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2-{[4-(Pyridin-2-yl)pyrimidin-2-yl]sulfanyl}acetic acid

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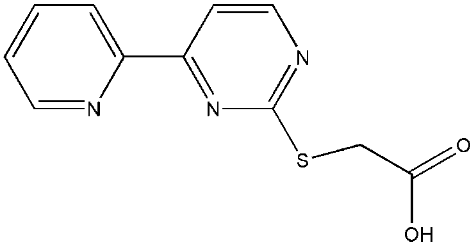
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.096; data-to-parameter ratio = 16.3.

In the title molecule, $C_{11}H_9N_3O_2S$, the pyridine and pyrimidine rings are almost parallel [dihedral angle = 6.7 (1)°]. In the crystal, adjacent molecules are joined by O—H···N and C—H···O hydrogen bonds, leading to the formation of a sheet parallel to $(10\overline{2})$.

Related literature

For details of the synthesis and general background, see: Dong *et al.* (2009); Wang (2011). For the crystal structures of coordination complexes with related ligands, see: Du *et al.* (2004); Zhu *et al.* (2009).



Experimental

Crystal data

$C_{11}H_9N_3O_2S$
M_r = 247.28
Monoclinic, $P2_1/c$
a = 6.5722 (2) Å
b = 22.4650 (8) Å
c = 7.4314 (2) Å
β = 93.237 (2)°
V = 1095.45 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 291 K
0.28 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.920, T_{max} = 0.950
10868 measured reflections
2524 independent reflections
2116 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.096
S = 1.05
2524 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N2^{i}	0.82	1.87	2.694 (2)	178
C2—H2A···O1^{ii}	0.93	2.58	3.230 (2)	127
C8—H8···O2^{iii}	0.93	2.48	3.392 (2)	165
C9—H9···O1^{iv}	0.93	2.45	3.296 (2)	151

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: KJ2186).

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supporting information

Acta Cryst. (2011). E**67**, o2916 [doi:10.1107/S1600536811039791]

2-{[4-(Pyridin-2-yl)pyrimidin-2-yl]sulfanyl}acetic acid

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S1. Comment

The rational dsign and assembly of new coordination polymers with with thioethers derived from 4-pyridinyl pyrimidine-2-thiol have received considerable attention in recent years (Dong *et al.*, 2009; Du *et al.*, 2004; Wang, 2011; Zhu *et al.*, 2009). Here we report the crystal structure of a newly synthesized compound derived from 4-(4-pyridinyl)pyrimidine-2-thiol.

The molecular structure of title compound is shown in Fig. 1 together with the atom-numbering scheme. The pyridine and pyrimidine rings are almost parallel with a dihedral angle of 6.7 (1)°. Molecules are linked by O-H···N hydrogen bonds into a chain running in direction [2 0 1]. C-H···O interactions join these chains into a two-dimensional network with base vectors [2 0 1] and [0 1 0] (equivalent to a sheet parallel to the (1 0 -2) lattice planes). Geometrical details are given in Table 1; a plot is given in Fig. 2.

S2. Experimental

All solvents and chemicals were of analytical grade and were used without further purification. The title compound was prepared by a similar procedure as reported in the literature (Dong *et al.*, 2009). To a solution of 4-(4-pyridinyl)pyrimidine-2-thiol (3.78 g, 20 mmol) and sodium hydroxide (0.80 g, 20 mmol) in water (30 ml), 2-bromoacetic acid (2.78 g, 20 mmol) in water (30 ml) was added. The mixture was stirred at room temperature for 4 h. Dilute hydrochloric acid was added to the reacted solution until the pH was about 4. Precipitates were filtered, washed by water and ethanol, and dried in vacuum. Single crystals suitable for X-ray diffraction were grown from a methanol solution by slow evaporation in air at room temperature.

S3. Refinement

All hydrogen atoms were geometrically positioned (C—H 0.93–0.97 Å) and refined as riding, with U_{iso}(H)=1.2–1.5 U_{eq} of the parent atom.

