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trans-1,4-Dimethylcyclohexane

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.001 Å
R factor = 0.044
wR factor = 0.091
Data-to-parameter ratio = 66.2

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

trans-1,4-Dimethylcyclohexane, C_8H_{16}, was studied as part of a project to develop a computer-controlled low-temperature crystal-growing device. The liquid crystallizes with the molecule lying on a centre of symmetry, leading to $Z' = \frac{1}{2}$.

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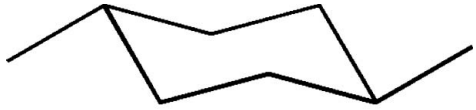
Comment

trans-1,4-Dimethylcyclohexane, (I) (Fig. 1), was one of eight alkylcyclohexanes whose thermodynamic properties were published in 1949 (Huffman *et al.*, 1949). That work reported a melting point of 236.217 K and showed no evidence for phase changes in the range down to liquid-nitrogen temperatures.



(I)

The sample used for the present study was one of several sealed in 0.2 mm Lindeman tubes for preliminary work carried out in 1979. Data had been collected at that time on a Stoe Weissenberg diffractometer and the structure solved, but it was not of a publishable quality (Courseille *et al.*, 1979).

The sample solidified spontaneously to a polycrystalline mass on flash cooling to 150 K. The temperature was then raised to 230 K and the sample zone-refined into a single-crystal using tandem computer-controlled heating elements. The temperature was then slowly reduced to 150 K for data collection.

The structure of (I) consists of molecules lying on centres of symmetry. This leads to the packing consisting of columns of molecules lying along the *b* axis (Fig. 2), with the mean plane of the molecule inclined at 145° to that axis (Fig. 3).

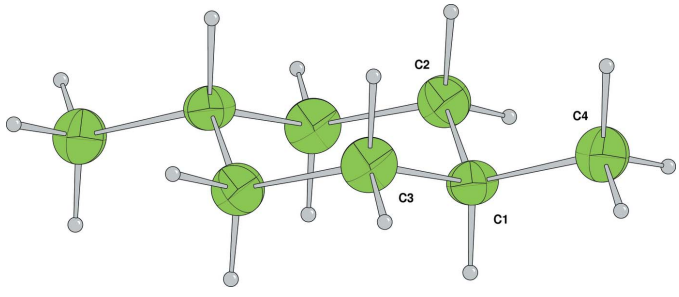


Figure 1
The structure of (I), with displacement ellipsoids drawn at the 50% probability level and H atoms shown as spheres of arbitary radii. Unlabelled atoms are related to labelled atoms by a centre of symmetry.

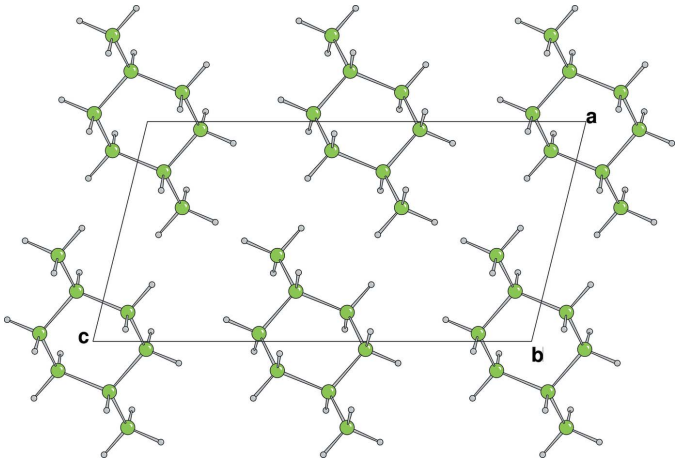


Figure 2
A projection of (I) along the *b* axis. The low specific gravity (0.98 Mg m^{-3}) is explained by the open texture of the structure.

Experimental

The material was used as supplied by Aldrich Chemical Company Inc. in 1979.

Crystal data

C_8H_{16}
M_r = 112.22
Monoclinic, $P2_1/c$
a = 6.0843 (2) Å
b = 5.4818 (2) Å
c = 11.7629 (5) Å
β = 103.8918 (18)°
V = 380.85 (2) Å^3
Z = 2
D_x = 0.978 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 882 reflections
θ = 1–27°
μ = 0.05 mm^{-1}
T = 150 K
Cylinder, colourless
1.00 (length) × 0.20 mm (diameter)

Data collection

Nonius KappaCCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*DENZO*/*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.758, T_{max} = 1.000
4141 measured reflections
862 independent reflections
861 reflections with $I > 3\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.6°
$h = -7 \rightarrow 7$
$k = -7 \rightarrow 6$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.091
S = 0.99
861 reflections
13 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F^2) + (0.03P)^2 + 0.07P]$ where $P = (\max(F_o^2,0) + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

The H atoms were all located in a difference map and then repositioned geometrically. The H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry, with C—H distances in the range 0.93–0.98 Å, and on the displacement parameters, with U_{iso}(H) = 1.2–1.5 times U_{eq} of the parent atom, after which their positions were refined with riding constraints.

Data collection: *COLLECT* (Nonius, 2001).; cell refinement: *DENZO*/*SCALEPACK*; data reduction: *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *CRYSTALS*.

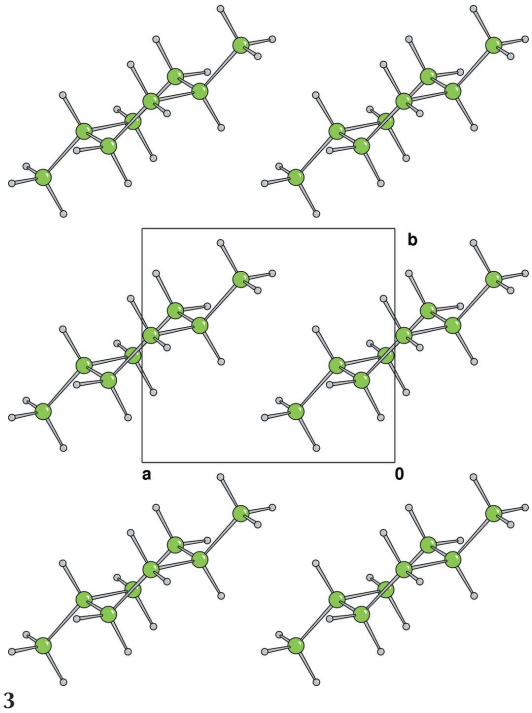


Figure 3
A projection of (I) along the *c* axis, showing the molecular stacks parallel to the *b* axis.

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