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(1*R*)-(−)-Fenchone

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.005 Å
R factor = 0.056
wR factor = 0.156
Data-to-parameter ratio = 8.0

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

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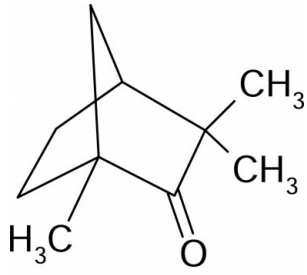
The crystal structure of (1*R*)-(−)-fenchone, $C_{10}H_{16}O$, has been determined at 150 (2) K following *in situ* crystal growth from the liquid.

Comment

Fenchone (I) occurs in nature and may be extracted from fennel oil and thuja oil. An account of its history and the determination of its structure using the techniques of classical organic chemistry is given by Simonsen & Owen (1947). This work forms part of a continuing study devoted to improving the techniques for determining the crystal structures of substances which are liquids at room temperature (see, for example, Davies & Bond, 2001).



(I)

Experimental

(1*R*)-(−)-Fenchone (98%) was obtained from the Aldrich company and used without further purification. The crystal was grown in a 0.3 mm glass capillary tube at 260 K (a temperature only slightly less than the melting point of the solid in the capillary tube). With the axis of the capillary parallel to the φ axis and horizontal on the instrument, the crystal was obtained by moving a plug of solid material up and down the tube (the movement being controlled with the standard height adjustment of the goniometer head). The length of the cylindrical crystal was not estimated, but it exceeded the 0.35 mm diameter of the collimator. Data were collected at 150 K.

Crystal data

$C_{10}H_{16}O$
M_r = 152.23
Monoclinic, $P2_1$
a = 6.0520 (7) Å
b = 10.2748 (7) Å
c = 7.1621 (9) Å
β = 91.335 (4)°
V = 445.24 (8) Å^3
Z = 2
D_x = 1.135 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2665 reflections
θ = 1.0–25.0°
μ = 0.07 mm^{-1}
T = 150 (2) K
Cylinder, colourless
0.15 mm (radius)

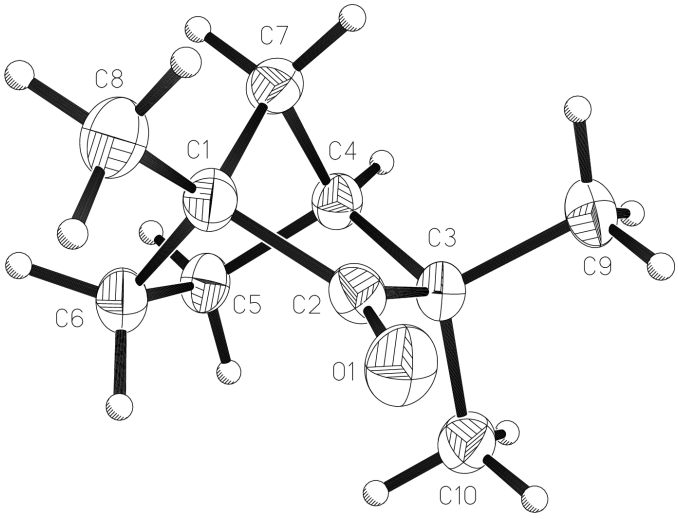


Figure 1
Molecular structure of (I), showing displacement ellipsoids at the 50% probability level (*XP*; Sheldrick, 1993).

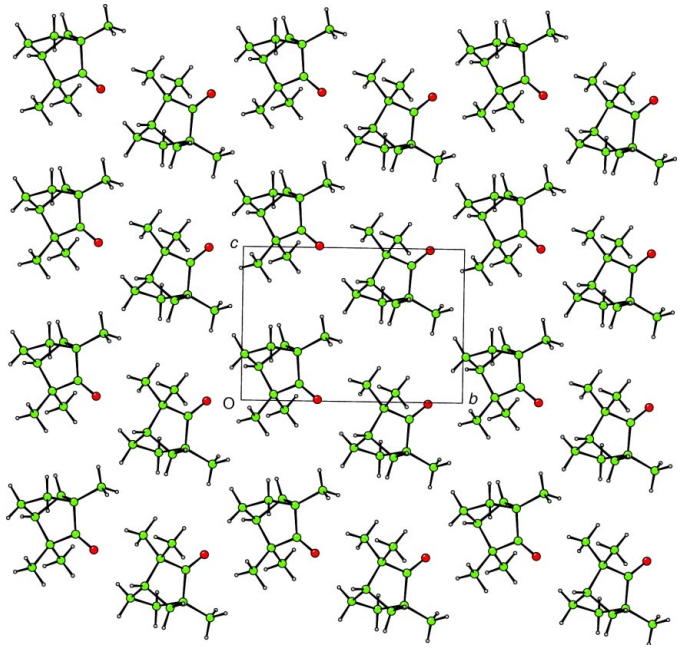


Figure 2
Projection of the structure of (I) onto (100) (*CAMERON*; Watkin *et al.*, 1996).

Data collection

Nonius KappaCCD diffractometer	757 reflections with $I > 2\sigma(I)$
Thin-slice ω and φ scans	$R_{int} = 0.078$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)	$\theta_{max} = 25.0^\circ$
$T_{min} = 0.783$, $T_{max} = 1.000$	$h = -7 \rightarrow 7$
2506 measured reflections	$k = -12 \rightarrow 10$
821 independent reflections	$l = -6 \rightarrow 8$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1005P)^2 + 0.0865P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.056$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.157$	$\Delta\rho_{max} = 0.19$ e Å^{-3}
$S = 1.10$	$\Delta\rho_{min} = -0.22$ e Å^{-3}
821 reflections	
103 parameters	
H-atom parameters constrained	

H atoms were placed geometrically and refined using a riding model with an isotropic displacement parameter fixed at 1.2 times U_{eq} for the C atom to which they are attached. The absolute configuration could not be determined reliably and was assigned according to the known configuration of the sample. Friedel pairs were merged prior to merging in $P2_1$; the reported value of R_{int} corresponds to subsequent refining of equivalent reflections in this space group.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; 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.

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