Crystallographic Characterization of 2,2,7,7-Tetraphenyl-6-oxabicyclo[3.2.1]octan-5-ol, C₃₁H₂₈O₂ – Reaction Product of 4,4-Diphenylcyclohex-2-en-1-one and the Radical Anion of Benzophenone

By Chin Hsuan Wei

Biology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, USA*

and Stuart W. Hawkinson

*Department of Biochemistry, The University of Tennessee, Knoxville, Tennessee 37916, USA*

The reaction product of 4,4-diphenylcyclohex-2-en-1-one and the radical anion of benzophenone has been characterized by the analysis of three-dimensional X-ray film data. The results provide detailed crystal and molecular structure for the reaction product (which had previously been assigned an incorrect formula with ring formula C_3O-C_6), thereby unambiguously establishing the correct formula as 2,2,7,7-tetraphenyl-6-oxabicyclo[3.2.1]octan-5-ol (ring formula C_4O-C_6). The compound crystallizes with 16 molecules in a tetragonal unit cell of symmetry $I4_1/a$ with parameters $a = b = 27.58$ (2) and $c = 12.09$ (2) Å. The structure was solved by direct methods and refined by the rigid-group least-squares method to $R(F) = 0.068$ based on 710 intensity data observed. Each molecule is hydrogen-bonded to two neighboring molecules *via* O–H···O bonds.

Introduction

In an attempt to investigate the molecular rearrangement of 4,4-diphenylcyclohex-2-en-1-one by the use of a radical anion of benzophenone, Peterson & Zimmerman (Peterson, 1966) treated 4,4-diphenylcyclohex-2-en-1-one (I) with two equivalents of the radical anion of benzophenone (II) in tetrahydrofuran under nitrogen. On the basis of chemical analyses and IR data for the new compound thus obtained, augmented with some

detailed analyses involving IR and NMR spectra of the acid hydrolysis and thermal degradation products, they tentatively assigned structure III for the reaction product.

The structural analysis by X-ray diffraction of the reaction product revealed that structure III was incorrect; the correct structure is as shown in IV (ring formula C_4O-C_6) or in an arrangement (V) in which the standard numbering scheme adopted in this paper is also given (*The Ring Index*, 1960).
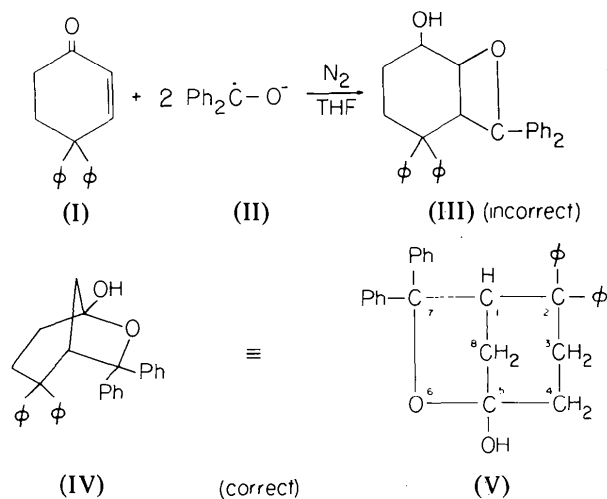
Experimental

Colorless transparent crystals of $C_{31}H_{28}O_2$ (M_r 432.565) were kindly supplied by Dr R. G. Peterson and Professor H. E. Zimmerman at the University of Wisconsin. A single crystal in the shape of a rectangular prism with dimensions 0.15 × 0.23 × 0.38 mm was mounted inside a thin-walled glass capillary so that the longest dimension, corresponding to the c axis, was nearly coincident with the capillary axis. Unit-cell parameters were determined from an $h0l$ precession photograph. The observed density of 1.26 g cm⁻³ (obtained by flotation) agrees satisfactorily with the calculated value of 1.249 g cm⁻³ based on 16 formula units of $C_{31}H_{28}O_2$ in a unit cell. The crystals are tetragonal with $a = b = 27.58$ (2) and $c = 12.09$ (2) Å (lattice-parameter errors were estimated on the basis of reproducibility of the measurements). The volume of the unit cell is 9196 Å³. The total number of electrons

