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5,6-Dimethoxy-1-indanone

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Abstract. $C_{11}H_{12}O_3$, $M_r = 192{\cdot}22$, monoclinic, $P2_1/c$, $a = 8{\cdot}173$ (2), $b = 6{\cdot}003$ (1), $c = 20{\cdot}034$ (4) Å, $\beta = 96{\cdot}75$ (3)°, $V = 976{\cdot}1$ (5) Å^3, $Z = 4$, $D_x = 1{\cdot}307$ g cm^{-3}, Cu $K\alpha$ radiation, $\lambda = 1{\cdot}5418$ Å, $\mu = 7{\cdot}4$ cm^{-1}, $F(000) = 408$, $T = 293$ K, final $R = 0{\cdot}043$ for 1078 observed reflections. The aromatic ring is planar, but not the five-membered ring. The methoxy group attached to C(6) is oriented out of the plane of the benzene ring, with a torsion angle C(11)–O(3)–C(6)–C(7) of −10·9 (4)°.

Experimental. The title compound (Fig. 1) was purchased from the Aldrich Chemical Company. Crystals were grown from acetone solution. Data were collected on an Enraf–Nonius CAD-4 diffractometer, graphite monochromator. The crystal had dimensions 0·3 × 0·3 × 0·25 mm. Cell parameters were measured on the diffractometer using 25 reflections in the 2θ range 20–40°. Range of indices $0 \le h \le 9$, $0 \le k \le 6$, $-22 \le l \le 22$ ($\theta \le 60°$). Three standard reflections 10,0,$\bar{2}$, 10,2,$\bar{1}$, $\bar{6}2\bar{1}$, measured after every 200 reflections showed a variation of 0·4%. Absorption corrections were considered unnecessary because of the almost equidimensional shape of the crystal and the small value of μ. Lorentz and polarization corrections. 1337 unique reflections measured; 1078 observed reflections with $I > 3{\cdot}0\sigma(I)$. Direct methods (*MULTAN*11/82; Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) were used for structure determination. H atoms located by difference Fourier synthesis. Anisotropic full-matrix least-squares refinement (on F) for non-H atoms, isotropic for H atoms. In the last cycle the H atoms were placed at idealized positions with fixed Debye–Waller temperature parameters at 4·0 Å^2. $\sum w(|F_o| - |F_c|)^2$ minimized. $wR = 0{\cdot}043$, max. $\Delta/\sigma = 0{\cdot}07$. Max. peak height in the final difference Fourier map 0·45 e Å^{-3}.

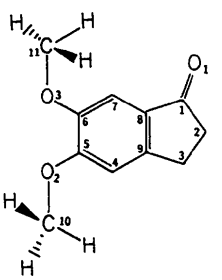

Fig. 1. Numbering of atoms and conformation of the molecule.

Table 1. *Final fractional coordinates and equivalent isotropic temperature factors for non-*H *atoms with e.s.d.'s in parentheses*

$B_{eq} = \frac{4}{3}\sum_i\sum_j B_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}(Å^2)
O(1)	0·6988 (3)	0·2037 (4)	0·5191 (1)	6·01 (6)
O(2)	0·1720 (2)	0·5230 (4)	0·7143 (1)	4·69 (5)
O(3)	0·1373 (2)	0·1789 (3)	0·6408 (1)	4·46 (5)
C(1)	0·6751 (4)	0·3540 (5)	0·5571 (1)	4·14 (7)
C(2)	0·7925 (4)	0·5463 (6)	0·5763 (2)	4·78 (7)
C(3)	0·7090 (4)	0·6914 (5)	0·6259 (2)	4·87 (8)
C(4)	0·4352 (4)	0·6228 (5)	0·6772 (1)	4·01 (7)
C(5)	0·2988 (3)	0·4875 (5)	0·6771 (1)	3·58 (6)
C(6)	0·2784 (3)	0·2944 (5)	0·6356 (1)	3·40 (6)
C(7)	0·3957 (3)	0·2402 (5)	0·5945 (1)	3·48 (6)
C(8)	0·5330 (3)	0·3799 (5)	0·5948 (1)	3·30 (6)
C(9)	0·5532 (3)	0·5682 (5)	0·6349 (1)	3·64 (6)
C(10)	0·1850 (4)	0·7107 (6)	0·7588 (2)	5·32 (8)
C(11)	0·0951 (4)	0·0100 (6)	0·5918 (2)	5·00 (8)

Table 2. *Bond lengths* (Å), *angles* (°), *selected torsion angles* (°) *and shortest non-bonded distances* (Å) *with e.s.d.'s in parentheses*

