OP   ON   oO   OC |0___.___.._.._.|5 Å

Fig. 4. Projection of the crystal structure down **a** with inter-molecular distances (Å). E.s.d.'s of the distances are all <0·01 Å.

4. The following contacts between molecules related by the **a** lattice translation are omitted from the diagram: $O(2)\cdots C(4)(1 + x, y, z)$ 3·82 and $C(2)\cdots C(4)(1 + x, y, z)$ 3·69 Å. The shortest contacts of each type are: $O\cdots O$ 3·59, $CH_3\cdots CH_3$ 3·68, $O\cdots CH_3$ 3·23 Å. The corresponding shortest contacts found in the crystal of isomer (2) are 3·58, 3·57, and 3·10 Å respectively.

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The Structure of (2*R*,5*S*,8*R*,11*S*)-1,4,7,10-Tetrabenzyl-2,5,8,11-tetraethyl-1,4,7,10-tetraazacyclododecane

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Abstract

$C_{44}H_{60}N_4$, tetragonal, $P4_2/n$, $a = 27\cdot949$ (14), $c = 12\cdot505$ (8) Å, $U = 9768$ (12) Å^3, $Z = 10$, $D_c = 1\cdot096$, $D_o = 1\cdot04$ Mg m^{-3}. $R = 7\cdot3\%$ for 3837 independent reflections. The 12-membered ring has a tub form with the methylene groups at the corners. The chirality of the asymmetric carbon has a significant effect on the form of the ring.

Introduction

A series of investigations on the polymerization of chiral aziridines have been performed in our Institute.

In the presence of $BF_3.Et_2O$, (R)-1-benzyl-2-ethyl-aziridine (1) reacts to give a cyclic tetramer (2) or the corresponding polymer depending on the reaction conditions (Tsuboyama, Tsuboyama, Higashi & Yanagita, 1970). Only one isomer of the tetramer was found, which means that the ring cleavage of the aziridine takes place preferentially at the methylene—nitrogen linkage.

CH₂——C(R)H–Et
  \ /
   N   Et   CH₂Ph
   | | |
  CH₂Ph ⟶ [CH₂–C(R)H–N]₄

(1)   (2)
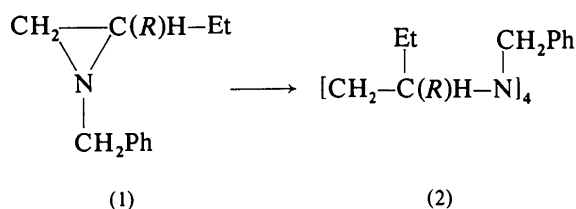
Therefore, starting from the racemic monomer, six different configurations are possible. Corresponding to these configurations, four geometrical isomers exist (Fig. 1). The separation of these isomers was carried out by fractional recrystallization from an appropriate solvent and/or by selecting them with tweezers under a low-power microscope. Of these configurations, A_R and A_S crystallize with solvent of recrystallization, and the resultant crystal system depends on the solvent of crystallization. B_R and B_S were not obtained as single crystals. Good single crystals were obtained for C, D and the racemic forms A; $(A_R + A_S)$ and B; $(B_R + B_S)$ (Tsuboyama, Tsuboyama, Uzawa & Higashi, 1974). The structures of isomer A (Sakurai, Kobayashi, Tsuboyama & Tsuboyama, 1978b), B (Sakurai, Hiramatsu, Tsuboyama & Tsuboyama, 1980) and C (Hiramatsu, Sakurai, Tsuboyama & Tsuboyama, 1979) have been reported. This paper describes the structure of isomer D.

Experimental and structure determination

Single crystals were obtained by recrystallization from ethyl acetate solution. A clear, colourless needle crystal $1.2 \times 0.07 \times 0.05$ mm was used for the X-ray study. The crystal data are in the *Abstract*. Intensity data were measured on a Rigaku AFC four-circle diffractometer, with graphite-monochromatized Mo $K\alpha$ radiation. The intensities were corrected for Lorentz and polarization factors, but no absorption correction was applied. Within the range of $2\theta \leq 45°$, 3837 independent reflections with $|F| \geq 3\sigma(F)$ were obtained.

