Investigation of the Structure, Stability, and Atmospheric Significance of N_2 and O_2 Polyhydrates

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There exists a great volume of literature detailing the contributions of water dimers, trimers and other high-order polymers of water to the atmosphere's absorption spectrum. Also thoroughly investigated is the N_2 and O_2 monohydrates, specifically H_2O's various stretching and bending modes. Less well-known is the contribution of the N_2 and O_2 stretching modes (circa 2000 cm^{-1} and 1500 cm^{-1}, respectively) and some of the intermolecular modes to the IR absorption spectrum for larger hydrates. For $N_2(H_2O)_n$ and $O_2(H_2O)_n$ where n = 1 - 4, we first used genetic algorithm with PM7, HF-3c and B3LYP methods to generate an ensemble of low energy structures. We optimized these structures with MP2/aug-cc-pVDZ and estimated their binding energy using the MP2-F12/VTZ-F12 method. We looked for trends in the data as we added waters, focusing on the binding energy of the clusters and the frequencies and intensity of their IR vibrational modes.

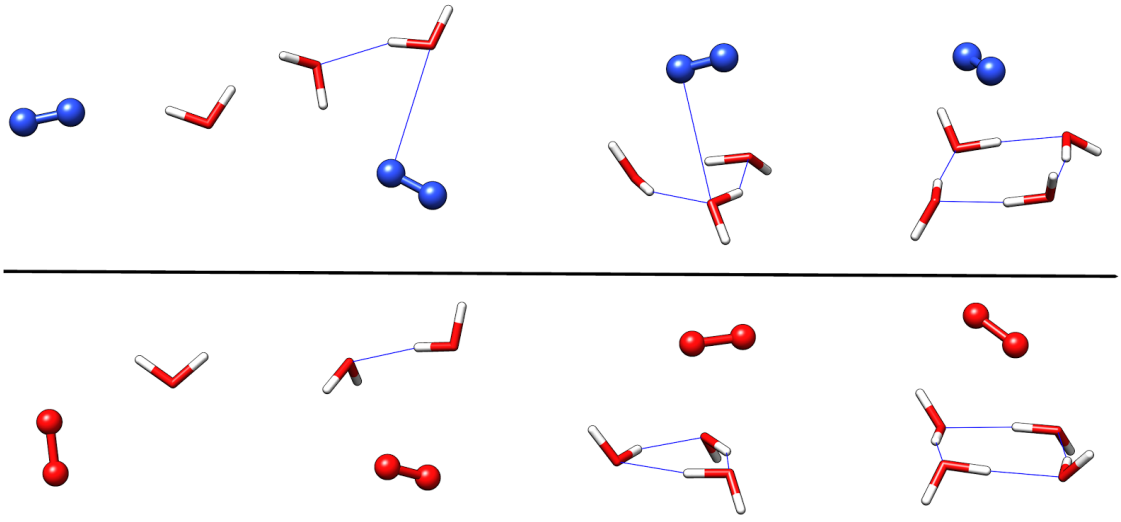

Figure 1. The MP2-F12/VTZ-F12//MP2/aug-cc-pVDZ global minima of $N_2(H_2O)_n$ and $O_2(H_2O)_n$ for n=1-4.