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1,4-Dibenzylbenzene

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Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.109; data-to-parameter ratio = 16.3.

The title molecule, $C_{20}H_{18}$, lies on a crystallographic inversion centre. The dihedral angle between the unique phenyl ring and the central benzene ring is 88.39 (11)°.

Related literature

For the synthetic procedure, see: Serres & Fields (1960).

Experimental

Crystal data

$C_{20}H_{18}$	b = 7.8736 (17) Å
M_r = 258.34	c = 18.379 (4) Å
Orthorhombic, *Pbca*	V = 1460.1 (6) Å^3
a = 10.090 (2) Å	Z = 4
Mo $K\alpha$ radiation	T = 294 (2) K
μ = 0.07 mm^{-1}	0.26 × 0.22 × 0.14 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	7693 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	1486 independent reflections
T_{min} = 0.983, T_{max} = 0.991	973 reflections with $I > 2\sigma(I)$
	R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040	91 parameters
$wR(F^2)$ = 0.109	H-atom parameters constrained
S = 1.01	$\Delta\rho_{max}$ = 0.14 e Å^{-3}
1486 reflections	$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2423).

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supplementary materials

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1,4-Dibenzylbenzene

Y.-J. Cui, G. Li, F.-X. Ren, Z.-Y. Duan and **W.-J. Zhang**

Comment

Although the synthesis of the title compound, has been reported previously (Serres *et al.*, 1960) the crystal structure has not. The compound is an important precursor in the synthesis of a flame retardant (Richard *et al.*, 1999). The molecular is shown in Fig. 1 and the bond lengths and angles are within normal ranges. The molecule lies on a crystallographic center of symmetry. Both phenyl rings are twisted from the plane of the central benzene ring by 88.39 (11)°. In the crystal structure molecules pack in a herring-bone arrangement with phenyl groups pointing towards each other (Fig. 2).

Experimental

The title compound was synthesized in 35% yield by alkylation of benzene with α,α'-dichloro-*p*-xylene. 210 g (2.7 mol) benzene, 28.9 g (0.165 mol)α,α'-dichloro-*p*-xylene and 0.24 g anhydrous ferric chloride as catalyst, were added to 500 ml flask equipped with a stirrer, a thermometer and a reflux condenser. The mixture was stirred for 2 h. The temperature was maintained at 323–328 K and then the mixture was hydrolysed with cold water. The resulting two-phase mixture was transferred to a separation funnel and extracted with 200 ml benzene. The combined organic layers were washed with three 100-ml portions of aqueous 10% sodium carbonate, dried over anhydrous calcium chloride, and filtered into a $1 - 1$ flask. The benzene was removed and the residue was transferred to a 250-ml flask, distilled under reduced pressure to give 15.5 g 1,4-dibenzylbenzene, b.p. 431–434 K/0.15 m mH g. Crystals form as colourless blocks upon slow evaporation of a solution of the title compound in ethanol. In addition to the crystal structure, the compound was also characterized by ^{1}HNMR [($CDCl_3$, 400MHZ): δ 7.321, 7.302, 7.284 (t, 4H), 7.230, 7.218, 7.199 (t, 6H)], 7.133 (s, 4H), 2.973(s, 4H). ^{13}C NMR ($CDCl_3$, δ, p.p.m.):141.166, 138.805, 128.954, 128.877, 128.407, 125.993, 41.492.

Refinement

H atoms were included in calculated positions and refined using a riding-model approximation. Constrained C—H bond lengths and isotropic U parameters: 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for Csp^2—H; 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for methylene C—H.

Figures

Fig. 1. The molecular structure, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level·H atoms are represented by circles of arbitrary size. Unlabelled atoms are realted by the symmetry operator ($1 - x$, $1 - y$, $1 - z$).

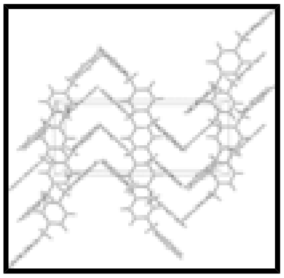

Fig. 2. The molecular packing viewed along the *a* axis.

