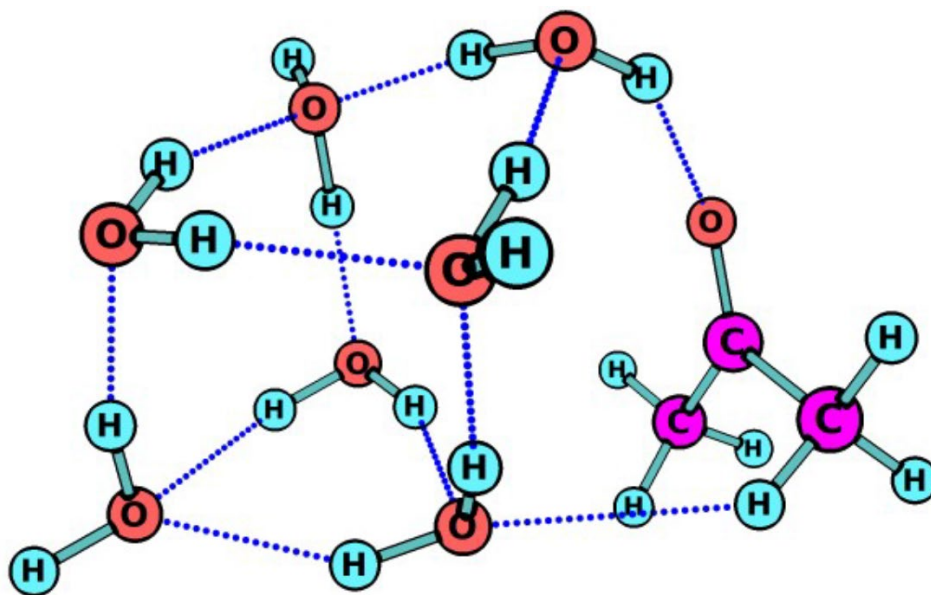


Sampling and Analyzing Noncovalent Interactions in Water Cluster–Organic Molecule Complexes

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In search of cheaper and sustainable alternatives to organic solvents in chemistry, the development and research of synthetic procedures in the presence of water have increasingly become an active topic of interest. In particular, the study and analysis of water-organic molecule complexes are central to understanding the complexities arising in water-organic systems. In this work, we analyzed the interactions present in complexes that small organic molecules such as acetone, azomethane, dimethylamine, dimethyl ether, methyl acetate, and oxirane form with 39 different $(\text{H}_2\text{O})_n$ clusters ($n = 1-10$). A random generation of configurations and a subsequent screening procedure were employed to sample representative interactions. Then, we calculated the associated binding energies using high-level quantum chemical computations, ranging from -0.19 to -10.76 kcal/mol at the DLPNO-CCSD(T)/CBS level. We rationalized the binding energies in terms of various factors, including the water cluster size, the nature of the organic molecule, and the type of hydrogen bond donor. In general, small water clusters and organic molecules can form a diverse set of noncovalent interactions. We found that the most stable complexes often arise from a combination of a strong hydrogen bond plus a secondary interaction between the organic molecule and the water cluster.



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