Computing rotational, rovibrational, and vibrational spectra for astronomical observations: high accuracy line lists for high temperatures, limited line lists for biosignature molecules, and PAH emission spectra

Timothy J. Lee

Space Science and Astrobiology Division,
NASA Ames Research Center, Moffett Field, CA, USA

Over the last several years, our group has been involved in developing approaches to compute highly accurate spectroscopic constants and vibrational frequencies for small transient molecules that may be used in the interpretation and assignment of high-resolution laboratory experiments as well as high-resolution astronomical spectra. Additionally, we have used the computed spectroscopic constants to simulate purely rotational and rovibrational spectra so that these may be compared directly with high-resolution astronomical observations, and we have worked on developing approaches that can be applied to much larger molecules, such as PAHs, where we can explicitly determine anharmonic corrections to vibrational modes as well as take into account intensity sharing due to resonances. Another part of our work in spectroscopic signatures involves computing highly accurate line lists for common molecules, such as CO_2, SO_2, and NH_3, which occur in many astrophysical environments, including the atmospheres of exoplanents, and often need to have their lines identified in high-resolution observations in order to determine which lines are due to other molecules. In order to characterize the atmospheres of hot exoplanets, these line lists need to be very accurate and extend to very high energies. I will discuss our latest work in these areas of astrochemical spectroscopy research.