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Structure of 7-Thiabicyclo[4.2.1]nona-2,4-diene 7,7-Dioxide

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Abstract. $C_8H_{10}O_2S$, $M_r = 170{\cdot}23$, monoclinic, $P2_1/n$, $a = 11{\cdot}256\,(1)$, $b = 5{\cdot}951\,(1)$, $c = 13{\cdot}099\,(1)$ Å, $\beta = 114{\cdot}44\,(1)°$, $V = 798{\cdot}8\,(2)$ Å^3, $Z = 4$, $D_x = 1{\cdot}42$ g cm^{-3}, $\lambda(\text{Cu}\,K\alpha) = 1{\cdot}5418$ Å, $\mu = 31{\cdot}01$ cm^{-1}, $F(000) = 360$, $T = 293$ K, $R = 0{\cdot}063$ for 1003 unique observed $[I/\sigma(I) > 2{\cdot}0]$ reflections. This analysis confirms the earlier structural assignment. The significantly non-planar diene moiety, with torsion angle C(2)—C(3)—C(4)—C(5) −5·7 (7)°, exhibits marked opening of its angles C(1)—C(2)—C(3) 128·3 (6), C(2)—C(3)—C(4) 129·6 (6), C(3)—C(4)—C(5) 129·6 (6) and C(4)—C(5)—C(6) 126·3 (6)°. The conformation of the five-membered ring in the crystal is characterized by torsion angle C(1)—C(8)—S(7)—C(6) −8·4 (4)°.

Experimental. Light brown, platy crystals, m.p. 333·7–334·7 K, were obtained by recrystallization from benzene/CS_2. A crystal of dimensions 0·2 × 0·2 × 0·1 mm was used for the measurement of 1512 unique X-ray intensities by ω–2θ scan on a Nonius CAD-4 diffractometer, these comprising all possible reflections with $\sin\theta/\lambda < 0{\cdot}61$ Å^{-1} in the index ranges $0 < h < 13$, $0 < k < 7$, $-15 < l < 15$. Two standard reflections showed no appreciable intensity variation. 1003 reflections having $I > 2\sigma(I)$ were considered observed. $R_{\text{int}} = 0{\cdot}13$ from merging 79 pairs of equivalent reflections. Intensities were not corrected for absorption or extinction. Lattice parameters were determined from setting angles for 25 reflections with $21 < \theta < 30°$. The structure was solved with the *MULTAN* program (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978). Anisotropic least-squares refinement gave a final R value (on F) of 0·063, with $wR = 0{\cdot}077$, $S = 11{\cdot}5$, $w = 1/\sigma^2(F_o)$. The H atoms were located in difference syntheses and refined isotropically, with the exception of H(1), which was placed in a calculated position assuming a C—H bond length of 1·073 Å and allowed to ride on C(1). After the final refinement cycle $(\Delta/\sigma)_{\max} = 0{\cdot}2$, $(\Delta\rho)_{\max} = 0{\cdot}6$, $(\Delta\rho)_{\min} = -0{\cdot}6$ e Å^{-3}. Computations were carried out with the *GX* crystallographic package (Mallinson & Muir, 1985). Atomic

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2), *with standard deviations in the least significant digits in parentheses*

$$U_{\text{eq}} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
C(1)	0·8295 (5)	0·3507 (8)	0·5176 (4)	0·052
C(2)	0·8206 (5)	0·2279 (11)	0·4166 (4)	0·068
C(3)	0·7491 (6)	0·0463 (13)	0·3694 (4)	0·075
C(4)	0·6691 (6)	−0·0871 (9)	0·4060 (5)	0·068
C(5)	0·6527 (5)	−0·0758 (9)	0·5003 (6)	0·061
C(6)	0·7073 (4)	0·1010 (8)	0·5897 (4)	0·049
C(8)	0·9436 (5)	0·2669 (9)	0·6225 (4)	0·056
C(9)	0·7099 (5)	0·3337 (8)	0·5422 (5)	0·051
S(7)	0·87790 (11)	0·05501 (22)	0·68123 (9)	0·049
O(7a)	0·9223 (3)	−0·1634 (6)	0·6664 (3)	0·078
O(7b)	0·9002 (4)	0·1229 (9)	0·7925 (3)	0·091

