Related literature. During the course of our studies on plant growth regulators, some heteroaromatic ureas, such as *N*-(2-chloro-4-pyridyl)-*N'*-phenylurea and *N*-(4-pyridyl)-*N'*-phenylurea showed a strong cytokinin activity (Takahashi, Shudo, Okamoto, Yamada & Isogai, 1978). Crystallographic studies on several urea cytokinins have been carried out (Yamaguchi & Shudo, 1991).

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Structures of (I) 5a,10b-*cis*- and (II) 5a,10b-*trans*-10-Methoxy-3,3,4-trimethyl-1,2a,3,4,5,5a,6,10b-octahydrobenzo[*g*][1,3]oxazolidino[2,3,4-*de*][2,4a]naphthyridine

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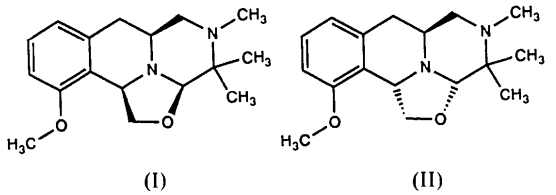
Abstract. (I) $C_{17}H_{24}N_2O_2$, $M_r = 288.39$, monoclinic, $P2_1/c$, $a = 13.033$ (2), $b = 17.763$ (4), $c = 6.761$ (1) Å, $\beta = 104.96$ (1)°, $V = 1512.0$ (5) Å^3, $Z = 4$, $D_x = 1.27$ g cm^{-3}, λ(Cu $K\alpha$) = 1.5418 Å, $\mu = 6.7$ cm^{-1}, $F(000) = 624$, $T = 115$ K, $R = 0.053$, $wR = 0.066$ for 1671 unique observed reflections. (II) $C_{17}H_{24}N_2O_2$, $M_r = 288.39$, monoclinic, $P2_1/n$, $a = 12.872$ (4), $b = 17.279$ (4), $c = 13.619$ (2) Å, $\beta = 96.59$ (2)°, $V = 3009$ (1) Å^3, $Z = 8$, $D_x = 1.27$ g cm^{-3}, λ(Mo $K\alpha$) = 0.7107 Å, $\mu = 0.8$ cm^{-1}, $F(000) = 1248$, $T = 148$ K, $R = 0.067$, $wR = 0.067$ for 3747 unique observed reflections. The stereoisomeric compounds are heterotricyclic about an N bridgehead atom.

Experimental. Crystals (colorless prisms) of (I) and (II) were obtained from hexane solutions by Dr Tomasz Glinka and Professor Robert M. Williams (Colorado State University). For (I), crystal size 0.48 × 0.47 × 0.26 mm; for (II), crystal size 0.24 × 0.21 × 0.50 mm. Nicolet *R*3*m* diffractometer, unit-cell constants from least-squares fit of setting angles for 25 reflections [$2\theta_{av} = 53.97°$ for (I), 16.34° for (II)]. Data collected for (I) ($\theta/2\theta$ scans) to $(\sin\theta)/\lambda = 0.5313$ Å^{-1}, $-8 \le h \le 0$, $0 \le k \le 19$, $-14 \le l \le 14$. Data collected for (II) (Wyckoff ω scans) to $(\sin\theta)/\lambda = 0.5947$ Å^{-1}, $0 \le h \le 16$, $0 \le k \le 21$, $-17 \le l \le 17$. Three standard reflections [400, 020, 005 for (I); 400, 040, 004 for (II)] every 97 reflections, no trend in intensity observed; Lorentz and polarization corrections; no absorption correction applied for either crystal due to low absorption coefficients; 1887 unique reflections measured for (I), 5310 unique reflections measured for (II), 1671 reflections with $F_o > 2.5\sigma(F_o)$ observed for (I), 3747 for (II).



