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(1,3-Dithiol-2-ylidene)propanedinitrile

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In the crystal structure of the title compound, $C_6H_2N_2S_2$, there is a tape structure, as a result of C—H···N hydrogen bonds is found. The molecules stack along the [120] direction in a head-to-tail fashion.

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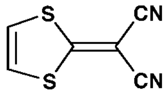
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.008 Å
R factor = 0.048
wR factor = 0.139
Data-to-parameter ratio = 15.9

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

Comment

New push–pull chromophores containing electron-donor and electron-acceptor groups have been thoroughly explored in the development of efficient second-order non-linear optical (NLO) materials (Denning, 1995; Marks & Ratner, 1995). The use of the 1,3-dithiol-2-ylidene group as an electron donor in NLO materials has been reported (Gompper *et al.*, 1968; Katz *et al.*, 1987; Moore *et al.*, 1998, 2001; Nguyen *et al.*, 1998; Andreu *et al.*, 2003). Compound (I) is the first and the simplest push–pull system involving the 1,3-dithiol-2-ylidene donor (Mayer & Gebhardt, 1964). However, only two examples (Komarova *et al.*, 1990; Tomura & Yamashita, 2001) of structures containing this framework were found in the Cambridge Structural Database (CSD, Version 5.24; Allen, 2002). Therefore, we report here the molecular and crystal structure of (I).



(I)

The molecular structure is shown in Fig. 1, and selected geometric parameters are given in Table 1. The molecule of (I) is planar, with an r.m.s deviation of 0.0308 Å from the least-squares plane for the fitted non-H atoms. No bond alternation is observed in the C1═C4 and C2═C3 double bonds. The geometric parameters of the dicyanomethylene group in (I) are almost the same as those of tetracyanoquinodimethane (Long *et al.*, 1965).

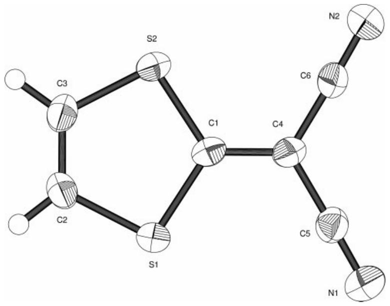


Figure 1
The molecular structure of (I), with the atomic numbering scheme. Displacement ellipsoids are shown at the 50% probability level.

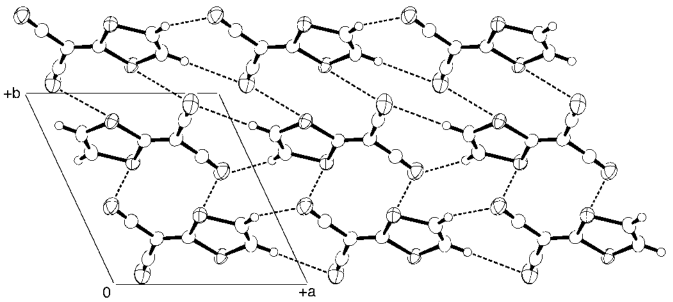


Figure 2
Packing diagram of (I), viewed along the *c* axis. Dashed lines show the intermolecular S···N and C—H···N contacts.

Fig. 2 shows the packing diagram of (I), viewed along the *c* axis. The molecules form a one-dimensional molecular-tape structure along the [101] direction and are connected *via* intermolecular C—H···N hydrogen bonds (Taylor & Kennard, 1982). The geometry of the C—H···N hydrogen bonds (Table 2) is almost the same as previously reported (Drück & Littke, 1978; Dhurjati *et al.*, 1991; Reddy *et al.*, 1993; Langley *et al.*, 1998; Thaimattam *et al.*, 1998). This type of molecular-tape structure has been found in the crystals of 1,2-dicyanobenzene (Janczak & Kubiak, 1995) and 2,3-dicyanonaphthalene (Janczak & Kubiak, 2000). Short intermolecular S···N contacts [3.089 (5) Å for S1···N1(1 − *x*, 1 − *y*, 1 − *z*) and 3.117 (5) Å for S2···N2(1 − *x*, −*y*, 1 − *z*)] are observed between adjacent molecular tapes (Yamashita & Tomura, 1998). The S···N distances are 7.0–7.8% shorter than the sum of the corresponding van der Waals radii (Pauling, 1960). The molecules form an alternating stack along the [120] direction, where the distances between the molecular planes are 3.381 (6) and 3.474 (6) Å. The shortest intermolecular S···S contact [3.619 (3) Å for S2···S2(1 − *x*, −*y*, −*z*)] is observed within the stack.

Experimental

The title compound, (I), was synthesized according to the literature method of Mayer & Gebhardt (1964). Colorless crystals of (I) suitable for X-ray analysis were grown from a chloroform solution.

Crystal data

$C_6H_2N_2S_2$
$M_r = 166.22$
Triclinic, $P\overline{1}$
$a = 8.2420\ (10)$ Å
$b = 8.8190\ (13)$ Å
$c = 5.6400\ (6)$ Å
$\alpha = 104.325\ (11)^\circ$
$\beta = 107.919\ (9)^\circ$
$\gamma = 108.320\ (11)^\circ$
$V = 342.37\ (9)$ Å^3
$Z = 2$
$D_x = 1.612$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 25 reflections
$\theta = 12.6$–14.5°
$\mu = 0.69$ mm^{-1}
$T = 296\ (2)$ K
Plate, colorless
0.20 × 0.13 × 0.03 mm

Data collection

Rigaku AFC-7*R* diffractometer
ω–2θ scans
1678 measured reflections
1571 independent reflections
738 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.054$
$\theta_{\max} = 27.5^\circ$
$h = 0 \rightarrow 10$
$k = -11 \rightarrow 10$
$l = -7 \rightarrow 6$
3 standard reflections
every 150 reflections
intensity decay: 0.9%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.139$
$S = 0.95$
1571 reflections
99 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.38$ e Å^{-3}
$\Delta\rho_{\min} = -0.39$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C1	1.732 (5)	N2—C6	1.135 (7)
S1—C2	1.739 (6)	C1—C4	1.358 (7)
S2—C1	1.726 (5)	C2—C3	1.312 (7)
S2—C3	1.734 (5)	C4—C6	1.427 (7)
N1—C5	1.140 (6)	C4—C5	1.434 (7)
C1—S1—C2	95.7 (2)	C2—C3—S2	117.3 (4)
C1—S2—C3	96.0 (2)	C6—C4—C5	118.5 (4)
S2—C1—S1	113.9 (3)	N1—C5—C4	177.5 (6)
C3—C2—S1	117.1 (4)	N2—C6—C4	178.3 (6)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···N1^{i}	0.93 (6)	2.79 (6)	3.692 (7)	164 (5)
C3—H3···N2^{i}	0.99 (5)	2.70 (5)	3.651 (7)	162 (4)

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

Both H atoms were located in a difference Fourier map and their positional and isotropic displacement parameters were refined freely. Owing to the large number of weak high-angle reflections, the ratio of observed to unique reflections is low (47%).

Data collection: *MSC*/*AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988); cell refinement: *MSC*/*AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation & Rigaku, 2000); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL*97.

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