Acta Cryst. (1985). C**41**, 137–140

A 1:1 Complex between 1,4,7,10,13,16-Hexaoxacyclooctadecane (18-Crown-6) and Phenacylammonium Hexafluorophosphate, $C_{12}H_{24}O_6.C_6H_5COCH_2NH_3^+.PF_6^-$

By John M. Maud† and J. Fraser Stoddart

Department of Chemistry, The University, Sheffield S3 7HF, England

and David J. Williams

Department of Chemistry, Imperial College, London SW7 2AY, England

(*Received* 13 *April* 1984; *accepted* 18 *September* 1984)

Abstract. $M_r = 545{\cdot}4$, monoclinic, $P2_1/n$, $a = 11{\cdot}189\,(2)$, $b = 17{\cdot}461\,(4)$, $c = 13{\cdot}449\,(3)$ Å, $\beta = 99{\cdot}72\,(2)°$, $V = 2590$ Å^3, $Z = 4$, $D_x = 1{\cdot}40$ g cm^{-3}, Cu $K\alpha$, $\lambda = 1{\cdot}54178$ Å, $\mu = 1{\cdot}7$ mm^{-1}, $F(000) = 1144$, room temperature, $R = 0{\cdot}095$ for 2162 unique observed reflections with $|F_o| > 3\sigma(|F_o|)$. On account of steric interactions with the guest, the host molecule adopts a conformation that is slightly distorted from that 'all-*gauche*' conformation with approximate D_{3d} symmetry that is usually observed for complexes of 18-crown-6 with primary alkylammonium ions. The sequence of torsion angles (O–C, C–C, C–O) starting from O(1) in the host is ag^+a ag^-a [−121 (3), −16 (3), −120 (2)°]* ag^-a ag^+a ag^-a around the ring with disorder * evident in the C(8)–C(9) region. The guest phenacylammonium ion is complexed principally by three [N—H···O] hydrogen bonds to the nearer triangle of alternate oxygen atoms in the host in a face-to-face type of complex where the carbonyl oxygen atom of the guest resides over the region of disorder identified in the host.

Introduction. Although the crystal structures of many complexes between 18-crown-6 (18C6) and cationic and neutral guest species have been determined (Goldberg, 1980; Vögtle, Sieger & Müller, 1981), relatively few cases involving RNH_3^+ ions as the guest cation have been reported. To our knowledge, examples are limited to 1:1 complexes with $NH_4Br(2H_2O)$ (Nagano, Kobayashi & Sasaki, 1978), $HONH_3ClO_4$-$(0{\cdot}5H_2O)$, $H_2NNH_3ClO_4$ and $MeNH_3ClO_4$ (Trueblood, Knobler, Lawrence & Stevens, 1982) and $PhCH_2$-NH_3SCN (Bovill, Chadwick, Sutherland & Watkin, 1980). In all these cases, 18C6 adopts an 'all-*gauche*' conformation with pseudo D_{3d} symmetry (Wipff, Weiner & Kollman, 1982; Wipff, Kollman & Lehn, 1983) such that the guest cation is bound principally through [N$^+$—H···O] hydrogen bonding to the host with the NH_3^+ group in either of the so-called (Trueblood *et al.*, 1982) *perching* (R = H, Me, and $PhCH_2$) or *nesting* ($R = NH_2$) positions, or, in one case (R = OH), between these two extreme positions.

We investigated the ability of the $PhCOCH_2NH_3^+$ ion to complex with 18C6 because of its potential for chemical modification while bound to the host, *i.e.* it is a potentially reactive substrate. Early on in our investigations, we isolated a crystalline 1:1 complex of $[PhCOCH_2NH_3.18C6][PF_6]$. Here, we report on this isolation and the subsequent crystal structure analysis of the 1:1 complex, which reveals an interesting consequence for the preferred complexing conformation of 18C6 when a steric interaction occurs with a bound RNH_3^+ ion.

