# COMBINING THEORY AND EXPERIMENT TO COMPUTE HIGHLY ACCURATE LINE LISTS FOR STABLE MOLECULES, AND PURELY AB INITIO THEORY TO COMPUTE ACCURATE ROTATIONAL AND ROVIBRATIONAL LINE LISTS FOR TRANSIENT MOLECULES

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Theoretical chemists have been computing vibrational and rovibrational spectra of small molecules for more than 40 years, but over the last decade the interest in this application has grown significantly. The increased interest in computing accurate rotational and rovibrational spectra for small molecules could not come at a better time, as NASA and ESA have begun to acquire a mountain of high-resolution spectra from the Herschel mission, and soon will from the SOFIA and JWST missions. In addition, the ground-based telescope, ALMA, has begun to acquire high-resolution spectra in the same time frame. Hence the need for highly accurate line lists for many small molecules, including their minor isotopologues, will only continue to increase. I will present the latest developments from our group on using the ”Best Theory + High-Resolution Experimental Data” strategy to compute highly accurate rotational and rovibrational spectra for small molecules, including NH3, CO2, and SO2. I will also present the latest work from our group in producing purely *ab initio* line lists and spectroscopic constants for small molecules thought to exist in various astrophysical environments, but for which there is either limited or no high-resolution experimental data available. These more limited line lists include purely rotational transitions as well as rovibrational transitions for bands up through a few combination/overtones.