

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

Yong-Tao Wang,\* Zhen-Wei  
Qiang, Wen-Zhu Wan and  
Gui-Mei TangDepartment of Chemical Engineering, Shandong  
Institute of Light Industry, Jinan, Shandong  
250353, People's Republic of China

Correspondence e-mail: ceswyt@sohu.com

## Key indicators

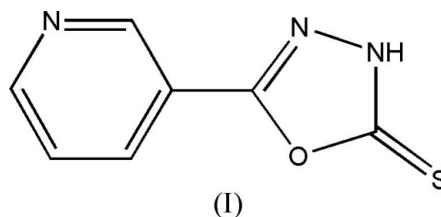
Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.036  
 $wR$  factor = 0.098  
Data-to-parameter ratio = 14.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the title compound,  $\text{C}_7\text{H}_5\text{N}_3\text{OS}$ , the dihedral angle between the pyridyl and oxadiazole rings is  $9.32(2)^\circ$ . In the crystal structure, a combination of intermolecular  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds and  $\pi-\pi$  stacking interactions forms a two-dimensional network.

Received 27 October 2006  
Accepted 8 November 2006

## Comment

The design and assembly of supramolecular architectures with variable cavities or channels are currently of great interest owing to their novel topologies and potential applications (Wang *et al.*, 2005*a,b*; Wang, Tong *et al.*, 2005). The geometry of the organic ligands has a great effect on the structural frameworks of such coordination polymers and hence much effort has been devoted to the modification of the building blocks and the control of the assembled motifs for the required products through the selection of different organic ligands. Previous studies have shown that mostly symmetric rigid bridging ligands are used in the construction of versatile networks and other porous coordination polymers (Robin & Fromm, 2006). However, there are fewer studies on the coordination chemistry of unsymmetric organic ligands (Wang, Tang & Qin, 2006; Wang, Tang, Wu *et al.*, 2006). We have recently discussed some coordination complexes of 5-(4-pyridyl)-1,3,4-oxadiazole-2-thione (Wang & Tang 2006*a,b*) and reported the crystal structure of the free ligand (Wang, Tang, Ma *et al.*, 2006). To further expand this area of research, we have synthesized the title compound, (I), by the reaction of nicotinoylhydrazide and carbon disulfide in the presence of KOH in ethanol and its crystal structure is presented here.



The molecular structure of (I) is shown in Fig. 1. All bond lengths and angles are within the expected ranges (Allen *et al.*, 1987). In the crystal structure, one-dimensional chains are formed *via* intermolecular  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds (Table 2). In addition,  $\pi-\pi$  stacking interactions [ $\text{Cg}1\cdots\text{Cg}2(1+x, y, z) = 3.591(2)^\circ$  Å, where  $\text{Cg}1$  and  $\text{Cg}2$  are the centroids of the ring atoms  $\text{O}1/\text{C}6/\text{N}2/\text{N}3/\text{C}7$  and  $\text{N}1/\text{C}1-\text{C}5$ , respectively] connect one-dimensional chains into a two-dimensional network (Fig. 2).

## Experimental

The title compound was synthesized according to a literature method (Wang, Tang, Ma *et al.*, 2006). Pale-yellow plate-shaped single crystals suitable for X-ray diffraction were obtained from an ethanol solution of (I). Analysis found (%): C 46.80, H 2.82, N 23.40; requires (%): C 46.92, H 2.81, N 23.45.

### Crystal data

$C_7H_5N_3OS$	$Z = 4$
$M_r = 179.20$	$D_x = 1.503 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 5.1351(2) \text{ \AA}$	$\mu = 0.36 \text{ mm}^{-1}$
$b = 18.1940(7) \text{ \AA}$	$T = 293(2) \text{ K}$
$c = 8.5727(4) \text{ \AA}$	Plate, pale yellow
$\beta = 98.694(3)^\circ$	$0.30 \times 0.20 \times 0.10 \text{ mm}$
$V = 791.73(6) \text{ \AA}^3$	

