Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2*Z*)-2-Methylsulfanyl-1,4-di-2-thienylbut-2-ene-1,4-dione

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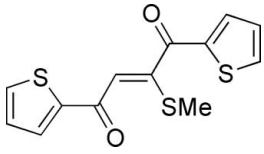
Received 8 November 2007; accepted 15 November 2007

Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.129; data-to-parameter ratio = 17.9.

The asymmetric unit of the title compound, $C_{13}H_{10}O_2S_3$, contains two independent molecules, which exhibit different conformations [C=C(SMe)—C(O)—C torsion angles of 81.4 (3) and 80.2 (2)°], normal bond lengths and angles, and short intramolecular S···O distances [2.768 (3) Å in both molecules]. The crystal packing exhibits weak intermolecular C—H···O hydrogen bonds.

Related literature

For details of the preparation of the title compound, see: Yin *et al.* (2006, 2007). For the crystal structures of similar compounds, see: Chen *et al.* (2007); Gao *et al.* (2007). For applications of the title compound, see: Ellison *et al.* (1973); Yuguchi *et al.* (2004).



Experimental

Crystal data

$C_{13}H_{10}O_2S_3$
M_r = 294.41
Monoclinic, $P2_1/c$
a = 9.7994 (14) Å
b = 27.571 (4) Å
c = 10.8814 (16) Å
β = 113.816 (2)°
V = 2689.6 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.54 mm^{-1}
T = 297 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.900, T_{max} = 0.948
29719 measured reflections
5868 independent reflections
5087 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.129
S = 1.06
5868 reflections
327 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O4^{i}	0.93	2.52	3.448 (3)	172
C5—H5···O4^{i}	0.93	2.54	3.416 (3)	157
C20—H20···O4^{ii}	0.93	2.54	3.438 (3)	162

Symmetry codes: (i) $x, y, z+1$; (ii) $x+1, y, z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

The authors are grateful to Central China Normal University and Dr Guo-Dong Yin.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2356).

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  doi:10.1107/S1600536807059533

supplementary materials

Acta Cryst. (2007). E**63**, o4810 [**doi:10.1107/S1600536807059533**]

(2*Z*)-2-Methylsulfanyl-1,4-di-2-thienylbut-2-ene-1,4-dione

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Comment

1,4-Dicarbonyl compounds are widely used as synthetic building blocks for further elaboration into substituted cyclopentenones, such as jasmones, rethorolones, cuparenones, prostaglandins, and five-membered heterocyclic compounds, such as furans, pyrroles, thiophenes, pyridazines (Ellison *et al.*, 1973; Yuguchi *et al.*, 2004). As a continuation of our previous studies in this area, (Chen *et al.*, 2007; Gao *et al.*, 2007; Yin *et al.*, 2007). We herein report the structure of the title compound (I) (Fig. 1).

There are two independent molecules in the asymmetric unit. The bond lengths of the C1—C2 and C14—C15 in two molecules are 1.339 (2) and 1.341 (2) Å, respectively, supporting their double-bond character. The torsion angles C2—C1—C8—C9 and C15—C14—C21—C22 are −81.4 (3) and 80.2 (2) %A, respectively, showing the difference in conformations of two molecules. In both molecules, there is a short intramolecular S···O distance of 2.768 (3) Å.

The crystal packing exhibits weak intermolecular C—H···O hydrogen bonds (Table 1).

Experimental

The title compound was prepared according to the method described by Yin *et al.* (2006). Crystals appropriate for data collection were obtained by slow evaporation from a CH_2Cl_2/CH_3OH (1:1, *v*/*v*) solution at 283 K.

Refinement

All H atoms were geometrically positioned (C—H 0.93–0.96 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$ (methyl C).

Figures

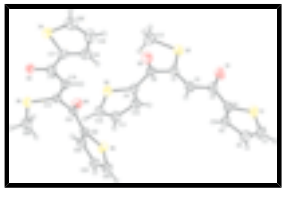


Fig. 1. The content of asymmetric unit of (I) showing the atom-labelling scheme and displacement ellipsoids drawn at the 30% probability level.

