

## (2Z,3E)-2,3-Bis(2-thienylmethylene)-succinic acid methanol hemisolvate

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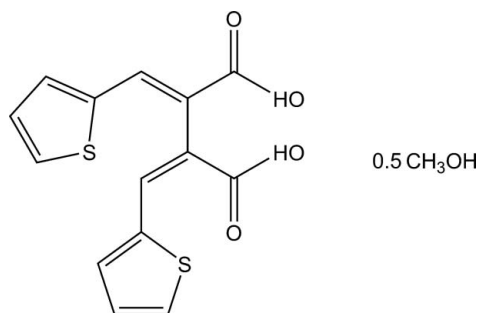
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Key indicators: single-crystal X-ray study;  $T = 290$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å; disorder in solvent or counterion;  $R$  factor = 0.072;  $wR$  factor = 0.233; data-to-parameter ratio = 14.7.

In the title compound,  $\text{C}_{14}\text{H}_{10}\text{O}_4\text{S}_2 \cdot 0.5\text{CH}_3\text{OH}$ , the molecule adopts a *gauche* conformation around the central C—C bond. Intermolecular O—H...O hydrogen bonds between carboxyl groups link the molecules into zigzag chains. Between chains, the thiophene rings form  $\pi$ — $\pi$  stacking interactions with a centroid—centroid distance of 3.98 Å. The methanol solvent molecule forms an O—H...O hydrogen bond to one carboxyl group and is disordered about a crystallographic centre of inversion.

### Related literature

For related literature, see: Abdel-Wahhab & El-Rayyes (1971); Bonham & Momany (1963); Nakanishi *et al.* (1970); Vasu (2007); Windholz (1976).



### Experimental

#### Crystal data

$\text{C}_{14}\text{H}_{10}\text{O}_4\text{S}_2 \cdot 0.5\text{CH}_4\text{O}$   
 $M_r = 322.36$   
Monoclinic,  $C2/c$   
 $a = 15.042$  (7) Å  
 $b = 13.295$  (6) Å

$c = 16.219$  (7) Å  
 $\beta = 101.792$  (7)°  
 $V = 3175$  (2) Å<sup>3</sup>  
 $Z = 8$   
Mo  $K\alpha$  radiation

$\mu = 0.35$  mm<sup>-1</sup>  
 $T = 290$  (2) K

0.25 × 0.20 × 0.15 mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.902$ ,  $T_{\max} = 0.950$   
14721 measured reflections  
2783 independent reflections  
2407 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.029$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.072$   
 $wR(F^2) = 0.233$   
 $S = 1.12$   
2783 reflections  
189 parameters  
1 restraint  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 1.01$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.31$  e Å<sup>-3</sup>

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

D—H...A	D—H	H...A	D...A	D—H...A
O5—H5O...O1	0.82	2.06	2.88 (2)	171
O3—H3O...O1 <sup>i</sup>	0.82	1.84	2.650 (3)	168
O2—H2O...O2 <sup>ii</sup>	0.82	1.81	2.620 (5)	167
O4—H4O...O4 <sup>ii</sup>	0.82	1.83	2.624 (5)	164

Symmetry codes: (i)  $-x + \frac{1}{2}, -y + \frac{3}{2}, -z$ ; (ii)  $-x + 1, y, -z + \frac{1}{2}$ .

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SIR92 (Altomare *et al.*, 1993); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1999) and CAMERON (Pearce *et al.*, 1993); software used to prepare material for publication: PLATON (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2212).

### References

- Abdel-Wahhab, S. M. & El-Rayyes, N. R. (1971). *J. Chem. Soc. C*, pp. 3171–3173.  
Altomare, A., Casciarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.  
Bonham, R. A. & Momany, F. A. (1963). *J. Phys. Chem.* **67**, 2474–2477.  
Bruker (2000). SMART (Version 5.628) and SAINT (Version 6.45a). Bruker AXS Inc., Madison, Wisconsin, USA.  
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.  
Nakanishi, M., Emamura, H. & Maruyama, Y. (1970). *Arzneim. Forsch. (Drug. Res.)*, **20**, 998–1002.  
Pearce, L., Watkin, D. J. & Prout, C. K. (1993). CAMERON. Chemical Crystallography Laboratory, University of Oxford, England.  
Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.  
Sheldrick, G. M. (1997). SHELXL97. University of Göttingen, Germany.  
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.  
Vasu (2007). PhD Thesis, Bangalore University.  
Windholz, M. (1976). *Merck Index*, 9th ed., pp. 1147–1149. Boca Raton: Merck & Co Inc.

