

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

FUMIE X. SUNAHORI, GUOCHUN YANG, ELENA N. KITOVA, JOHN S. KLASSEN, AND YUNJIE XU,

Department of Chemistry, University of Alberta, Edmonton, Canada T6G 2G2.

Serine is an amino acid which has long been known to form magic-number ionic clusters, serine octamer $[\text{Ser}_8 + \text{H}]^+$. It has been shown^a that serine octamers exhibit strong preference for homochirality, but its structure is still unclear. We have used infrared multiphoton dissociation (IRMPD) spectroscopic technique coupled with a Fourier transform ion cyclotron (FRICR) mass spectrometer to investigate the structures of protonated serine octamer and dimer as well as the chiral recognition in these clusters. With the use of ICR cell, the ions can be stored for a sufficient time so that measurements of IRMPD spectra become possible with a CW OPO laser in the 3000-4000 cm^{-1} region. As an aid to interpret the observed spectra, molecular structures and vibrational frequencies of the octamer and dimer have been predicted by using the B3LYP/6-311++G** calculations. Differences in chiral selectivity between the serine octamer and dimer will be discussed.

^aS. C. Nanita and R. G. Cooks *Angew. Chem. Int. Ed.* **45**(554), 2006.