(2*Z*)-2-Methylsulfanyl-1,4-di-2-thienylbut-2-ene-1,4-dione

Crystal data

$C_{13}H_{10}O_2S_3$ $F_{000} = 1216$

M_r = 294.41	D_x = 1.454 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P2ybc	Cell parameters from 6482 reflections
a = 9.7994 (14) Å	θ = 2.3–28.3º
b = 27.571 (4) Å	μ = 0.54 mm^{-1}
c = 10.8814 (16) Å	T = 297 (2) K
β = 113.816 (2)º	Block, colourless
V = 2689.6 (7) Å^3	0.20 × 0.20 × 0.10 mm
Z = 8	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	5868 independent reflections
Radiation source: fine-focus sealed tube	5087 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.022
T = 297(2) K	θ_{max} = 27.0º
φ and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	h = −12→12
T_{min} = 0.900, T_{max} = 0.948	k = −35→32
29719 measured reflections	l = −12→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H-atom parameters constrained
$wR(F^2)$ = 0.129	$w = 1/[\sigma^2(F_o^2) + (0.0723P)^2 + 0.9173P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max}$ = 0.001
5868 reflections	$\Delta\rho_{max}$ = 0.41 e Å^{-3}
327 parameters	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculat-

ing *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8777 (2)	0.77555 (7)	0.9581 (2)	0.0472 (4)
C2	0.7685 (2)	0.77154 (8)	1.0017 (2)	0.0514 (5)
H2	0.7468	0.7983	1.0426	0.062*
C3	0.6814 (3)	0.72716 (8)	0.9882 (2)	0.0538 (5)
C4	0.5584 (2)	0.72918 (8)	1.0320 (2)	0.0514 (5)
C5	0.5266 (3)	0.76375 (9)	1.1109 (2)	0.0546 (5)
H5	0.5797	0.7924	1.1414	0.066*
C6	0.4014 (3)	0.74909 (11)	1.1383 (3)	0.0700 (7)
H6	0.3636	0.7670	1.1899	0.084*
C7	0.3450 (3)	0.70635 (11)	1.0805 (3)	0.0771 (8)
H7	0.2631	0.6918	1.0879	0.093*
C8	0.9616 (2)	0.82346 (8)	0.9849 (2)	0.0484 (5)
C9	0.8910 (2)	0.86269 (7)	0.8925 (2)	0.0455 (4)
C10	0.7624 (3)	0.86089 (9)	0.7771 (2)	0.0592 (6)
H10	0.7021	0.8336	0.7487	0.071*
C11	0.7326 (3)	0.90526 (11)	0.7067 (3)	0.0746 (8)
H11	0.6503	0.9106	0.6265	0.089*
C12	0.8367 (3)	0.93903 (10)	0.7685 (3)	0.0777 (8)
H12	0.8345	0.9702	0.7351	0.093*
C13	1.0565 (3)	0.76053 (11)	0.8186 (3)	0.0706 (7)
H13A	1.0041	0.7867	0.7605	0.106*
H13B	1.0911	0.7382	0.7698	0.106*
H13C	1.1402	0.7732	0.8937	0.106*
C14	0.8364 (2)	0.93124 (7)	0.28464 (19)	0.0406 (4)
C15	0.9289 (2)	0.91501 (8)	0.4059 (2)	0.0460 (4)
H15	0.8959	0.8903	0.4452	0.055*
C16	1.0792 (2)	0.93429 (7)	0.4794 (2)	0.0447 (4)
C17	1.1705 (2)	0.91180 (7)	0.6088 (2)	0.0441 (4)
C18	1.1315 (3)	0.87987 (9)	0.6871 (2)	0.0560 (5)
H18	1.0360	0.8676	0.6642	0.067*
C19	1.2562 (3)	0.86837 (11)	0.8071 (2)	0.0734 (7)
H19	1.2510	0.8478	0.8729	0.088*
C20	1.3836 (3)	0.89032 (10)	0.8162 (2)	0.0702 (7)
H20	1.4755	0.8861	0.8878	0.084*
C21	0.6899 (2)	0.90491 (7)	0.21273 (19)	0.0410 (4)
C22	0.5692 (2)	0.91621 (7)	0.25324 (18)	0.0402 (4)
C23	0.5668 (2)	0.94842 (8)	0.3484 (2)	0.0468 (4)
H23	0.6487	0.9667	0.4027	0.056*
C24	0.4256 (2)	0.95063 (9)	0.3547 (2)	0.0539 (5)
H24	0.4038	0.9705	0.4134	0.065*
C25	0.3249 (2)	0.92002 (9)	0.2642 (2)	0.0556 (5)
H25	0.2265	0.9168	0.2544	0.067*

