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Key indicators

Single-crystal X-ray study

$T = 293\text{ K}$

Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$

R factor = 0.045

wR factor = 0.092

Data-to-parameter ratio = 14.8

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

5-(4-Pyridyl)-1,3,4-oxadiazole-2(3H)-thione

In the crystal structure of the title compound, $\text{C}_7\text{H}_5\text{N}_3\text{OS}$, the H atom of the thiol group is transferred to the neighboring N atom of the five-membered oxadiazole ring. Intermolecular $\text{N}-\text{H}\cdots\text{N}$ interactions exist between adjacent molecules, resulting in a one-dimensional (1D) supramolecular structure; $\pi-\pi$ stacking interactions also exist between these 1D motifs.

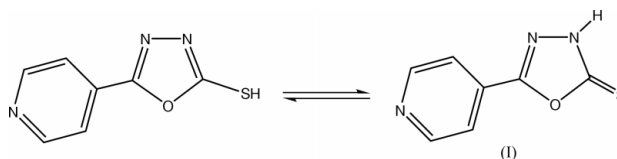
Received 12 January 2004

Accepted 26 January 2004

Online 7 February 2004

Comment

Recently, we have initiated a research project to construct coordination polymers or supramolecules with novel topological structures and interesting properties, based on oxadiazole-containing dipyridyl bridging ligands (Du *et al.*, 2002, 2003; Du & Zhao, 2003). The title compound, (I), consisting of a 1,3,4-oxadiazole ring system substituted with a pyridyl ring and a thiol group, is an interesting building block for generating novel supramolecular architectures upon metal complexation.



In the crystal structure of (I), as depicted in Fig. 1, the H atom of the thiol group is transferred to the neighboring N atom of the five-membered oxadiazole ring; this situation is reflected by the structural parameters listed in Table 1. The $\text{C1}-\text{N1}$ bond length [1.328 (3) Å], which is intermediate between standard single $\text{C}-\text{N}$ (1.47 Å) and double $\text{C}=\text{N}$ (1.28 Å) bonds, is significantly longer than the $\text{C2}-\text{N2}$ bond length [1.278 (3) Å]. In the crystal structures of other oxadiazole-containing compounds (Stockhouse *et al.*, 2001; Du & Zhao, 2004), the two corresponding $\text{C}-\text{N}$ bond lengths are almost equivalent (*ca.* 1.29 Å). In addition, the compressed $\text{C}=\text{S}$ bond length [1.642 (2) Å] is consistent with a double bond. The dihedral angle between the pyridyl ring and the oxadiazole system is $7.8(2)^\circ$.

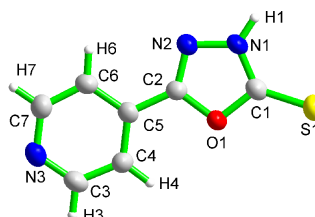


Figure 1

View of the molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

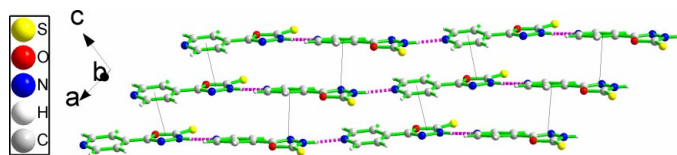


Figure 2

Packing diagram of (I). Hydrogen bonds are indicated by purple dashed lines and aromatic stacking interactions are represented by black solid lines.

Analysis of the crystal packing of the title compound reveals the existence of $N-H \cdots N^i$ [symmetry code: (i) $x - \frac{3}{2}, \frac{3}{2} - y, z - \frac{1}{2}$] intermolecular hydrogen bonds between the NH groups of the oxadiazole rings and the pyridyl N-atom acceptors. These bonds connect adjacent molecules to form a one-dimensional (1D) hydrogen-bonded chain, as shown in Fig. 2. The relevant geometrical details are listed in Table 2. Additionally, significant inter-chain face-to-face π - π stacking interactions (see Fig. 2) are observed between the oxadiazole and pyridyl rings in different 1D motifs, the closest separation being 3.285 (3) Å [center-to-center separation = 3.737 (3) Å]. Examination of the structure with *PLATON* (Spek, 2003) indicates that there are no solvent-accessible voids in the crystal structure of (I).

Experimental

Well shaped yellow single crystals of (I), suitable for X-ray diffraction, were obtained by recrystallizing the commercial product (Aldrich, 97%) from a hot CH_3OH solution.

Crystal data

$C_7H_5N_3OS$	$D_x = 1.500 \text{ Mg m}^{-3}$
$M_r = 179.20$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 683 reflections
$a = 4.869$ (2) Å	$\theta = 2.3$ – 24.1°
$b = 13.902$ (5) Å	$\mu = 0.36 \text{ mm}^{-1}$
$c = 11.839$ (4) Å	$T = 293$ (2) K
$\beta = 97.930$ (6) $^\circ$	Prism, yellow
$V = 793.6$ (5) Å ³	$0.24 \times 0.12 \times 0.10 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART 1000 diffractometer	1616 independent reflections
ω scans	1112 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1997)	$R_{\text{int}} = 0.040$
$T_{\text{min}} = 0.955, T_{\text{max}} = 0.968$	$\theta_{\text{max}} = 26.4^\circ$
4439 measured reflections	$h = -6 \rightarrow 4$
	$k = -17 \rightarrow 17$
	$l = -14 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0325P)^2 + 0.1604P]$
$R[F^2 > 2\sigma(F^2)] = 0.045$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.092$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.09$	$\Delta\rho_{\text{max}} = 0.21 \text{ e } \text{Å}^{-3}$
1616 reflections	$\Delta\rho_{\text{min}} = -0.22 \text{ e } \text{Å}^{-3}$
109 parameters	
H-atom parameters constrained	

Table 1

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

S1—C1	1.642 (2)	N2—C2	1.278 (3)
N1—C1	1.328 (3)	N3—C7	1.325 (3)
N1—N2	1.373 (2)	N3—C3	1.330 (3)
C2—O1—C1	105.59 (16)	C7—N3—C3	117.5 (2)
C1—N1—N2	112.78 (18)	N1—C1—S1	130.91 (17)
C2—N2—N1	103.71 (18)	O1—C1—S1	124.33 (17)

Table 2

Hydrogen-bonding geometry (Å, $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N1—H1 \cdots N3 ⁱ	0.86	1.88	2.737 (3)	177

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

Although all H atoms were visible in difference maps, they were placed in geometrically calculated positions ($C-H = 0.93$ Å and $N-H = 0.86$ Å) and included in the final refinement in the riding-model approximation, with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(\text{carrier atom})$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINTE* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Berndt, 1999); software used to prepare material for publication: *SHELXTL* (Bruker, 1998).

We gratefully acknowledge the financial support from the Natural Science Foundation of Tianjin (No. 033609711) and the Starting Funding of Tianjin Normal University (to MD).

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