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Tetrathiafulvalene with a fused pyrazine ring

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.016 Å
R factor = 0.079
wR factor = 0.198
Data-to-parameter ratio = 16.0

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

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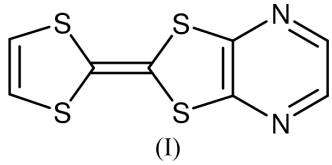
The title compound, 2-(1,3-dithiol-2-ylidene)-2,3-dihydro-1,3-dithia-4,7-diazaindene (pyrazinotetrathiafulvalene), $C_8H_4N_2S_4$, forms a head-to-tail type of π–π-stacking centrosymmetric dimer with an interplanar distance of 3.59 (1) Å. The dimers form a two-dimensional column along the [101] direction.

Comment

It is known that S···N inter-heteroatom contacts work to construct unique molecular networks (Yamashita & Tomura, 1998). In the title compound, (I) (Fig. 1), short S···N inter-heteroatom contacts [3.10 (1) Å for S2···N1(x, $y+1$, z)] are observed between the two π–π dimers, as shown in Fig. 2. Two molecules in a dimer are related by an inversion center. A planar π-conjugated molecule prefers to overlap with a single molecule at both sides of the molecular plane to form a one-dimensional column. In the two-dimensional column of (I), however, one dimer bridges two other dimers through the overlap of the pyrazine and 1,3-dithiole rings (Fig. 3). The angle between the dimers is 111 (1)°. This type of unique multi-dimensional structure is important for the construction of organic conducting materials (Barclay *et al.*, 2000; Kato *et al.*, 1988; Morimoto & Inabe, 1995; Tomura & Yamashita, 2000; Yamashita *et al.*, 1997, 1998).



(I)

Experimental

The title compound (I) was synthesized according to the literature method of Papavassiliou *et al.* (1988). Crystals of (I) were grown from a dichloromethane solution.

Crystal data

$C_8H_4N_2S_4$
M_r = 256.37
Monoclinic, $P2_1/n$
a = 8.481 (2) Å
b = 9.1928 (9) Å
c = 12.8980 (14) Å
β = 96.89 (2)°
V = 998.4 (3) Å^3
Z = 4
D_x = 1.706 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 24 reflections
θ = 9.7–42.8°
μ = 8.39 mm^{-1}
T = 296 (2) K
Needle, orange
0.40 × 0.05 × 0.05 mm

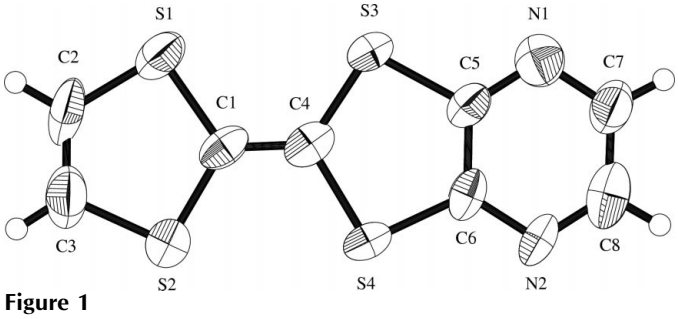


Figure 1
The molecular structure of (I) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.134, T_{max} = 0.679
2060 measured reflections
2026 independent reflections
663 reflections with $I > 2\sigma(I)$

R_{int} = 0.084
θ_{max} = 74.2°
$h = -10 \rightarrow 10$
$k = 0 \rightarrow 11$
$l = 0 \rightarrow 16$
3 standard reflections
frequency: 120 min
intensity decay: 4.9%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.198
S = 1.07
2026 reflections
127 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

All H atoms were placed in geometrically calculated positions and refined by using a riding model with C—H distances set to 0.93 Å.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1992); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *HELENA* (Spek, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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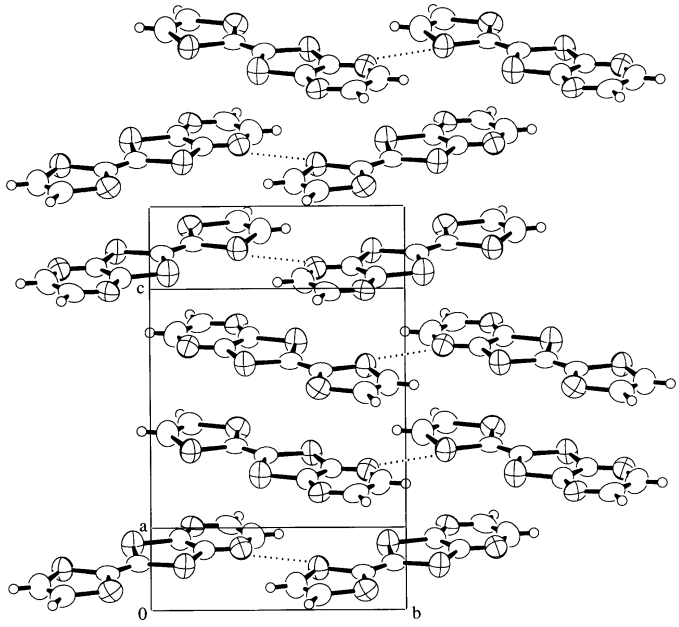

Figure 2
Packing diagram of (I). Short S···N inter-heteroatom contacts are indicated by dotted lines.

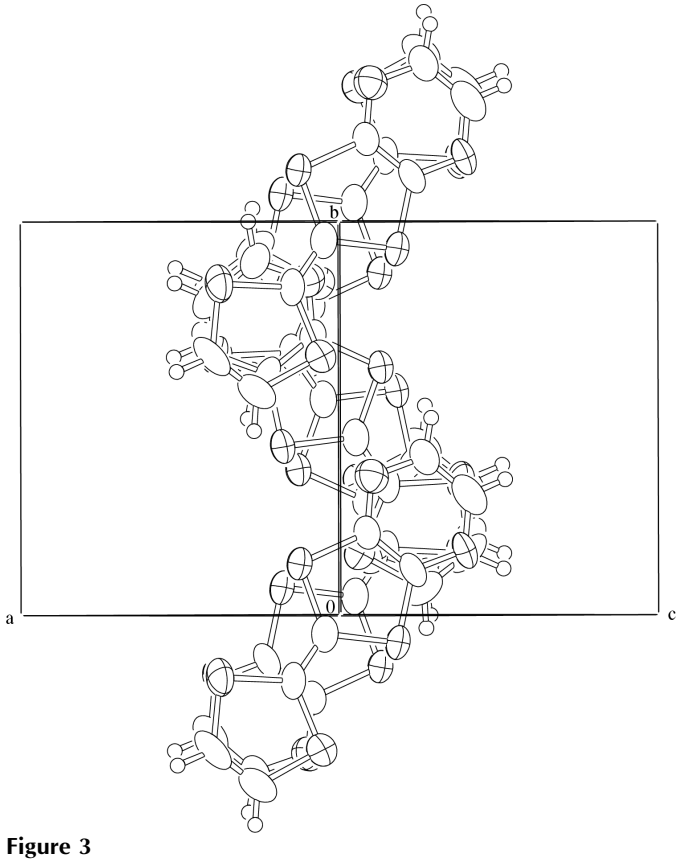

Figure 3
Packing diagram of (I) viewed along the [101] direction. Three dimers (six molecules) are indicated.

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