Experimental. A solution of $PhCOCH_2NH_3PF_6$ (69·5 mg) in MeOH (1·5 ml) was added to a solution of 18C6 (65·3 mg) in MeOH (1·5 ml). The resulting solution was filtered immediately and warmed to remove the turbidity. On cooling to room temperature, the turbidity did not reappear and Et_2O (12 ml) was layered on top of the methanolic solution. After 19 days, small crystals of $[PhCOCH_2NH_3.18C6][PF_6]$ (found: C 44·0; H 6·0; N 2·8%. $C_{20}H_{34}F_6NO_7P$ requires C 44·0; H 6·3; N 2·6%), which had m.p. 456–459 K, were isolated and found to be suitable for X-ray structural investigation. Crystal size 0·2 × 0·2 × 0·3 mm. Refined unit-cell parameters obtained by centring 20 reflections, Nicolet $R3m$ diffractometer. 2660 independent reflections ($\theta \leq 50°$) measured, Cu $K\alpha$ radiation (graphite monochromator), ω scan. 2162 [$|F_o| > 3\sigma(|F_o|)$] considered observed, index range h −11/10, k 0/17, l 0/13; two check reflections measured every 50 reflections, net count constant; data brought to uniform scale, Lorentz and polarization corrections, no absorption correction. Structure solved by direct methods; non-hydrogen atoms refined anisotropically; positions of phenyl and methylene H atoms calculated (C—H = 0·96 Å), assigned isotropic thermal parameters, $U(H) = 1{\cdot}2\ U_{eq}(C)$, allowed to ride on parent C atoms; ammonium H atoms clearly resolved

---

† Present address: Edward Davies Chemical Laboratories, University College of Wales, Aberystwyth, Dyfed SY23 1NE, Wales.

0108-2701/85/010137-04$01.50

in ΔF map, group refined as rigid body. $\bar{2}02$ had $|F_o| << |F_c|$ and was suspected as being affected by extinction and was removed. Refinement using F magnitudes by blocked cascade full-matrix least squares; $R = 0.095$, $R_w = 0.11$ $[w^{-1} = \sigma^2(F) + 0.0005F^2]$. $\Delta/\sigma = 0.05$; residual electron density in difference map within -0.3 and $+0.5$ e Å^{-3}; atomic scattering factors and dispersion corrections from *International Tables for X-ray Crystallography* (1974). Computations carried out on an Eclipse S140 computer using the *SHELXTL* program system (Sheldrick, 1983).

Discussion. Table 1* lists the fractional atomic coordinates of the non-hydrogen atoms, Table 2 the bond lengths and angles and the C–C and C–O torsion angles in the host and selected ones in the guest.

Table 1. *Atom coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors* (Å^2 $\times 10^3$) *with e.s.d.'s in parentheses*