(I) (II)

Both structures solved by direct methods (*SOLV*; Sheldrick, 1985); block-diagonal [max. 103 parameters/block; 202 parameters (I), 403 (II); data/parameters ratio = 8.3 (I), 9.3 (II)] weighted $\{w = [\sigma^2(F) + gF^2]^{-1}$, $g = 1.38 \times 10^{-3}$ for (I), 6.40×10^{-3} for (II)$\}$ least-squares refinement on *F*. H atoms in idealized positions [C—H = 0.96 Å, U(H) = 1.2 × U_{iso}(C)]. Non-H atoms refined with anisotropic thermal parameters. At convergence $[(\Delta/\sigma)_{max} = 0.062$ (I), 0.209 (II), $(\Delta/\sigma)_{mean} = 0.017$ for last two cycles

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Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* ($Å^2 \times 10^3$) *for* (I)

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
O(1)	0.4031 (1)	0.4378 (1)	0.6150 (2)	37 (1)
O(2)	0.3669 (1)	0.6387 (1)	0.9534 (2)	38 (1)
N(1)	0.2586 (1)	0.5004 (1)	0.4466 (3)	26 (1)
N(2)	0.2402 (2)	0.4245 (1)	0.0837 (3)	32 (1)
C(1)	0.3133 (2)	0.5540 (1)	0.5992 (3)	28 (1)
C(2)	0.2336 (2)	0.6025 (1)	0.6667 (3)	27 (1)
C(3)	0.2626 (2)	0.6457 (1)	0.8472 (3)	29 (1)
C(4)	0.1897 (2)	0.6910 (1)	0.9047 (4)	34 (1)
C(5)	0.0863 (2)	0.6935 (1)	0.7826 (4)	37 (1)
C(6)	0.0580 (2)	0.6537 (1)	0.6032 (3)	33 (1)
C(7)	0.1312 (2)	0.6087 (1)	0.5400 (3)	28 (1)
C(8)	0.0976 (2)	0.5686 (1)	0.3361 (4)	33 (1)
C(9)	0.1884 (2)	0.5331 (1)	0.2666 (3)	29 (1)
C(10)	0.1523 (2)	0.4712 (1)	0.1096 (3)	33 (1)
C(11)	0.3020 (2)	0.3881 (1)	0.2768 (3)	31 (1)
C(12)	0.3437 (2)	0.4560 (1)	0.4126 (3)	30 (1)
C(13)	0.3849 (2)	0.4986 (1)	0.7470 (4)	33 (1)
C(14)	0.2367 (2)	0.3364 (1)	0.3758 (4)	38 (1)
C(15)	0.3958 (2)	0.3454 (1)	0.2369 (4)	41 (1)
C(16)	0.2023 (2)	0.3730 (1)	−0.0878 (4)	41 (1)
C(17)	0.4039 (2)	0.6852 (1)	1.1300 (4)	41 (1)

Table 2. *Bond lengths* (Å) *and angles* (°) *for* (I)

