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1,2-Bis(3-methyl-2-thienyl)ethane-1,2-dione

Stefanie A. Cantalupo and Guy Crundwell*

Department of Chemistry, Central Connecticut State University, New Britain, CT 06053, USA

Correspondence e-mail: crundwellg@mail.ccsu.edu

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Key indicators

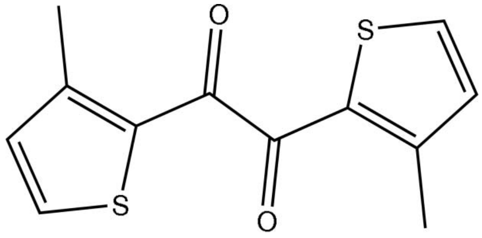
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.047
wR factor = 0.052
Data-to-parameter ratio = 10.2

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

The molecule of the title compound, $C_{12}H_{10}O_2S_2$, is disposed about a centre of inversion and is essentially planar.

Comment

We have investigated the crystal structures of 2- and 3-thenils (Crundwell, Sullivan *et al.*, 2003), as well as bromo-substituted 2-thenils which, along with other benzil analogs, have been shown to inhibit liver carboxylesterases (Hyatt *et al.*, 2005). The structural similarities between thenils and benzil have led our laboratory to investigate inclusion of thienyl-containing guest molecules into growing benzil crystals and the resulting effects on benzil crystal morphology. Ethanediones are also reactants used by our laboratories to make 2,3-disubstituted quinoxalines (Crundwell, Sayers *et al.*, 2003) and tetra-substituted cyclopentadienones (Linehan *et al.*, 2003). As a part of this program, the structure of the title compound, (I), was determined.



(I)

The molecule of (I) (Fig. 1) sits on an inversion center and is planar. The S atom in the thienyl ring is *trans* to the nearest keto O atom. All bond lengths and angles (Table 1) are in agreement with those of other published thienyl-containing compounds and thienyl ring geometries, and difference maps show no evidence of thienyl ring flip disorders. The molecular geometry is analogous to that of 2,2′-thenil, which also packs in a completely planar configuration (Crundwell, Sullivan *et al.*, 2003).

Experimental

The title compound was purchased from Acros Chemicals and was recrystallized from many solvents in attempts to grow crystals suitable for diffraction studies. Slow evaporation from a ethanol solution of the compound, over a period of three weeks, yielded the best crystals. A small, laminar, yellow plate that displayed homogeneous birefringence was mounted for diffraction studies. ^{1}H NMR and UV–vis spectroscopies as well as melting points of the title compound agree with literature values (Lee *et al.*, 1995).

Crystal data

$C_{12}H_{10}O_2S_2$
$M_r = 250.34$
Monoclinic, $P2_1/n$
$a = 9.605$ (3) Å
$b = 5.0901$ (16) Å
$c = 12.193$ (4) Å
$\beta = 101.37$ (2)°
$V = 584.4$ (3) Å^3
$Z = 2$

$D_x = 1.423$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3871 reflections
$\theta = 3.7$–$29.6°$
$\mu = 0.44$ mm^{-1}
$T = 293$ K
Plate, yellow
0.26 × 0.15 × 0.01 mm

Data collection

Oxford Diffraction Sapphire3 diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{\min} = 0.865$, $T_{\max} = 1$
3871 measured reflections

1452 independent reflections
743 reflections with $I > 3\sigma(I)$
$R_{\rm int} = 0.051$
$\theta_{\max} = 29.7°$
$h = -13 \rightarrow 13$
$k = -6 \rightarrow 6$
$l = -15 \rightarrow 14$

Refinement

Refinement on F
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.052$
$S = 1.13$
743 reflections
73 parameters
H-atom parameters constrained
$w = [1 - (F_o - F_c)^2/36\sigma^2(F_o)]^2/[0.352T_0(x) + 0.362T_1(x) + 0.186T_2(x) + 0.0821T_3(x)]$, where $T_i(x)$ are Chebychev polynomials and $x = F_c/F_{\max}$ (Watkin, 1994; Prince, 1982)
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.21$ e Å^{-3}
$\Delta\rho_{\min} = -0.23$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C2	1.741 (3)	C1—C1$^{\rm i}$	1.542 (6)
S1—C5	1.701 (4)	C3—C4	1.405 (5)
C2—C1	1.468 (5)	C3—C6	1.511 (5)
C2—C3	1.394 (5)	C4—C5	1.370 (5)
O1—C1	1.227 (4)		
C2—S1—C5	91.31 (17)	C2—C1—O1	121.4 (3)
S1—C2—C1	123.6 (2)	C2—C3—C4	111.8 (3)
S1—C2—C3	111.1 (3)	C2—C3—C6	125.9 (3)
C1—C2—C3	125.3 (3)	C6—C3—C4	122.3 (3)
C1$^{\rm i}$—C1—O1	119.3 (4)	C3—C4—C5	113.2 (3)
C1$^{\rm i}$—C1—C2	119.3 (3)	S1—C5—C4	112.6 (3)

Symmetry code: (i) $-x + 2, -y + 1, -z + 1$.

Owing to the thin nature of the crystal, *SADABS* (Sheldrick, 2003) was applied to the data in order to account for absorption effects. The nature of the crystal also had the consequence that $\theta_{\max}$ was only 22.3°. H atoms were constrained during refinement at ideal locations so that C—H = 0.93 Å (aromatic H) and 0.096 Å (methyl H), and with $U_{\rm iso}$(H) = 0.05 Å^2.

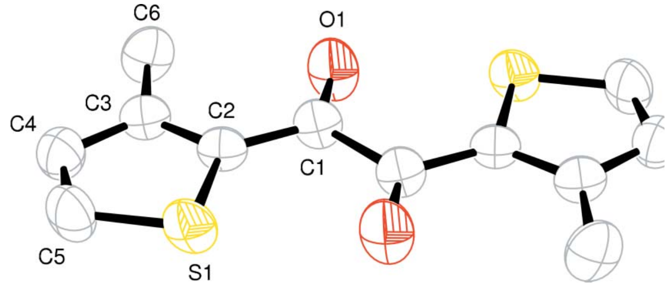


Figure 1
A view of (I); displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2005); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2005); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CRYSTALS*.

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