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2,2′-(*p*-Phenylene)di-2-propanol

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Abstract. $C_{12}H_{18}O_2$ (PDHIPB), M_r = 194·26, triclinic, $P\bar{1}$, a = 10·269 (4), b = 14·369 (4), c = 6·276 (6) Å, α = 98·21 (3), β = 96·62 (4), γ = 70·15 (10)°, Z = 3, D_x = 1·125, D_m = 1·10 (3) g cm^{-3} (by flotation), μ = 0·807 cm^{-1} for Mo $K\alpha$ radiation; R = 0·068 for 1211 observed reflexions. A hydrogen-bonding system connects the O atoms of three adjacent molecules and produces spirals parallel to the **c** direction. The spirals link the molecules into sheets parallel to the (110) plane.

Introduction. The aim of the structure determination was (*a*) a comparison of the structure with that of the Si-analogue compound 1,1′-(*p*-phenylene)bis(dimethylsilanol) (DHMSB), which is the monomer of disilanol type of poly[oxy(dimethylsilyl)-*p*-phenylene-(dimethylsilyl)] (Alexander, Northolt & Engmann, 1967), and (*b*) to obtain a key to the interpretation of the vibration spectra of PDHIPB (Zelei & Dobos, 1979). The sample was prepared by Dr B. Zelei in the Institute of Inorganic Chemistry of the Hungarian Academy of Sciences by the method of Mitin (1958). The crystals form plates elongated in the **c** direction. One of the linear dimensions of the specimen was about 0·01 mm and so only 1746 independent reflexions could be collected on an Enraf–Nonius CAD-4 diffractometer; 535 of these with zero intensities were excluded from the final data set. No absorption corrections were made. The phases for 196 reflexions having $E \geq 1·7$ were obtained by *MULTAN* (Germain, Main & Woolfson, 1971). The E map calculated with these signs revealed the positions of all non-hydrogen atoms (R = 0·37). A full-matrix least-squares refinement procedure resulted in R = 0·072 for the observed reflexions. At the stage when anisotropic temperature factors were used the refinement proceeded separately for the two parts of the asymmetric unit. A difference Fourier map gave the positions of all H atoms and the subsequent refinement cycles resulted in a final R = 0·068 for the 1211 observed and R = 0·103 for all reflexions.* All calculations were performed on a PDP

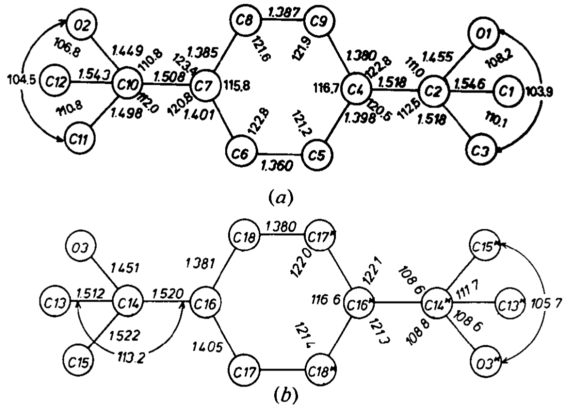

Fig. 1. Schematic drawings of (*a*) molecule *A* and (*b*) molecule *B*, with bond lengths (Å) and bond angles (°) for the non-hydrogen atoms. For both molecules the e.s.d.'s of bond lengths vary from 0·006 to 0·009 Å, those for the bond angles from 0·7 to 0·9°.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36591 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Final atomic parameters with standard deviations in parentheses*

The fractional positional parameters of C and O have been multiplied by 10^4, those of H by 10^3. For non-hydrogen atoms $B_{eq} = \frac{4}{3}\sum_i\sum_j b_{ij}(\mathbf{a}_i\mathbf{a}_j)$. The e.s.d.'s of B_{iso} are not greater than 0·9 Å^2.

