$wR = 0.047$
$S = 1.49$
906 reflections
137 parameters
H atoms were refined with one overall U_{iso}
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *SHELX*76 (Sheldrick, 1976)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$B_{eq} = (4/3)\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
Cl	0.6410 (1)	0.0435 (3)	0.5583 (1)	6.04 (5)
N	1.0358 (3)	−0.0072 (6)	0.6319 (2)	3.3 (1)
O(1)	0.9848 (3)	0.3551 (6)	0.7022 (2)	4.4 (1)
O(2)	1.2610 (3)	0.2545 (7)	0.7665 (2)	5.5 (1)
O(3)	0.9000 (3)	−0.2222 (7)	0.5490 (2)	5.9 (1)
C(2)	1.0612 (4)	0.1833 (9)	0.6855 (2)	3.6 (1)
C(3)	1.2090 (4)	0.1287 (9)	0.7174 (2)	4.0 (1)
C(4)	1.3891 (5)	−0.206 (1)	0.6820 (2)	4.7 (2)
C(5)	1.4137 (5)	−0.410 (1)	0.6353 (3)	5.0 (2)
C(6)	1.3092 (5)	−0.4888 (9)	0.5857 (2)	4.8 (2)
C(7)	1.1803 (4)	−0.3712 (8)	0.5802 (2)	4.1 (2)
C(8)	1.1576 (4)	−0.1680 (8)	0.6270 (2)	3.5 (1)
C(9)	1.2607 (4)	−0.0892 (8)	0.6768 (2)	3.7 (1)
C(10)	0.9112 (4)	−0.0469 (9)	0.5917 (2)	3.8 (1)
C(11)	0.7953 (4)	0.1402 (9)	0.6066 (2)	4.2 (1)

Table 2. *Selected geometric parameters* (Å, °)

Cl—C(11)	1.768 (4)	N—C(2)	1.408 (5)
N—C(8)	1.442 (5)	N—C(10)	1.398 (5)
O(1)—C(2)	1.196 (5)	O(2)—C(3)	1.209 (5)
O(3)—C(10)	1.198 (5)	C(2)—C(3)	1.542 (6)
C(3)—C(9)	1.452 (6)	C(4)—C(5)	1.390 (7)
C(4)—C(9)	1.376 (6)	C(5)—C(6)	1.393 (7)
C(6)—C(7)	1.382 (6)	C(7)—C(8)	1.385 (6)
C(8)—C(9)	1.386 (6)	C(10)—C(11)	1.510 (6)
C(2)—N—C(8)	109.1 (3)	C(6)—C(7)—C(8)	117.0 (4)
C(2)—N—C(10)	126.3 (3)	N—C(8)—C(7)	128.7 (4)
C(8)—N—C(10)	124.5 (3)	N—C(8)—C(9)	110.5 (3)
N—C(2)—O(1)	127.2 (4)	C(7)—C(8)—C(9)	120.7 (4)
N—C(2)—C(3)	105.9 (3)	C(3)—C(9)—C(4)	129.1 (4)
O(1)—C(2)—C(3)	126.9 (4)	C(3)—C(9)—C(8)	108.6 (4)
O(2)—C(3)—C(2)	122.4 (4)	C(4)—C(9)—C(8)	122.2 (4)
O(2)—C(3)—C(9)	131.8 (4)	N—C(10)—O(3)	120.5 (4)
C(2)—C(3)—C(9)	105.8 (3)	N—C(10)—C(11)	115.8 (3)
C(5)—C(4)—C(9)	117.8 (4)	O(3)—C(10)—C(11)	123.6 (4)
C(4)—C(5)—C(6)	119.6 (4)	Cl—C(11)—C(10)	110.4 (3)
C(5)—C(6)—C(7)	122.7 (4)		

Data were corrected for Lorentz, polarization and absorption effects. The structure was solved by direct methods. H atoms were found in a difference synthesis and included as fixed contributors with an overall isotropic displacement factor that refined to $U_{iso} = 0.081$ (6) Å^2. Programs used were: *SHELXS*86 (Sheldrick, 1985), *SHELX*76 (Sheldrick, 1976) and *ORTEP* (Johnson, 1965). Most of the calculations were performed on a MicroVAX 3600 computer at the Weizmann Institute of Science, Israel.

