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5,6-Dimethoxyindole

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Abstract. $C_{10}H_{11}NO_2$, $M_r = 177{\cdot}21$, orthorhombic, $P2_12_12_1$, $a = 5{\cdot}805\ (1)$, $b = 11{\cdot}195\ (2)$, $c = 13{\cdot}533\ (2)$ Å, $V = 879{\cdot}5\ (2)$ Å^3, $Z = 4$, $D_x = 1{\cdot}34$ g cm^{-3}, Cu $K\alpha$ radiation, $\lambda = 1{\cdot}5418$ Å, $\mu = 7{\cdot}7$ cm^{-1}, $F(000) = 376$, $T = 293$ K, final $R = 0{\cdot}036$ for 693 observed reflections. The molecule is nearly planar with the exception of C(11) which is out of the plane by $-0{\cdot}257\ (4)$ Å. The torsion angles C(11)–O(2)–C(4) and C(10)–O(1)–C(6)–C(7) are $-6{\cdot}0\ (5)$ and $-1{\cdot}5\ (5)°$, respectively.

Experimental. The title compound (Fig. 1) was purchased from the Aldrich Chemical Company. Crystals grown from acetonitrile solution. Data collected on an Enraf–Nonius CAD-4 diffractometer, graphite monochromator. The crystal had dimensions $0{\cdot}2 \times 0{\cdot}3 \times 0{\cdot}3$ mm. Cell parameters measured on the diffractometer using 25 reflections in the 2θ range 20–40°. Range of indices $0 < h < 6$, $0 < k < 12$, $0 < l < 15$ ($\theta < 60°$). Three standards 101, 024, 131, measured after every 200 reflections, showed a variation of 0·2%. No absorption corrections. Lorentz and polarization corrections. 785 unique reflections measured; 693 observed reflections with $I > 3{\cdot}0\sigma(I)$. Direct methods (*MULTAN*11/82; Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) used for structure determination. H atoms located by difference Fourier synthesis. Anisotropic full-matrix least-squares refinement (on F) for non-H atoms,

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)	0·3447 (5)	−0·0990 (2)	−0·0039 (2)	4·00 (5)
O(2)	0·0080 (5)	−0·0059 (2)	−0·1005 (2)	4·14 (5)
N(1)	0·1533 (6)	0·1664 (3)	0·2746 (2)	4·13 (7)
C(2)	−0·0167 (8)	0·2515 (4)	0·2815 (3)	4·49 (9)
C(3)	−0·1350 (7)	0·2588 (3)	0·1945 (3)	4·43 (8)
C(4)	−0·0852 (6)	0·1341 (3)	0·0327 (3)	3·61 (8)
C(5)	0·0439 (6)	0·0434 (3)	−0·0077 (2)	3·20 (7)
C(6)	0·2260 (6)	−0·0097 (3)	0·0457 (2)	3·23 (7)
C(7)	0·2778 (7)	0·0248 (3)	0·1413 (2)	3·43 (7)
C(8)	0·1410 (7)	0·1161 (3)	0·1811 (2)	3·37 (7)
C(9)	−0·0356 (7)	0·1714 (3)	0·1295 (2)	3·48 (7)
C(10)	0·5318 (7)	−0·1534 (3)	0·0488 (3)	4·65 (9)
C(11)	−0·1929 (7)	0·0354 (4)	−0·1519 (3)	4·52 (9)

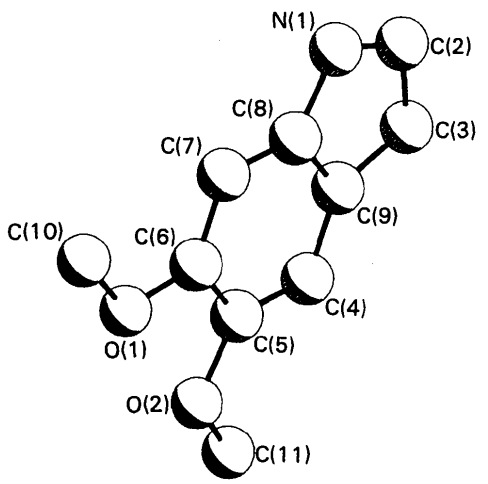

Fig. 1. Numbering of atoms and conformation of the molecule.