CONFIGURATION

┌R┐ ┌S┐ ┌R┐ ┌S┐ ┌R┐ ┌R┐
R│ S│ S│ R│ S│ S│
└R┘ └S┘ └R┘ └S┘ └S┘ └R┘
 L R   L S   L R   L S   L R   L S

GEOMETRICAL ISOMER

Aᴿ   Aˢ   Bᴿ   Bˢ
└─┬─┘   └─┬─┘
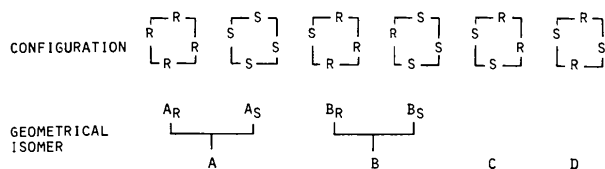 A   B   C   D

Fig. 1. Configurations and isomers of the cyclic chiral tetramer.

Table 1. *Atomic parameters*

Positional parameters are multiplied by 10^4. Atoms belonging to the molecule (I) are indicated by A at the end of the atom name.
$B_{eq} = \frac{4}{3} \sum_i \sum_j B_{ij} \mathbf{a}_i . \mathbf{a}_j.$

	x	y	z	B_{eq} (Å²)
N(1)A	3280 (1)	2378 (1)	2961 (3)	3·4
C(2)A	3125 (2)	2209 (2)	1883 (4)	3·4
C(12)A	3291 (2)	2904 (2)	3047 (4)	3·6
C(2)1A	3539 (2)	2219 (2)	1049 (5)	4·9
C(2)2A	3337 (3)	2181 (3)	−95 (5)	7·1
C(1)1A	3742 (2)	2168 (2)	3320 (4)	4·2
C(1)2A	3779 (2)	2187 (2)	4536 (5)	4·3
C(1)3A	4091 (2)	2507 (2)	5041 (5)	5·6
C(1)4A	4105 (3)	2531 (3)	6143 (6)	7·7
C(1)5A	3814 (3)	2237 (3)	6737 (5)	8·8
C(1)6A	3506 (3)	1899 (3)	6266 (6)	9·0
C(1)7A	3489 (3)	1880 (3)	5134 (6)	6·7
N(1)	615 (2)	5810 (2)	2991 (3)	3·9
N(4)	1142 (2)	4861 (1)	1972 (3)	3·4
N(7)	2103 (1)	5366 (2)	2986 (3)	3·6
N(10)	1578 (2)	6324 (2)	1985 (3)	3·7
C(2)	625 (2)	5593 (2)	1888 (4)	3·9
C(3)	650 (2)	5046 (2)	1947 (4)	3·9
C(5)	1360 (2)	4865 (2)	3059 (4)	3·5
C(6)	1909 (2)	4878 (2)	2998 (4)	3·8
C(8)	2089 (2)	5590 (2)	1906 (4)	3·6
C(9)	2071 (2)	6135 (2)	1965 (4)	3·9
C(11)	1357 (2)	6309 (2)	3075 (4)	4·0
C(12)	812 (2)	6301 (2)	3009 (5)	4·1
C(2)1	186 (2)	5755 (2)	1202 (5)	5·2
C(2)2	258 (2)	5671 (3)	−7 (5)	6·0
C(5)1	1189 (2)	4432 (2)	3745 (5)	5·0
C(5)2	1320 (3)	4499 (3)	4952 (5)	6·6
C(8)1	2519 (2)	5429 (2)	1188 (5)	4·7
C(8)2	2421 (2)	5506 (3)	−12 (5)	6·1
C(11)1	1519 (2)	6737 (2)	3774 (5)	5·6
C(11)2	1425 (3)	6651 (3)	4983 (6)	7·7
C(1)1	125 (2)	5790 (2)	3460 (5)	5·0
C(1)2	147 (2)	5876 (2)	4667 (5)	5·0
C(1)3	−115 (2)	6244 (2)	5139 (5)	5·4
C(1)4	−98 (3)	6318 (3)	6243 (6)	6·7
C(1)5	174 (3)	6025 (3)	6863 (6)	7·3
C(1)6	428 (3)	5638 (3)	6435 (6)	8·6
C(1)7	417 (3)	5572 (3)	5305 (6)	7·7
C(4)1	1171 (2)	4389 (2)	1447 (4)	4·2
C(4)2	1166 (2)	4426 (2)	222 (4)	4·4
C(4)3	1066 (2)	4007 (2)	−364 (5)	5·5
C(4)4	1086 (3)	4017 (3)	−1474 (6)	6·9
C(4)5	1192 (3)	4440 (3)	−1982 (5)	7·7
C(4)6	1284 (3)	4871 (3)	−1431 (5)	6·7
C(4)7	1269 (2)	4854 (2)	−300 (5)	5·3
C(7)1	2587 (2)	5386 (2)	3468 (5)	5·0
C(7)2	2560 (2)	5296 (2)	4677 (5)	4·8
C(7)3	2860 (3)	4952 (3)	5151 (6)	7·5
C(7)4	2824 (3)	4901 (3)	6282 (7)	9·4
C(7)5	2516 (3)	5170 (3)	6854 (6)	9·0
C(7)6	2222 (4)	5504 (3)	6397 (6)	9·6
C(7)7	2255 (3)	5569 (3)	5292 (6)	8·0
C(10)1	1556 (2)	6803 (2)	1487 (5)	5·1
C(10)2	1616 (2)	6767 (2)	276 (5)	4·8
C(10)3	1939 (3)	7056 (3)	−261 (6)	7·4
C(10)4	1992 (3)	7010 (3)	−1376 (7)	8·7
C(10)5	1724 (3)	6698 (3)	−1929 (6)	8·4
C(10)6	1387 (4)	6422 (4)	−1428 (7)	10·3
C(10)7	1344 (3)	6456 (3)	−317 (6)	9·3

