AB INITIO PREDICTIONS FOR HO_2^+: THEORETICAL GUIDANCE FOR AN ASTRONOMICAL DETECTABILITY STUDY

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The protonated form of molecular oxygen, HO_2^+, could potentially serve as a good tracer of its parent molecule, O_2, which is difficult to detect. Theoretical predictions for various properties of HO_2^+ are critical inputs both for a preliminary assessment of its astronomical detectability as well as for guiding experimental study. *Ab initio* quantum chemical calculations were performed to generate predictions of the rotational constants, vibrational frequencies, dipole moment components, spin-rotation constants, and other properties of ground state HO_2^+ ($^3A''$), along with parallel benchmark values for ground state $HO_2(^2A'')$. Both multireference configuration interaction (MRCI) and single reference coupled cluster theory [full singles and doubles and perturbative triples, RCCSD(T)] were employed, in conjunction with basis sets as large as aug-cc-pV5Z (with extra *sp* functions included in all-electron calculations). Full quartic forcefields were computed from grids of 84 points in order to include anharmonic corrections via perturbation theory analysis. In addition to the spectroscopic properties, we computed the reaction enthalpy for $H_3^+ + O_2 \rightarrow HO_2^+ + H_2$ to be 127 cm^{-1} with anharmonic vibrational zero-point energy (ZPE) corrections; the value is 64 cm^{-1} once experimental numbers for the rotational ZPE corrections are also incorporated. This prediction agrees very well with the latest result of 50 ± 12 cm^{-1} from the Active Thermochemical Tables (ATcT) analysis of the underlying thermochemical network.

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