factors or the equivalent values of the anisotropic temperature factors for the non-H atoms are given in Table 1.* Bond lengths and angles are given in Table 2.

Related literature. A distorted pseudopentagonal bipyramid around Te is formed as in dimethyltellurium dichloride (Ziolo & Troup, 1983). As in dimethylammonium picrate (Walkinshaw, 1986) the geometry of the picrate ring shows significant distortions from the standard benzene ring with C—C 1·395 Å and C—C—C 120°. Lattice-energy calculations with the program *PCK*83 (Williams, 1983) using the potential curves given by Mirsky (1978) show that the lattice energies for the crystal structure with the conformation F(1), F(2) and F(3) and the crystal structure with the conformation F(1′), F(2′) and F(3′) differ only by 1·0 kJ mol^{-1}.

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* Lists of H-atom coordinates, anisotropic thermal parameters, structure-factor amplitudes and least-squares planes and dihedral angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44524 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Diméthylamino-3 Diméthyl-5,8 Carbazolecarbaldéhyde-4

Par B. Viossat

Laboratoire de Chimie minérale, UFR de Médecine et de Pharmacie, 34 *rue du Jardin des Plantes,*
86034 *Poitiers CEDEX, France*

N. Rodier

Laboratoire de Chimie minérale, Faculté des Sciences pharmaceutiques et biologiques, rue J.-B. Clément,
92296 *Châtenay-Malabry CEDEX, France*

et C. Gansser et C. Viel

Laboratoire de Chimie thérapeutique UA 496 *CNRS, Faculté des Sciences pharmaceutiques et biologiques,*
rue J.-B. Clément, 92296 *Châtenay-Malabry CEDEX, France*

(*Reçu le* 29 *avril* 1987, *accepté le* 2 *novembre* 1987)

Abstract. $C_{17}H_{18}N_2O$, $M_r = 266{\cdot}3$, monoclinic, $P2_1/c$, $a = 8{\cdot}397$ (1), $b = 13{\cdot}506$ (2), $c = 13{\cdot}656$ (3) Å, $\beta = 117{\cdot}01(1)°$, $V = 1379{\cdot}8(8)$ Å^3, $Z = 4$, $D_m = 1{\cdot}24$, $D_x = 1{\cdot}282$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}7107$ Å, $\mu = 0{\cdot}075$ mm^{-1}, $F(000) = 568$, room temperature. $R = 0{\cdot}035$ for 1641 independent reflections $[I > 3\sigma(I)]$. The Vilsmeier–Haack formylation of 3-dimethylamino-5,8-dimethylcarbazole leads to several carbaldehydes depending on the pH of the medium. One of them, the title compound, has been analysed by X-ray crystallography to determine with certainty the position of the formyl group. The usual planar geometry of the carbazole group is distorted in this molecule with the largest deviation from the mean plane being 0·186 (2) Å. The molecules are linked together by N—H···O hydrogen bonds and form layers which spread out along the $y = \pm\frac{1}{4}$ planes.

Partie expérimentale. Masse volumique par flottaison. Cristal prismatique: 0,25 × 0,30 × 0,40 mm. Dimensions de la maille déterminées sur monocristal avec 25 réflexions telles que $7{,}79 \le \theta \le 19{,}38°$. Diffractomètre Enraf–Nonius CAD-4. $0{,}039 \le (\sin\theta)/\lambda \le 0{,}595$ Å^{-1}; $0 \le h \le 9$, $0 \le k \le 16$, $-16 \le l \le 14$. Réflexions de

0108-2701/88/030581-03$03.00

Tableau 1. *Coordonnées atomiques relatives, facteurs de température isotropes équivalents et écarts-type*

$B_{éq} = \frac{4}{3}(\beta_{11}a^2 + \beta_{22}b^2 + \beta_{33}c^2 + \beta_{12}ab\cos\gamma + \beta_{13}ac\cos\beta + \beta_{23}bc\cos\alpha)$.