	x	y	z	U_{eq}*
O(1)	3387 (5)	3868 (3)	1936 (4)	97 (2)
C(2)	4508 (8)	3931 (5)	1619 (6)	104 (4)
C(3)	4712 (8)	4756 (5)	1424 (7)	116 (4)
O(4)	4772 (5)	5165 (3)	2320 (5)	105 (3)
C(5)	5042 (9)	5932 (5)	2277 (8)	138 (5)
C(6)	5247 (8)	6278 (5)	3257 (8)	136 (5)
O(7)	4182 (6)	6282 (3)	3662 (5)	133 (3)
C(8)	4354 (16)	6441 (9)	4639 (7)	264 (10)
C(9)	4190 (14)	6164 (8)	5357 (9)	223 (8)
O(10)	3327 (7)	5487 (4)	5283 (4)	162 (4)
C(11)	2431 (10)	5613 (6)	5720 (6)	145 (5)
C(12)	1708 (9)	4834 (6)	5768 (7)	141 (5)
O(13)	1403 (5)	4503 (4)	4775 (5)	140 (3)
C(14)	1162 (9)	3739 (8)	4859 (10)	146 (6)
C(15)	893 (10)	3419 (7)	3793 (11)	153 (6)
O(16)	1943 (6)	3462 (3)	3343 (5)	125 (3)
C(17)	1975 (9)	3061 (5)	2530 (8)	142 (5)
C(18)	3178 (8)	3093 (4)	2196 (7)	119 (4)
C(19)	5794 (7)	1000 (4)	3871 (5)	82 (3)
C(20)	6851 (8)	1290 (5)	4441 (6)	109 (4)
C(21)	7476 (7)	1867 (4)	4060 (7)	97 (4)
C(22)	7060 (6)	2156 (4)	3137 (6)	74 (3)
C(23)	6006 (5)	1878 (3)	2563 (5)	61 (2)
C(24)	5369 (5)	1292 (3)	2944 (4)	53 (2)
C(25)	4249 (5)	1003 (3)	2309 (5)	52 (2)
O(25)	3858 (4)	1281 (3)	1508 (4)	80 (2)
C(26)	3589 (5)	326 (3)	2678 (4)	63 (2)
N	2560 (4)	93 (3)	1897 (4)	58 (2)
P	1980 (2)	6346 (1)	−680 (2)	92 (1)
F(1)	1759 (8)	6727 (4)	289 (6)	232 (5)
F(2)	649 (5)	6022 (5)	−889 (5)	189 (4)
F(3)	1607 (10)	7067 (5)	−1222 (8)	295 (7)
F(4)	3284 (6)	6640 (5)	−484 (7)	226 (5)
F(5)	2303 (8)	5632 (4)	−90 (6)	234 (5)
F(6)	2233 (7)	5956 (5)	−1608 (5)	220 (4)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

The structure of the 1:1 complex is illustrated in Fig. 1(*a*) and (*b*). Fig. 1(*a*) includes the atomic numbering scheme. The analysis of the structure was marred by severe thermal anisotropy and disorder in both the host macrocycle and the PF_6^- anion. These effects are most pronounced in the C(8)—C(9) region of the crown-ether ring and result in artificial shortening of the bonds in this region of the macrocycle and perturbation of the torsion angles (see Table 2). A consequence of this disorder is the rather poor value of R obtained in the refinement of the structure. It was not possible to identify

Table 2. *Bond lengths* (Å), *bond angles and selected torsion angles* (°)

O(1)–C(2)	1·396 (11)	O(1)–C(18)	1·426 (9)
C(2)–C(3)	1·489 (12)	C(3)–O(4)	1·393 (11)
O(4)–C(5)	1·375 (11)	C(5)–C(6)	1·433 (15)
C(6)–O(7)	1·392 (13)	O(7)–C(8)	1·326 (12)
C(8)–C(9)	1·122 (18)	C(9)–O(10)	1·519 (16)
O(10)–C(11)	1·264 (13)	C(11)–C(12)	1·590 (15)
C(12)–O(13)	1·442 (11)	O(13)–C(14)	1·369 (15)
C(14)–C(15)	1·520 (19)	C(15)–O(16)	1·411 (14)
O(16)–C(17)	1·304 (12)	C(17)–C(18)	1·490 (14)
C(19)–C(20)	1·391 (10)	C(19)–C(24)	1·356 (8)
C(20)–C(21)	1·374 (12)	C(21)–C(22)	1·348 (11)
C(22)–C(23)	1·384 (8)	C(23)–C(24)	1·394 (8)
C(24)–C(25)	1·481 (8)	C(25)–O(25)	1·195 (8)
C(25)–C(26)	1·522 (9)	C(26)–N	1·478 (7)
P–F(1)	1·520 (9)	P–F(2)	1·573 (7)
P–F(3)	1·480 (9)	P–F(4)	1·527 (7)
P–F(5)	1·489 (7)	P–F(6)	1·490 (8)

