HELIUM NANODROPLET ISOLATION SPECTROSCOPY OF METHANOL AND METHANOL-WATER CLUSTERS IN THE SYMMETRIC METHYL STRETCHING BAND

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The mid-infrared spectra of helium solvated methanol and methanol-water clusters have been investigated in the symmetric CD_3 stretching band of CD_3OH and CD_3OD . We find that the position of this band provides a useful signature of the general type of hydrogen-bonded cluster it is associated with. Our results are consistent with those previously reported in the OH stretching region [1], in that methanol clusters from the trimer to the pentamer are cyclic, and that mixed clusters with one water molecule (and at least two methanol molecules) are also cyclic. We additionally provide evidence that the methanol trimer adopts a chair-like structure (as opposed to bowl-like), that mixed clusters with a larger number of water molecules are also cyclic, and that branched methanol clusters contribute to the depletion signal in larger methanol clusters. We performed DFT calculations which support these interpretations.

[1] Sulaiman, M. I., Yang, S., Ellis, A. M., J. Phys. Chem. A, 2017, 121, 771-776.