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4-(Pyridin-2-yl)-1,3-dithiol-2-one

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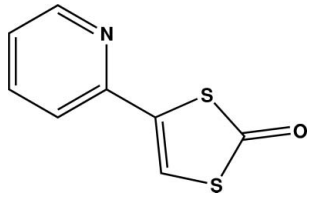
Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.005 Å; R factor = 0.032; wR factor = 0.081; data-to-parameter ratio = 11.0.

In the title compound, $C_8H_5NOS_2$, the non-H atoms are approximately coplanar [maxium deviation = 0.060 (3) Å]. The dihedral angle between the least-squares planes of the pyridine and 1,3-dithiol-2-one rings is 5.96 (17)°. The crystal packing is stabilized by weak intermolecular C—H···O hydrogen bonds and by an S···S close contact [3.510 (5) Å].

Related literature

For background to the chemistry of pyridine-based tetrathiafulvalenes, see: Fabre (2004); Zhu *et al.* (2010). For the preparation and crystal structures of related compounds, see: Zhu *et al.* (2010); Han *et al.* (2007).



Experimental

Crystal data

$C_8H_5NOS_2$
M_r = 195.27
Orthorhombic, $Pna2_1$
a = 11.157 (2) Å
b = 5.3216 (10) Å
c = 13.689 (3) Å
V = 812.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.60 mm^{-1}
T = 223 K
0.60 × 0.25 × 0.20 mm

Data collection

Rigaku Saturn CCD diffractometer
Absorption correction: multi-scan (REQAB; Jacobson, 1998)
T_{min} = 0.564, T_{max} = 0.887
2825 measured reflections
1215 independent reflections
1144 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.081
S = 1.10
1215 reflections
110 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack (1983), 430 Friedel pairs
Flack parameter: −0.09 (11)

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O1^{i}	0.94	2.46	3.3486	158

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2379).

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supporting information

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4-(Pyridin-2-yl)-1,3-dithiol-2-one

Guoquan Zhou and Xinzhi Chen

S1. Comment

Bifunctional molecules featuring a TTF (tetrathiafulvalene) unit with a pyridine, TTF-py, have been explored and a series of new TTF compounds with transition metal centers have been synthesized. The title compound is an intermediate for synthesis of this type of TTF derivative and also a donor-acceptor ligand.

In the title compound (Fig. 1), all bonds lengths and angles are found to be within the range for 4-pyridine-4-yl-1,3-dithiol-2-one (Han *et al.*, 2007). In addition, the non-H atoms are approximately planar [maxium deviation = 0.060 (3) Å] (Fig. 1). There are short S···S contacts [3.510 (5) Å] and weak C—H···O intermolecular hydrogen bonds in the crystal structure (Table 1, Fig.2).

S2. Experimental

The title compound was synthesized according to a literature procedure (Han *et al.*, 2007). Slow evaporation of a solution in THF gave single crystals suitable for *X*-ray analysis.

S3. Refinement

All H atoms were placed geometrically (C—H = 0.94 Å) with $U_{iso} = 1.2U_{eq}$ of the parent atom.

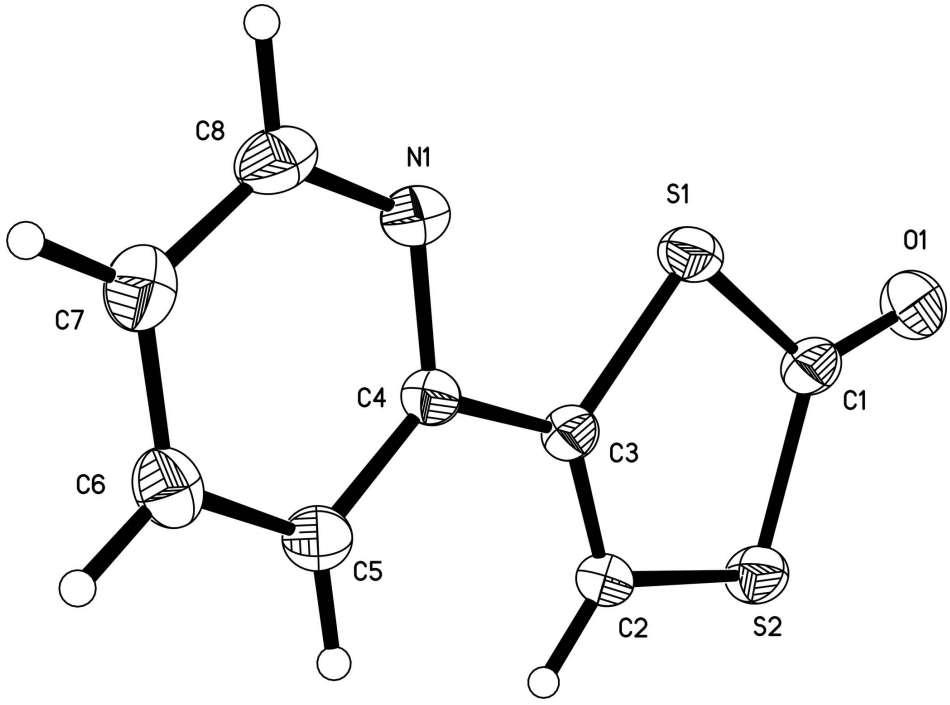

Figure 1

The molecular structure of the title compound. Displacement ellipoids are drawn at the 30% probability level.

