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Key indicators

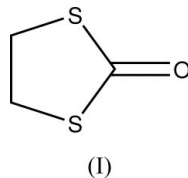
Single-crystal X-ray study
 $T = 110$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.020
 wR factor = 0.052
Data-to-parameter ratio = 15.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

1,3-Dithiolan-2-one

The title compound, $\text{C}_3\text{H}_4\text{OS}_2$, possesses pseudo-twofold symmetry and consists of a twisted five-membered ring of three C and two S atoms, with a ketone O atom in an equatorial position.

Comment

We report here, for the first time, the crystal and molecular structure of 1,3-dithiolan-2-one, (I). The molecule consists of a five-membered ring of three C and two S atoms, with a ketone O atom in an equatorial position (Fig. 1). Selected geometric parameters are given in Table 1.



Atoms O1, C1, S1 and S2 are in a distorted trigonal planar arrangement, but atoms C2 and C3 are in slightly distorted tetrahedral environments. The ring is in a twist (T) conformation, less typical of five-membered rings, with puckering parameters $\varphi = 127^\circ$ and $q = 0.431$ Å (Cremer & Pople, 1975). The puckering is best described by twisting the groups on C2 and C3 (Evans & Boeyens, 1989). The molecule has approximate C_2 symmetry. In the crystal structure, symmetry-related molecules are held together by very weak hydrogen bonds between the keto O atoms and the methylene H atoms (Fig. 2 and Table 2).

Experimental

The title compound, (I), was prepared by stirring a solution of vinylene trithiocarbonate (3.5 g) and mercuric acetate (19.4 g) in chloroform/acetic acid (3:1 v/v , 100 ml) under an atmosphere of N_2

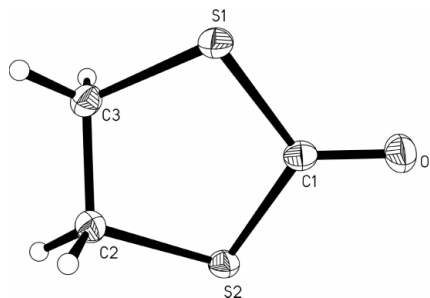


Figure 1
View of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as circles of arbitrary radius.

for 12 h. The solution was filtered in air through celite and washed with chloroform. The organic phases were refluxed under N_2 with activated charcoal for 2 h. The solution was filtered and washed with aqueous $NaHCO_3$ and dried over $MgSO_4$. The solution was allowed to evaporate and large crystals grew in the solution over a period of 5 d.

Crystal data

$C_3H_4OS_2$	$D_x = 1.687 \text{ Mg m}^{-3}$
$M_r = 120.18$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3398 reflections
$a = 8.0397 (16) \text{ \AA}$	$\theta = 2.0\text{--}27.5^\circ$
$b = 5.2020 (10) \text{ \AA}$	$\mu = 0.96 \text{ mm}^{-1}$
$c = 11.318 (2) \text{ \AA}$	$T = 110 (2) \text{ K}$
$\beta = 90.426 (4)^\circ$	Prism, light yellow
$V = 473.31 (16) \text{ \AA}^3$	$0.28 \times 0.24 \times 0.22 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART 1K CCD diffractometer	1078 independent reflections
ω scans	985 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2003)	$R_{\text{int}} = 0.024$
$T_{\text{min}} = 0.775$, $T_{\text{max}} = 0.817$	$\theta_{\text{max}} = 27.6^\circ$
3916 measured reflections	$h = -10 \rightarrow 10$
	$k = -5 \rightarrow 6$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.020$	$w = 1/[\sigma^2(F_o^2) + (0.0369P)^2]$
$wR(F^2) = 0.052$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{\text{max}} = 0.001$
1078 reflections	$\Delta\rho_{\text{max}} = 0.56 \text{ e \AA}^{-3}$
71 parameters	$\Delta\rho_{\text{min}} = -0.24 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

S1—C1	1.7725 (11)	S2—C2	1.8143 (12)
S1—C3	1.8128 (11)	O1—C1	1.2068 (14)
S2—C1	1.7779 (11)	C3—C2	1.5274 (15)
C1—S1—C3	96.60 (5)	S1—C1—S2	113.42 (6)
C1—S2—C2	96.57 (5)	C2—C3—S1	108.32 (7)
O1—C1—S1	124.10 (8)	C3—C2—S2	108.29 (8)
O1—C1—S2	122.48 (8)		

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C2-H2B\cdots O1^i$	0.965 (13)	2.635 (13)	3.3455 (14)	130.7 (10)
$C3-H3B\cdots O1^{ii}$	0.947 (15)	2.613 (15)	3.3342 (14)	133.3 (12)
$C3-H3A\cdots O1^{iii}$	0.948 (15)	2.635 (15)	3.5087 (15)	153.4 (11)

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

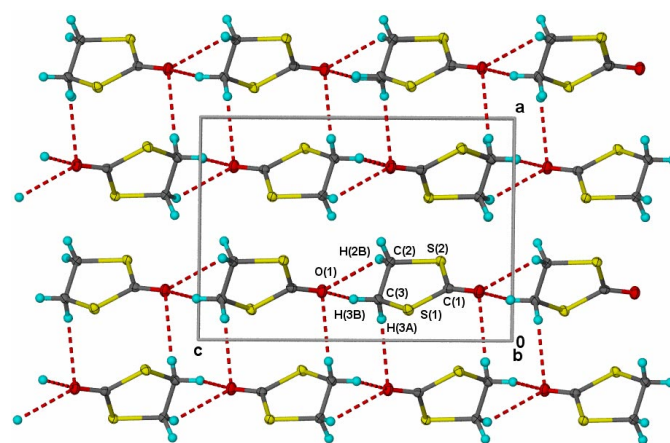


Figure 2

Projection of the molecular packing of (I) on the ac plane, showing the hydrogen bonding (dashed lines).

All the H atoms were located in difference electron-density maps and refined isotropically.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *X-SEED* (Barbour, 2001) and *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *PLATON* (Spek, 2003).

We gratefully acknowledge the service provided by Dr Joseph Reibenspies and the X-ray facility at Texas A&M University. We thank the National Science Foundation for PI and NIRT grants (CHE-9906583 and DMR-0103455) and for equipment grants for the CCD X-ray equipment (CHE-9807975). We thank the Department of Energy for a PI grant (DE-FG03-02ER45999). Support from the Welch Foundation (A-1449) and from a Telecommunications and Informatics Task Force (TITF) Grant from Texas A&M University is also gratefully acknowledged.

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