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Methylcyclopentane

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Key indicators

Single-crystal X-ray study
T = 110 K
Mean σ(C–C) = 0.002 Å
R factor = 0.070
wR factor = 0.097
Data-to-parameter ratio = 25.6

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

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Methylcyclopentane, C_6H_{12}, a liquid at room temperature, was studied as part of a project to develop a computer-controlled low-temperature crystal-growing device. A single crystal was obtained at 115 K. The ring has an envelope conformation, with a pseudo-equatorial methyl substituent on the flap atom.

Comment

The melting point of methylcyclopentane is noted by the CRC Handbook of Chemistry and Physics as being −142.4° C (130.8 K) (Weast, 1978). A sample solidified spontaneously to a polycrystalline mass on flash-cooling to 115 K, and was then zone refined into a single crystal using tandem computer-controlled heating elements. Data collection was completed at 110 K

(I)

The molecule is in the envelope conformation (Fig. 1), with the four atoms C2—C5 almost coplanar (maximum deviation 0.04 Å) and a pseudo-equatorial methyl group attached to the flap atom C1. The crystal structure consists of molecular stacks formed by unit-cell translations along the a axis (Figs. 2 and 3).

The calculated density is not unlike that of the ordered monoclinic phase of cyclohexane (0.996 Mg m^{-3}), suggesting that a low density may be a feature of small cyclic hydrocarbons (Kahn *et al.*, 1973).

Experimental

The material was used as supplied by Acros Organics. A 2.0 mm column was flame-sealed in a 0.3 mm diameter Lindemann tube and crystallized as described above.

Crystal data

C_6H_{12}
M_r = 84.16
Monoclinic, $P2_1/n$
a = 5.3934 (2) Å
b = 11.1439 (5) Å
c = 9.7047 (5) Å
β = 98.0288 (17)°
V = 577.57 (5) Å^3
Z = 4
D_x = 0.968 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1447 reflections
θ = 5–28°
μ = 0.05 mm^{-1}
T = 110 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} = 0.69, T_{max} = 0.98
7788 measured reflections
1412 independent reflections
1408 reflections with $I > 3\sigma(I)$
R_{int} = 0.063
θ_{max} = 28.3°
$h = -7 \rightarrow 7$
$k = -14 \rightarrow 14$
$l = -12 \rightarrow 12$

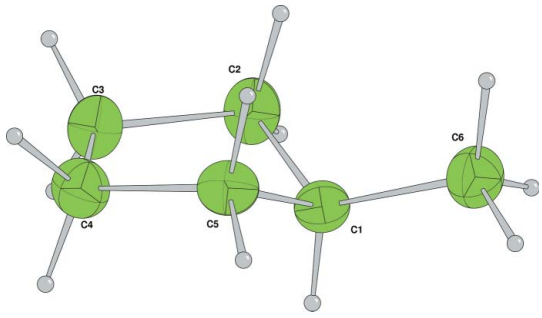

Figure 1
The title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitary radius.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F^2) + (0.03P)^2 + 0.1P]$ where $P = [\max(F_o^2,0) + 2F_c^2]/3$
$R[F^2 > 2\sigma(F^2)] = 0.070$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.097$	$\Delta\rho_{max} = 0.28$ e Å^{-3}
$S = 0.94$	$\Delta\rho_{min} = -0.22$ e Å^{-3}
1408 reflections	
55 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.5290 (14)	C2—C3	1.5344 (14)
C1—C5	1.5274 (14)	C3—C4	1.5402 (15)
C1—C6	1.5171 (14)	C4—C5	1.5286 (14)
C2—C1—C5	101.82 (8)	C2—C3—C4	105.88 (8)
C2—C1—C6	114.77 (8)	C3—C4—C5	105.39 (8)
C5—C1—C6	115.00 (8)	C4—C5—C1	104.05 (8)
C1—C2—C3	105.28 (8)		

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 (C–H in the range 0.93–0.98 Å) and displacement parameters [U_{iso}(H) in the range 1.2–1.5 times U_{eq} of the parent atom], after which they 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*.

