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Trona at extreme conditions: A pollutant-sequestering material at high pressures and low temperatures

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Abstract

Single-crystal X-ray diffraction of trona, $Na_3CO_3HCO_3 \cdot 2H_2O$, was measured between 100 and 340 K at ambient pressures, and the infrared and Raman spectra of this material characterized to ~25 GPa. The thermal expansion of trona is greatest in the *b* direction, which is due to a particularly large expansion of the long Na_2-O_1 and the short Na_2-O_4 bonds within the sodium septahedron in the trona structure. This crystallographic direction is associated with the distance between neighboring carbonate groups and neighboring water molecules within the structure. The dimensions of the carbonate group undergo no systematic changes over this temperature range, and the disordered hydrogen atom within the structure does not order at temperatures down to 100 K. Thus, detailed changes in the geometry of the sodium polyhedra primarily modulate the response of trona to decreases in temperature. The infrared and Raman spectra undergo discontinuous and reversible changes at ~7 and ~14.5 GPa: the former of these phase transitions is likely associated with a shift primarily in the sodium-oxygen polyhedra, while the latter also involves shifts in bonding of the carbonate groups. New assignments are suggested for portions of the vibrational spectrum based on the high-pressure results. Resonance effects between different vibrational modes are observed, including the observation of a transmission maximum associated with a resonant interaction between the carbonate symmetric stretching vibration and a broad mode at similar frequencies. The behavior of trona under extreme conditions is useful for understanding CO_2-vapor-saturated alkali-rich systems, and late-stage peralkaline magmatic processes and, in its usage as both a sorbent and scrubber of SO_2 and CO_2 in flue gasses and lignite coals.

Keywords: Trona, high pressure, low temperature, single-crystal diffraction, vibrational spectroscopy