

## Styrene at 120 K

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## Key indicators

Single-crystal X-ray study

$T = 120$  K

Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å

$R$  factor = 0.038

$wR$  factor = 0.100

Data-to-parameter ratio = 13.4

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

The crystal structure of styrene,  $\text{C}_8\text{H}_8$ , has been determined at 120 (2) K following *in situ* crystal growth from the liquid. Molecules crystallize in the orthorhombic space group *Pbcn* and contains intermolecular  $\text{C}-\text{H}\cdots\pi$  interactions, with both the phenyl ring and the alkene unit acting as acceptors.

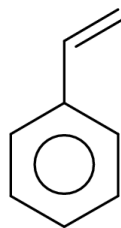
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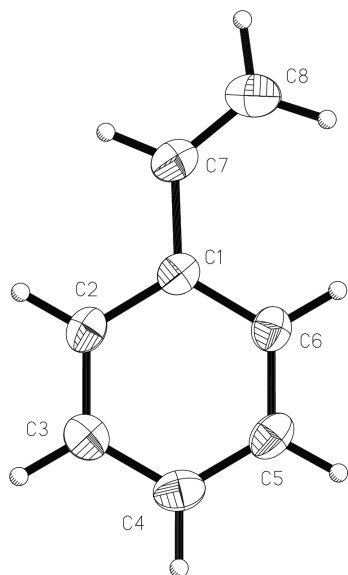
## Comment

Styrene occurs in nature in *Liquidambar orientalis* and oil of *Xanthorrhoea hastilis*. It is an important industrial chemical (*ca* 4.01 million tons per year produced in the USA), manufactured mainly by the dehydrogenation of ethylbenzene. It is used to produce polystyrene and is a component of SBR synthetic rubber, ABS terpolymer and styrene/butadiene and styrene/acrylonitrile copolymers. From a study of Debye–Scherrer patterns recorded from frozen styrene at 93 K, Roy (1958) determined correctly that the crystal structure of styrene is orthorhombic and suggested a possible (although unfortunately incorrect) set of unit-cell parameters. We report here the results of a full determination of the crystal structure of styrene at 120 (2) K. This work forms part of a study devoted to improving techniques for determining the crystal structures of substances that are liquid at room temperature (see, for example, Bond & Davies, 2001*a,b*).

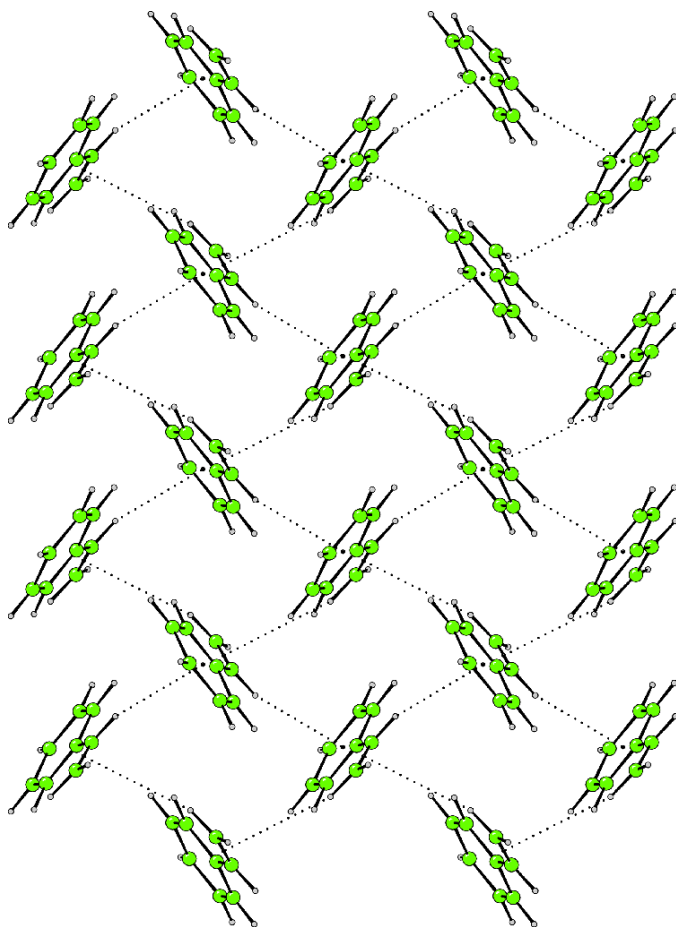


(I)

