

Lorentz and *CPT* violation and the hydrogen and antihydrogen molecular ions. II. Hyperfine-Zeeman spectrum

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(Received 22 May 2025; accepted 22 July 2025; published 15 September 2025)

Fundamental principles of quantum field theory (QFT) such as Lorentz invariance, *CPT* symmetry, and locality may be tested to extremely high precision in atomic and molecular spectroscopy. The narrow natural linewidth of rovibrational states in the hydrogen molecular ion H_2^+ and its antimatter counterpart $\bar{H}_2^-$ make these ideal candidates, and give $O(m_p/m_e)$ increased sensitivity to Lorentz and *CPT* violation in the proton sector compared to H and $\bar{H}$ atoms. In a previous paper, we presented a detailed analysis of the rovibrational spectrum of H_2^+ and $\bar{H}_2^-$ in an effective QFT encoding Lorentz and *CPT* violation, focusing on spin-independent effects. Here, we extend this analysis to include the full hyperfine-Zeeman spectrum and include spin-dependent Lorentz and *CPT* violating operators in the effective theory. The results demonstrate how constraints on these symmetry-violating couplings may be extracted from specific rovibrational transitions between hyperfine-Zeeman states in the presence of an applied magnetic field.

DOI: [10.1103/vby7-p924](https://doi.org/10.1103/vby7-p924)

I. INTRODUCTION

The extremely narrow natural linewidth of rovibrational states in the hydrogen molecular ion H_2^+ [1], together with recent theoretical and experimental developments [2,3], opens up the possibility of testing fundamental physics principles such as Lorentz and *CPT* symmetry with high-precision rovibrational spectroscopy at levels potentially approaching 1 part in 10^{17} . Meanwhile, the increasing precision of 1S-2S spectroscopy in atomic antihydrogen [4,5] further raises the prospect of future high-precision rovibrational spectroscopy with the antimolecular ion $\bar{H}_2^-$ [6–8].

In a recent paper [9] (hereafter referred to as Paper I), we presented a detailed investigation of the potential effects of Lorentz and *CPT* violation on the rovibrational spectrum of H_2^+ and $\bar{H}_2^-$ [10,11]. In particular, we showed how, in addition to improved experimental precision, rovibrational spectroscopy of the H_2^+ and $\bar{H}_2^-$ molecular ions permits an enhancement of $O(m_p/m_e)$ in sensitivity to Lorentz and *CPT* violation in the proton sector compared to the corresponding H and $\bar{H}$ atomic spectroscopy [11–13].

Our analysis was conducted in the framework of the effective theory of Lorentz and *CPT* violation known as the

Standard Model extension (SME) [14,15]. Here, the standard QED Lagrangian is augmented by Lorentz tensor operators with couplings which, if nonzero, would break Lorentz invariance and in some cases also *CPT*. In the form we use in this paper, the Lagrangian for a single Dirac fermion field $\psi(x)$ is taken to be

$$\begin{aligned} \mathcal{L}_{\text{SME}} = & \frac{1}{2} \int d^4x \left[\bar{\psi} (i\gamma^\mu \partial_\mu - m) \psi - a_\mu \bar{\psi} \gamma^\mu \psi + i c_{\mu\nu} \bar{\psi} \gamma^\mu \partial^\nu \psi \right. \\ & + a_{\mu\nu\lambda} \bar{\psi} \gamma^\mu \partial^\nu \partial^\lambda \psi - b_\mu \bar{\psi} \gamma^5 \gamma^\mu \psi + i d_{\mu\nu} \bar{\psi} \gamma^5 \gamma^\mu \partial^\nu \psi \\ & \left. - \frac{1}{2} H_{\mu\nu} \bar{\psi} \sigma^{\mu\nu} \psi + \frac{1}{2} i g_{\mu\nu\lambda} \bar{\psi} \sigma^{\mu\nu} \partial^\lambda \psi + \dots \right] \\ & + \text{H.c.} \end{aligned} \quad (1.1)$$

While the SME does not by any means exhaust the possibilities for Lorentz and *CPT* violation—for example, it remains a local Lagrangian quantum field theory built from causal fields and respecting the equality of masses for particles and antiparticles—it is especially valuable in showing in a systematic way how Lorentz and *CPT* violating effects may manifest themselves in many different ways, e.g. appearing in certain spectroscopic transitions but not others. Further motivation and discussion of our approach is given in Paper I.

