

Author's Accepted Manuscript

Thermal expansion and structural complexity of Ba silicates with tetrahedrally coordinated Si atoms

Liudmila A. Gorelova, Rimma S. Bubnova, Sergey V. Krivovichev, Maria G. Krzhizhanovskaya, Stanislav K. Filatov



PII: S0022-4596(15)30280-2
DOI: <http://dx.doi.org/10.1016/j.jssc.2015.12.012>
Reference: YJSSC19201

To appear in: *Journal of Solid State Chemistry*

Received date: 8 October 2015
Revised date: 8 December 2015
Accepted date: 10 December 2015

Cite this article as: Liudmila A. Gorelova, Rimma S. Bubnova, Sergey V. Krivovichev, Maria G. Krzhizhanovskaya and Stanislav K. Filatov, Thermal expansion and structural complexity of Ba silicates with tetrahedrally coordinated Si atoms, *Journal of Solid State Chemistry*, <http://dx.doi.org/10.1016/j.jssc.2015.12.012>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Thermal expansion and structural complexity of Ba silicates with tetrahedrally coordinated Si atoms

Liudmila A. Gorelova^{a,b,*}, Rimma S. Bubnova^{a,b}, Sergey V. Krivovichev^{a,b},
Maria G. Krzhizhanovskaya^b, Stanislav K. Filatov^b

^a*Institute of Silicate Chemistry, Russian Academy of Sciences, Makarova Emb. 6, 199034 St. Petersburg, Russia*

^b*Department of Crystallography, Institute of Earth Sciences, Saint-Petersburg State University, University Emb. 7/9, 199034 St. Petersburg, Russia*

Abstract

Thermal expansion of Ba silicates with tetrahedrally coordinated Si atoms in the temperature range of 25–1100 °C had been studied by high-temperature X-ray powder diffraction. The volume thermal expansion coefficients (TECs) are in the range $41\text{--}50 \times 10^{-6} \text{ }^\circ\text{C}^{-1}$ with an average value of $\langle \alpha_V \rangle = 45 \times 10^{-6} \text{ }^\circ\text{C}^{-1}$. In the structures with chain and layered silicate anions, thermal expansion is anisotropic: the direction of maximal TEC is parallel to the extension of the *zweier* chains of silicate tetrahedra, which are strained owing to the interactions with Ba^{2+} . The strain is released during thermal expansion due to the increasing effective size of Ba^{2+} cations induced by thermal vibrations. Information-theoretic analysis of the structural and topological complexities of Ba silicates indicates that their structural complexity is a function of the topological complexity of their silicate anions. The latter displays a non-linear behaviour with increasing SiO_2 content (= the increasing degree of polymerization and increasing dimensionality): it starts from simple topologies, reaches a maximum at topologies of intermediate complexity, and ends up at simple topologies again. The specificity of the interactions of Ba^{2+} with the silicate anions results in higher complexity of high-temperature $\alpha\text{-BaSi}_2\text{O}_5$ compared to that of low-temperature $\beta\text{-BaSi}_2\text{O}_5$. This uncommon behaviour may be explained by

*Corresponding author

Email address: gorelova.ljudmila@gmail.com (Liudmila A. Gorelova)

Download English Version:

<https://daneshyari.com/en/article/7758385>

Download Persian Version:

<https://daneshyari.com/article/7758385>

[Daneshyari.com](https://daneshyari.com)