

**Related literature.** 2-[ $\alpha$ -(Methylthio)benzylidene-amino]-2-phenyl-1,1-ethylenedicarbonitrile (Balcazar, Florencio & García-Blanco, 1985; Yeh, Moriarty, Yeh & Ramey, 1972).

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## Benzyl-9 Diméthyl-1,4 Diméthylamino-6 Carbazoledicarbaldéhyde-3,5

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**Abstract.**  $C_{25}H_{24}N_2O_2$ ,  $M_r = 384.5$ , triclinic,  $P\bar{1}$ ,  $a = 9.860$  (3),  $b = 10.953$  (2),  $c = 12.304$  (2) Å,  $\alpha = 125.60$  (2),  $\beta = 95.25$  (2),  $\gamma = 105.54$  (2)°,  $V = 987.5$  Å<sup>3</sup>,  $Z = 2$ ,  $D_m = 1.27$ ,  $D_x = 1.293$  Mg m<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.7107$  Å,  $\mu = 0.077$  mm<sup>-1</sup>,  $F(000) = 408$ , room temperature,  $R = 0.051$  for 1536 independent reflections [ $I > 3\sigma(I)$ ]. The structure was solved as it was impossible to infer the positions occupied by the two formyl groups from the NMR spectroscopy. The steric hindrance entails a distortion of the carbazole group which is not as planar as it is in the carbazole molecule. The distances from the atoms of the carbazole group to its mean plane are  $\leq 0.216$  (4) Å. The phenyl ring of the benzyl group and the pyrrole ring are almost perpendicular [ $85.7$  (2)°]. The molecules form columns parallel to the [010] axis.

**Partie expérimentale.** Masse volumique par flottaison. Cristal prismatique:  $0,12 \times 0,20 \times 0,30$  mm. Dimensions de la maille déterminées sur monocristal avec 25 réflexions telles que  $6,23 \leq \theta \leq 13,64^\circ$ . Diffractomètre Enraf-Nonius CAD-4.  $0 \leq (\sin \theta) / \lambda \leq 0,550$  Å<sup>-1</sup>;  $-10$

$\leq h \leq 10$ ,  $0 \leq k \leq 11$ ,  $-13 \leq l \leq 10$ . Réflexions de contrôle:  $\bar{3}35$ , 120 et  $23\bar{3}$ .  $\sigma(I)/I$  (contrôle) =  $6 \times 10^{-3}$ . Diminution de  $I$ : 1,0%. 2751 réflexions indépendantes mesurées, 1215 réflexions inobservées [ $I \leq 3\sigma(I)$ ].

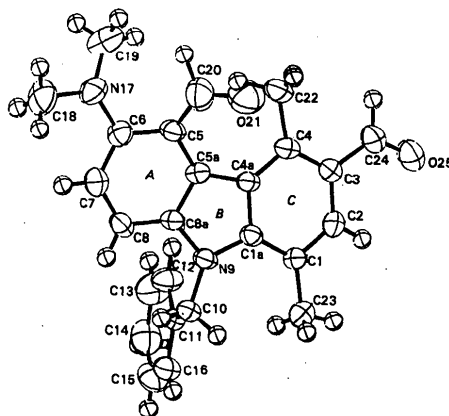


Fig. 1. Vue de la molécule en perspective, numérotation des atomes et lettres utilisées pour désigner les cycles.