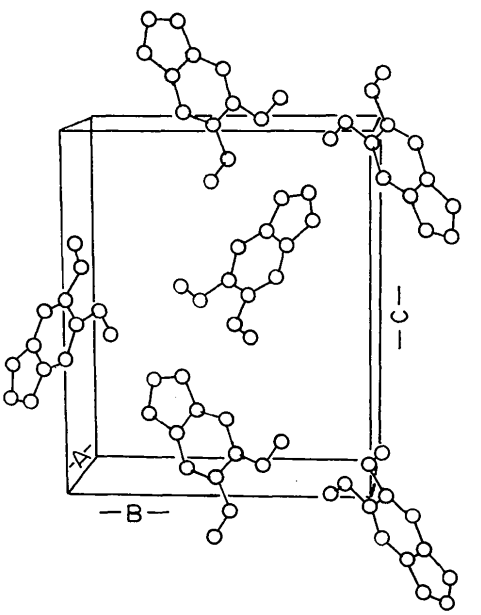

Fig. 2. Molecular packing diagram.

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Table 2. *Bond distances* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

O(1)	C(6)	1·387 (4)	C(3)	C(9)	1·436 (5)
O(1)	C(10)	1·434 (5)	C(4)	C(5)	1·375 (5)
O(2)	C(5)	1·387 (4)	C(4)	C(9)	1·404 (5)
O(2)	C(11)	1·433 (5)	C(5)	C(6)	1·411 (5)
N(1)	C(2)	1·373 (5)	C(6)	C(7)	1·383 (5)
N(1)	C(8)	1·387 (4)	C(7)	C(8)	1·402 (5)
C(2)	C(3)	1·365 (5)	C(8)	C(9)	1·385 (5)

C(6)	O(1)	C(10)	116·2 (3)	O(1)	C(6)	C(7)	123·1 (3)
C(5)	O(2)	C(11)	115·7 (3)	C(5)	C(6)	C(7)	121·7 (3)
C(2)	N(1)	C(8)	107·9 (3)	C(6)	C(7)	C(8)	116·1 (3)
N(1)	C(2)	C(3)	110·1 (3)	N(1)	C(8)	C(7)	128·1 (3)
C(2)	C(3)	C(9)	106·6 (3)	N(1)	C(8)	C(9)	108·5 (3)
C(5)	C(4)	C(9)	118·6 (3)	C(7)	C(8)	C(9)	123·4 (3)
O(2)	C(5)	C(4)	124·9 (3)	C(3)	C(9)	C(4)	133·7 (3)
O(2)	C(5)	C(6)	114·1 (3)	C(3)	C(9)	C(8)	107·0 (3)
C(4)	C(5)	C(6)	120·9 (3)	C(4)	C(9)	C(8)	119·3 (3)
O(1)	C(6)	C(5)	115·3 (3)				

isotropic for H atoms. $\sum w(|F_o| - |F_c|)^2$ minimized. $R = wR = 0{\cdot}036$, max. $\Delta/\sigma = 0{\cdot}12$. Max. peak height in the final difference Fourier map 0·28 e Å^{-3}, $S = 0{\cdot}51$. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Enraf–Nonius *SDP* (Frenz, 1984).

Atomic parameters are given in Table 1,* bond distances and bond angles are presented in Table 2. Atomic numbering is shown in Fig. 1 and packing in Fig. 2.

Related literature. The methoxy group has the same non-planar conformation as in 5,6-dimethoxy-1-indanone (Shoja, 1988).

* 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 51232 (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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