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4,4′,5,5′-Tetrakis(methylsulfanyl)tetrathiafulvalene

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.031
wR factor = 0.079
Data-to-parameter ratio = 21.6

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

The title compound, $C_{10}H_{12}S_8$, crystallizes in a monoclinic space group with one molecule in the asymmetric unit. All bond lengths and angles in the molecule are normal. The crystal packing is stabilized by van der Waals forces.

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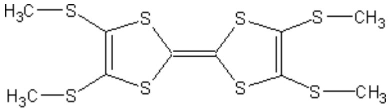
Comment

Tetrathiafulvalene (TTF) and its derivatives have been studied intensively since the 1970s (Narita *et al.*, 1976; Andreu *et al.*, 2000). In the past, they were widely used in the preparation of charge-transfer salts, possessing transport properties (Williams *et al.*, 1992). Nowadays, they are also much utilized as versatile functionalized building blocks. TTF has stimulated much effort in the preparation of its derivatives, possessing various electron-donating properties.



(I)

We report here the crystal structure of the title compound, (I) (Fig. 1). All bond lengths and angles in (I) are normal (Table 1) and comparable with those in previously reported analogues (Katayama *et al.*, 1985). The crystal packing (Fig. 2) is mainly stabilized by van der Waals forces, though relatively short intermolecular S···S [3.512 (2)–3.528 (2) Å] contacts are also observed.

Experimental

The title compound was synthesized according to the method of Tsujimoto *et al.* (1985). Crystals of (I) suitable for single-crystal X-ray diffraction were obtained by recrystallization from CH_2Cl_2.

Crystal data

$C_{10}H_{12}S_8$
M_r = 388.68
Monoclinic, $P2_1/n$
a = 14.0010 (2) Å
b = 7.0811 (1) Å
c = 15.6584 (3) Å
β = 106.213 (1)°
V = 1490.67 (4) Å^3
Z = 4

D_x = 1.732 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 19 853 reflections
θ = 3.4–27.5°
μ = 1.18 mm^{-1}
T = 296 (2) K
Block, orange
0.45 × 0.35 × 0.27 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{\min}$ = 0.620, $T_{\max}$ = 0.742
33 274 measured reflections
3521 independent reflections

2515 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.058
$\theta_{\max}$ = 27.9°
$h = -18 \rightarrow 18$
$k = -9 \rightarrow 9$
$l = -20 \rightarrow 20$

doi:10.1107/S1600536804031769

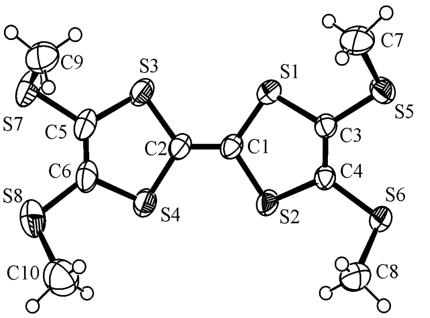


Figure 1
A view of (I), showing displacement ellipsoids at the 50% probability level.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.079$
$S = 1.05$
3521 reflections
163 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0383P)^2 + 0.2485P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0134 (9)

Table 1
Selected geometric parameters (Å, °).

S1—C1	1.669 (2)	S6—C4	1.7305 (19)
S1—C3	1.763 (2)	S6—C8	1.777 (3)
S2—C1	1.678 (2)	S7—C9	1.665 (3)
S2—C4	1.703 (2)	S7—C5	1.697 (2)
S3—C2	1.687 (2)	S8—C6	1.727 (2)
S3—C5	1.760 (2)	S8—C10	1.743 (3)
S4—C2	1.672 (2)	C1—C2	1.348 (3)
S4—C6	1.720 (2)	C3—C4	1.255 (3)
S5—C7	1.671 (2)	C5—C6	1.261 (3)
S5—C3	1.6849 (19)		
C1—S1—C3	95.30 (9)	S4—C2—S3	110.02 (12)
C1—S2—C4	99.15 (10)	C4—C3—S5	121.42 (16)
C2—S3—C5	95.23 (11)	C4—C3—S1	117.39 (16)
C2—S4—C6	98.23 (11)	S5—C3—S1	120.75 (11)
C7—S5—C3	96.58 (12)	C3—C4—S2	113.43 (16)
C4—S6—C8	100.45 (11)	C3—C4—S6	123.64 (16)
C9—S7—C5	97.78 (12)	S2—C4—S6	122.38 (12)
C6—S8—C10	102.90 (13)	C6—C5—S7	122.4 (2)
C2—C1—S1	125.86 (16)	C6—C5—S3	116.81 (18)
C2—C1—S2	124.06 (17)	S7—C5—S3	120.52 (15)
S1—C1—S2	110.09 (12)	C5—C6—S4	113.89 (19)
C1—C2—S4	123.30 (16)	C5—C6—S8	124.03 (19)
C1—C2—S3	126.68 (17)	S4—C6—S8	121.91 (15)

All H atoms were positioned geometrically and refined as riding atoms, with C—H distances of 0.96 Å and U_{iso}(H) values of $1.5U_{eq}$(C)

Data collection: *COLLECT* (Nonius, 1997–2000); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Bruker, 1998); software used to prepare material for publication: *SHELXL*97.

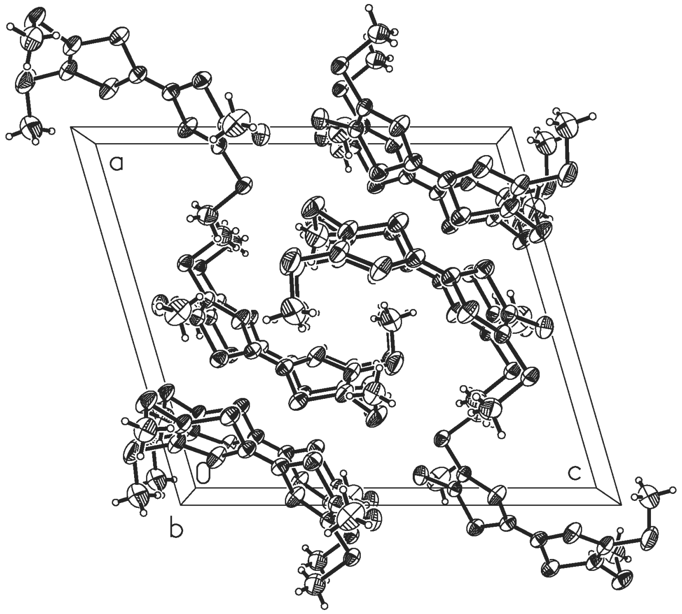


Figure 2
The crystal packing of (I), viewed along the *b* axis.

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