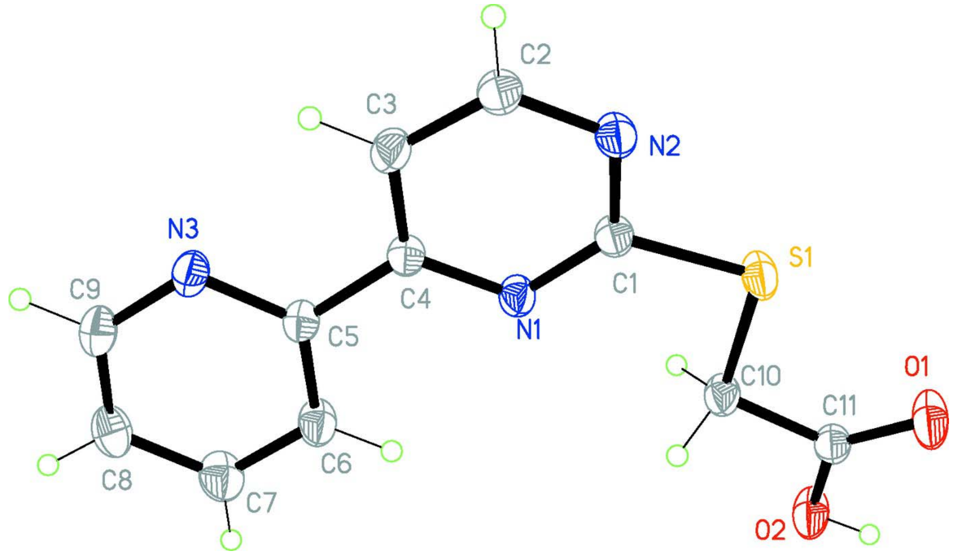

Figure 1

The structure of the title compound, showing 30% probability displacement ellipsoids.

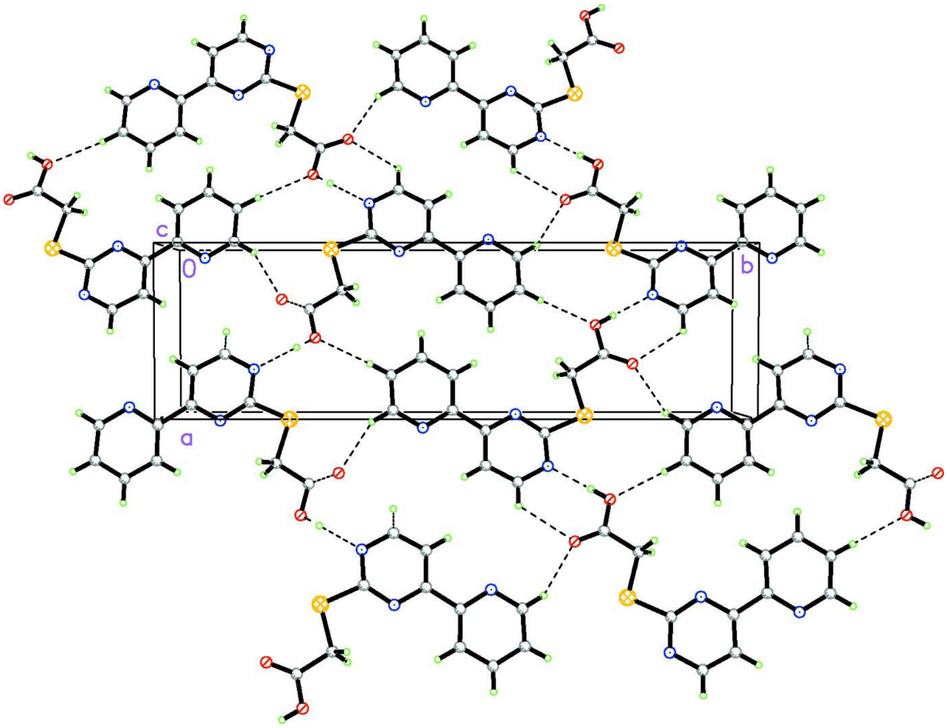

Figure 2

Perspective view of the crystal packing. Hydrogen bonding interactions are indicated with dashed lines.