C(1)–O(1)	1·211 (4)	C(5)–C(6)	1·425 (4)
C(1)–C(2)	1·521 (4)	C(6)–C(7)	1·376 (4)
C(1)–C(8)	1·468 (4)	C(6)–O(3)	1·361 (3)
C(2)–C(3)	1·541 (5)	C(7)–C(8)	1·401 (4)
C(3)–C(9)	1·503 (4)	C(8)–C(9)	1·385 (4)
C(4)–C(5)	1·380 (4)	C(10)–O(2)	1·432 (4)
C(4)–C(9)	1·397 (4)	C(11)–O(3)	1·424 (4)
C(5)–O(2)	1·364 (4)		

O(1)–C(1)–C(2)	125·5 (3)	O(3)–C(6)–C(7)	125·7 (2)
O(1)–C(1)–C(8)	126·7 (3)	C(6)–C(7)–C(8)	118·1 (3)
C(2)–C(1)–C(8)	107·7 (2)	C(1)–C(8)–C(7)	128·1 (3)
C(1)–C(2)–C(3)	106·1 (3)	C(1)–C(8)–C(9)	109·7 (2)
C(2)–C(3)–C(9)	104·3 (2)	C(7)–C(8)–C(9)	122·2 (3)
C(5)–C(4)–C(9)	118·5 (3)	C(3)–C(9)–C(4)	127·9 (3)
O(2)–C(5)–C(4)	125·0 (3)	C(3)–C(9)–C(8)	112·1 (3)
O(2)–C(5)–C(6)	113·7 (2)	C(4)–C(9)–C(8)	120·0 (3)
C(4)–C(5)–C(6)	121·3 (3)	C(5)–O(2)–C(10)	117·3 (2)
C(5)–C(6)–C(7)	120·0 (3)	C(6)–O(3)–C(11)	116·7 (2)
O(3)–C(6)–C(5)	114·3 (2)		

C(8)–C(1)–C(2)–C(3)	−1·7 (3)	C(1)–C(2)–C(3)–C(9)	2·8 (3)
C(2)–C(3)–C(9)–C(8)	−3·0 (3)	C(3)–C(9)–C(8)–C(1)	2·0 (3)
C(9)–C(8)–C(1)–C(2)	−0·1 (3)	C(4)–C(5)–O(2)–C(10)	−2·4 (4)

O(1)–O′(1)	4·069 (3)	C(10)–C′(10)	4·247 (5)
C(11)–C′(11)	3·822 (4)		

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Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Enraf–Nonius *SDP* (Frenz, 1984).

Atomic parameters are given in Table 1,* selected bond lengths, bond angles and relevant torsion angles are presented in Table 2. Atomic numbering is shown in Fig. 1.

Related literature. The structure of 5,7-dimethoxy-1-indanone has been reported by Gupta, Lenstra & Geise (1984). The main difference between the two structures is the non-planar conformation of the C(6) methoxy group in the title compound.

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44930 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Molecular Structure of Haemanthamine, an Alkaloid from *Narcissus confusus*

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Abstract. $C_{17}H_{19}NO_4$, $M_r = 301{\cdot}34$, orthorhombic, $P2_12_12_1$, $a = 14{\cdot}055\ (4)$, $b = 11{\cdot}056\ (5)$, $c = 9{\cdot}608\ (3)$ Å, $V = 1493\ (2)$ Å^3, $Z = 4$, $D_x = 1{\cdot}341$ Mg m^{-3}, $F(000) = 640$, Mo $K\alpha$ radiation, $\lambda = 0{\cdot}71069$ Å, μ(Mo $K\alpha$) $= 0{\cdot}057$ mm^{-1}. The structure was solved by direct methods and refined to a final R value of 0·041 for 1369 observed reflections, confirming the *anti* position of C(11)–OH with respect to the aromatic ring, and the half-chair conformation of ring *C*.

Experimental. Platy white crystals, 0·07 × 0·09 × 0·10 mm. Philips PW 1100 computer-controlled single-crystal diffractometer, graphite-monochromated Mo $K\alpha$ radiation. ω–2θ scan. Cell parameters from setting angles of 25 reflections having $10 < \theta < 15°$. Data collection at 293 K: index range $2 \le h \le 16$, $0 \le k \le 13$, $0 \le l \le 11$ with $2\theta \le 50°$, three standard reflections (800, 040, 004) measured every 60 min showed only random deviations from mean intensity, 1524 unique measured reflections of which 1369 observed with $I(hkl) \ge 1{\cdot}5\sigma(I)$.

Structure solved by *XMY*84 (Debaerdemaeker, 1984). The least-squares refinement used *SHELX*76 (Sheldrick, 1976). $\sum w(|F_o| - |F_c|)^2$ minimized where $w = 1/[\sigma^2(F) + 0{\cdot}0202(F)^2]$. 275 parameters refined: atom coordinates, anisotropic temperature factors for all non-H atoms, isotropic temperature factors for all H, $(\Delta/\sigma)_{max}$ (for non-H atoms) = 0·034, max. and min. in final $\Delta\rho$ map 0·20 and −0·32 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Table 1* gives the final atomic

* Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44911 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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