

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 &

\* 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.

Geise (1984). The main difference between the two structures is the non-planar conformation of the C(6) methoxy group in the title compound.

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

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**Abstract.**  $C_{17}H_{19}NO_4$ ,  $M_r = 301.34$ , orthorhombic,  $P2_12_12_1$ ,  $a = 14.055$  (4),  $b = 11.056$  (5),  $c = 9.608$  (3) Å,  $V = 1493$  (2) Å<sup>3</sup>,  $Z = 4$ ,  $D_x = 1.341$  Mg m<sup>-3</sup>,  $F(000) = 640$ , Mo  $K\alpha$  radiation,  $\lambda = 0.71069$  Å,  $\mu(\text{Mo } K\alpha) = 0.057$  mm<sup>-1</sup>. 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,  $0.07 \times 0.09 \times 0.10$  mm. Philips PW 1100 computer-controlled single-crystal diffractometer, graphite-monochromated Mo  $K\alpha$  radiation.  $\omega$ – $2\theta$  scan. Cell parameters from setting angles of 25 reflections having  $10 < \theta < 15^\circ$ . Data collection at 293 K: index range  $2 \leq h \leq 16$ ,  $0 \leq k \leq 13$ ,  $0 \leq l \leq 11$  with  $2\theta \leq 50^\circ$ , 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  $I(hkl) \geq 1.5\sigma(I)$ .

Structure solved by XMY84 (Debaerdemaeker, 1984). The least-squares refinement used SHELX76 (Sheldrick, 1976).  $\sum w(|F_o| - |F_c|)^2$  minimized where  $w = 1/[\sigma^2(F) + 0.0202(F)^2]$ . 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<sup>-3</sup>. 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.

Table 1. Atomic coordinates ( $\times 10^4$ ) and temperature coefficients ( $\text{\AA}^2 \times 10^3$ )

The equivalent isotropic  $U$  is defined as one-third of the trace of the orthogonalized  $U_{ij}$  tensor.

	$x$	$y$	$z$	$U_{eq}$
O(1)	8303 (2)	3793 (2)	6276 (3)	56 (5)
O(211)	9834 (2)	4379 (2)	13018 (2)	41 (16)
O(3)	7952 (2)	5800 (3)	5733 (2)	57 (12)
O(4)	12981 (2)	5253 (2)	10958 (3)	57 (20)
C(1)	10826 (2)	3829 (2)	10451 (3)	38 (11)
C(2)	11698 (2)	3786 (3)	11007 (4)	42 (11)
C(3)	12173 (2)	4822 (3)	11753 (4)	44 (7)
C(4)	11515 (2)	5888 (3)	12013 (4)	42 (9)
C(4a)	10789 (2)	6085 (2)	10843 (3)	35 (9)
N	10047 (2)	6979 (2)	11232 (3)	36 (13)
C(5)	13769 (3)	4465 (5)	11001 (5)	44 (14)
C(6)	9605 (2)	7402 (2)	9929 (3)	43 (14)
C(6a)	9339 (2)	6383 (2)	8936 (3)	42 (14)
C(7)	8798 (2)	6681 (3)	7762 (3)	42 (13)
C(8)	8514 (2)	5754 (3)	6923 (3)	42 (11)
C(9)	8729 (2)	4553 (3)	7242 (3)	41 (5)
C(10)	9271 (2)	4243 (3)	8358 (3)	38 (7)
C(10a)	9605 (2)	5190 (2)	9232 (3)	32 (5)
C(10b)	10205 (2)	4936 (2)	10537 (3)	31 (9)
C(11)	9483 (2)	4914 (2)	11785 (3)	33 (5)
C(12)	9352 (2)	6291 (3)	12092 (3)	39 (2)
C(13)	7988 (3)	4590 (4)	5183 (4)	58 (25)

Table 2. Bond lengths ( $\text{\AA}$ ) and angles ( $^\circ$ )