C(2)–O(1)–C(18)	110·0 (6)	O(1)–C(2)–C(3)	107·6 (7)
C(2)–C(3)–O(4)	109·3 (7)	C(3)–O(4)–C(5)	116·2 (7)
O(4)–C(5)–C(6)	112·0 (9)	C(5)–C(6)–O(7)	110·3 (8)
C(6)–O(7)–C(8)	113·4 (10)	O(7)–C(8)–C(9)	138·2 (15)
C(8)–C(9)–O(10)	118·3 (12)	C(9)–O(10)–C(11)	112·3 (9)
O(10)–C(11)–C(12)	108·6 (9)	C(11)–C(12)–O(13)	110·4 (7)
C(12)–O(13)–C(14)	109·5 (8)	O(13)–C(14)–C(15)	106·9 (10)
C(14)–C(15)–O(16)	109·8 (8)	C(15)–O(16)–C(17)	118·3 (8)
O(16)–C(17)–C(18)	112·8 (8)	O(1)–C(18)–C(17)	107·6 (6)
C(20)–C(19)–C(24)	120·2 (7)	C(19)–C(20)–C(21)	120·0 (7)
C(20)–C(21)–C(22)	120·0 (7)	C(21)–C(22)–C(23)	120·8 (7)
C(22)–C(23)–C(24)	119·5 (6)	C(19)–C(24)–C(23)	119·5 (5)
C(19)–C(24)–C(25)	122·3 (6)	C(23)–C(24)–C(25)	118·2 (5)
C(24)–C(25)–O(25)	121·9 (5)	C(24)–C(25)–C(26)	119·1 (5)
O(25)–C(25)–C(26)	119·0 (5)	C(25)–C(26)–N	110·1 (5)
F(1)–P–F(2)	91·4 (4)	F(1)–P–F(3)	88·6 (5)
F(2)–P–F(3)	92·2 (5)	F(1)–P–F(4)	89·6 (5)
F(2)–P–F(4)	178·5 (5)	F(3)–P–F(4)	88·9 (5)
F(1)–P–F(5)	88·2 (4)	F(2)–P–F(5)	86·0 (4)
F(3)–P–F(5)	176·4 (6)	F(4)–P–F(5)	92·9 (5)
F(1)–P–F(6)	178·0 (4)	F(2)–P–F(6)	89·7 (4)
F(3)–P–F(6)	93·1 (6)	F(4)–P–F(6)	89·3 (5)
F(5)–P–F(6)	90·1 (4)		

C(18)–O(1)–C(2)–C(3)	−176·3 (6)
O(1)–C(2)–C(3)–O(4)	+63·0 (8)
C(2)–C(3)–O(4)–C(5)	+175·6 (7)
C(3)–O(4)–C(5)–C(6)	−172·0 (7)
O(4)–C(5)–C(6)–O(7)	−66·2 (10)
C(5)–C(6)–O(7)–C(8)	+166·4 (10)
C(6)–O(7)–C(8)–C(9)	−120·8 (25)
O(7)–C(8)–C(9)–O(10)	−15·6 (33)
C(8)–C(9)–O(10)–C(11)	−119·6 (16)
C(9)–O(10)–C(11)–C(12)	−170·4 (7)
O(10)–C(11)–C(12)–O(13)	−53·4 (9)
C(11)–C(12)–O(13)–C(14)	+159·8 (8)
C(12)–O(13)–C(14)–C(15)	−178·0 (8)
O(13)–C(14)–C(15)–O(16)	+65·4 (10)
C(14)–C(15)–O(16)–C(17)	+164·5 (9)
C(15)–O(16)–C(17)–C(18)	173·9 (8)
O(16)–C(17)–C(18)–O(1)	−63·6 (10)
C(17)–C(18)–O(1)–C(2)	+179·8 (7)
C(19)–C(24)–C(25)–O(25)	+177·3 (6)
C(23)–C(24)–C(25)–O(25)	−3·3 (9)
C(24)–C(25)–C(26)–N	−175·3 (5)
O(25)–C(25)–C(26)–N	+3·7 (8)
C(25)–C(26)–N–H_a	−175·9