(I)   (II)   (III) (incorrect)

(IV)   (correct)   (V)

per unit cell, $F(000)$, is 3680. Systematic absences of hkl for $h + k + l$ odd, $hk0$ for h or k odd, and $00l$ for $l \neq 4n$ are uniquely characteristic of the space group $I4_1/a$ (C_{4h}^6, No. 88), which was later confirmed by a successful refinement of the structure.

Multiple-film equi-inclination Weissenberg data ($hk0$ through $h,k,10$) and multiple-exposure precession data ($h0l$) were obtained with Zr-filtered Mo $K\alpha$ radiation ($\lambda = 0.7107$ Å). The crystal was found to be stable to X-irradiation. Intensities were estimated visually by comparison with a standard set of intensities prepared with the same crystal, and then corrected for Lorentz and polarization effects. Although corrections for spot extension were applied to the Weissenberg data, no corrections were made for absorption or extinction. With the linear absorption coefficient of 0.824 cm^{-1} for Mo $K\alpha$ radiation, the variation of absorption correction factors with θ is not appreciable. Reflections appearing in both Weissenberg and precession photographs were used to assign initial individual relative scale factors for the 12 reciprocal levels; these scale factors were subsequently varied in the rigid-group least-squares refinement based on a total of 710 unique intensity data observed. Minimum observed intensities, I_o(min), were estimated for each reciprocal level, and variable weights were assigned to individual reflections according to the following scheme: $\sqrt{w}(F_o) = 20/F_o$ if $I_o \geq 4I_o$(min); $\sqrt{w}(F_o) = 1.25I_o^2/F_o[I_o(min)]^2$ if $I_o < 4I_o$(min).

Solution and refinement of the structure

The 710 reflections represent only a small fraction of the 3188 possible in a sin θ/λ range of 0.050 to 0.549. In order to obtain an appropriate representation of the intensity distribution, the unobserved reflections were each assigned a value of $\frac{1}{2}F_o$(min) for their structure amplitudes, and were merged with those collected by the film methods. Since two reflections, 200 and 101 (with sin θ/λ values of 0.036 and 0.045 respectively), were cut off in the films, they were excluded from the initial treatment of the data. A Wilson plot (including

the unobserved reflections) gave an overall temperature factor of 2.8 Å^2; a set of normalized structure amplitudes (E) was obtained using program $NORMAL$ [part of the program $MULTAN$ (Germain, Main & Woolfson, 1971)].

$MULTAN$ was then applied for the multiple-solution problem. There were 250 reflections with $E > 1.70$ that were used for phase generation. Of eight phase sets thus generated, only one was plausible on the basis of various figures of merit. The corresponding E map yielded 33 peaks interpretable as the C and O atoms on the basis of normal chemical criteria. Among them, 24 peaks interpretable as four phenyl ring C atoms were then adjusted, with the aid of program $BMFIT$ (Nyburg, 1974), to their best idealized positions as the starting model.

Table 1. *Positional, thermal, and group parameters for* $C_{31}H_{28}O_2$

Least-squares-derived standard deviations of the least significant figures are given in parentheses in all the tables and in the text. All the H atoms were assigned isotropic temperature factors of 5.0 Å^2, which were not varied. In the final rigid-group refinement, positional parameters for all the H atoms were also fixed (see text).

