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Key indicators
Single-crystal X-ray study
T = 110 K
Mean σ(C–C) = 0.002 Å
R factor = 0.020
wR factor = 0.052
Data-to-parameter ratio = 15.2

1,3-Dithiolan-2-one

The title compound, C₃H₄OS₂, 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 N₂.

Received 11 June 2004
Accepted 14 June 2004
Online 19 June 2004

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.

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DOI: 10.1107/S1600536804014382
for 12 h. The solution was filtered in air through celite and washed with chloroform. The organic phases were refluxed under N₂ with activated charcoal for 2 h. The solution was filtered and washed with aqueous NaHCO₃ and dried over MgSO₄. The solution was allowed to evaporate and large crystals grew in the solution over a period of 5 d.

Crystal data

\[ \text{C}_{3}\text{H}_4\text{O}_2 \]

Monoclinic, \( P2_1/c \)

\( a = 8.0397 \) (16) Å

\( b = 5.2020 \) (10) Å

\( c = 11.318 \) (2) Å

\( \beta = 90.426 \) (4)°

\( V = 473.31 \) (16) Å³

\( Z = 4 \)

\( \mu = 0.96 \) mm⁻¹

\( T = 110 (2) \) K

\( \text{Mr} = 120.18 \)

Data collection

Bruker SMART 1K CCD diffractometer

Absorption correction: multi-scan

\( R_{	ext{int}} = 0.024 \)

\( h = -10 \rightarrow 10 \)

\( k = -5 \rightarrow 6 \)

\( l = -14 \rightarrow 14 \)

Refinement

Refinement on \( F^2 \)

\( R(F^2 > 2\sigma(F^2)) = 0.020 \)

\( wR(F) = 0.052 \)

\( S = 1.02 \)

1078 reflections

71 parameters

Table 1

Selected geometric parameters (Å, °).

<table>
<thead>
<tr>
<th></th>
<th>( D-H \cdot A )</th>
<th>( D-H \cdot A )</th>
<th>( D-A \cdot A )</th>
<th>( D-H \cdot A )</th>
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</thead>
<tbody>
<tr>
<td>C2-H2B 1 - O1’</td>
<td>0.965 (13)</td>
<td>2.635 (13)</td>
<td>3.3455 (14)</td>
<td>130.7 (10)</td>
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<tr>
<td>C3-H3B 1 - O1’</td>
<td>0.947 (15)</td>
<td>2.613 (15)</td>
<td>3.3342 (14)</td>
<td>133.3 (12)</td>
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<tr>
<td>C3-H3A 1 - O1’</td>
<td>0.948 (15)</td>
<td>2.635 (15)</td>
<td>3.5087 (15)</td>
<td>153.4 (11)</td>
</tr>
</tbody>
</table>

Symmetry codes: (i) \( x, -y, -z \); (ii) \( x, -y, -z \); (iii) \( -x, y, -z \).

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: SADABS (Bruker, 2003); data reduction: SAINT; 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.

References


