000
C6	0.0403 (11)	0.0632 (13)	0.0277 (9)	0.000	-0.0041 (8)	0.000
C5	0.0416 (10)	0.0624 (14)	0.0299 (9)	0.000	0.0075 (8)	0.000

Geometric parameters (\AA , $^\circ$)

S1—C3	1.7507 (19)	C2—H2B	0.9700
S1—C2	1.7976 (19)	C3—N1	1.326 (2)
O2—C1	1.316 (2)	C4—C5	1.372 (3)
O2—H1	0.89 (3)	C4—H4	0.9300
O1—C1	1.202 (2)	N1—C6	1.337 (2)
N2—C4	1.336 (2)	C6—C5	1.374 (3)
N2—C3	1.343 (2)	C6—H6	0.9300
C2—C1	1.501 (3)	C5—H5	0.9300
C2—H2A	0.9700		

supplementary materials

C3—S1—C2	100.92 (9)	N2—C4—H4	119.2
C1—O2—H1	111 (2)	C5—C4—H4	119.2
C4—N2—C3	116.72 (16)	O1—C1—O2	123.91 (17)
C1—C2—S1	108.51 (13)	O1—C1—C2	124.65 (16)
C1—C2—H2A	110.0	O2—C1—C2	111.44 (16)
S1—C2—H2A	110.0	C3—N1—C6	115.33 (17)
C1—C2—H2B	110.0	N1—C6—C5	123.38 (18)
S1—C2—H2B	110.0	N1—C6—H6	118.3
H2A—C2—H2B	108.4	C5—C6—H6	118.3
N1—C3—N2	126.17 (17)	C4—C5—C6	116.72 (18)
N1—C3—S1	120.70 (14)	C4—C5—H5	121.6
N2—C3—S1	113.13 (13)	C6—C5—H5	121.6
N2—C4—C5	121.68 (18)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H1 \cdots N2 ⁱ	0.89 (3)	1.78 (3)	2.663 (2)	178 (3)
C6—H6 \cdots O1 ⁱⁱ	0.93	2.44	3.266 (3)	148
C5—H5 \cdots O2 ⁱⁱⁱ	0.93	2.47	3.403 (3)	178

Symmetry codes: (i) $x-1/2, y, -z+1/2$; (ii) $x, y, z-1$; (iii) $x+1/2, -y+1/2, -z-1/2$.

Fig. 1

