\( P, T \)-Odd and Magnetic Hyperfine Interaction Constants and Excited-State Lifetime for HfF\(^+\)

Timo Fleig\(^1\)

\(^1\)Laboratoire de Chimie et Physique Quantiques, IRSAMC, Université Paul Sabatier Toulouse III, 118 Route de Narbonne, F-31062 Toulouse, France

(Dated: February 27, 2018)

Parity- and time-reversal-symmetry violating interaction constants required for the interpretation of a recent measurement (arXiv:1704.07928 [physics.atom-ph]) of corresponding symmetry violations in the \( \Omega = 1 \) \((^3\Delta_1)\) science state of the HfF\(^+\) molecular ion are reported. Using a relativistic four-component all-electron multi-reference configuration interaction model the nucleon-electron scalar-pseudoscalar interaction constant is determined as \( W_S = 20.0 \) [kHz]. An updated result for the electron electric-dipole-moment effective electric field of \( |E_{\text{eff}}| = 22.7 \) [GV cm] is obtained. Further results of relevance in the context of the search for leptonic charge-parity violation such as magnetic hyperfine interaction constants and electronic \( G \)-tensor for HfF\(^+\) are presented.

INTRODUCTION

Electric dipole moments (EDMs) are a powerful probe of physics beyond the standard model (SM) of elementary particles in the regime of low energies \cite{1}. The underlying \( CP \) (charge-parity)-violating interactions \cite{2,3} give rise to \( T \) (time-reversal)-odd energy shifts which can be strongly enhanced in atomic matter including heavy nuclei \cite{4,5}. In polar molecules sensitive to lepton EDMs this enhancement can be several orders of magnitude larger than in corresponding heavy atoms \cite{6}. Such molecular systems thus hold great promise for the detection of a \( P, T \)-odd energy shift which in turn could help unravel observations in the universe yet unexplained by the SM, in particular related to its matter and energy content \cite{7-9}.

HfF\(^+\) is a paramagnetic system where the major sources of a potential \( P, T \)-odd molecular EDM are the electron EDM, \( d_e \), and the nucleon-electron scalar-pseudoscalar (ne-SPS) interaction, \( C_S \) \cite{10}. The sensitivity of HfF\(^+\) to these two \( CP \)-violating parameters allows for interpreting a null measurement and the upper bound to the molecular EDM through the corresponding interaction constants, \( W_d \) for the electron EDM and \( W_S \) for the ne-SPS interaction, respectively. The main objective of the present work is, therefore, the accurate calculation of \( W_S \) and a reassessment of \( W_d \) for the \( \Omega = 1 \) \((^3\Delta_1)\) state in which a recent measurement yielded an EDM-sensitive frequency shift of \( f^{BD} = 0.10 \pm 0.87_{\text{stat}} \pm 0.20_{\text{sys}} \) [mHz] \cite{11,12}. The measured shift is consistent with zero and this result and the presently calculated interaction constants for HfF\(^+\) are likely \cite{13} to lead to stronger constraints on \( d_e \) and \( C_S \), since the tightest upper bound on an EDM shift in a paramagnetic system thus far has been obtained from measurements on the ThO molecule \cite{14,15} where the heavy atom has a significantly larger proton number.

The following section briefly reviews definitions of interaction constants, the electronic \( G \)-tensor, and the method for calculating the lifetime of the relevant excited state in which the EDM experiment has been carried out. In the final section electronic-structure methods and technical parameters are defined, followed by a discussion of the present results and their consequences in view of further constraining \( CP \)-violation in the lepton sector.
THEORY

\( \mathcal{P}, \mathcal{T} \)-odd interaction constants

The electron EDM interaction constant is evaluated as proposed in stratagem II of Lindroth et al. [16] as an effective one-electron operator via the squared electronic momentum operator,

\[
E_{\text{eff}} = \frac{2ie\hbar}{c} \langle \Psi_{\Omega} | \sum_{j=1}^{n} \gamma_{j}^0 \gamma_{j}^5 \vec{p}_{j}^2 | \Psi_{\Omega} \rangle
\]

(1)

with \( n \) the number of electrons and \( j \) an electron index, as described in greater detail in reference [17]. The EDM effective electric field is related to the electron EDM interaction constant \( W_d = -\frac{i}{\Omega} E_{\text{eff}} \).