In this sequel, we extend the analysis of Paper I in two main directions. First, we take fully into account the hyperfine and Zeeman structure of the H_2^+ spectrum, including the mixing of states in an applied magnetic field. We consider in detail both high and low magnetic field

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regimes, keeping in mind that while current measurements with H_2^+ are carried out in small fields, future $\bar{\text{H}}_2^-$ spectroscopy will most probably be conducted in a high-field regime [2,6,7].

Second, whereas in Paper I we considered only the spin-independent couplings in the SME Hamiltonian derived from (1.1) [15–17], [see Eqs. (3.1) and (3.2) below], here we extend our analysis to the full set of SME couplings including those $(b_\mu, g_{\mu\nu\lambda}, d_{\mu\nu}, H_{\mu\nu})$ which couple to the electron and proton spins. While these are more tightly constrained [18] by existing spin-precession experiments than the spin-independent couplings $(c_{\mu\nu}, a_{\mu\nu\lambda})$, the rich structure and high measurement precision possible with the molecular ion motivates their study in this context.

In a recent paper [19], the issue of testing Lorentz and *CPT* symmetry with H_2^+ and $\bar{\text{H}}_2^-$ spectroscopy was also addressed within the SME framework, though with a rather different focus and application from the work presented here. In particular, a main focus of [19] is the possibility of constraining SME couplings through sidereal variations, emphasizing the nonminimal SME, though only considering some of the leading-order effects in the molecular dynamics described here and in Paper I.¹ Together, these papers should provide complementary insights and help provide theoretical input into the design of an experimental program of high-precision rovibrational spectroscopy tailored to provide maximum sensitivity to potential Lorentz and *CPT* violation.

The paper is organized as follows. In Sec. II, we review the hyperfine-Zeeman structure of the spectrum of H_2^+ , emphasizing the dependence of the energy levels on the rovibrational quantum numbers (v, N) . Then, in Sec. III, we summarize the application of the Born-Oppenheimer approximation to H_2^+ in the presence of both spin-independent and spin-dependent Lorentz and *CPT* violating operators in the Hamiltonian giving the effective Schrödinger equations in the electron and proton sectors.

Sections IV and V contain the main physics development in the paper. The extended Born-Oppenheimer analysis, described in detail in Paper I, shows that Lorentz and *CPT* violation affects the rovibrational spectrum in two ways—directly through the SME couplings in the Schrödinger equation describing the rovibrational motion of the protons, and indirectly through the modifications of the internucleon potential due to the binding electron (but note this is also

sensitive to the proton SME couplings). The analysis of Paper I for the spin-independent couplings is extended to include the hyperfine-Zeeman mixing and magnetic field dependence in Sec. IV, while an extensive study of the effects of the spin-dependent couplings is given in Sec. V.

This development is taken up again in Sec. VII, while meanwhile Sec. VI and Appendix A present an equivalent analysis using the SME Hamiltonian in the widely-used spherical tensor formalism, extended and adapted to the dynamics of the molecular ion. This would provide the basis for an extension of our results to the nonminimal SME. These sections may be omitted by readers interested primarily in the physics results for the rovibrational spectrum.

In Sec. VII, our results for the SME-modified internucleon potential are translated into energy-level shifts in the rovibrational spectrum using the general methods developed in Paper I. We present our results in the form of an expansion of the rovibrational energy levels as

$$\begin{aligned} \Delta E_{vNJM_J}^{\text{SME}} = & \mathcal{E}_{\text{SME}} + \delta_{\text{SME}} \left(v + \frac{1}{2} \right) \omega_0 + B_{\text{SME}} N(N+1) \omega_0 \\ & - x_{\text{SME}} \left(v + \frac{1}{2} \right)^2 \omega_0 - \alpha_{\text{SME}} \left(v + \frac{1}{2} \right) N(N+1) \omega_0 \\ & - D_{\text{SME}} (N(N+1))^2 \omega_0 + \dots \end{aligned} \quad (1.2)$$

where ω_0 is the fundamental vibration frequency. We give explicit expressions for $\mathcal{E}_{\text{SME}}$ and the coefficients $\delta_{\text{SME}}, B_{\text{SME}}, \dots$ for each hyperfine-Zeeman state in terms of the rovibrational and angular momentum quantum numbers and corresponding SME couplings.

Two further appendixes provide a collection of useful relations involving Clebsch-Gordan coefficients, and a brief summary of the implications of our results for the potential detection of Lorentz violation through annual, and sidereal, variations of the transition frequencies.

