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α-Methylstyrene

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Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.005 Å
R factor = 0.085
wR factor = 0.250
Data-to-parameter ratio = 10.8

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

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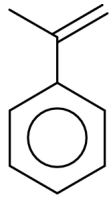
The crystal structure of α-methylstyrene, C_9H_{10}, has been determined at 180 (2) K following *in situ* crystal growth from the liquid. In space group $P2_1/n$, the structure consists of herring-bone-packed layers within which intermolecular C—H···π interactions are evident.

Comment

As part of a study devoted to improving techniques for determining the crystal structures of substances that are liquid at room temperature, we have recently reported the structure of styrene, C_8H_8 (Bond & Davies, 2001; Yasuda *et al.*, 2001). We report here the crystal structure of the α-methyl derivative, C_9H_{10}, determined at 180 (2) K following *in situ* crystal growth from the liquid.



(I)

α–Methylstyrene, (I), crystallizes in the monoclinic space group $P2_1/n$ with one whole molecule in the asymmetric unit (Fig. 1). The propenyl substituent lies approximately coplanar with the phenyl ring [the angle between the least-squares planes through C1–C6 and C7–C9 is 1.8 (3)°]. Molecules of (I) form herring-bone-packed layers parallel to (001) (Fig. 2). These layers may be considered to stack in an *ABAB* arrangement (Fig. 3). C—H···π interactions are evident between molecules within layers [H5···cent(C7–C8)^{i} = 3.06 Å, C5—H5···cent(C7–C8)^{i} = 153°; H6···cent(C1–C6)^{i} = 3.06 Å, C6—H6···cent(C1–C6)^{i} = 137°; H8*B*···cent(C1–C6)^{ii} = 3.03 Å, C8—H8*B*···cent(C1–C6)^{ii} = 138°; symmetry codes: (i) −1/2−*x*, 1/2+*y*, 1/2−*z*; (ii) 1/2−*x*, −1/2+*y*, 1/2−*z*; cent denotes the centroid of the indicated ring]. A similar arrangement is observed in styrene itself, but in that case, the α-hydrogen also acts as a C—H···π donor; this interaction is clearly prohibited in (I).

Experimental

The sample (99%) was obtained from the Lancaster company and used without further purification. The crystal was grown in a 0.3 mm glass capillary tube at *ca* 247.4 K (a temperature only slightly less than the melting point of the solid in the capillary) using a technique described earlier (Davies & Bond, 2001). Once grown, the crystal was

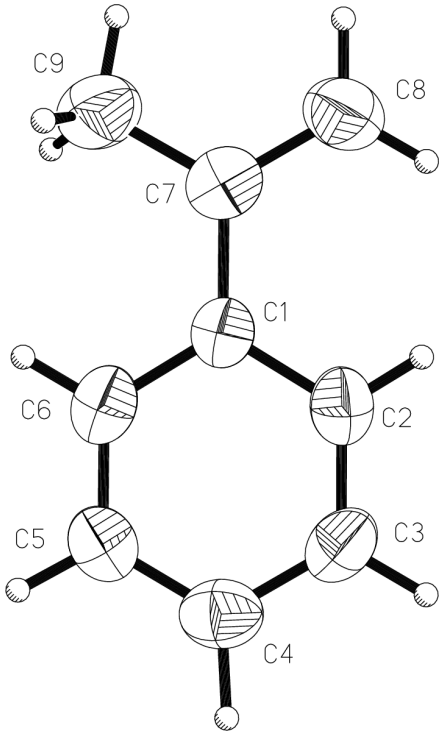


Figure 1
The molecular unit in (I), showing displacement ellipsoids at the 50% probability level for non-H atoms (*XP*; Sheldrick, 1993).

cooled to 180 (2) K for data collection. The length of the cylindrical crystal was not estimated, but it exceeded the diameter of the collimator (0.35 mm).

