

ACCURATE AB INITIO QUARTIC FORCE FIELDS FOR HO₂⁺

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Purely *ab initio* CCSD(T) quartic force fields have been determined for the lowest triplet and singlet states of HO₂⁺ ion with TZ-, QZ- and 5Z-level one-particle basis sets. After extrapolating to complete basis-set limit, small correction terms have now been incorporated, including core-correlation, scalar relativistic, and others. Anharmonic vibrational fundamentals and ro-vibrational spectroscopic constants are computed with perturbational and variational methods. Our best computed force field should give fundamentals to within ± 5 cm⁻¹. In this talk we will present the procedure details and compare our results with previous work on this ion. Effects of small corrections and benchmark results on H₂O will also be discussed.