PROGRESS TOWARDS THE ROTATIONAL SPECTRUM OF H_5^+ AND ITS ISOTOPOLOGUES

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The reaction of H_3^+ with H_2, arguably the most common bimolecular reaction in the universe, proceeds through the H_5^+ collisional complex. This reaction, and consequently H_5^+, greatly influence the chemical and physical processes in the interstellar medium, playing crucial roles in such varied processes as isotopic fractionation and the formation of complex organic molecules. A thorough understanding of the role of H_5^+ in interstellar chemistry is contingent upon its definitive astronomical detection, necessitating the acquisition of a laboratory rotational spectrum. Rotationally-resolved spectra of H_5^+ in the terahertz region have not yet been observed experimentally. The prediction of this spectrum based on a high-level theoretical study is therefore an important first step to guide experiment. The highly fluxional nature of H_5^+ presents major challenges for theory, especially for the pure rotational spectrum due to the difficulties in determining an accurate dipole moment from a correct description of the highly delocalized zero-point wavefunction. We have now completed this work using the most recent potential energy and dipole moment surfaces for H_5^+ and its isotopologues DH_4^+, $D_2H_3^+$, $D_3H_2^+$, D_4H^+, and D_5^+. Pure rotational spectra have been predicted for these species based on the optimized minimum-energy geometries and the zero-point averaged dipole moments calculated from our potential energy surface. We will discuss the implications of these results for the detection of each ion's rotational spectrum, show preliminary predictions of the rotational spectrum for those species possessing permanent dipole moments, and comment on the degree of expected spectral splitting arising from internal motion. Finally, we will report on progress toward the laboratory spectroscopic investigation of these species in the terahertz region.