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4,4′-Bipyridine–5-amino-1,3,4-thiadiazole-2(3*H*)-thione (1/2)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.109
Data-to-parameter ratio = 15.7

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

In the title complex, $C_{10}H_8N_2\cdot 2C_2H_3N_3S_2$, the 4,4′-bipyridine (bpy) molecule, lying on an inversion centre, is connected to two 5-amino-1,3,4-thiadiazole-2(3*H*)-thione (tdz) molecules through N—H···N hydrogen bonds. The tdz planes are slightly twisted with respect to the bpy plane, with a dihedral angle of 2.1 (2)°. Further intermolecular N—H···N and N—H···S hydrogen bonds result in a three-dimensional network structure.

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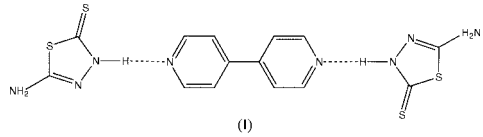
Comment

The title compound, (I), was prepared as part of our ongoing studies of hydrogen-bonding interactions in crystal structures (Sun *et al.*, 2004). We report here the structure of 4,4′-bipyridine–5-amino-1,3,4-thiadiazole-2(3*H*)-thione (1/2), (I).



(I)

In (I), the 4,4′-bipyridine (bpy) molecules, lying on an inversion centre, is connected to two 5-amino-1,3,4-thiadiazole-2(3*H*)-thione (tdz) molecules through N—H···N hydrogen bonds (Fig. 1 and Table 1). The tdz planes are slightly twisted with respect to the bpy plane, with a dihedral angle of only 2.1 (2)°. The bpy–tdz (1/2) units are linked by N—H···N hydrogen bonds to form a one-dimensional stair-like chain (Fig. 2). These chains are further interconnected by N—H···S hydrogen bonds, leading to a three-dimensional network (Fig. 3).

Experimental

4,4′-Bipyridine (0.1 mmol) and 5-amino-1,3,4-thiadiazole-2(3*H*)-thione (0.2 mmol) were dissolved in a water–ethanol (4:1 *v*/*v*, 10 ml) mixture. The solution was stirred for 1 h at 313 K and then filtered.

Figure 1
The structure of (I), showing the atom-labelling scheme and the interconnection between the bpy and tdz molecules (dashed lines). Ellipsoids are drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by the symmetry code (−2 − *x*, 1 − *y*, −*z*).

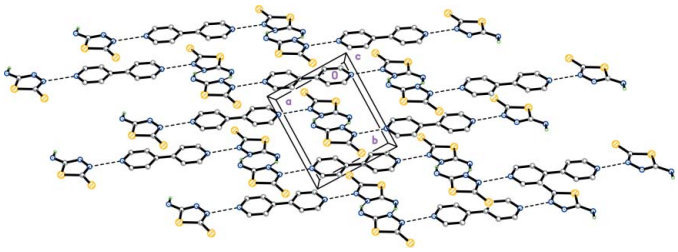


Figure 2
Perspective view, along the *c* axis, of the chains. Hydrogen bonds shown as dashed lines.

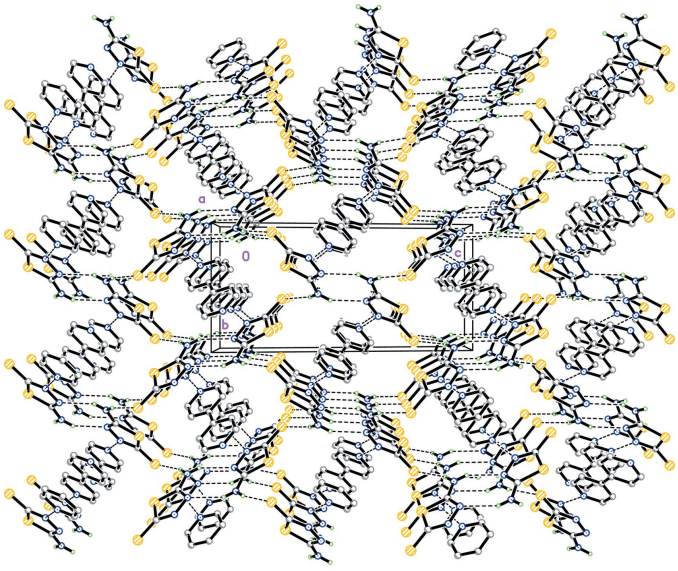


Figure 3
Packing diagram of (I). Dashed lines indicate hydrogen bonds.

The resulting solution was allowed to stand in air at room temperature for two days and yielded pale-yellow crystals.

Crystal data

$C_{10}H_8N_2{\cdot}2C_2H_3N_3S_2$
M_r = 422.57
Monoclinic, $P2_1/n$
a = 7.020 (3) Å
b = 8.121 (4) Å
c = 16.888 (7) Å
β = 100.74 (4)°
V = 945.9 (7) Å^3
Z = 2
D_x = 1.484 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 2–7°
μ = 0.52 mm^{-1}
T = 293 (2) K
Block, pale yellow
0.46 × 0.38 × 0.32 mm

Data collection

Siemens *R3m* diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.796, T_{max} = 0.852
2007 measured reflections
1852 independent reflections
1330 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 26.0°
$h = 0 \rightarrow 8$
$k = 0 \rightarrow 10$
$l = -20 \rightarrow 20$
2 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.109
S = 1.01
1852 reflections
118 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 0.5922P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N4	0.86	1.94	2.792 (3)	172
N3—H3A···N2^{i}	0.86	2.28	3.079 (4)	155
N3—H3B···S2^{ii}	0.86	2.57	3.412 (3)	165

Symmetry codes: (i) $-x, -y+2, -z$; (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

H atoms were positioned geometrically (C—H = 0.93 Å and N—H = 0.86 Å) and refined as riding on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C, N).

Data collection: *R3m Software* (Siemens, 1990); cell refinement: *R3m Software*; data reduction: *R3m Software*; program(s) used to solve structure: *SHELXTL* (Bruker, 1999); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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