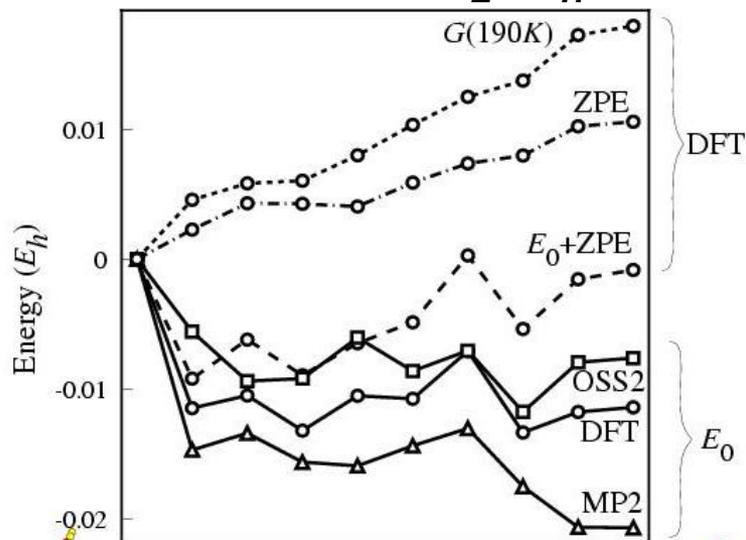


Pilot-6 Highlight

Ohio State U.

Protonated water clusters: $H^+(H_2O)_n$



The cations of the lower ionosphere are almost exclusively protonated water clusters, $H^+(H_2O)_n$. These ions have also been studied in molecular beam experiments, and provide important models of fundamental acid/base chemistry. *Ab initio* studies performed at MSCF reveal that $H^+(H_2O)_8$, a typical size found in the ionosphere, can exist in many stable arrangements, from the linear arrangement shown on the left to the compact cubes on the right. These studies show that electronic energy (E_0) favors the compact structures, but vibrational zero point energy (ZPE) favors the open structures. These two effects balance, making these clusters nearly equal in stability. [Ciobanu *et al.*, *J. Chem. Phys.* **113**:5321 (2000)]. Statistical simulations of $H^+(H_2O)_8$ demonstrated that linear or tree-like arrangements dominate at high temperature, and that, in the temperature range found in the stratosphere, $H^+(H_2O)_8$ is actively isomerizing between compact and extended structures [Singer *et al.*, *J. Chem. Phys.* **112**:710 (2000)].