Méthodes directes, programme *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982). Coordonnées des H: série de Fourier des  $\Delta F$ . Facteurs de diffusion des *International Tables for X-ray Crystallography* (1974). Affinement sur  $F$ . Paramètres affinés:  $x, y, z$  de tous les atomes et  $\beta_{ij}$  de O, N et C.  $R=0,052$ ,  $wR=0,061$ ,  $w=1/\sigma^2(F)$ ,  $S=2,01$ ,  $(\Delta/\sigma)_{\max}=0,48$ ,  $|\Delta\rho|_{\max}=0,20$  (5) e  $\text{\AA}^{-3}$ . Programmes de calcul du système *SDP* (Frenz, 1982) et *Best-Plane Program* (Ito & Sugawara, 1983). Dessin de la molécule (Fig. 1): programme *ORTEP* (Johnson, 1965). La Fig. 2 montre la structure vue parallèlement à l'axe  $b$ . Les paramètres atomiques sont rassemblés dans le Tableau 1, les distances et les angles dans le Tableau 2.\*

**Littérature.** Structure du benzyl-9 diméthyl-5,8 diméthylamino-3 carbazolecarbaldéhyde-4 (Viossat, Rodier, Gansser & Viel, 1987). Structure du carbazole (Kurahashi, Fukuyo, Shimada, Furusaki & Nitta, 1969). Structure du diméthyl-5,11 6*H*-pyrido[4,3-*b*]-carbazole (Courseille, Busetta & Hospital, 1974).

\* Les listes des facteurs de structure, des plans moyens, des distances C—H, des angles de torsion, des facteurs d'agitation thermique anisotrope et des paramètres des atomes d'hydrogène ont été déposées au dépôt d'archives de la British Library Document Supply Centre (Supplementary Publication No. SUP 43824: 20 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.

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

$$B_{\text{eq}} = \frac{1}{3}(\beta_{11}a^2 + \beta_{22}b^2 + \beta_{33}c^2 + \beta_{12}ab\cos\gamma + \beta_{13}accos\beta + \beta_{23}bccos\alpha).$$

	$x$	$y$	$z$	$B_{\text{eq}}(\text{\AA}^2)$
C(1)	0,9729 (4)	0,2920 (3)	0,6067 (3)	3,0 (1)
C(1a)	0,8789 (4)	0,1255 (3)	0,5242 (3)	2,8 (1)
C(2)	0,9534 (4)	0,3923 (4)	0,7347 (3)	3,6 (1)
C(3)	0,8437 (4)	0,3397 (4)	0,7812 (3)	3,4 (1)
C(4)	0,7501 (4)	0,1752 (4)	0,6984 (3)	3,2 (1)
C(4a)	0,7743 (4)	0,0653 (3)	0,5718 (3)	2,72 (9)
C(5)	0,5958 (4)	-0,2399 (4)	0,4469 (4)	3,4 (1)
C(5a)	0,6991 (4)	-0,1093 (3)	0,4606 (3)	3,0 (1)
C(6)	0,5272 (4)	-0,3948 (4)	0,3121 (3)	3,7 (1)
C(7)	0,5808 (5)	-0,4204 (4)	0,2022 (4)	4,3 (1)
C(8)	0,6941 (4)	-0,3012 (4)	0,2193 (3)	3,9 (1)
C(8a)	0,7521 (4)	-0,1449 (3)	0,3490 (3)	2,88 (9)
N(9)	0,8647 (3)	-0,0043 (3)	0,3893 (2)	3,07 (8)
C(10)	0,9338 (4)	0,0006 (4)	0,2918 (3)	3,4 (1)
C(11)	0,8613 (4)	0,0571 (4)	0,2246 (3)	3,3 (1)
C(12)	0,9304 (5)	0,0970 (4)	0,1505 (4)	4,6 (1)
C(13)	0,8664 (5)	0,1459 (4)	0,0863 (3)	5,5 (1)
C(14)	0,7334 (5)	0,1569 (4)	0,0963 (4)	5,8 (1)
C(15)	0,6643 (5)	0,1185 (5)	0,1695 (4)	6,0 (1)
C(16)	0,7273 (4)	0,0691 (4)	0,2325 (3)	4,5 (1)
N(17)	0,4137 (4)	-0,5214 (3)	0,2913 (3)	4,9 (1)
C(18)	0,3681 (6)	-0,6890 (4)	0,1623 (4)	6,1 (2)
C(19)	0,3067 (5)	-0,4905 (5)	0,3661 (4)	6,2 (1)
C(20)	0,6048 (5)	-0,2444 (5)	0,5646 (4)	5,9 (2)
O(21)	0,6977 (4)	-0,1336 (3)	0,6842 (3)	7,2 (1)
C(22)	0,6161 (4)	0,1182 (4)	0,7332 (4)	4,5 (1)
C(23)	1,0844 (4)	0,3647 (4)	0,5632 (4)	4,3 (1)
C(24)	0,8279 (5)	0,4632 (4)	0,9139 (4)	4,5 (1)
O(25)	0,8962 (3)	0,6103 (3)	0,9850 (3)	5,8 (1)

