

THEORETICAL RESULTS FOR $(\text{H}_2\text{O})_n\text{H}^+$ AND $(\text{H}_2\text{O})_n$: QMC FOR H_5O_2^+ , GRAPH THEORETICAL ENUMERATION OF DISTINCT HYDROGEN-BONDED ARRANGEMENTS, COMPACT TO EXTENDED PHASE TRANSITIONS IN $(\text{H}_2\text{O})_n\text{H}^+$

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Our recent progress in the study of protonated and neutral water clusters, $(\text{H}_2\text{O})_n\text{H}^+$ AND $(\text{H}_2\text{O})_n$, is reviewed. Both variational and diffusion Monte Carlo calculations have been performed, leading to a prediction of the fundamental frequency for motion of the central proton in H_5O_2^+ . *Ab initio* electronic structure calculations suggest this absorption feature will be intense. Extensive Monte Carlo simulations of larger hydrated proton clusters indicate there is a transition between compact and extended phases. Local minima of the potential energy surface for $(\text{H}_2\text{O})_n\text{H}^+$ AND $(\text{H}_2\text{O})_n$ are studied. The number of topologically distinct hydrogen-bonded arrangements can be enumerated using graph theory, leading to a prediction of the number of distinct local minima of the potential energy surface in compact geometries, including dodecahedral clathrate structures.