

**K<sub>2</sub>CaSi<sub>4</sub>O<sub>10</sub> – A PREVIOUSLY UNKNOWN CRYSTALLINE PHASE IN THE TERNARY SYSTEM K<sub>2</sub>O-CaO-SiO<sub>2</sub>**

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In the course of a systematic re-investigation of the ternary oxide system K<sub>2</sub>O-CaO-SiO<sub>2</sub> a new potassium calcium silicate with the chemical composition K<sub>2</sub>CaSi<sub>4</sub>O<sub>10</sub> was discovered within the products of solid state reactions aimed at the synthesis of K<sub>4</sub>CaSi<sub>6</sub>O<sub>15</sub>. By applying direct methods the crystal structure of K<sub>2</sub>CaSi<sub>4</sub>O<sub>10</sub> was solved from single-crystal X-ray diffraction data. The compound crystallizes in the triclinic space group *P*-1. Its unit cell is defined by the following lattice parameters: *a* = 7.0915(7) Å, *b* = 8.4211(9) Å, *c* = 10.2779(12) Å,  $\alpha$  = 104.491(10)°,  $\beta$  = 100.570(9)° and  $\gamma$  = 113.738(11)°. K<sub>2</sub>CaSi<sub>4</sub>O<sub>10</sub> is isotypic with the minerals litidionite, fenaksite and manaksite (BRANDAO et al., 2009). Loop-branched *dreier* double-chains of [SiO<sub>4</sub>]-tetrahedra running along [100] are connected via dimers of irregularly coordinated edge-sharing [CaO<sub>5</sub>]-polyhedra. Potassium cations are located within cavities of the heteropolyhedral framework. However, the channels within the silicate double-chains remain unoccupied.

K<sub>2</sub>CaSi<sub>4</sub>O<sub>10</sub> further enlarges the knowledge of the system K<sub>2</sub>O-CaO-SiO<sub>2</sub>, which is of interest for process technology in the fields of biomass combustion (BERJONNEAU et al., 2009).

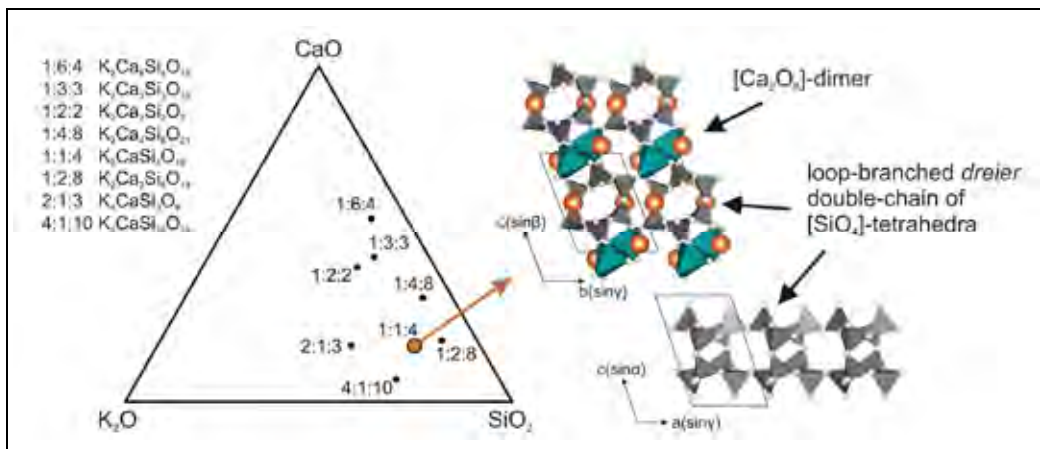


Figure 1. Ternary plot of the system K<sub>2</sub>O-CaO-SiO<sub>2</sub> showing the composition [in mol%] of all ternary phases with known crystal structure and details of the crystal structure of K<sub>2</sub>CaSi<sub>4</sub>O<sub>10</sub>.

BERJONNEAU, J., COLOMBEL, L., POIRIER, J., PICHAVANT, M., DEFOORT, F., SEILER, J.-M. (2009): Energy Fuels, 23, 6231-6241.

BRANDAO, P., ROCHA, J., REIS, M.S., DOS SANTOS, A.M., JIN, R. (2009): J. Solid State Chem., 182, 253-258.