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trans-1,2-Dimethylcyclohexane

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.083
wR factor = 0.149
Data-to-parameter ratio = 23.0

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

The title compound, C_8H_{16}, a liquid at room temperature, was studied as part of a project to develop a computer-controlled low-temperature crystal-growing device. Single crystals, in $P21/n$, were obtained at 167 K. The molecule adopts a chair conformation and possesses a non-crystallographic twofold axis of symmetry.

Comment

trans-1,2-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 184.994 K and showed no evidence for phase changes in the range down to liquid nitrogen temperatures.

(I)

The sample we used 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 was not of a publishable quality (Courseille *et al.*, 1979).

The sample solidified spontaneously to a polycrystalline mass on flash cooling to 120 K. The temperature was then raised to 167 K and the sample was 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 molecules are in the chair conformation with the two methyl groups *trans*-equatorial [τ = −58.0 (2)]. The molecule has an excellent internal twofold axis (r.m.s. positional

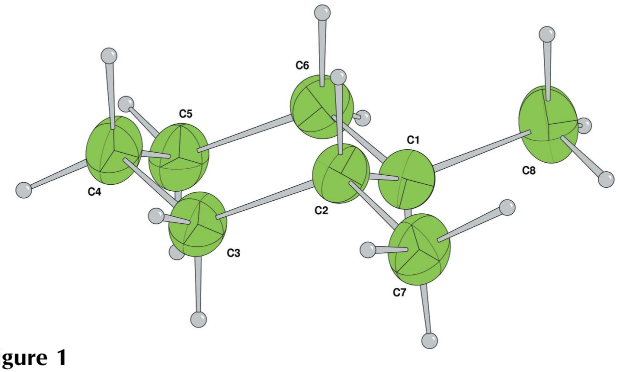

Figure 1
The title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitary radius.

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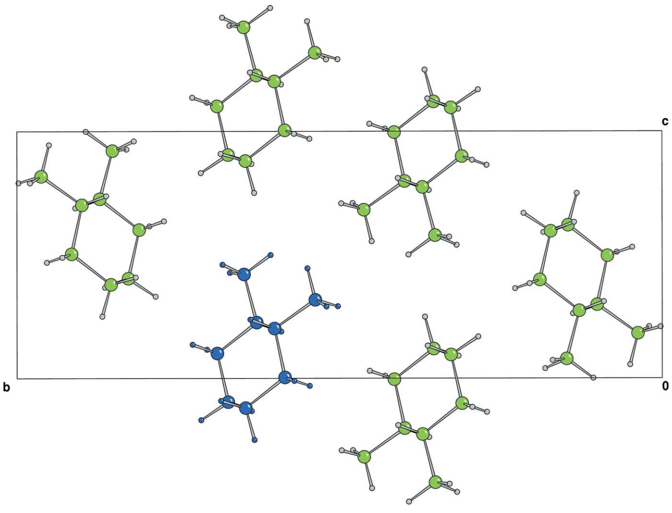

Figure 2
An *a* axis projection of the title compound. One column of molecules has been highlighted in blue for comparison with Fig. 3.

deviation 0.03 Å, r.m.s. bond length deviation 0.01 Å and r.m.s. torsion angle deviation 1.6° including the refined H atoms). The van der Waals surface is in the form of a slightly elongated disk with alternate layers inclined to each other. The calculated density is not unlike that of the ordered monoclinic phase of cyclohexane (0.996 Mg m^{-3}), suggesting that a low specific gravity may be a feature of small chain cyclic hydrocarbons (Kahn *et al.*, 1973).

Experimental

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

Crystal data

C_8H_{16}
$M_r = 112.22$
Monoclinic, $P2_1/n$
$a = 5.3403$ (4) Å
$b = 19.4410$ (15) Å
$c = 7.4446$ (7) Å
$\beta = 92.378$ (4)°
$V = 772.24$ (11) Å^3
$Z = 4$
$D_x = 0.965$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1440 reflections
$\theta = 5$–27°
$\mu = 0.05$ mm^{-1}
$T = 150$ K
Cylinder, colourless
1.00 × 0.20 (radius) mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (*DENZO*/*SCALEPACK*; Otwinowski & Minor, 1997)
$T_{\min} = 0.86$, $T_{\max} = 0.97$
2938 measured reflections
1679 independent reflections
1677 reflections with $I > -3\sigma(I)$
$R_{\rm int} = 0.039$
$\theta_{\max} = 27.4°$
$h = -6 \rightarrow 6$
$k = -25 \rightarrow 22$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.083$
$wR(F^2) = 0.149$
$S = 1.01$
1677 reflections
73 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F^2) + (0.05P)^2 + 0.29P]$ where $P = [\max(F_o^2,0) + 2F_c^2]/3$
$(\Delta/\sigma)_{\max} = 0.004$
$\Delta\rho_{\max} = 0.23$ e Å^{-3}
$\Delta\rho_{\min} = -0.20$ e Å^{-3}

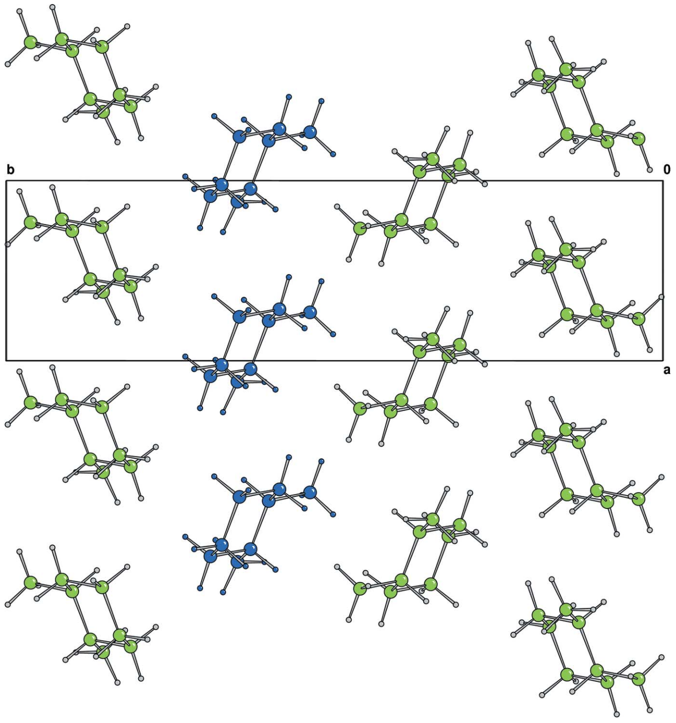

Figure 3
A projection along the *c* axis, showing the molecular stacks parallel to the *a* axis.

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.531 (2)	C2—C7	1.531 (2)
C1—C6	1.531 (2)	C3—C4	1.526 (2)
C1—C8	1.529 (2)	C4—C5	1.521 (2)
C2—C3	1.529 (2)	C5—C6	1.526 (2)
C2—C1—C6	110.81 (12)	C3—C2—C7	110.38 (12)
C2—C1—C8	113.12 (13)	C2—C3—C4	112.76 (12)
C6—C1—C8	110.15 (12)	C3—C4—C5	110.67 (12)
C1—C2—C3	110.76 (12)	C4—C5—C6	111.00 (13)
C1—C2—C7	112.87 (12)	C1—C6—C5	112.93 (12)

The H atoms were all located in a difference map and then repositioned geometrically. They were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C—H = 0.93–0.98 Å) and displacement parameters [$U_{\rm iso}({\rm H}) = 1.2$–$1.5U_{\rm eq}({\rm C})$], 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*.

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