Ab initio Spectroscopic Investigation of Hydrogen Fluoride

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Hydrogen fluoride (HF) is a chemically simple but astrophysically significant molecule, with strong rovibrational features that make it a useful probe in exoplanetary atmospheres. It has been detected in various astronomical environments, including sunspots, the atmosphere of Venus, red giant stars, and the interstellar medium. In this study, we perform a detailed ab initio investigation of the rovibronic spectroscopy of the HF molecule. High-level quantum methods are used to model the electronic structure of the HF molecule, including potential energy curves, transition dipole moments, and allowed couplings for relevant excited states. These data are then combined with accurate nuclear motion calculations to characterize the rovibronic structure and spectral features of HF. The resulting theoretical spectra provide reliable molecular data that is applicable to astrophysical modeling, particularly in the context of exoplanetary atmospheres and interstellar chemistry. This work contributes to a deeper understanding of molecular signatures in the ultraviolet (UV) region and supports the interpretation of spectroscopic data from current and future space-based observatories.