2-{[4-(Pyridin-2-yl)pyrimidin-2-yl]sulfanyl}acetic acid

Crystal data

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b = 22.4650 (8) Å

c = 7.4314 (2) Å
β = 93.237 (2)°
V = 1095.45 (6) Å^3
Z = 4
$F(000)$ = 512.0
D_x = 1.499 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 2524 reflections
θ = 1.8–27.5°
μ = 0.29 mm^{-1}
T = 291 K
Block, pale yellow
0.28 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min}$ = 0.920, $T_{\max}$ = 0.950

10868 measured reflections
2524 independent reflections
2116 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
$\theta_{\max}$ = 27.5°, $\theta_{\min}$ = 1.8°
$h = -8 \rightarrow 8$
$k = -24 \rightarrow 29$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.096
S = 1.05
2524 reflections
155 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
$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 0.289P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 0.21 e Å^{-3}
$\Delta\rho_{\min}$ = −0.24 e Å^{-3}

Special details

Experimental. The structure was solved by direct methods (Bruker, 2000) and successive difference Fourier syntheses.

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 (Å^2)

	x	y	z	$U_{\text{iso}}*/U_{\text{eq}}$
C1	−0.0901 (2)	0.34978 (6)	0.26132 (19)	0.0342 (3)
C2	−0.3668 (2)	0.39680 (7)	0.1300 (2)	0.0412 (4)
H2A	−0.4973	0.3959	0.0747	0.049*
C3	−0.2718 (2)	0.45062 (7)	0.1562 (2)	0.0391 (3)
H3	−0.3370	0.4860	0.1229	0.047*
C4	−0.0745 (2)	0.45042 (6)	0.23433 (19)	0.0327 (3)
C5	0.0431 (2)	0.50633 (6)	0.25998 (19)	0.0333 (3)
C6	0.2462 (2)	0.50591 (7)	0.3208 (2)	0.0427 (4)
H6	0.3120	0.4702	0.3493	0.051*

C7	0.3493 (3)	0.55934 (8)	0.3385 (2)	0.0511 (4)
H7	0.4862	0.5602	0.3778	0.061*
C8	0.2464 (3)	0.61115 (7)	0.2972 (2)	0.0493 (4)
H8	0.3113	0.6478	0.3096	0.059*
C9	0.0444 (3)	0.60757 (7)	0.2367 (3)	0.0490 (4)
H9	−0.0242	0.6428	0.2078	0.059*
C10	0.2527 (2)	0.30146 (7)	0.4321 (2)	0.0380 (3)
H10A	0.3269	0.3242	0.3463	0.046*
H10B	0.2369	0.3259	0.5380	0.046*
C11	0.3674 (2)	0.24555 (7)	0.4832 (2)	0.0365 (3)
N1	0.01710 (17)	0.39939 (5)	0.28821 (16)	0.0340 (3)
N2	−0.27844 (18)	0.34541 (6)	0.18112 (18)	0.0391 (3)
N3	−0.0580 (2)	0.55666 (6)	0.21748 (19)	0.0432 (3)
O1	0.30963 (19)	0.19622 (5)	0.4458 (2)	0.0623 (4)
O2	0.53762 (17)	0.25707 (5)	0.57657 (19)	0.0544 (3)
H2	0.5945	0.2257	0.6057	0.082*
S1	0.00702 (6)	0.280700 (17)	0.33349 (6)	0.04496 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0331 (7)	0.0315 (7)	0.0371 (8)	−0.0008 (6)	−0.0044 (6)	0.0020 (6)
C2	0.0329 (7)	0.0395 (8)	0.0500 (9)	0.0000 (6)	−0.0100 (6)	0.0044 (7)
C3	0.0357 (7)	0.0329 (8)	0.0477 (9)	0.0046 (6)	−0.0053 (6)	0.0035 (6)
C4	0.0344 (7)	0.0297 (7)	0.0338 (7)	0.0004 (5)	0.0004 (6)	0.0001 (5)
C5	0.0373 (7)	0.0279 (7)	0.0345 (7)	0.0011 (6)	−0.0004 (6)	−0.0005 (6)
C6	0.0425 (8)	0.0330 (8)	0.0512 (9)	−0.0010 (6)	−0.0106 (7)	0.0027 (7)
C7	0.0470 (9)	0.0454 (10)	0.0591 (11)	−0.0091 (7)	−0.0137 (8)	−0.0012 (8)
C8	0.0612 (10)	0.0321 (8)	0.0543 (10)	−0.0104 (7)	0.0000 (8)	−0.0057 (7)
C9	0.0564 (10)	0.0281 (8)	0.0628 (11)	0.0042 (7)	0.0045 (8)	−0.0008 (7)
C10	0.0340 (7)	0.0297 (8)	0.0491 (9)	0.0002 (6)	−0.0078 (6)	0.0004 (6)
C11	0.0324 (7)	0.0313 (8)	0.0452 (8)	0.0003 (6)	−0.0041 (6)	−0.0005 (6)
N1	0.0328 (6)	0.0284 (6)	0.0399 (7)	−0.0004 (5)	−0.0052 (5)	0.0024 (5)
N2	0.0347 (6)	0.0331 (7)	0.0482 (7)	−0.0028 (5)	−0.0096 (5)	0.0040 (5)
N3	0.0418 (7)	0.0286 (7)	0.0587 (8)	0.0041 (5)	0.0000 (6)	0.0007 (6)
O1	0.0526 (7)	0.0291 (6)	0.1011 (11)	−0.0001 (5)	−0.0329 (7)	−0.0024 (6)
O2	0.0424 (6)	0.0322 (6)	0.0852 (9)	0.0028 (5)	−0.0269 (6)	−0.0038 (6)
S1	0.0384 (2)	0.0272 (2)	0.0670 (3)	−0.00354 (15)	−0.01691 (18)	0.00762 (17)

