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Key indicators

Single-crystal X-ray study
 $T = 213\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.043
 wR factor = 0.124
Data-to-parameter ratio = 13.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

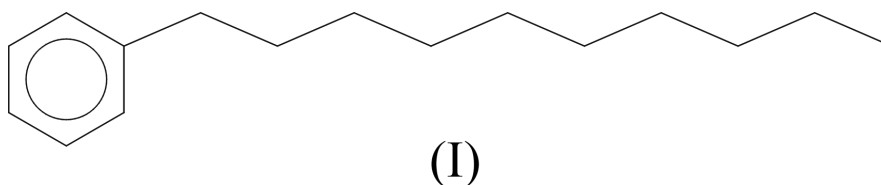
1-Phenyldecane

In the crystal structure of the title compound, $\text{C}_{16}\text{H}_{26}$, the crystal packing is formed by a herring-bone arrangement of the phenyl rings.

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Comment

Long-chain linear alkylbenzenes have been identified in wastes (Valls *et al.*, 1989), sediments (Ishiwatari *et al.*, 1983) and suspended particles (Takada & Ishiwatari, 1987); these compounds are produced industrially as precursors for the anionic surfactants linear alkylbenzene sulfonates. The long-chain linear alkylbenzenes have both an aliphatic and aromatic nature because of their unique structure. This results in their having physical properties in the same range as other hydrocarbon atoms of interest, such as saturated hydrocarbon atoms, polynuclear aromatic hydrocarbon atoms and polychlorinated biphenyls (Sherblom & Eganhouse, 1991). We report here the structure and the crystal packing of 1-phenyldecane, (I), which has a melting point about 259 K and crystallizes in space group $P2_12_12_1$.



The molecular structure is shown in Fig. 1. As 1-phenyldecane is a liquid, a special crystal growth technique was used. The title compound was first purified by distillation in high vacuum, and then transferred into an attached capillary. The sealed capillary was transferred to the diffractometer with a detachable cooling device. Single crystals suitable for X-ray diffraction were grown *in situ* using a computer-controlled device that applied a focused CO_2 laser beam along the capillary (Boese *et al.*, 1999). The molecular structure of (I) has a planar arrangement of the alkane carbon skeleton. The mean $\text{C}(\text{H}_3)-\text{C}(\text{H}_2)$ and $\text{C}(\text{H}_2)-\text{C}(\text{H}_2)$ distances, and the mean $\text{C}(\text{H}_3)-\text{C}(\text{H}_2)-\text{C}$ and $\text{C}(\text{H}_2)-\text{C}(\text{H}_2)-\text{C}$ angles, are in good agreement with those determined for *n*-alkanes [1.521 (1) \AA and 112.8 (1)–113.5 (1) $^\circ$, respectively; Boese *et al.*, 1999]. In the molecule, the phenyl ring and the alkane carbon skeleton are oriented at 84.73 (8) $^\circ$ with respect to each other. A search of the October 2001 release of the Cambridge Structural Database (Allen *et al.*, 1983) for structures containing the $\text{C}_6\text{H}_5(\text{CH}_2)_n\text{CH}_3$ fragment with $n > 1$ revealed no long-chain linear alkylbenzenes. In contrast to *n*-alkanes

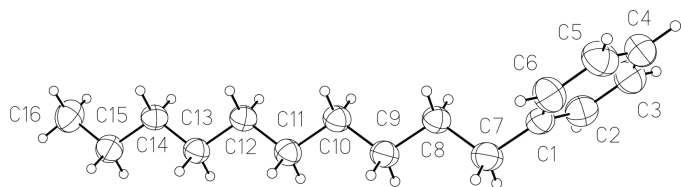


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids.

and most end-substituted *n*-alkanes (Kitaigorodskii, 1973), the long-chain linear alkylbenzenes do not show remarkable variation in their melting points. The crystal packing of 1-phenyldecane is shown in Fig. 2. This exhibits a herring-bone arrangement and the overall packing is similar to that of benzene, in the manner of 2-aminophenol, another *o*-disubstituted benzene (Allen *et al.*, 1997). The CH₂ groups fit into the hollows of the neighbouring chains.