II. THE ROVIBRATIONAL, HYPERFINE, AND ZEEMAN SPECTRUM OF H_2^+ AND $\bar{\text{H}}_2^-$

We begin with a brief review of the main features of the hyperfine-Zeeman spectrum for H_2^+ [20–22], and equivalently $\bar{\text{H}}_2^-$, which we need later to describe the Lorentz and *CPT* violating effects. We focus here on the simplest case, Para- H_2^+ , since this is sufficient to illustrate all the main principles and is the main subject of current experiments, but comment on the more complicated case of Ortho- H_2^+ where relevant.

In general, the energy eigenstates of H_2^+ at zero applied magnetic field are described by the quantum numbers $|vNSIFJM_J\rangle$. Before including spin, the rovibrational energy levels are described by $|vN\rangle$, where v is the vibrational quantum number and N is the molecular orbital angular momentum, with quantum numbers N, M_N . The electron spin is S , with quantum numbers $S = 1/2$ and M_S . The nucleon spin is I and we define the total molecular spin

¹Notably, Ref. [19] does not consider the terms here proportional to $\text{tr}_Y(p_a p_b)$, and therefore their associated SME couplings. This expectation value is nonzero because the molecule only has cylindrical and not spherical symmetry, and is smaller but comparable in magnitude to $\text{tr}(p_a p_b)$. Another important approximation in [19] is the neglect of terms beyond δ_{SME} in the expansion (1.2), in particular the leading $N(N+1)$ dependence. On the other hand, [19] includes contributions to the energy levels of fourth order in momentum associated with higher-dimension SME operators, which we do not consider here.

by $\mathbf{F} = \mathbf{I} + \mathbf{S}$. Spin-statistics requires that for $I = 0$ (Para- H_2^+), N is even, while $I = 1$ (Ortho- H_2^+) requires N odd. The total angular momentum is then $\mathbf{J} = \mathbf{N} + \mathbf{F}$.

For Para- H_2^+ therefore, since $I = 0$ and $F = S = 1/2$ always, we characterize the molecular rovibrational-spin states simply by $|vNJM_J\rangle$. It will also be useful to consider the alternative representation with states $|vNM_NM_S\rangle$, which are the eigenstates at large applied magnetic field $\mathbf{B}$.

A. Hyperfine-Zeeman Hamiltonian

The hyperfine and Zeeman interactions for Para- H_2^+ are then

$$H_{\text{HFS}} = c_e(v, N) \mathbf{N} \cdot \mathbf{S} = \frac{1}{2} c_e(v, N) (\mathbf{J}^2 - \mathbf{N}^2 - \mathbf{S}^2), \quad (2.1)$$

and

$$H_Z = g_e \mu_B \mathbf{S} \cdot \mathbf{B} - g_m(v, N) \mu_B \mathbf{N} \cdot \mathbf{B} = \mu_B B (g_e S_3 - g_m(v, N) N_3), \quad (2.2)$$

in the EXP frame with 3-axis aligned with the applied magnetic field.

H_{HFS} describes the spin-orbit interaction between the electron spin and the molecular orbital angular momentum.² Evidently, J and M_J are good quantum numbers for this interaction, so at zero magnetic field the energy eigenstates are naturally labeled as $|vNJM_J\rangle$. The coupling $c_e(v, N)$ depends on the rovibrational state and can be calculated at $O(\alpha^2)$ in nonrelativistic QED. Explicit values are given in Table 1 of [20], which includes a very detailed discussion of the hyperfine structure of both Para- and Ortho- H_2^+ . For illustration, a typical value for a low-lying rovibrational state is (in $h = 1$ units) $c_e(0, 2) = 42.1625$ MHz.

The form of the Zeeman interaction (2.2) requires some justification. Although the electron is in the $1s\sigma_g$ ground state, its orbital angular momentum $\mathbf{N}_e$ is not exactly zero because unlike the hydrogen atom the molecular ion only possesses cylindrical and not spherical symmetry. Compared to the orbital angular momentum $\mathbf{N}_p$ of the proton it is of $O(m_e/m_p)$, but this is compensated by the g -factor

coefficients such that both $\mathbf{N}_p$ and $\mathbf{N}_e$ contribute approximately equally to the Zeeman energy.