The ne-SPS interaction constant is defined and implemented [18] as

\[
W_S = \frac{i}{\Omega} \frac{G_F}{\sqrt{2}} Z \langle \Psi_{\Omega} | \sum_{j=1}^{n} \gamma_{j}^0 \gamma_{j}^5 \rho_K(\vec{r}_j) | \Psi_{\Omega} \rangle
\]

(2)

where \( G_F \) is the Fermi constant, \( Z \) is the proton number and \( \rho_K(\vec{r}_j) \) is the nuclear charge density at position \( \vec{r}_j \), normalized to unity.

Magnetic hyperfine interaction

The parallel component of the magnetic hyperfine interaction tensor is defined as follows (a.u.):

\[
A_{||}(K) = \frac{\mu_K[\mu_N]}{2eIm_p \Omega} \langle \Psi_{\Omega} | \sum_{i=1}^{n} \left( \vec{\alpha}_i \times \vec{r}_{iK} \right) \frac{z}{\vec{r}_{iK}} | \Psi_{\Omega} \rangle
\]

(3)

where \( \mu_K[\mu_N] \) is the magnetic moment of nucleus \( K \) in Bohr magnetons, \( \vec{\alpha} \) is a vector of Dirac matrices and \( \vec{r}_{iK} \) is the position vector relative to nucleus \( K \). Further details can be found in reference [19].

Excited-State Lifetime

The decay rate of an electronically excited state \( \psi_k \) to a state \( \psi_a \) via spontaneous emission of photons reads in electric-dipole (E1) approximation

\[
\Gamma_{ka} = \frac{4}{3} \frac{(\varepsilon_k - \varepsilon_a)^3}{\hbar^4 c^3} |D_{ak}|^2
\]

(4)

where \( \varepsilon_k - \varepsilon_a \) is the transition energy, \( D_{ak} \) is an electric transition dipole matrix element between states \( \Psi_a \) and \( \Psi_k \) and \( \hat{D} \) is the electronic electric dipole moment vector operator.

The ensuing lifetime \( \tau \) of the state \( \psi_k \) is determined as

\[
\tau_k = \frac{1}{\Gamma_{ka}}
\]

(5)

where only decay into state \( \psi_a \) (usually the electronic ground state) has been taken into account.

Electronic G-Tensor

The parallel component of the electronic G-tensor for a linear molecule is defined as

\[
G_{||} = \frac{1}{\Omega} \left\langle \Psi_{\Omega} | \hat{L}_n^e + g_s \hat{S}_n^e | \psi_{\Omega} \right\rangle
\]

(6)
with \( \hat{L}_n^6 = \hat{L} \cdot \hat{n} \) where \( \hat{n} \) is a unit vector along the molecular axis and \( g_s = -g_e = 2.00231930436182 \) is the free-electron g-factor. 

Thus, for a molecule in a \( ^3\Delta_1 \) state \( \Omega = 1 \), \( \Lambda = \pm 2 \), and \( \Sigma = \mp 1 \), so \( G_{||}(^3\Delta_1) \approx 0 \). However, spin-orbit interaction will mix states with deviant \( \Lambda \) and \( \Sigma \) quantum numbers into the state denoted \( ^3\Delta_1 \), e.g., a higher-lying \( ^1\Pi_1 \) state via

\[
\langle ^3\Delta_1 | \hat{H}_{SO} | ^1\Pi_1 \rangle \neq 0
\]

where \( \hat{H}_{SO} \) is a generic spin-orbit interaction Hamiltonian. It is, therefore, of importance to numerically determine \( G_{||}(^3\Delta_1) \) using molecular electronic wavefunctions including the effects of spin-orbit interaction.