	x	y	z	B (Å^2)
C(1)	0.3710 (4)	0.6338 (4)	0.9388 (7)	2.6 (2)
C(2)	0.3988 (4)	0.5865 (4)	0.9000 (8)	3.1 (2)
C(3)	0.4538 (4)	0.5971 (4)	0.9040 (8)	3.3 (2)
C(4)	0.4723 (4)	0.6217 (4)	1.0077 (8)	3.4 (3)
C(5)	0.4377 (4)	0.6639 (4)	1.0319 (8)	3.0 (3)
O(6)	0.4333 (3)	0.6925 (2)	0.9308 (5)	3.0 (2)
C(7)	0.3855 (4)	0.6830 (4)	0.8832 (8)	2.9 (2)
C(8)	0.3878 (4)	0.6453 (4)	1.0565 (8)	2.7 (2)
O(5)	0.4554 (3)	0.6956 (3)	1.1165 (5)	3.6 (2)
H(1)	0.336	0.631	0.992	
H(3a)	0.474	0.558	0.897	
H(3b)	0.459	0.618	0.844	
H(4a)	0.502	0.637	0.995	
H(4b)	0.470	0.602	1.079	
H(8a)	0.382	0.621	1.116	
H(8b)	0.366	0.673	1.090	
H(5)	0.491	0.695	1.111	

Table 1 (*cont.*)

Group*	x_c	y_c	z_c	φ	θ	ρ
PH(1)†	0.3723 (2)	0.5019 (2)	1.0379 (4)	1.037 (5)	−2.798 (4)	2.546 (5)
PH(2)	0.3677 (2)	0.5535 (2)	0.6791 (4)	1.707 (5)	−2.777 (4)	−1.870 (5)
PH(3)	0.3895 (2)	0.6836 (2)	0.6410 (4)	1.703 (4)	3.124 (3)	−1.560 (4)
PH(4)	0.3238 (2)	0.7653 (2)	0.9407 (4)	−0.928 (5)	3.024 (4)	2.924 (4)

* x_c, y_c, and z_c are fractional coordinates of the origins for the rigid phenyl-ring groups. The rigid-body positional coordinates are defined relative to right-handed orthogonal axes x', y', and z' with origins at the centers of the phenyl rings. In the PH(1), PH(2), PH(3), and PH(4) groups, C(14), C(24), C(34), and C(44) lie on the $+x'$ axes, and the $+y'$ axes intersect the midpoints of C(15)–C(16), C(25)–C(26), C(35)–C(46), and C(45)–C(46). For each phenyl group, the three angular parameters φ, θ, and ρ (in radians) define the orientation of the rigid-body axial system with respect to the right-handed orthogonal crystal axes a, b, and c. Three successive rotations bring the crystal axes into parallel coincidence with rigid-body axes as follows. A positive rotation φ about c brings a to a_1 and b to b_1; next, a positive rotation θ about a_1 brings b_1 to b' and c to c_1; lastly, a positive rotation ρ about b' brings a_1 to a' and c_1 to c'.

† PH(1) and PH(2) are bonded to C(2), and PH(3) and PH(4) are bonded to C(7).

Three cycles of isotropic full-matrix least-squares refinement (Busing, Martin & Levy, 1962), in which the function minimized was $\Sigma w(|F_o| - |F_c|)^2$, converged to give an $R(F)$ value of 0·111. A difference Fourier synthesis calculated [program ORFFP (Levy, 1975)] at this stage showed seven strong peaks which were unambiguously identified as nonphenyl H atoms with reasonable positions based on chemical grounds. One strong peak corresponding to $H(8b)$, however, was approximately 1·5 Å away from C(8) in the neighborhood of the expected position. Hence, this