O(1)—C(12)	1.424 (2)	O(1)—C(13)	1.458 (3)
O(2)—C(3)	1.370 (2)	O(2)—C(17)	1.429 (3)
N(1)—C(1)	1.449 (3)	N(1)—C(9)	1.442 (2)
N(1)—C(12)	1.427 (3)	N(2)—C(10)	1.462 (3)
N(2)—C(11)	1.492 (3)	N(2)—C(16)	1.459 (3)
C(1)—C(2)	1.508 (3)	C(1)—C(13)	1.535 (3)
C(2)—C(3)	1.409 (3)	C(2)—C(7)	1.391 (3)
C(3)—C(4)	1.374 (3)	C(4)—C(5)	1.388 (3)
C(5)—C(6)	1.370 (3)	C(6)—C(7)	1.395 (3)
C(7)—C(8)	1.512 (3)	C(8)—C(9)	1.520 (3)
C(9)—C(10)	1.516 (3)	C(11)—C(12)	1.527 (3)
C(11)—C(14)	1.520 (4)	C(11)—C(15)	1.521 (4)
C(12)—O(1)—C(13)	106.7 (2)	C(3)—O(2)—C(17)	117.4 (2)
C(1)—N(1)—C(9)	115.2 (2)	C(1)—N(1)—C(12)	102.6 (2)
C(9)—N(1)—C(12)	115.9 (2)	C(10)—N(2)—C(11)	113.8 (2)
C(10)—N(2)—C(16)	109.6 (2)	C(11)—N(2)—C(16)	114.8 (2)
N(1)—C(1)—C(2)	109.8 (2)	N(1)—C(1)—C(13)	98.5 (2)
C(2)—C(1)—C(13)	121.3 (2)	C(1)—C(2)—C(3)	121.5 (2)
C(1)—C(2)—C(7)	119.0 (2)	C(3)—C(2)—C(7)	119.4 (2)
O(2)—C(3)—C(2)	114.3 (2)	O(2)—C(3)—C(4)	124.7 (2)
C(2)—C(3)—C(4)	120.9 (2)	C(3)—C(4)—C(5)	119.1 (2)
C(4)—C(5)—C(6)	120.5 (2)	C(5)—C(6)—C(7)	121.2 (2)
C(2)—C(7)—C(6)	118.7 (2)	C(2)—C(7)—C(8)	122.0 (2)
C(6)—C(7)—C(8)	119.3 (2)	C(7)—C(8)—C(9)	114.3 (2)
N(1)—C(9)—C(8)	106.3 (2)	N(1)—C(9)—C(10)	108.3 (2)
C(8)—C(9)—C(10)	113.1 (2)	N(2)—C(10)—C(9)	112.6 (2)
N(2)—C(11)—C(12)	102.2 (2)	N(2)—C(11)—C(14)	114.2 (2)
C(12)—C(11)—C(14)	111.4 (2)	N(2)—C(11)—C(15)	109.7 (2)
C(12)—C(11)—C(15)	108.9 (2)	C(14)—C(11)—C(15)	110.2 (2)
O(1)—C(12)—N(1)	102.9 (2)	O(1)—C(12)—C(11)	114.8 (2)
N(1)—C(12)—C(11)	111.3 (2)	O(1)—C(13)—C(1)	104.1 (2)

(I), 0.030 for last four cycles (II)] $R = 0.053$ for (I) and 0.067 for (II), $wR = 0.066$ for (I) and 0.067 for (II), $S = 1.43$ for (I) and 1.38 for (II), slope of normal probability plot = 1.28 for (I) and 1.14 for (II), $(\Delta\rho)_{max} = 0.27$ for (I) and 0.34 e $Å^{-3}$ for (II), $(\Delta\rho)_{min} = -0.26$ for (I) and -0.38 e $Å^{-3}$ for (II). Neutral-atom scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974, Vol. IV); all calculations performed using *SHELXTL* program library (Sheldrick, 1985). Tables 1 and 2* contain atomic coordinates, and bond lengths and angles for (I). Fig. 1 shows the structure of (I), as well as the numbering scheme used. Tables 3 and 4 contain atomic coordinates, and bond lengths and angles for (II). Fig. 2 shows the structure of one of the two crystallographically independent molecules (the numbering scheme for the second molecule can be obtained by adding 17, 2 and 2 to the numbers shown for the C, N and O atoms, respectively) in the asymmetric unit of (II).

Table 3. *Atomic coordinates and equivalent isotropic thermal parameters* ($Å^2 \times 10^3$) *for* (II)