The number of molecules in the unit cell is 10, and the number of general equivalent positions is 8. Therefore, the unit cell must contain two independent molecules, one being at the general position, and the other at the special position with point symmetry 4̄. The structure analysis was not straightforward. Several attempts to solve the structure by the direct method, the Patterson method, or the model-building method were not successful. In some cases a fairly good molecular shape was found from *MULTAN* (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), but was not refined. Finally, the Monte Carlo method (Furusaki, 1979) was applied with 22 initial sets, and a reasonable solution was obtained. The structure was refined by the block-diagonal least-squares method with anisotropic temperature factors for all the non-hydrogen atoms. Unit weight was given to all reflections. Among 75 H atoms, 57 were located from the difference Fourier synthesis. The final R index is 7·3%. The atomic coordinates of the non-hydrogen atoms are shown in Table 1, and the numbering scheme is the same as that in previous papers (cf. Fig. 3).*

Discussion

(a) Crystal and molecular structure

The packing of the molecules in the crystal is shown in Fig. 2. There are two independent molecules, (I) and

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* Lists of structure factors, hydrogen atom coordinates and anisotropic temperature factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35759 (25 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
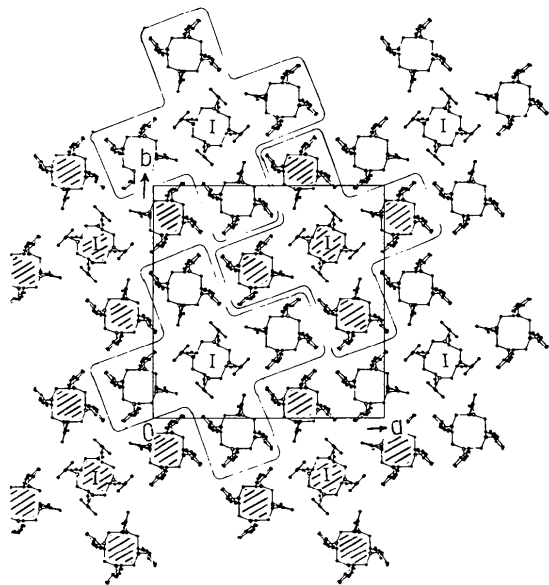

Fig. 2. The crystal structure projected along c. Molecule (I) is surrounded by four molecules (II). The shadowed molecules are centrosymmetrically related to the others.