	x	y	z	$B_{éq}$(Å^2)
C(1)	0,5590 (2)	0,1603 (1)	0,0507 (1)	3,60 (4)
C(1a)	0,5615 (2)	0,2470 (1)	0,1057 (1)	2,98 (4)
C(2)	0,4242 (2)	0,1461 (1)	−0,0538 (1)	3,62 (4)
C(3)	0,2844 (2)	0,2144 (1)	−0,1044 (1)	3,08 (4)
C(4)	0,2818 (2)	0,3006 (1)	−0,0460 (1)	2,76 (4)
C(4a)	0,4309 (2)	0,3205 (1)	0,0573 (1)	2,63 (3)
C(5)	0,4293 (2)	0,5017 (1)	0,1335 (1)	3,07 (4)
C(5a)	0,4831 (2)	0,4017 (1)	0,1358 (1)	2,71 (3)
C(6)	0,5189 (2)	0,5556 (1)	0,2288 (1)	3,86 (4)
C(7)	0,6583 (2)	0,5162 (2)	0,3240 (1)	4,07 (5)
C(8)	0,7215 (2)	0,4220 (1)	0,3276 (1)	3,39 (4)
C(8a)	0,6350 (2)	0,3679 (1)	0,2301 (1)	2,93 (4)
N(9)	0,6809 (2)	0,2756 (1)	0,2100 (1)	3,39 (3)
N(10)	0,1436 (2)	0,1941 (1)	−0,2077 (1)	3,91 (4)
C(11)	0,1171 (3)	0,0916 (2)	−0,2459 (2)	5,45 (6)
C(12)	0,1098 (3)	0,2641 (2)	−0,2955 (1)	5,36 (6)
C(13)	0,1169 (2)	0,3531 (1)	−0,0706 (1)	3,27 (4)
O(14)	−0,0233 (2)	0,3534 (1)	−0,1549 (1)	4,57 (3)
C(15)	0,2916 (2)	0,5532 (1)	0,0333 (1)	3,88 (4)
C(16)	0,8707 (3)	0,3776 (2)	0,4275 (1)	4,38 (5)

Tableau 2. *Distances interatomiques* (Å), *angles valenciels* (°) *et écarts-type*

C(1)–C(1a)	1,386 (3)	C(5)–C(15)	1,502 (2)
C(1)–C(2)	1,374 (2)	C(5a)–C(8a)	1,415 (2)
C(1a)–C(4a)	1,402 (2)	C(6)–C(7)	1,401 (2)
C(1a)–N(9)	1,374 (2)	C(7)–C(8)	1,370 (3)
C(2)–C(3)	1,404 (2)	C(8)–C(8a)	1,400 (2)
C(3)–C(4)	1,417 (2)	C(8)–C(16)	1,496 (2)
C(3)–N(10)	1,396 (2)	C(8a)–N(9)	1,368 (2)
C(4)–C(4a)	1,424 (2)	N(9)···O(14^{i})	2,906 (2)*
C(4)–C(13)	1,452 (2)	N(10)–C(11)	1,461 (3)
C(4a)–C(5a)	1,455 (2)	N(10)–C(12)	1,450 (3)
C(5)–C(5a)	1,420 (2)	C(13)–O(14)	1,218 (2)
C(5)–C(6)	1,379 (2)		
C(1a)–C(1)–C(2)	118,9 (2)	C(4a)–C(5a)–C(5)	135,6 (1)
C(1)–C(1a)–C(4a)	121,8 (1)	C(4a)–C(5a)–C(8a)	105,8 (1)
C(1)–C(1a)–N(9)	128,6 (1)	C(5)–C(5a)–C(8a)	118·2 (1)
C(4a)–C(1a)–N(9)	109,6 (1)	C(5)–C(6)–C(7)	122,9 (2)
C(1)–C(2)–C(3)	122,0 (2)	C(6)–C(7)–C(8)	122,2 (2)
C(2)–C(3)–C(4)	119,1 (1)	C(7)–C(8)–C(8a)	115,2 (1)
C(2)–C(3)–N(10)	120,2 (2)	C(7)–C(8)–C(16)	123,7 (2)
C(4)–C(3)–N(10)	120,5 (1)	C(8a)–C(8)–C(16)	121,1 (2)
C(3)–C(4)–C(4a)	118,8 (1)	C(5a)–C(8a)–C(8)	124,2 (2)
C(3)–C(4)–C(13)	121,9 (1)	C(5a)–C(8a)–N(9)	109,3 (1)
C(4a)–C(4)–C(13)	117,0 (2)	C(8)–C(8a)–N(9)	126,5 (1)
C(1a)–C(4a)–C(4)	118,8 (1)	C(1a)–N(9)–C(8a)	109,0 (1)
C(1a)–C(4a)–C(5a)	106,1 (1)	C(3)–N(10)–C(11)	118,0 (1)
C(4)–C(4a)–C(5a)	135,0 (1)	C(3)–N(10)–C(12)	117,8 (2)
C(5a)–C(5)–C(6)	116,8 (1)	C(11)–N(10)–C(12)	112,5 (2)
C(5a)–C(5)–C(15)	124,5 (1)	C(4)–C(13)–O(14)	129,1 (2)
C(6)–C(5)–C(15)	118,6 (2)	N(9)–H(9)···O(14^{i})	174 (2)*

