

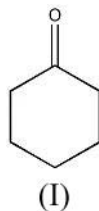
Cyclohexanone at 150 K

Howard A. Shallard-Brown,*
David J. Watkin and Andrew
R. CowleyChemical Crystallography Laboratory, Chemistry
Research Laboratory, Mansfield Road, Oxford
University, Oxford OX1 3TA, EnglandCorrespondence e-mail:
howard.shallard-brown@lmh.ox.ac.uk

Key indicators

Single-crystal X-ray study
 $T = 150$ K
Mean $\sigma(C-C) = 0.003$ Å
 R factor = 0.046
 wR factor = 0.119
Data-to-parameter ratio = 12.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.The structure of cyclohexanone, $C_6H_{10}O$, at 150 K is that of
discrete molecules, with no strong intermolecular interactions.Received 12 May 2005
Accepted 19 May 2005
Online 9 July 2005

Comment

Many of the esters and ketones used in the flavours and
fragrances industry are liquid at room temperature, meaning
that, in the past, crystalline derivatives have had to be
prepared for X-ray analysis. As part of a programme to
systematize *in situ* crystal growth from liquids, we have
examined a range of commercially available chemicals. Low-
molecular weight organic ketones are liquid at room
temperature. The molecules of cyclohexanone, (I), exist in the
crystal structure at 150 K as discrete entities, with no strong
intermolecular interactions.

Experimental

A 3 mm column of the title material, which is a liquid at room
temperature, was sealed in a 0.3 mm Lindemann tube. The Linde-
mann tube was not precisely parallel to the φ axis. A single crystal of
the compound was grown by keeping the compound under a cold
nitrogen gas stream (Oxford Cryostream 600) at 180 K and slowly
moving a small liquid zone, created by a micro-heating coil, up and
down the sample. Once a suitable approximately single-crystal
specimen had been obtained, the main data collection was carried out
at 150 K. Because not all of the data were collected with the
Lindemann tube perpendicular to the X-ray beam, the multi-scan
corrections applied by *DENZO/SCALEPACK* (Otwinowski &
Minor, 1997) also contain contributions due to changes in the illu-
minated volume of the cylindrical sample, which affects the value of
 T_{\min}/T_{\max} .

Crystal data

 $C_6H_{10}O$
 $M_r = 98.14$
Orthorhombic, $P2_12_12_1$
 $a = 5.3736$ (2) Å
 $b = 7.0394$ (3) Å
 $c = 15.1910$ (7) Å
 $V = 574.63$ (4) Å³
 $Z = 4$
 $D_x = 1.134$ Mg m⁻³Mo $K\alpha$ radiation
Cell parameters from 784
reflections
 $\theta = 5-27^\circ$
 $\mu = 0.08$ mm⁻¹
 $T = 150$ K
Cylinder, colourless
 $0.70 \times 0.30 \times 0.30$ mm

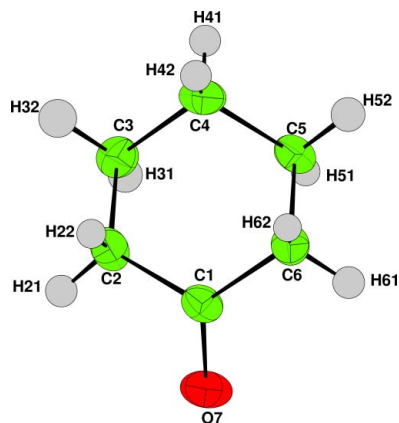


Figure 1

The title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms are of arbitrary radii.

Data collection

Nonius KappaCCD diffractometer	775 independent reflections
ω scans	693 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (<i>DENZO/SCALEPACK</i> ; Otwinowski & Minor, 1997)	$R_{\text{int}} = 0.085$
$T_{\text{min}} = 0.74$, $T_{\text{max}} = 0.98$	$\theta_{\text{max}} = 27.4^\circ$
9235 measured reflections	$h = -6 \rightarrow 6$
	$k = -9 \rightarrow 9$
	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.046$	$w = 1/[\sigma^2(F) + 0.08 + 0.07P]$,
$wR(F^2) = 0.119$	where $P = (\max(F_o^2, 0) + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{\text{max}} = 0.009$
774 reflections	$\Delta\rho_{\text{max}} = 0.21 \text{ e } \text{\AA}^{-3}$
64 parameters	$\Delta\rho_{\text{min}} = -0.17 \text{ e } \text{\AA}^{-3}$

Table 1

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

C1—C2	1.501 (2)	C3—C4	1.520 (3)
C1—C6	1.513 (2)	C4—C5	1.523 (3)
C1—O7	1.213 (2)	C5—C6	1.533 (2)
C2—C3	1.532 (3)		
C2—C1—C6	115.45 (14)	C2—C3—C4	111.63 (15)
C2—C1—O7	122.61 (15)	C3—C4—C5	110.85 (16)
C6—C1—O7	121.93 (15)	C4—C5—C6	111.04 (15)
C1—C2—C3	112.29 (15)	C5—C6—C1	111.65 (13)

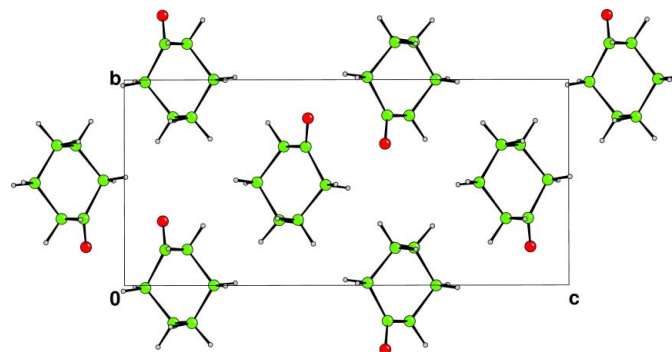


Figure 2

The crystal structure, viewed down the a axis.

All H atoms were located in a difference map and were repositioned geometrically. The H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry [$\text{C—H} = 0.97\text{--}1.01 \text{ \AA}$, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$], after which they were refined with riding constraints. In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: *COLLECT* (Nonius, 1997); cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK*; 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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