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Anharmonic Vibrational Spectra of Hydrogen Bonded Clusters[1]

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We report anharmonic vibrational spectra for a variety of hydrogen bonded clusters such as $(H_2O)_n$ and $(HF)_n$, n=1-5. We investigate the convergence of the hydrogen bonded frequencies with basis set and level of electron correlation and compare with the available experimental data. For this purpose we employ the correlation-consistent basis sets up to quintuple zeta (5z) quality and compute the spectra at the second order Møller-Plesset (MP2) and Coupled Cluster plus Single and Double with perturbative estimate of Triple excitations [CCSD(T)]. The correlation between the calculated elongations in the hydrogen bonding stretches and the corresponding computed/observed vibrational frequencies suggest an extension of Badger's rule for these hydrogen bonded systems.

[1]Battelle operates the Pacific Northwest National Laboratory for the US Department of Energy

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