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Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: LI1118). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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7,10-Dimethoxybenzo[*b*]carbazole†

J. Seetharaman and S. S. Rajan*

Department of Crystallography and Biophysics, University of Madras, Madras 600025, India

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Abstract

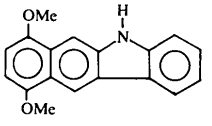
The asymmetric unit of the title compound, $C_{18}H_{15}NO_2$, contains two crystallographically independent molecules with similar conformations. Each molecule consists of a carbazole ring system and a fused substituted benzene ring. The molecules are highly planar and their conformations are similar to that of ellipticine [Courseille, Busetta & Hospital (1974). *Acta Cryst.* B**30**, 2628–2631], which is a DNA-intercalating molecule.

Comment

Preliminary studies of carbazole derivatives have shown that the presence of oxygenated substituents increases their biological activity (Hewlins, Oliveira-Campos & Shannon, 1984). Their structures are analogous to that of ellipticine (Courseille, Busetta & Hospital, 1974), a plant alkaloid having pronounced anti-tumour activity (Hartwell & Abbott, 1969), and they have been found to have DNA-intercalating properties (Neidle, 1979; Gale, Cundliffe, Reynolds,

† DCB contribution No. 837.

Richmond & Waring, 1981; Aggarwal, Neidle & Sainsbury, 1983). Ellipticine derivatives with various substituents have been synthesized and their DNA affinity and anti-tumour activities have been tested (Le Pecq, Xuong, Gosse & Paoletti, 1974; Paoletti, Cros, Xuong, Lecointe & Moisand, 1979). The title compound, (I), a carbazole derivative similar to ellipticine, was synthesized by means of the reductive condensation method (Rajeswaran & Srinivasan, 1994) and was crystallized from acetone.



(I)

A perspective view (*PLUTO*; Motherwell & Clegg, 1976) of the molecule is shown in Fig. 1. The mean values of the C(sp^2)—C(sp^2) bond lengths in molecules *A* and *B* are 1.397 (2) and 1.397 (1) Å, respectively, and they agree well with those in related compounds (Aggarwal, Neidle & Sainsbury, 1983; Reimers, Guth & Wang, 1984). The molecules are highly planar [$\sum(\Delta/\sigma)^2 = 32$ and 39 for molecules *A* and *B*, respectively], as found in ellipticine derivatives such as 5-*n*-butyl-11-dimethylellipticine and 9-methoxyellipticine (Aggarwal, Neidle & Sainsbury, 1983), 7-methylellipticine (Kuroda & Sainsbury, 1984) and ellipticine-iodoCpG$^+$ (Jain, Bhandary & Sobell, 1979). This planarity is said to be essential for intercalation with DNA (Neidle, 1979; Gale, Cundliffe, Reynolds, Richmond & Waring, 1981; Aggarwal, Neidel & Sainsbury, 1983). The deviations of the methoxy C atoms from the plane of the benzene ring are 0.038 (9) and 0.050 (10) Å in molecule *A* and 0.194 (8) and 0.109 (10) Å in molecule *B*. The molecules in the unit cell are held together by van der Waal's forces.

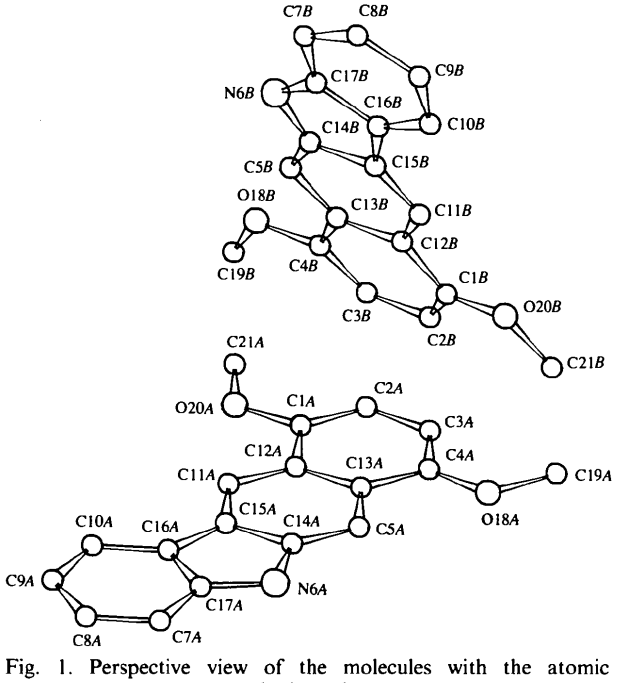


Fig. 1. Perspective view of the molecules with the atomic numbering scheme.