Table 2. *Derived parameters of group atoms for* $C_{31}H_{28}O_2$

Group		x	y	z	B (Å²)
PH(1)	C(11)	0·3854	0·5428	0·9769	3·0 (2)
	C(12)	0·3433	0·5434	1·0410	4·3 (3)
	C(13)	0·3303	0·5025	1·1020	5·6 (3)
	C(14)	0·3593	0·4610	1·0989	4·9 (3)
	C(15)	0·4013	0·4605	1·0348	4·9 (3)
	C(16)	0·4144	0·5014	0·9738	3·8 (3)
	H(12)	0·3226	0·5731	1·0433	*
	H(13)	0·3001	0·5029	1·1480	*
	H(14)	0·3499	0·4317	1·1426	*
	H(15)	0·4221	0·4308	1·0325	*
	H(16)	0·4445	0·5010	0·9278	*
PH(2)	C(21)	0·3828	0·5706	0·7821	3·9 (3)
	C(22)	0·3347	0·5565	0·7663	4·7 (3)
	C(23)	0·3196	0·5394	0·6633	5·8 (3)
	C(24)	0·3526	0·5364	0·5761	4·7 (3)
	C(25)	0·4007	0·5505	0·5920	4·4 (3)
	C(26)	0·4158	0·5676	0·6950	3·8 (3)
	H(22)	0·3110	0·5587	0·8287	*
	H(23)	0·2851	0·5293	0·6519	*
	H(24)	0·3418	0·5241	0·5023	*
	H(25)	0·4244	0·5483	0·5295	*
	H(26)	0·4502	0·5777	0·7063	*
PH(3)	C(31)	0·3887	0·6829	0·7564	3·2 (3)
	C(32)	0·3456	0·6775	0·6969	4·3 (3)
	C(33)	0·3465	0·6781	0·5816	3·9 (3)
	C(34)	0·3903	0·6843	0·5256	4·2 (3)
	C(35)	0·4333	0·6897	0·5851	4·3 (3)
	C(36)	0·4325	0·6890	0·7004	3·4 (3)
	H(32)	0·3142	0·6731	0·7370	*
	H(33)	0·3156	0·6742	0·5390	*
	H(34)	0·3909	0·6847	0·4429	*
	H(35)	0·4647	0·6941	0·5450	*
	H(36)	0·4633	0·6929	0·7430	*
PH(4)	C(41)	0·3524	0·7250	0·9160	2·6 (2)
	C(42)	0·3729	0·7712	0·9166	3·3 (2)
	C(43)	0·3443	0·8115	0·9413	4·0 (3)
	C(44)	0·2952	0·8056	0·9654	4·2 (3)
	C(45)	0·2747	0·7594	0·9648	5·6 (3)
	C(46)	0·3032	0·7191	0·9401	4·7 (3)
	H(42)	0·4081	0·7755	0·8993	*
	H(43)	0·3590	0·8447	0·9417	*
	H(44)	0·2747	0·8345	0·9832	*
	H(45)	0·2395	0·7552	0·9821	*
	H(46)	0·2885	0·6860	0·9397	*

* All H atoms were assigned isotropic temperature factors of 5·0 Å², which were not varied.

particular H atom was added at its calculated position and was not varied in the subsequent refinements. Each of a total of 61 nonhydrogen and H atoms was found to be located on the 16-fold set of general positions (16*f*): $(0,0,0; \frac{1}{2},\frac{1}{2},\frac{1}{2}) \pm (x,y,z; -x, \frac{1}{2} - y, z; \frac{3}{4} - y, \frac{1}{4} + x, \frac{1}{4} + z; \frac{1}{4} + y, \frac{1}{4} - x, \frac{1}{4} + z)$.

With the use of a rigid-group refinement program, kindly supplied by Professor L. F. Dahl of the University of Wisconsin, the four phenyl rings were next constrained to possess idealized symmetry in order to improve the ratio of the number of observations to the number of varied parameters. The orthogonal axes for the rigid phenyl groups (C—C distances 1·395 Å; C—H distances 1·0 Å) were as defined in Table 1 (first footnote). Four cycles of isotropic refinement, in which the thermal parameters for all 28 hydrogen atoms (each assigned a value of 5·0 Å²) and positional parameters for $H(8b)$ were not varied, were next carried out. Although at this stage of the refinement the $R(F)$ value had dropped to 0·069, some positional parameters for the nonphenyl H atoms were still shifting as much as twice the corresponding standard deviations.