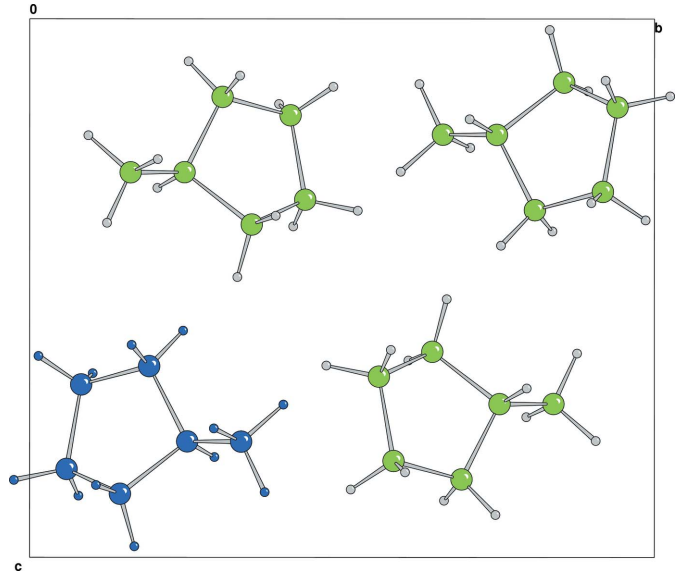

Figure 2
An *a*-axis projection of the title compound. One column of molecules has been highlighted in blue for comparison with Fig. 3.

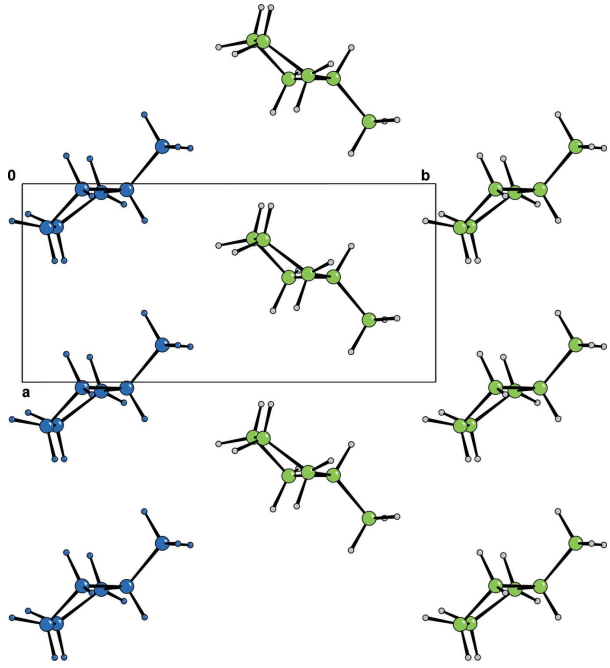

Figure 3
A projection along the *c* axis, showing the molecular stacks parallel to the *a* axis.

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$\beta = 98.0288$ (17)°
$V = 577.57$ (5) Å^3
$Z = 4$
$F(000) = 192$
$D_x = 0.968$ Mg m^{-3}
Melting point: 130.8 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1447 reflections
$\theta = 5$–28°
$\mu = 0.05$ mm^{-1}
$T = 110$ K
Cylinder, colourless
1.00 × 0.20 (radius) mm

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Graphite monochromator
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$\theta_{max} = 28.3°$, $\theta_{min} = 5.3°$
$h = -7 \rightarrow 7$
$k = -14 \rightarrow 14$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.070$
$wR(F^2) = 0.097$
$S = 0.94$
1408 reflections
55 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F^2) + (0.03P)^2 + 0.1P]$ where $P = [\max(F_o^2,0) + 2F_c^2]/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.03029 (18)	0.25222 (9)	0.78471 (10)	0.0284
C2	1.0448 (2)	0.19129 (9)	0.64490 (11)	0.0347
C3	1.2171 (2)	0.08259 (10)	0.67904 (11)	0.0350
C4	1.22182 (19)	0.05906 (10)	0.83578 (11)	0.0343

