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Structural variations across the nepheline ($NaAlSiO_4$)–kalsilite ($KAlSiO_4$) series

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Abstract

The crystal structures of 19 samples from the nepheline ($NaAlSiO_4$; Ne)–kalsilite ($KAlSiO_4$; Ks) series, previously prepared via ion-exchange, were examined using synchrotron high-resolution powder X-ray diffraction (HRPXRD) data and Rietveld structure refinements. Parent materials for the three series include a natural Monte Somma nepheline (series-1), synthetic Na nepheline (series-2), and high-Si synthetic nepheline (series-3), having excess Si mole percentages of 5.2, 1.7, and 12.5%, respectively. Three different structure-types were found to occur among the samples examined: nepheline ($P6_3$), tetrakalsilite ($P6_3$), and kalsilite (both $P6_3$ and $P31c$ intergrowth). Trikalsilite was not observed in this study. Vacancies (□) at the K site as well as Ca and K atoms at the Na1 site play an important role in the crystal-chemical behavior of nepheline solid solutions. Vacancies cause an elongation in the average <K-O>[9] distance in nepheline. When K atoms enter the Na1 site in nepheline, the average <(Na,K)-O>[7] distance increases linearly and is parallel to the average <(Na,K)-O>[9] distance in kalsilite and the grand mean of such distances in trikalsilite and tetrakalsilite. Before K atoms enter the Na1 site, the average <(Na,K)-O>[7] distance is constant because of the full occupancy of the Na1 site with Na atoms. Ca atoms at the Na1 site in the Monte Somma sample-1 cause a contraction in the <(Na,K)-O>[7] distance. In Na-rich nepheline samples, Na atoms in the large channels occupy a Na(K) site that is off the 6_3 axis and close to the usual K site. In natural nepheline samples, the K site in most cases contains K atoms and □, and the Na1 site is filled mainly with Na, minor Ca, and K atoms in K-rich samples. Nepheline from Monte Somma (sample-1) contains weak satellite reflections that are also present in some other kalsilite samples. Average <*T*-O> distances indicate a high degree of Al-Si disorder in nepheline but increasing Al-Si order in tetrakalsilite and kalsilite. Increasing the amount of K atoms beyond the ideal composition of $K_{0.25}Na_{0.75}[AlSiO_4]$ causes expansion in multiple structural parameters because of the larger size of K^+ relative to Na^+.

Keywords: Nepheline-kalsilite series, crystal structure, Al-Si order, HRPXRD, satellite reflections