$C(2^i)$—N—C(2)—C(3)	−172.84 (6)	C(6)—N—C(2)—C(3)	−58.11 (11)
B—N—C(2)—C(3)	69.11 (12)	N—C(2)—C(3)—C(4)	56.12 (13)
C(2)—C(3)—C(4)—C(5)	−52.07 (13)	C(3)—C(4)—C(5)—C(6)	54.44 (13)
C(4)—C(5)—C(6)—$C(5^i)$	174.46 (8)	C(4)—C(5)—C(6)—N	−58.93 (13)
C(2)—N—C(6)—$C(5^i)$	−172.89 (9)	$C(2^i)$—N—C(6)—$C(5^i)$	−58.68 (12)
B—N—C(6)—$C(5^i)$	64.21 (9)	C(2)—N—C(6)—C(5)	58.68 (12)
$C(2^i)$—N—C(6)—C(5)	172.89 (9)	B—N—C(6)—C(5)	−64.21 (9)

Symmetry code: (i) $x, \frac{1}{2} - y, z$.

An empirical extinction parameter to cover both primary and secondary extinction was refined (Sheldrick, 1993; Larson, 1970). The structure was solved by direct methods using *SHELXS*86 (Sheldrick, 1985).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AS1111). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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6-Methyl-2-oxabicyclo[4.3.0]non-4-en-3,7-dione, $C_9H_{10}O_3$

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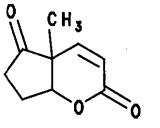
Abstract

The pyrone ring adopts a C(1)-sofa conformation and the *cis*-fused five-membered ring is in a C(9)-envelope conformation. The Me group is in a pseudo-axial position. The molecular packing involves C—H···O intermolecular contacts.

Comment

The title compound, (I), was synthesized as a model compound for natural products isolated from *Otoba parvifolia* (Boscaini, 1991). In order to establish unambiguously its stereochemistry, a crystal structure determination was undertaken.



(I)

The pyrone ring is in a sofa conformation with C(1) 0.470 (2) Å out of the plane formed by atoms O(1) and C(3)–C(6); the carbonyl atom O(2) lies 0.101 (1) Å out of the plane. As in other pyrones (Selladurai & Subramanian, 1992, and references therein) the angle O(2)—C(3)—O(1) is smaller than the angle O(2)—C(3)—C(4). The five-membered ring is in an envelope conformation with C(1), C(6), C(7) and C(8) coplanar to within experimental error and C(9) lying 0.514 (2) Å out of the plane. The dihedral angle between the best least-squares planes through the rings is 66.19 (7)°. The molecular packing involves intermolecular C—H···O interactions as listed in Table 3.

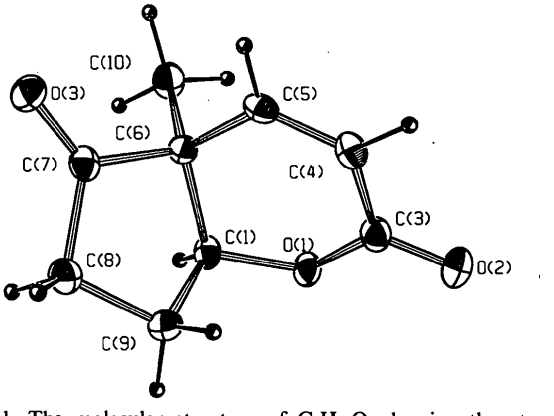


Fig. 1. The molecular structure of $C_9H_{10}O_3$ showing the atom labelling; 50% probability displacement ellipsoids are shown for non-H atoms.

Experimental

Crystal data

$C_9H_{10}O_3$	Mo $K\alpha$ radiation
M_r = 166.18	λ = 0.71073 Å
Orthorhombic	Cell parameters from 25 reflections
Pbca	θ = 9–20°
a = 8.151 (1) Å	μ = 0.97 mm^{-1}
b = 10.648 (1) Å	T = 83 K
c = 18.330 (2) Å	Irregular
V = 1590.9 (5) Å^3	

$Z = 8$	$0.30 \times 0.20 \times 0.11$ mm
$D_x = 1.388$ Mg m^{-3}	Colourless
	Crystal source: from ethyl acetate/*n*-hexane

Data collection

Rigaku AFC-5*R* diffractometer	$\theta_{max} = 28°$
ω scans	$h = 0 \rightarrow 10$
Absorption correction: none	$k = 0 \rightarrow 13$
1686 measured reflections	$l = 0 \rightarrow 23$
1686 independent reflections	3 standard reflections
1176 observed reflections $[I > 3\sigma(I)]$	frequency: 15 min
	intensity variation: ±0.3%

