INFRARED-ULTRAVIOLET PHOTOIONIZATION AND DEPLETION SPECTROSCOPY OF AL- AND CU-ETHYLENEDIAMINE COMPLEXES

YUXIU LEI, JUNG SUP LEE, and DONG-SHENG YANG, *Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055*.

Al- and Cu-ethylenediamine ($C_2N_2H_8$) complexes were generated in supersonic molecular beams, and their C-H and N-H stretching modes were measured by resonant infrared-ultraviolet two-photon ionization and depletion spectroscopy. The spectrum of Al-ethylenediamine displayed three C-H stretching frequencies of 2880, 2936, and 2946 cm^{-1}, whereas that of Cu-ethylenediamine exhibited five such vibrations with frequencies of 2880, 2921, 2931, 2951, and 2967 cm^{-1}. In contrast, only two N-H stretches were identified for each of the two complexes, which were 3320 and 3392 cm^{-1} for Al and 3275 and 3360 cm^{-1} for Cu. These experimental spectra were compared to the prediction of density functional theory calculations and to the infrared spectrum of the free ligand. From these comparisons, a cyclic bidentate structure was identified for Al-ethylenediamine, and a hydrogen-bonded monodentate structure was determined for the corresponding Cu species. This study was consistent with the previous work of pulsed-field ionization electron spectroscopy of these complexes.[ab]

[a] S. Li, J. F. Fuller, X. Wang, B. R. Sohnlein, P. Bhowmik, and D.-S. Yang, J. Chem Phys. 121, 7692 (2004).
[b] X. Wang and D.-S. Yang, J. Phys. Chem. A 110, 7568 (2006).