

## DFT and Ab Initio Computational Study of Structural Properties and Vibrational Spectra for Protonated Water Clusters

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Protonated water clusters are the subjects of increasing interest, both experimental [1-3] and theoretical [4-6]. Ionized water clusters constitute the most abundant ionic species in the low stratosphere [7]; water ions are important in atmospheric nucleation and chemical reactions.

The geometrical parameters and spectral properties of different conformers of protonated water clusters  $H^+(H_2O)_{n=1-4}$  are investigated with Density Functional Theory and ab initio methods. Results of Hartree-Fock and hybrid DFT methods: BVP86, B3LYP, PBEPBE, MPW1PW91, HTCH and THCTH with 6-311G++(2d,2p) and 6-311G++(3df,3pd) basis sets and high levels of ab initio computational studies with the quadratic complete basis set (CBS-Q) were compared with experimental data of vibrational modes. Some differences in spectral features between Eigen ( $H_3O^+$ ) and Zundel ( $H_5O_2^+$ ) conformers among different experiments as well as between experiments and theory are denoted.

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