A COMPUTATIONAL AND EXPERIMENTAL VIEW OF HYDROGEN BONDING IN POLYOL WATER CLUSTERS

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Polyol water clusters can act as a proxy for alcohol water ices in the interstellar medium. By studying these clusters, conclusions can be drawn about ionization and solvation processes of atmospheric and interstellar chemical interest, as was done with the polyols ethylene glycol, 1,2 propylene glycol, and 1,3 propylene glycol. These polyol water clusters are generated in a continuous supersonic jet expansion, then photionized with synchrotron based tunable vacuum ultraviolet light, and detected by a reflectron time-of-flight mass spectrometer. Polyol water cluster fragments are observed and the appearance energies for these clusters as well as water clusters are determined. To explain the experimentally obtained mass spectra, theoretical calculations are performed on neutral and ionized polyol water clusters as well as the detected fragments and fragment clusters. From these calculations, interaction and ionization energies are determined and hydrogen bond networks may be visualized.