MICROWAVE SPECTRA OF O_2–HF AND O_2–DF AND GLOBAL FITTING WITH IR DATA: INSIGHT INTO THE NATURE OF HYPERFINE INTERACTIONS

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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[a] 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[b] 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.

[a] E. M. Grumstrup, G. Sedo and K. R. Leopold, *The 61st Symposium on Molecular Spectroscopy* **TE08** (2006)
[b] W. A. Fawzy, C. M. Lovejoy, D. J. Nesbitt, and J. T. Hougen *J. Chem. Phys.* **117**, 693(2002)