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2,2,2-Triphenylethanol: a Hydrogen-Bonded Tetramer Based upon a Centrosymmetric $R_4^4(8)$ Motif

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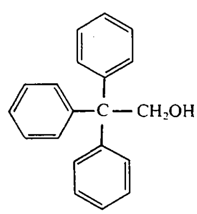
Abstract

2,2,2-Triphenylethanol, $C_{20}H_{18}O$, crystallizes as hydrogen-bonded tetrameric aggregates which are centrosymmetric. The resulting planar O_4 ring is almost square with O···O distances of 2.786 (2) and 2.822 (2) Å; the hydroxyl H atoms are fully ordered, one along each O···O edge of the O_4 parallelogram

Comment

The crystal structures of sterically congested monoalcohols display a wide variety of hydrogen-bonding patterns. The compounds Ph_3MOH (M = C, Si, Ge) all crystallize as hydrogen-bonded tetramers but while Ph_3COH forms an almost perfectly tetrahedral tetramer (Ferguson, Gallagher, Glidewell, Low & Scrimgeour, 1992), the tetramers of both Ph_3SiOH (Puff, Braun & Reuter, 1991) and Ph_3GeOH (Ferguson, Gallagher, Murphy, Spalding, Glidewell & Holden, 1992) contain puckered O-atom rings of approximate $\bar{4}$ (S_4) symmetry; $Ph_2(C_2H_5)COH$ forms similar $\bar{4}$ tetramers (Sultanov, Shnulin & Mamedov, 1985*a*). Although the dimers of Ph_2(ferrocenyl)COH are formed by O—H···O hydrogen bonds giving four-membered OHOH rings (Ferguson, Gallagher, Glidewell & Zakaria, 1993*a*), by contrast, in $Ph_2(PhCH_2)COH$ the sole intermolecular interactions leading to dimer formation are O—H···π(arene) hydrogen bonds (Ferguson, Gallagher, Glidewell & Zakaria, 1994), while the dimers of $Ph_2(PhCHF)COH$ depend upon O—H···F hydrogen bonds (DesMarteau, Xu & Witz, 1992). The structure of $Ph_2(CH_3)COH$ also contains O—H···π(arene) interactions, but these are intramolecular and the compound is monomeric (Sultanov, Shnulin & Mamedov, 1985*b*). In contrast to both Ph_3COH and $Ph_2(PhCH_2)COH$, the introduction of further methylene spacer groups between the phenyl rings and the quaternary C atom in $Ph(PhCH_2)_2COH$ and $(PhCH_2)_3COH$ leads to structures which contain no hydrogen bonds (Ferguson, Gallagher, Glidewell & Zakaria, 1993*b*). We have now extended the series $Ph_x(PhCH_2)_{3-x}COH$ to 2,2,2-triphenylethanol, $Ph_3C—CH_2—OH$ (I), in which the methylene spacer group has been placed between the quaternary C atom and the hydroxyl group; the structure of this compound shows yet another hydrogen-bonding pattern.



(I)

In the structure of 2,2,2-triphenylethanol there are two molecules, labelled *A* and *B*, in the asymmetric unit; these two molecules, together with a similar pair of molecules related to them by a centre of inversion, form a hydrogen-bonded tetrameric array (see Figs. 1 and 2). The centrosymmetry requires that all four O atoms in the tetramer are coplanar. The closest O···O distances are 2.786 (2)