In the final refinement, therefore, all nonphenyl H atoms were fixed at their current positions, which appeared reasonable, and only parameters for non-phenyl C and O atoms were varied along with the group parameters. At the end of two cycles, all parameter shifts were less than 21% of the corresponding standard deviations. The $R(F)$ and $R_w(F)$ values remained at 0·068 and 0·066 respectively. The final standard deviation of an observation of unit weight – defined as $[\Sigma w||F_o| - |F_c||^2/(n - p)]^{1/2}$, where n is the number of observations and p the number of parameters fitted to the data set – was 1·012. The atomic scattering factors used were those of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenen-daal (1955) for C and O, and those of Stewart, Davidson & Simpson (1965) for H.

The final parameters for nongroup atoms and rigid groups, together with the corresponding standard deviations, are given in Table 1. The derived parameters for the group atoms are shown in Table 2.*

Description of the structure

The X-ray-derived molecular structure of $C_{31}H_{28}O_2$ corresponds to a 6-oxabicyclo[3.2.1]octane derivative instead of the structure as assigned by Peterson (1966). Fig. 1 shows a stereoscopic view of the molecule. The 6-oxabicyclo[3.2.1]octan-5-ol fragment is formed from the addition of the radical ion of benzophenone to the enone system of cyclohexenone, resulting in tetra-

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32897 (2 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.
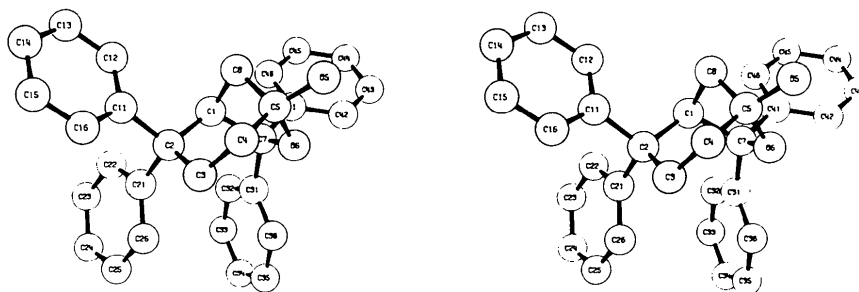
Fig. 1. Stereoscopic view of the molecule showing the atom-labeling scheme used in the text. For the sake of clarity, H atoms are not included. All drawings were prepared by the use of program ORTEP-II (Johnson, 1976).
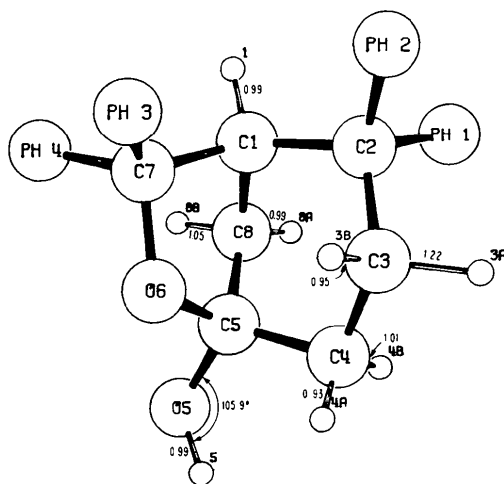

Fig. 2. Perspective view of the 6-oxabicyclo[3.2.1]octan-5-ol moiety. H atoms are represented by small spheres.

hedral configuration for all seven C atoms in the heterocyclic ring sː tem. The framework of the 6-oxabicyclo[3.2.1]octan-5-ol moiety of the molecule is shown in Fig. 2, and the bond distances and angles for nonhydrogen atoms are given in Table 3.

