Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2-Pyridyl)bis(1,3,4-thiadiazol-2-ylamino)methane

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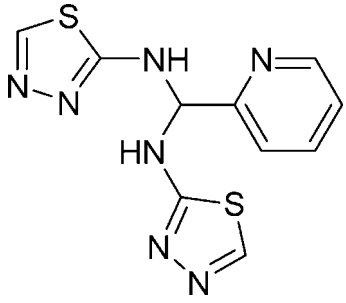
Received 15 September 2007; accepted 17 September 2007

Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.095; data-to-parameter ratio = 17.2.

In the title compound, $C_{10}H_9N_7S_2$, the dihedral angle between the aminothiazole rings is 80.91 (10)°. In the crystal structure, the molecules are linked into chains by N—H···N hydrogen bonds

Related literature

The title compound was synthesized according to a similar method reported by Hopkinson *et al.* (1991).



Experimental

Crystal data

$C_{10}H_9N_7S_2$
M_r = 291.36
Monoclinic, $P2_1/n$
a = 11.283 (2) Å
b = 8.7613 (18) Å
c = 13.151 (3) Å
β = 97.13 (3)°
V = 1290.0 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.41 mm^{-1}
T = 153 (2) K
0.20 × 0.18 × 0.16 mm

Data collection

Bruker $P4$ diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.983, T_{max} = 1.000
(expected range = 0.921–0.937)
5688 measured reflections
2953 independent reflections
1908 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.095
S = 1.03
2953 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1^{i}	0.86	2.13	2.866 (2)	143
N5—H5A···N3^{i}	0.86	2.27	2.949 (2)	136

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

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: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

YXZ gratefully acknowledges the financial support of the Science Foundation of Henan Province in China (grant No. 0511020400).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2543).

References

Bruker (1998). *SMART*, *SAINT*, *SADABS* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Hopkinson, C., Meakins, G. D. & Purcell, R. J. (1991). *Synthesis*, pp. 621–624.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

  doi:10.1107/S1600536807045473

supplementary materials

Acta Cryst. (2007). E**63**, o4128 [**doi:10.1107/S1600536807045473**]

(2-Pyridyl)bis(1,3,4-thiadiazol-2-ylamino)methane

Y.-X. Zhang and P. Liu

Comment

The molecule of the title compound, (I) (Fig. 1), consists of two aminothiadiazolyl rings and a pyridyl group bridged by a carbon atom with the N donors of the pyridyl and thiadiazolyl groups extending toward the same direction. Dihedral angles between rings (identified by one atom) are S1/S2 = 80.91 (10)°, S1/N1 = 87.08 (9)°, S2/N1 = 73.65 (9)°.

In the crystal, adjacent molecules are linked by N—H···N hydrogen bonds (Table 1) to generate a one-dimensional supramolecular network, as shown in Fig. 2. There are no aromatic π-π stacking interactions involving the thiadiazolyl and pridyl rings.

Experimental

The title compound, was obtained by the reaction of 2-aminothiadiazole (5.05 g, 0.05 mmol) and 2-pyridylaldehyde (6.5 g, 0.06 mmol) in 100 ml me thanol solution with ten drops of 6 *M* HCl. The colorless block crystals of (I) were grown *via* recrystallization in methanol at room temperature.

Refinement

The H atoms were positionedg geometrically (C—H = 0.93 Å, N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier).

Figures

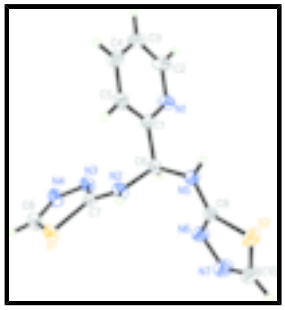


Fig. 1. The molecular structure of (I), with 50% probability displacement ellipsoids for the non-H atoms.

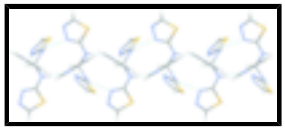


Fig. 2. The packing of (I), viewed down the *a* axis, showing intermolecular N—H···N hydrogen bonds (dashed lines).

