Theoretical Characterization of Amorphous Solids and Carbonic Acid Clusters in the UV

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Ices in the interstellar medium largely exist as amorphous solids composed of small molecules including ammonia, water, and carbon dioxide. Gas-phase molecules can be readily analyzed with current high-level quantum chemical computations including crystalline solids. Differently, amorphous solids require more novel approaches. The present work describes a method for generating amorphous structures and constructing electronic spectra through a combination of quantum chemical calculations and statistical mechanics. The methodology can produce experimentally-comparable electronic spectra for ice analogs and can be used to predict electronic spectra for other ices. Most notably, the experimental UV spectrum of carbonic acid ice has not been fully explained. This work shows that amorphous carbonic acid appears to play a role in the experimental spectral behavior, but other cluster isomers, non-minimum perpendicular motifs in particular, provide the best comparisons to experiment for lower-energy transitions than the ribbon, helix, or even amorphous clusters of carbonic acid.