

Raman spectroscopy and vibrational analyses of albite: From 25 °C through the melting temperature

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ABSTRACT

Raman spectra were collected for crystalline albite from 25 °C to above the 1118 °C melting temperature, where vibrational assignments for the crystal spectra were determined by lattice dynamics (LD). The Raman spectra and associated vibrational assignments are reported for triclinic albite ($\text{NaAlSi}_3\text{O}_8$) at 25 °C and monoclinic albite at 1060 °C. The 25 °C calculations determined that localized T-O stretch and O-T-O bend modes are above 900 cm^{-1} (where T = Si,Al), while motions from the aluminosilicate tetrahedral cage mixed with Na displacements occur in modes as high as 814 cm^{-1} . Vibrational modes for the most prominent peaks in the spectrum, between 350 and 550 cm^{-1} , are dominated by four-membered tetrahedral ring deformations. For completeness, calculated infrared mode frequencies and their atomic displacements are reported for the 25 °C structure and compared with normal mode calculation results and observed infrared mode frequencies presented by von Stengel (1977). At higher temperatures, modes above 550 cm^{-1} broaden and shift to lower frequencies by 15 to 27 cm^{-1} ; modes below 550 cm^{-1} broaden, but experience little, if any frequency shifts. Albite melted sluggishly, was completely liquid at 1320 °C, and remained amorphous upon cooling to room temperature. At frequencies above 550 cm^{-1} , the crystalline albite peaks, and possibly their vibrational assignments, can be correlated to Raman bands for albite glass. Spectral differences below 550 cm^{-1} between crystal and glass correspond to changes of average tetrahedral ring type upon melting, as shown by Taylor and Brown (1979).