Tableau 2. Distances interatomiques ( $\text{\AA}$ ), angles valentiels ( $^\circ$ ) et écarts-type

C(1)—C(1a)	1,408 (4)	C(6)—N(17)	1,393 (5)
C(1)—C(2)	1,370 (5)	C(7)—C(8)	1,361 (6)
C(1)—C(23)	1,504 (7)	C(8)—C(8a)	1,390 (3)
C(1a)—C(4a)	1,428 (6)	C(8a)—N(9)	1,394 (4)
C(1a)—N(9)	1,378 (3)	N(9)—C(10)	1,453 (6)
C(2)—C(3)	1,412 (6)	C(10)—C(11)	1,516 (7)
C(3)—C(4)	1,391 (4)	C(11)—C(12)	1,380 (7)
C(3)—C(24)	1,452 (5)	C(11)—C(16)	1,369 (6)
C(4)—C(4a)	1,403 (4)	C(12)—C(13)	1,375 (8)
C(4)—C(22)	1,514 (6)	C(13)—C(14)	1,359 (8)
C(4a)—C(5a)	1,444 (3)	C(14)—C(15)	1,360 (8)
C(5)—C(5a)	1,421 (6)	C(15)—C(16)	1,364 (9)
C(5)—C(6)	1,410 (3)	N(17)—C(18)	1,458 (4)
C(5)—C(20)	1,474 (8)	N(17)—C(19)	1,443 (7)
C(5a)—C(8a)	1,388 (6)	C(20)—O(21)	1,248 (4)
C(6)—C(7)	1,399 (7)	C(24)—O(25)	1,218 (4)
C(1a)—C(1)—C(2)	114,7 (4)	C(7)—C(6)—N(17)	120,9 (3)
C(1a)—C(1)—C(23)	125,6 (3)	C(6)—C(7)—C(8)	122,7 (3)
C(2)—C(1)—C(23)	119,6 (3)	C(7)—C(8)—C(8a)	118,4 (4)
C(1)—C(1a)—C(4a)	122,6 (3)	C(5a)—C(8a)—C(8)	121,7 (3)
C(1)—C(1a)—N(9)	129,3 (4)	C(5a)—C(8a)—N(9)	109,9 (2)
C(4a)—C(1a)—N(9)	108,0 (2)	C(8)—C(8a)—N(9)	128,4 (4)
C(1)—C(2)—C(3)	124,4 (3)	C(1a)—N(9)—C(8a)	108,6 (3)
C(2)—C(3)—C(4)	120,4 (3)	C(1a)—N(9)—C(10)	127,8 (3)
C(2)—C(3)—C(24)	117,9 (3)	C(8a)—N(9)—C(10)	122,8 (2)
C(4)—C(3)—C(24)	121,7 (4)	N(9)—C(10)—C(11)	113,2 (3)
C(3)—C(4)—C(4a)	117,4 (4)	C(10)—C(11)—C(12)	119,8 (4)
C(3)—C(4)—C(22)	121,7 (3)	C(10)—C(11)—C(16)	122,7 (4)
C(4a)—C(4)—C(22)	120,5 (3)	C(12)—C(11)—C(16)	117,5 (5)
C(1a)—C(4a)—C(4)	120,0 (3)	C(11)—C(12)—C(13)	121,2 (5)
C(1a)—C(4a)—C(5a)	106,9 (3)	C(12)—C(13)—C(14)	119,9 (5)
C(4)—C(4a)—C(5a)	132,6 (4)	C(13)—C(14)—C(15)	119,5 (6)
C(5a)—C(5)—C(6)	118,7 (4)	C(14)—C(15)—C(16)	120,6 (5)
C(5a)—C(5)—C(20)	121,6 (3)	C(11)—C(16)—C(15)	121,3 (5)
C(6)—C(5)—C(20)	114,4 (4)	C(6)—N(17)—C(18)	119,8 (4)
C(4a)—C(5a)—C(5)	134,9 (3)	C(6)—N(17)—C(19)	121,4 (3)
C(4a)—C(5a)—C(8a)	106,3 (3)	C(18)—N(17)—C(19)	115,5 (3)
C(5)—C(5a)—C(8a)	118,8 (2)	C(5)—C(20)—O(21)	123,6 (5)
C(5)—C(6)—C(7)	118,4 (4)	C(3)—C(24)—O(25)	125,1 (5)
C(5)—C(6)—N(17)	120,5 (4)		

