## MICROWAVE SPECTRA OF O<sub>2</sub>–HF AND O<sub>2</sub>–DF AND GLOBAL FITTING WITH IR DATA: INSIGHT INTO THE NATURE OF HYPERFINE INTERACTIONS

## SHENGHAI WU, GALEN SEDO, ERIK M. GRUMSTRUP AND KENNETH R. LEOPOLD, Department of Chemistry, University of Minnesota, Minneapolis, MN 55455.

Understanding intermolecular interactions involving open shell systems is important to both combustion and atmospheric research. In this talk, we present microwave spectra of  $O_2$ -HF and  $O_2$ -DF, and analysis of their hyperfine structure. Last year, spectra were reported<sup>*a*</sup> for six different pure rotational transitions of  $O_2$ -HF, though at the time, the analysis of the hyperfine structure was still incomplete. A simultaneous fit of microwave and infrared<sup>*b*</sup> data was also described. In this talk, we report a complete analysis of the hyperfine structure for  $O_2$ -HF and a new global fit including microwave and infrared frequencies. New assignments for the  $F_1$  quantum numbers, together with complete assignment of *F* quantum numbers has allowed all observed transitions of  $O_2$ -HF to be fully analyzed with confidence. Calculated spectral intensities are also consistent with experimental observation. The Fermi contact parameters for the two nuclei are found to have opposite signs, consistent with a simple model based on spin polarization. Progress on analysis of magnetic and nuclear quadrupole hyperfine structure in  $O_2$ -DF and global fit with IR data will be reported. The derived hyperfine parameters unambiguously establish the correspondence between the magnetic hyperfine constants and the two nuclei of the H(D)F.

<sup>&</sup>lt;sup>a</sup>E. M. Grumstrup, G. Sedo and K. R. Leopold, The 61<sup>st</sup> Symposium on Molecular Spectroscopy TE08 (2006)

<sup>&</sup>lt;sup>b</sup>W. A. Fawzy, C. M. Lovejoy, D. J. Nesbitt, and J. T. Hougen J. Chem. Phys. 117, 693(2002)