Experimental

Crystal data

C ₁₆ H ₂₆	Mo K α radiation
$M_r = 218.37$	Cell parameters from 95 reflections
Orthorhombic, $P2_12_12_1$	$\theta = 2.8\text{--}18.7^\circ$
$a = 5.1428(16) \text{ \AA}$	$\mu = 0.06 \text{ mm}^{-1}$
$b = 8.908(3) \text{ \AA}$	$T = 213(2) \text{ K}$
$c = 31.687(11) \text{ \AA}$	Cylinder, colourless
$V = 1451.7(8) \text{ \AA}^3$	0.4 (length) \times 0.2 mm (diameter)
$Z = 4$	
$D_x = 0.999 \text{ Mg m}^{-3}$	

Data collection

Bruker AXS CCD 1000 diffractometer	1941 independent reflections
ω scans	1287 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (Blessing, 1995)	$R_{\text{int}} = 0.037$
$T_{\text{min}} = 0.970$, $T_{\text{max}} = 0.991$	$\theta_{\text{max}} = 25.0^\circ$
6337 measured reflections	$h = -2 \rightarrow 7$
	$k = -10 \rightarrow 11$
	$l = -33 \rightarrow 37$

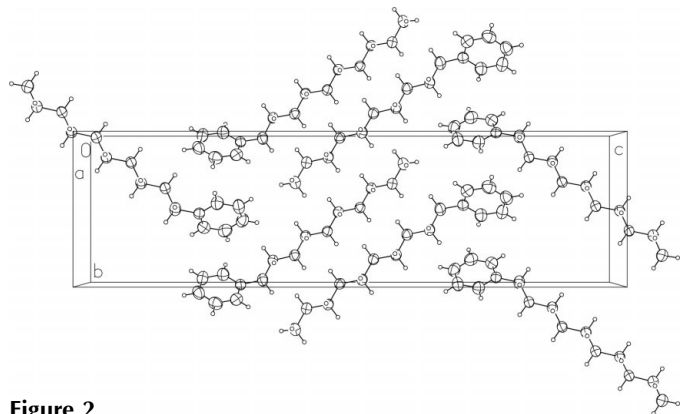


Figure 2
The crystal packing of (I), showing the herring-bone packing of the molecules.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2 + 0.1408P]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.124$	$(\Delta/\sigma)_{\text{max}} = 0.002$
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.11 \text{ e \AA}^{-3}$
1941 reflections	$\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$
145 parameters	H-atom parameters constrained

Table 1

Selected geometric parameters (\AA , $^\circ$).

C12—C13	1.511 (3)	C15—C16	1.519 (3)
C12—C11	1.521 (3)	C1—C6	1.376 (3)
C10—C11	1.515 (3)	C1—C2	1.389 (3)
C10—C9	1.523 (3)	C1—C7	1.501 (3)
C14—C15	1.505 (3)	C3—C4	1.362 (3)
C14—C13	1.518 (3)	C3—C2	1.375 (3)
C8—C9	1.512 (3)	C5—C4	1.364 (4)
C8—C7	1.529 (3)	C5—C6	1.372 (3)
C13—C12—C11	114.05 (17)	C6—C1—C7	120.9 (2)
C11—C10—C9	113.74 (17)	C2—C1—C7	121.6 (2)
C15—C14—C13	113.95 (17)	C1—C7—C8	112.70 (17)
C10—C11—C12	113.93 (17)	C4—C3—C2	119.9 (2)
C12—C13—C14	113.87 (17)	C3—C2—C1	121.2 (2)
C9—C8—C7	113.28 (18)	C4—C5—C6	120.5 (2)
C8—C9—C10	113.60 (18)	C5—C6—C1	121.1 (2)
C14—C15—C16	113.7 (2)	C3—C4—C5	119.8 (2)
C6—C1—C2	117.4 (2)		

All H atoms, visible in difference maps, were positioned geometrically and included as riding atoms in the refinement. Friedel pairs were merged, because of the absence of significant anomalous scattering effects.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Siemens, 1996); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

References

- Allen, F. H., Hoy, V. J., Howard, J. A. K., Thalladi, V. R., Desiraju, G. R., Wilson, C. C. & McIntyre, G. J. J. (1997). *J. Am. Chem. Soc.* **119**, 3477–3480.
- Allen, F. H., Kennard, O. & Taylor, R. (1983). *Acc. Chem. Res.* **16**, 146–153.
- Blessing, R. H. (1995). *Acta Cryst.* **A51**, 33–38.
- Boese, R., Weiss, H.-C. & Blaeser, D. (1999). *Angew. Chem. Int. Ed.* **38**, 988–992.
- Ishiwatari, R., Takada, H., Yun, S. J. & Matsumoto, E. (1983). *Nature (London)*, **301**, 599–600.
- Kitaigorodskii, A. I. (1973). *Molecular Crystals and Molecules*. New York: Academic Press.
- Sherblom, P. M. & Eganhouse, R. P. (1991). *Organic Substances and Sediments in Water*, Vol. 3, *Biological*, edited by R. A. Baker, pp. 139–158. Chelsea, Michigan: Lewis Publishers.
- Siemens (1996). *SHELXTL* (Version 5.10/DOS/WIN95/NT). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Takada, H. & Ishiwatari, R. (1987). *Environ. Sci. Technol.* **21**, 875–883.
- Valls, M., Bayona, J. M. & Albaiges, J. (1989). *Nature (London)*, **337**, 722–724.