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(1*S*)-(−)-α-Pinene

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Key indicators

Single-crystal X-ray study
T = 203 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.103
Data-to-parameter ratio = 14.5

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

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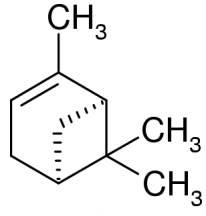
The crystal structure of (1*S*)-(−)-α-pinene, $C_{10}H_{16}$, has been determined at 203 (2) K by *in situ* crystal growth from the liquid.

Comment

α-Pinene, (I), is very widely distributed in nature. It is present in the majority of essential oils derived from the Coniferae and it is the principal constituent of oil of turpentine. 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*S*)-(−)-α-Pinene (99%) was obtained from the Aldrich Company and used without further purification. The crystal was grown in a 0.4 mm glass capillary tube at 203 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 *Z* (height) adjustment of the goniometer head]. The data are 90.2% complete because the crystal melted during an attempt to move it into a different orientation for the final set of frames. Previous attempts to reduce the temperature further for data collection resulted in the crystals being destroyed. Data were collected therefore at 203 (2) K.

Crystal data

$C_{10}H_{16}$
M_r = 136.23
Orthorhombic, $P2_12_12_1$
a = 7.1944 (6) Å
b = 7.5920 (3) Å
c = 15.9190 (15) Å
V = 869.49 (11) Å^3
Z = 4
D_x = 1.041 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2466 reflections
θ = 1.0–25.0°
μ = 0.06 mm^{-1}
T = 203 (2) K
Cylinder, colourless
0.20 mm (radius)

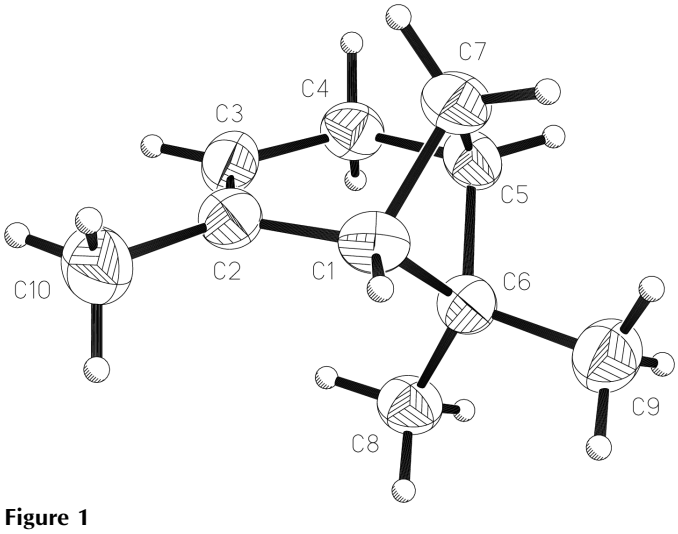


Figure 1
The asymmetric unit in (I) showing displacement ellipsoids at the 50% probability level (*XP*; Sheldrick, 1993).

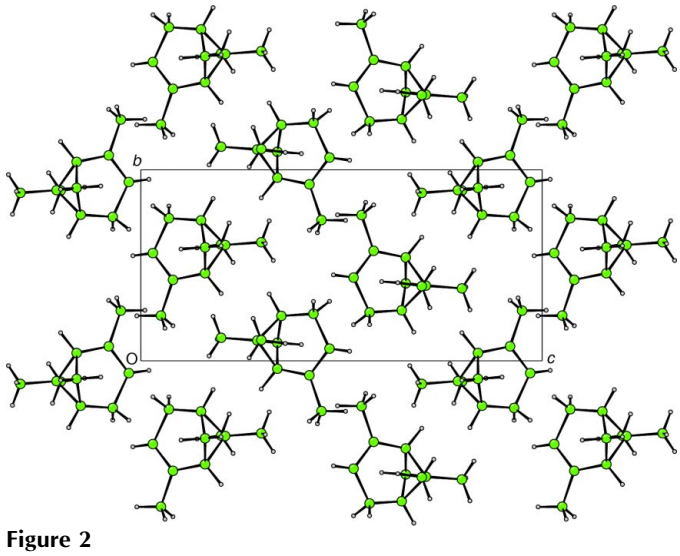


Figure 2
Projection onto (100) of the crystal structure of (I) (*CAMERON*; Watkin *et al.*, 1996).

Data collection

Nonius KappaCCD diffractometer	$R_{int} = 0.050$
Thin-slice ω and φ scans	$\theta_{max} = 25.0°$
3727 measured reflections	$h = -5 \rightarrow 8$
1379 independent reflections	$k = -7 \rightarrow 7$
1194 reflections with $I > 2\sigma(I)$	$l = -16 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0279P)^2 + 0.1574P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.046$	
$wR(F^2) = 0.103$	
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
1379 reflections	$\Delta\rho_{max} = 0.13$ e Å^{-3}
95 parameters	$\Delta\rho_{min} = -0.15$ e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXL*97
	Extinction coefficient: 0.096 (12)

H atoms were placed geometrically and refined using a riding model with an isotropic displacement parameter fixed at $1.2U_{eq}$ of the carbon 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, therefore, prior to merging of other equivalent reflections in $P2_12_12_1$; the reported value of R_{int} corresponds to merging 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); software used to prepare material for publication: *SHELXL*97.

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