In view of the limited quantity and quality of the data, the average e.s.d.'s for bond lengths and angles associated with nonhydrogen atoms are fairly large (Busing, Martin & Levy, 1964), 0·01 Å and 0·8° respectively, as estimated from the least-squares refinement. The $C(sp^3)-C(sp^3)$ bond distances range from 1·50 to 1·59 Å (average 1·54 Å), and the C—O distances are 1·43, 1·46, and 1·46 Å (Table 3). All these values are in agreement with those given in *Tables of Interatomic Distances and Configuration in Molecules and Ions* (1965). Seven C—H bonds associated with nonphenyl groups vary from 0·93 to 1·05 Å (average 1·02 Å) with an exceptionally large value of 1·22 Å for C(3)—H(3b), while the O(5)—H(5) distance is 0·99 Å (Fig. 2). The C—C—H and H—C—H angles for the nonphenyl groups are in the range 96–122° (average of 18 values, 110°).

Table 3. *Bond distances and angles for non-hydrogen atoms*

Standard deviations involving members of the rigid groups and non-phenyl-ring H atoms were not calculated and are not given.

C(1)—C(2)	1·59 (1) Å		C(8)—C(5)	1·50 (1) Å
C(2)—C(3)	1·55 (1)		C(5)—O(5)	1·43 (1)
C(3)—C(4)	1·51 (1)			
C(4)—C(5)	1·53 (1)		C(2)—C(11)	1·57
C(5)—O(6)	1·46 (1)		—C(21)	1·56
O(6)—C(7)	1·46 (1)		C(7)—C(31)	1·54
C(7)—C(1)	1·56 (1)		—C(41)	1·53
C(1)—C(8)	1·53 (1)		O(5)···O(5')*	2·75 (1)

C(1)—C(2)—C(3)	108·2 (9)°	C(1)—C(2)—C(11)	110·1°
C(2)—C(3)—C(4)	116·1 (9)	—C(21)	111·4
C(3)—C(4)—C(5)	106·7 (9)	C(3)—C(2)—C(11)	111·0
C(4)—C(5)—C(8)	110·6 (9)	—C(21)	111·2
C(5)—C(8)—C(1)	99·4 (8)	C(11)—C(2)—C(21)	105·0
C(8)—C(1)—C(2)	107·4 (8)	C(1)—C(7)—C(31)	116·3
C(8)—C(1)—C(7)	98·2 (8)	—C(41)	113·2
C(1)—C(7)—O(6)	102·5 (8)	O(6)—C(7)—C(31)	109·9
C(7)—O(6)—C(5)	107·8 (8)	—C(41)	107·6
O(6)—C(5)—C(8)	106·0 (8)	C(31)—C(7)—C(41)	107·1
C(4)—C(5)—O(5)	112·8 (8)		
O(6)—C(5)—O(5)	107·2 (8)	C(2)—C(11)—C(12)	121·2
C(2)—C(1)—C(7)	117·5 (8)	—C(16)	118·6
C(4)—C(5)—O(6)	107·5 (8)	—C(21)—C(22)	118·4
		—C(26)	121·5
		C(7)—C(31)—C(32)	117·7
		—C(36)	122·2
		—C(41)—C(42)	116·9
		—C(46)	123·1

* The prime refers to the transformation of (x,y,z) into atomic position $(1·25 - y, 0·25 + x, 2·25 - z)$ or $(-0·25 + y, 1·25 - x, 2·25 - z)$.

The best molecular planes, calculated for atoms of the two nonphenyl rings, are given in Table 4. The six-membered ring (plane *A*) has a chair conformation with C(3) and C(8) displaced to opposite sides of the plane. The five-membered ring is in the twist conformation with C(1) and C(8) located 0·523 Å above and 0·293 Å below the mean plane formed by C(5), O(6), and C(7) (plane *B*). This is reflected in calculations of the torsion angles C(1)—C(7)—O(6)—C(5) and C(8)—C(5)—O(6)—C(7), the former (−20°) being 8° larger

Table 4. *Equations of best molecular planes and perpendicular distances (Å) of constituent atoms from these planes:* $lX + mY + nZ = p$

Calculations were performed with the program written by Smith (1962). X,Y,Z are orthogonal coordinates (in Å) along the **a,b,c** directions respectively.