C5	1.02749 (18)	0.14454 (9)	0.88184 (11)	0.0313
C6	0.81288 (19)	0.33855 (10)	0.78504 (12)	0.0360
H11	1.1857	0.2957	0.8138	0.0340*
H21	1.1039	0.2457	0.5789	0.0431*
H22	0.8742	0.1633	0.6054	0.0443*
H31	1.3876	0.1010	0.6582	0.0454*
H32	1.1534	0.0141	0.6260	0.0435*
H41	1.3888	0.0781	0.8855	0.0414*
H42	1.1882	−0.0251	0.8563	0.0421*
H51	1.0629	0.1677	0.9795	0.0402*
H52	0.8593	0.1062	0.8656	0.0385*
H61	0.8146	0.3762	0.8788	0.0540*
H62	0.8215	0.4062	0.7163	0.0519*
H63	0.6522	0.2949	0.7605	0.0531*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0268 (5)	0.0270 (5)	0.0316 (6)	−0.0033 (4)	0.0046 (4)	0.0004 (4)
C2	0.0411 (6)	0.0343 (6)	0.0297 (6)	0.0059 (5)	0.0078 (4)	0.0033 (4)
C3	0.0380 (6)	0.0309 (6)	0.0366 (6)	0.0042 (5)	0.0067 (4)	0.0009 (4)
C4	0.0341 (5)	0.0316 (5)	0.0364 (6)	0.0002 (4)	0.0024 (4)	0.0058 (5)
C5	0.0320 (5)	0.0333 (5)	0.0286 (6)	−0.0044 (4)	0.0044 (4)	0.0021 (4)
C6	0.0348 (6)	0.0338 (6)	0.0405 (6)	0.0017 (5)	0.0085 (4)	−0.0023 (5)

Geometric parameters (Å, º)

C1—C2	1.5290 (14)	C3—H32	0.957
C1—C5	1.5274 (14)	C4—C5	1.5286 (14)
C1—C6	1.5171 (14)	C4—H41	0.984
C1—H11	0.975	C4—H42	0.981
C2—C3	1.5344 (14)	C5—H51	0.975
C2—H21	0.967	C5—H52	0.995
C2—H22	0.996	C6—H61	1.001
C3—C4	1.5402 (15)	C6—H62	1.013
C3—H31	0.990	C6—H63	0.993
C2—C1—C5	101.82 (8)	C3—C4—C5	105.39 (8)
C2—C1—C6	114.77 (8)	C3—C4—H41	109.6
C5—C1—C6	115.00 (8)	C5—C4—H41	109.9
C2—C1—H11	109.2	C3—C4—H42	112.6
C5—C1—H11	107.1	C5—C4—H42	112.5
C6—C1—H11	108.5	H41—C4—H42	106.8
C1—C2—C3	105.28 (8)	C4—C5—C1	104.05 (8)
C1—C2—H21	111.8	C4—C5—H51	113.6
C3—C2—H21	113.1	C1—C5—H51	112.0
C1—C2—H22	108.7	C4—C5—H52	109.5
C3—C2—H22	109.6	C1—C5—H52	109.1

H21—C2—H22	108.3	H51—C5—H52	108.5
C2—C3—C4	105.88 (8)	C1—C6—H61	111.0
C2—C3—H31	110.1	C1—C6—H62	111.4
C4—C3—H31	110.5	H61—C6—H62	107.0
C2—C3—H32	110.6	C1—C6—H63	109.8
C4—C3—H32	110.5	H61—C6—H63	108.7
H31—C3—H32	109.2	H62—C6—H63	109.0