(2-Pyridyl)bis(1,3,4-thiadiazol-2-ylamino)methane

Crystal data

$C_{10}H_9N_7S_2$	F_{000} = 600
M_r = 291.36	D_x = 1.500 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 12640 reflections
a = 11.283 (2) Å	θ = 3.4–27.5º
b = 8.7613 (18) Å	μ = 0.41 mm^{-1}
c = 13.151 (3) Å	T = 153 (2) K
β = 97.13 (3)º	Block, colourless
V = 1290.0 (5) Å^3	0.20 × 0.18 × 0.16 mm
Z = 4	

Data collection

Bruker P4 diffractometer	2953 independent reflections
Radiation source: fine-focus sealed tube	1908 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 153(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.4º
Absorption correction: multi-scan (SADABS; Bruker, 1998)	h = −14→14
T_{min} = 0.983, T_{max} = 1.000	k = −11→11
5688 measured reflections	l = −17→17

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
$wR(F^2)$ = 0.095	$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
2953 reflections	$\Delta\rho_{max}$ = 0.29 e Å^{-3}
172 parameters	$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	y	z	U_{iso}*/U_{eq}

C1	0.39112 (15)	0.06831 (18)	0.76159 (12)	0.0325 (4)
C2	0.55007 (17)	−0.0844 (2)	0.82008 (16)	0.0514 (5)
H2	0.5793	−0.1714	0.8552	0.062*
C3	0.62985 (18)	0.0092 (2)	0.77961 (16)	0.0526 (5)
H3	0.7109	−0.0138	0.7871	0.063*
C4	0.58714 (18)	0.1363 (2)	0.72823 (15)	0.0508 (5)
H4	0.6389	0.2016	0.6996	0.061*
C5	0.46582 (17)	0.1680 (2)	0.71879 (13)	0.0429 (5)
H5	0.4353	0.2549	0.6843	0.052*
C6	0.25742 (15)	0.09060 (19)	0.75500 (12)	0.0345 (4)
H6	0.2199	−0.0105	0.7517	0.041*
C7	0.17955 (14)	0.10493 (19)	0.57373 (13)	0.0345 (4)
C8	0.1164 (2)	0.0319 (2)	0.40249 (15)	0.0539 (5)
H8	0.0864	0.0218	0.3337	0.065*
C9	0.11296 (16)	0.1562 (2)	0.86842 (13)	0.0381 (4)
C10	−0.0725 (2)	0.1710 (3)	0.93144 (19)	0.0695 (7)
H10	−0.1392	0.1909	0.9644	0.083*
N1	0.43237 (13)	−0.05732 (15)	0.81182 (12)	0.0411 (4)
N2	0.20837 (14)	0.17587 (16)	0.66401 (11)	0.0410 (4)
H2A	0.1978	0.2728	0.6682	0.049*
N3	0.20509 (14)	−0.03795 (17)	0.55573 (11)	0.0433 (4)
N4	0.16735 (16)	−0.07900 (18)	0.45482 (12)	0.0534 (4)
N5	0.22648 (13)	0.16712 (16)	0.84586 (11)	0.0388 (4)
H5A	0.2792	0.2184	0.8846	0.047*
N6	0.03642 (14)	0.05646 (18)	0.82607 (13)	0.0496 (4)
N7	−0.07234 (16)	0.0652 (2)	0.86360 (15)	0.0657 (5)
S1	0.10722 (5)	0.20038 (6)	0.46841 (4)	0.04768 (17)
S2	0.05728 (5)	0.27312 (7)	0.95736 (4)	0.06054 (19)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0361 (10)	0.0303 (9)	0.0306 (9)	−0.0021 (7)	0.0020 (7)	−0.0041 (7)
C2	0.0401 (12)	0.0420 (11)	0.0689 (14)	0.0063 (9)	−0.0055 (10)	0.0012 (10)
C3	0.0323 (11)	0.0615 (14)	0.0632 (14)	−0.0034 (10)	0.0028 (10)	−0.0130 (11)
C4	0.0488 (13)	0.0568 (13)	0.0484 (12)	−0.0155 (10)	0.0119 (10)	−0.0039 (10)
C5	0.0491 (12)	0.0382 (10)	0.0414 (11)	−0.0061 (9)	0.0052 (9)	0.0050 (8)
C6	0.0380 (10)	0.0303 (9)	0.0344 (10)	0.0012 (7)	0.0018 (7)	−0.0035 (7)
C7	0.0313 (10)	0.0363 (10)	0.0358 (10)	0.0020 (7)	0.0033 (7)	0.0017 (8)
C8	0.0639 (14)	0.0591 (13)	0.0366 (11)	−0.0043 (11)	−0.0022 (10)	−0.0014 (10)
C9	0.0411 (11)	0.0380 (10)	0.0348 (10)	0.0012 (8)	0.0026 (8)	−0.0023 (8)
C10	0.0451 (14)	0.0941 (18)	0.0721 (16)	−0.0046 (12)	0.0190 (11)	−0.0144 (14)
N1	0.0385 (9)	0.0324 (8)	0.0506 (9)	−0.0012 (7)	−0.0011 (7)	0.0057 (7)
N2	0.0530 (10)	0.0298 (8)	0.0382 (9)	0.0069 (7)	−0.0023 (7)	−0.0019 (7)
N3	0.0527 (10)	0.0382 (9)	0.0376 (9)	0.0060 (7)	−0.0001 (7)	−0.0035 (7)
N4	0.0708 (12)	0.0486 (10)	0.0386 (10)	−0.0010 (9)	−0.0016 (8)	−0.0094 (8)
N5	0.0344 (9)	0.0441 (9)	0.0375 (9)	−0.0054 (7)	0.0024 (7)	−0.0114 (7)
N6	0.0388 (9)	0.0554 (10)	0.0542 (10)	−0.0067 (8)	0.0042 (8)	−0.0112 (8)