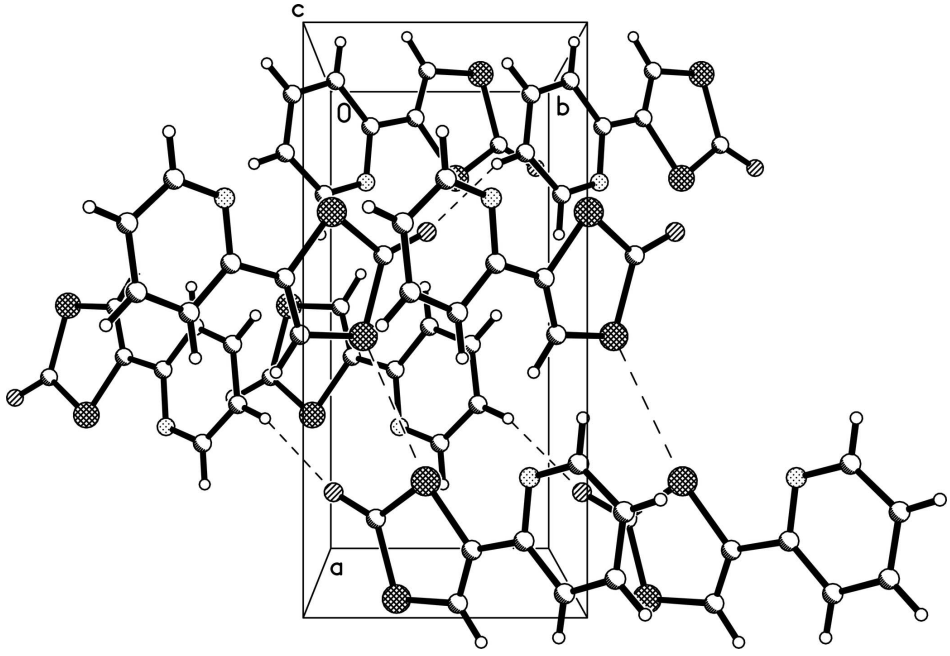

Figure 2

A crystal packing diagram viewed down the *c* axis. Dashed lines indicate the weak C—H···O interactions.

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Crystal data

$C_8H_5NOS_2$
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Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 11.157$ (2) Å
$b = 5.3216$ (10) Å
$c = 13.689$ (3) Å
$V = 812.8$ (3) Å^3
$Z = 4$
$F(000) = 400$
$D_x = 1.596$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Cell parameters from 2396 reflections
$\theta = 3.5$–$27.5°$
$\mu = 0.60$ mm^{-1}
$T = 223$ K
Block, colorless
0.60 × 0.25 × 0.20 mm

Data collection

Rigaku Saturn CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 14.63 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (REQAB; Jacobson, 1998)
$T_{min} = 0.564$, $T_{max} = 0.887$
2825 measured reflections
1215 independent reflections
1144 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 25.5°$, $\theta_{min} = 3.9°$
$h = -10 \rightarrow 13$
$k = -6 \rightarrow 5$
$l = -15 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.081$
$S = 1.10$
1215 reflections
110 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0458P)^2 + 0.0545P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Absolute structure: Flack (1983), **430 Friedel pairs**
Absolute structure parameter: −0.09 (11)

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	0.29937 (7)	1.06740 (15)	0.65200 (6)	0.0415 (2)
S2	0.53107 (7)	1.18329 (17)	0.55954 (7)	0.0439 (2)
O1	0.3307 (3)	1.4374 (5)	0.52711 (19)	0.0562 (7)