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	1.0641 (2)	0.8317 (2)	0.2293 (2)	20 (1)
C(2)	0.9948 (2)	0.8834 (2)	0.2657 (2)	23 (1)
C(3)	0.9373 (2)	0.9360 (2)	0.2054 (2)	28 (1)
C(4)	0.9511 (3)	0.9371 (2)	0.1054 (2)	32 (1)
C(5)	1.0194 (2)	0.8877 (2)	0.0676 (2)	29 (1)
C(6)	1.0760 (2)	0.8338 (2)	0.1285 (2)	23 (1)
C(7)	1.1452 (2)	0.7747 (2)	0.0881 (2)	26 (1)
C(8)	1.1509 (2)	0.7027 (2)	0.1515 (2)	21 (1)
C(9)	1.2150 (3)	0.6381 (2)	0.1141 (2)	29 (1)
C(10)	1.2603 (2)	0.5886 (2)	0.2819 (2)	24 (1)
C(11)	1.2045 (2)	0.6590 (2)	0.3184 (2)	21 (1)
C(12)	1.1215 (2)	0.7742 (2)	0.2985 (2)	20 (1)
C(13)	0.9195 (3)	0.9268 (2)	0.4090 (3)	41 (1)
C(14)	1.0500 (2)	0.7153 (2)	0.3441 (2)	24 (1)
C(15)	1.2410 (3)	0.5202 (2)	0.3487 (2)	32 (1)
C(16)	1.3784 (2)	0.6061 (2)	0.2911 (2)	32 (1)
C(17)	1.2600 (3)	0.5037 (2)	0.1356 (3)	40 (1)
N(1)	1.2157 (2)	0.5714 (1)	0.1793 (2)	26 (1)
N(2)	1.1966 (2)	0.7256 (1)	0.2520 (2)	19 (1)
O(1)	1.1006 (2)	0.6419 (1)	0.3385 (1)	24 (1)
O(2)	0.9891 (2)	0.8764 (1)	0.3661 (1)	29 (1)
C(18)	0.5655 (2)	0.9340 (2)	0.2412 (2)	20 (1)
C(19)	0.4952 (2)	0.8800 (2)	0.2712 (2)	20 (1)
C(20)	0.4385 (2)	0.8319 (2)	0.2041 (2)	23 (1)
C(21)	0.4551 (2)	0.8360 (2)	0.1050 (2)	27 (1)
C(22)	0.5253 (2)	0.8883 (2)	0.0739 (2)	24 (1)
C(23)	0.5809 (2)	0.9379 (2)	0.1416 (2)	21 (1)
C(24)	0.6540 (2)	0.9972 (2)	0.1086 (2)	23 (1)
C(25)	0.6614 (2)	1.0655 (2)	0.1789 (2)	21 (1)
C(26)	0.7317 (2)	1.1297 (2)	0.1511 (2)	26 (1)
C(27)	0.7660 (2)	1.1726 (2)	0.3228 (2)	23 (1)
C(28)	0.7075 (2)	1.1003 (2)	0.3499 (2)	21 (1)
C(29)	0.6232 (2)	0.9865 (2)	0.3175 (2)	18 (1)
C(30)	0.4223 (3)	0.8221 (2)	0.4069 (2)	30 (1)
C(31)	0.5511 (2)	1.0435 (2)	0.3666 (2)	24 (1)
C(32)	0.7423 (3)	1.2380 (2)	0.3922 (2)	32 (1)
C(33)	0.8841 (2)	1.1544 (2)	0.3392 (2)	31 (1)
C(34)	0.7782 (3)	1.2625 (2)	0.1832 (3)	39 (1)
N(3)	0.7284 (2)	1.1942 (1)	0.2197 (2)	25 (1)
N(4)	0.7013 (2)	1.0370 (1)	0.2789 (2)	19 (1)
O(3)	0.6021 (2)	1.1172 (1)	0.3660 (1)	24 (1)
O(4)	0.4874 (2)	0.8794 (1)	0.3712 (1)	25 (1)

Related literature. Several tricyclic compounds with amino-bridgehead N atoms have been studied: 1,2a,3,3a,4,11a-hexahydro-3-(2-methoxy-2-oxoethyl)-3a-methyl-2*H*-[1]benzothiopyrano[3,4-*b*]pyrrolo-

* Lists of anisotropic thermal parameters, H-atom coordinates and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54376 (49 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 4. *Bond lengths* (Å) *and angles* (°) *for* (II)

