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2-(2-Pyridylsulfanyl)acetic acid

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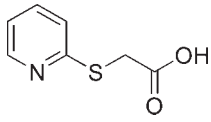
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.050; wR factor = 0.140; data-to-parameter ratio = 12.0.

All non-H atoms of the title compound, $C_7H_7NO_2S$, lie on a crystallographic mirror plane, with the two methylene H atoms bisected by this plane. The crystal packing is characterized by intermolecular C—H···O and O—H···N contacts, which link the molecules into infinite zigzag chains parallel to [010].

Related literature

For background to the design of similar ligands, see: Akrivos (2001); Ye *et al.* (2005). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_7H_7NO_2S$
M_r = 169.20
Orthorhombic, *Pnma*
a = 14.5521 (19) Å
b = 6.6774 (13) Å
c = 7.7212 (19) Å
V = 750.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 293 K
0.37 × 0.35 × 0.27 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.875, T_{max} = 0.906
1160 measured reflections
805 independent reflections
473 reflections with $I > 2\sigma(I)$
R_{int} = 0.066

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.140
S = 1.00
805 reflections
67 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2B···N1^{i}	0.82	1.79	2.606 (5)	175
C2—H2A···O2^{ii}	0.93	2.50	3.410 (6)	167
C3—H3A···O1^{iii}	0.93	2.46	3.229 (5)	140

Symmetry codes: (i) $x-\frac{1}{2}, y, -z+\frac{1}{2}$; (ii) $x+\frac{1}{2}, y, -z+\frac{3}{2}$; (iii) $x, y, z+1$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2712).

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supporting information

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2-(2-Pyridylsulfanyl)acetic acid

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S1. Comment

Compounds involving heterocyclic thiolate groups are ambidentate ligands which can form various metal-organic coordination structures *via* coordination of the exocyclic sulfur or the endocyclic nitrogen atoms (Akrivos, 2001). Similarly, carboxylic acids also exhibit diverse coordination modes in different metal complexes (Ye *et al.*, 2005). In attempts to develop novel coordination frameworks, we have designed and synthesized the title compound, 2-(pyridin-2-ylthio)acetic acid (I), as a potentially multidentate ligand. Its crystal structure is reported here.

The single-crystal X-ray analysis of I reveals that all the bond lengths in compound I are within normal ranges (Allen *et al.*, 1987). All the non-hydrogen atoms in each molecule are coplanar with the methylene hydrogen atoms related by mirror symmetry (Fig. 1). In the crystal structure molecules are linked into infinite, one dimensional, zigzag chains due to intermolecular H-bonding (Fig. 2, Table 2).

S2. Experimental

The title compound was prepared by heating a mixture of 2-pyridinethione (0.335 g, 3 mmol), chloroacetic acid (0.292 g, 3.1 mmol) and sodium hydroxide (0.248 g, 6.2 mmol) in ethanol at 353 K with magnetic stirring for 8 h. The pH of the solution was adjusted to 6 with hydrochloric acid. Yellow crystals were obtained after being recrystrallized twice from the ethanol solution (yield 78%). Analysis, calculated for $C_7H_7NO_2S$: C 49.69, H 4.17, N 8.28%; Found: C 50.06, H 4.27, N 8.06%.

S3. Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C-H) = 0.93Å, U_{iso}=1.2U_{eq} (C) for aromatic 0.97Å, U_{iso} = 1.2U_{eq} (C) for CH_2, and 0.82Å, U_{iso} = 1.5U_{eq} (O) for the OH group.