### Data collection

Bruker SMART APEX CCD diffractometer	4047 measured reflections
$\varphi$ and $\omega$ scans	1804 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1371 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.900$ , $T_{\max} = 0.965$	$R_{\text{int}} = 0.021$
	$\theta_{\text{max}} = 27.6^\circ$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0475P)^2 + 0.162P]$
$R[F^2 > 2\sigma(F^2)] = 0.036$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.098$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.00$	$\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$
1804 reflections	$\Delta\rho_{\text{min}} = -0.25 \text{ e \AA}^{-3}$
129 parameters	
All H-atom parameters refined	

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

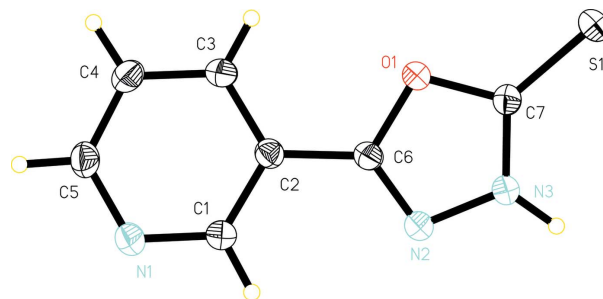
$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N3-H1A\cdots N1^i$	0.94 (2)	1.86 (2)	2.800 (2)	172 (2)

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

All H atoms were refined independently with isotropic displacement parameters, giving  $N-H = 0.94(2) \text{ \AA}$  and  $C-H = 0.924(18)-0.95(2) \text{ \AA}$ .

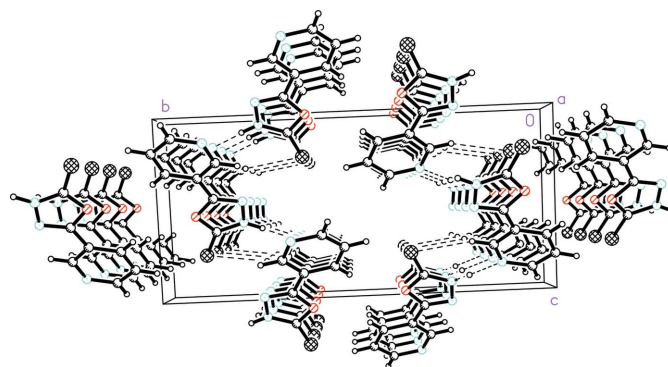
Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Sheldrick, 1999); software used to prepare material for publication: SHELXTL.

This work was supported by the Starting Fund of Shandong Institute of Light Industry (YTW).



**Figure 1**

The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level.



**Figure 2**

Part of the crystal structure of (I), showing hydrogen bonding interactions as dashed lines.

## 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.
- Bruker (2001). SMART and SAINT, Bruker AXS Inc., Madison, Wisconsin, USA.
- Robin, A. Y. & Fromm, K. M. (2006). *Coord. Chem. Rev.* **250**, 2127–2157.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). SHELXS97 and SHELXL97, University of Göttingen, Germany.
- Sheldrick, G. M. (1999). SHELXTL. University of Göttingen, Germany.
- Wang, Y.-T., Fan, H.-H., Wang, H.-Z. & Chen, X.-M. (2005a). *Inorg. Chem.* **44**, 4148–4150.
- Wang, Y.-T., Fan, H.-H., Wang, H.-Z. & Chen, X.-M. (2005b). *J. Mol. Struct.* **740**, 61–67.
- Wang, Y.-T. & Tang, G.-M. (2006a). *Inorg. Chem. Commun.* In the press.
- Wang, Y.-T. & Tang, G.-M. (2006b). *J. Coord. Chem.* Accepted.
- Wang, Y.-T., Tang, G.-M., Ma, W.-Y. & Wan, W.-Z. (2006). *Polyhedron*. In the press.
- Wang, Y.-T., Tang, G.-M. & Qin, D.-W. (2006). *Aust. J. Chem.* pp. 647–652.
- Wang, Y.-T., Tang, G.-M., Wu, Y., Qin, X.-Y. & Qin, D.-W. (2006). *J. Mol. Struct.* In the press.
- Wang, Y.-T., Tong, M.-L., Fan, H.-H., Wang, H.-Z. & Chen, X.-M. (2005). *J. Chem. Soc. Dalton Trans.* pp. 424–426.