	l	*m*	*n*	*p*
Plane *A*	0·3037	0·4680	−0·8299	1·8761
Plane *B*	0·3804	−0·7596	−0·5276	−15·8964
Plane PH(1)	−0·5254	−0·3415	−0·7793	−19·9015
Plane PH(2)	−0·2337	0·9325	−0·2755	9·6034
Plane PH(3)	0·1320	−0·9912	−0·0108	−17·3526
Plane PH(4)	−0·2215	0·1040	−0·9696	−10·8092

Plane *A*	Distance	Plane *B*	Distance
C(1)	−0·006	C(5)	0
C(2)	0·006	O(6)	0
C(4)	−0·006	C(7)	0
C(5)	0·006	C(1)*	0·523
C(3)*	0·563	C(8)*	−0·293
C(8)*	−0·898		

* Atoms excluded from the plane calculations.

Fig. 4. View of the structure projected down the [001] direction, showing four hydrogen-bonded molecules related by the $\bar{4}$ axis.

than the latter (−12°). The displacements of C(2) from the two planes of phenyl rings PH(1) and PH(2) are 0·119 and 0·087 Å, respectively, whereas C(7) is fairly close to the planes of PH(3) and PH(4), the displacements being 0·029 and 0·061 Å respectively.

The centroids of PH(1) and PH(2) are equidistant from C(2) within experimental error (2·96 and 2·95 Å respectively), and the angle subtended at C(2) is 101·2°. The dihedral angle between the vectors normal to the planes PH(1) and PH(2) is 89° (Table 4), indicating that the two phenyl rings are not related by mirror symmetry. It is interesting to compare the conformational angles associated with bonds between PH(1) and PH(2), and C(2) (Fig. 3). The torsion angle C(26)—C(21)—C(2)—C(3) is −1° (Fig. 3b), in sharp contrast to the value −45° for C(16)—C(11)—C(2)—C(3) (Fig. 3a). These orientations for PH(1) and PH(2) presumably alleviate the steric repulsions between neighboring H atoms − in particular

H(16)···H(3a), H(26)···H(3b), H(12)···H(1), and H(12)···H(8a). The H(16)···H(3a) contact of 1·80 Å, much shorter than the sum (2·4 Å) of its van der Waals radii (Pauling, 1960), seems to be due to inaccurate location of H(3a) [which appears to be 1·22 Å from C(3)].

For the two phenyl rings, PH(3) and PH(4), bonded to C(7), the C(7)—centroid distances are 2·92 and 2·93 Å, and the centroid—C(7)—centroid angle is 104·8°. The dihedral angle between the vectors normal to the planes of PH(3) and PH(4) is 97° (Table 4). Although for PH(3), C(36) is in a nearly eclipsed position with respect to O(6) [the torsion angle C(36)—C(31)—C(7)—O(6) is 3°] (Fig. 3c), C(46) of PH(4) is twisted away from C(1) in order to minimize the steric interaction between H(46) and H(1), in a manner similar to that shown in Fig. 3(a) for C(16) and C(3).
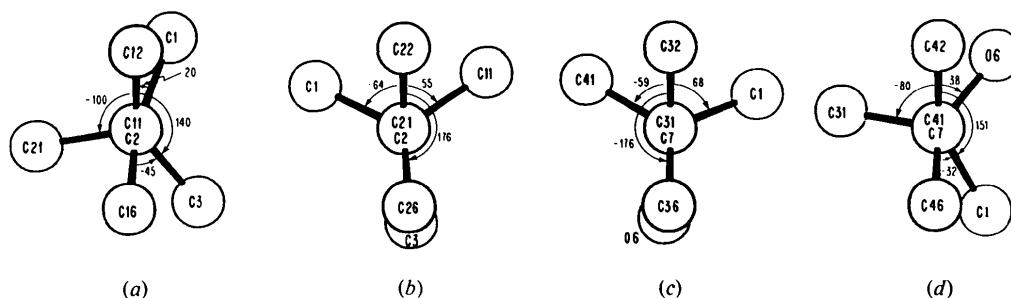

