S—C1—N2	116,0 (3)	N4—C7—C3	110,8 (4)
S—C1—N3	121,1 (4)	N4—C7—C14	119,6 (4)
N2—C1—N3	122,9 (4)	C3—C7—C14	129,5 (4)
O—C2—N3	116,4 (4)		
C4—N1—N2—C5	−151,13	C1—N3—C2—C3	36,65
C4—N1—N2—C1	76,83	C1—N3—C2—O	−145,44
N1—N2—C1—N3	−68,61	N3—C2—C3—C4	4,60
N1—N2—C1—S	113,99	O—C2—C3—C4	−173,41
N2—C1—N3—C2	−2,48	C2—C3—C4—N1	−36,60
S—C1—N3—C2	174,79		

L'enregistrement a été effectué à l'aide d'un diffractomètre équipé d'un monochromateur en graphite balayage $\omega/2\theta$; $\Delta\omega = (0{,}80 + 0{,}34\tan\theta)^\circ$; vitesse de balayage variable de 1,8 à 20,1° min^{-1} en ω en fonction de l'intensité du pic de diffraction.

Les atomes S, O, N et C ont été localisés par les méthodes directes à l'aide du programme *SHELXS*86 (Sheldrick, 1985). La structure a été résolue par des synthèses de Fourier différence successives et affinements par moindres carrés en matrice totale, en utilisant le programme *CRYSTALS* (Watkin, Carruthers & Betteridge, 1988). En raison de la faible valeur de μ, aucune correction d'absorption n'a été appliquée. Après l'affinement anisotrope de tous le atomes, les coordonnées des atomes d'hydrogène ont été calculées. Un facteur d'agitation thermique isotrope commun à ces atomes a été introduit dans l'affinement. Au total, 255 paramètres variables ont été considérés: facteur d'échelle, facteur d'extinction secondaire (Larson, 1970), coordonnées atomiques, facteurs d'agitation thermique, isotrope pour les atomes d'hydrogène et anisotropes pour les autres atomes.

Les listes des facteurs de structure, des facteurs d'agitation thermique anisotrope, des coordonnées des atomes d'hydrogène, des distances et des angles ont été déposées au dépôt d'archives de l'UICr (Référence: DU1140). On peut en obtenir des copies en s'adressant à: The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, Angleterre.

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Structure-Based Rationalization of the Ionophore Character of Lead-Selective Amide–Ether–Amine-Containing Macrocycles: 2,3-Benzo-1,4-dioxa-7,11,15-triazacycloheptadec-2-ene-6,16-dione and 2,3-Benzo-1,4-dioxa-7,10,13-triazacyclopentadec-2-ene-6,14-dione–Water (1/2)

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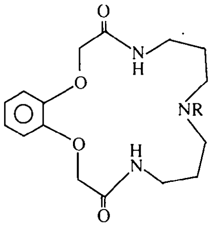
Abstract

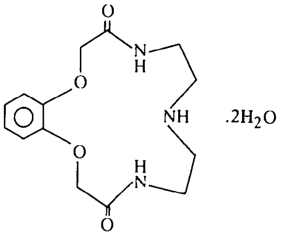
2,3-Benzo-1,4-dioxa-7,11,15-triazacycloheptadec-2-ene-6,16-dione, $C_{16}H_{23}N_3O_4$, has a 17-membered ring with an envelope conformation in which amide N and ether O atoms form one plane and the amine N atom lies on the flap. 2,3-Benzo-1,4-dioxa-7,10,13-triazacyclopentadec-2-ene-6,14-dione–water (1/2), $C_{14}H_{19}N_3O_4.2H_2O$, has a 15-membered ring with all the donor atoms in an approximately planar arrangement. The amide groups of this macrocycle are hydrogen bonded to the water molecules. It appears that the availability of the unsubstituted amine N atom is crucial for the extraction and transport of Pb^{2+} ions. Substitution of a side arm on the amine N atom significantly alters the coordination ability of this N atom in the 17-membered ring and decreases the extraction and transport ability of the macrocycle.