C(1)—C(2)	1.394 (4)	C(1)—C(6)	1.399 (4)
C(1)—C(12)	1.503 (4)	C(2)—C(3)	1.381 (4)
C(2)—O(2)	1.384 (4)	C(3)—C(4)	1.393 (5)
C(4)—C(5)	1.369 (4)	C(5)—C(6)	1.395 (4)
C(6)—C(7)	1.500 (4)	C(7)—C(8)	1.512 (4)
C(8)—C(9)	1.510 (4)	C(8)—N(2)	1.480 (3)
C(9)—N(1)	1.455 (4)	C(10)—C(11)	1.525 (4)
C(10)—C(15)	1.529 (4)	C(10)—C(16)	1.540 (4)
C(10)—N(1)	1.479 (4)	C(11)—N(2)	1.460 (4)
C(11)—O(1)	1.427 (4)	C(12)—C(14)	1.550 (4)
C(12)—N(2)	1.477 (4)	C(13)—O(2)	1.422 (4)
C(14)—O(1)	1.432 (3)	C(17)—N(1)	1.458 (4)
C(18)—C(19)	1.394 (4)	C(18)—C(23)	1.395 (4)
C(18)—C(29)	1.509 (4)	C(19)—C(20)	1.380 (4)
C(19)—O(4)	1.376 (3)	C(20)—C(21)	1.392 (4)
C(21)—C(22)	1.379 (4)	C(22)—C(23)	1.395 (4)
C(23)—C(24)	1.495 (4)	C(24)—C(25)	1.515 (4)
C(25)—C(26)	1.507 (4)	C(25)—N(4)	1.483 (3)
C(26)—N(3)	1.458 (4)	C(27)—C(28)	1.526 (4)
C(27)—C(32)	1.527 (4)	C(27)—C(33)	1.544 (4)
C(27)—N(3)	1.480 (4)	C(28)—N(4)	1.456 (4)
C(28)—O(3)	1.429 (3)	C(29)—C(31)	1.555 (4)
C(29)—N(4)	1.473 (4)	C(30)—O(4)	1.419 (4)
C(31)—O(3)	1.433 (3)	C(34)—N(3)	1.456 (4)

C(2)—C(1)—C(6)	118.6 (3)	C(2)—C(1)—C(12)	119.3 (3)
C(6)—C(1)—C(12)	122.1 (3)	C(1)—C(2)—C(3)	122.2 (3)
C(1)—C(2)—O(2)	113.8 (2)	C(3)—C(2)—O(2)	124.0 (3)
C(2)—C(3)—C(4)	118.0 (3)	C(3)—C(4)—C(5)	121.3 (3)
C(4)—C(5)—C(6)	120.5 (3)	C(1)—C(6)—C(5)	119.5 (3)
C(1)—C(6)—C(7)	118.6 (2)	C(5)—C(6)—C(7)	121.8 (3)
C(6)—C(7)—C(8)	110.0 (2)	C(7)—C(8)—C(9)	114.1 (2)
C(7)—C(8)—N(2)	107.2 (2)	C(9)—C(8)—N(2)	109.5 (2)
C(8)—C(9)—N(1)	110.2 (2)	C(11)—C(10)—C(15)	107.9 (2)
C(11)—C(10)—C(16)	108.2 (2)	C(15)—C(10)—C(16)	109.3 (2)
C(11)—C(10)—N(1)	108.8 (2)	C(15)—C(10)—N(1)	109.6 (2)
C(16)—C(10)—N(1)	112.9 (2)	C(10)—C(11)—N(2)	115.4 (2)
C(10)—C(11)—O(1)	112.6 (2)	N(2)—C(11)—O(1)	106.3 (2)
C(1)—C(12)—C(14)	114.4 (2)	C(1)—C(12)—N(2)	113.9 (2)
C(14)—C(12)—N(2)	104.2 (2)	C(12)—C(14)—O(1)	105.4 (2)
C(9)—N(1)—C(10)	113.0 (2)	C(9)—N(1)—C(17)	111.3 (2)
C(10)—N(1)—C(17)	114.8 (2)	C(8)—N(2)—C(11)	110.7 (2)
C(8)—N(2)—C(12)	109.8 (2)	C(11)—N(2)—C(12)	100.7 (2)
C(11)—O(1)—C(14)	105.6 (2)	C(2)—O(2)—C(13)	117.4 (2)
C(19)—C(18)—C(23)	119.2 (2)	C(19)—C(18)—C(29)	119.0 (2)
C(23)—C(18)—C(29)	121.8 (3)	C(18)—C(19)—C(20)	121.4 (3)
C(18)—C(19)—O(4)	114.8 (2)	C(20)—C(19)—O(4)	123.9 (3)
C(19)—C(20)—C(21)	118.9 (3)	C(20)—C(21)—C(22)	120.6 (3)
C(21)—C(22)—C(23)	120.3 (3)	C(18)—C(23)—C(22)	119.6 (3)
C(18)—C(23)—C(24)	119.3 (2)	C(22)—C(23)—C(24)	121.1 (3)
C(23)—C(24)—C(25)	109.9 (2)	C(24)—C(25)—C(26)	114.2 (2)
C(24)—C(25)—N(4)	108.2 (2)	C(26)—C(25)—N(4)	108.7 (2)
C(25)—C(26)—N(3)	109.9 (2)	C(28)—C(27)—C(32)	108.5 (2)
C(28)—C(27)—C(33)	107.6 (2)	C(32)—C(27)—C(33)	109.0 (2)
C(28)—C(27)—N(3)	108.7 (2)	C(32)—C(27)—N(3)	109.5 (2)
C(33)—C(27)—N(3)	113.4 (2)	C(27)—C(28)—N(4)	116.4 (2)
C(27)—C(28)—O(3)	111.9 (2)	N(4)—C(28)—O(3)	105.9 (2)
C(18)—C(29)—C(31)	113.9 (2)	C(18)—C(29)—N(4)	114.3 (2)
C(31)—C(29)—N(4)	104.2 (2)	C(29)—C(31)—O(3)	105.2 (2)
C(26)—N(3)—C(27)	112.6 (2)	C(26)—N(3)—C(34)	110.8 (2)
C(27)—N(3)—C(34)	114.8 (2)	C(25)—N(4)—C(28)	110.3 (2)
C(25)—N(4)—C(29)	110.2 (2)	C(28)—N(4)—C(29)	101.2 (2)
C(28)—O(3)—C(31)	105.3 (2)	C(19)—O(4)—C(30)	117.2 (2)

