Anharmonic IR Absorption and Emission Spectra of Polycyclic Aromatic Hydrocarbons

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In order to provide a foundation for the analysis of new high-fidelity JWST data, computational tools have been developed at NASA Ames to produce fully anharmonic IR absorption and cascade emission spectra of PAHs. The computational spectra are validated and benchmarked with new and existing laboratory measurements. Gas-phase polycyclic aromatic hydrocarbons (PAHs) are ubiquitous throughout the universe, and their emission dominates the near- and mid-infrared (IR) spectrum of various astronomical sources such as molecular clouds, protoplanetary disks, and galaxies. This emission is used as a tracer for the temperature, density, and radiative characteristics of the local chemical and physical environment. These data are then utilized as input for astrochemical and astrophysical models that are integral to understanding the lifecycle (or evolutionary) dynamics of these sources. Focusing on astrochemistry, PAH molecules provide a rich source of accessible carbon while PAH clustering and stacking provide precursors of carbonaceous dust grains that participate in the subsequent growth of pebbles, boulders, and ultimately planets. Carbon based dust also acts as the medium on which interstellar ices composed of H_2O and CO_2, among other molecules, accumulate. Chemistry within these ices produces new molecules, seeding the chemical complexity that is found in geological features on Earth. 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 interpretation of astronomical PAH data from missions such as JWST, Spitzer, ISO, and RST.