Geometric parameters (Å, º)

C1—N1	1.3276 (18)	C7—C8	1.372 (2)
C1—N2	1.3466 (18)	C7—H7	0.9300
C1—S1	1.7507 (15)	C8—C9	1.380 (2)
C2—N2	1.3377 (19)	C8—H8	0.9300
C2—C3	1.369 (2)	C9—N3	1.331 (2)
C2—H2A	0.9300	C9—H9	0.9300
C3—C4	1.3909 (19)	C10—C11	1.503 (2)

C3—H3	0.9300	C10—S1	1.7964 (14)
C4—N1	1.3453 (17)	C10—H10A	0.9700
C4—C5	1.4815 (19)	C10—H10B	0.9700
C5—N3	1.3401 (18)	C11—O1	1.1991 (18)
C5—C6	1.385 (2)	C11—O2	1.3085 (17)
C6—C7	1.381 (2)	O2—H2	0.8200
C6—H6	0.9300		

N1—C1—N2	126.48 (13)	C7—C8—C9	118.45 (15)
N1—C1—S1	121.11 (10)	C7—C8—H8	120.8
N2—C1—S1	112.41 (10)	C9—C8—H8	120.8
N2—C2—C3	122.31 (13)	N3—C9—C8	123.84 (15)
N2—C2—H2A	118.8	N3—C9—H9	118.1
C3—C2—H2A	118.8	C8—C9—H9	118.1
C2—C3—C4	117.60 (13)	C11—C10—S1	108.22 (10)
C2—C3—H3	121.2	C11—C10—H10A	110.1
C4—C3—H3	121.2	S1—C10—H10A	110.1
N1—C4—C3	121.20 (13)	C11—C10—H10B	110.1
N1—C4—C5	117.57 (12)	S1—C10—H10B	110.1
C3—C4—C5	121.23 (13)	H10A—C10—H10B	108.4
N3—C5—C6	122.60 (14)	O1—C11—O2	123.76 (14)
N3—C5—C4	115.89 (12)	O1—C11—C10	124.47 (13)
C6—C5—C4	121.49 (13)	O2—C11—C10	111.76 (12)
C7—C6—C5	118.94 (15)	C1—N1—C4	116.48 (12)
C7—C6—H6	120.5	C2—N2—C1	115.86 (12)
C5—C6—H6	120.5	C9—N3—C5	117.29 (14)
C8—C7—C6	118.87 (15)	C11—O2—H2	109.5
C8—C7—H7	120.6	C1—S1—C10	101.46 (7)
C6—C7—H7	120.6		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N2^{i}	0.82	1.87	2.694 (2)	178
C2—H2*A*···O1^{ii}	0.93	2.58	3.230 (2)	127
C8—H8···O2^{iii}	0.93	2.48	3.392 (2)	165
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Symmetry codes: (i) *x*+1, −*y*+1/2, *z*+1/2; (ii) *x*−1, −*y*+1/2, *z*−1/2; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) −*x*, *y*+1/2, −*z*+1/2.