N7	0.0417 (11)	0.0844 (14)	0.0713 (13)	−0.0134 (10)	0.0086 (9)	−0.0122 (11)
S1	0.0522 (3)	0.0472 (3)	0.0414 (3)	0.0072 (2)	−0.0028 (2)	0.0083 (2)
S2	0.0534 (4)	0.0723 (4)	0.0590 (4)	−0.0035 (3)	0.0191 (3)	−0.0240 (3)

Geometric parameters (Å, °)

C1—N1	1.337 (2)	C7—N2	1.344 (2)
C1—C5	1.382 (2)	C7—S1	1.7330 (18)
C1—C6	1.513 (2)	C8—N4	1.284 (2)
C2—N1	1.340 (2)	C8—S1	1.722 (2)
C2—C3	1.373 (3)	C8—H8	0.9300
C2—H2	0.9300	C9—N6	1.304 (2)
C3—C4	1.360 (3)	C9—N5	1.354 (2)
C3—H3	0.9300	C9—S2	1.7307 (18)
C4—C5	1.387 (3)	C10—N7	1.287 (3)
C4—H4	0.9300	C10—S2	1.714 (2)
C5—H5	0.9300	C10—H10	0.9300
C6—N5	1.450 (2)	N2—H2A	0.8600
C6—N2	1.460 (2)	N3—N4	1.390 (2)
C6—H6	0.9800	N5—H5A	0.8600
C7—N3	1.313 (2)	N6—N7	1.380 (2)
N1—C1—C5	121.96 (17)	N2—C7—S1	121.42 (13)
N1—C1—C6	114.72 (14)	N4—C8—S1	115.44 (15)
C5—C1—C6	123.32 (16)	N4—C8—H8	122.3
N1—C2—C3	123.64 (19)	S1—C8—H8	122.3
N1—C2—H2	118.2	N6—C9—N5	123.27 (16)
C3—C2—H2	118.2	N6—C9—S2	114.12 (14)
C4—C3—C2	118.21 (19)	N5—C9—S2	122.60 (13)
C4—C3—H3	120.9	N7—C10—S2	116.03 (17)
C2—C3—H3	120.9	N7—C10—H10	122.0
C3—C4—C5	119.58 (18)	S2—C10—H10	122.0
C3—C4—H4	120.2	C1—N1—C2	117.80 (16)
C5—C4—H4	120.2	C7—N2—C6	120.86 (14)
C1—C5—C4	118.80 (18)	C7—N2—H2A	119.6
C1—C5—H5	120.6	C6—N2—H2A	119.6
C4—C5—H5	120.6	C7—N3—N4	111.77 (15)
N5—C6—N2	109.47 (14)	C8—N4—N3	112.31 (15)
N5—C6—C1	110.65 (14)	C9—N5—C6	118.61 (14)
N2—C6—C1	112.76 (14)	C9—N5—H5A	120.7
N5—C6—H6	107.9	C6—N5—H5A	120.7
N2—C6—H6	107.9	C9—N6—N7	112.40 (16)
C1—C6—H6	107.9	C10—N7—N6	111.47 (18)
N3—C7—N2	124.47 (16)	C8—S1—C7	86.39 (10)
N3—C7—S1	114.09 (13)	C10—S2—C9	85.96 (11)
N1—C2—C3—C4	0.0 (3)	S1—C7—N3—N4	0.01 (19)
C2—C3—C4—C5	0.4 (3)	S1—C8—N4—N3	0.0 (2)
N1—C1—C5—C4	0.1 (3)	C7—N3—N4—C8	0.0 (2)
C6—C1—C5—C4	−179.31 (15)	N6—C9—N5—C6	14.7 (3)
C3—C4—C5—C1	−0.4 (3)	S2—C9—N5—C6	−165.92 (13)