To justify (2.2) therefore, we have to demonstrate that the elementary Zeeman Hamiltonian in terms of $\mathbf{N}_e$ and $\mathbf{N}_p$ satisfies

$$\begin{aligned} \mu_B B \langle vNJ'M_J | \left(N_{e3} - \frac{2m_e}{m_p} N_{p3} \right) | vNJM_J \rangle \\ = -g_m(v, N) \mu_B B \langle vNJ'M_J | N_3 | vNJM_J \rangle, \end{aligned} \quad (2.3)$$

where the factor 2 is due to the reduced mass $m_p/2$ of the protons.

Now, inspection of (2.1)–(2.3) shows that M_J remains a good quantum number in the presence of an applied magnetic field but J is not. The Zeeman interaction induces mixing between the states with $J = N \pm \frac{1}{2}$ for fixed M_J [as indicated in (2.3)], except for the unique (“stretched”) states where $M_J = \pm(N + \frac{1}{2})$ which occur only for $J = N + \frac{1}{2}$. To justify the identification (2.3) and find the effective g -factor $g_m(v, N)$, we therefore need to compare the matrix elements on both sides for $J', J = N \pm \frac{1}{2}$ including the off-diagonal elements.

To evaluate these, first write the $|vNJM_J\rangle$ states in terms of the $|vNM_NM_S\rangle$ basis states as follows:

$$|vNJM_J\rangle = \sum_{M_S} C_{NM_N, \frac{1}{2}M_S}^{JM_J} |vNM_NM_S\rangle, \quad (2.4)$$

where $M_N = M_J - M_S$. We will make extensive use of these Clebsch-Gordan coefficients in what follows, so it is convenient to record them here, for $J = N \pm \frac{1}{2}$:

$$\begin{aligned} C_{NM_J \mp \frac{1}{2}, \frac{1}{2} \pm \frac{1}{2}}^{N + \frac{1}{2} M_J} &= \frac{1}{\sqrt{2N+1}} \sqrt{N + \frac{1}{2} \pm M_J}, \\ C_{NM_J \mp \frac{1}{2}, \frac{1}{2} \pm \frac{1}{2}}^{N - \frac{1}{2} M_J} &= \mp \frac{1}{\sqrt{2N+1}} \sqrt{N + \frac{1}{2} \mp M_J}. \end{aligned} \quad (2.5)$$

The matrix elements of S_3 are readily evaluated in the $|vNM_NM_S\rangle$ basis [see (B4)], giving

$$\begin{aligned} \langle vNJ' = N \pm \frac{1}{2} M_J | S_3 | vNJ = N \pm \frac{1}{2} M_J \rangle &= \pm \frac{1}{2N+1} M_J, \\ \langle vNJ' = N \mp \frac{1}{2} M_J | S_3 | vNJ = N \pm \frac{1}{2} M_J \rangle &= -\frac{1}{2N+1} \sqrt{\left(N + \frac{1}{2}\right)^2 - M_J^2}, \end{aligned} \quad (2.6)$$

²We follow the common nomenclature and refer to all the spin and angular momentum interactions, perhaps loosely, as “hyperfine,” even though (2.1) is a spin-orbit interaction. For Ortho- H_2^+ there are five such couplings including $b_p(v, N) \mathbf{I} \cdot \mathbf{S}$ and $c_I(v, N) \mathbf{N} \cdot \mathbf{I}$ together with two more complicated interactions amongst $\mathbf{N}$, $\mathbf{I}$, and $\mathbf{S}$. See Ref. [20] for details and values for the coefficients $b_F, c_e, c_I, \dots$

and the matrix elements of N_3 follow directly using $N_3 = J_3 - S_3$. Explicitly,

$$\langle vNJ'M_J|N_3|vNJM_J\rangle = \frac{1}{2N+1} \begin{cases} 2NM_J, & (J' = J = N + \frac{1}{2}) \\ 2(N+1)M_J, & (J' = J = N - \frac{1}{2}) \\ \sqrt{(N + \frac{1}{2})^2 - M_J^2}, & (J' = N \mp \frac{1}{2}, J = N \pm \frac{1}{2}). \end{cases} \quad (2.7)$$