1,4-dibenzylbenzene

Crystal data

$C_{20}H_{18}$

$M_r = 258.34$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 10.090$ (2) Å

$b = 7.8736$ (17) Å

$c = 18.379$ (4) Å

$V = 1460.1$ (6) Å^3

$Z = 4$

$F_{000} = 552$

$D_x = 1.175$ Mg m^{-3}

Mo *Kα* radiation
$\lambda = 0.71073$ Å

Cell parameters from 1782 reflections

$\theta = 2.2$–25.2°

$\mu = 0.07$ mm^{-1}

$T = 294$ (2) K

Block, colourless

0.26 × 0.22 × 0.14 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 294(2)$ K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.983$, $T_{\max} = 0.991$

7693 measured reflections

1486 independent reflections

973 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.046$

$\theta_{\max} = 26.4$°

$\theta_{\min} = 2.2$°

$h = -9\rightarrow 12$

$k = -6\rightarrow 9$

$l = -22\rightarrow 22$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.109$

$S = 1.01$

1486 reflections

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.1629P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.14$ e Å^{-3}

91 parameters	$\Delta\rho_{\min} = -0.20$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.59364 (16)	0.00124 (18)	0.32979 (7)	0.0520 (4)
H1	0.6851	0.0025	0.3237	0.062*
C2	0.51761 (18)	−0.1021 (2)	0.28591 (8)	0.0589 (4)
H2	0.5581	−0.1704	0.2511	0.071*
C3	0.38309 (17)	−0.10439 (19)	0.29345 (8)	0.0578 (4)
H3	0.3315	−0.1743	0.2641	0.069*
C4	0.32456 (16)	−0.00224 (18)	0.34494 (9)	0.0572 (4)
H4	0.2329	−0.0024	0.3500	0.069*
C5	0.40087 (14)	0.10059 (18)	0.38913 (8)	0.0495 (4)
H5	0.3599	0.1690	0.4237	0.059*
C6	0.53707 (14)	0.10314 (16)	0.38264 (7)	0.0429 (4)
C7	0.62560 (15)	0.20681 (18)	0.43237 (9)	0.0561 (4)
H7A	0.6586	0.1329	0.4705	0.067*
H7B	0.7014	0.2456	0.4045	0.067*
C8	0.56130 (13)	0.35893 (17)	0.46745 (8)	0.0448 (4)
C9	0.53593 (15)	0.50516 (19)	0.42826 (8)	0.0515 (4)
H9	0.5596	0.5101	0.3794	0.062*
C10	0.47629 (15)	0.64359 (18)	0.46017 (8)	0.0511 (4)
H10	0.4610	0.7406	0.4326	0.061*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0529 (9)	0.0530 (10)	0.0501 (9)	0.0058 (7)	0.0065 (7)	−0.0008 (7)
C2	0.0742 (11)	0.0569 (10)	0.0456 (9)	0.0087 (8)	0.0019 (8)	−0.0090 (7)
C3	0.0690 (11)	0.0495 (9)	0.0548 (10)	0.0009 (8)	−0.0133 (8)	−0.0053 (7)
C4	0.0482 (9)	0.0524 (10)	0.0712 (10)	−0.0001 (7)	−0.0067 (8)	−0.0011 (8)
C5	0.0498 (9)	0.0428 (8)	0.0559 (9)	0.0061 (7)	0.0035 (7)	−0.0051 (7)
C6	0.0493 (9)	0.0338 (7)	0.0458 (8)	0.0043 (6)	0.0008 (7)	0.0020 (6)

C7	0.0497 (9)	0.0513 (9)	0.0672 (10)	0.0053 (7)	−0.0036 (8)	−0.0109 (8)
C8	0.0409 (8)	0.0416 (8)	0.0519 (8)	−0.0020 (6)	−0.0052 (7)	−0.0065 (6)
C9	0.0612 (10)	0.0510 (9)	0.0421 (7)	−0.0013 (7)	0.0029 (7)	−0.0006 (7)
C10	0.0617 (9)	0.0398 (8)	0.0518 (9)	−0.0001 (7)	−0.0043 (7)	0.0059 (7)