N1—C1—C6—N5	85.31 (18)	N2—C6—N5—C9	74.84 (19)
C5—C1—C6—N5	−95.21 (18)	C1—C6—N5—C9	−160.28 (14)
N1—C1—C6—N2	−151.70 (15)	N5—C9—N6—N7	178.40 (17)
C5—C1—C6—N2	27.8 (2)	S2—C9—N6—N7	−1.1 (2)
C5—C1—N1—C2	0.2 (3)	S2—C10—N7—N6	0.5 (3)
C6—C1—N1—C2	179.69 (15)	C9—N6—N7—C10	0.4 (3)
C3—C2—N1—C1	−0.3 (3)	N4—C8—S1—C7	0.04 (17)
N3—C7—N2—C6	−8.6 (3)	N3—C7—S1—C8	−0.03 (15)
S1—C7—N2—C6	173.28 (12)	N2—C7—S1—C8	178.31 (15)
N5—C6—N2—C7	−151.96 (15)	N7—C10—S2—C9	−0.9 (2)
C1—C6—N2—C7	84.40 (19)	N6—C9—S2—C10	1.09 (16)
N2—C7—N3—N4	−178.27 (15)	N5—C9—S2—C10	−178.39 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···N1^{i}	0.86	2.13	2.866 (2)	143
N5—H5A···N3^{i}	0.86	2.27	2.949 (2)	136

Symmetry codes: (i) −*x*+1/2, *y*+1/2, −*z*+3/2.

Fig. 1

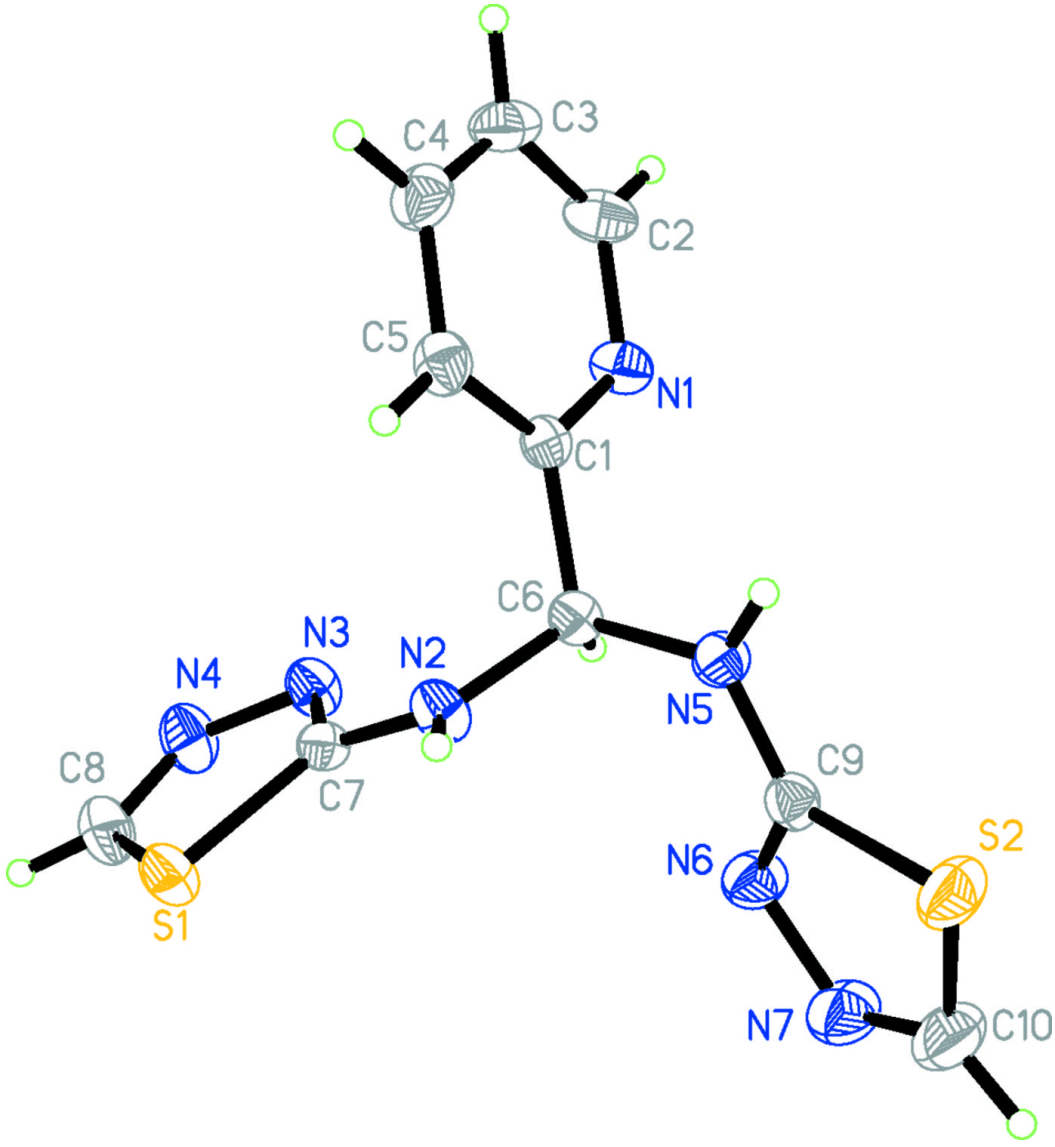


Fig. 2