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and 2.822 (2) Å, and the O···O···O angles are 92.8 (1) and 87.2 (1)°; thus the parallelogram of O atoms is only slightly distorted from a square. The O atoms are linked by fully ordered H atoms to give a motif with graph set $R_4^4(8)$ (Etter, 1990; Etter, MacDonald & Bernstein, 1990). In neither Ph_3SiOH nor Ph_3GeOH were the hydroxyl H atoms located, possibly owing to disorder, although they were located in $Ph_2C(C_2H_5)OH$. The hydroxyl H atoms in the two independent molecules of (I), HO*A* and HO*B*, are displaced from the O_4 plane by only 0.12 (3) and −0.06 (3) Å, respectively; thus the entire $(OH)_4$ ring is virtually planar. The torsion angles *OB*′···*OA*···*OB*—C1*B* and *OA*···*OB*···*OA*′—C1*A*′ are −154.4 (1) and −177.3 (1)°, respectively, indicating only minor displacements of C1*A* and C1*B* from the O_4 plane. Similarly, the torsion angles *OB*···*OA*—C1*A*—C2*A* and *OA*′···*OB*—C1*B*—C2*B*, which have values of 14.1 (1) and −23.4 (1)°, respectively, indicate firstly that C2*A* and C2*B* are also close to the O_4 plane and secondly that the central $(HO—C1—C2)_4$ framework has close to four-fold symmetry. The conformations about the two independent C1—C2 bonds are extremely similar with torsion angles *OA*—C1*A*—C2*A*—C*n*1*A* of 167.3 (2), −76.3 (1) and 47.4 (1)° for *n* = 1, 2 and 3, respectively, and values of 166.4 (2), −75.2 (1) and 48.4 (1)° for the corresponding angles *OB*—C1*B*—C2*B*—C*n*1*B*; the bonds C2*A*—C21*A* and C2*B*—C21*B* therefore each project at almost right angles to the O_4 plane.

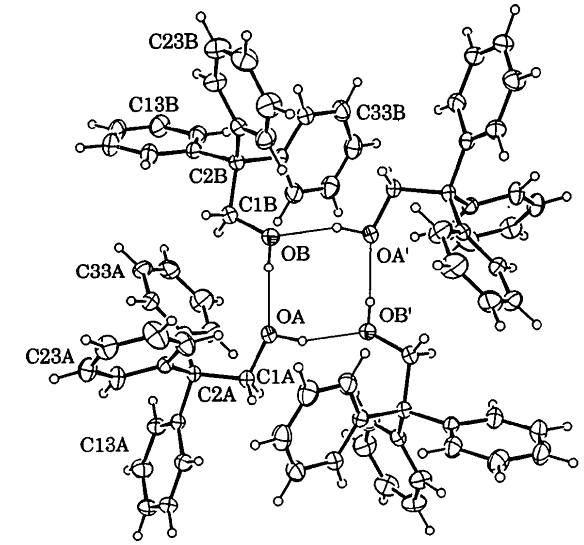

Fig. 1. A view of 2,2,2-triphenylethanol as a hydrogen-bonded tetrameric aggregate. The non-H atoms are shown as displacement ellipsoids drawn at the 35% probability level. For clarity, H atoms are drawn as small spheres of arbitrary size.

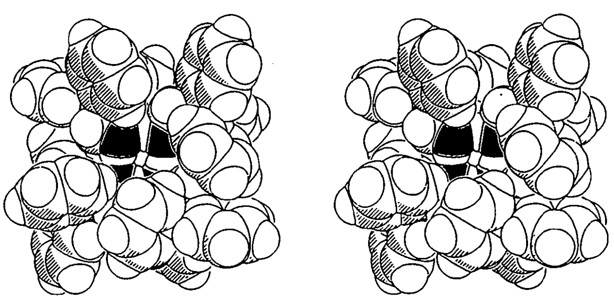

Fig. 2. A stereoview of the tetrameric aggregate of 2,2,2-triphenylethanol with atoms depicted as their van der Waals spheres.

Within the two independent molecules of 2,2,2-triphenylethanol, the C—O distances of 1.426 (2) and 1.429 (2) Å are close to the mean C—O bond length of 1.426 (11) Å in alcohols of type $R—CH_2—OH$ (Allen, Kennard, Watson, Brammer, Orpen & Taylor, 1987). The distances between the four-coordinate C atoms, C1*A*—C2*A* and C1*B*—C2*B*, are 1.549 (2) and 1.547 (2) Å, respectively, both above the upper quartile value of 1.541 Å for C—C bonds of type $R_3C—CH_2X$; this is presumably a reflection of the steric congestion around C2*A* and C2*B*. Similarly, the C—C bonds to the phenyl rings range from 1.535 (2) to 1.549 (2) Å with a mean value of 1.543 Å, again above the upper quartile value for bonds of type $R_3C—C(aryl)$.