**supplementary materials**

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## (2*Z*,3*E*)-2,3-Bis(2-thienylmethylene)succinic acid methanol hemisolvate

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### Comment

Compounds containing the succinyl group are known for their promising biological activities. Succinyl peroxide is used as a germicide and antiseptic. Compounds such as succinylsulfathiazole and succisulfone exhibit antibacterial activity (Windholz, 1976). Amongst heterocyclic systems, thiophene derivatives exhibit diversity in biological applications, namely antibacterial, anti-inflammatory and antifungal activities (Nakanishi *et al.*, 1970). The crystal and molecular structures of thiophene-containing compounds have recently been analyzed in detail (Vasu, 2007).

The title molecule (Fig. 1) is non-planar. It is evident from the torsion angles C10/C7/C6/C5 = 77.3 (4)° and C9/C6/C7/C8 = 73.6 (4)° that the thiophene rings and the carboxyl groups exist in a *gauche* arrangement. The thiophene bond lengths and bond angles are similar to those in unsubstituted thiophene (Bonham & Momany, 1963). The C6—C7 bond length [1.492 (4) Å] is slightly shorter than a typical single bond, suggesting the possibility of extended conjugation.

The crystal structure contains O—H···O carboxylic acid dimers, which link the molecules into zigzag chains. Between these chains,  $\pi$ - $\pi$  stacking interactions are formed involving the thiophene ring [S1/C1—C4], with a centroid-centroid distance of 3.98 Å (Fig. 2) [symmetry code:  $-x + 1, y, -z + 1/2$ ]. The methanol solvent molecule forms an O—H···O hydrogen bond to one carboxylic acid group, and is disordered over two equivalent sites.

### Experimental

The compound was made in accordance with the literature procedure (Abdel-Wahhab & El-Rayyes, 1971) and was recrystallized from methanol.

### Refinement

H atoms bound to C atoms were placed in calculated positions with C—H = 0.93–0.96 Å and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2$  or  $1.5 U_{\text{eq}}(\text{C})$ . The H atoms of the carboxyl groups were placed so as to form the best hydrogen bond (AFIX 83) with O—H = 0.82 Å, and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$ . In the case of C9/O1/O3, the hydrogen-bonded dimer is formed about a centre of inversion and the hydroxyl group could be distinguished by the longer C9—O3 bond length. For C8/O2/O4, the hydrogen bonded dimer is formed about a 2-fold rotation axis and the C8—O2 and C8—O4 bonds do not differ significantly, requiring the H atom to be disordered equally over atoms O2 and O4. The methanol molecule forms a hydrogen bond to the C9=O1 group, and atom H50 was placed along the O50···O1 vector with O—H = 0.82 Å and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$ . The methanol molecule is disordered equally over two equivalent sites related by a centre of inversion, with the C—O distance restrained to be 1.40 (1) Å.

## Figures

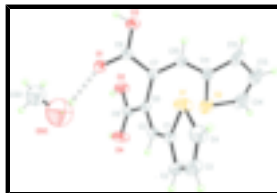


Fig. 1. Molecular structure of the title compound showing displacement ellipsoids at 30% probability for non-H atoms. The dashed line indicates an O—H...O hydrogen bond.

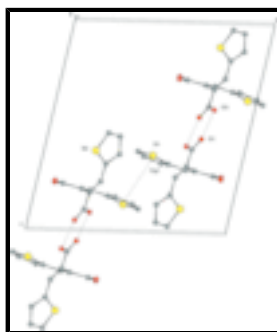


Fig. 2. Partial packing diagram of the title compound showing the  $\pi$ - $\pi$  stacking interaction between adjacent [S1/C1-C4] rings. The centroids (denoted Cg1) are joined by dotted lines.

