SPECTROSCOPY AND DYNAMICS OF THE JET-COOLED SELENOKETENYL (HCCSe) RADICAL

SHENG-GUI HE, DAVID A. HOSTUTLER and DENNIS J. CLOUTHIER, *Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055*.

The previously observed [a] 418 - 402 nm LIF spectra of the jet-cooled HCCSe and DCCSe free radicals have been vibrationally and rotationally analyzed as a $^2\Pi_i$ - $^2\Pi_i$ electronic transition. The upper electronic state has a very large HCC bending mode Renner-Teller effect although the CCSe bend is nearly harmonic, in accord with our analysis of the electronic spectra of the HCCS and DCCS radicals, which are found to be quasi-linear in the excited state. Based on ab initio calculations, the ground state vibrational energy levels obtained from wave-length resolved emission spectra have also been assigned for both HCCSe and DCCSe. The LIF and emission spectra of HCCSe/DCCSe are not as complex as those of HCCS/DCCS because the selenium-containing radicals have a very large spin-orbit splitting which decreases the Renner-Teller complications. HCCSe exhibits field-free molecular quantum beats in collision-free single rotational level fluorescence decays due to coupling with high vibrational levels of the ground state.

[a] D. A. Hostutler and D. J. Clouthier, Presentation TA 10, 55-th International Symposium on the Molecular Spectroscopy, 2000.