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Key indicators

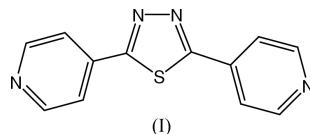
Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.042
 wR factor = 0.146
Data-to-parameter ratio = 13.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

2,5-Bis(4-pyridyl)-1,3,4-thiadiazole

In the structure of the title compound, $\text{C}_{12}\text{H}_8\text{N}_4\text{S}$, the molecule has crystallographic C_2 symmetry. The two pyridine rings make dihedral angles of $21.8(2)^\circ$ with the mean plane of the central thiadiazole system, and the dihedral angle between the pyridine rings is $43.0(2)^\circ$.

Comment

Polypyridyl bridging ligands derived from the appropriate modification of 4,4'-bipyridine have been widely employed due to their application as the building blocks in supramolecular assemblies to produce a wide variety of solid-state coordination architectures (Blake *et al.*, 1999). The nature of such ligands (*e.g.* the length and the steric interaction) is crucial to the final observed coordination frameworks (Withersby *et al.*, 1999). The title compound, 2,5-bis(4-pyridyl)-1,3,4-thiadiazole, (*L*), an angular dipyridyl ligand, has attracted our attention and we recently determined the structure of the complex $[\text{Co}(\text{SCN})_2(\text{L})_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$ (Du & Zhao, 2004). The central thiadiazole ring of this ligand introduces a rigid 156° angle between the directions of coordination of the two pyridyl N atoms, and therefore the ligand could potentially provide both discrete and infinite products upon metal complexation under appropriate conditions. In this paper, we report the crystal structure of compound (I).



In the molecular structure of (I), as depicted in Fig. 1, there is half a molecule in the asymmetric unit and the other half is related by a crystallographic twofold axis. The two pyridyl rings make dihedral angles of $21.8(2)^\circ$ with the mean plane of the central five-membered thiadiazole system, and the dihedral angle between the two pyridyl rings is $43.0(2)^\circ$. In the pyridyl rings, the C1–N1 and C5–N1 bond lengths [$1.334(4)$ and $1.322(4)\text{ \AA}$] are within the range of values normally

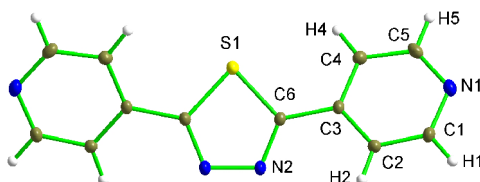


Figure 1

View of the molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. Unlabelled atoms are related by the symmetry code $(-x, y, \frac{1}{2} - z)$.

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considered standard for single C–N (1.47 Å) and double C=N (1.28 Å) bonds. The C6–N2 bond in the thiadiazole ring is 1.305 (3) Å. All bond lengths and angles are in the normal range (Table 1). The angle subtended at the center of the thiadiazole ring by the two pyridyl N-donors is 156°, and the separation of the two N-donors is 10.763 (4) Å.

Analysis of the crystal packing of (I) reveals that no significant weak interactions, such as hydrogen bonds or face-to-face π – π stacking interactions, exist in this structure. Examination of the crystal structure of (I) with *PLATON* (Spek, 2003) indicates that the unit cell contains no solvent-accessible voids.

Experimental

Well shaped colorless single crystals of the title compound, (I), suitable for X-ray diffraction were obtained by recrystallizing the commercial product from a hot CH₃OH–H₂O solution.

Crystal data

C ₁₂ H ₈ N ₄ S	$D_x = 1.518 \text{ Mg m}^{-3}$
$M_r = 240.28$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 629 reflections
$a = 26.179 (9) \text{ \AA}$	$\theta = 3.6\text{--}26.2^\circ$
$b = 5.8223 (17) \text{ \AA}$	$\mu = 0.29 \text{ mm}^{-1}$
$c = 7.169 (3) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 105.855 (9)^\circ$	Block, colorless
$V = 1051.1 (6) \text{ \AA}^3$	$0.20 \times 0.18 \times 0.12 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART 1000 diffractometer	1081 independent reflections
ω scans	854 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.026$
$T_{\text{min}} = 0.945$, $T_{\text{max}} = 0.966$	$\theta_{\text{max}} = 26.4^\circ$
2924 measured reflections	$h = -28 \rightarrow 32$
	$k = -7 \rightarrow 6$
	$l = -8 \rightarrow 8$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0872P)^2 + 0.0744P]$
$R[F^2 > 2\sigma(F^2)] = 0.042$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.146$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.19$	$\Delta\rho_{\text{max}} = 0.38 \text{ e \AA}^{-3}$
1081 reflections	$\Delta\rho_{\text{min}} = -0.33 \text{ e \AA}^{-3}$
78 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

S1–C6	1.725 (2)	N2–C6	1.305 (3)
C1–N1	1.334 (4)	N2–N2 ⁱ	1.371 (4)
N1–C5	1.322 (4)		
C6 ⁱ –S1–C6	86.02 (16)	N1–C5–C4	124.3 (2)
C2–C3–C4	117.9 (2)	C5–C4–C3	118.4 (2)
N1–C1–C2	124.0 (3)	C6–N2–N2 ⁱ	112.12 (13)
C1–C2–C3	118.8 (2)	N2–C6–S1	114.87 (17)
C5–N1–C1	116.7 (2)		

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

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

Data collection: *SMART-NT* (Bruker, 1998); cell refinement: *SMART-NT*; data reduction: *SAINT-NT* (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: *SHELXL97*.

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