Comment

Metal-cation-selective ionophores have shown great potential for the development of adequately sensitive sensors and cost-effective separation technology for solving environmental problems caused by toxic metals such as Pb, Cd, Hg, *etc.* The versatility of the design of multidentate macrocycles has remarkable potential for creating such ionophores (Lehn, 1988; Takagi & Nakamura, 1986). Recently, we described two Pb^{2+}-selective ether–amide–amine macrocycles, (I) and (II), but surprisingly their amine-derived lariats lacked the selectivity of the parent compounds (Kumar, Singh & Singh, 1992). The structure analysis (Hundal, Hundal, Kumar, Singh & Sanz-Aparicio, 1995) of the lariat (III) indicated the presence of a centrally bound water molecule and an exterior spatial disposition of the amine N atom, rendering it incapable of coordination. In order to identify the spatial disposition of the ligating sites in compounds (I) and (II) and to rationalize structural and spatial parameters for Pb^{2+} selectivity, the structural analyses of the title compounds were performed. It has been found that the appropriate placement of the amine N atom in these macrocycles is conducive to cavity formation along with other ligating sites.



(I) R = H
(III) R = $-CH_2CH_2CN$



(II)

All bond distances and angles are as expected. In both ring systems, the cavities have five potential donors, *i.e.* two ether O atoms, two amide N atoms and an amine N atom. In both ring systems, the amide O atoms point towards the outer side of the macrocycle. Compound (I) possesses a mirror plane (Fig. 1) which passes through the amine N2 atom and bisects the phenyl ring. Torsion-angle studies (Nardelli, 1976) indicate that the macrocycle possesses an envelope conformation. This feature of the ring system is expected because the presence of a fused phenyl group along with the two amide groups makes the ring system rigid in such a way that the four potential donor atoms, O1, N1, N1*A* and O1*A* (where *A* refers to atoms generated by mirror symmetry), are planar. The amine N2 atom lies in the flap of the envelope. The remaining part of the ring system, $-(CH_2)_3$—NH—$(CH_2)_3-$, adjusts the torsion angles to accommodate the restraints imposed by the fused phenyl ring and the amide groups. The substitution of a long chain or a bulky group at the amine N atom is likely to alter the torsion angles only in this segment of the macrocycle, thus fulfilling the requirement that the host should be relatively rigid so that complexation should involve the minimum amount of conformational change so as to minimize the effect of conformational entropy change on binding with the guest (Hunter, 1995; Izaat, Pawlak, Bradshaw & Bruening, 1991).

Compound (II) (Fig. 2) has a 15-membered macrocycle and two water molecules present in its lattice. The structure shows extensive hydrogen bonding between the water molecules and the macrocycle. The O5 water molecule acts as a hydrogen-bond donor towards the amide $O3^{i}$ and $O2^{iii}$ atoms [symmetry codes: (i) x, y, $z+1$; (iii) $x-\frac{1}{2}$, $-y$, z], whereas it behaves as an acceptor towards the second O6 water molecule forming an intramolecular contact. The O6 atom donates its other H atom to the $O3^{ii}$ atom [symmetry code: (ii) x, $-y-\frac{1}{2}$, $z+\frac{1}{2}$]. These water molecules, however, do not occupy the centre of the macrocycle and the extraction profile (Kumar, Singh & Singh, 1992) for the extraction of Pb^{2+} ion is not significantly affected by their presence, indicating that the amount of energy spent on desolvation of the ring is very little. Because of the constraints imposed by the rigid segment of the molecule, the ring acquires a more flattened conformation in which the ether O atoms, the amide N atoms and the amine N atom lie within ±0.06 Å of the mean plane defined by the five donor atoms.

