THE ELECTRONIC SPECTRUM AND MOLECULAR STRUCTURE OF CuSH

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The electronic spectrum of the jet-cooled copper hydrosulfide molecule has been observed for the first time by pulsed electric discharge and laser-induced fluorescence techniques. High resolution studies of the $0_0^0$ bands of the $\tilde{A}^1A'' - \tilde{X}^1A'$ transition of CuSH and its various isotopomers ($^{65}$CuSH, $^{63}$CuSD, and $^{65}$CuSD) have allowed us to obtain the excited state molecular structure and refine the previously reported ground state structure[a]. Single vibronic level emission spectra have also been recorded to measure the ground state vibrational frequencies. Some of the excited state vibrational frequencies have been obtained from an analysis of the vibronic structure in the LIF spectra. *Ab initio* Franck-Condon simulations of the absorption and emission spectra are in accord with experiment.

[a] A. Janczyk, S. K. Walter and L. M. Ziurys *Chem. Phys. Lett.* **401**(211), 2005.