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

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.111
Data-to-parameter ratio = 16.0

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

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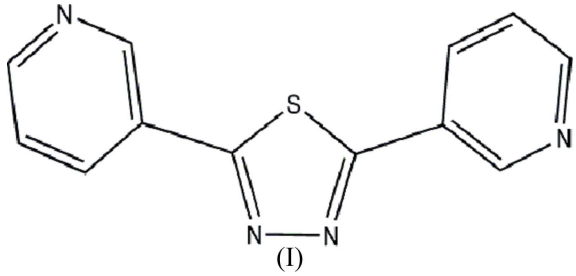
The title molecule, $C_{12}H_8N_4S$, possesses antibacterial properties and is a potential ligand for metal complexes. The dihedral angles between the pyridyl rings and the central thiadiazole ring are less than 10°.

Comment

The X-ray crystallographic structure of the title compound, (I) (Fig. 1), has not been published previously, although the structures of two closely related isomers, namely 2,5-bis(4-pyridyl)-1,3,4-thiadiazole (Du *et al.* 2004; Zhao *et al.*, 2005) and 2,5-bis(2-pyridyl)-1,3,4-thiadiazole (Bentiss *et al.*, 2004), have been characterized.



(I)

In (I), the two pyridyl rings make dihedral angles with the central thiadiazole ring of 9.63 (6) (pyridyl ring N1/C1–C5) and 7.60 (6)° (pyridyl ring N4/C8–C12). This twisting of the molecule is significantly reduced compared to that of ca 30° found in some coordination complexes containing 4-pyridyl- or 2-pyridylthiadiazole derivatives cited above (Huang *et al.*, 2004; Bentiss *et al.*, 2004).

Experimental

Compound (I) (0.024 g, 0.1 mmol) and 2,3-dimethylpyrazine (0.012 g, 0.1 mmol) dissolved in chloroform (5 ml) was added to a methanol solution (10 ml) of zinc acetate (0.022 g, 0.1 mmol) with

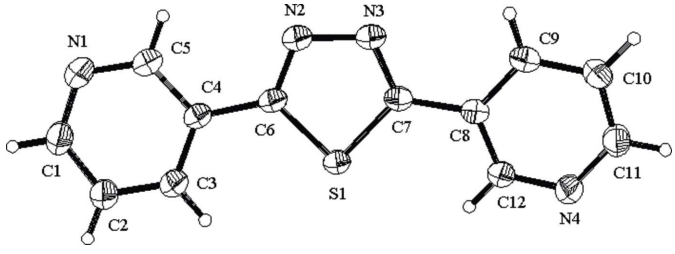


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

stirring. An ammonium hexafluorophosphate (0.033 g, 0.2 mmol) solution in water (5 ml) was added dropwise after 20 min. Suitable colourless needle-shaped crystals were obtained by slow evaporation of the solvents over a period of about 30 d (yield 35%).

Crystal data

$C_{12}H_8N_4S$
$M_r = 240.29$
Monoclinic, $P2_1/c$
$a = 12.872$ (2) Å
$b = 11.0157$ (19) Å
$c = 7.8170$ (13) Å
$\beta = 100.405$ (2)°
$V = 1090.2$ (3) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.28$ mm^{-1}
$T = 291$ (2) K
0.36 × 0.24 × 0.07 mm

Data collection

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.907$, $T_{max} = 0.981$
7069 measured reflections
2480 independent reflections
1607 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.111$
$S = 1.03$
2480 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

H atoms were placed at calculated positions (C—H = 0.93 Å), and were included in the refinement in the riding-model approximation, with $U_{iso}(H)$ values set at $1.2U_{eq}(C)$.

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* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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