ACCURATE FUNDAMENTAL FREQUENCIES AND SPECTROSCOPIC CONSTANTS FOR CCH^-, NH_2^- AND THEIR ISOTOPOMERS

TIMOTHY J. LEE, CHRISTOPHER E. DATEO and GALINA CHABAN, *MST27B-1, NASA Ames Research Center, Moffett Field, CA 94035-1000*.

Accurate quartic force fields have been determined for the CCH^- and NH_2^- molecular anions using the singles and doubles coupled-cluster method that includes a perturbational estimate of the effects of connected triple excitations, CCSD(T). Very large one-particle basis sets have been used including diffuse functions and up through g-type functions. Correlation of the nitrogen and carbon core electrons has also been included. The fundamental vibrational frequencies have been computed using second-order perturbation theory and exact variational methods. Results for NH_2^- are in excellent agreement with previous experiments, but for CCH^- our results support low-resolution photoelectron experiments by Ervin and Lineberger that indicated the high-resolution studies by Gruebele, Polak, and Saykally error in their assignment for the CC stretch. The implications of our research for the astronomical observation of molecular anions will be discussed.