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1,2-Di-2-pyridyl-1,2-bis(1,3,4-thiadiazol-2-ylamino)ethane

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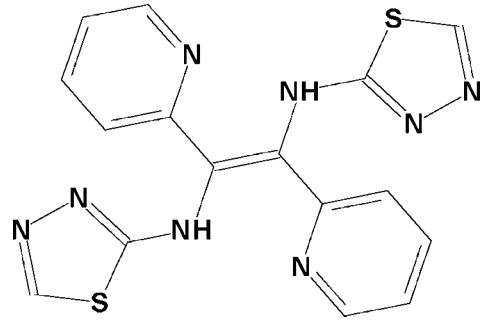
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.101; data-to-parameter ratio = 12.3.

The title compound, $C_8H_6N_4S$, was obtained *via* the reaction of 2-aminothiadiazole with pyridine-2-carbaldehyde in methanol solution in a 1:1 stoichiometry. The molecule consists of two aminothiazolyl and two pyridyl groups linked by a C=C double bond which lies on a crystallographic centre of symmetry. Adjacent molecules are linked by N—H···S hydrogen bonds to generate a one-dimensional supramolecular chain structure.

Related literature

For related literature, see: Zhang & Liu (2007).



Experimental

Crystal data

$C_{16}H_{12}N_8S_2$
M_r = 380.46
Triclinic, $P\overline{1}$
a = 5.4720 (11) Å
b = 7.9623 (16) Å
c = 9.7363 (19) Å
α = 91.01 (3)°
β = 93.96 (3)°
γ = 105.57 (3)°
V = 407.38 (15) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 153 (2) K
0.20 × 0.18 × 0.14 mm

Data collection

Bruker $P4$ diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.926, T_{max} = 0.943
2787 measured reflections
1447 independent reflections
1032 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.101
S = 1.02
1447 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···S1^{i}	0.86	2.79	3.513 (2)	143

Symmetry code: (i) $x-1, y, z$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Bruker, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2232).

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supplementary materials

Acta Cryst. (2007). E**63**, o4179 [**doi:10.1107/S1600536807046673**]

1,2-Di-2-pyridyl-1,2-bis(1,3,4-thiadiazol-2-ylamino)ethane

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Comment

The molecule of the title compound consists of two aminothiazolyl and two pyridyl groups linked by a C═C double bond which lies on a crystallographic centre of symmetry (Fig. 1).

The adjacent molecules are linked by N3—H3A···S1^{i} (Table 1) hydrogen bonds to generate a one dimensional supramolecular network strcucture (Fig. 2). There are no aromatic π–π stacking interactions.

Experimental

The title compound, $C_{10}H_9N_7S_2$, was synthesized *via* the reflux reaction of 2-aminothiazole (10.711 g, 0.1 mol) and 2-pyridylaldehyde (10.113 g, 0.1 mol) in 1:1 stoichiometry in 200 ml me thanol solution with 1 ml HCl (6 *M*) for 24 h. The block crystals suitable for single-crystal X-ray diffraction were obtained *via* recrystallization of the powder in methanol at room temperature.

Refinement

All H atoms attached to C and N atom were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic) and N—H = 0.86 Å with U_{iso}(H) = 1.2U_{eq}(C or N).

Figures

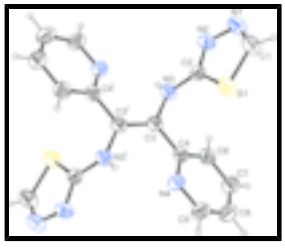

Fig. 1. The molecular structure of (I), with the vatom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii. [Symmetry code: (i) −*x* + 1, −*y* + 1, −*z* + 1]

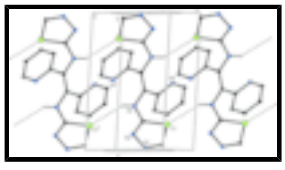

Fig. 2. Partial packing view of (I) showing intermolecular N—H···S hydrogen bonds (dashed lines). H atoms not involved in hydrogen bondings have been omitted for carity. [Symmetry code: (i) −*x* + 1, −*y* + 1, −*z* + 1; (ii) *x* − 1, *y*, *z*]

1,2-Di-2-pyridyl-1,2-bis(1,3,4-thiadiazol-2-ylamino)ethane

Crystal data

$C_{16}H_{12}N_8S_2$	$Z = 1$
$M_r = 380.46$	$F_{000} = 196$
Triclinic, $P\overline{1}$	$D_x = 1.551$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.4720$ (11) Å	Cell parameters from 4677 reflections
$b = 7.9623$ (16) Å	$\theta = 3.4$–27.5°
$c = 9.7363$ (19) Å	$\mu = 0.35$ mm^{-1}
$\alpha = 91.01$ (3)°	$T = 153$ (2) K
$\beta = 93.96$ (3)°	Block, colourless
$\gamma = 105.57$ (3)°	0.20 × 0.18 × 0.14 mm
$V = 407.38$ (15) Å^3	

