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Phase Transitions and Water Interactions in Uranyl Fluoride ANDREW MISKOWIEC, MARIE KIRKEGAARD, JOHN LANGFORD, BRIAN ANDERSON, Oak Ridge National Laboratory — Uranyl fluoride (UO2F2) is a hygroscopic powder resulting from the hydrolysis of uranium hexafluoride (UF6). Crystal hydrates of the form UO2F2*x(H2O) have previously been identified with X-ray and neutron scattering, but phase transitions between different crystal hydrate structures have not been directly observed. In this work, we present a combined experimental and theoretical approach to determining crystal structures and vibrational modes. We use inelastic neutron scattering to probe vibrational frequencies of powder samples of anhydrous uranyl fluoride (x = 0, anh-UO2F2), and the most stable crystal hydrate (x = 0.4, partially hydrated (ph-UO2F2)). Combined with density functional theory (DFT), we identify and differentiate crystalline phonons and water-coupled phonon modes. Significant shifts in water O-H stretching frequencies are observed as well as lower-energy water librational modes due to water-crystal interactions. Finally, we use temperature-dependent Raman scattering with a custom sample cell, providing constant relative humidity environments, to observe phase transitions between the anhydrous and hydrated states of uranyl fluoride in situ.

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