From Interstellar Ices to Polycyclic Aromatic Hydrocarbons
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Computing Anharmonic Vibrational Spectra for Polycyclic Aromatic Hydrocarbons: Naphthalene, Anthracene, and Tetracene

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It is now widely accepted that polycyclic aromatic hydrocarbons (PAHs) are ubiquitous throughout the galaxy. The vibrational frequencies of PAH molecules in the infrared (IR) have been shown to be an excellent fingerprint for their existence and for assessing the physical conditions of the astrophysical environment in which they are observed. The Ames PAH database is now used routinely by astronomers to understand the specific PAH features, enabling them to determine the importance of ionized PAHs, nitrogen-containing PAHs (PANHs) etc. for a specific object. While the laboratory spectra and theoretical calculations that make up the PAH database have been enormously useful, it is becoming clear that future space telescopes will be high-resolution and thus there is a need for high-resolution gas-phase experiments and theoretical calculations that explicitly include anharmonic effects and rotational structure in a given vibrational band. In this presentation, recent studies focused on explicitly computing anharmonic spectroscopic constants and vibrational spectra for the linear PAH molecules, naphthalene, anthracene, and tetracene, will be discussed. Some of the details to be discussed include advances in manipulating normal coordinate quartic force fields which are used together with vibrational second-order perturbation theory to compute the anharmonic spectroscopic constants and vibrational spectra, the importance of resonances, especially in the C-H stretching region, an improved method for distributing the IR intensity across the bands of a polyad resonance, and the importance of anharmonic IR intensities, especially in regions of the spectrum where no resonances occur. Where available, comparison to recent experiments will be discussed as well.