

Structure, stability and thermoelastic properties of CO₂-IV

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The study of solid CO₂ at elevated pressures and temperatures is important in geology, condensed matter physics and material science. Studies of high pressure, high temperature phases of solid CO₂ help to understand the forms that carbon may adopt at the pressures and temperatures of planetary interiors. Knowledge of these forms gives insight into the possible composition of carbon reservoirs in the deep earth, icy bodies of the outer solar system, and icy exoplanets. We conducted neutron diffraction experiments on CO₂-ice at high pressures and temperatures to determine its structure, stability and thermoelastic properties. These experiments used novel resistive heating techniques at the high pressure beamline at the Spallation Neutron Source at Oak Ridge National Laboratory (SNAP instrument). CO₂-IV was synthesized from CO₂-I starting material at ~18 GPa and 625 K, and found to be stable down to 300 K and up to pressure of 26 GPa, for run durations of up to 12 hours. This study confirmed the rhombohedral *R-3c* structure of CO₂-IV. Our measurements of lattice volumes in situ at high pressures and temperatures enable a high-precision determination of the thermoelastic properties including bulk modulus and thermal expansivity of CO₂-IV ice with respect to the CO₂-I starting material. The results indicate that resistively heated DAC experiments are possible using neutron diffraction and encourage the further development of heating systems for DAC experiments in these settings. This study is a first step toward expanding the range of DAC neutron diffraction experiments and compiling data to yield definitive thermoelastic properties for CO₂ phases.