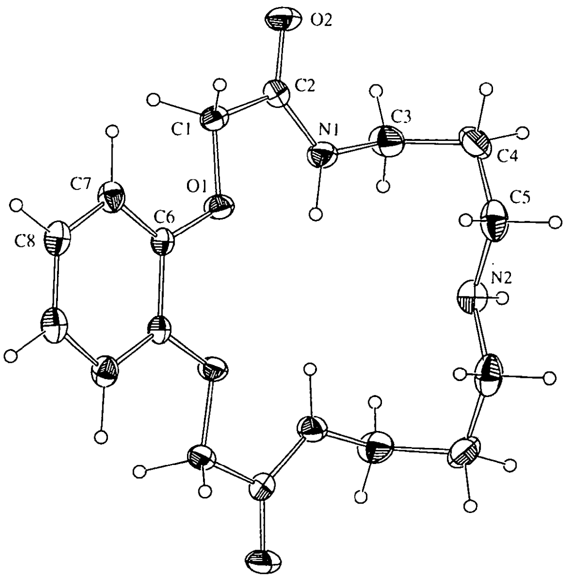


Fig. 1. An *ORTEP* drawing (Johnson, 1965) of compound (I) showing the atomic labelling scheme. The non-H atoms are shown with displacement ellipsoids drawn at the 30% probability level. H-atom labels have been omitted for clarity.

Comparison of compound (I) with the results obtained for compound (III) (Hundal *et al.*, 1995), a lariat of compound (I) wherein a $-(CH_2)_2CN$ group has been substituted on the amine N atom, indicates that the conformation is envelope type in the latter. The presence of a substituent at the amine N atom alters the torsion angles significantly. The torsion angle C3—C4—C5—N2 of −49.4 (8)° in compound (I) changes to values of −56.3 (8) and −106.9 (14)° in compound (III). The presence of a substituent at the amine N atom causes flattening of the ring system. This flattening increases the distance between the ether O and amine N atoms. Consequently, the amine N atom moves out of the spatial cavity constituted by the other heteroatoms and becomes non-available for complex formation. This effect is quite evident from the decreased extraction of cations by compound (III) compared with compounds (I) and (II) (Hundal *et al.*, 1995). Also, in compound (III), the cavity is such that a water molecule remains in the cavity and binds the macrocycle from a side opposite to the amine group. The desolvation of this water molecule probably requires a lot of energy and also leads to the poor extraction and transport properties of compound (III). Structurally, compounds (I) and (III), with three-carbon interceptions, exist in envelope-type conformations, but compound (II), with two-carbon interceptions, acquires a nearly planar conformation. Despite the conformational differences in compounds (I) and (II), the amine N atom is available for ligation in both cases, whereas in the case of compound (III), it is not. The selectivity, and hence transportation ability, of compounds (I) and (II) towards Pb^{2+} could, therefore, be attributed to the ligation of the amine N atom, which is lacking in the case of compound (III).

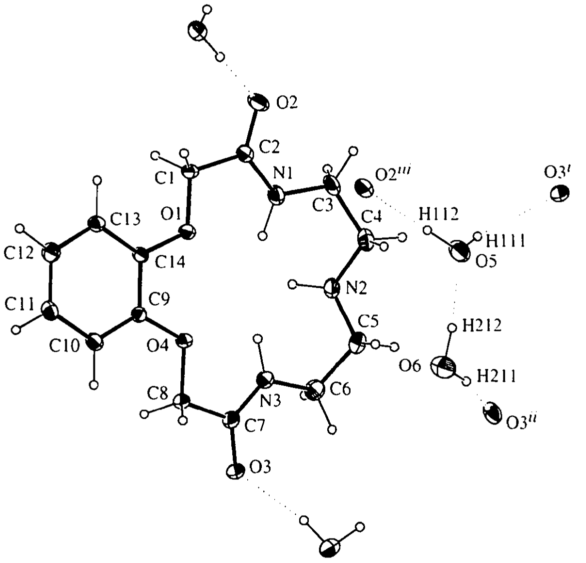


Fig. 2. An *ORTEP* drawing (Johnson, 1965) of compound (II) showing the atomic labelling and hydrogen-bonding schemes. The non-H atoms are shown with displacement ellipsoids drawn at the 30% probability level. H-atom labels have been omitted for clarity.

Experimental

Compounds (I) and (II) were supplied by the Department of Chemistry, Guru Nanak Dev University, Amritsar 143 005, India.