C26	0.7093 (3)	0.98422 (12)	0.0489 (3)	0.0780 (8)
H26A	0.6983	0.9558	−0.0052	0.117*
H26B	0.7164	1.0123	−0.0003	0.117*
H26C	0.6244	0.9873	0.0711	0.117*
O1	0.7101 (2)	0.68979 (6)	0.9424 (2)	0.0768 (5)
O2	1.08117 (19)	0.82733 (7)	1.07963 (18)	0.0719 (5)
O3	1.12945 (16)	0.96742 (6)	0.43439 (16)	0.0576 (4)
O4	0.67672 (18)	0.87642 (6)	0.12342 (16)	0.0575 (4)
S1	0.43580 (8)	0.68155 (2)	0.99352 (7)	0.0719 (2)
S2	0.97234 (7)	0.91905 (2)	0.91322 (7)	0.06458 (19)
S3	0.93242 (7)	0.72952 (2)	0.87829 (7)	0.06165 (17)
S4	1.35647 (6)	0.92628 (2)	0.68299 (6)	0.06146 (18)
S5	0.39848 (6)	0.88857 (2)	0.17198 (5)	0.05342 (16)
S6	0.87586 (6)	0.97902 (2)	0.20071 (6)	0.05825 (17)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0487 (10)	0.0406 (10)	0.0460 (10)	−0.0015 (8)	0.0126 (8)	0.0032 (8)
C2	0.0557 (12)	0.0405 (11)	0.0569 (12)	−0.0059 (9)	0.0218 (10)	−0.0017 (9)
C3	0.0598 (12)	0.0433 (11)	0.0563 (12)	−0.0070 (9)	0.0212 (10)	0.0011 (9)
C4	0.0528 (11)	0.0419 (11)	0.0524 (11)	−0.0109 (8)	0.0141 (9)	0.0034 (9)
C5	0.0510 (11)	0.0528 (12)	0.0610 (13)	−0.0143 (9)	0.0235 (10)	−0.0053 (10)
C6	0.0630 (15)	0.0737 (17)	0.0787 (17)	−0.0072 (13)	0.0342 (13)	−0.0016 (14)
C7	0.0554 (14)	0.084 (2)	0.0864 (19)	−0.0167 (13)	0.0234 (13)	0.0172 (15)
C8	0.0455 (10)	0.0469 (11)	0.0490 (11)	−0.0066 (8)	0.0150 (9)	0.0013 (9)
C9	0.0414 (9)	0.0425 (10)	0.0521 (11)	−0.0059 (8)	0.0184 (8)	0.0000 (8)
C10	0.0500 (12)	0.0547 (13)	0.0604 (13)	−0.0071 (10)	0.0094 (10)	0.0107 (10)
C11	0.0472 (12)	0.0768 (17)	0.0822 (17)	−0.0016 (12)	0.0081 (12)	0.0322 (14)
C12	0.0544 (14)	0.0590 (15)	0.114 (2)	0.0032 (11)	0.0285 (14)	0.0331 (15)
C13	0.0684 (15)	0.0782 (18)	0.0718 (16)	−0.0030 (13)	0.0351 (13)	−0.0022 (13)
C14	0.0384 (9)	0.0375 (9)	0.0482 (10)	−0.0016 (7)	0.0198 (8)	−0.0032 (8)
C15	0.0439 (10)	0.0453 (11)	0.0489 (10)	−0.0059 (8)	0.0189 (8)	0.0008 (8)
C16	0.0397 (9)	0.0454 (11)	0.0492 (10)	0.0013 (8)	0.0183 (8)	−0.0006 (8)
C17	0.0414 (9)	0.0443 (10)	0.0451 (10)	−0.0011 (8)	0.0159 (8)	−0.0064 (8)
C18	0.0534 (12)	0.0670 (14)	0.0454 (11)	−0.0072 (10)	0.0178 (9)	0.0005 (10)
C19	0.0780 (17)	0.0847 (19)	0.0460 (12)	−0.0150 (14)	0.0132 (12)	0.0078 (12)
C20	0.0662 (15)	0.0754 (17)	0.0485 (12)	−0.0043 (13)	0.0020 (11)	−0.0006 (12)
C21	0.0413 (9)	0.0376 (9)	0.0421 (9)	−0.0026 (7)	0.0147 (7)	0.0006 (8)
C22	0.0371 (9)	0.0395 (9)	0.0399 (9)	−0.0050 (7)	0.0113 (7)	0.0010 (7)
C23	0.0453 (10)	0.0438 (11)	0.0484 (10)	−0.0015 (8)	0.0158 (8)	−0.0029 (8)
C24	0.0508 (11)	0.0574 (13)	0.0571 (12)	0.0043 (9)	0.0254 (10)	−0.0018 (10)
C25	0.0418 (10)	0.0674 (14)	0.0584 (12)	0.0021 (9)	0.0212 (9)	0.0077 (11)
C26	0.0602 (14)	0.0858 (19)	0.0701 (16)	−0.0064 (13)	0.0077 (12)	0.0305 (14)
O1	0.0985 (14)	0.0438 (9)	0.1046 (15)	−0.0114 (9)	0.0580 (12)	−0.0118 (9)
O2	0.0556 (9)	0.0694 (11)	0.0649 (10)	−0.0141 (8)	−0.0023 (8)	0.0120 (8)
O3	0.0433 (8)	0.0595 (9)	0.0660 (9)	−0.0073 (7)	0.0177 (7)	0.0125 (7)
O4	0.0603 (9)	0.0547 (9)	0.0599 (9)	−0.0101 (7)	0.0269 (7)	−0.0186 (7)