---

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39747 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

discrete alternative sites for C(8) and C(9) consistent with two different conformations in this, or in any other regions displaying high thermal anisotropy. Despite these observations, the conformation of the ring is such that it does display the classic three-point binding characteristic of a 1:1 complex of 18C6 with an RNH_3^+ guest cation. Ignoring the O(7)–O(10) region, the observed bond lengths (average C—O 1·38 Å; average C—C 1·50 Å), bond angles (average C—O—C 113·5°; average C—C—O 109·5°) (Table 2), and torsion angles (average C—O—C—C 171·6°; average O—C—C—O 62·3°) (Table 2) are similar to those commonly found (Goldberg, 1980) in 18C6 when it is involved in complex formation. An upper triangle of oxygen atoms, which can be identified as O(1), O(7) and O(13) form [N^+—H···O] hydrogen bonds with (N^+···O) distances of 2·96 (1), 2·86 (1) and 2·89 (1) Å, respectively. The corresponding N—H—O angles at H_a, H_c and H_b, respectively, are 165, 172 and 170°. The angles between the COC planes and the HO vectors are 35, 34 and 29° for H_a, H_c and H_b, respectively. The (N^+···O) distances to the lower triangle of oxygen atoms O(4), O(10) and O(16) are 2·98 (1), 3·01 (1) and 2·93 (1) Å, respectively. The nitrogen atom is displaced 1·15 (1) Å from the best mean plane of the six oxygen atoms in the macrocycle and the angle between the C(26)–N axis and this plane is 88·4 (1)°. [The nitrogen atom is displaced by 0·80 (1) Å from the plane defined by the upper triangle of oxygen atoms with the C(26)–N axis inclined at 80·7 (1)° to this plane.] Thus, in the vicinity of the binding site, and ignoring the region of disorder in the host, the molecular structure of [$PhCOCH_2NH_3$.18C6][PF_6] bears a resemblance to [NH_4.18C6.2H_2O][Br] (Nagano *et al.*, 1978), [$MeNH_3$.18C6][ClO_4] (Trueblood *et al.*, 1982) and [$PhCH_2NH_3$.18C6][SCN] (Bovill *et al.*, 1980), where the N atom is displaced by 1·0, 0·84 and 0·86 Å, respectively, from the mean plane of the macrocyclic ring O atoms. The conformation of the guest $PhCOCH_2NH_3^+$ cation is such that the carbonyl and phenyl groups are almost coplanar (Fig. 1*b* and Table 2), presumably because of the stabilization of this conformation by efficient π–π conjugation. The refined orientation of the NH_3^+ group with respect to the $PhCOCH_2$ unit shows that they adopt a nearly ideal staggered relationship. Interestingly, the carbonyl oxygen atom O(25) in the guest resides over that portion of the macrocycle, from O(7) to O(10), that exhibits the most severe disorder. The non-bonded distances of O(25) to O(7), C(8), C(9) and O(10) of 3·37 (1), 3·67 (2), 3·88 (2) and 3·42 (1) Å, respectively, suggest that steric interactions between guest and host may be partly responsible for this disorder. However, it should be noted that these distances are of the same order as the shortest inter-complex non-bonded distances, *e.g.* C(20)–O(1$^{\text{i}}$) 3·51 (1) Å and C(18)–O(25$^{\text{i}}$) 3·42 (1) Å.

There are several short inter-complex contacts to the PF_6^- ion. Most notable are contacts of 3·27 (2) Å between C(2) and F(4) and 3·29 (2) Å between C(6) and F(3). In the case of the latter, one of the hydrogen atoms on C(6) is only 2·39 (2) Å from F(3) indicating a possible weak [C—H···F] interaction, with the angle at H equal to 155°.