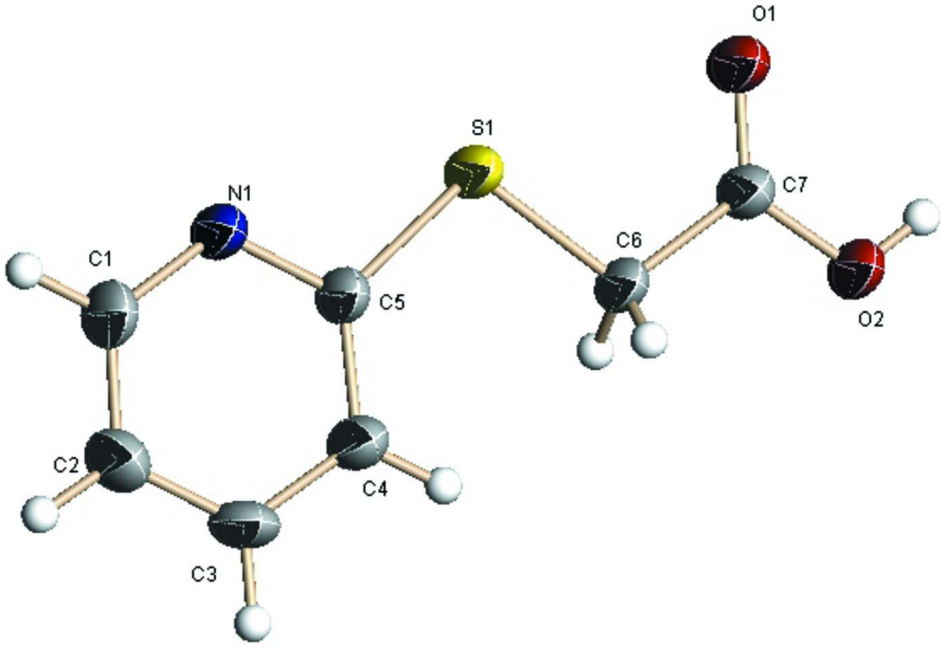

Figure 1

View of the structure of I. Displacement ellipsoids are drawn at the 30% probability level.

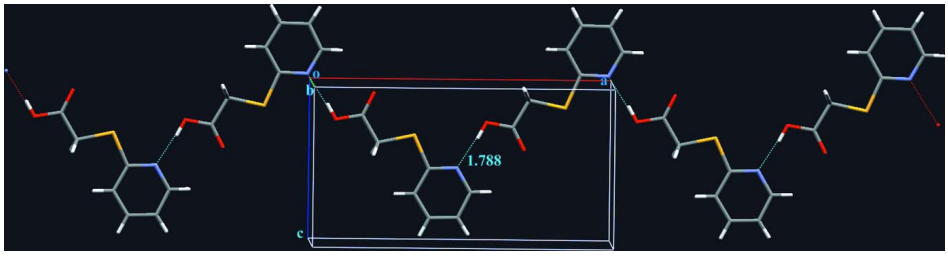

Figure 2

Crystal packin of the title compound viewed down the *b* axis.

2-(2-Pyridylsulfanyl)acetic acid

Crystal data

$C_7H_7NO_2S$
M_r = 169.20
Orthorhombic, *Pnma*
Hall symbol: -P 2ac 2n
a = 14.5521 (19) Å
b = 6.6774 (13) Å
c = 7.7212 (19) Å
V = 750.3 (3) Å^3
Z = 4
F(000) = 352
D_x = 1.498 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 343 reflections
θ = 2.8–28.0°
μ = 0.37 mm^{-1}
T = 293 K
Block, yellow
0.37 × 0.35 × 0.27 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.875, T_{max} = 0.906

