APPLICATION OF INFRARED MULTIPHOTON DISSOCIATION SPECTROSCOPY FOR THE STUDY OF CHIRAL RECOGNITION IN THE PROTONATED SERINE CLUSTERS: PART II

FUMIE X. SUNAHORI, ELENA N. KITOVA, JOHN S. KLASSEN, AND YUNJIE XU, *Department of Chemistry, University of Alberta, Edmonton, Canada T6G 2G2*; GUOCHUN YANG, *Department of Chemistry, Northeast Normal University, Changchun 130024, Jilin, P.R. China.*.

Serine is an amino acid which has long been known to form the magic-number serine octamer $[Ser_8 + H]^+$. It has been shown[a] that the serine octamer exhibits strong preference for homochirality. Although a few possible structures for the homochiral serine octamer have been proposed, no definite conclusion has so far been drawn. Last year at this conference, we reported on the study of the protonated serine octamer and dimer as well as the chiral recognition in these clusters using infrared multiphoton dissociation (IRMPD) spectroscopic technique coupled with a Fourier transform ion cyclotron (FTICR) mass spectrometer. Here we present our latest results on the search for the infrared signatures of chiral recognition in the serine octamer and the dimer using a mixture of the deuterated 2,3,3-d_3-*L*-serine and normal *D*-serine solution. Using the isotopic labeled species, we could isolate the heterochiral species and obtain their IRMPD spectra which can be directly compared with those of the homochiral species. As an aid to interpret the observed spectra, molecular structures and vibrational frequencies of both homochiral and heterochiral octamer and dimer have been predicted by ab initio calculations. New insights into the hitherto undetermined structure of the serine octamer will be discussed.

[a] S. C. Nanita and R. G. Cooks *Angew. Chem. Int. Ed.* **45**(554), 2006.