

Table 1. Fractional coordinates of atoms with e.s.d.'s

$$U_{eq} = \frac{1}{3}(U_{11} + U_{22} + U_{33}).$$

	x	y	z	$U_{eq}(\text{\AA}^2)$
Si(1)	0.2947 (6)	0.0490 (4)	0.2500	0.065 (4)
Si(2)	0.2056 (5)	0.2116 (4)	0.329 (2)	0.065 (4)
Si(3)	0.5000	0.2257 (6)	0.725 (3)	0.063 (6)
Si(4)	0.5000	0.1234 (6)	0.225 (3)	0.063 (6)
O(11)	0.2722 (15)	0.9815 (12)	0.461 (3)	0.070 (12)
O(12)	0.2285 (13)	0.1203 (10)	0.323 (4)	0.073 (10)
O(14)	0.4059 (12)	0.0731 (10)	0.278 (4)	0.066 (11)
O(22)	0.2722 (14)	0.2580 (14)	0.118 (4)	0.073 (13)
O(23)	0.4075 (12)	0.2780 (10)	0.776 (4)	0.077 (12)
O(34)	0.5000	0.1554 (16)	0.917 (5)	0.069 (16)
O(43)	0.5000	0.1966 (15)	0.423 (4)	0.063 (16)

all atoms, and weights $1/[\sigma^2(F) + 0.00012F^2]$, giving, for the larger data set, *i.e.* the merged data for two orientations, $R = 0.116$ ($wR = 0.13$) for 394 reflections with $F > 6\sigma(F)$. Atom parameters are listed in Table 1.* An alternative refinement, using the first data set, *i.e.* for the crystal of lower rocking width only, gave $R = 0.080$ ($wR = 0.09$), but the atom parameters were not significantly different and the e.s.d.'s were larger.

The relatively high R values can be explained by a number of factors, including the large mosaic spread and the camera geometry (Andrews *et al.*, 1988).

Results, comparison with powder diffraction study

Our results are in agreement, within 0.1–0.15 Å, with the structure as illustrated in the *c*-axis projection by Highcock, Smith & Wood (1985), but indicate substantial revision of some of the *z* coordinates, Si(3) and Si(4) by 0.5 Å, O(22), O(34) and O(43) by up to 1.5 Å. This does not alter the description of the structure as a three-

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52102 (5 pp.). Copies may be obtained through the Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Acta Cryst. (1990). **C46**, 173

Structure of α -trans-cinnamic acid. Addendum. By DERK A. WIERDA, TIMOTHY L. FENG and ANDREW R. BARRON,* *Department of Chemistry, Harvard University, Cambridge, Massachusetts 02138, USA*

(Received 2 October 1989)

Abstract

An addendum [Wierda, Feng & Barron (1989). *Acta Cryst.* **C45**, 838] of a recent report of a determination of the structure of the title compound [Wierda, Feng & Barron (1989). *Acta Cryst.* **C45**, 338–339] drew attention to a reference

* To whom correspondence should be addressed.

Table 2. Selected bond lengths (Å) and angles (°)

Si(1)—O(11)	1.61 (2)	Si(3)—O(23)	1.59 (2)
Si(1)—O(11 ^{iv})	1.58 (2)	Si(3)—O(23 ^v)	1.59 (2)
Si(1)—O(12)	1.59 (2)	Si(3)—O(34)	1.56 (2)
Si(1)—O(14)	1.60 (2)	Si(3)—O(43)	1.61 (2)
Si(2)—O(12)	1.62 (2)	Si(4)—O(14)	1.59 (2)
Si(2)—O(22)	1.62 (2)	Si(4)—O(14 ^{iv})	1.65 (2)
Si(2)—O(22 ^{iv})	1.59 (2)	Si(4)—O(34 ^{iv})	1.62 (2)
Si(2)—O(23)	1.60 (2)	Si(4)—O(43)	1.65 (2)
Si(1)—O(11)—Si(1 ⁱ)	144.3 (1.3)	Si(2)—O(22 ^{iv})—Si(2 ^{iv})	151.7 (1.5)
Si(1)—O(12)—Si(2)	152.2 (1.4)	Si(2 ^{iv})—O(23)—Si(3)	151.5 (1.4)
Si(1)—O(14)—Si(4)	156.1 (1.3)	Si(3)—O(34)—Si(4 ^{iv})	148.1 (1.5)
		Si(3)—O(43)—Si(4)	146.4 (1.4)

Symmetry code: (i) $x, -y, \frac{1}{2} + z$; (ii) $\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} + z$; (iii) $x, y, 1 + z$; (iv) $x, -y, -\frac{1}{2} + z$; (v) $1 - x, y, z$; (vi) $x, y, -1 + z$.

dimensional network of SiO₄ tetrahedra, sharing all corners, in such a way that there are large channels parallel to *c*. The revised Si and O atom positions do not differ significantly from those derived in a single-crystal study of silica-ZSM-22, 24SiO₂(C₂H₅)₂NH (Marler, 1987), but the present material contains no organic guest molecules. Selected bond lengths and angles are given in Table 2.

We are grateful to SERC Daresbury Laboratory for the provision of synchrotron-radiation facilities, and to Dr J. R. Helliwell for helpful advice.

References

- ANDREWS, S. J., PAPIZ, M. Z., McMEEKING, R., BLAKE, A. J., LOWE, B. M., FRANKLIN, K. R., HELLIWELL, J. R. & HARDING, M. M. (1988). *Acta Cryst.* **B44**, 73–77.
 HIGHCOCK, R. M., SMITH, G. W. & WOOD, D. (1985). *Acta Cryst.* **C41**, 1391–1394.
 MARLER, B. (1987). *Zeolites*, **7**, 393–397.
 MESSERSCHMIDT, A. & PFLUGRATH, J. W. (1987). *J. Appl. Cryst.* **20**, 306–315.
 SHELDRIK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.
 SHELDRIK, G. M. (1986). *SHELX86*. Program for crystal structure determination. Univ. of Göttingen, Federal Republic of Germany.

[Bryan & Freyberg (1975). *J. Chem. Soc. Perkin Trans. 2*, pp. 1835–1840] overlooked by the authors in their original report. The addendum failed to make clear that this reference contained a report of a complete room-temperature determination of the crystal structure in question. The two structures are in good agreement, except for variations attributed to differences in temperature.

All relevant information is contained in the *Abstract*.

International Union of Crystallography

Acta Cryst. (1990). C46, 174

Commission on Journals

Criteria for Acceptance in Sections B and C of *Acta Crystallographica*

Papers submitted for publication in Section B of *Acta Crystallographica* should meet the following general criteria:

1. The paper must contain a major structural element. Some examples of this component are: an original determination of one or more structures, along with significant discussion of the structural implications; a structure studied at more than one pressure or temperature; a theoretical structural investigation including new methodology; or a study of structural relationships based on a search of the literature.
2. The paper should also present a significant experimental and/or theoretical contribution to one of the natural sciences.
3. The paper should combine the above types of contribution to provide new structural insight.
4. Papers reporting work on a **single compound** are suitable for Section B as long as criteria 2 and 3 are met.
5. Papers reporting work on **more than one compound** are acceptable either in Section B if criteria 2 and 3 are met or in Section C otherwise.