

Styrene at 83 K

Nobuhiro Yasuda, Hidehiro Uekusa* and Yuji Ohashi

Department of Chemistry and Materials Science,
Tokyo Institute of Technology, O-okayama,
Meguro-ku, Tokyo 152-8551, Japan

Correspondence e-mail:
uekusa@cms.titech.ac.jp

Key indicators

Single-crystal X-ray study

$T = 83$ K

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

R factor = 0.039

wR factor = 0.099

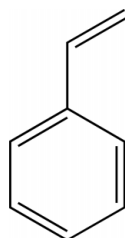
Data-to-parameter ratio = 13.5

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

The single crystal of the title compound, C_8H_8 , was obtained by *in situ* crystallization. The torsion angle between the phenyl ring and the vinyl group is 7.82 (17)°. The double-bond length in the vinyl group is 1.3245 (16) Å, which is slightly shorter than a normal $\text{C}=\text{C}$ double bond.

Comment

Styrene, (I), is one of the most widely used compounds in synthetic polymer science and theoretical calculations. Thus, determination of the crystal structure of styrene is very important to establish its chemical properties and to compare it with the structure derived by theoretical calculation. However, the crystal structure has not yet been reported because styrene is liquid at room temperature (m.p. 242.5 K). In this study, a single crystal of styrene was obtained by the *in situ* crystallization method, and the crystal structure was determined by the single-crystal X-ray diffraction method at 83 K.



(I)

The molecular structure is nearly planar, the torsion angle between the phenyl ring and the vinyl group being 7.82 (17)°. The $\text{C}7=\text{C}8$ vinyl double bond is 1.3245 (16) Å. These values are almost the same as those in 4-vinylbenzoic acid, 9.06 (16)° and 1.3248 (14) Å at 108 K, respectively (Yasuda *et al.*, 2000). However, these vinyl bond lengths are slightly shorter than the normal $\text{C}=\text{C}$ double-bond length of 1.34 Å.

Note added to proof: this work and the following study of Bond & Davies (2001) were carried out independently.

Experimental

The title compound, (I), was purchased from Aldrich Chemical Company Inc. A single crystal was obtained by the *in situ* crystallization method (Boese & Nussbaumer, 1994) in a 0.3 mm diameter glass capillary and was cooled to 83 K by the nitrogen gas flow method for data collection.

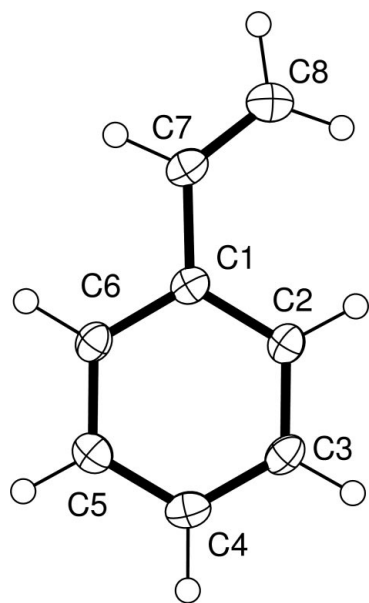


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

Crystal data

C_8H_8
 $M_r = 104.14$
 Orthorhombic, $Pbcn$
 $a = 15.6757$ (12) Å
 $b = 10.4805$ (8) Å
 $c = 7.5277$ (6) Å
 $V = 1236.72$ (17) Å³
 $Z = 8$
 $D_x = 1.119$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 11 393 reflections
 $\theta = 3.6$ – 27.5°
 $\mu = 0.06$ mm⁻¹
 $T = 83$ (2) K
 Cylindrical, colorless
 Radius: 0.3 mm

Data collection

Rigaku R-AXIS RAPID Imaging
 Plate diffractometer
 φ scans
 Absorption correction: none
 11 393 measured reflections
 1417 independent reflections

1255 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.059$
 $\theta_{max} = 27.5^\circ$
 $h = -19 \rightarrow 20$
 $k = -13 \rightarrow 12$
 $l = -9 \rightarrow 9$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.099$
 $S = 1.04$
 1417 reflections
 105 parameters
 All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0404P)^2 + 0.3865P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.19$ e Å⁻³
 $\Delta\rho_{min} = -0.18$ e Å⁻³

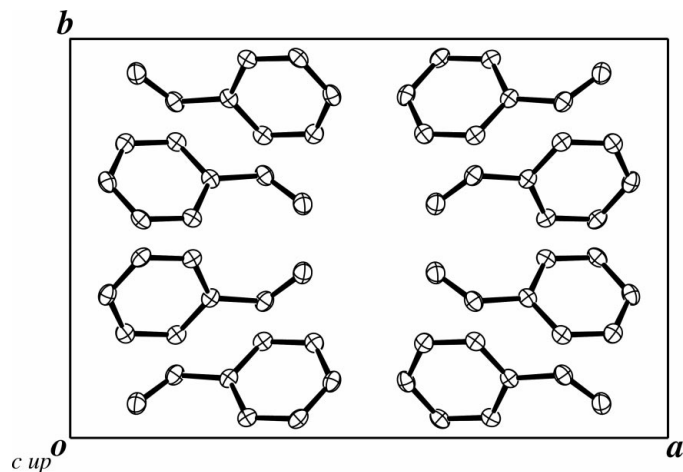


Figure 2
The crystal packing of (I), viewed along the c axis. H atoms have been omitted.

Table 1

Selected geometric parameters (Å, °).

C1–C6	1.3951 (14)	C3–C4	1.3922 (16)
C1–C2	1.4017 (14)	C4–C5	1.3882 (15)
C1–C7	1.4737 (14)	C5–C6	1.3901 (14)
C2–C3	1.3878 (14)	C7–C8	1.3245 (16)
C2–C1–C7–C8	7.82 (17)		

All H atoms were located from difference Fourier maps. Their positional and isotropic displacement parameters were refined. The C–H bond lengths are 0.968 (16)–1.008 (14) Å.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *TEXSAN* (Rigaku, 1999); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* for Windows (Farrugia, 1998); software used to prepare material for publication: *SHELXL97*.

References

- Altomare, A., Burla, M. C., Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
- Boese, R. & Nussbaumer, M. (1994). *Correlations, Transformations, and Interactions in Organic Crystal Chemistry*, edited by D. W. Jones and A. Katrusiak, pp. 20–37. Oxford: Oxford University Press.
- Bond, A. D. & Davies, J. E. (2001). *Acta Cryst.* **E57**, o1191–o1193.
- Farrugia, L. J. (1998). *ORTEP3* for Windows. University of Glasgow, Scotland.
- Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
- Rigaku (1999). *TEXSAN*. Version 1.10. Rigaku Corporation, Tokyo, Japan.
- Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
- Yasuda, N., Uekusa, H. & Ohashi, Y. (2000). *Acta Cryst.* **C56**, 1364–1366.