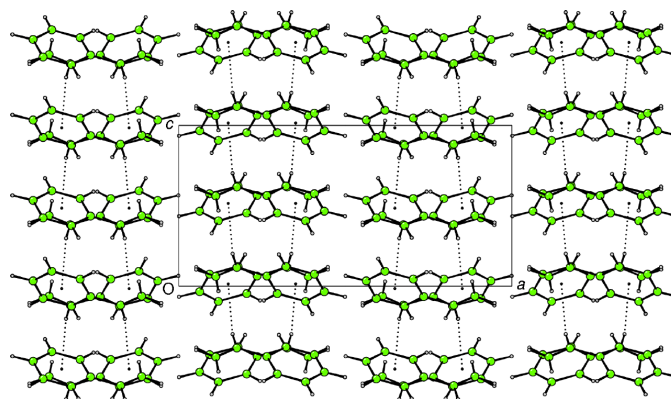
Styrene, (I), crystallizes in the orthorhombic space group *Pbcn* with one whole molecule in the asymmetric unit (Fig. 1). The terminal  $\text{CH}_2$  group of the alkene unit is displaced slightly from the plane of the phenyl ring, giving a  $\text{C6}-\text{C1}-\text{C7}-\text{C8}$  torsion angle of  $6.5(2)^\circ$ . Between molecules,  $\text{C}-\text{H}\cdots\pi$  interactions exist in which the  $\alpha\text{-C}-\text{H}$  group of the alkene unit acts as a hydrogen-bond donor and the phenyl ring of an adjacent molecule acts as an acceptor [ $\text{H7}\cdots\text{centroid}(\text{C1}-\text{C6})^i = 2.76$  Å,  $\text{C7}-\text{H7}\cdots\text{centroid}(\text{C1}-\text{C6}) = 161.7^\circ$ ; symmetry code: (i)  $3/2-x, 1/2-y, 1/2+z$ ]. In addition, edge-to-face arrangements between adjacent molecules give rise to further  $\text{C}-\text{H}\cdots\pi$  interactions in which the double bond of the alkene unit acts as an acceptor [ $\text{H8A}\cdots\text{centroid}(\text{C7}-\text{C8})^{ii} = 3.26$  Å,



**Figure 1**  
The molecular structure and atom-labelling scheme showing displacement ellipsoids for non-H atoms at the 50% probability level (*XP*; Sheldrick, 1993).



**Figure 2**  
Projection on to (100) of a single layer of (I), showing C—H... $\pi$  interactions as dotted lines (*CAMERON*; Watkin *et al.*, 1996).



**Figure 3**  
Projection of (I) on to (010) (*CAMERON*; Watkin *et al.*, 1996).

$C8-H8A \cdots \text{centroid}(C7-C8)^{ii} = 160.6^\circ$ ; symmetry code: (ii)  $x, -y, 1/2+z$ . The directional nature of C—H... $\pi$  interactions in organic crystals has been established previously (Umezawa *et al.*, 1998). The two sets of interactions may be considered to link the molecules into layers parallel to the (100) plane (Fig. 2). Adjacent layers are stacked along the *a* direction (Fig. 3).

*Note added to proof:* this work and the preceding study of Yasuda *et al.* (2001) were carried out independently.

## Experimental

The sample (99%) was obtained from the Aldrich company and was used without further purification. The crystal was grown in a 0.3 mm glass capillary tube at *ca* 220 K (a temperature only slightly less than the melting point of the solid in the capillary tube) using a technique described previously (Davies & Bond, 2001). Once grown, the crystal was cooled to 120 (2) K for data collection. The length of the cylindrical crystal could not be measured accurately but it exceeded the diameter of the collimator (0.35 mm).

### Crystal data

$C_8H_8$   
 $M_r = 104.14$   
Orthorhombic, *Pbcn*  
 $a = 15.6898$  (6) Å  
 $b = 10.5854$  (4) Å  
 $c = 7.5745$  (2) Å  
 $V = 1257.99$  (8) Å<sup>3</sup>  
 $Z = 8$   
 $D_x = 1.100$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
Cell parameters from 4669 reflections  
 $\theta = 1.0$ – $27.5^\circ$   
 $\mu = 0.06$  mm<sup>-1</sup>  
 $T = 120$  (2) K  
Cylinder, colourless  
0.15 mm (radius)

### Data collection

Nonius KappaCCD diffractometer  
Thin-slice  $\omega$  and  $\varphi$  scans  
Absorption correction: none  
2559 measured reflections  
1411 independent reflections  
1111 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.020$   
 $\theta_{max} = 27.4^\circ$   
 $h = -20 \rightarrow 20$   
 $k = -13 \rightarrow 13$   
 $l = -9 \rightarrow 9$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.038$   
 $wR(F^2) = 0.100$   
 $S = 1.06$   
1411 reflections  
105 parameters  
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0488P)^2 + 0.1803P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.14$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.14$  e Å<sup>-3</sup>

All H atoms were located in difference Fourier maps and allowed to refine freely with independent isotropic displacement parameters.

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: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Sheldrick, 1993) and *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *SHELXL97*.

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