

INFRARED SPECTROSCOPY OF  $((\text{CH}_3)_3\text{N})_n\text{-H}^+\text{-H}_2\text{O}$  ( $n=1-3$ ): STRUCTURES AND DISSOCIATION CHANNELS OF PROTONATED MIXED CLUSTERS AROUND A MAGIC NUMBER

RYUNOSUKE SHISHIDO, ASUKA FUJII, *Department of Chemistry, Graduate School of Science, Tohoku University, Sendai 980-8578, Japan*; JER-LAI KUO, *Institute of Atomic and Molecular Science, Academia Sinica, Taipei 10617, Taiwan*.

The magic number behavior of  $((\text{CH}_3)_3\text{N})_n\text{-H}^+\text{-H}_2\text{O}$  clusters at  $n = 3$  is investigated by applying infrared spectroscopy to the clusters of  $n = 1-3$ .<sup>a</sup> Structures of these clusters are determined in conjunction with density functional theory calculations. Dissociation channels upon infrared excitation are also measured, and their correlation with the cluster structures is examined. It is demonstrated that the magic number cluster has a closed-shell structure, in which the water moiety is surrounded by three  $(\text{CH}_3)_3\text{N}$  molecules. Large rearrangement of the cluster structures of  $n = 2$  and 3 before dissociation, which has been suggested in the mass spectrometric study,<sup>b</sup> is confirmed on the basis of the structure determination by infrared spectroscopy.

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<sup>a</sup>R. Shishido, J. -L. Kuo and A. Fujii *J. Phys. Chem. A* **116**, 6740, 2012.

<sup>b</sup>S. Wei, W. B. Tzeng, R. G. Keese and A. W. Castleman, Jr. *J. Am. Chem. Soc.* **113**, 1960, 1991.