Refinement

Refinement on F	$(\Delta/\sigma)_{max} = 0.001$
$R = 0.038$	$\Delta\rho_{max} = 0.25$ e Å^{-3}
$wR = 0.039$	$\Delta\rho_{min} = -0.27$ e Å^{-3}
$S = 1.42$	Extinction correction: none
1176 reflections	Atomic scattering factors from *SHELX*76 (Sheldrick, 1976)
140 parameters	
$w = 1/[\sigma^2(\lvert F_o\rvert) + 0.0001(\lvert F_o\rvert)^2]$	

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$B_{eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
O(1)	0.1565 (2)	0.9448 (1)	0.0971 (1)	1.62 (4)
O(2)	−0.0057 (2)	1.1083 (1)	0.1007 (1)	2.28 (5)
O(3)	−0.0144 (2)	0.5313 (1)	0.1682 (1)	1.90 (4)
C(1)	0.1845 (2)	0.8167 (2)	0.1214 (1)	1.36 (6)
C(3)	0.0066 (3)	0.9954 (2)	0.1052 (1)	1.60 (5)
C(4)	−0.1330 (3)	0.9112 (2)	0.1152 (1)	1.56 (6)
C(5)	−0.1171 (2)	0.7882 (2)	0.1130 (1)	1.37 (6)
C(6)	0.0456 (2)	0.7253 (2)	0.1043 (1)	1.25 (5)
C(7)	0.0615 (2)	0.6281 (2)	0.1658 (1)	1.39 (6)
C(8)	0.1815 (3)	0.6740 (2)	0.2221 (1)	1.68 (6)
C(9)	0.2108 (3)	0.8117 (2)	0.2036 (1)	1.68 (6)
C(10)	0.0556 (3)	0.6626 (2)	0.0294 (1)	1.82 (6)

Table 2. *Selected geometric parameters* (Å, °)

O(1)—C(1)	1.453 (2)	O(1)—C(3)	1.344 (3)
O(2)—C(3)	1.209 (2)	O(3)—C(7)	1.203 (2)
C(1)—C(6)	1.526 (3)	C(1)—C(9)	1.523 (3)
C(3)—C(4)	1.460 (3)	C(4)—C(5)	1.317 (3)
C(5)—C(6)	1.494 (3)	C(6)—C(7)	1.536 (3)
C(6)—C(10)	1.529 (3)	C(7)—C(8)	1.504 (3)
C(8)—C(9)	1.524 (3)		
C(1)—O(1)—C(3)	119.0 (1)	C(1)—C(6)—C(7)	102.5 (1)
O(1)—C(1)—C(6)	114.8 (1)	C(1)—C(6)—C(10)	115.1 (2)
O(1)—C(1)—C(9)	111.0 (1)	C(5)—C(6)—C(7)	107.4 (1)
C(6)—C(1)—C(9)	106.6 (2)	C(5)—C(6)—C(10)	109.8 (2)
O(1)—C(3)—O(2)	117.8 (2)	C(7)—C(6)—C(10)	111.1 (2)
O(1)—C(3)—C(4)	118.4 (2)	O(3)—C(7)—C(6)	124.1 (2)
O(2)—C(3)—C(4)	123.7 (2)	O(3)—C(7)—C(8)	126.0 (2)
C(3)—C(4)—C(5)	122.0 (2)	C(6)—C(7)—C(8)	109.9 (2)
C(4)—C(5)—C(6)	122.4 (2)	C(7)—C(8)—C(9)	105.2 (2)
C(1)—C(6)—C(5)	110.5 (2)	C(1)—C(9)—C(8)	103.4 (2)

Table 3. *Hydrogen-bonding geometry* (Å, °)

D	H	A	D—H	H···A	D···A	D—H···A
C(8)	H′(C8)	O(2^i)	1.01 (2)	2.76 (2)	3.525 (3)	133 (1)
C(4)	H(C4)	O(3^{ii})	0.98 (2)	2.34 (2)	3.292 (2)	163 (1)
C(9)	H(C9)	O(3^{iii})	1.01 (2)	2.74 (2)	3.681 (2)	154 (1)

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

Data were corrected for Lorentz and polarization effects. The structure was solved by direct methods. H atoms were found in difference syntheses and refined with an overall isotropic temperature factor [$U_{iso} = 0.027$ (2) Å^2]. Refinement was by full-matrix least-squares methods. Programs used were *SHELXS*86 (Sheldrick, 1985), *SHELX*76 (Sheldrick, 1976) and *ORTEP* (Johnson, 1965). Most of the calculations were performed at the Weizmann Institute of Science, Israel.

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Lists of structure factors and anisotropic displacement parameters have been deposited with the IUCr (Reference: LI1083). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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A 5,6-Dihydroimidazo[2,1-*b*]thiazole Derivative

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Abstract

In 6-benzyl-5-methyl-5-(1-pyrazolyl)-5,6-dihydroimidazo[2,1-*b*]thiazol-6-ol, $C_{16}H_{16}N_4OS$, the phenyl,