	x	y	z	B_{eq}/B_{iso} (Å^2)
O(1)	5163 (3)	2606 (2)	5640 (5)	3·5 (2)
O(2)	3173 (3)	6948 (2)	667 (5)	3·4 (2)
O(3)	6797 (3)	1762 (2)	2218 (5)	3·6 (2)
C(1)	3138 (5)	2199 (4)	3967 (9)	4·0 (3)
C(2)	3663 (5)	3018 (3)	5259 (8)	2·9 (3)
C(3)	3143 (6)	3264 (4)	7508 (9)	4·0 (3)
C(4)	3259 (5)	3928 (3)	4047 (8)	2·9 (3)
C(5)	1863 (5)	4487 (4)	3658 (9)	4·0 (3)
C(6)	1488 (5)	5340 (4)	2699 (10)	4·4 (3)
C(7)	2456 (5)	5699 (3)	1995 (9)	3·0 (3)
C(8)	3836 (5)	5129 (3)	2337 (9)	3·2 (3)
C(9)	4224 (5)	4264 (3)	3333 (9)	3·5 (3)
C(10)	1991 (5)	6666 (3)	1003 (9)	3·2 (3)
C(11)	1282 (6)	6578 (4)	−1204 (10)	5·8 (4)
C(12)	1058 (6)	7529 (4)	2477 (10)	5·2 (4)
C(13)	6067 (5)	728 (4)	−702 (9)	4·0 (3)
C(14)	7109 (5)	746 (3)	1199 (8)	3·4 (3)
C(15)	6989 (5)	142 (4)	2926 (9)	4·2 (3)
C(16)	8601 (5)	370 (3)	571 (8)	2·8 (3)
C(17)	8998 (5)	−242 (3)	−1359 (9)	3·5 (3)
C(18)	9643 (5)	598 (3)	1907 (8)	3·7 (3)
H(O1)	553 (4)	231 (3)	408 (7)	6
H(O2)	378 (4)	691 (3)	198 (7)	6
H(O3)	689 (5)	208 (3)	100 (8)	8
H(1*A*)	219 (5)	243 (3)	378 (8)	7
H(1*B*)	358 (4)	206 (3)	247 (7)	6
H(1*C*)	344 (6)	157 (4)	457 (9)	11
H(3*A*)	346 (5)	261 (4)	821 (9)	10
H(3*B*)	351 (4)	378 (3)	860 (7)	6
H(3*C*)	209 (4)	349 (3)	743 (7)	6
H(5)	121 (4)	429 (3)	447 (7)	6
H(6)	55 (5)	565 (3)	241 (8)	9
H(8)	445 (5)	535 (3)	162 (7)	7
H(9)	522 (4)	387 (3)	360 (7)	6
H(11*A*)	184 (4)	606 (3)	−221 (7)	6
H(11*B*)	65 (5)	631 (3)	−90 (8)	9
H(11*C*)	100 (6)	709 (4)	−185 (9)	12
H(12*A*)	26 (4)	735 (3)	289 (7)	5
H(12*B*)	167 (5)	758 (3)	387 (8)	7
H(12*C*)	84 (5)	822 (3)	244 (8)	9
H(13*A*)	613 (5)	9 (3)	−147 (8)	8
H(13*B*)	610 (6)	118 (4)	−215 (9)	11
H(13*C*)	513 (4)	108 (3)	−43 (7)	4
H(15*A*)	726 (4)	−60 (3)	215 (6)	4
H(15*B*)	767 (4)	18 (3)	422 (7)	5
H(15*C*)	609 (5)	39 (3)	378 (8)	6
H(17)	827 (4)	−39 (2)	−247 (6)	3
H(18)	932 (4)	104 (3)	330 (7)	5

11/34 minicomputer with the Enraf–Nonius SDP-34 system. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974). The final atomic parameters are given in Table 1. Fig. 1 contains the bond lengths and angles. Fig. 2 shows a projection of the structure along [001].

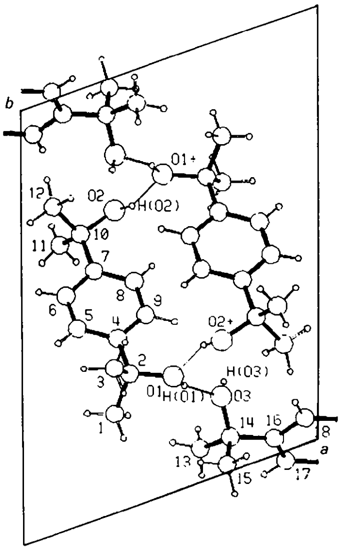

Fig. 2. Projection of the structure along [001].

Discussion. The asymmetric part of the unit cell consists of one molecule in a general position (molecule *A*) and one half-molecule located at the centre of inversion coinciding with the origin (molecule *B*). In the hydroxyisopropyl groups a major deviation from the regular tetrahedral value is observed for only one angle involving the O atom. In the benzene rings the inner bond angles are less than 120° by about 3° at the C atoms where the substituents are attached. This is an effect occurring in *p*-disubstituted benzene derivatives with donor-type substituents (Domenicano, Vaciago & Coulson, 1975; Domenicano, Mazzeo & Vaciago, 1976). The averages of the aromatic and aliphatic C—C bond lengths are normal: 1·387 and 1·520 Å, respectively. In the benzene rings no significant differences exist between the bond lengths parallel to the long axes of the molecules and those inclined to these directions by about 60°, in contrast to DHMSB, where the lateral bonds show considerable shortenings (Alexander, Northolt & Engmann, 1967). The best plane of the aromatic ring in molecule *A* (*P*1) and that of molecule *B* (*P*2) form almost a right angle with each other [89·2 (4)°]. The O atoms in molecule *A* are in *cis* arrangement and deviate only slightly ($\Delta = 0{\cdot}2$ Å) from *P*1, while the distance of O(3) from *P*2 is 0·8 Å.