(II), in the asymmetric unit. Molecule (I) is situated around the special position at ¼, ¼, ¼, and has exact 4̄ symmetry. It is surrounded by four molecules of (II) with almost the same z coordinates. Therefore, this group of five molecules forms a cross-shaped rod along the c axis, and the whole structure consists of close-packed cross-shaped rods. Neighbouring rods are related by the centre of symmetry.

Molecules (I) and (II) have a similar conformation. Viewed down the longest principal axis of the ring, the conformation appears as a square with the methylene groups at the corners. The torsion angles, bond lengths and bond angles of the 12-membered ring are shown in Fig. 3. The ethyl and benzyl groups are axial to the ring. At each side of the square, the direction of the benzyl group is opposite to the ethyl group, the directions of the ethyl groups at neighbouring sides are opposite to each other (Fig. 4), and the skeletal 12-membered ring takes the tub form (Fig. 5). The methylene groups [C(3), C(6), C(9), C(12)] are at the 'tips' of the tub.

The conformation energy for the benzyl group has been calculated with respect to the rotation about the two single bonds in the benzyl group (Fig. 6). Throughout the calculation, the torsion angles about the four groups were changed simultaneously. For the S sides, the torsion angles have opposite signs from those of the others. The resultant energy map shows the
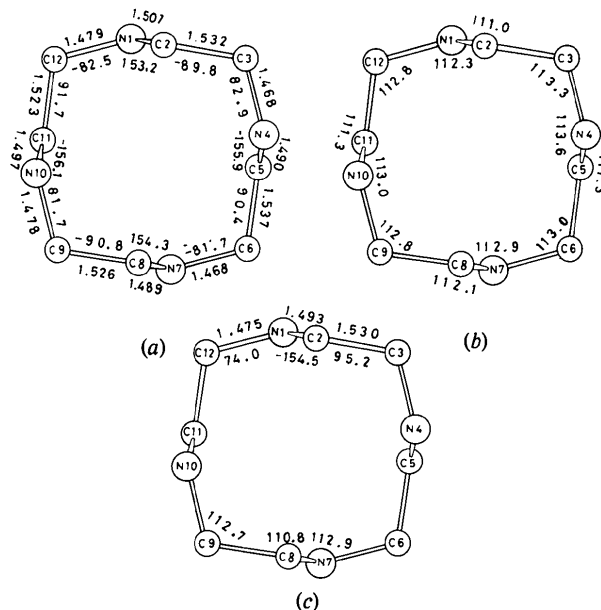

Fig. 3. The bond parameters in the 12-membered ring. Standard deviations are 0·007 Å for N—C, 0·008 Å for C—C, 0·4° for bond angles, and 0·5° for torsion angles. (a) Bond lengths (Å) and torsion angles (°) of molecule (II). The torsion angles are given by the values inside the ring. (b) Bond angles (°) of molecule (II). (c) Bond parameters of molecule (I). The bond lengths (Å) are at the top, the torsion angles (°) are below the bond lengths, and the bond angles (°) are at the bottom.
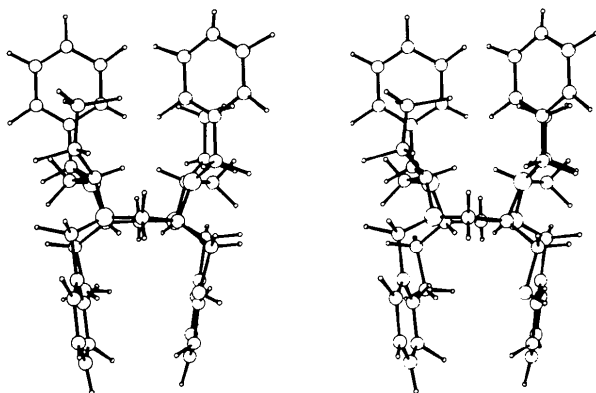
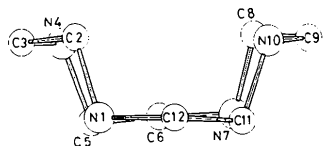Fig. 4. A stereoscopic drawing of molecule (II).