S1	0.0713 (4)	0.0563 (4)	0.0768 (4)	−0.0220 (3)	0.0182 (3)	−0.0003 (3)
S2	0.0508 (3)	0.0491 (3)	0.0863 (4)	−0.0106 (2)	0.0198 (3)	0.0032 (3)
S3	0.0664 (4)	0.0504 (3)	0.0718 (4)	−0.0007 (2)	0.0317 (3)	−0.0043 (3)
S4	0.0456 (3)	0.0647 (4)	0.0631 (3)	−0.0076 (2)	0.0105 (2)	0.0019 (3)
S5	0.0424 (3)	0.0632 (4)	0.0513 (3)	−0.0128 (2)	0.0155 (2)	−0.0078 (2)
S6	0.0483 (3)	0.0567 (3)	0.0638 (3)	−0.0093 (2)	0.0164 (2)	0.0152 (3)

Geometric parameters (Å, °)

C1—C2	1.339 (3)	C14—C15	1.340 (3)
C1—C8	1.521 (3)	C14—C21	1.514 (3)
C1—S3	1.740 (2)	C14—S6	1.733 (2)
C2—C3	1.465 (3)	C15—C16	1.463 (3)
C2—H2	0.9300	C15—H15	0.9300
C3—O1	1.225 (3)	C16—O3	1.230 (2)
C3—C4	1.465 (3)	C16—C17	1.467 (3)
C4—C5	1.400 (3)	C17—C18	1.382 (3)
C4—S1	1.714 (2)	C17—S4	1.716 (2)
C5—C6	1.433 (3)	C18—C19	1.417 (3)
C5—H5	0.9300	C18—H18	0.9300
C6—C7	1.345 (4)	C19—C20	1.355 (4)
C6—H6	0.9300	C19—H19	0.9300
C7—S1	1.683 (3)	C20—S4	1.686 (3)
C7—H7	0.9300	C20—H20	0.9300
C8—O2	1.213 (3)	C21—O4	1.215 (2)
C8—C9	1.448 (3)	C21—C22	1.453 (3)
C9—C10	1.375 (3)	C22—C23	1.372 (3)
C9—S2	1.719 (2)	C22—S5	1.7225 (18)
C10—C11	1.410 (3)	C23—C24	1.414 (3)
C10—H10	0.9300	C23—H23	0.9300
C11—C12	1.344 (4)	C24—C25	1.368 (3)
C11—H11	0.9300	C24—H24	0.9300
C12—S2	1.691 (3)	C25—S5	1.692 (2)
C12—H12	0.9300	C25—H25	0.9300
C13—S3	1.808 (3)	C26—S6	1.799 (3)
C13—H13A	0.9600	C26—H26A	0.9600
C13—H13B	0.9600	C26—H26B	0.9600
C13—H13C	0.9600	C26—H26C	0.9600
C2—C1—C8	116.85 (19)	C14—C15—C16	123.25 (18)
C2—C1—S3	124.61 (17)	C14—C15—H15	118.4
C8—C1—S3	118.52 (16)	C16—C15—H15	118.4
C1—C2—C3	123.4 (2)	O3—C16—C15	121.94 (18)
C1—C2—H2	118.3	O3—C16—C17	120.60 (18)
C3—C2—H2	118.3	C15—C16—C17	117.45 (18)
O1—C3—C2	121.6 (2)	C18—C17—C16	130.37 (19)
O1—C3—C4	121.2 (2)	C18—C17—S4	111.33 (16)
C2—C3—C4	117.3 (2)	C16—C17—S4	118.29 (15)
C5—C4—C3	129.90 (19)	C17—C18—C19	111.1 (2)
C5—C4—S1	111.32 (17)	C17—C18—H18	124.4