* Liaison hydrogène; (i) $1+x, \frac{1}{2}-y, \frac{1}{2}+z$.

contrôle $\bar{3}35$, 053 et 421; $\sigma(I)/I$ (contrôle) = 2×10^{-3}. 2419 réflexions indépendantes mesurées, 778 réflexions inobservées [$I < 3\sigma(I)$]. Pas de correction d'absorption. Méthodes directes, programme *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982). Coordonnées des H: série de Fourier des ΔF. Facteurs de diffusion des *International Tables for X-ray Crystallography* (1974). Affinement sur F. Paramètres affinés: x, y, z de tous les atomes et β_{ij} de O, N et C. $R = 0{,}035$, $wR = 0{,}042$, $w = 1/\sigma^2(F)$, $S = 1{,}55$, $(\Delta/\sigma)_{\max} = 0{,}00$. $|\Delta\rho|_{\max} = 0{,}12$ (3) e Å^{-3}. Programmes de calcul du système *SDP* (Frenz, 1982). Angles des plans moyens: *Best-Plane Program* (Ito & Sugawara, 1983). Dessin de la molécule (Fig. 1): programme *ORTEP* (Johnson, 1965).

Les paramètres atomiques sont rassemblés dans le Tableau 1, les distances et les angles dans le Tableau 2.* La Fig. 2 montre une représentation de la structure vue parallèlement à l'axe *a*.

Littérature. Structure du benzyl-9 diméthylamino-3 diméthyl-5,8 carbazolecarbaldéhyde-4 (Viossat,

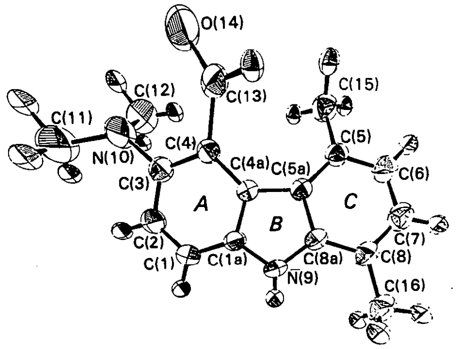

Fig. 1. Vue de la molécule en perspective, numérotation des atomes et lettres utilisées pour désigner les cycles.

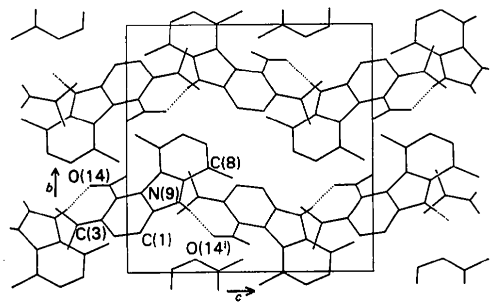

Fig. 2. Représentation de la structure vue parallèlement à l'axe *a*.