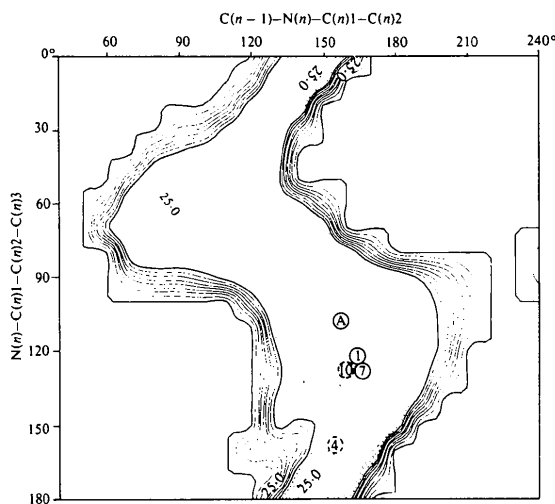
Fig. 5. Skeleton of the 12-membered ring.

$C(n-1)-N(n)-C(n)1-C(n)2$

Fig. 6. The conformation-energy map for the benzyl-group rotation. The contour lines are drawn at intervals of 1 kcal mol^{-1} (1 kcal mol^{-1} ≡ 4·2 kJ mol^{-1}). The observed values are circled. Ⓐ corresponds to molecule (I). For the S-side substituents, the signs of the observed values are the opposite of those shown. These are represented by broken circles.

stable for the 12-membered hydrocarbon ring. This is also confirmed by strain-energy calculations (Wiberg, 1965; Bixon & Lifson, 1967; Dale, 1976).

The skeleton of the present series of molecules also has a square conformation. However, the resultant molecular shape is considerably affected by the chirality of the asymmetric C atoms.

For the heterocyclic ring, even for the square conformation, three different arrangements are possible according to the kind of corner atom (Fig. 7). The observed structures are, except for $RRRR$ where N atoms appear at the corners, methylene corners. The asymmetric C atom is always on the side of the square. There are two possible bonding directions for the ethyl group at this C atom, one towards the inside of the ring, and the other towards the outside. For the four ethyl groups, the inside of the ring is too crowded; therefore, they must dispose themselves towards the outside of the ring (Fig. 8a). Thus, the chirality of the C atom has a significant effect on the form of the ring. If the chirality is R, the torsion angles along the side of the square are $-sc$, $+ap$,$-sc$, while if the chirality is S, they are $+sc$, $-ap$, $+sc$. The skeletal conformations and the direction of the ethyl groups are shown schematically in Fig. 8(b). In the actual structure, the torsion angles adjacent to the junction of the R side and the S side are near |90°|, and are sometimes in the anticlinal region. The benzyl group extends from the ring opposite to the ethyl group. For $RRRR$, if all the benzyl groups are at the same side of the ring the phenyl groups will be too crowded. In order to avoid this situation, the N atoms appear at the corners, and the benzyl groups extend toward the side of the ring. [Elimination of the benzyl groups gives the methylene-corner conformation (Sakurai, Kobayashi, Tsuboyama & Tsuboyama, 1978a).] Because of this open conformation, the $RRRR$ molecule forms a variety of clathrate crystals with the crystalline solvent.

The average values of the bond lengths and angles within the ring for all the observed isomers are: C—C = 1·533 (2), C—N = 1·478 (2) Å, C—N—C = 113·3 (2), and N—C—C = 112·3 (3)°.

Although the square conformation with methylene corners seems to be the most stable, the energy differences from other conformations may not be so large. Thus, a variety of ring conformations are observed for metal complexes (Table 2). A square with

broad low-energy region. One of the benzyl groups, attached to N(4) in molecule (II), appears different from the others, but it still belongs to the same low-energy region as shown by ⚃ in the region.