Experimental

Crystal data

$C_{18}H_{15}NO_2$
$M_r = 277.31$
Trigonal
$P3_1$
$a = 12.294$ (3) Å
$c = 15.945$ (3) Å
$V = 2087$ (3) Å^3
$Z = 6$
$D_x = 1.324$ Mg m^{-3}
Cu $K\alpha$ radiation
$\lambda = 1.5418$ Å
Cell parameters from 20 reflections
$\theta = 20$–$30°$
$\mu = 0.62$ mm^{-1}
$T = 293$ K
Rectangular
0.35 × 0.25 × 0.20 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: empirical
$T_{min} = 0.84$, $T_{max} = 0.97$
2258 measured reflections
2258 independent reflections
1525 observed reflections [$I > 3\sigma(I)$]
$\theta_{max} = 70°$
$h = -14 \rightarrow 14$
$k = 0 \rightarrow 13$
$l = 0 \rightarrow 19$
3 standard reflections monitored every 100 reflections
intensity decay: <2%

Refinement

Refinement on F
$R = 0.043$
$wR = 0.046$
$S = 0.97$
1525 reflections
499 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F) + 0.00259F^2]$
$(\Delta/\sigma)_{max} = 0.041$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *SHELX*76 (Sheldrick, 1976)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
C1*A*	0.6973 (5)	0.3160 (6)	−0.0946 (4)	0.051 (5)
C2*A*	0.6500 (6)	0.3910 (7)	−0.0710 (5)	0.061 (6)
C3*A*	0.7057 (7)	0.5143 (7)	−0.1015 (5)	0.074 (7)
C4*A*	0.8069 (6)	0.5633 (6)	−0.1521 (4)	0.052 (5)
C5*A*	0.9675 (5)	0.5377 (5)	−0.2284 (4)	0.043 (5)
N6*A*	1.1167 (5)	0.4863 (5)	−0.3012 (4)	0.055 (5)
C7*A*	1.2182 (6)	0.3635 (7)	−0.3500 (5)	0.069 (7)
C8*A*	1.2112 (7)	0.2498 (8)	−0.3441 (5)	0.079 (8)
C9*A*	1.1174 (7)	0.1528 (7)	−0.2966 (6)	0.080 (7)
C10*A*	1.0292 (6)	0.1687 (6)	−0.2520 (5)	0.063 (6)
C11*A*	0.8551 (5)	0.2863 (5)	−0.1713 (4)	0.046 (5)
C12*A*	0.8039 (5)	0.3615 (6)	−0.1487 (4)	0.046 (5)
C13*A*	0.8620 (5)	0.4884 (6)	−0.1764 (4)	0.048 (5)
C14*A*	1.0131 (5)	0.4601 (5)	−0.2500 (4)	0.045 (5)

C15*A*	0.9589 (5)	0.3335 (5)	−0.2228 (4)	0.046 (5)
C16*A*	1.0342 (6)	0.2846 (6)	−0.2580 (4)	0.051 (5)
C17*A*	1.1288 (6)	0.3802 (6)	−0.3057 (4)	0.053 (5)
O18*A*	0.8688 (4)	0.6830 (4)	−0.1833 (3)	0.071 (4)
C19*A*	0.8227 (7)	0.7627 (7)	−0.1584 (6)	0.090 (8)
O20*A*	0.6516 (4)	0.1940 (4)	−0.0680 (3)	0.065 (4)
C21*A*	0.5447 (7)	0.1404 (8)	−0.0142 (6)	0.080 (7)
C1*B*	1.1408 (5)	0.7573 (5)	0.0314 (4)	0.048 (5)
C2*B*	1.0217 (6)	0.6721 (6)	0.0118 (5)	0.063 (5)
C3*B*	0.9648 (6)	0.5486 (5)	0.0437 (5)	0.052 (5)
C4*B*	1.0305 (5)	0.5118 (5)	0.0945 (4)	0.043 (4)
C5*B*	1.2242 (5)	0.5650 (5)	0.1731 (4)	0.046 (5)
N6*B*	1.4302 (5)	0.6457 (4)	0.2470 (4)	0.054 (4)
C7*B*	1.6466 (6)	0.7979 (6)	0.3003 (5)	0.057 (5)
C8*B*	1.7390 (6)	0.9234 (7)	0.2955 (5)	0.065 (6)
C9*B*	1.7260 (6)	1.0098 (6)	0.2483 (5)	0.064 (6)
C10*B*	1.6211 (5)	0.9730 (5)	0.1997 (4)	0.050 (5)
C11*B*	1.3360 (5)	0.8145 (5)	0.1122 (4)	0.045 (4)
C12*B*	1.2125 (5)	0.7260 (5)	0.0882 (4)	0.044 (5)
C13*B*	1.1558 (5)	0.6000 (5)	0.1195 (4)	0.043 (4)
C14*B*	1.3461 (6)	0.6551 (5)	0.1954 (4)	0.052 (5)
C15*B*	1.4001 (5)	0.7801 (5)	0.1647 (4)	0.042 (4)
C16*B*	1.5246 (5)	0.8468 (5)	0.2026 (4)	0.045 (4)
C17*B*	1.5388 (5)	0.7609 (5)	0.2525 (4)	0.045 (4)
O18*B*	0.9837 (4)	0.3928 (4)	0.1263 (3)	0.051 (3)
C19*B*	0.8640 (6)	0.2988 (6)	0.0969 (5)	0.062 (6)
O20*B*	1.2049 (4)	0.8773 (4)	0.0020 (3)	0.060 (3)
C21*B*	1.1417 (7)	0.9157 (7)	−0.0542 (6)	0.077 (7)