Compound (I)

Crystal data

$C_{16}H_{23}N_3O_4$
$M_r = 321.39$
Orthorhombic
Pnma
$a = 19.825 (5)$ Å
$b = 16.714 (2)$ Å
$c = 4.905 (1)$ Å
$V = 1625.3 (6)$ Å^3
$Z = 4$
$D_x = 1.313$ Mg m^{-3}
$D_m = 1.321$ Mg m^{-3}
D_m measured by flotation in benzene/bromoform

Cu $K\alpha$ radiation
$\lambda = 1.5418$ Å
Cell parameters from 25 reflections
$\theta = 2–40°$
$\mu = 0.79$ mm^{-1}
$T = 293$ K
Needle
0.3 × 0.2 × 0.1 mm
Colourless

Data collection

Seifert XRD 3000*S* diffractometer
$\omega–2\theta$ scans
Absorption correction: none
1511 measured reflections
1263 independent reflections
456 observed reflections [$F > 4\sigma(F)$]

$R_{int} = 0.003$
$\theta_{max} = 60.06°$
$h = 0 \rightarrow 22$
$k = 0 \rightarrow 18$
$l = 0 \rightarrow 5$
2 standard reflections monitored every 100 reflections
intensity decay: none

Refinement

Refinement on F
$R = 0.039$
$wR = 0.039$
$S = 1.219$
456 reflections
107 parameters
H-atom parameters not refined
Unit weights applied
$(\Delta/\sigma)_{max} = 0.222$

$\Delta\rho_{max} = 0.535$ e Å^{-3}
$\Delta\rho_{min} = -0.473$ e Å^{-3}
Extinction correction: Zachariasen (1968)
Extinction coefficient: 1487 (131)
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

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

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

	x	y	z	U_{eq}
O1	0.4464 (2)	0.1728 (2)	0.6676 (9)	0.053 (3)
O2	0.4003 (2)	−0.0079 (2)	0.992 (1)	0.076 (3)
N1	0.3652 (2)	0.1196 (3)	1.035 (1)	0.056 (3)
N2	0.2412 (4)	1/4	1.113 (1)	0.058 (5)
C1	0.4527 (3)	0.0887 (3)	0.713 (1)	0.051 (4)
C2	0.4036 (3)	0.0629 (3)	0.930 (1)	0.052 (4)
C3	0.3139 (4)	0.1044 (4)	1.243 (1)	0.070 (5)
C4	0.2434 (4)	0.1027 (4)	1.121 (2)	0.081 (6)
C5	0.2259 (3)	0.1766 (5)	0.958 (1)	0.075 (5)
C6	0.4903 (2)	0.2080 (3)	0.490 (1)	0.040 (3)
C7	0.5324 (3)	0.1672 (4)	0.315 (1)	0.052 (4)
C8	0.5743 (3)	0.2085 (3)	0.134 (1)	0.057 (4)

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

O1—C6	1.363 (7)	C1—C2	1.508 (9)
O1—C1	1.428 (6)	C3—C4	1.52 (1)
O2—C2	1.223 (7)	C4—C5	1.51 (1)
N1—C2	1.321 (8)	C6—C7	1.381 (8)
N1—C3	1.461 (9)	C6—C6^i	1.404 (7)
N2—C5	1.473 (9)	C7—C8	1.396 (8)
N2—C5^i	1.473 (9)	C8—C8^i	1.389 (8)
C6—O1—C1	117.9 (4)	N2—C5—C4	111.3 (6)
C2—N1—C3	123.3 (5)	O1—C6—C7	124.9 (5)
C5—N2—C5^i	112.9 (6)	O1—C6—C6^i	115.6 (5)
O2—C2—N1	124.5 (6)	C7—C6—C6^i	119.6 (5)
O2—C2—C1	119.1 (5)	C6—C7—C8	120.9 (5)
N1—C2—C1	116.3 (5)	C8^i—C8—C7	119.6 (5)
C5—C4—C3	113.8 (5)		
C6—O1—C1—C2	175.5 (5)	C1—C2—N1—C3	178.4 (6)
O1—C1—C2—O2	178.0 (5)	O2—C2—N1—C3	0 (1)
O1—C1—C2—N1	0.2 (8)	N1—C3—C4—C5	−54.2 (8)
C2—N1—C3—C4	−101.9 (7)	C7—C6—O1—C1	12.1 (8)
C3—C4—C5—N2	−49.4 (8)		

Symmetry code: (i) $x, \frac{1}{2} - y, z$.