**APPLICATION TO HFF**

**Technical details**

Atomic basis sets are of triple-\( \zeta \) quality \cite{21, 22} including core- and valence-correlating functions. The molecular spinor basis is obtained in Hartree-Fock approximation using the Dirac-Coulomb Hamiltonian (here in a.u.)

\[
\hat{H}^{DC} = \sum_i \left[ c_i \alpha_i \cdot p_i + \beta_i c^2 + \sum_j \frac{Z_A}{r_{ij}} \mathbb{1}_4 \right] + \sum_{i,j>i} \frac{1}{r_{ij}} \mathbb{1}_4 + V_{AB}
\]

where \( \alpha \) and \( \beta \) are Dirac matrices, \( Z_A \) is the proton number for nucleus \( A \), \( i, j \) are electron indices and \( V_{AB} \) is the classical electrostatic potential energy for the clamped nuclei. For the Fock operator in the Dirac-Coulomb-Hartree-Fock calculation valence configurations are averaged over Hf(6\( s^2 \)), Hf(6\( s^15\delta^1 \)), and Hf(5\( d^5 \)). For correlated calculations the wavefunction model MR\(_{12}\)-CISD(20) is used in the present. It corresponds to the parameter settings for the model MR-CISD(20) in ref. \cite{17}, however, using a larger active spinor space by adding four \( \pi \)-type and two \( \sigma \)-type Kramers pairs (all of Hf atomic character) from the virtual into the next lower space. Since for the eEDM effective electric field it has been shown that the inclusion of higher excitation ranks and the correlation of Hf outer-core electrons leads to only minor corrections which even largely cancel each other, the current model with 20 correlated electrons is considered sufficiently accurate. Further technical details on molecular wavefunctions can be found in reference \cite{17}.

For the determination of parallel magnetic hyperfine interaction constants \( (A_{J}) \) the following nuclear magnetic moments have been used \cite{23}: \( \mu = 0.7936 \mu_N \) for \(^{177}\)Hf with nuclear spin \( I = 7/2 \) and \( \mu = 2.62887 \mu_N \) for \(^{19}\)F with nuclear spin \( I = 1/2 \).

**Results and discussion**

All calculated constants for Hf\(^{+} \) are given in Table 1.

The g-tensor component \( G_{||}(\Omega = 1) \approx 0.013 \) a.u. is small but still roughly an order of magnitude larger than \( g_s \approx 0.00232 \). Since spin-orbit interaction is treated rigorously in the present approach, neither \( \Lambda \) nor \( \Sigma \) (or \( S \), for that matter) are exact quantum numbers of the CI state. Therefore, the state denoted \( \Omega = 1 \) is a mixture of terms \( ^3\Delta_1, ^1\Pi_1 \), and others. The determined value for \( G_{||}(\Omega = 1) \) indicates that a small contribution to the science state from a low-lying \( ^1\Pi_1 \) state, arising from an excitation \( 6s^1 \rightarrow 6p^1 \) on Hf is likely to be the main source of "contamination", since \( G_{||}(^1\Pi_1) = +1 \).

For the calculation of the excited-state lifetime from the decay rate (Eq. (4)) into the electronic ground state (\( \Omega = 0 \)) the experimental excitation energy of 991.83 cm\(^{-1} \) \cite{24} has been used. The required electric transition-dipole matrix element is with the model \( \nablaTZ/\text{MR}_{12}\)-CISD(20) calculated as \( \left| \psi_{\Omega=1} \right\rangle \left\langle \psi_{\Omega=0} \right| \hat{D} \left| \psi_{\Omega=0} \right\rangle \approx 0.0349 \) [Debye], yielding a lifetime of \( \tau_{\Omega=1} \approx 2.7 \) [s] which agrees well with the measured lifetime of \( \tau_{\exp} = 2.1(1) \) [s] \cite{11}.
The magnetic hyperfine interaction constant for the $^{19}$F nucleus agrees qualitatively with the value of $-62.0(2)$ [MHz] measured in reference [11]. However, the present electronic-structure model has not been designed with a focus on properties depending on spin density in the vicinity of the fluorine nucleus. On the other hand, the calculated hyperfine interaction constant for the $^{177}$Hf nucleus allows for an assessment of the accuracy of the molecular wavefunction for the electron EDM and ne-SPS interaction constants. At present, the author is not aware of a measurement of $A_{||}(^{177}$Hf) in the $\Omega = 1$ state of HfF$^+$ to compare with.

