MONOETHANOLAMINE-(H2O)N, N=1-7, AND -(CO2)M, M=1-4, CLUSTERS CHARACTERIZED BY ROTATIONAL SPECTROSCOPY

FAN XIE, WENHAO SUN, *FS-SMP, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany*; PABLO PINACHO, *Physical Chemistry, University of the Basque Country (UPV/EHU), Bilbao, Spain*; MELANIE SCHNELL, *FS-SMP, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany*.

In this study, we present the structures of MEA-H2O and MEA-CO2 complexes identified in pulsed jet expansion using the broadband chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy COMPACT that operated in the 2-18 GHz range[1]. We reveal the microhydration processes of MEA from these observed MEA-H2O clusters and show that the structures of MEA-(H2O)n are closely analogous to the pure water clusters (H2O)n+2. For example, the MEA monohydrate, dihydrate, and trihydrate adopt cyclic topologies similar to water trimer, tetramer, and pentamer, respectively. With four water molecules participating, we identified two isomers of MEA-(H2O)4, named Cage and Prism. In the observed MEA-H2O clusters, the intramolecular OH-NH2 H-bond of MEA is broken to form an energetically favorable intermolecular H-bond with water. In contrast, without the presence of water, CO2 is unable to break the intramolecular H-bond based on the observed MEA-CO2 complexes[2]. Interestingly, we discovered that the OH lone pair-CO2 interaction has higher energetic priority than the NH2 lone pair-CO2 interaction, which is in sharp contrast to the results from aqueous solutions. How would the CO2 bind to MEA with the presence of a few water molecules? A short discussion on the topic will be made based on what we learned from the observed structures of MEA-H2O and MEA-CO2.

[1] D. Schmitz, V. A. Shubert, T. Betz, M. Schnell, J. Mol. Spectrosc. 2012, 280, 77–84. [2] F. Xie, W. Sun, P. Pinacho, M. Schnell, Angew. Chem. Int. Ed. 2023, e202218539; Angew. Chem. 2023, e202218539.