

High-temperature Raman spectroscopy of $\text{K}_2\text{Ca}(\text{CO}_3)_2$ bütschliite and $\text{Na}_2\text{Ca}_2(\text{CO}_3)_3$ shortite

GARRETT ZEFF^{1,*} AND QUENTIN WILLIAMS²

¹Shock & Detonation Physics, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, U.S.A.

²Department of Earth and Planetary Sciences, University of California, Santa Cruz, California 95064, U.S.A.

ABSTRACT

Raman spectra of $\text{Na}_2\text{Ca}_2(\text{CO}_3)_3$ shortite and $\text{K}_2\text{Ca}(\text{CO}_3)_2$ bütschliite were measured to 715 and 740 °C, respectively, under vacuum. The vibrational spectra demonstrate that shortite converts to nyerereite [$\text{Na}_2\text{Ca}(\text{CO}_3)_2$] and calcite at 535 °C. This assemblage remains stable up to ~700 °C, at which point nyerereite begins to decompose. Bütschliite converts to the isochemical phase fairchildite at 570 °C, which is stable to 665 °C, where it decomposes to an assemblage of K_2CO_3 and CaO. The variation of anharmonicity between different vibrational modes of each of the low-temperature phases is assessed, and these yield insights into inter-carbonate group couplings. Both fairchildite and nyerereite exhibit spectral features consistent with extensive disordering.

Keywords: Carbonate, high-temperature, Raman spectroscopy, carbonatite