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1,2-Bis(1,3-dithiolan-2-ylidene)hydrazine

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Key indicators

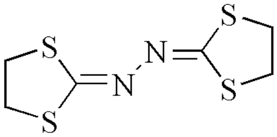
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.046
wR factor = 0.130
Data-to-parameter ratio = 17.7

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

The title molecule, $C_6H_8N_2S_4$, possesses a crystallographically imposed center of symmetry. The two five-membered rings are in half-chair conformations. The crystal packing is stabilized mainly by van der Waals forces.

Comment

As an important type of fungicide, heterocyclic compounds are highly efficient in view of their low toxicity (Shi *et al.*, 1995; Xu *et al.*, 2002). In this paper, we report the crystal structure of the title compound, (I) (Fig. 1).



(I)

In the solid state, the molecule of (I) possesses a crystallographically imposed center of symmetry. All bond lengths and angles are normal (Table 1). The 1,3-dithiolane rings are each in a half-chair conformation. The deviations of atoms C2 and C3 from the plane fromed by S1, S2 and C1 are 0.226 (7) and −0.442 (6) Å, respectively. The crystal packing (Fig. 2) is stabilized mainly by van der Waals forces.

Experimental

The title compound, (I), was prepared according to the method of Mayer & Schaefer (1964) and was crystallized from a mixture of ethanol and petroleum ether.

Crystal data

$C_6H_8N_2S_4$
M_r = 236.38
Monoclinic, $P2_1/n$
a = 6.300 (2) Å
b = 7.737 (2) Å
c = 10.386 (3) Å
β = 106.712 (4)°
V = 484.9 (2) Å^3
Z = 2
D_x = 1.619 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1494 reflections
θ = 2.6–26.4°
μ = 0.92 mm^{-1}
T = 293 (2) K
Prism, colorless
0.30 × 0.28 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan, (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.708, $T_{\max}$ = 0.816
2712 measured reflections
992 independent reflections
834 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.023
$\theta_{\max}$ = 26.4°
$h = -7 \rightarrow 7$
$k = -9 \rightarrow 9$
$l = -12 \rightarrow 8$

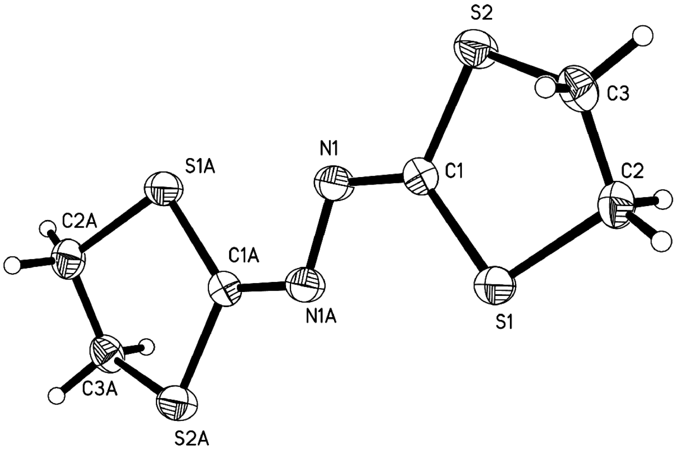


Figure 1
View of the molecule of (I), with displacement ellipsoids drawn at the 30% probability level. The suffix A corresponds to symmetry code (i) in Table 1.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.130$
$S = 1.04$
992 reflections
56 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0675P)^2 + 0.6306P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.0001$
$\Delta\rho_{\max} = 1.06$ e Å^{-3}
$\Delta\rho_{\min} = -0.37$ e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.161 (16)

Table 1
Selected geometric parameters (Å, °).

S1—C1	1.757 (3)	N1—C1	1.287 (4)
S1—C2	1.816 (3)	N1—N1^i	1.396 (5)
S2—C1	1.749 (3)	C2—C3	1.506 (5)
S2—C3	1.803 (3)		
C1—S1—C2	95.5 (2)	N1—C1—S1	125.8 (2)
C1—S2—C3	94.9 (2)	S2—C1—S1	115.3 (2)
C1—N1—N1^i	111.2 (3)	C3—C2—S1	108.1 (2)
N1—C1—S2	118.9 (2)	C2—C3—S2	108.8 (2)
N1^i—N1—C1—S2	179.1 (3)	C2—S1—C1—S2	-7.2 (2)
N1^i—N1—C1—S1	-2.6 (5)	C1—S1—C2—C3	31.4 (3)
C3—S2—C1—N1	164.3 (3)	S1—C2—C3—S2	-45.2 (3)
C3—S2—C1—S1	-14.2 (2)	C1—S2—C3—C2	36.0 (3)
C2—S1—C1—N1	174.4 (3)		

Symmetry codes: (i) $-x+2, -y, -z$.

All H atoms were placed in calculated positions, with C—H distances of 0.97 Å, and included in the final cycles of refinement using a riding model, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). The maximum electron-density peak was located 0.83 Å from atom S2.

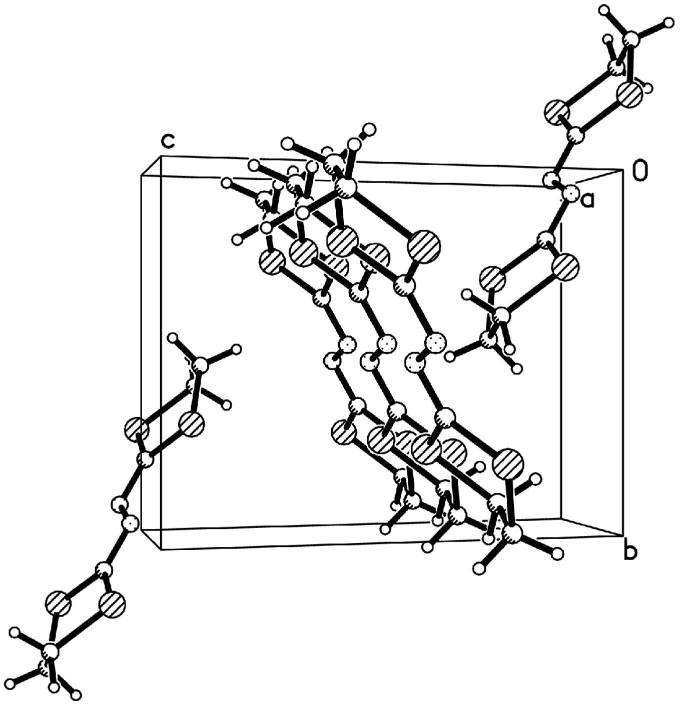


Figure 2
Packing diagram of the title compound, viewed along the *a* axis.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); 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, 1999); software used to prepare material for publication: *SHELXTL*.

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