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### Crystal data

$C_{14}H_{10}O_4S_2 \cdot 0.5CH_4O$

$M_r = 322.36$

Monoclinic,  $C2/c$

Hall symbol:  $-C\ 2yc$

$a = 15.042\ (7)\ \text{\AA}$

$b = 13.295\ (6)\ \text{\AA}$

$c = 16.219\ (7)\ \text{\AA}$

$\beta = 101.792\ (7)^\circ$

$V = 3175\ (2)\ \text{\AA}^3$

$Z = 8$

$F_{000} = 1336$

$D_x = 1.349\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 560 reflections

$\theta = 1.4\text{--}26.4^\circ$

$\mu = 0.35\ \text{mm}^{-1}$

$T = 290\ (2)\ \text{K}$

Block, yellow

$0.25 \times 0.20 \times 0.15\ \text{mm}$

### Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 290\ (2)\ \text{K}$

$\phi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.902$ ,  $T_{\max} = 0.950$

14721 measured reflections

2783 independent reflections

2407 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 25.0^\circ$

$\theta_{\min} = 2.1^\circ$

$h = -17 \rightarrow 17$

$k = -15 \rightarrow 15$

$l = -19 \rightarrow 19$

*Refinement*

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.072$	H-atom parameters constrained
$wR(F^2) = 0.233$	$w = 1/[\sigma^2(F_o^2) + (0.1453P)^2 + 4.5426P]$
$S = 1.12$	where $P = (F_o^2 + 2F_c^2)/3$
2783 reflections	$(\Delta/\sigma)_{\max} < 0.001$
189 parameters	$\Delta\rho_{\max} = 1.01 \text{ e } \text{\AA}^{-3}$
1 restraint	$\Delta\rho_{\min} = -0.31 \text{ e } \text{\AA}^{-3}$
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  $F^2 > 2\sigma(F^2)$  is used only for calculating  $R$ -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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
S1	0.04546 (7)	0.51459 (8)	0.13193 (8)	0.0698 (4)	
S2	0.24373 (9)	0.57706 (9)	0.38316 (7)	0.0762 (4)	
O1	0.2673 (2)	0.63802 (19)	0.05018 (16)	0.0654 (8)	
O2	0.41114 (17)	0.62150 (18)	0.22940 (18)	0.0600 (7)	
H2O	0.4661	0.6119	0.2424	0.090*	0.50
O3	0.2015 (2)	0.7757 (2)	0.08846 (18)	0.0820 (10)	
H3O	0.2083	0.7946	0.0420	0.123*	
O4	0.41109 (17)	0.45447 (18)	0.2387 (2)	0.0704 (9)	
H4O	0.4660	0.4646	0.2508	0.106*	0.50
C1	0.1300 (2)	0.4297 (2)	0.1708 (2)	0.0440 (7)	
C2	0.0941 (3)	0.3337 (3)	0.1680 (3)	0.0592 (9)	
H2	0.1288	0.2768	0.1857	0.071*	
C3	0.0010 (3)	0.3306 (3)	0.1359 (3)	0.0698 (11)	
H3	-0.0332	0.2718	0.1307	0.084*	
C4	-0.0342 (3)	0.4212 (4)	0.1134 (3)	0.0747 (12)	
H4	-0.0952	0.4323	0.0903	0.090*	
C5	0.2252 (2)	0.4518 (2)	0.19699 (19)	0.0416 (7)	