Geometric parameters (Å, °)

C1—C2	1.379 (2)	C6—C7	1.516 (2)
C1—C6	1.3831 (18)	C7—C8	1.5071 (19)
C1—H1	0.9300	C7—H7A	0.9700
C2—C3	1.364 (2)	C7—H7B	0.9700
C2—H2	0.9300	C8—C9	1.382 (2)
C3—C4	1.375 (2)	C8—C10^{i}	1.384 (2)
C3—H3	0.9300	C9—C10	1.376 (2)
C4—C5	1.381 (2)	C9—H9	0.9300
C4—H4	0.9300	C10—C8^{i}	1.384 (2)
C5—C6	1.380 (2)	C10—H10	0.9300
C5—H5	0.9300		
C2—C1—C6	121.57 (15)	C1—C6—C7	119.50 (13)
C2—C1—H1	119.2	C8—C7—C6	115.60 (12)
C6—C1—H1	119.2	C8—C7—H7A	108.4
C3—C2—C1	120.12 (14)	C6—C7—H7A	108.4
C3—C2—H2	119.9	C8—C7—H7B	108.4
C1—C2—H2	119.9	C6—C7—H7B	108.4
C2—C3—C4	119.30 (15)	H7A—C7—H7B	107.4
C2—C3—H3	120.3	C9—C8—C10^{i}	117.54 (13)
C4—C3—H3	120.3	C9—C8—C7	121.26 (13)
C3—C4—C5	120.54 (15)	C10^{i}—C8—C7	121.20 (13)
C3—C4—H4	119.7	C10—C9—C8	121.24 (13)
C5—C4—H4	119.7	C10—C9—H9	119.4
C6—C5—C4	120.86 (14)	C8—C9—H9	119.4
C6—C5—H5	119.6	C9—C10—C8^{i}	121.21 (13)
C4—C5—H5	119.6	C9—C10—H10	119.4
C5—C6—C1	117.61 (14)	C8^{i}—C10—H10	119.4
C5—C6—C7	122.85 (12)		
C6—C1—C2—C3	0.7 (2)	C5—C6—C7—C8	−24.6 (2)
C1—C2—C3—C4	0.2 (2)	C1—C6—C7—C8	157.73 (13)
C2—C3—C4—C5	−0.6 (2)	C6—C7—C8—C9	−75.04 (17)
C3—C4—C5—C6	0.0 (2)	C6—C7—C8—C10^{i}	104.00 (16)
C4—C5—C6—C1	0.9 (2)	C10^{i}—C8—C9—C10	0.4 (2)
C4—C5—C6—C7	−176.76 (13)	C7—C8—C9—C10	179.50 (13)
C2—C1—C6—C5	−1.3 (2)	C8—C9—C10—C8^{i}	−0.4 (2)
C2—C1—C6—C7	176.49 (13)		

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

Fig. 1

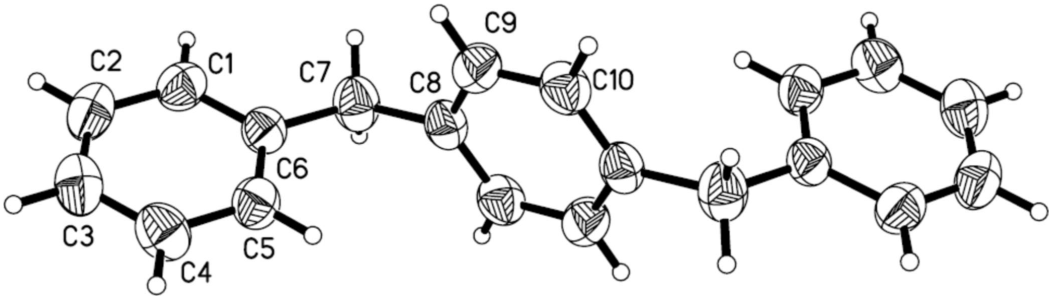

Fig. 2