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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.072
 wR factor = 0.161
Data-to-parameter ratio = 17.6

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

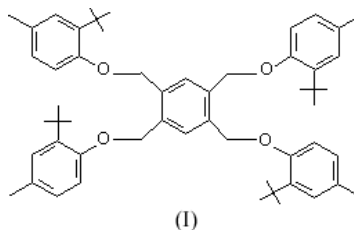
1,2,4,5-Tetrakis(2-*tert*-butyl-4-methylphenoxy-methyl)benzene

The centrosymmetric title compound, $\text{C}_{54}\text{H}_{70}\text{O}_4$, contains a benzene ring at the centre and four 2-*tert*-butyl-4-methylphenoxy-methyl substituents. In the structure of the molecule, some of the benzene rings are coplanar. The title compound displays intramolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds. The crystal structure is stabilized by $\text{C}-\text{H}\cdots\pi$ interactions.

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Comment

1,2,4,5-Tetrakis(2-*tert*-butyl-4-methylphenoxy-methyl)benzene, (I), and similar compounds are generally used for the synthesis of polystyrene polymers. These polymers have become of interest in recent years because of their unique properties and important applications (Kuriyama & Otsu, 1984; Kwon *et al.*, 2003).



The structure of the centrosymmetric molecule consists of a benzene ring (ring *A*, C13–C27) at the centre with four 2-*tert*-butyl-4-methylphenoxy-methyl substituents at C13, C13ⁱ, C14 and C14ⁱ [Fig. 1; symmetry code: (i) $-x, 1 - y, 1 - z$]. Rings *A* and *B* (C1–C6) are coplanar. Atom C26 attached to ring *C* (C16–C21) has a larger displacement parameter than usual. The torsion angles C1–O1–C12–C13 (between rings *A* and *B*) and C14–C15–O2–C16 (between rings *A* and *C*) are 179.0 (2) and 93.2 (3)°, respectively. The C–O bond lengths are in the range 1.378 (3)–1.434 (3)° (Table 1). The crystal structure of the title compound is stabilized by $\text{C}-\text{H}\cdots\pi$ interactions and there are also weak intramolecular $\text{C}-\text{H}\cdots\text{O}$ interactions (Table 2).

Experimental

A solution of 2-*tert*-butyl-4-methylphenol (1.48 g, 9.01 mmol) and K_2CO_3 (2.5 g, 18.12 mmol) in dry dimethylformamide (DMF, 50 ml) was heated and stirred at 313 K under N_2 for 1 h. To this mixture, a solution of 1,2,4,5-tetrakis(bromomethyl)benzene (1.00 g, 2.22 mmol) in dry DMF (20 ml) was added dropwise under N_2 over a period of 2–3 h. The reaction mixture was stirred for 2 d at 313 K and poured into iced water (150 g). The product was filtered off and washed with (10% *w/w*) NaOH solution and water until the filtrate was neutral. Recrystallization from an ethanol solution gave a white product (yield 0.06 g, 3.45%). Single crystals were obtained from absolute ethanol at room temperature *via* slow evaporation (m.p. 406 K);

elemental analysis calculated for $C_{54}H_{70}O_4$: C 82.82, H 9.01%; found: C 82.92, H 9.10%.

Crystal data

$C_{54}H_{70}O_4$
 $M_r = 783.10$
 Monoclinic, $P2_1/n$
 $a = 10.1833$ (9) Å
 $b = 21.5350$ (16) Å
 $c = 11.5029$ (11) Å
 $\beta = 107.725$ (7)°
 $V = 2402.8$ (4) Å³
 $Z = 2$

$D_x = 1.082$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 23 574 reflections
 $\theta = 1.9$ – 28.8 °
 $\mu = 0.07$ mm⁻¹
 $T = 293$ (2) K
 Prism, colourless
 $0.40 \times 0.22 \times 0.04$ mm

Data collection

Stoe IPDS-2 diffractometer
 ω scans
 Absorption correction: by integration (*X-RED32*; Stoe & Cie, 2002)
 $T_{\min} = 0.983$, $T_{\max} = 0.997$
 24 464 measured reflections

4725 independent reflections
 2611 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.092$
 $\theta_{\text{max}} = 26.0$ °
 $h = -12 \rightarrow 12$
 $k = -26 \rightarrow 26$
 $l = -14 \rightarrow 14$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.072$
 $wR(F^2) = 0.161$
 $S = 1.04$
 4725 reflections
 268 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.7513P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.009$
 $\Delta\rho_{\text{max}} = 0.17$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.19$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

O1—C1	1.378 (3)	O2—C16	1.383 (4)
O1—C12	1.425 (3)	O2—C15	1.433 (3)
C1—O1—C12—C13	179.0 (2)	C16—O2—C15—C14	93.2 (3)

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C9—H9B \cdots O1	0.96	2.38	3.012 (4)	123
C10—H10C \cdots O1	0.96	2.31	2.956 (4)	124
C12—H12A \cdots O2	0.97	2.39	2.920 (3)	114
C24—H24A \cdots O2	0.96	2.32	2.953 (5)	123
C25—H25C \cdots O2	0.96	2.39	3.012 (5)	123
C27—H27 \cdots O1	0.93	2.36	2.726 (4)	103
C12—H12B \cdots Cg1 ⁱⁱ	0.97	2.75	3.572 (3)	143

Symmetry code: (ii) $1 - x, 1 - y, 1 - z$. Cg1 is the centroid of ring C (C16–C21).

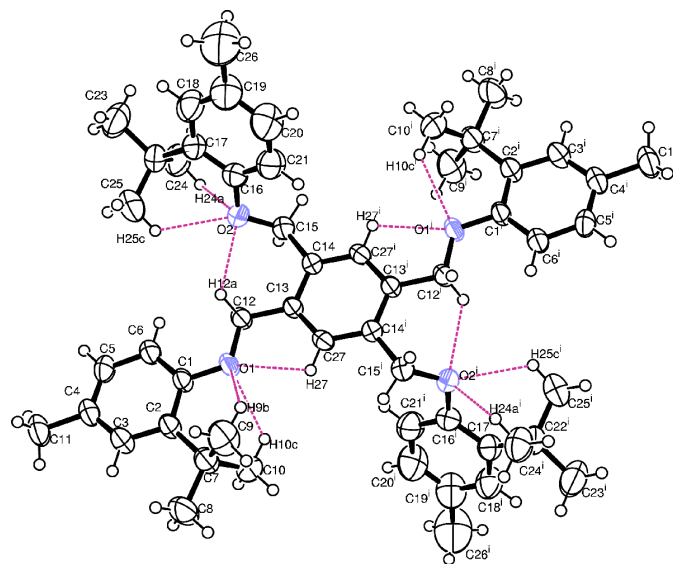


Figure 1

An *ORTEP-3* (Farrugia, 1997) view of the title compound, showing the atom-numbering scheme, 50% probability displacement ellipsoids and intramolecular hydrogen bonds. [Symmetry code: (i) $-x, 1 - y, 1 - z$.]

All H atoms were refined using a riding model, with C—H = 0.93 (aromatic H), 0.97 (methylene H) or 0.96 Å (methyl H). U_{iso} (aromatic and methylene H) values were set at $1.2U_{\text{eq}}(\text{C})$, while U_{iso} (methyl H) values were set at $1.5U_{\text{eq}}(\text{C})$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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