C3—C4—S1	118.65 (17)	C19—C18—H18	124.4
C4—C5—C6	110.9 (2)	C20—C19—C18	113.2 (2)
C4—C5—H5	124.5	C20—C19—H19	123.4
C6—C5—H5	124.5	C18—C19—H19	123.4
C7—C6—C5	112.0 (3)	C19—C20—S4	112.3 (2)
C7—C6—H6	124.0	C19—C20—H20	123.9
C5—C6—H6	124.0	S4—C20—H20	123.9
C6—C7—S1	114.1 (2)	O4—C21—C22	122.99 (18)
C6—C7—H7	123.0	O4—C21—C14	119.72 (17)
S1—C7—H7	123.0	C22—C21—C14	117.27 (16)
O2—C8—C9	123.44 (19)	C23—C22—C21	129.21 (17)
O2—C8—C1	120.08 (19)	C23—C22—S5	111.39 (15)
C9—C8—C1	116.48 (17)	C21—C22—S5	119.35 (14)
C10—C9—C8	127.74 (19)	C22—C23—C24	112.33 (19)
C10—C9—S2	110.96 (16)	C22—C23—H23	123.8
C8—C9—S2	121.18 (15)	C24—C23—H23	123.8
C9—C10—C11	112.2 (2)	C25—C24—C23	112.0 (2)
C9—C10—H10	123.9	C25—C24—H24	124.0
C11—C10—H10	123.9	C23—C24—H24	124.0
C12—C11—C10	112.4 (2)	C24—C25—S5	112.74 (17)
C12—C11—H11	123.8	C24—C25—H25	123.6
C10—C11—H11	123.8	S5—C25—H25	123.6
C11—C12—S2	113.1 (2)	S6—C26—H26A	109.5
C11—C12—H12	123.4	S6—C26—H26B	109.5
S2—C12—H12	123.4	H26A—C26—H26B	109.5
S3—C13—H13A	109.5	S6—C26—H26C	109.5
S3—C13—H13B	109.5	H26A—C26—H26C	109.5
H13A—C13—H13B	109.5	H26B—C26—H26C	109.5
S3—C13—H13C	109.5	C7—S1—C4	91.68 (13)
H13A—C13—H13C	109.5	C12—S2—C9	91.37 (12)
H13B—C13—H13C	109.5	C1—S3—C13	102.81 (12)
C15—C14—C21	118.14 (17)	C20—S4—C17	92.08 (12)
C15—C14—S6	124.49 (15)	C25—S5—C22	91.55 (10)
C21—C14—S6	117.31 (14)	C14—S6—C26	103.40 (11)
C8—C1—C2—C3	−177.6 (2)	C16—C17—C18—C19	−178.5 (2)
S3—C1—C2—C3	0.5 (3)	S4—C17—C18—C19	0.4 (3)
C1—C2—C3—O1	4.3 (4)	C17—C18—C19—C20	−1.1 (4)
C1—C2—C3—C4	−175.8 (2)	C18—C19—C20—S4	1.3 (4)
O1—C3—C4—C5	165.1 (2)	C15—C14—C21—O4	−101.2 (2)
C2—C3—C4—C5	−14.8 (4)	S6—C14—C21—O4	76.3 (2)
O1—C3—C4—S1	−10.4 (3)	C15—C14—C21—C22	80.2 (2)
C2—C3—C4—S1	169.69 (17)	S6—C14—C21—C22	−102.33 (18)
C3—C4—C5—C6	−175.1 (2)	O4—C21—C22—C23	−177.7 (2)
S1—C4—C5—C6	0.7 (3)	C14—C21—C22—C23	0.8 (3)
C4—C5—C6—C7	−0.7 (3)	O4—C21—C22—S5	−0.2 (3)
C5—C6—C7—S1	0.4 (3)	C14—C21—C22—S5	178.31 (14)
C2—C1—C8—O2	98.6 (3)	C21—C22—C23—C24	177.5 (2)
S3—C1—C8—O2	−79.6 (3)	S5—C22—C23—C24	−0.2 (2)
C2—C1—C8—C9	−81.4 (3)	C22—C23—C24—C25	0.0 (3)