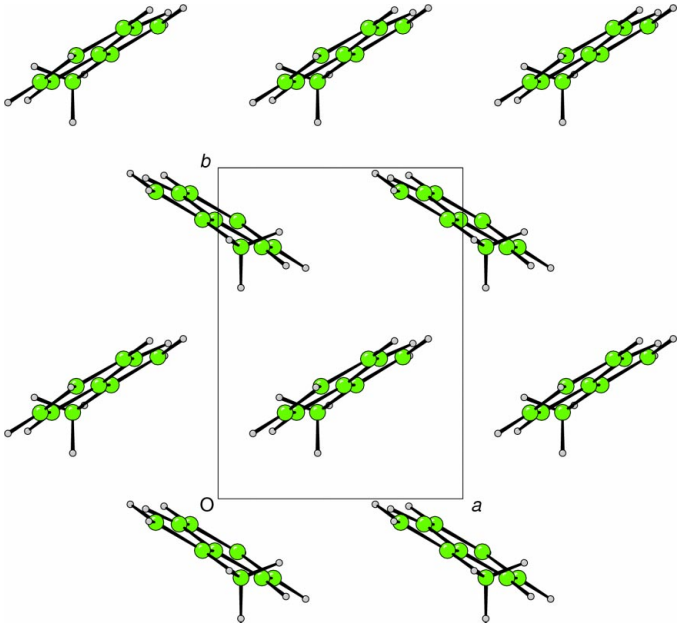


Figure 2
Projection on to (001) of a single layer of (I), showing the herring-bone packing arrangement (*CAMERON*; Watkin *et al.*, 1996).

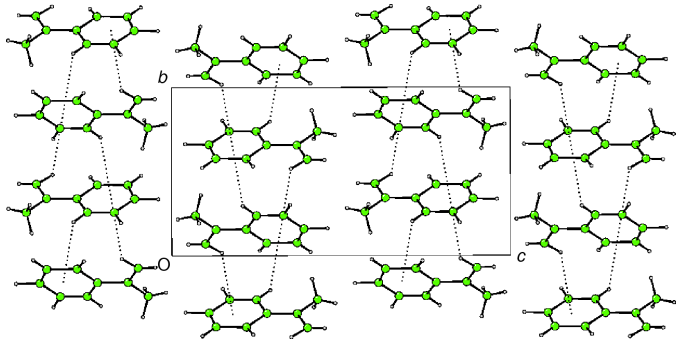


Figure 3
Projection of (I) on to (100). C—H$\cdots\pi$ interactions are indicated by dotted lines (*CAMERON*; Watkin *et al.*, 1996).

Crystal data

C_9H_{10}	D_x = 1.095 Mg m^{-3}
M_r = 118.17	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 2680 reflections
a = 5.795 (1) Å	θ = 1.0–22.5°
b = 7.829 (1) Å	μ = 0.06 mm^{-1}
c = 15.820 (1) Å	T = 180 (2) K
β = 93.23 (1)°	Cylinder, colourless
V = 716.60 (16) Å^3	0.15 mm (radius)
Z = 4	

Data collection

Nonius KappaCCD diffractometer	R_{int} = 0.089
Thin-slice ω and φ scans	θ_{max} = 22.3°
Absorption correction: none	$h = -5 \rightarrow 6$
3208 measured reflections	$k = -7 \rightarrow 8$
895 independent reflections	$l = -15 \rightarrow 16$
676 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1448P)^2 + 0.2267P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.085	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.250	$\Delta\rho_{max}$ = 0.37 e Å^{-3}
S = 1.15	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
895 reflections	
83 parameters	
H-atom parameters constrained	

H atoms were placed geometrically and allowed to ride during subsequent refinement with $U_{iso}(H) = xU_{eq}(C)$ (x = 1.2 for alkene and phenyl H, and 1.5 for methyl H). The methyl group was allowed to rotate about its local threefold axis. No significant diffracted intensity was observed beyond 22.5° in θ (equivalent to 0.93 Å resolution) and the data were truncated at this point; the precision of the result is reduced accordingly.

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