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Sodalite: High-temperature structures obtained from synchrotron radiation and Rietveld refinements

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ABSTRACT

The structural behavior of sodalite, ideally $Na_8[Al_6Si_6O_{24}]Cl_2$, at room pressure and from 28 to 982 °C on heating, was determined by using in situ synchrotron X-ray powder diffraction data (λ = 0.92007(4) Å) and Rietveld refinement. The sample was heated at a rate of about 9.5 °C/min and X-ray spectra were collected at intervals of about 15 °C. The cubic unit-cell parameter for sodalite increases smoothly and non-linearly to 982 °C. The percent volume change between 28 and 982 °C is 4.8(2)%. Between 28 and 982 °C, the Al-O and Si-O distances are constant, while the Al-O-Si angle increases from 138.29(1) to 146.35(2)° by 5.06(2)°. Simultaneously, the angle of rotation of the AlO_4 tetrahedron, φ_{Al}, decreases from 22.1 to 16.9°, a difference of 5.2°, while the angle of rotation of the SiO_4 tetrahedron, φ_{Si}, decreases from 23.6 to 18.0°, a difference of 5.6°. Moreover, the $[Na_4Cl]^{3+}$ clusters expand with increases in the Na-Cl bond length by 0.182(4) Å, and corresponding increases in the short Na-O bond length by 0.093(2) Å, and decreases in the longer Na-O* distance by 0.108(1) Å. Large displacement parameters occur for the Na and Cl atoms, and as the weaker Na-Cl bond expands with temperature, the Na atoms move toward the plane of the framework six-membered rings, which causes the framework tetrahedra to rotate and results in a relatively high rate of expansion of the structure. The framework TO_4 tetrahedra distort slightly with temperature. If the Na atom reaches approximately the plane of the six-membered ring, the expansion will be retarded, but sodalite melts before this occurs. Sodalite melts at about 1079 °C and begins to lose NaCl. The NaCl component is lost in two stages: about 4.5 wt% of NaCl is lost slowly at about 1150 °C, and about 7.0 wt% of NaCl is lost at a faster rate at about 1284 °C.