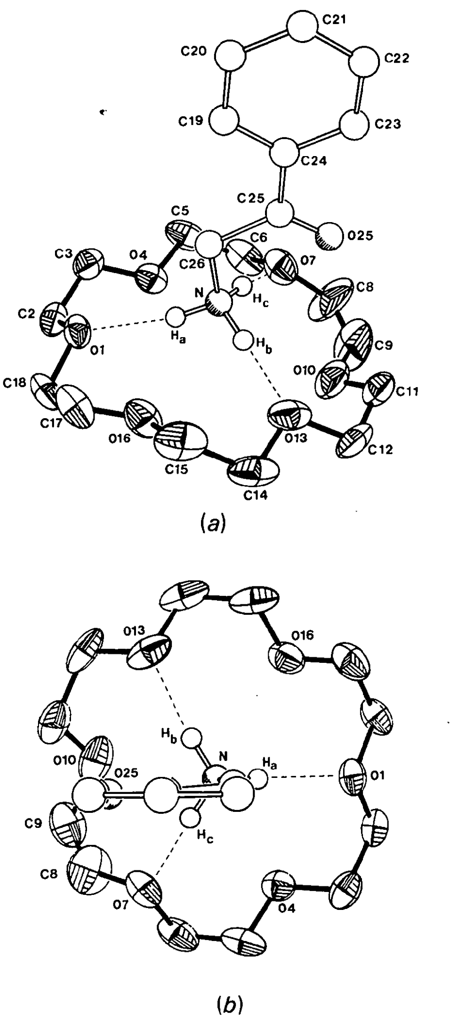


Fig. 1. (*a*) Plot showing a side-on view of the 1:1 complex and the atomic numbering scheme. The thermal ellipsoids correspond to 20% probability. The H atoms, other than on the NH_3^+ centre, have been omitted for clarity. H bonds are indicated by dashed lines. (*b*) Plot showing a view of the 1:1 complex from above.

We thank the Science and Engineering Research Council and Imperial Chemical Industries PLC for financial support under their Joint Research Scheme.

References

Bovill, M. J., Chadwick, D. J., Sutherland, I. O. & Watkin, D. (1980). *J. Chem. Soc. Perkin Trans.* 2, pp. 1529–1543.

Goldberg, I. (1980). *The Chemistry of Functional Groups. Supplement E: The Chemistry of Ethers, Crown Ethers, Hydroxyl Groups and their Sulphur Analogues.* Part 1, edited by S. Patai, pp. 175–214. Chichester: John Wiley.
International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press.
Nagano, O., Kobayashi, A. & Sasaki, I. (1978). *Bull. Chem. Soc. Jpn*, **51**, 790–793.
Sheldrick, G. M. (1983). *SHELXTL*, revision 4·0, January 1983. *An Integrated System for Solving, Refining and Displaying Crystal Structures from Diffraction Data.* Univ. of Göttingen.
Trueblood, K. N., Knobler, C. B., Lawrence, D. S. & Stevens, R. V. (1982). *J. Am. Chem. Soc.* **104**, 1355–1362.
Vögtle, F., Sieger, H. & Müller, W. M. (1981). *Topics in Current Chemistry* 98. *Host Guest Complex* I, edited by F. Vögtle, pp. 107–161. Berlin: Springer-Verlag.
Wipff, G., Kollman, P. A. & Lehn, J. M. (1983). *J. Mol. Struct.* **93**, 153–165.
Wipff, G., Weiner, P. & Kollman, P. (1982). *J. Am. Chem. Soc.* **105**, 3249–3258.