(b) *Comparison with other structures*

The square [3333] conformation, first found for cyclododecane (Dunitz & Shearer, 1960), will be most
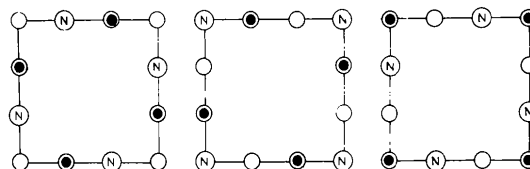

Fig. 7. Three possible arrangements of the corner groups; from left to right: methylene corners, N corners, and ethyl corners. The asymmetric carbon is represented by ⬤.

Table 2. *Conformation of the* 12-*membered ring*

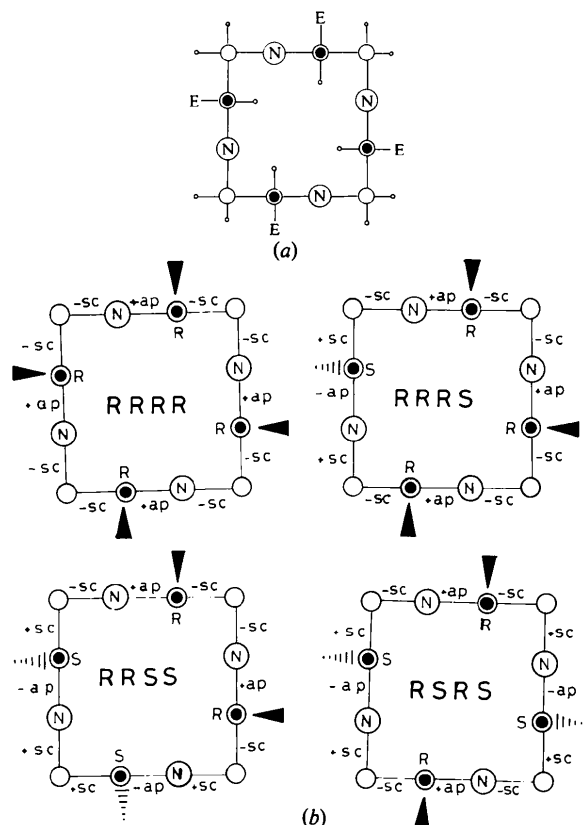| Ring form	Corner	Molecule		Metal complex	
		te	tbte	te	tbte
Square [3333]	CH₂	RRRR	RRRS RRSS RSRS	[Cu^{II}Cl-RRRR]Cl	
Square [3333]	N		RRRR		
Square [3333]	CHEt				[Cu^{II}Cl-RRRR]Cl [Co^{II}Cl-RRRR]Cl
Rectangular [2424]	CH₂, CHEt			[Co^{III}Br(Br₂H₂O)-RRRR]	[Cu^{II}Cl-RSRS]Cl

Fig. 8. Fundamental conformations. (*a*) Direction of the ethyl groups. (*b*) Conformations for the four configurations.

ethyl corners appears for Co^{II} and Cu^{II} complexes of tbte-*RRRR** (Sakurai, Kobayashi, Hasegawa, Tsuboyama & Tsuboyama, 1981), while the rectangular [2424] conformation is observed for [Co^{III}Br(Br₂H₂O) (te-*RRRR*)] (Sakurai, Tsuboyama & Tsuboyama, 1980), and [Cu^{II}Cl(tbte-*RSRS*)]Cl (Kobayashi, Sakurai, Hasegawa, Tsuboyama & Tsuboyama, 1981). A quantitative analysis by a

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* Abbreviations: tbte-*RRRR*: (2R,5R,8R,11R)-1,4,7,10-tetra-benzyl-2,5,8,11-tetraethyl-1,4,7,10-tetraazacyclododecane; te-*RRRR*: (2R,5R,8R,11R)-2,5,8,11-tetraethyl-1,4,7,10-tetraaza-cyclododecane.

molecular-mechanics calculation is now in progress (Tsuboyama, Tsuboyama & Sakurai, 1980).

The benzyl groups have the flexibilities of the two single bonds connecting the phenyl group to the 12-membered ring. The conformation-energy calculation shows a broad low-energy region with 30 ∼ 60 degrees of freedom for each bond. Thus the shape of the molecule is easily changed within this region, in order to satisfy the packing requirements of the molecules in the crystal.