Experimental

Samples of 2,2,2-triphenylethanol were prepared by reduction of triphenylacetic acid with lithium aluminium hydride. ^{13}C NMR ($CDCl_3$ solution): 58.9(*q*), 70.4(*t*), 126.6(*d*), 128.2(*d*), 129.4(*d*), 145.2(*s*). Crystals were grown by slow evaporation of a solution in light petroleum, b.p. 313-333 K.

Crystal data

$C_{20}H_{18}O$
M_r = 274.36
Monoclinic
$P2_1/c$
a = 9.2287 (9) Å
b = 14.1910 (12) Å
c = 23.2013 (15) Å
β = 95.835 (6)°
V = 3022.8 (4) Å^3
Z = 8
D_x = 1.206 Mg m^{-3}

Mo *Kα* radiation
λ = 0.71067 Å
Cell parameters from 25 reflections
θ = 9.50-20.00°
μ = 0.07 mm^{-1}
T = 293 K
Multifaceted gem-like block
0.77 × 0.50 × 0.44 mm
Colourless

Data collection

Nonius CAD-4 diffractometer
θ/2θ scans
Absorption correction: none
6979 measured reflections
6583 independent reflections
4233 observed reflections [$I > 3.0\sigma(I)$]

R_{int} = 0.011
θ_{max} = 26.92°
h = −11 → 11
k = 0 → 18
l = 0 → 29
3 standard reflections
frequency: 60 min
intensity variation: 1.0%

Refinement

Refinement on F
$R = 0.041$
$wR = 0.061$
$S = 1.51$
4233 reflections
388 parameters
$w = 1/[\sigma^2(F) + 0.0010F^2]$
$(\Delta/\sigma)_{max} = 0.006$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Extinction correction: Larson (1970)
Extinction coefficient: $0.67 (16) \times 10^4$
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

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

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

	x	y	z	U_{eq}
OA	0.38890 (15)	0.44755 (9)	0.42700 (6)	0.0549 (7)
C1A	0.33626 (19)	0.38452 (12)	0.38177 (7)	0.0445 (8)
C2A	0.22859 (16)	0.43273 (10)	0.33530 (7)	0.0351 (8)
C11A	0.21135 (16)	0.36270 (11)	0.28392 (7)	0.0357 (8)
C12A	0.24082 (19)	0.38482 (12)	0.22824 (8)	0.0462 (9)
C13A	0.21594 (22)	0.31970 (15)	0.18360 (8)	0.0570 (11)
C14A	0.16118 (21)	0.23252 (13)	0.19350 (8)	0.0545 (10)
C15A	0.13211 (21)	0.20919 (12)	0.24867 (9)	0.0529 (10)
C16A	0.15644 (20)	0.27297 (12)	0.29333 (7)	0.0465 (9)
C21A	0.07702 (17)	0.44675 (11)	0.35576 (7)	0.0363 (8)
C22A	−0.04469 (18)	0.45282 (14)	0.31530 (7)	0.0485 (10)
C23A	−0.18226 (20)	0.46804 (14)	0.33143 (9)	0.0551 (11)
C24A	−0.20299 (21)	0.47623 (15)	0.38884 (9)	0.0588 (12)
C25A	−0.0861 (3)	0.46774 (18)	0.42930 (9)	0.0727 (14)
C26A	0.05328 (21)	0.45372 (15)	0.41320 (8)	0.0571 (12)
C31A	0.29134 (17)	0.52758 (11)	0.31714 (7)	0.0367 (8)
C32A	0.20986 (18)	0.60904 (12)	0.31045 (7)	0.0433 (9)
C33A	0.26750 (23)	0.69199 (12)	0.29153 (8)	0.0546 (11)
C34A	0.40998 (25)	0.69587 (14)	0.27981 (9)	0.0638 (12)
C35A	0.49264 (23)	0.61576 (16)	0.28647 (12)	0.0781 (16)
C36A	0.43468 (20)	0.53335 (14)	0.30504 (11)	0.0637 (13)
OB	0.38599 (15)	0.61433 (9)	0.49024 (5)	0.0519 (7)
C1B	0.33210 (20)	0.69107 (12)	0.45434 (8)	0.0473 (9)
C2B	0.38926 (18)	0.78820 (11)	0.47669 (7)	0.0389 (8)
C11B	0.35028 (19)	0.85603 (11)	0.42511 (7)	0.0412 (8)
C12B	0.45324 (21)	0.90868 (13)	0.40037 (8)	0.0506 (9)
C13B	0.4134 (3)	0.96870 (15)	0.35439 (9)	0.0635 (12)
C14B	0.2702 (3)	0.97632 (15)	0.33228 (9)	0.0668 (13)
C15B	0.16601 (24)	0.92453 (15)	0.35624 (9)	0.0662 (12)
C16B	0.20532 (21)	0.86526 (14)	0.40235 (8)	0.0554 (10)
C21B	0.31294 (18)	0.82077 (11)	0.52933 (7)	0.0395 (8)
C22B	0.26487 (23)	0.91266 (13)	0.53491 (8)	0.0557 (11)
C23B	0.1988 (3)	0.94126 (15)	0.58307 (10)	0.0676 (12)
C24B	0.17904 (25)	0.87906 (17)	0.62653 (9)	0.0684 (13)
C25B	0.2257 (3)	0.78846 (16)	0.62202 (9)	0.0683 (13)
C26B	0.29175 (22)	0.75958 (13)	0.57427 (8)	0.0544 (10)
C31B	0.55585 (18)	0.78538 (11)	0.49174 (7)	0.0392 (8)
C32B	0.62489 (19)	0.84347 (12)	0.53423 (8)	0.0472 (9)
C33B	0.77566 (22)	0.84599 (14)	0.54476 (9)	0.0570 (11)
C34B	0.86050 (21)	0.78927 (16)	0.51409 (9)	0.0614 (12)
C35B	0.79419 (23)	0.73037 (16)	0.47227 (9)	0.0617 (12)
C36B	0.64440 (21)	0.72854 (14)	0.46087 (8)	0.0518 (10)
HOA	0.457 (3)	0.4118 (17)	0.4534 (10)	0.092 (8)
HOB	0.388 (3)	0.5648 (18)	0.4678 (10)	0.091 (8)

