

## SINGLE-CRYSTAL X-RAY DIFFRACTION STUDY OF Cs<sub>2</sub>Er[Si<sub>6</sub>O<sub>14</sub>]F AND Cs<sub>2</sub>Er[Si<sub>4</sub>O<sub>10</sub>]F

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Single-crystal growth experiments in the system CsF-Er<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> resulted in the simultaneous crystallization of two chemically related compounds within the same run: Cs<sub>2</sub>Er[Si<sub>6</sub>O<sub>14</sub>]F (phase I) and Cs<sub>2</sub>Er[Si<sub>4</sub>O<sub>10</sub>]F (phase II). They represent the first examples for cesium erbium silicates containing fluorine.

Basic crystallographic data of the two structures at ambient conditions are as follows: phase I: space group *Cmca*,  $a = 17.2556(6)$  Å,  $b = 24.6565(7)$  Å,  $c = 14.4735(5)$  Å,  $V = 6157.9(3)$  Å<sup>3</sup>,  $Z = 16$ ; phase II: space group *Pnma*,  $a = 22.3748(7)$  Å,  $b = 8.8390(2)$  Å,  $c = 11.9710(4)$  Å,  $V = 2367.5(1)$  Å<sup>3</sup>,  $Z = 8$ . The structures were determined by direct methods and refined to residuals of  $R(|F|) = 0.0229$  for 2920 (phase I) and 0.0231 for 2314 (phase II) independent observed reflections with  $I > 2\sigma(I)$ .

The structure of phase I forms a three dimensional tetrahedral framework consisting of Q<sup>3</sup> and Q<sup>4</sup> groups in the ratio 2:1. Basic building units of the network are unbranched *sechser* single-chains running parallel to [001]. The network can be conveniently built up from the condensation of tetrahedral layers parallel to (010) or (100), respectively.

The crystal structure of phase II can be classified as a *tubular* or *columnar* chain silicate indicating that the backbones of the structure are multiple chains of silicate tetrahedra. The multiplicity of the loop-branched chains is two. The periodicity of the chains has a value of four which is also reflected in the translation periods parallel to the chain direction:  $t_{(010)} = 8.839$  Å.

Alternatively, both compounds can be described as mixed octahedral-tetrahedral frameworks, which can be classified according to their *polyhedral microensembles*. A topological analysis of both nets is presented.