[2,1,5-*cd*]pyrrolizine-3,10,11-tricarboxylic acid trimethyl ester (Lamm, Andersen & Aurel, 1983), 2,2a,4,4a,6,6a-hexahydro-1,3,5-trithia-7-azacyclopenta[*cd*]pentalene (Stein, Baker, Lewis & White, 1984), 1,1′,1″-(dodecahydro-1,4,7,9b-tetraazaphenalene-2,5,8-triyl)tris(1,2-propanediyl) hexaacetate–acetic acid (Martin *et al.*, 1981), nirurine (Petchnaree *et al.*, 1986), dodecahydro-1,4,7,9b-tetraazaphenalene trihydrochloride hemihydrate (Smith, 1965), 2,6,10-trioxa-13-azatricyclo[7.3.1.$0^{5,13}$]tridecane (Fritz, Gebauer, Huttner, Frank & Lorenz, 1976).

The bond lengths between the amino-bridgehead N atom and adjacent C atoms are significantly shorter in (I) than in either molecule of (II). As a result, the pyramidalization as measured by the distance from the plane formed by adjacent C atoms about the amino-bridgehead N atom is smaller in (I) [0.435 (1) Å for N(1)] than in (II) [0.545 (2) for N(2), 0.540 (2) Å for N(4)].

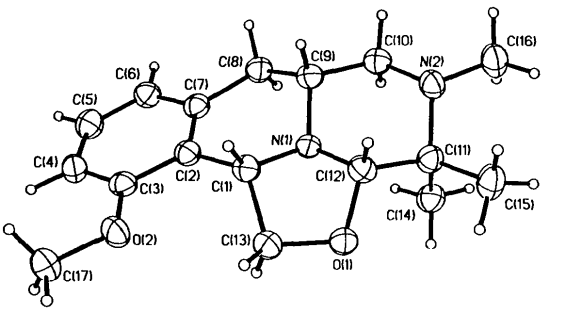

Fig. 1. The structure of (I) (50% probability thermal ellipsoids).

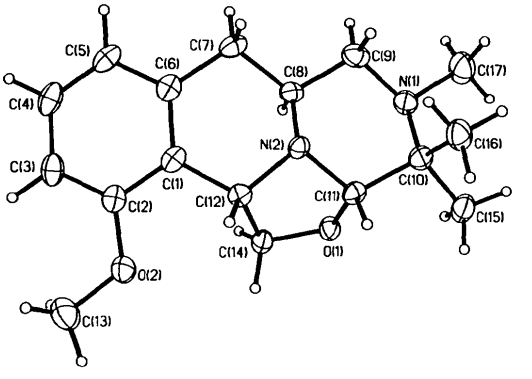

Fig. 2. The structure of a molecule of (II) (50% probability thermal ellipsoids).

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