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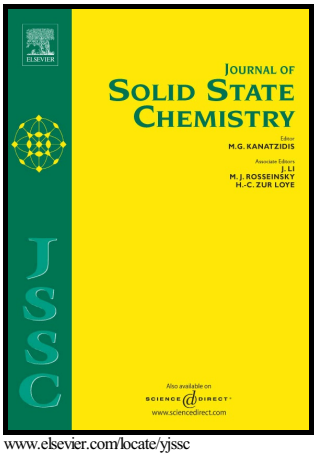

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Thermal expansion and structural complexity of Ba silicates with tetrahedrally coordinated Si atoms

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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 41–50×10^{-6} °C^{-1} with an average value of $<\alpha_V> = 45\times10^{-6}$ °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 α-$BaSi_2O_5$ compared to that of low-temperature β-$BaSi_2O_5$. This uncommon behaviour may be explained by

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