Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

n-Decane

Andrew D. Bond* and John E. Davies

Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, England

Correspondence e-mail: adb29@cam.ac.uk

Received 8 January 2002
Accepted 21 January 2002
Online 31 January 2002

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.054
wR factor = 0.181
Data-to-parameter ratio = 12.5

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

The crystal structure of *n*-decane, $C_{10}H_{22}$, has been determined at 150 (2) K following *in situ* crystal growth from the liquid. In space group $P\overline{1}$, the molecule is sited on a crystallographic centre of symmetry, and has a fully extended conformation.

Comment

It has been known for well over a century that the melting points of the straight-chain aliphatic acids display an odd-even alternation effect, the melting points of those with an even number of C atoms being high compared with those with an odd number of C atoms (Baeyer, 1877). Since the boiling points of these compounds show a monotonic increase with chain length, this phenomenon must be attributed to differences in the crystal structures. A plausible explanation for the effect has been proposed only recently: from precise single-crystal X-ray diffraction data, Boese *et al.* (1999) established that the melting point alternation for the short- and intermediate-chain *n*-alkanes (C_nH_{2n+2}, n = 2–10) mirrors an alternation in crystal density. For *n*-hexane to *n*-nonane, which crystallize in space group $P\overline{1}$, this density alternation may be attributed to the interaction between the terminal methyl groups. Even-numbered *n*-alkanes adopt optimal intermolecular contacts at both ends of the molecules while odd-numbered *n*-alkanes must adopt longer intermolecular distances at one end, resulting in a lower crystal density.

(I)

The elegant study of Boese *et al.* (1999) was facilitated by examination of crystals grown *in situ* from the liquid (obtained where necessary by condensation of the gas), by application of a CO_2 laser beam along a sealed capillary. This technique proved successful for *n*-propane to *n*-nonane. It was not possible, however, to obtain a crystal of *n*-decane suitable for data collection. Recently, we have been pursuing a programme of research intended to improve techniques for determining the crystal structures of compounds that are liquid at room temperature (see, for example, Bond & Davies, 2001*a*,*b*,*c*), and report here the crystal structure of *n*-decane at 150 (2) K. The crystal was grown *in situ* from the liquid using a technique described earlier (Davies & Bond, 2001). In space group $P\overline{1}$, the molecule is sited on a crystallographic centre of symmetry, and the unit-cell parameters are consistent with those of the rest of the series, and also with values determined previously

DOI: 10.1107/S1600536802001332

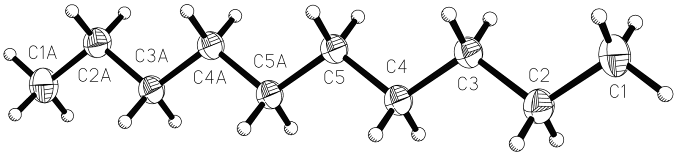

Figure 1
The molecular unit showing displacement ellipsoids at the 50% probability level for C atoms. Atoms related by the centre of symmetry are denoted by the suffix *A* (*XP*; Sheldrick, 1993).

from powder X-ray diffraction measurements (Norman & Mathisen, 1972).

Experimental

The sample (99%) was obtained from the Aldrich Company and used without further purification. The crystal was grown in a 0.3 mm glass capillary tube at *ca* 241.5 K (a temperature only slightly less than the melting point of the solid in the capillary). Once grown, the crystal was cooled to 150 (2) K for data collection. The length of the cylindrical crystal was not estimated, but it exceeded the diameter of the collimator (0.35 mm).

Crystal data

$C_{10}H_{22}$
$M_r = 142.28$
Triclinic, $P\bar{1}$
$a = 4.1741$ (4) Å
$b = 4.7239$ (6) Å
$c = 13.5066$ (15) Å
$\alpha = 85.974$ (1)°
$\beta = 81.463$ (7)°
$\gamma = 74.652$ (6)°
$V = 253.85$ (5) Å^3

$Z = 1$
$D_x = 0.931$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3994 reflections
$\theta = 1.0$–27.5°
$\mu = 0.05$ mm^{-1}
$T = 150$ (2) K
Cylinder, colourless
0.15 mm (radius)

Data collection

Nonius KappaCCD diffractometer
Thin-slice ω and φ scans
Absorption correction: none
2851 measured reflections
1122 independent reflections
865 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.069$
$\theta_{\rm max} = 27.4°$
$h = -4 \rightarrow 5$
$k = -6 \rightarrow 6$
$l = -15 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.181$
$S = 1.09$
1122 reflections
90 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0856P)^2 + 0.0416P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.22$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.18$ e Å^{-3}

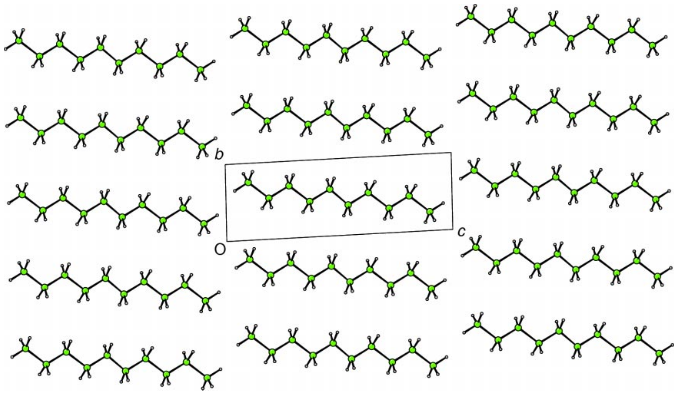

Figure 2
Projection on to (100) (*CAMERON*; Watkin *et al.*, 1996).

All H atoms were located from a difference Fourier map and refined freely with independent isotropic displacement parameters.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Sheldrick, 1993) and *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *SHELXL*97.

We thank the EPSRC for financial assistance towards the purchase of the Nonius CCD diffractometer.

References

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Baeyer, A. (1877). *Ber. Chem. Ges.* **10**, 1286.
Boese, R., Bläser, D. & Weiss, H.-C. (1999). *Angew. Chem. Int. Ed.* **38**, 988–992.
Bond, A. D. & Davies, J. E. (2001*a*). *Acta Cryst.* E**57**, o1039–o1040.
Bond, A. D. & Davies, J. E. (2001*b*). *Acta Cryst.* E**57**, o1087–o1088.
Bond, A. D. & Davies, J. E. (2001*c*). *Acta Cryst.* E**57**, o1191–o1193.
Davies, J. E. & Bond, A. D. (2001). *Acta Cryst.* E**57**, o947–o949.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Norman, N. & Mathisen, H. (1972). *Acta Chem. Scand.* **26**, 3913–3916.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter and R. M. Sweet, pp. 307–326. London: Academic Press.
Sheldrick, G. M. (1993). *XP*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.