Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

A double mesogen based on linked *p*-terphenyl units

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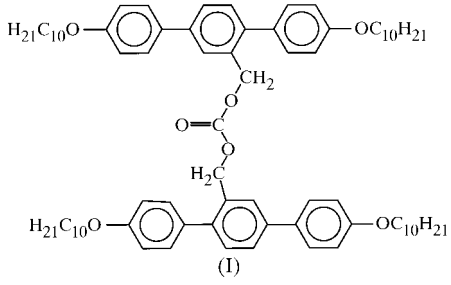
Received 14 February 2000
Accepted 1 March 2000

Data validation number: IUC0000054

The structure of bis(4,4′′-decyloxy-*p*-terphenyl-2′-ylmethyl) carbonate, $C_{79}H_{110}O_7$, (I), has been determined at 123 K. It is a new type of twin mesogen. No two adjacent aromatic rings are coplanar and the four decyloxy side chains are maximally extended. Molecules of the compound are packed along the crystallographic *a* axis. The molecular arrangement is a precursor of a smectic A phase.



(I)

Experimental

Transparent plate-shaped crystals were obtained by means of slow evaporation from a solution of the compound in methanol at 298 K.

Crystal data

$C_{79}H_{110}O_7$
M_r = 1171.67
Monoclinic, $P2_1/c$
a = 33.654 (9) Å
b = 30.229 (8) Å
c = 6.798 (2) Å
β = 94.74 (1)°
V = 6892.3 (3) Å^3
Z = 4
D_x = 1.129 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4620 reflections
θ = 1.21–26.37°
μ = 0.070 mm^{-1}
T = 123 (2) K
Plate, colourless
0.4 × 0.10 × 0.02 mm
Crystal source: Andersch & Tschierske (1996)

Data collection

Bruker 1 K CCD area-detector diffractometer
φ and ω scans
79 109 measured reflections
17 107 independent reflections
6169 reflections with $I > 2\sigma(I)$
R_{int} = 0.179
θ_{max} = 29.12°
$h = -45 \rightarrow 45$
$k = -40 \rightarrow 40$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.130
S = 1.160
14 105 reflections
775 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0576P)^2 + 3.1481P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = -0.085$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Dihedral angles (°) formed between normals to least-squares mean planes.

Planes†	Θ	Planes†	Θ
*P*1^*P*2	33.01 (7)	*P*3^*P*8	12.56 (8)
*P*2^*P*3	41.68 (8)	*P*4^*P*9	75.77 (9)
*P*4^*P*5	53.14 (8)	*P*6^*P*10	2.40 (9)
*P*5^*P*6	21.36 (9)	*P*2^*P*11	28.45 (6)
*P*1^*P*7	26.44 (9)	*P*5^*P*11	63.64 (6)

† Definition of planes: *P*1 = C41–C46; *P*2 = C47–C52; *P*3 = C53–C58; *P*4 = C59–C64; *P*5 = C65–C70; *P*6 = C71–C76; *P*7 = O1, C1–C10; *P*8 = O2, C11–C20; *P*9 = O3, C21–C30; *P*10 = O4, C31–C40; *P*11 = O5, O6, O7, C77, C78, C79.

The independent reflections included 181 Friedel-related data. The H atoms were allowed to ride on their parent atom with $U_{iso} = xU_{eq}$ (parent), where x = 1.5 for methyl and x = 1.2 for all others.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SHELXTL* (Bruker, 1998); program(s) used to solve structure: *SHELXS*93 (Sheldrick, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai & Huttner, 1994); software used to prepare material for publication: *SHELXL*97.

We are grateful to CSIR (New Delhi, India) for financial assistance.

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