THEORETICAL ROVIBRATIONAL SPECTRA FOR MOLECULES CONTAINING A LARGE-AMPLITUDE MOTION: AMMONIA

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Molecules with large amplitude motions possess significant complexity in their rovibrational and purely rotational spectra. Because of this complexity, they are ideal molecules to be used to characterize the physical conditions of the celestial objects and galactic environments in which they are observed, which was noted more than two decades ago by Ho and Townes. The simplest and best characterized molecule with a large amplitude motion of interest in astronomy is ammonia. The available experimental data for even this molecule, however, is not sufficient to generate a synthetic spectrum that compares well with observations from the Spitzer Space Telescope of one of the coolest known T dwarfs Gl570D, and this is likely to be the case for any celestial environments above 400K. The IRS instrument on the Spitzer Space Telescope has already recorded spectra that cannot be well modeled and interpreted using the available experimental data for ammonia. In response to the urgent need for better line lists, including intensities, we have used the tools of theoretical spectroscopy to obtain a highly accurate potential energy surface (PES) and dipole surface for the ammonia. I will report on our progress to date. Ultimately, the resulting highly accurate PES and dipole moment surface will be used to solve the nuclear Schroedinger equation to generate the necessary line lists.