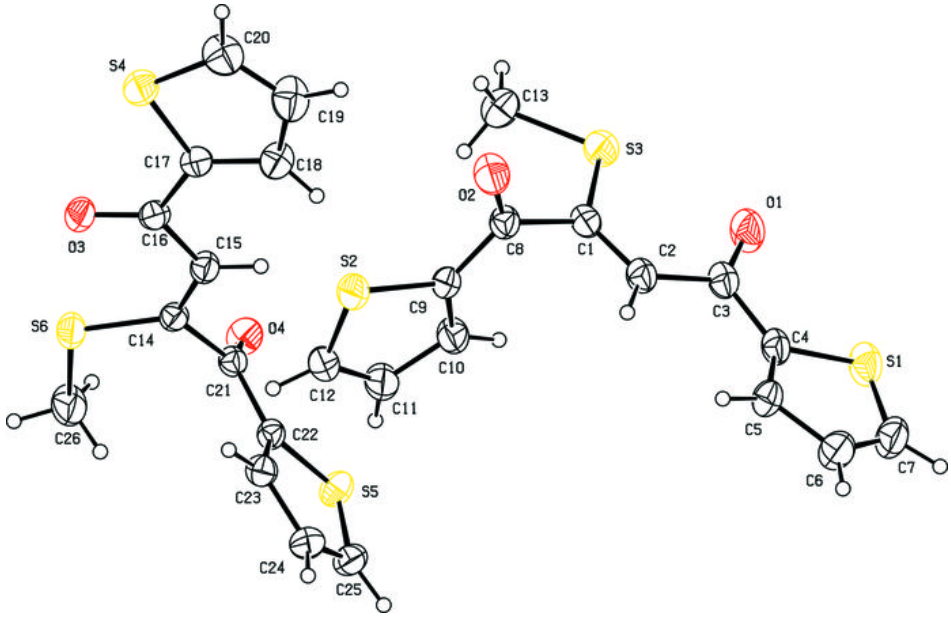
S3—C1—C8—C9	100.4 (2)	C23—C24—C25—S5	0.1 (3)
O2—C8—C9—C10	174.5 (2)	C6—C7—S1—C4	0.0 (2)
C1—C8—C9—C10	−5.5 (3)	C5—C4—S1—C7	−0.39 (19)
O2—C8—C9—S2	−1.2 (3)	C3—C4—S1—C7	175.9 (2)
C1—C8—C9—S2	178.76 (15)	C11—C12—S2—C9	0.7 (3)
C8—C9—C10—C11	−175.6 (2)	C10—C9—S2—C12	−0.7 (2)
S2—C9—C10—C11	0.5 (3)	C8—C9—S2—C12	175.7 (2)
C9—C10—C11—C12	0.1 (4)	C2—C1—S3—C13	169.9 (2)
C10—C11—C12—S2	−0.6 (4)	C8—C1—S3—C13	−12.07 (19)
C21—C14—C15—C16	173.87 (18)	C19—C20—S4—C17	−0.9 (2)
S6—C14—C15—C16	−3.4 (3)	C18—C17—S4—C20	0.30 (19)
C14—C15—C16—O3	0.9 (3)	C16—C17—S4—C20	179.33 (18)
C14—C15—C16—C17	−177.61 (19)	C24—C25—S5—C22	−0.19 (19)
O3—C16—C17—C18	169.2 (2)	C23—C22—S5—C25	0.21 (17)
C15—C16—C17—C18	−12.3 (3)	C21—C22—S5—C25	−177.70 (17)
O3—C16—C17—S4	−9.7 (3)	C15—C14—S6—C26	−178.4 (2)
C15—C16—C17—S4	168.90 (15)	C21—C14—S6—C26	4.32 (19)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O4^{i}	0.93	2.52	3.448 (3)	172
C5—H5···O4^{i}	0.93	2.54	3.416 (3)	157
C20—H20···O4^{ii}	0.93	2.54	3.438 (3)	162

Symmetry codes: (i) *x*, *y*, *z*+1; (ii) *x*+1, *y*, *z*+1.

Fig. 1


C20
S4
C19
C17
C18
O3
C16
C15
S6
C14
O4
C21
C26
C22
C23
S5
C24
C25
C13
S3
O2
C8
C1
C2
O1
S2
C9
C3
C4
S1
C10
C12
C11
C5
C6
C7