## supplementary materials

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H5	0.2617	0.3959	0.2134	0.050*	
C6	0.2700 (2)	0.5393 (2)	0.20167 (19)	0.0402 (7)	
C7	0.2259 (2)	0.6395 (2)	0.18277 (19)	0.0402 (7)	
C8	0.3698 (2)	0.5376 (2)	0.2245 (2)	0.0456 (8)	
C9	0.2323 (2)	0.6863 (2)	0.1019 (2)	0.0482 (8)	
C10	0.1832 (2)	0.6901 (2)	0.2356 (2)	0.0437 (7)	
H10	0.1527	0.7481	0.2137	0.052*	
C11	0.1786 (2)	0.6665 (2)	0.3211 (2)	0.0503 (8)	
C12	0.1206 (4)	0.7246 (3)	0.3669 (3)	0.0761 (13)	
H12	0.0806	0.7761	0.3455	0.091*	
C13	0.1383 (5)	0.6852 (4)	0.4523 (3)	0.0934 (18)	
H13	0.1089	0.7096	0.4934	0.112*	
C14	0.2006 (4)	0.6106 (4)	0.4678 (3)	0.0879 (16)	
H14	0.2182	0.5803	0.5203	0.105*	
C50	0.4751 (10)	0.5542 (11)	0.0075 (10)	0.122 (4)*	0.50
H50A	0.4454	0.5847	-0.0445	0.184*	0.50
H50B	0.5201	0.5075	-0.0032	0.184*	0.50
H50C	0.5038	0.6054	0.0456	0.184*	0.50
O50	0.4124 (13)	0.5001 (14)	0.0413 (13)	0.233 (8)*	0.50
H50	0.3689	0.5348	0.0468	0.349*	0.50

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0508 (6)	0.0504 (6)	0.1032 (9)	0.0079 (4)	0.0038 (5)	0.0053 (5)
S2	0.1012 (9)	0.0771 (8)	0.0530 (7)	-0.0035 (6)	0.0217 (6)	0.0110 (5)
O1	0.101 (2)	0.0519 (15)	0.0530 (14)	0.0236 (14)	0.0386 (14)	0.0142 (11)
O2	0.0514 (14)	0.0375 (13)	0.0911 (19)	-0.0048 (10)	0.0145 (12)	0.0030 (12)
O3	0.138 (3)	0.0505 (16)	0.0713 (18)	0.0392 (17)	0.0534 (18)	0.0279 (13)
O4	0.0459 (14)	0.0369 (13)	0.124 (3)	0.0054 (10)	0.0060 (14)	0.0080 (14)
C1	0.0482 (17)	0.0401 (16)	0.0459 (17)	0.0012 (13)	0.0149 (13)	0.0058 (13)
C2	0.057 (2)	0.0457 (18)	0.075 (2)	-0.0067 (16)	0.0145 (18)	0.0125 (17)
C3	0.058 (2)	0.066 (2)	0.086 (3)	-0.0200 (19)	0.017 (2)	0.007 (2)
C4	0.046 (2)	0.077 (3)	0.099 (3)	-0.0014 (19)	0.009 (2)	0.002 (2)
C5	0.0464 (16)	0.0330 (15)	0.0463 (17)	0.0059 (12)	0.0119 (13)	0.0062 (12)
C6	0.0473 (17)	0.0333 (14)	0.0419 (16)	0.0031 (12)	0.0132 (13)	0.0059 (12)
C7	0.0470 (16)	0.0323 (14)	0.0430 (16)	0.0003 (12)	0.0138 (13)	0.0037 (12)
C8	0.0472 (17)	0.0348 (16)	0.0559 (19)	0.0017 (13)	0.0126 (14)	0.0028 (13)
C9	0.064 (2)	0.0372 (16)	0.0470 (17)	0.0094 (14)	0.0199 (15)	0.0074 (13)
C10	0.0489 (17)	0.0320 (15)	0.0531 (18)	-0.0015 (12)	0.0174 (14)	0.0019 (13)
C11	0.063 (2)	0.0427 (17)	0.0512 (18)	-0.0132 (15)	0.0260 (15)	-0.0065 (14)
C12	0.119 (4)	0.064 (2)	0.059 (2)	-0.038 (2)	0.049 (2)	-0.0141 (19)
C13	0.146 (5)	0.083 (3)	0.067 (3)	-0.033 (4)	0.059 (3)	-0.022 (2)
C14	0.134 (5)	0.084 (3)	0.052 (2)	-0.030 (3)	0.034 (3)	-0.001 (2)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