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

OA—C1A	1.426 (2)	C1B—C2B	1.547 (2)
OA—HOA	0.97 (3)	C2B—C11B	1.549 (2)
C1A—C2A	1.549 (2)	C2B—C21B	1.542 (2)
C2A—C11A	1.548 (2)	C2B—C31B	1.542 (2)
C2A—C21A	1.535 (2)	C11B—C12B	1.379 (3)
C2A—C31A	1.541 (2)	C11B—C16B	1.394 (2)
C11A—C12A	1.383 (2)	C12B—C13B	1.385 (3)
C11A—C16A	1.396 (2)	C13B—C14B	1.373 (3)
C12A—C13A	1.390 (3)	C14B—C15B	1.372 (4)
C13A—C14A	1.365 (3)	C15B—C16B	1.380 (3)
C14A—C15A	1.375 (3)	C21B—C22B	1.388 (3)
C15A—C16A	1.377 (2)	C21B—C26B	1.386 (2)
C21A—C22A	1.391 (2)	C22B—C23B	1.387 (3)
C21A—C26A	1.376 (2)	C23B—C24B	1.366 (3)
C22A—C23A	1.377 (3)	C24B—C25B	1.363 (3)
C23A—C24A	1.370 (3)	C25B—C26B	1.380 (3)
C24A—C25A	1.362 (3)	C31B—C32B	1.389 (2)
C25A—C26A	1.389 (3)	C31B—C36B	1.396 (3)
C31A—C32A	1.379 (2)	C32B—C33B	1.389 (3)
C31A—C36A	1.382 (3)	C33B—C34B	1.371 (3)
C32A—C33A	1.382 (3)	C34B—C35B	1.376 (3)
C33A—C34A	1.371 (3)	C35B—C36B	1.381 (3)
C34A—C35A	1.369 (3)	OA···OB	2.7863 (18)
C35A—C36A	1.373 (3)	OA···OB^i	2.8218 (17)
OB—C1B	1.429 (2)	OA···HOB	1.91 (3)
OB—HOB	0.88 (3)	OB···HOA^i	1.89 (3)
OB···OA···OB^i	87.24 (5)		

Symmetry code: (i) $1 - x, 1 - y, 1 - z$.