Next, consider the matrix elements of N_{e3} in (2.3). In this case, remembering that N_{e3} does not act on the electron spin states, we can use the Wigner-Eckart theorem to write

$$\langle vNNM_N|N_{e3}|vNM_NM_S\rangle = C_{NM_N,10}^{NM_N} \langle vN||N_e||vN\rangle, \quad (2.8)$$

where $C_{NM_N,10}^{NM_N} = 1/\sqrt{N(N+1)}$. Using the Clebsch-Gordan coefficients in (2.5) we can then express the required matrix elements for N_{e3} in terms of these reduced matrix elements involving only the rovibrational quantum numbers. We find

$$\begin{aligned} \langle vNJ'M_J|N_{e3}|vNJM_J\rangle &= \frac{1}{2N+1} \frac{1}{\sqrt{N(N+1)}} \langle vN||N_e||vN\rangle \\ &\times \begin{cases} 2NM_J, & (J' = J = N + \frac{1}{2}) \\ 2(N+1)M_J, & (J' = J = N - \frac{1}{2}) \\ \sqrt{(N + \frac{1}{2})^2 - M_J^2}, & (J' = N \mp \frac{1}{2}, J = N \pm \frac{1}{2}) \end{cases} \end{aligned} \quad (2.9)$$

with a similar result for N_{p3} .

Comparing (2.7) and (2.9), we verify the proposed identification (2.2) for the Zeeman Hamiltonian in terms of the total molecular orbital angular momentum $\mathbf{N}$ with the identification,

$$g_m(v, N) = \frac{1}{\sqrt{N(N+1)}} \left(-\langle vN||N_e||vN\rangle + \frac{2m_e}{m_p} \langle vN||N_p||vN\rangle \right). \quad (2.10)$$

The reduced matrix elements have been calculated using precision variational estimates for the rovibrational wave functions for H_2^+ and are given in [22] for low values of (v, N) .³ The identification is $g_m(v, N) = g_{\text{rot}}(v, N)m_e/m_p$, with $g_{\text{rot}}(v, N)$ given in Table 1 of [22]. For illustration, a typical value is $g_m(0, 2) = 0.9198m_e/m_p$.

³As evident from (2.14) below, the off-diagonal matrix elements only contribute to the energies at $O(B^2)$ and can be neglected in the weak-field approximation. Noting from above that the diagonal matrix elements are all proportional to M_J , the Zeeman Hamiltonian may be approximated at weak field, only, by

$$H_Z \simeq g_J(v, N, J)\mu_B \mathbf{J} \cdot \mathbf{B},$$

with an effective Landé g -factor,

$$g_J(v, N, J) = \begin{cases} \frac{1}{2N+1}(g_e - 2Ng_m(v, N)), & (J = N + \frac{1}{2}) \\ -\frac{1}{2N+1}(g_e + 2(N+1)g_m(v, N)), & (J = N - \frac{1}{2}) \end{cases}$$

as realized in the diagonal elements of (2.14). This may be compared with [22], where these two contributions to g_J are denoted $g_1(N, J)$ and $g_3(v, N, J)$ respectively. Note however that our derivation here determines the angular momentum g -factor $g_m(v, N)$ independently of being in the weak or strong magnetic field regime.

A similar analysis may be made for Ortho- H_2^+ , starting from the representation (2.12) of the relevant states. In this case there are three contributions to the Landé g -factor corresponding to the three terms in the Zeeman Hamiltonian (2.11), and they each depend additionally on the total spin quantum number F . Full details are given in [22].

For Ortho- H_2^+ , the proton spins are aligned so that $I = 1$ and spin-statistics implies N is odd. The Zeeman interaction is generalized to

$$H_Z = g_e \mu_B \mathbf{S} \cdot \mathbf{B} - g_p \mu_p \mathbf{I} \cdot \mathbf{B} - g_m(v, N) \mu_B \mathbf{N} \cdot \mathbf{B}, \quad (2.11)$$

with $\mu_p = (m_e/m_p)\mu_B$. Since $I = 1$, $S = 1/2$ always, we abbreviate the notation for the states here to $|vNFM_J\rangle$. Again, M_J remains a good quantum number for both the hyperfine and Zeeman interactions, but the energy levels are now split in both J and F .

The effective orbital angular momentum g -factor $g_m(v, N)$ in (2.11) is naturally unchanged and is still given in terms of reduced matrix elements by (2.10). To see this explicitly, and evaluate the weak-field g -factors described in footnote 3, it is convenient first to reexpress the states in the form

$$|vNFM_J\rangle = \sum_{M_F, M_S} C_{NM_N, Fm_F}^{JM_J} C_{1M_I, \frac{1}{2}M_S}^{FM_F} |vNM_J M_F M_S\rangle, \quad (2.12)$$

where of course $M_I = M_F - M_S$ and $M_N = M_J - M_F$. The analysis above can then be carried through using orthonormality relations to simplify the additional Clebsch-Gordan factors and verify (2.10) still holds. A complete set of values for the Landé g -factors for Ortho- H_2^+ is given in [22].