Data collection

Bruker P4 diffractometer	1447 independent reflections
Radiation source: fine-focus sealed tube	1032 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.024$
$T = 153$(2) K	$\theta_{max} = 25.2^\circ$
ω scans	$\theta_{min} = 3.5^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -6 \rightarrow 6$
$T_{min} = 0.926$, $T_{max} = 0.943$	$k = -9 \rightarrow 9$
2787 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.101$	$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 0.0338P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
1447 reflections	$\Delta\rho_{max} = 0.34$ e Å^{-3}
118 parameters	$\Delta\rho_{min} = -0.41$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.7059 (5)	0.2732 (3)	0.9578 (3)	0.0497 (7)
H1	0.8187	0.2333	1.0159	0.060*
C2	0.4851 (4)	0.3957 (3)	0.7878 (2)	0.0314 (5)
C3	0.5411 (4)	0.5333 (3)	0.5653 (2)	0.0312 (5)
C4	0.7705 (4)	0.6802 (3)	0.6017 (2)	0.0317 (5)
N4	0.9649 (3)	0.7030 (3)	0.5189 (2)	0.0363 (5)
C5	1.1725 (4)	0.8343 (3)	0.5528 (3)	0.0423 (6)
H5	1.3071	0.8511	0.4966	0.051*
C6	1.1987 (5)	0.9445 (3)	0.6642 (3)	0.0463 (7)
H6	1.3481	1.0327	0.6842	0.056*
C7	0.9988 (5)	0.9226 (3)	0.7473 (3)	0.0452 (7)
H7	1.0098	0.9973	0.8233	0.054*
N1	0.4702 (4)	0.2465 (3)	0.9794 (2)	0.0489 (6)
N2	0.3381 (4)	0.3183 (3)	0.8806 (2)	0.0405 (5)
N3	0.3944 (3)	0.4696 (3)	0.67620 (18)	0.0348 (5)
H3	0.2404	0.4775	0.6737	0.042*
C8	0.7827 (4)	0.7882 (3)	0.7156 (2)	0.0386 (6)
H8	0.6462	0.7705	0.7705	0.046*
S1	0.79840 (11)	0.38809 (9)	0.81359 (7)	0.0459 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0555 (17)	0.0585 (18)	0.0389 (15)	0.0214 (14)	0.0033 (13)	0.0134 (13)
C2	0.0307 (12)	0.0341 (13)	0.0278 (12)	0.0059 (10)	0.0037 (10)	−0.0023 (10)
C3	0.0262 (11)	0.0370 (14)	0.0317 (11)	0.0102 (10)	0.0042 (9)	0.0053 (10)
C4	0.0284 (12)	0.0354 (14)	0.0313 (13)	0.0087 (10)	0.0006 (10)	0.0078 (10)
N4	0.0277 (10)	0.0418 (12)	0.0378 (11)	0.0064 (9)	0.0041 (9)	0.0044 (9)
C5	0.0292 (12)	0.0432 (15)	0.0507 (16)	0.0024 (11)	0.0057 (11)	0.0040 (13)
C6	0.0378 (14)	0.0378 (15)	0.0573 (18)	0.0015 (11)	−0.0024 (13)	0.0002 (14)
C7	0.0497 (15)	0.0376 (15)	0.0447 (15)	0.0070 (12)	−0.0012 (13)	−0.0038 (12)
N1	0.0583 (15)	0.0548 (14)	0.0349 (12)	0.0153 (11)	0.0095 (10)	0.0140 (10)
N2	0.0397 (11)	0.0457 (13)	0.0354 (11)	0.0076 (9)	0.0112 (9)	0.0076 (10)
N3	0.0263 (10)	0.0490 (13)	0.0300 (10)	0.0102 (9)	0.0060 (8)	0.0077 (9)
C8	0.0385 (14)	0.0432 (15)	0.0341 (14)	0.0103 (11)	0.0053 (11)	0.0019 (12)
S1	0.0346 (4)	0.0632 (5)	0.0426 (4)	0.0163 (3)	0.0060 (3)	0.0156 (3)

Geometric parameters (Å, °)