Compound (II)

Crystal data

$C_{14}H_{19}N_3O_4.2H_2O$
$M_r = 329.352$

Cu $K\alpha$ radiation
$\lambda = 1.5418$ Å

Monoclinic
Ia
$a = 7.3684$ (9) Å
$b = 22.641$ (3) Å
$c = 10.479$ (2) Å
$\beta = 110.44$ (1)°
$V = 1638.1$ (4) Å^3
$Z = 4$
$D_x = 1.35$ Mg m^{-3}
$D_m = 1.342$ Mg m^{-3}
D_m measured by flotation in benzene/bromoform

Cell parameters from 30 reflections
$\theta = 2$–40°
$\mu = 0.84$ mm^{-1}
$T = 293$ K
Prism
0.3 × 0.3 × 0.1 mm
Colourless

Data collection

Seifert XRD 3000*S* diffractometer
ω–2θ scans
Absorption correction: none
1506 measured reflections
1363 independent reflections
1144 observed reflections [$F > 4\sigma(F)$]

$R_{\rm int} = 0.005$
$\theta_{\rm max} = 64.86°$
$h = -8 \rightarrow 7$
$k = 0 \rightarrow 26$
$l = 0 \rightarrow 12$
2 standard reflections monitored every 100 reflections
intensity decay: none

Refinement

Refinement on F
$R = 0.041$
$wR = 0.045$
$S = 1.128$
1144 reflections
207 parameters
H-atom parameters not refined
Unit weights applied
$(\Delta/\sigma)_{\rm max} = 0.491$

$\Delta\rho_{\rm max} = 0.217$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.256$ e Å^{-3}
Extinction correction: Zachariasen (1968)
Extinction coefficient: 3525 (108)
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for (II)*

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

	x	y	z	$U_{\rm eq}$
O1	0.39886	0.0247 (1)	0.33506	0.046 (2)
O2	0.6907 (10)	0.0378 (2)	0.6821 (6)	0.063 (3)
O3	0.1016 (10)	−0.1777 (2)	−0.0283 (6)	0.064 (2)
O4	0.1995 (9)	−0.0378 (2)	0.1304 (6)	0.046 (2)
O5	0.1346 (10)	−0.1573 (2)	0.7168 (6)	0.069 (3)
O6	−0.0869 (11)	−0.2130 (2)	0.4761 (6)	0.075 (3)
N1	0.5832 (11)	−0.0410 (2)	0.5424 (6)	0.049 (3)
N2	0.5235 (11)	−0.1565 (2)	0.4582 (7)	0.051 (3)
N3	0.2763 (11)	−0.1472 (2)	0.1856 (7)	0.053 (3)
C1	0.5166 (12)	0.0570 (3)	0.4496 (7)	0.045 (3)
C2	0.6037 (11)	0.0165 (3)	0.5683 (7)	0.043 (3)
C3	0.6608 (12)	−0.0872 (3)	0.6451 (7)	0.056 (3)
C4	0.5454 (12)	−0.1431 (3)	0.5972 (8)	0.056 (4)
C5	0.3862 (13)	−0.2029 (3)	0.3953 (8)	0.060 (4)
C6	0.3458 (14)	−0.2054 (3)	0.2445 (8)	0.065 (4)
C7	0.1645 (12)	−0.1387 (3)	0.0577 (7)	0.045 (3)
C8	0.1092 (11)	−0.0749 (3)	0.0157 (7)	0.045 (3)
C9	0.1874 (11)	0.0224 (2)	0.1086 (7)	0.037 (3)
C10	0.0801 (11)	0.0492 (3)	−0.0116 (7)	0.045 (3)
C11	0.1920 (12)	0.1440 (3)	0.0862 (8)	0.051 (3)
C12	0.0833 (11)	0.1111 (3)	−0.0226 (7)	0.050 (3)
C13	0.3017 (11)	0.1170 (2)	0.2090 (7)	0.044 (3)
C14	0.2992 (11)	0.0564 (2)	0.2202 (7)	0.036 (3)

