

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

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The identification of  $\text{HfF}^+$  as a possible candidate for a  $d_e$  measurement has stimulated new interest in the spectroscopy of both  $\text{HfF}^+$  <sup>a, b, c</sup> and neutral  $\text{HfF}$  <sup>a, d</sup>. 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  $\text{HfF}^+$  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  $^{177}\text{HfF}$ ,  $^{179}\text{HfF}$ , and  $^{180}\text{HfF}$  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  $^{180}\text{HfF}$  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.

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