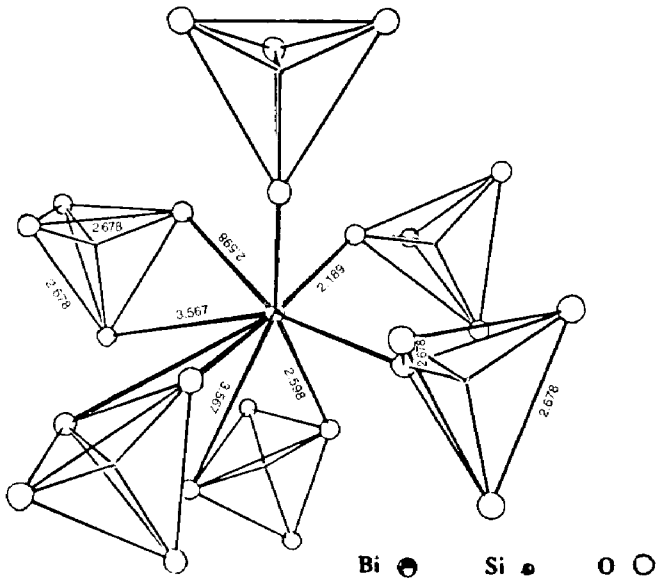
Crystal structure of bismuth(III) silicate, $Bi_4(SiO_4)_3$

H. Liu and C. Kuo

Chinese Academy of Sciences, Shanghai Institute of Ceramics, Shanghai, 200050, P. R. China

Received December 12, 1995, transferred to 1st update of database ICSD in 1997, CSD-No. 402349



Source of material: The sample was synthesized by solid reaction of Bi_2O_3 and SiO_2 at 1273 K. The specimen for diffraction study was prepared by grinding the powder manually and passing it through a 400 mesh sieve.

Eulytite, $Bi_4(SiO_4)_3$, isostructural with $Bi_4(GeO_4)_3$, is promised to be a latent scintillation crystal. However, both crystal structures have not been revealed clearly. Two possible structures were proposed by Menzer (see ref. 1). Segal (see ref. 2) showed one of them was correct by Neutron powder diffraction. The displacement parameters and details of the structure were not reported.

In this structure, the SiO_4 tetrahedra are isolated but distorted, although the bond lengths of the four Si–O bonds are equal (1.613 Å). Two of the O–O bond lengths in the tetrahedra are 2.678 Å as labelled, and the other two are 2.595 Å (unlabelled); thus, two of the O–Si–O angles are 107.13° and 114.26° in the tetrahedra. This distortion may be attributed to the stereochemically active lone pair $6s^2$ of Bi^{3+} ion.

Table 1. Parameters used for the X-ray data collection

Powder:	white
Wavelength:	Cu K_α radiation (1.54183 Å)
μ:	1203.4 cm^{-1}
Diffractometer:	RIGAKU D/MAXIIIB
Sample geometry:	Flat
Scan mode:	2θ
Stepwidth:	0.02°
$T_{measurement}$:	293 K
$2\theta_{max}$:	120°
$N((points))_{meas}$:	5000
$N(param)_{refined}$:	25
Profile function:	Pseudo-Voigt
Background correction:	4th order polynomial
Program:	Rietveld DBWS9411

Table 2. Final atomic coordinates and displacement parameters (in $Å^2$)

Atom	Site	x	y	z	U_{iso}
O	48*e*	0.0590(7)	0.1310(6)	0.2889(6)	0.53(1)
Si	12*a*	3/8	0	1/4	0.180(8)
Bi	16*c*	0.0849	x	x	0.68(1)

$Bi_4O_{12}Si_3$, cubic, $I\bar{4}3d$ (No. 220), a =10.2867(5) Å, V =1088.5 $Å^3$, Z =4, Rp =0.084, R_w =0.118, R_{Bragg} =0.047, R_{exp} =0.048.

References

1. Menzer, G.: Die Kristallstruktur von Eulytin. Z. Kristallogr. **78** (1931) 136-163.
2. Segal, D. J.; Santoro, R.-P.; Newnham, R. E.: Neutron-diffraction study of $Bi_4(SiO_4)_3$. Z. Kristallogr. **123** (1966) 73-76.
3. Vickovic, I.: ORTEP92 program - an improved PC version. J. Appl. Crystallogr. **27** (1994) 437.