Table 4. *Selected geometric parameters (Å, °) for (II)*

O1—C14	1.373 (6)	N3—C6	1.470 (8)
O1—C1	1.414 (7)	C1—C2	1.497 (9)
O2—C2	1.238 (9)	C3—C4	1.509 (10)
O3—C7	1.231 (8)	C5—C6	1.504 (12)
O4—C9	1.379 (6)	C7—C8	1.522 (9)
O4—C8	1.427 (8)	C9—C10	1.374 (9)
N1—C2	1.327 (8)	C9—C14	1.403 (8)
N1—C3	1.467 (9)	C10—C12	1.407 (8)
N2—C4	1.441 (11)	C11—C12	1.364 (9)
N2—C5	1.447 (9)	C11—C13	1.399 (9)
N3—C7	1.319 (9)	C13—C14	1.379 (8)
C14—O1—C1	117.1 (4)	O3—C7—C8	118.4 (6)
C9—O4—C8	117.3 (5)	N3—C7—C8	116.1 (5)
C2—N1—C3	124.2 (6)	O4—C8—C7	108.4 (5)
C4—N2—C5	115.2 (7)	C10—C9—O4	124.9 (6)
C7—N3—C6	124.0 (5)	C10—C9—C14	120.3 (5)
O1—C1—C2	110.3 (5)	O4—C9—C14	114.8 (5)
O2—C2—N1	124.3 (6)	C9—C10—C12	119.7 (6)
O2—C2—C1	119.3 (5)	C12—C11—C13	120.8 (5)
N1—C2—C1	116.5 (6)	C11—C12—C10	119.9 (6)
N1—C3—C4	108.9 (5)	C14—C13—C11	119.5 (6)
N2—C4—C3	111.3 (7)	O1—C14—C13	125.2 (5)
N2—C5—C6	110.9 (7)	O1—C14—C9	115.0 (4)
N3—C6—C5	108.6 (6)	C13—C14—C9	119.9 (6)
O3—C7—N3	125.5 (6)		
O1—C14—C9—O4	−2 (1)	C8—O4—C9—C14	−172.1 (8)
C1—O1—C14—C9	178.8 (7)		

Table 5. *Hydrogen-bonding geometry (Å, °) for (II)*

D—H$\cdots A$	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O5—H111$\cdots$O3$^{\rm i}$	1.968 (6)	2.80 (1)	130.0 (4)
O5—H112$\cdots$O2$^{\rm ii}$	1.826 (5)	2.779 (7)	171.2 (5)
O6—H211$\cdots$O3$^{\rm iii}$	1.988 (6)	2.844 (8)	160.9 (6)
O6—H212$\cdots$O5	1.845 (5)	2.782 (8)	173.3 (4)

Symmetry codes: (i) $x, y, 1 + z$; (ii) $x - \frac{1}{2}, -y, z$; (iii) $x, -\frac{1}{2} - y, \frac{1}{2} + z$.

All H atoms were fixed geometrically. For compound (II), the systematic extinctions indicated space group *I*2/*a* or *Ia*. Attempts to solve the structure in *I*2/*a* were unsuccessful. All the non-H atoms were revealed in the first *E* map when space group *Ia* was chosen. The water H atoms were located by difference Fourier synthesis.

For both compounds, data reduction: *Xtal*3.2 *DIFDAT SORTRF ADDREF* (Hall, Flack & Stewart, 1992); program(s) used to solve structures: *SIR*92 (Altomare *et al.*, 1992); program(s) used to refine structures: *Xtal*3.2 *CRYLSQ*; software used to prepare material for publication: *Xtal*3.2 *BONDLA CIFIO*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: PA1212). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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4,4-Dibenzyl-1,4-dihydroisoquinoline

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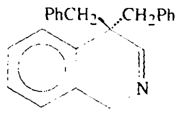
Abstract

The title compound, 4,4-dibenzyl-1,4-dihydroisoquinoline, $C_{23}H_{21}N$, is one of the few stable derivatives of 1,4-dihydroisoquinoline for which structures have been reported so far. In the solid state the compound exhibits an interesting conformation with both benzyl groups at C4 folded symmetrically toward the heterocyclic system.

