DETECTION OF THE H_2PS FREE RADICAL BY LASER SPECTROSCOPY

ROBERT A. GRIMMINGER, DENNIS J. CLOUTHIER, *Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055, USA*; RICCARDO TARRONI, *Dipartimento di Chimica Fisica ed Inorganica, Università di Bologna, 40136 Bologna, Italy*.

The previously unobserved H_2PS free radical has been detected by laser-induced fluorescence (LIF) techniques. H_2PS (and D_2PS) were produced in a pulsed discharge jet using a precursor gas mixture of Cl_3PS vapor and hydrogen (or deuterium) in high pressure argon. Our *ab initio* predictions of the ground and excited state frequencies and excitation energy are in good agreement with the results obtained by vibrational analysis of the LIF and single vibronic level (SVL) emission spectra. High-resolution spectra of the hybrid 0_0^0 bands of H_2PS and D_2PS were analyzed by band contour methods to obtain approximate ground and excited state rotational constants and molecular structures. The electronic transition involves promotion of an electron from the π to the π^* orbital and is assigned as $\tilde{B}^2\mathrm{A}' - \tilde{X}^2\mathrm{A}'$. The results will be discussed in comparison to *ab initio* predictions and the spectra of other X_2PS radicals recently studied in our laboratory.