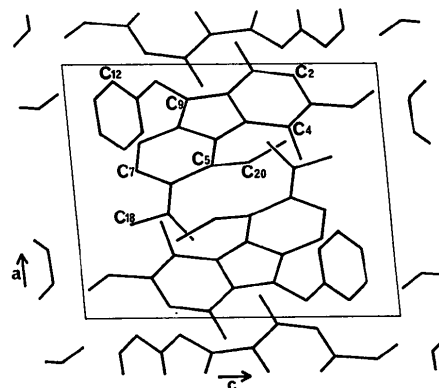


Fig. 2. Représentation de la structure vue parallèlement à l'axe  $b$ .

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## International Union of Crystallography

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### The Ewald Prize

The first Ewald Prize for outstanding contributions to the science of crystallography has been awarded jointly to Professor J. M. Cowley and Dr A. F. Moodie, for their outstanding achievements in electron diffraction and microscopy, especially for their fundamental contributions to the theory and technique of direct imaging of crystal structures and structure defects by high-resolution electron microscopy.

Their pioneering work on the dynamical scattering of electrons was reported in a series of papers in *Acta Crystallographica* and other journals from 1957 onwards. A theory of Fourier images led them to the multi-slice formulation of the scattering of an electron wave in its passage through a crystal. This formulation is able to take into account many hundreds of scattered beams, and has become the basis of widely used computer programs. The theory allows electron micrographs, obtained with modern high-resolution instruments, to be reliably and quantitatively interpreted, and used for the determination of the structures of both perfect crystals and crystals containing defects.

Professor Cowley and Dr Moodie, together and separately, have made many further contributions to theory, methods and results in electron diffraction and microscopy.

Their work has often stressed a unified approach to diffraction and microscopy through physical optics. An overview of the whole field may be found in Professor Cowley's book *Diffraction Physics* [(1981). Amsterdam: North-Holland].

John Maxwell Cowley, born in Australia in 1923 and a graduate of Adelaide University, was formerly a Chief Research Scientist at the Division of Chemical Physics, CSIRO, Melbourne, Australia. Later he was Professor of Physics at the University of Melbourne, and since 1970 has been the Galvin Professor of Physics at Arizona State University, Tempe, USA.

Alexander Forbes Moodie, born in Scotland in 1923, graduated from St Andrews University in 1948. Since then he has been a member of CSIRO in Australia where he is a Chief Research Scientist at the Division of Chemical Physics. This Division was incorporated into the Division of Materials Science and Technology at the end of 1986.

The presentation of the Ewald Prize, which consists of a medal and a certificate for each awardee and a shared award of US \$20 000, will take place at the Opening Ceremony of the XIV International Congress of Crystallography at Perth, Western Australia, on 12 August 1987. An honorary medal will also be presented to the Ewald family during the ceremony.