1160 measured reflections
805 independent reflections
473 reflections with $I > 2\sigma(I)$
$R_{int} = 0.066$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.8°$
$h = -17 \rightarrow 1$
$k = -1 \rightarrow 8$
$l = -9 \rightarrow 1$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.140$
$S = 1.00$
805 reflections
67 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0634P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.34558 (7)	0.2500	0.33858 (14)	0.0562 (6)	
C1	0.5342 (3)	0.2500	0.6916 (6)	0.0583 (19)	
H1A	0.5981	0.2500	0.6879	0.070*	
C2	0.4919 (3)	0.2500	0.8503 (6)	0.0560 (17)	
H2A	0.5262	0.2500	0.9520	0.067*	
C3	0.3973 (3)	0.2500	0.8547 (6)	0.0545 (17)	
H3A	0.3668	0.2500	0.9605	0.065*	
C4	0.3481 (3)	0.2500	0.7029 (5)	0.0484 (15)	
H4A	0.2842	0.2500	0.7050	0.058*	
C5	0.3950 (3)	0.2500	0.5463 (5)	0.0452 (15)	
C6	0.2251 (2)	0.2500	0.3861 (5)	0.0459 (15)	
H6A	0.2093	0.1322	0.4533	0.055*	0.50
H6B	0.2093	0.3678	0.4533	0.055*	0.50
C7	0.1723 (3)	0.2500	0.2160 (6)	0.0454 (15)	
N1	0.4877 (2)	0.2500	0.5405 (5)	0.0474 (13)	
O1	0.2095 (2)	0.2500	0.0775 (4)	0.0638 (13)	
O2	0.08419 (18)	0.2500	0.2437 (4)	0.0557 (12)	
H2B	0.0569	0.2500	0.1508	0.084*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0240 (6)	0.1177 (15)	0.0269 (6)	0.000	−0.0001 (5)	0.000
C1	0.025 (2)	0.109 (6)	0.041 (3)	0.000	−0.0074 (19)	0.000
C2	0.042 (3)	0.095 (5)	0.031 (2)	0.000	−0.007 (2)	0.000
C3	0.041 (3)	0.099 (5)	0.023 (2)	0.000	0.006 (2)	0.000
C4	0.028 (2)	0.086 (5)	0.031 (2)	0.000	0.0029 (18)	0.000
C5	0.023 (2)	0.083 (5)	0.030 (2)	0.000	−0.0021 (17)	0.000
C6	0.0196 (19)	0.088 (5)	0.030 (2)	0.000	−0.0003 (17)	0.000
C7	0.027 (2)	0.080 (5)	0.029 (2)	0.000	0.0009 (18)	0.000
N1	0.0240 (17)	0.088 (4)	0.0304 (18)	0.000	−0.0001 (15)	0.000
O1	0.0268 (15)	0.134 (4)	0.0310 (16)	0.000	−0.0006 (13)	0.000
O2	0.0211 (16)	0.112 (4)	0.0345 (16)	0.000	−0.0018 (13)	0.000

Geometric parameters (Å, º)

S1—C5	1.757 (4)	C4—C5	1.389 (6)
S1—C6	1.791 (4)	C4—H4A	0.9300
C1—N1	1.348 (5)	C5—N1	1.350 (5)
C1—C2	1.372 (6)	C6—C7	1.522 (6)
C1—H1A	0.9300	C6—H6A	0.9700
C2—C3	1.377 (6)	C6—H6B	0.9700
C2—H2A	0.9300	C7—O1	1.198 (5)
C3—C4	1.374 (6)	C7—O2	1.301 (5)
C3—H3A	0.9300	O2—H2B	0.8200
C5—S1—C6	102.31 (19)	N1—C5—S1	112.3 (3)
N1—C1—C2	123.2 (4)	C4—C5—S1	126.4 (3)
N1—C1—H1A	118.4	C7—C6—S1	108.5 (3)
C2—C1—H1A	118.4	C7—C6—H6A	110.0
C1—C2—C3	118.1 (4)	S1—C6—H6A	110.0
C1—C2—H2A	121.0	C7—C6—H6B	110.0
C3—C2—H2A	121.0	S1—C6—H6B	110.0
C4—C3—C2	120.0 (4)	H6A—C6—H6B	108.4
C4—C3—H3A	120.0	O1—C7—O2	126.3 (4)
C2—C3—H3A	120.0	O1—C7—C6	122.9 (4)
C3—C4—C5	119.1 (4)	O2—C7—C6	110.8 (4)
C3—C4—H4A	120.4	C1—N1—C5	118.3 (4)
C5—C4—H4A	120.4	C7—O2—H2B	109.5
N1—C5—C4	121.3 (4)		
N1—C1—C2—C3	0.000 (1)	C5—S1—C6—C7	180.0
C1—C2—C3—C4	0.000 (1)	S1—C6—C7—O1	0.0
C2—C3—C4—C5	0.000 (1)	S1—C6—C7—O2	180.0
C3—C4—C5—N1	0.0	C2—C1—N1—C5	0.0
C3—C4—C5—S1	180.0	C4—C5—N1—C1	0.0
C6—S1—C5—N1	180.0	S1—C5—N1—C1	180.0

C6—S1—C5—C4	0.0

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*B*···N1^{i}	0.82	1.79	2.606 (5)	175
C2—H2*A*···O2^{ii}	0.93	2.50	3.410 (6)	167
C3—H3*A*···O1^{iii}	0.93	2.46	3.229 (5)	140

Symmetry codes: (i) $x-1/2, y, -z+1/2$; (ii) $x+1/2, y, -z+3/2$; (iii) $x, y, z+1$.