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The Anharmonic Infrared Spectra of Polycyclic Aromatic Hydrocarbons

- i Accounting for translation and rotation eigenvectors simplify the analysis of the quartic force field of a molecule. (Chapter 2)
- ii Anharmonic calculations improve greatly the theoretical infrared spectrum of polycyclic aromatic hydrocarbons. (Chapters 3, 4, and 5)
- iii Fermi resonances dominate the CH-stretching region of the infrared spectrum of PAHs and PAH derivatives, and need to be handled simultaneously in so-called polyads, which must take into account the redistribution of intensities. (Chapters 3, 4, and 5)
- iv A polyad treatment of resonances can be easily incorporated into anharmonic temperature dependent calculations, and are necessary to account for changes in the spectrum due to waxing and waning of resonant effects. (Chapter 6)
- v A full theoretical anharmonic infrared cascade model is necessary to understand the emission process of interstellar PAHs, however a full theoretical anharmonic infrared cascade model may *not* be necessary to model the emission process of interstellar PAHs. (Chapter 7)
- vi The standard 15 cm^{-1} shift applied to current PAH emission models was adopted in err, and should be dropped. (Chapter 7)
- vii Low-temperature absorption spectra of PAHs can be used to reproduce the emission spectra of interstellar PAHs. (Chapter 7)
- viii The James Webb Space Telescope should answer many long-standing PAH related questions. If it does not, the PAH hypothesis itself should be reevaluated.
- ix Theoretical chemistry can answer many questions that experiments cannot, but without experiments theory is useless.
- x Anharmonic calculations of molecular properties will soon become routine, and replace standard harmonic calculations.
- xi The latent carcinogenic potential of nanomaterials may limit their usefulness in society.
- xii The monotony of data production and analysis is analogous to the “farming” and “grinding” seen in many videogames. The latter has trained me well for the former.