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* Les listes des facteurs de structure, des facteurs d'agitation thermique anisotrope, des paramètres des atomes d'hydrogène, des distances intermoléculaires, des distances des atomes aux plans moyens et des angles de torsion ont été déposées au dépôt d'archives de la British Library Document Supply Centre (Supplementary Publication No. SUP 44508: 17 pp.). On peut en obtenir des copies en s'adressant à: The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, Angleterre.

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Acta Cryst. (1988). C**44**, 583–584

Structure of (1*R*,3*R*)- and (1*S*,3*S*)-1-(1-Methylindol-2-yl)-1,3-diphenylbutane-1,3-diol

By F. H. Cano and C. Foces-Foces

Instituto de Química Física 'Rocasolano', Serrano 119, *Madrid* 28006, *Spain*

T. Aznar-Saliente and J. Sepulveda-Arques

Facultad de Farmacia, Universidad de Valencia, Valencia 46010, *Spain*

and R. A. Jones

*School of Chemical Sciences, University of East Anglia, Norwich NR*4 *7TJ, England*

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Abstract. $C_{25}H_{25}NO_2$, $M_r = 371{\cdot}478$, monoclinic, Pc, $a = 8{\cdot}3906\,(4)$, $b = 13{\cdot}4356\,(8)$, $c = 8{\cdot}9449\,(3)$ Å, $\beta = 91{\cdot}518\,(7)°$, $V = 1008{\cdot}03\,(8)$ Å^3, $Z = 2$, $D_x = 1{\cdot}2239$ g cm^{-3}, $\lambda(\mathrm{Cu}\ K\alpha) = 1{\cdot}5418$ Å, $\mu = 5{\cdot}698$ cm^{-1}, $F(000) = 396$, room temperature, $R = 0{\cdot}042$ for 1498 reflections with $I > 2\sigma(I)$. The lattice cell comprises a pair of the *R,R* and *S,S* enantiomers with the planes of the two phenyl rings of each stereoisomer orientated at *ca* 90° to the coplanar structure of the indole ring and attached carbon chain. Intramolecular hydrogen bonding is evident in the crystal structure between the proton of the 1-hydroxy group and the O atom of the 3-hydroxy group within each enantiomer, whilst the enantiomeric pairs are linked by weak hydrogen bonds between the proton of the 3-hydroxy group of one stereoisomer and the O atom of the 1-hydroxy group of the second isomer.

Experimental. An enantiomeric mixture of the (*S,S*)- and (*R,R*)-diols was obtained as a by-product of the reaction of 1-methylindol-2-yl lithium and acetophenone (Jones, Fresneda, Aznar-Saliente & Sepulveda-Arques, 1984). A transparent, colourless, prismatic crystal of the racemate was obtained from cyclohexane, with dimensions of *ca* 0·40 × 0·13 × 0·08 mm. Intensities were measured on a Philips PW1100 diffractometer, with graphite-monochromated Cu *Kα* radiation, with $\omega/2\theta$ scans and 1·5° width. Lattice parameters were obtained from a least-squares fit of the angular 2θ positions of 40 reflections, with $\theta < 45°$. Of the 1724 independent data, 1498 were considered as

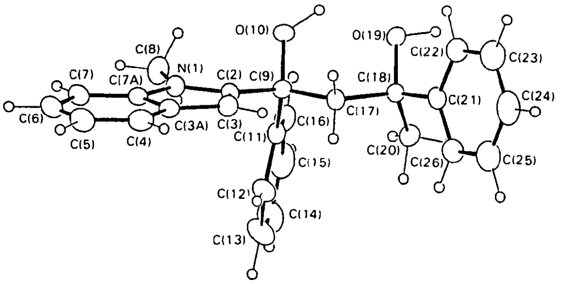

Fig. 1. *ORTEP*II (Johnson, 1976) view of the *R,R* stereoisomer showing atomic numbering.