Crystal structure of the new barium zinc silicate $Ba_2ZnSi_2O_7$

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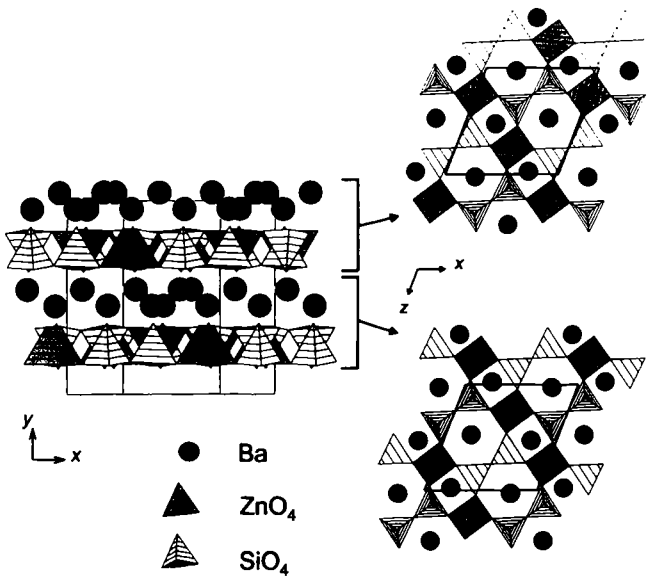

Abstract

$Ba_2O_7Si_2Zn$, monoclinic, $C12/c1$ (No. 15), $a = 8.434(2)$ Å, $b = 10.722(2)$ Å, $c = 8.436(2)$ Å, $\beta = 111.30(3)°$, $V = 710.8$ Å^3, $Z = 4$, $R_{gt}(F) = 0.020$, $wR_{ref}(F^2) = 0.048$, $T = 293$ K.

Source of material

$Ba_2ZnSi_2O_7$ was prepared in the presence of a salt flux (NaCl/KCl) by heating 0.5 g of a mixture of the oxides BaO, ZnO, and SiO_2 with the atomic ratio 2:1:2 with 2 g of the flux in an open silica tube for 3 days at 1073 K. The salt-matrix was dissolved in water. An energy dispersive X-ray fluorescence analysis for elements heavier than sodium revealed only barium, zinc, and silicon.

Discussion

The structure consists of ZnO_4 tetrahedra which share their oxygen atoms with those of the Si_2O_7 groups, thus forming two-dimensionally infinite sheets which are separated by the barium atoms. The barium atoms have eight oxygen neighbors with Ba—O distances ranging from 268.9(1) pm to 293.8(1) pm with an average distance of 281.3 pm. The Zn—O distances amount to 194.9(1) pm and 197.2(1) pm with an average of 196.0 pm. The Si—O distances are in between 160.3(1) pm and 167.3(1) pm with an average of 163.0 pm. All of these average distances are in good agreement with the corresponding distances calculated from the data given by Shannon [1] with Ba—O: 280 pm, Zn—O: 198 pm, Si—O: 164 pm. All of the four different oxygen atoms have four cationic neighbors: O1 (1Si + 3Ba), O2 (1Si + 1Zn + 2Ba), O3 (1Si + 1Zn + 2Ba), and O4 (2Si + 2Ba). $Ba_2ZnSi_2O_7$ is only the third compound with this monoclinic layered structure. The others are $Ba_2CoSi_2O_7$ [2] and $Ba_2CuSi_2O_7$ [3]. Most disilicates with the analogous composition $A_2TSi_2O_7$ (A = alkaline earth metal, T = late transition metal) crystallize with melilite $(Ca,Na,K)_2(Mg,Fe,Al)[(Si,Al)_2O_7]$ type structure, e.g., $Ca_2CoSi_2O_7$ [4], $Sr_2CoSi_2O_7$ [4], and $Ca_2ZnSi_2O_7$ [5].

Table 1. Data collection and handling.

Crystal:	white, irregular, size 0.04 × 0.04 × 0.04 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	146.4 cm^{-1}
Diffractometer, scan mode:	Enraf-Nonius CAD4, $\omega/2\theta$
$2\theta_{max}$:	70.24°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4890, 1565
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1408
$N(param)_{refined}$:	57
Programs:	SHELXL-97 [6], DIAMOND [7], STRUCTURE TIDY [8]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ba(1)	8*f*	0.22600(1)	0.042667(7)	0.473812(9)	0.00942(3)	0.00676(3)	0.00904(2)	0.00002(2)	0.00367(2)	-0.00050(2)
Zn(1)	4*e*	0	0.74136(2)	1/4	0.00859(8)	0.00787(9)	0.00758(6)	0	0.00295(6)	0
Si(1)	8*f*	0.11403(5)	0.28212(4)	0.13705(4)	0.0070(1)	0.0053(1)	0.0064(1)	-0.0001(1)	0.00289(9)	-0.0002(1)
O(1)	8*f*	0.1099(1)	0.1327(1)	0.1321(1)	0.0139(4)	0.0060(4)	0.0137(3)	0.0005(3)	0.0068(3)	0.0003(3)
O(2)	8*f*	0.3002(1)	0.3431(1)	0.2344(1)	0.0068(3)	0.0086(4)	0.0109(3)	-0.0009(3)	0.0013(3)	-0.0011(3)
O(3)	8*f*	0.4716(1)	0.1472(1)	0.0439(1)	0.0126(4)	0.0086(4)	0.0071(3)	0.0004(3)	0.0022(3)	-0.0005(3)
O(4)	4*e*	0	0.3332(2)	1/4	0.0154(5)	0.0098(6)	0.0139(4)	0	0.0109(4)	0

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