Comment

The nitrogen-containing ring of the 1,4-dihydroisoquinoline moiety is in the flattened boat conformation with C1 and C4 deviating from the least-squares plane by 0.183 and 0.124 Å, respectively. The deviation of the remaining atoms ranges from 0.036 to 0.077 Å.



Almost all C—C and C—N bond distances as well as intra-annular bond and torsion angles in the 1,4-dihydroisoquinoline moiety do not differ significantly from the corresponding distances and angles in other compounds reported (Gieren, Burger & Einhellig, 1973; Weidner, Maas & Würthwein, 1989; Vogel, Delavier, Jones & Doring, 1991; Richter-Addo, Knight, Dewey, Arif & Gladysz, 1993; Pich, Bishop, Craig & Scudder, 1994). The most noticeable difference in the geometry of the 1,4-dihydroisoquinoline system is the significant enlargement of the intra-annular bond angle N2—C3—C4 to 129.0 (2)° *versus* 121.5–125.0° reported for other structures. The relative enlargement of the angle may result from the presence of two bulky benzyl groups at the adjacent C atom (C4).

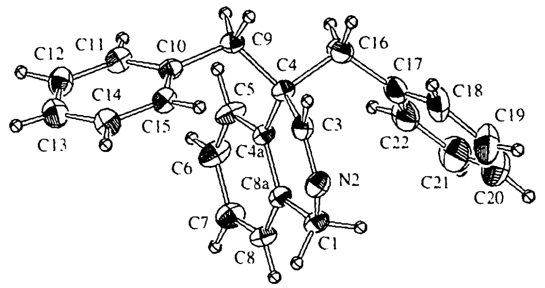


Fig. 1. Molecular structure showing 30% probability displacement ellipsoids. Displacement ellipsoids for H atoms are of arbitrary size.

Both benzyl substituents at C4 are twisted toward the isoquinoline moiety in a similar fashion, yet they are not equivalent. The C4—C9 bond is shorter by 0.015 Å (5σ) than the C4—C16 bond. Also, the C4—C16—C17 angle is significantly smaller (3.2° or 16σ) than its counterpart, C4—C9—C10. The two phenyl rings of the benzyl groups are twisted differently with respect to the isoquinoline system. Whereas the torsion angles around the first single bond (*i.e.* C4—C9 and C4—C16) are virtually equivalent for both groups, the torsion angles around the second bond (C9—C10 and C16—C17) differ by about 20°. Thus, the dihedral angle between the benzene ring and the plane dissecting the methylene group is 68.1° for one benzyl substituent (C9–C15) and 89.0° for the other (C16–C22). The planes dissecting the methylene groups are almost perpendicular to the isoquinoline moiety for both benzyl substituents. The discussed angular differences between the two benzyl groups can be rationalized by different packing interactions acting on both phenyl rings.

The isoquinoline moieties are arranged in a parallel pattern in the crystal (Fig. 2) with the distance between

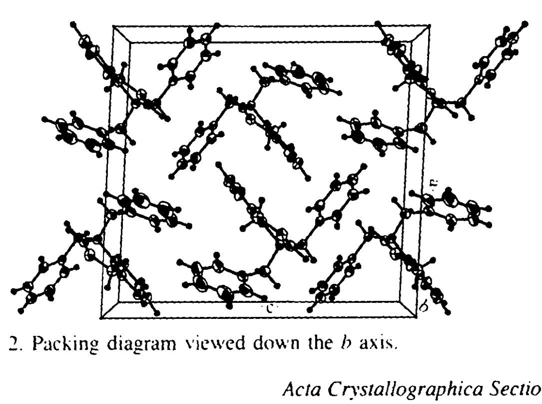


Fig. 2. Packing diagram viewed down the *b* axis.