Acta Cryst. (1985). C**41**, 140–142

The Structure of Dispiro(tricyclo[3.3.1.1^{3,7}]decane-2,6′-6′*H*,12′*H*-dibenzo[*b*,*f*][1,5]dioxocin-12′,2′′-tricyclo[3.3.1.1^{3,7}]decane), $C_{32}H_{36}O_2$

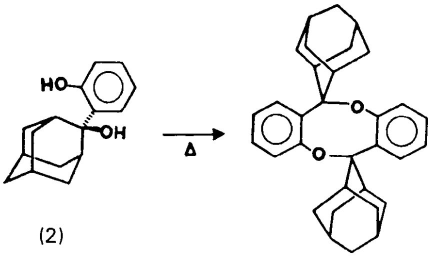
By Mary F. Garbauskas, Irene A. Evans and John J. Talley

General Electric Corporate Research and Development, PO Box 8, *Schenectady, NY* 12301, *USA*

(*Received* 30 *May* 1984; *accepted* 18 *September* 1984)

Abstract. $M_r = 456{\cdot}7$, monoclinic, $P2_1/a$, $a = 13{\cdot}961$ (8), $b = 11{\cdot}189$ (6), $c = 16{\cdot}208$ (9) Å, $\beta = 107{\cdot}94$ (4)°, $V = 2408{\cdot}7$ Å^3, $Z = 4$, $D_x = 1{\cdot}26$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71079$ Å, $\mu = 0{\cdot}8$ cm^{-1}, $F(000) = 495{\cdot}94$, approximately 303 K, $R = 0{\cdot}0635$, 1901 unique observed reflections. The central 1,5-dioxocin ring adopts a tub shape to minimize non-bonded interactions between the two very bulky adamantane moieties. This conformation leads to bridgehead carbons that are shift inequivalent in the proton-decoupled ^{13}C NMR spectrum and explains the presence of the nine aliphatic NMR resonances observed for this molecule.

Introduction. A sample of (1) was prepared by the thermolysis of (2) (Talley & Evans, 1984) in the melt at 443 K. As (2) melted, 437 K, it acquired an orange color; continued heating resulted in the evolution of water vapor and the resolidification of (1) as a white solid with m.p. 500–501 K.



(2)

(1)

The solution ^{13}C NMR of (1) contained four resonances in the aromatic region and nine resonances in the aliphatic region. Since the ^{13}C NMR of (2) showed only seven aliphatic resonances in addition to four aromatic signals, the formation of an unusual structure or conformation was suspected. The field desorption mass spectrum of (1) confirmed that a dimer with a molecular formula of $C_{32}H_{36}O_2$ had been formed.

In order to establish unequivocally the structure of the dimer, we performed a single-crystal X-ray analysis of (1).

Experimental. Rectangular thin plates obtained by crystallization from acetone. Data collected on Nicolet P3/F automated diffractometer, monochromated Mo $K\alpha$ radiation, crystal dimensions $0{\cdot}2 \times 0{\cdot}3 \times 0{\cdot}05$ mm. Lattice parameters from 12 reflections with 5 to 14° 2θ. $h = 0$ to 15, $k = 0$ to 12, $l = -16$ to 16, max. $\sin\theta/\lambda = 0{\cdot}54$ Å^{-1}. Two standard reflections, $00\bar{3}$ and $\bar{1}1\bar{2}$, monitored with s.d. in intensity of 1% in both cases. 3524 reflections collected; 1901 unique observed with $F \geq 3\sigma(F)$. Structure solved by direct methods using *SHELXTL* (Sheldrick, 1981). Refinement based on F. Hydrogen positions located by difference Fourier synthesis. In final stages of refinement, C—H bond lengths and H—C—H angles fixed at 0·96 Å and 109·5°. Fixed isotropic temperature factor of 0·06 Å^2 for all H atoms. All non-hydrogen atoms anisotropic. 307 parameters refined, final $R_w = 0{\cdot}0488$, $R = 0{\cdot}0635$. $w^{-1} = \sigma^2(F) + (0{\cdot}00026)F^2$. In final difference Fourier map, max. and min. 0·24 and $-0{\cdot}25$ e Å^{-3}. Max.