Calculations were performed on a FACOM 230-75 computer of this Institute using the *UNICS* III program system (Sakurai & Kobayashi, 1979) for the crystallographic and MMB 80 (Sakurai, 1978) for the conformation-energy calculations. The authors thank Miss K. Kobayashi for her assistance in the direct-method calculation.

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Sels Diastéréoisomères de Phényl-1 Ethylamine et d'Acides Phénylacétiques α Substitués p et n. Séparation ou Syncristallisation: une Explication Cristallographique

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Abstract

The crystal structures of several diastereoisomer salts are compared. The molecular forms and arrangements allow elucidation of the crystallographic factors which determine whether syncrystallization or separation of the *p* and *n* salts will occur.

Introduction

Dans le cadre d'une étude des sels diastéréoisomères utilisés dans le dédoublement des racémiques, nous avons étudié, sur le plan cristallographique, les sels diastéréoisomères de phényl-1 éthylamine (α-phényl-éthylamine) et d'acide phénylacétique α substitués *p* et *n*, pour lesquels les substituants $R = CH_3$, OH, C_2H_5; ces différents sels correspondent à des diagrammes de solubilité différents entre les sels *p* et *n*:

$R = CH_3$ séparation spontanée
$R = C_2H_5$ miscibilité partielle
$R = OH$ miscibilité totale.

Nous pensions que l'étude cristallographique donnerait une explication aux différents types de diagrammes observés (Leclercq & Jacques, 1975). Cependant nous avons rencontré des problèmes de cristallisation; les sels *p* tels que $R = C_2H_5$ et $R = OH$ cristallisent en fibres très fines; bien que de mauvaise qualité, des fibres plus épaisses du sel $R = C_2H_5$ ont pu être utilisées aux rayons X (Brianso, 1980).

Nous ne comparerons donc que cinq sels (Brianso, 1976, 1978, 1980; Brianso, Leclercq & Jacques, 1979).

Comparaison des différentes structures

(1) *Comparaison des empilements moléculaires*

Dans un mémoire précédent, nous avions remarqué une similitude dans l'organisation cristalline (Brianso *et al.*, 1979).

(*a*) Les structures s'ordonnent toujours en colonnes rigides le long d'un axe binaire hélicoïdal 2_1 autour duquel s'organise le réseau de liaisons hydrogène entre les pôles $(-NH_3)^+$ et $(-COO)^-$ (Fig. 1).

(*b*) Les colonnes se disposent côte à côte en respectant les distances de van der Waals moyennes.

Tableau 1. *Comparaison des distances intramoléculaires* (Å) *des molécules d'acide et de base pour les différents sels*

	$R = CH_3$		$R = C_2H_5$		$R = OH$
	Sel *p*	Sel *n*	Sel *p*	Sel *n*	Sel *n*
Molécule d'acide					
$C-CO_2$	1,524	1,597	1,565	1,573	1,532
$C-R$	1,546	1,580	1,531	1,584	'1,412'
$C-\varphi$	1,502	1,537	1,525	1,549	1,513
$C-O$	{1,251 / 1,255	{1,251 / 1,213	{1,238 / 1,226	{1,268 / 1,218	{1,274 / 1,231
$\langle C=C\rangle, \varphi$	1,388	1,393	1,375	1,417	1,387
$\Delta(\langle C=C\rangle)$	0,057	0,019	0,128	0,045	0,023
Molécule de base					
$C-N$	1,506	1,535	1,511	1,547	1,526
$C-CH_3$	1,538	1,536	1,540	1,561	1,522
$C-\varphi$	1,511	1,497	1,491	1,554	1,493
$\langle C=C\rangle, \varphi$	1,436	1,400	1,387	1,407	1,378
$\Delta(\langle C=C\rangle)$	0,050	0,050	0,100	0,036	0,013
Liaisons hydrogène					
$N \cdots O$	{2,732 / 2,732 / 2,751	{2,798 / 2,723 / 2,810	{2,721 / 2,739 / 2,722	{2,780 / 2,761 / 2,734	{2,831 / 2,863 / 2,843