The electronic EDM effective electric field has been recalculated with the present slightly improved correlation model, and a small decrease of its value by $-0.6 \left[ \text{GV cm}^{-1} \right]$ (or 2.5%) relative to the result reported in reference [17] is observed. A related drop of $E_{\text{eff}}$ also occurs in the valence isoelectronic ThF$^+$ molecular ion [18] and its origin is explained in reference [19].

$\mathcal{P}, \mathcal{T}$-odd energy shifts are defined as $\Delta E_{\mathcal{P},\mathcal{T}} = -d_e E_{\text{eff}} = d_e W_d \Omega$ for the electron EDM, where $W_d = -E_{\text{eff}}/\Omega$, and $\Delta E_{\mathcal{P},\mathcal{T}} = C_S W_S \Omega$ for the ne-SPS interaction. Therefore, the ratio of the energy shifts due to leptonic ($W_d$) and semi-leptonic ($W_S$) interaction constants is proportional to the ratio of these interaction constants. Thus,

$$\frac{W_d}{W_S} = -\frac{E_{\text{eff}}}{\Omega W_S}. \quad (9)$$

With the interaction constants determined in the present work, $\frac{W_d}{W_S}(\text{HfF}^+) \approx 274.5 \left[ \text{GV cm}^{-1} \right]$ for the science state with $\Omega = 1$. This ratio differs significantly from the one for ThO ($\Omega = 1$) where $\frac{W_d}{W_S} \approx 172 \left[ \text{GV cm}^{-1} \right]$ [20], which is predominantly due to the large difference in proton number between Th ($Z = 92$) and Hf ($Z = 72$) [27, 28]. Consequently, accounting for both leading $\mathcal{P}, \mathcal{T}$-odd enhancements in the paramagnetic system HfF$^+$ and the result of the recent measurement [11] will likely lead to stronger constraints on the $\mathcal{CP}$-violating parameters $d_e$ and $C_S$ through the procedure of global fits [13, 29].

The more detailed discussion of electronic-structure models for HfF$^+$ in reference [17] suggests that the uncertainty for both $W_d$ and $W_S$ presented here remains at 5%, although a more accurate active-space model has been employed in the present work. The same applies to the heavy-atom magnetic hyperfine constant $A_{||}(^{177}$Hf) with reference to earlier studies of hyperfine interaction on valence isoelectronic systems [18, 26]. The uncertainties for $G_{||}$ and the molecule-frame EDM $D$ are estimated to be 10% and 15%, respectively, in accord with the discussion in reference [30].
TABLE I: Molecule-frame static electric dipole moment, electron EDM and ne-S-PS interaction constants, parallel component of electronic G tensor, excited-state lifetime, and magnetic hyperfine interaction constants for the $\Omega = 1 \left( ^3\Delta_1 \right)$ science state of HfF$^+$. All values are given for the Hf nucleus at the origin of the reference frame and the F nucleus at $-3.4384$ a.u. on the z axis. The molecule-frame dipole moment corresponds to an origin located at the center of mass.

| CI Wavefunction model | $D$ [Debye] | $E_{\text{eff}}$ [GV/cm] | $W_S$ [kHz] | $G_{||}$ [a.u.] | $\tau$ [s] | $A_{||}(^{177}\text{Hf})$ [MHz] | $A_{||}(^{19}\text{F})$ [MHz] |
|----------------------|------------|-----------------|-------------|----------------|----------|----------------------|----------------------|
| vTZ/MR12-CISD(20)    | 4.19       | -22.7           | 20.0        | 0.0127         | 2.7      | -1328                | -43.0                |
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