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γ-Terpinene

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.049
wR factor = 0.139
Data-to-parameter ratio = 15.7

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

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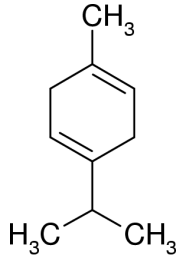
The crystal structure of γ-terpinene, $C_{10}H_{16}$, has been determined at 150 (2) K following *in situ* crystal growth from the liquid. The molecule lies on a mirror plane in the space group *Pnma* and forms stacks which pack in a herring-bone-type arrangement.

Comment

γ-Terpinene (I) occurs in nature and can be obtained, for example, from coriander oil, lemon oil and cumin 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

γ-Terpinene (97%) was obtained from the Aldrich company and used without further purification. The crystal was grown in a 0.3 mm glass capillary tube at 210 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 collimator diameter. Data were collected at 150 K.

Crystal data

$C_{10}H_{16}$
M_r = 136.23
Orthorhombic, *Pnma*
a = 18.1968 (13) Å
b = 7.2601 (5) Å
c = 6.7498 (3) Å
V = 891.72 (10) Å^3
Z = 4
D_x = 1.015 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4398 reflections
θ = 1.0–27.5°
μ = 0.06 mm^{-1}
T = 150 (2) K
Cylinder, colourless
0.15 mm (radius)

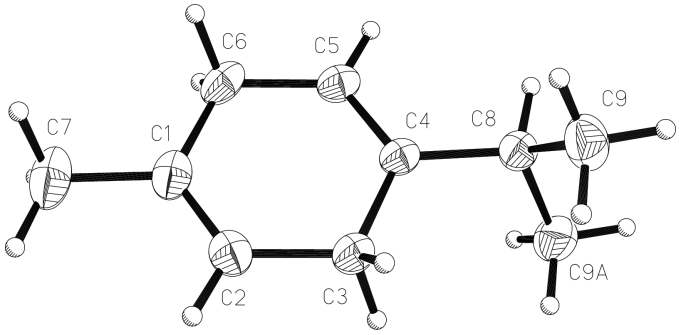


Figure 1
Molecular structure of (I), showing displacement ellipsoids at the 50% probability level (*XP*; Sheldrick, 1993).

Data collection

Nonius KappaCCD diffractometer
Thin-slice ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.809, T_{max} = 0.986
5877 measured reflections
1102 independent reflections
829 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 27.5°
$h = -21 \rightarrow 23$
$k = -7 \rightarrow 9$
$l = -8 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.139
S = 1.06
1102 reflections
70 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0688P)^2 + 0.1715P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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.

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.

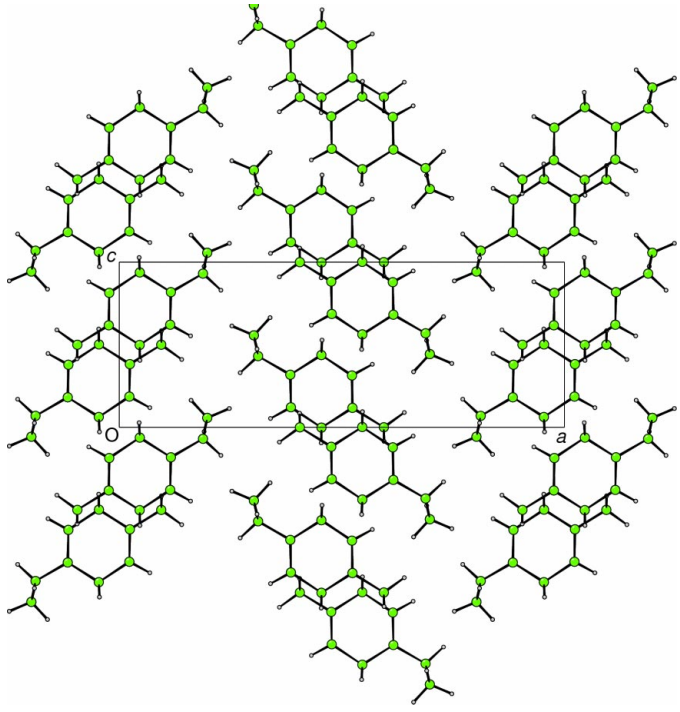


Figure 2
Projection onto (010), showing stacks of (I) packed in a herring-bone-type arrangement (*CAMERON*; Watkin *et al.*, 1996).

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