(a)   *(b)*   *(c)*   *(d)*

Fig. 3. Torsion angles about the C atoms having phenyl rings attached. The view directions are from atoms C(11) and C(21) down to atom C(2) in (*a*) and (*b*); from atoms C(31) and C(41) to atom C(7) in (*c*) and (*d*).
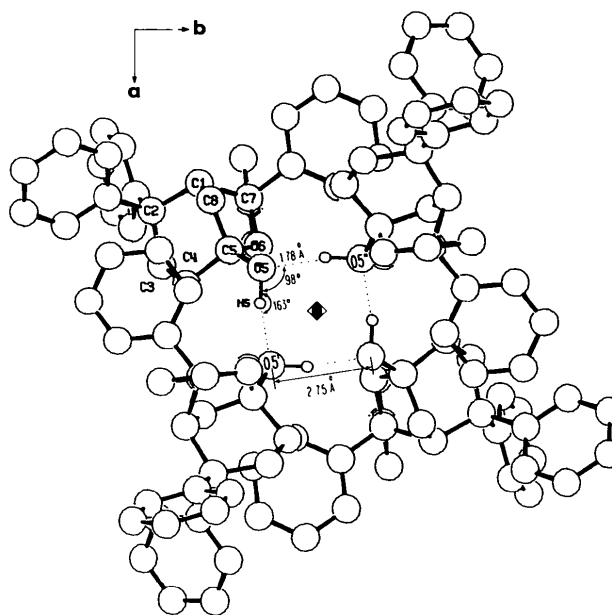
The molecule is hydrogen-bonded to two symmetry-equivalent, neighboring molecules *via* O(5)—H(5)···O(5') and O(5)···H(5'')—O(5'') around the $\bar{4}$ axes. The C(5)—O(5)—H(5) angle is 105·9°. Some other pertinent molecular parameters in the hydrogen-bond system are given in Fig. 4. The shortest intermolecular van der Waals contacts for C···H and H···H are 2·89 and 2·41 Å for C(25)···H(26) and H(26)···H(45) respectively.

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Structure Cristalline et Moléculaire du Biphényldicarboximide-2,2', C₁₄H₉NO₂

PAR P. CAILLET

Laboratoire de Chimie Minérale B, Laboratoire associé au CNRS n° 254, Université de Rennes, avenue du Général Leclerc, BP 25 A, 35031 Rennes CEDEX, France

ET J. Y. LE MAROUILLE

Laboratoire de Cristallochimie, Laboratoire associé au CNRS n° 254, Université de Rennes, avenue du Général Leclerc, BP 25 A, 35031 Rennes CEDEX, France

2,2'-Biphenyldicarboximide crystallizes in the monoclinic system, space group $P2_1/c$ with $Z = 4$, $a = 3\cdot868$ (3), $b = 14\cdot23$ (2), $c = 18\cdot78$ (2) Å, $\beta = 91\cdot7$ (2)°, $D_x = 1\cdot43$, $D_m = 1\cdot42$ g cm⁻³. From three-dimensional diffractometer data, the structure was solved with the *MULTAN* program; Fourier synthesis and full-matrix least-squares refinement gave a final R value of 0·065. The molecular structure consists of two benzene rings fused to a distorted seven-membered ring bearing the imide group. Except for one hydrogen bond, N—H···O, connecting two molecules, the interactions are only of the van der Waals type.

Une étude théorique de la molécule de biphénylcarboximide-2,2' avait amené Botrel & Guerillot (1974) à proposer une structure de ce composé dans laquelle le cycle à sept atomes porteur des groupements fonctionnels était distordu; il n'avait pu toutefois préciser la position des plans des deux cycles benzéniques l'un par rapport à l'autre. Dans le but de poursuivre cette étude et de la compléter à l'aide des résultats obtenus à partir des spectres de vibration, nous avons déterminé la structure de cette molécule à l'état solide.