# BINDING BETWEEN NOBEL GAS ATOMS AND PROTONATED WATER MONOMER AND DIMER

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$H_3O^+$ and $H_5O_2^+$, Eigen and Zundel forms of the excess proton, are the basic moieties of hydrated proton in aqueous media. Using vibrational pre-dissotion spectra, vibrational spectra of messenager-tagged species are often measured; however, only neat species have been studied in detail by theoretical and computational means. To bridge this gap, we carry out extensive CCSD(T)/aug-cc-pvTZ calculations to investigate the binding between commonly used noble gas (NG) messenagers (He, Ne and Ar) with $H_3O^+$ and $H_5O_2^+$ to get an accurate estimate on the binding energy which yields the upper limits of vibrational temperature of NG-tagged clusters. The binding sites of NG and low-lying transition states have also been searched to give a better description on the energy landscape. In addition, a few exchange/correlation functionals have been tested to access the accuracy of these methods for future and more sophisticated theoretical studies.