N1	0.2818 (2)	0.6783 (5)	0.7860 (2)	0.0407 (7)
C3	0.4232 (3)	0.8896 (6)	0.6876 (2)	0.0329 (7)
C4	0.3981 (3)	0.6970 (6)	0.7623 (2)	0.0328 (7)
C8	0.2525 (4)	0.5068 (7)	0.8529 (3)	0.0482 (9)
H8	0.1713	0.4931	0.8704	0.058*
C7	0.3323 (4)	0.3487 (7)	0.8980 (3)	0.0474 (9)
H7	0.3068	0.2274	0.9434	0.057*
C6	0.4513 (4)	0.3754 (7)	0.8740 (3)	0.0443 (8)
H6	0.5091	0.2738	0.9047	0.053*
C5	0.4867 (3)	0.5504 (6)	0.8052 (3)	0.0380 (8)
H5	0.5678	0.5695	0.7880	0.046*
C2	0.5273 (3)	0.9427 (6)	0.6451 (2)	0.0349 (7)
H2	0.5970	0.8523	0.6609	0.042*
C1	0.3772 (3)	1.2650 (6)	0.5707 (2)	0.0414 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0314 (4)	0.0446 (5)	0.0484 (5)	0.0045 (3)	−0.0023 (4)	0.0054 (5)
S2	0.0388 (5)	0.0469 (5)	0.0459 (4)	−0.0031 (4)	−0.0006 (4)	0.0105 (4)
O1	0.0569 (16)	0.0481 (15)	0.0636 (18)	0.0060 (12)	−0.0125 (14)	0.0169 (13)
N1	0.0335 (15)	0.0428 (17)	0.0456 (16)	−0.0022 (13)	0.0034 (13)	0.0024 (15)
C3	0.0306 (17)	0.0326 (16)	0.0354 (16)	−0.0010 (14)	−0.0022 (13)	−0.0021 (14)
C4	0.0295 (16)	0.0326 (17)	0.0362 (16)	0.0008 (14)	−0.0022 (14)	−0.0008 (14)
C8	0.0369 (18)	0.057 (2)	0.051 (2)	−0.0075 (19)	0.0089 (17)	−0.001 (2)
C7	0.057 (2)	0.0413 (19)	0.044 (2)	−0.0030 (19)	0.0045 (17)	0.0009 (17)
C6	0.051 (2)	0.0404 (18)	0.0418 (18)	0.0073 (17)	−0.0046 (16)	0.0032 (17)
C5	0.0345 (18)	0.041 (2)	0.0383 (18)	−0.0006 (17)	0.0015 (14)	−0.0001 (16)
C2	0.0292 (15)	0.0358 (16)	0.0397 (18)	0.0020 (13)	−0.0029 (17)	0.0013 (15)
C1	0.0367 (17)	0.0442 (18)	0.0433 (18)	−0.0036 (15)	−0.0062 (17)	−0.0061 (18)

Geometric parameters (Å, º)

S1—C3	1.744 (3)	C4—C5	1.390 (5)
S1—C1	1.760 (4)	C8—C7	1.372 (5)
S2—C2	1.736 (3)	C8—H8	0.9400
S2—C1	1.778 (4)	C7—C6	1.375 (6)
O1—C1	1.211 (4)	C7—H7	0.9400
N1—C8	1.334 (5)	C6—C5	1.382 (5)
N1—C4	1.342 (4)	C6—H6	0.9400
C3—C2	1.329 (5)	C5—H5	0.9400
C3—C4	1.474 (4)	C2—H2	0.9400
C3—S1—C1	96.32 (17)	C6—C7—H7	121.4
C2—S2—C1	95.66 (16)	C7—C6—C5	120.5 (4)
C8—N1—C4	117.0 (3)	C7—C6—H6	119.7
C2—C3—C4	128.1 (3)	C5—C6—H6	119.7
C2—C3—S1	117.0 (2)	C6—C5—C4	117.6 (3)

C4—C3—S1	114.8 (2)	C6—C5—H5	121.2
N1—C4—C5	123.0 (3)	C4—C5—H5	121.2
N1—C4—C3	113.8 (3)	C3—C2—S2	118.3 (2)
C5—C4—C3	123.2 (3)	C3—C2—H2	120.9
N1—C8—C7	124.7 (4)	S2—C2—H2	120.9
N1—C8—H8	117.6	O1—C1—S1	123.6 (3)
C7—C8—H8	117.6	O1—C1—S2	123.8 (3)
C8—C7—C6	117.1 (4)	S1—C1—S2	112.63 (19)
C8—C7—H7	121.4		

C1—S1—C3—C2	−2.3 (3)	C7—C6—C5—C4	0.3 (6)
C1—S1—C3—C4	177.7 (2)	N1—C4—C5—C6	1.2 (5)
C8—N1—C4—C5	−1.1 (5)	C3—C4—C5—C6	−179.7 (3)
C8—N1—C4—C3	179.7 (3)	C4—C3—C2—S2	−179.5 (2)
C2—C3—C4—N1	−175.8 (3)	S1—C3—C2—S2	0.5 (4)
S1—C3—C4—N1	4.3 (4)	C1—S2—C2—C3	1.5 (3)
C2—C3—C4—C5	5.1 (5)	C3—S1—C1—O1	−177.0 (3)
S1—C3—C4—C5	−174.9 (3)	C3—S1—C1—S2	3.1 (2)
C4—N1—C8—C7	−0.4 (5)	C2—S2—C1—O1	177.2 (3)
N1—C8—C7—C6	1.9 (6)	C2—S2—C1—S1	−2.9 (2)
C8—C7—C6—C5	−1.7 (6)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1^{i}	0.94	2.46	3.3486	158

Symmetry code: (i) −*x*+1/2, *y*−3/2, *z*+1/2.