ANHARMONICITY AND DEUTERATION IN THE IR ABSORPTION AND EMISSION SPECTRA OF PHENYLACETYLENE

VINCENT J. ESPOSITO, *Planetary Systems Branch, NASA Ames Research Center, Moffett Field, CA, USA*.

Emission from polycyclic aromatic hydrocarbons (PAHs) is believed to dominate the infrared (IR) spectra of a wide variety of astronomical objects and environments. Quantum chemically computed PAH spectra, combined with experimental studies, are indispencible to analyze and interpret astronomical observations. To provide a foundation for the analysis of the high-fidelity JWST data, new computational tools have been developed at NASA Ames to produce fully anharmonic IR absorption and cascade emission spectra of various PAHs, including deuterated species. The substituted, aromatic molecule, phenylacetylene, is used as a test case for validation of the newly developed theoretical methods via comparison with IR absorption and emission experiments. This work sets the stage for future implementation of the code as a tool for populating the NASA Ames PAH IR Spectroscopic Database (PAHdb) with anharmonic spectra of vast numbers of PAHs for use in the analysis of astronomical PAH data.