The molecule crystallized in the monoclinic system; space group $P2_1/c$ was determined by the systematic absences ($h0l$ absent if $l = 2n + 1$, $0k0$ absent if $k = 2n + 1$). All H atoms bonded to C atoms were clearly visible in difference maps; they were positioned geometrically (C—H 0.95 Å) and included as riding atoms in the structure-factor calculations. The hydroxyl H atoms were allowed to refine isotropically. Data collection and cell refinement was performed using *CAD*-4 *Software* (Enraf-Nonius, 1989). Data reduction, structure solution and refinement, and preparation of the material for publication were performed using *NRCVAX* (Gabe, Le Page, Charland, Lee & White, 1989). The displacement-ellipsoid diagram (Fig. 1) was prepared using *ORTEP*II (Johnson, 1976). The stereoview shown in Fig. 2 was prepared with the aid of *PLUTON* (Spek, 1992*a*). Examination of the structure with *PLATON* (Spek, 1992*b*) showed that there were no solvent-accessible voids in the crystal structure (there were four possible 'void' locations in the unit cell, but each had a volume of only 9 Å^3, too small to accommodate any solvent molecule).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1164). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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2,6-Bis[(4-methyl-1-piperazinyl)methyl]-4-nitrophenol

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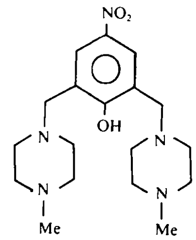
Abstract

In the title compound, $C_{18}H_{29}N_5O_3$, each piperazine ring assumes a 'perfect chair' conformation with the exocyclic methyl group in an equatorial position. The nitro group makes a dihedral angle of 5.5 (1)° with the mean plane of the phenyl ring. Best planes through the four non-N atoms of each of the two piperazine rings make a dihedral angle of 29.9 (1)° with one another.

† DCB contribution No. 829.

Comment

As part of a study of the chemistry of bidentate ligands containing N-atom donors the title compound (I) was synthesized by the Mannich reaction (Hodgkin, 1984) between *p*-nitrophenol, formaldehyde and *N*-methylpiperazine, and crystallized from light petroleum ether by slow evaporation. Bond lengths and angles have the expected values.



(I)

The methyl groups at N15 and N23 of the piperazine rings are in equatorial positions (Allinger, Carpenter & Karkowski, 1965). Both the piperazine rings (*A* and *B*) assume 'perfect chair' conformations (Bassi & Scordamaglia, 1977; Sbit, Dupont, Dideberg, Liegeois & Delarge, 1992). Packing of the molecules in the unit cell depends mainly on van der Waals forces. A short intermolecular contact distance of 3.203 (3) Å occurs between atoms C18 and O10(x, $y - 1$, $z + 1$).

An interesting aspect of the molecular conformation is that even though the two piperazine rings have similar bond geometry and are substituted symmetrically with respect to the phenyl ring, they adopt different relative orientations with respect to the phenyl ring. Atom N20 of piperazine ring *B* lies almost in the plane of the phenyl ring [torsion angle C3—C2—C19—N20 = 3.9 (3)°]. The intramolecular distance C3···N20 of 2.820 (3) Å is suggestive of a possible C—H···N interaction. On the other hand, ring *A* is rotated by about −36° to displace atom N12 significantly away from the plane of the phenyl

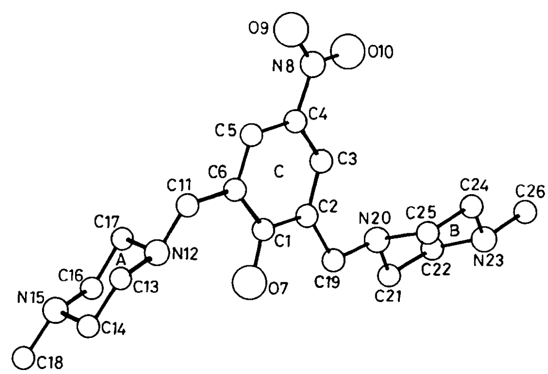


Fig. 1. Perspective view and numbering scheme of the title molecule.