S1—C4	1.708 (5)	C5—H5	0.930
S1—C1	1.721 (3)	C6—C8	1.470 (5)

S2—C14	1.693 (5)	C6—C7	1.492 (4)
S2—C11	1.728 (4)	C7—C10	1.351 (4)
O1—C9	1.254 (4)	C7—C9	1.472 (4)
O2—C8	1.272 (4)	C10—C11	1.436 (5)
O2—H2O	0.820	C10—H10	0.930
O3—C9	1.278 (4)	C11—C12	1.475 (6)
O3—H3O	0.820	C12—C13	1.454 (7)
O4—C8	1.266 (4)	C12—H12	0.930
O4—H4O	0.820	C13—C14	1.353 (8)
C1—C2	1.383 (5)	C13—H13	0.930
C1—C5	1.437 (5)	C14—H14	0.930
C2—C3	1.392 (6)	C50—O50	1.384 (9)
C2—H2	0.930	C50—H50A	0.960
C3—C4	1.336 (6)	C50—H50B	0.960
C3—H3	0.930	C50—H50C	0.960
C4—H4	0.930	O50—H50	0.820
C5—C6	1.340 (4)		
C4—S1—C1	91.6 (2)	O4—C8—C6	119.8 (3)
C14—S2—C11	91.5 (3)	O2—C8—C6	117.6 (3)
C8—O2—H2O	109.5	O1—C9—O3	123.2 (3)
C9—O3—H3O	109.5	O1—C9—C7	119.5 (3)
C8—O4—H4O	109.5	O3—C9—C7	117.2 (3)
C2—C1—C5	123.8 (3)	C7—C10—C11	128.8 (3)
C2—C1—S1	109.8 (3)	C7—C10—H10	115.6
C5—C1—S1	126.3 (2)	C11—C10—H10	115.6
C1—C2—C3	113.3 (3)	C10—C11—C12	121.5 (3)
C1—C2—H2	123.3	C10—C11—S2	125.4 (3)
C3—C2—H2	123.3	C12—C11—S2	113.0 (3)
C4—C3—C2	112.8 (4)	C13—C12—C11	106.2 (5)
C4—C3—H3	123.6	C13—C12—H12	126.9
C2—C3—H3	123.6	C11—C12—H12	126.9
C3—C4—S1	112.5 (3)	C14—C13—C12	115.2 (4)
C3—C4—H4	123.7	C14—C13—H13	122.4
S1—C4—H4	123.7	C12—C13—H13	122.4
C6—C5—C1	130.8 (3)	C13—C14—S2	114.1 (4)
C6—C5—H5	114.6	C13—C14—H14	122.9
C1—C5—H5	114.6	S2—C14—H14	122.9
C5—C6—C8	118.5 (3)	O50—C50—H50A	109.6
C5—C6—C7	124.5 (3)	O50—C50—H50B	107.3
C8—C6—C7	117.0 (3)	O50—C50—H50C	111.5
C10—C7—C9	118.7 (3)	H50A—C50—H50B	109.5
C10—C7—C6	124.3 (3)	H50A—C50—H50C	109.5
C9—C7—C6	116.9 (3)	H50B—C50—H50C	109.5
O4—C8—O2	122.6 (3)	C50—O50—H50	112.0
C4—S1—C1—C2	0.1 (3)	C5—C6—C8—O2	-179.4 (3)
C4—S1—C1—C5	175.9 (3)	C7—C6—C8—O2	2.3 (4)
C5—C1—C2—C3	-176.4 (3)	C10—C7—C9—O1	-176.1 (3)
S1—C1—C2—C3	-0.5 (4)	C6—C7—C9—O1	5.6 (5)

