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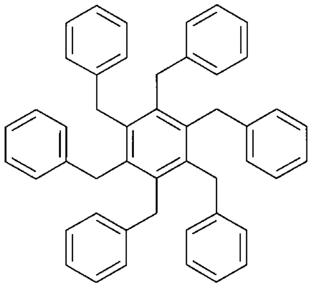
The title compound, (I), crystallizes unsolvated in the triclinic space group $P\overline{1}$, with one molecule per unit cell and a centrosymmetric ababab conformation (a and *b* denote side-chain units projecting, respectively, above and below the plane of the aromatic core), which possesses non-crystallographic $\overline{3}$ (S_6) symmetry. The CH_2 C atoms, in cyclic order, deviate from the mean plane of the central benzene ring by 0.042, −0.029, 0.050, −0.042, 0.029 and -0.050 Å (r.m.s. deviation 0.041 Å).



(I)

Experimental

The procedure employed $Co_2(CO)_8$ catalysed trimerization (*cf., e.g.*, Schore, 1991) of 1,4-diphenylbut-2-yne which was prepared by a literature method (Dupont *et al.*, 1954). Typically the acetylene (1 g, 4.9 mmol) was heated in a sealed tube under vacuum with $Co_2(CO)_8$ (0.1 g, 0.29 mmol) at 210°C for 3 h. The product was dissolved in chloroform, filtered and crystallized from this solvent, to give in near quantitative yield clear, colourless crystals (m.p. 580.5–581.5 K).

Crystal data

$C_{48}H_{42}$
$M_r = 618.82$
Triclinic, $P\overline{1}$
$a = 8.999$ (2) Å
$b = 10.456$ (4) Å
$c = 10.622$ (4) Å
$\alpha = 69.218$ (12)°
$\beta = 79.20$ (2)°
$\gamma = 67.07$ (2)°
$V = 859.2$ (5) Å^3
$Z = 1$
$D_x = 1.196$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7886 reflections
$\theta = 2.05$–29.00°
$\mu = 0.067$ mm^{-1}
$T = 123$ (1) K
Prism, colourless
0.45 × 0.35 × 0.30 mm

Data collection

Bruker 1 K CCD diffractometer
ω rotation with narrow frame scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{\min} = 0.970$, $T_{\max} = 1.000$
8524 measured reflections
3460 independent reflections
3077 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.016$
$\theta_{\max} = 26.37°$
$h = -11 \rightarrow 11$
$k = -13 \rightarrow 13$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.111$
$S = 1.008$
3460 reflections
238 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 0.250P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.234$ e Å^{-3}
$\Delta\rho_{\min} = -0.249$ e Å^{-3}

H atoms were placed geometrically and refined with a riding model with $U_{\rm iso}$ allowed to refine freely. Area-detector scaling and absorption corrections were performed by *SADABS.* This correction was used to scale the frames of data and to correct for absorption of the primary beam by the crystal support using the method of Blessing (1995). A correction for absorption of the primary beam by the crystal was not applied and as such the transmission factors quoted are not crystal dependant.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SMART* and *SAINT* (Bruker, 1999); data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1999); program(s) used to refine structure: *SHELXTL* (Sheldrick, 1999); molecular graphics: *SHELXTL* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 1999).

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