Table 2. *Selected geometric parameters* (Å, °)

C1*A*—O20*A*	1.379 (8)	C1*B*—O20*B*	1.362 (7)
C4*A*—O18*A*	1.368 (8)	C4*B*—O18*B*	1.374 (7)
N6*A*—C14*A*	1.408 (9)	N6*B*—C14*B*	1.371 (10)
N6*A*—C17*A*	1.387 (11)	N6*B*—C17*B*	1.380 (6)
O18*A*—C19*A*	1.412 (12)	O18*B*—C19*B*	1.421 (7)
O20*A*—C21*A*	1.425 (9)	O20*B*—C21*B*	1.421 (11)
C12*A*—C1*A*—O20*A*	114.0 (6)	C12*B*—C1*B*—O20*B*	113.9 (5)
C2*A*—C1*A*—O20*A*	124.7 (6)	C2*B*—C1*B*—O20*B*	125.4 (6)
C3*A*—C4*A*—O18*A*	126.3 (7)	C3*B*—C4*B*—O18*B*	124.6 (6)
C13*A*—C4*A*—O18*A*	113.7 (6)	C13*B*—C4*B*—O18*B*	115.1 (6)
C14*A*—N6*A*—C17*A*	109.0 (5)	C14*B*—N6*B*—C17*B*	109.6 (5)
C5*A*—C14*A*—N6*A*	128.7 (5)	C5*B*—C14*B*—N6*B*	130.0 (5)
N6*A*—C14*A*—C15*A*	107.6 (5)	N6*B*—C14*B*—C15*B*	109.5 (6)
N6*A*—C17*A*—C16*A*	109.1 (6)	N6*B*—C17*B*—C16*B*	108.4 (5)
N6*A*—C17*A*—C7*A*	128.5 (6)	N6*B*—C17*B*—C7*B*	130.1 (6)
C4*A*—O18*A*—C19*A*	116.3 (6)	C4*B*—O18*B*—C19*B*	117.1 (5)
C1*A*—O20*A*—C21*A*	117.9 (6)	C1*B*—O20*B*—C21*B*	117.6 (5)

Data collection, cell refinement and data reduction: *SDP* (Frenz, 1978). Structure solution: *SHELXS*86 (Sheldrick, 1985). Structure refinement: *SHELX*76 (Sheldrick, 1976). Calculation of geometrial parameters: *PARST* (Nardelli, 1983). Molecular graphics: *PLUTO* (Motherwell & Clegg, 1976). All H atoms were located from a difference Fourier map and were refined isotropically.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, bond distances involving H atoms, least-squares-planes data and torsion angles have been deposited with the IUCr (Reference: VJ1003). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1995). C**51**, 678–680

Absolute Configuration of *N*,*N*-{(1*S*)-1-[(1-Methoxy-1-methyl)ethyl]tetramethylene}-(1*R*,6*R*,7*R*)-9,9-diethoxy-1-methyl-2-oxobicyclo[4.3.0]nonane-7-sulfonamide

BERNARD TINANT AND JEAN-PAUL DECLERCQ

Laboratoire de Chimie Physique et de Cristallographie, Université Catholique de Louvain, 1 place Louis Pasteur, 1348 Louvain-la-Neuve, Belgium

CATHERINE HUART

Laboratoire de Chimie Organique de Synthèse, Université Catholique de Louvain, 1 place Louis Pasteur, 1348 Louvain-la-Neuve, Belgium

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Abstract

The title compound, $C_{22}H_{39}NO_6S$, is obtained by an intramolecular cyclization of the adduct resulting