## supplementary materials

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C1—C2—C3—C4	0.9 (6)	C10—C7—C9—O3	4.1 (5)
C2—C3—C4—S1	-0.8 (6)	C6—C7—C9—O3	-174.1 (3)
C1—S1—C4—C3	0.4 (4)	C9—C7—C10—C11	-171.1 (3)
C2—C1—C5—C6	178.7 (3)	C6—C7—C10—C11	7.0 (5)
S1—C1—C5—C6	3.5 (5)	C7—C10—C11—C12	-173.4 (3)
C1—C5—C6—C8	-175.0 (3)	C7—C10—C11—S2	11.6 (5)
C1—C5—C6—C7	3.1 (5)	C14—S2—C11—C10	175.0 (3)
C5—C6—C7—C10	77.3 (4)	C14—S2—C11—C12	-0.3 (3)
C8—C6—C7—C10	-104.5 (4)	C10—C11—C12—C13	-175.7 (3)
C5—C6—C7—C9	-104.5 (4)	S2—C11—C12—C13	-0.1 (4)
C8—C6—C7—C9	73.6 (4)	C11—C12—C13—C14	0.7 (6)
C5—C6—C8—O4	0.4 (5)	C12—C13—C14—S2	-1.1 (6)
C7—C6—C8—O4	-177.8 (3)	C11—S2—C14—C13	0.8 (4)

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O50—H50 $\cdots$ O1	0.82	2.06	2.88 (2)	171
O3—H3O $\cdots$ O1 <sup>i</sup>	0.82	1.84	2.650 (3)	168
O2—H2O $\cdots$ O2 <sup>ii</sup>	0.82	1.81	2.620 (5)	167
O4—H4O $\cdots$ O4 <sup>ii</sup>	0.82	1.83	2.624 (5)	164

Symmetry codes: (i)  $-x+1/2, -y+3/2, -z$ ; (ii)  $-x+1, y, -z+1/2$ .



Fig. 1

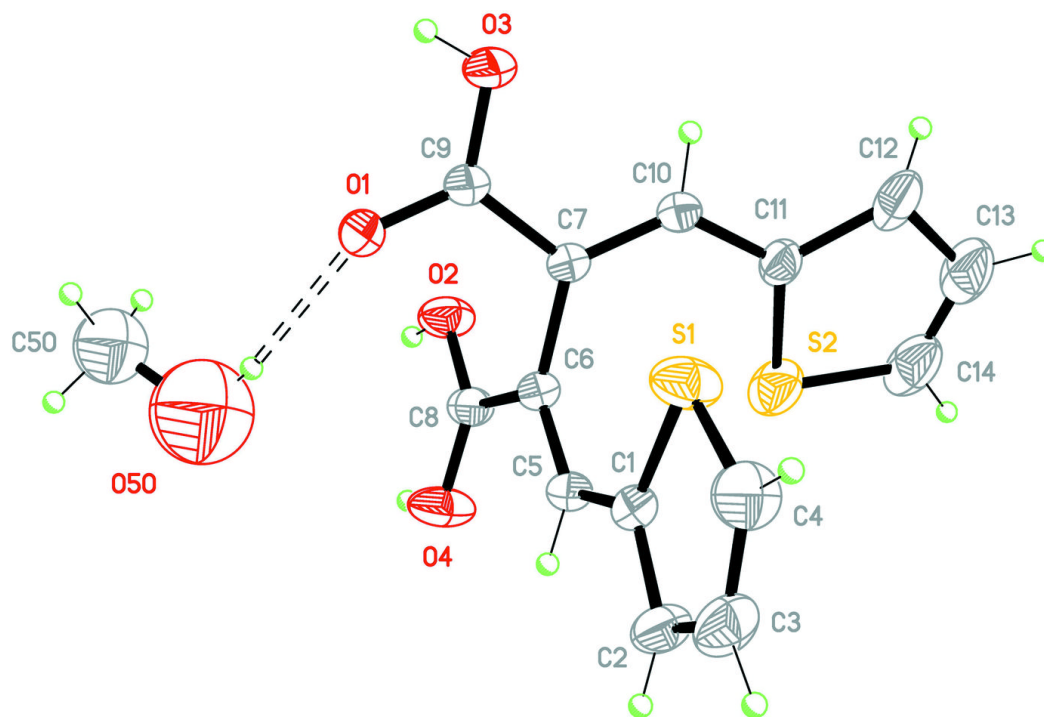


Fig. 2

