THE MOLECULAR FRAME ELECTRIC DIPOLE MOMENT AND HYPERFINE INTERACTIONS IN HAFNIUM FLUORIDE, HfF

ANH LE AND TIMOTHY C. STEIMLE, *Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287*; LEONID SKRIPNIKOV AND ANATOLY V. TITOV, *Petersburg Nuclear Physics Institute, Gatchina, 188300, Russia and Quantum Mechanics Division, St. Petersburg State University, St. Petersburg 198904, Russia*.

The identification of HfF^+ as a possible candidate for a d_e measurement has stimulated new interest in the spectroscopy of both HfF^+ [a, b, c] and neutral HfF [a, d]. Studies of the neutral are relevant because photoionization schemes can be used to produce the cations. More importantly, computational methodologies used to predict the electronic wavefunction of HfF^+ can be effectively assessed by making a comparison of predicted and experimental properties of the neutral, which are more readily determinable. The (1,0)[17.9]2.5 -$X^2\Delta_{3/2}$ band of hafnium monofluoride (HfF) has been recorded using high-resolution laser-induced fluorescence spectroscopy both field-free and in the presence of a static electric field. The field-free spectra of ^{177}HfF, ^{179}HfF, and ^{180}HfF were model to generate a set of fine and hyperfine parameters for the $X^2\Delta_{3/2}$ (v=0) and [17.9]2.5 (v=1) states. The observed optical Stark shifts for the ^{180}HfF isotopologue were analyzed to produce the molecular frame electric dipole moments of 1.66(1)D and 0.419(7)D for the $X^2\Delta_{3/2}$ and [17.9]2.5 states, respectively. A two-step *ab initio* calculation consisting of a two-component generalized relativistic effective core potential calculation (GRECP) followed by a restoration of the proper four-component wavefunction was performed to predict the properties of ground state HfF.

[a] B. J. Barker, I. O. Antonov, V. E. Bondybey, and M. C. Heaven, *J. Chem. Phys.*, **134**, 201102 (2011).

[b] K. C. Cossel, D. N. Gresh, L. C. Sinclair, T. Coffey, L. V. Skripnikov, A. N. Petrov, N. S. Mosyagin, A. V. Titov, R. W. Field, E. R. Meyer, E. A. Cornell and J. Ye, *Chem. Phys. Lett.*, **546**, 1 (2012).

[c] M. Grau, A. E. Leanhardt, H. Loh, L. C. Sinclair, R. P. Stutz, T. S. Yahn, and E. A. Cornell, *J. Mol. Spectroc.*, **272**, 32 (2012).

[d] H. Loh, R. P. Stutz, T. S. Yahn, H. Looser, R. W. Field, and E. A. Cornell, *J. Mol. Spectroc.*,**276-277**, 49 (2012).