Phthalate group			
C(8)—O(3)	1.390 (4)	O(1)—C(9)—C(8)	109.6 (3)
O(3)—C(13)	1.439 (5)	C(9)—C(8)—O(3)	109.8 (3)
C(13)—O(1)	1.441 (5)	C(8)—O(3)—C(13)	104.4 (3)
O(1)—C(9)	1.388 (4)	O(3)—C(13)—O(1)	108.1 (3)
		C(13)—O(1)—C(9)	104.5 (3)
Ring A			
C(6a)—C(7)	1.400 (4)	C(6a)—C(7)—C(8)	117.3 (3)
C(7)—C(8)	1.363 (5)	C(7)—C(8)—C(9)	121.5 (3)
C(8)—C(9)	1.396 (5)	C(8)—C(9)—C(10)	122.3 (3)
C(9)—C(10)	1.359 (4)	C(9)—C(10)—C(10a)	117.7 (3)
C(10)—C(10a)	1.421 (4)	C(10)—C(10a)—C(6a)	119.1 (3)
		C(10a)—C(6a)—C(7)	122.0 (3)
Ring B			
C(4a)—N	1.484 (4)	C(4a)—N—C(6)	107.1 (2)
N—C(6)	1.472 (4)	N—C(6)—C(6a)	113.7 (2)
C(6)—C(6a)	1.523 (4)	C(6)—C(6a)—C(10a)	120.3 (2)
C(6a)—C(10a)	1.401 (4)	C(6a)—C(10a)—C(10b)	118.9 (2)
C(10a)—C(10b)	1.537 (4)	C(10a)—C(10b)—C(4a)	107.3 (2)
C(10b)—C(4a)	1.540 (3)	C(10b)—C(4a)—N	102.9 (2)
Ring C			
C(1)—C(2)	1.338 (5)	C(1)—C(2)—C(3)	124.6 (3)
C(2)—C(3)	1.508 (5)	C(5)—C(7)—O(4)	108.0 (3)
C(3)—C(4)	1.518 (5)	C(2)—C(3)—O(4)	110.3 (3)
C(4)—C(4a)	1.534 (4)	C(3)—O(4)—C(5)	113.4 (3)
C(4a)—C(10b)	1.540 (3)	C(2)—C(3)—C(4)	113.5 (2)
C(10b)—C(1)	1.506 (4)	C(3)—C(4)—C(4a)	113.3 (3)
C(3)—O(4)	1.449 (4)	C(4)—C(4a)—C(10b)	112.1 (2)
O(4)—C(5)	1.408 (4)	C(4a)—C(10b)—C(1)	111.9 (2)
		C(10b)—C(1)—C(2)	122.5 (3)

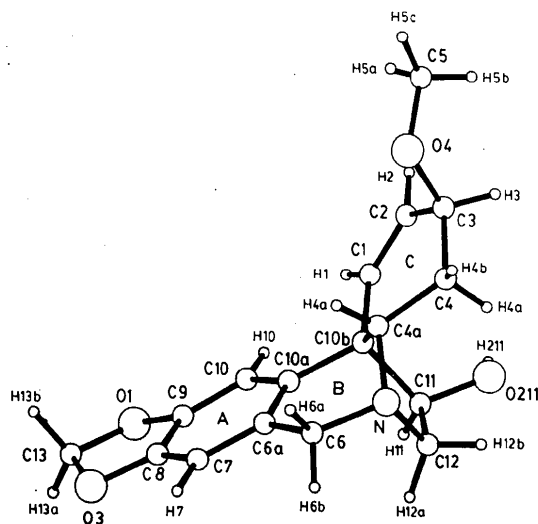


Fig. 1. The molecular structure of  $C_{17}H_{19}NO_4$  (Motherwell & Clegg, 1978).

coordinates. Bond lengths and angles are in Table 2. A drawing of the molecule with atomic numbering according to Ghosal, Saini & Razdan (1985) is shown in Fig. 1. The molecule is far from planar and can be regarded as consisting of a methoxy and a methylenedioxy group, a planar aromatic ring A and two non-planar rings B and C. The aromatic ring and the methylenedioxy group are fused at the C(8) and C(9) atoms. The *anti* position of C(11)—OH with respect to

the aromatic ring, the presence of an ethylidene bridge C(11)—C(12) and a half-chair conformation for ring C have been shown.

**Related literature.** The title compound is an alkaloid isolated from *Narcissus confusus* (Bastida, Viladomat, Llabres, Codina, Feliz & Rubiralta, 1987) collected in the Montserrat mountains (Barcelona, Spain).

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