Table 2. *Bond lengths* (Å)

C(1)—C(2)	1·478 (8)	C(1)—C(8)	1·525 (7)
C(1)—C(9)	1·512 (7)	C(2)—C(3)	1·337 (9)
C(3)—C(4)	1·425 (10)	C(4)—C(5)	1·325 (10)
C(5)—C(6)	1·503 (8)	C(6)—C(9)	1·524 (7)
C(6)—S(7)	1·815 (5)	C(8)—S(7)	1·789 (6)
S(7)—O(7a)	1·435 (4)	S(7)—O(7b)	1·432 (4)

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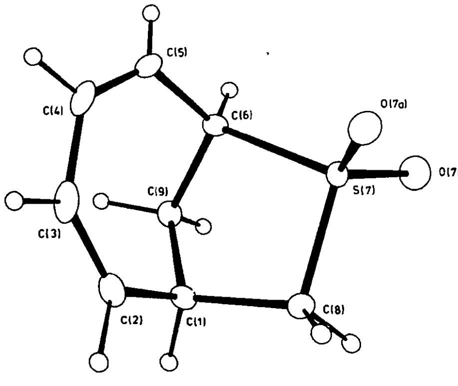


Fig. 1. A view of the molecular structure showing the atom labels.

scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Atomic coordinates and bond lengths are in Tables 1 and 2.* Fig. 1 shows the atom labels and Fig. 2 is a stereoview of the crystal packing.

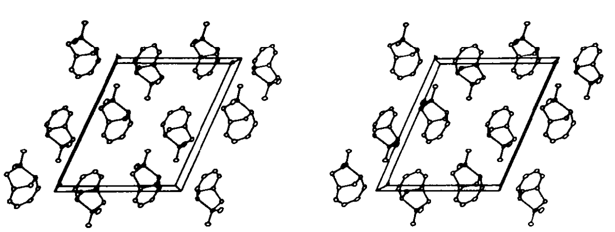
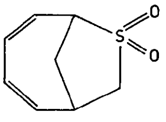


Fig. 2. A stereoview of the unit cell looking along the *b* axis. The *a* axis is across and the *c* axis down the page.

Related literature. The sulfone (I) was prepared in a novel reaction involving cyclopropane ring opening from 3,4-homotropilidene (bicyclo[5.1.0]octa-2,5-diene) as previously described (Dalling, Gall & MacNicol, 1979). (I) is also formed in high yield when the isomeric hydrocarbon bicyclo[5.1.0]octa-2,4-diene is heated with excess dry SO_2 in toluene-d_8. Interestingly, in this case ^1H NMR monitoring (unpublished results) shows the facile production of (I), even at room temperature.



(I)

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* Lists of structure factors, H-atom coordinates and anisotropic displacement parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51261 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of (*R*)-3-[(*R*)-(6,7-Dichloro-2,3-dihydrobenzofuran-2-yl)carbonyl]-4-phenyl-2-oxazolidone

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Abstract. $C_{18}H_{13}Cl_2NO_4$, $M_r = 378{\cdot}21$, orthorhombic, $P2_12_12_1$, $a = 13{\cdot}479\,(2)$, $b = 24{\cdot}885\,(3)$, $c = 4{\cdot}977\,(1)$ Å, $V = 1669{\cdot}5\,(4)$ Å^3, $Z = 4$, $D_x = 1{\cdot}505$ Mg m^{-3}, $\lambda(\text{Cu }K\alpha) = 1{\cdot}54178$ Å, $\mu = 3{\cdot}71$ mm^{-1}, $F(000) = 776$, $T = 295$ K, $R = 0{\cdot}046$ for 1742 observed reflections [$F_o > 3\sigma(F_o)$]. The absolute configuration of C(2) was determined as *R* based on the configuration of the (*R*)-4-phenyl-2-oxazolidone portion which was already known. All bond lengths and angles are normal.

Experimental. Colorless prism crystals obtained from dioxane. Crystal of dimensions 0·4 × 0·4 × 0·5 mm. Rigaku AFC-5R diffractometer, graphite-monochro-

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