## DETECTION OF THE H<sub>2</sub>PS FREE RADICAL BY LASER SPECTROSCOPY

## <u>ROBERT A. GRIMMINGER</u>, 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<sub>2</sub>PS free radical has been detected by laser-induced fluorescence (LIF) techniques. H<sub>2</sub>PS (and D<sub>2</sub>PS) were produced in a pulsed discharge jet using a precursor gas mixture of Cl<sub>3</sub>PS 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<sup>0</sup><sub>0</sub> bands of H<sub>2</sub>PS and D<sub>2</sub>PS 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  $\pi$  to the  $\pi^*$  orbital and is assigned as  $\tilde{B}^2A' - \tilde{X}^2A'$ . The results will be discussed in comparison to *ab initio* predictions and the spectra of other X<sub>2</sub>PS radicals recently studied in our laboratory.