The structure of the title compound is very similar to that of DHMSB (Alexander, Northolt & Engmann, 1967), though no isomorphism exists between the two crystals. An essential difference is that in DHMSB each of the three molecules in the unit cell is located at a centre of inversion, so the asymmetric part consists of three half-molecules.

Hydrogen-bond system. The O atoms of three adjacent molecules are linked by hydrogen bonds and a spiral parallel to the *c* axis evolves on both ends of the

Table 2. *Distances* (Å) *and angles* (°) *involving hydrogen bonds, with e.s.d.'s in parentheses*

O(2*) = O(2)(1 − *x*, 1 − *y*, 1 − *z*); O(3′) = O(3)(*x*, *y*, 1 + *z*).

O(1)···O(2*)	2·848 (4)	O(1)–H(O1)···O(3)	155·2 (2·7)
O(1)···O(3)	2·757 (4)	O(2*)–H(O2*)···O(1)	156·2 (2·7)
O(2*)···O(3′)	2·779 (5)	O(3′)–H(O3′)···O(2*)	160·8 (3·7)

molecules. By this, a two-dimensional network arises whose sheets are parallel to the (110) plane. The sheets can be regarded as consisting of zigzag chains running along [111] connected by the O(3)···O(1) and O(1)···O(2)(1 − *x*, 1 − *y*, 1 − *z*) hydrogen bonds; the chains are crosslinked by the hydrogen bond O(2)(1 − *x*, 1 − *y*, 1 − *z*)···O(3)(*x*, *y*, 1 + *z*). In DHMSB helices arise, also parallel to the **c** direction, but they connect the structure into a network in three dimensions. The bond data involving hydrogen bonds are in Table 2.

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2,2′-Dihydroxybenzophenone

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Abstract. $C_{13}H_{10}O_3$, monoclinic, $P2_1/n$, $a = 7{\cdot}865\ (1)$, $b = 12{\cdot}237\ (2)$, $c = 11{\cdot}253\ (3)$ Å, $\beta = 109{\cdot}73\ (2)°$, $U = 1019{\cdot}5\ (6)$ Å^3, $Z = 4$, $M_r = 214{\cdot}1$, $D_x = 1{\cdot}396\ (3)$ g cm^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 1{\cdot}07$ cm^{-1}, $T = 295\ (1)$ K. The three-dimensional X-ray diffraction data were measured by the θ–2θ scan technique with a scintillation detector. The structure was solved by direct methods and refined by full-matrix least-squares techniques to $R(F_o) = 0{\cdot}033$ and $R_w(F_o) = 0{\cdot}046$ for 1278 reflections above 2σ. The two planar six-membered rings are separated by a dihedral angle of 45·7 (5)°. Bond distances and angles are normal. Effects of ring substituents on the bond distances involving the carbonyl C atom are discussed. Both hydroxyl groups act as intramolecular hydrogen-bond donors to the carbonyl O atom [O(2)···O(1), 2·656 (2); O(3)···O(1), 2·602 (2); H(O2)···O(1), 1·87 (3); H(O3)···O(1), 1·77 (2) Å; O(2)–H(O2)···O(1), 141·7 (5); and O(3)–H(O3)···O(1), 148·6 (5)°]. The O(3)–H(O3) group is also involved in a weak intramolecular hydrogen bond with another carbonyl O atom.

Introduction. Intramolecular hydrogen bonding in 2-hydroxybenzophenones has been confirmed by several X-ray studies: (1) 2-hydroxy-4-methoxybenzophenone (HMB) (Liebich & Parthé, 1974); (2) 4′-chloro-2-hydroxy-4-methoxybenzophenone (HMCB) (Liebich, 1976); (3) 2,4-dihydroxybenzophenone (HHB) (Liebich, 1979); and (4) 2,2′,4,4′-tetrahydroxybenzophenone (THB) (Schlemper, 1982). The study of THB was undertaken to examine the possibility of intramolecular hydrogen bonding of both the 2 and 2′ hydroxyl groups to the carbonyl O. This was found to be the case, but the hydrogen bonding was further complicated by the 4 and 4′ hydroxy groups which are involved in intermolecular hydrogen bonds. Several IR and ^{1}H and ^{13}C NMR studies (Merrill, 1961; Maciel & Savitsky, 1964; Sopchik & Kingsbury, 1979) have been reported for 2,2′-dihydroxybenzophenone which suggested both O—H groups have intramolecular hydrogen bonds with the carbonyl group, but the equality of the bonds is disputed. For these reasons the present study of 2,2′-dihydroxybenzophenone (DHP) was performed.

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