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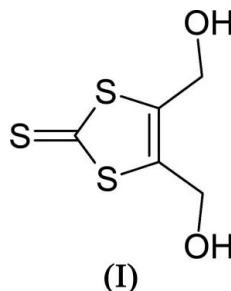
Key indicators

Single-crystal X-ray study
 $T = 180$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
Disorder in main residue
 R factor = 0.036
 wR factor = 0.082
Data-to-parameter ratio = 17.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

4,5-Bis(hydroxymethyl)-1,3-dithiole-2-thione

At 180 K, the title compound, $\text{C}_5\text{H}_6\text{O}_2\text{S}_3$, forms a three-dimensional hydrogen-bonded network in which the H atoms of the hydroxyl groups are disordered.Received 27 March 2006
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Comment

At 180 K, the crystal structure of the title compound, (I) (Fig. 1), contains planar 1,3-dithiole-2-thione units, with the O atom of one hydroxyl group (O1) lying approximately within this plane [torsion angle $\text{C}3-\text{C}2-\text{C}4-\text{O}1 = 169.8$ (2°)]. The O atom of the other hydroxyl group (O2) lies out of the plane, forming a $\text{C}2-\text{C}3-\text{C}5-\text{O}2$ torsion angle of -139.3 (2°).Adjacent molecules adopt centrosymmetric face-to-face arrangements, with a perpendicular interplanar separation of 3.56 (1) Å and no lateral offset (*i.e.* the vector joining the two centroids lies normal to the ring planes; Fig. 2).

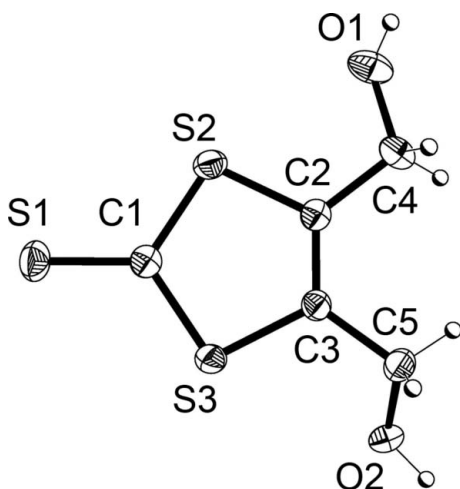
Both O1 and O2 lie in environments where two neighbouring hydroxyl groups offer potential hydrogen-bond acceptors (Table 1). The H atoms of the hydroxyl groups (located in difference Fourier maps) are disordered over two positions, in accordance with the two possibilities for hydrogen-bond formation. The resulting hydrogen-bond network (Fig. 3) is three-dimensional.

Experimental

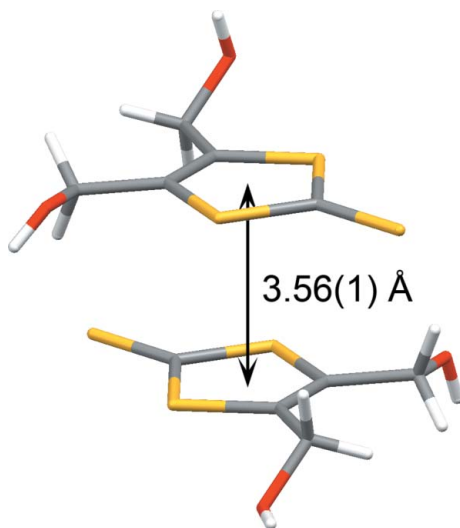
The title compound was prepared according to the literature procedure of Jeppesen *et al.* (1999). Recrystallization from CH_2Cl_2 -ethyl acetate (1:1) afforded yellow blocks of (I).

Crystal data

$\text{C}_5\text{H}_6\text{O}_2\text{S}_3$	$Z = 8$
$M_r = 194.28$	$D_x = 1.673$ Mg m $^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 13.7118$ (7) Å	$\mu = 0.89$ mm $^{-1}$
$b = 8.9540$ (5) Å	$T = 180$ (2) K
$c = 12.8244$ (6) Å	Block, yellow
$\beta = 101.558$ (2°)	$0.40 \times 0.40 \times 0.25$ mm
$V = 1542.59$ (14) Å 3	

**Figure 1**

The molecular unit of (I), showing displacement ellipsoids at the 50% probability level. H atoms are shown as spheres of arbitrary radii. Only one H-atom position is shown on each O atom.

**Figure 2**

Pairs of molecules forming centrosymmetric face-to-face arrangements. Only one H-atom position is shown on each O atom.

Data collection

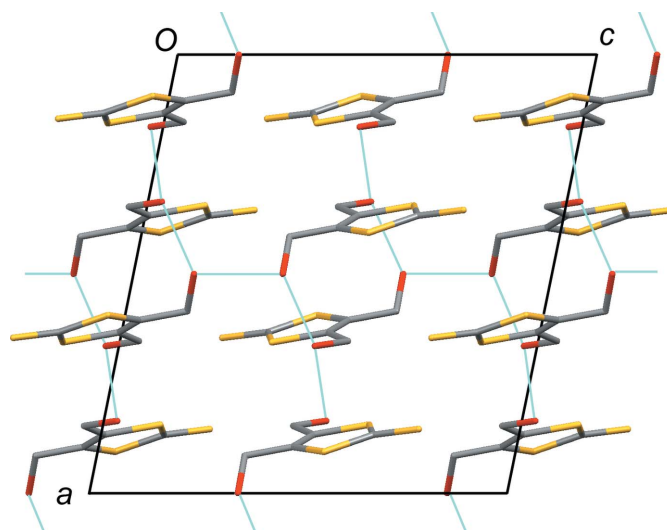
Bruker Nonius X8 APEX-II CCD
area-detector diffractometer
thin-slice ω and φ scans
Absorption correction: multi-scan
(SADABS; Sheldrick, 2003)
 $T_{\min} = 0.713$, $T_{\max} = 0.808$

9611 measured reflections
1894 independent reflections
1770 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$
 $\theta_{\text{max}} = 28.3^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.082$
 $S = 1.36$
1894 reflections
107 parameters

H atoms treated by a mixture of
independent and constrained
refinement
 $w = 1/[\sigma^2(F_o^2) + 4.478P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.37 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\text{min}} = -0.36 \text{ e } \text{Å}^{-3}$

**Figure 3**

A view of the structure of (I), along b , showing the hydrogen-bonding network (thin green lines). H atoms have been omitted.

Table 1

Hydrogen-bond geometry (Å , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1-H1B\cdots O1^i$	0.84 (1)	1.80 (1)	2.641 (4)	172 (6)
$O1-H1A\cdots O2^{ii}$	0.84 (1)	1.86 (1)	2.692 (3)	171 (5)
$O2-H2A\cdots O1^{iii}$	0.84 (1)	1.86 (1)	2.692 (3)	171 (5)
$O2-H2B\cdots O2^{iii}$	0.84 (1)	1.93 (3)	2.722 (3)	154 (6)

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

H atoms bound to C atoms were positioned geometrically and allowed to ride during subsequent refinement, with $C-H = 0.99 \text{ Å}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The H atoms of the hydroxyl groups were visible in difference Fourier maps. They were modelled as disordered over two sites, each with 50% occupancy, and their positions and isotropic displacement parameters were refined, with all O-H distances restrained to $0.84 (1) \text{ Å}$.

Data collection: APEX2 (Bruker Nonius, 2004); cell refinement: SAINT (Bruker, 2003); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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References

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