C1—N1	1.283 (3)	N4—C5	1.338 (3)
C1—S1	1.720 (3)	C5—C6	1.358 (4)
C1—H1	0.9300	C5—H5	0.9300
C2—N2	1.303 (3)	C6—C7	1.380 (4)
C2—N3	1.370 (3)	C6—H6	0.9300
C2—S1	1.733 (2)	C7—C8	1.378 (3)
C3—C3^{i}	1.367 (4)	C7—H7	0.9300
C3—N3	1.410 (3)	N1—N2	1.386 (3)
C3—C4	1.485 (3)	N3—H3	0.8600
C4—N4	1.354 (3)	C8—H8	0.9300
C4—C8	1.378 (3)		
N1—C1—S1	115.2 (2)	C5—C6—C7	118.6 (2)
N1—C1—H1	122.4	C5—C6—H6	120.7
S1—C1—H1	122.4	C7—C6—H6	120.7
N2—C2—N3	122.2 (2)	C8—C7—C6	118.8 (2)
N2—C2—S1	114.43 (18)	C8—C7—H7	120.6
N3—C2—S1	123.33 (16)	C6—C7—H7	120.6
C3^{i}—C3—N3	119.7 (2)	C1—N1—N2	112.67 (19)
C3^{i}—C3—C4	125.0 (2)	C2—N2—N1	111.6 (2)
N3—C3—C4	115.10 (19)	C2—N3—C3	123.21 (19)
N4—C4—C8	121.9 (2)	C2—N3—H3	118.4
N4—C4—C3	117.4 (2)	C3—N3—H3	118.4
C8—C4—C3	120.74 (19)	C4—C8—C7	119.4 (2)
C5—N4—C4	117.3 (2)	C4—C8—H8	120.3
N4—C5—C6	124.0 (2)	C7—C8—H8	120.3
N4—C5—H5	118.0	C1—S1—C2	86.18 (12)
C6—C5—H5	118.0		

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···S1^{ii}	0.86	2.79	3.513 (2)	143

Symmetry codes: (ii) *x*−1, *y*, *z*.

Fig. 1

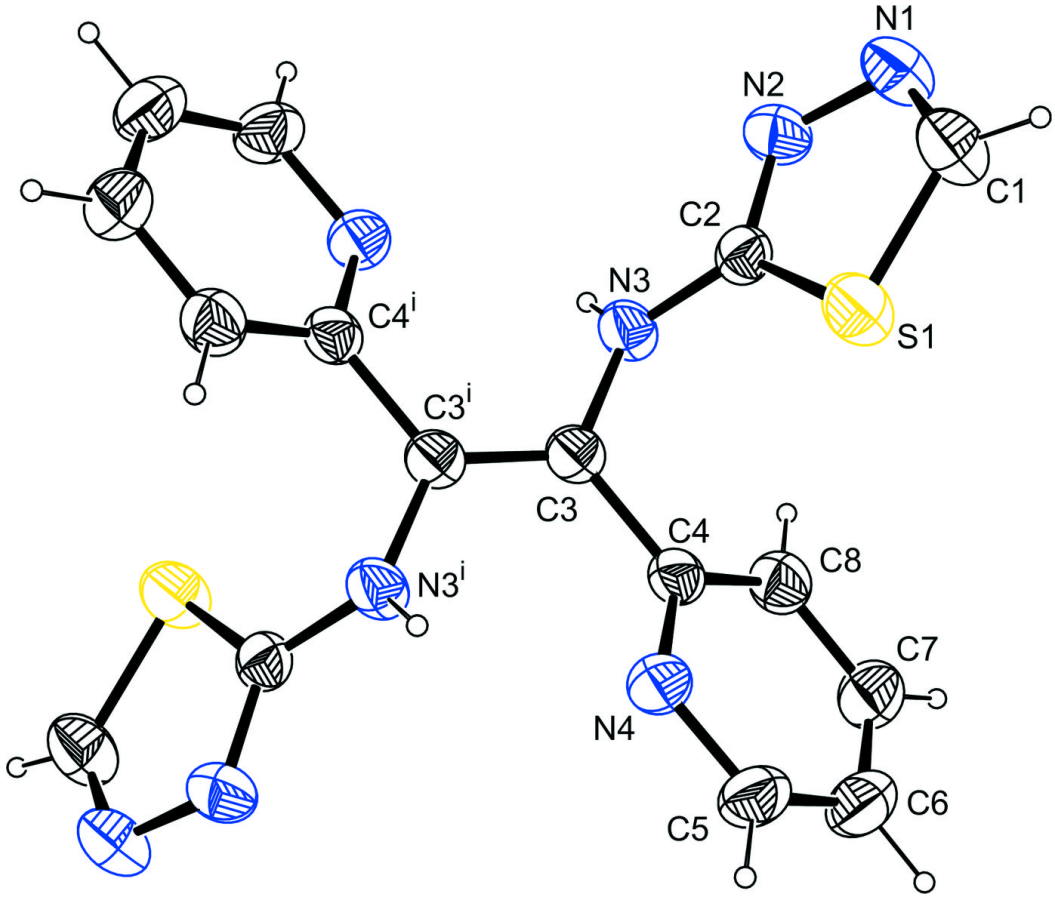

Fig. 2