B. Hyperfine-Zeeman energy spectrum

Given the hyperfine and Zeeman Hamiltonians in the form (2.1), (2.2), we can now readily evaluate the energy spectrum. With zero magnetic field, $|vNFM_J\rangle$ are eigenstates of H_{HFS} and we find immediately

$$\langle vNFM_J | H_{\text{HFS}} | vNFM_J \rangle = \begin{cases} \frac{1}{2} N c_e(v, N), & (J = N + \frac{1}{2}) \\ -\frac{1}{2} (N + 1) c_e(v, N), & (J = N - \frac{1}{2}) \end{cases} \quad (2.13)$$

with hyperfine energy splitting $(N + \frac{1}{2})c_e(v, N)$.

Combining with the results above for the matrix elements of H_Z , we can express the matrix elements of the full hyperfine-Zeeman Hamiltonian in the $|vNFM_J\rangle$ basis in the form

$$\begin{aligned} & \langle vNJ'M_J | H_{\text{HFS}} + H_Z | vNFM_J \rangle \\ &= \begin{pmatrix} \frac{1}{2} N c_e + \frac{1}{2N+1} (g_e - 2Ng_m) \mu_B B M_J & -\frac{1}{2N+1} \sqrt{\left(N + \frac{1}{2}\right)^2 - M_J^2} (g_e + g_m) \mu_B B \\ \text{Sym} & -\frac{1}{2} (N + 1) c_e(v, N) - \frac{1}{2N+1} (g_e + 2(N + 1)g_m) \mu_B B M_J \end{pmatrix} \end{aligned} \quad (2.14)$$

with rows/columns corresponding to $J = N \pm \frac{1}{2}$. Notice that for the states $J = N + \frac{1}{2}$, $M_J = \pm(N + \frac{1}{2})$ where there is no mixing, the off-diagonal elements here vanish. The energy eigenvalues in this case are simply read off from the top left element,

$$E(B)|_{M_J=\pm(N+\frac{1}{2})} = \frac{1}{2} N c_e(v, N) \pm \frac{1}{2} (g_e - 2Ng_m(v, N)) \mu_B B. \quad (2.15)$$

The energy eigenvalues $E(B)$ for the mixed states are given by the eigenvalues of this matrix, and after some algebra we find

$$E_{\pm}(B) = -\frac{1}{4} c_e(v, N) - g_m \mu_B B M_J \pm \frac{1}{2} \left[\left(N + \frac{1}{2}\right)^2 c_e^2 + 2c_e(g_e + g_m) \mu_B B M_J + (g_e + g_m)^2 (\mu_B B)^2 \right]^{\frac{1}{2}}. \quad (2.16)$$

For small B , the energies may be expanded as

$$\begin{aligned} E_+(B) &= \frac{1}{2} N c_e(v, N) + \frac{1}{2N+1} (g_e - 2Ng_m(v, N)) \mu_B B M_J, \\ E_-(B) &= -\frac{1}{2} (N + 1) c_e(v, N) - \frac{1}{2N+1} (g_e + 2(N + 1)g_m(v, N)) \mu_B B M_J, \end{aligned} \quad (2.17)$$

where the expansion parameter is $\mu_B B / c_e(v, N) \simeq B/3$ mT for small values of (v, N) . This defines the range of validity of the “small” or “large” B approximations.

For large B , we find

$$\begin{aligned} E_+(B) &= \left(\frac{1}{2} g_e - g_m(v, N) \left(M_J - \frac{1}{2} \right) \right) \mu_B B + \frac{1}{2} c_e(v, N) \left(M_J - \frac{1}{2} \right), \\ E_-(B) &= \left(-\frac{1}{2} g_e - g_m(v, N) \left(M_J + \frac{1}{2} \right) \right) \mu_B B - \frac{1}{2} c_e(v, N) \left(M_J + \frac{1}{2} \right), \end{aligned} \quad (2.18)$$

which we recognize as the eigenvalues corresponding to the high-field eigenstates $|v N M_N M_S\rangle$ with $M_S = \pm \frac{1}{2}$. The expansion parameter in this case is clearly $c_e(v, N) / \mu_B B$.

These results are illustrated for the particular case of the rovibrational level $v = 0, N = 2$ in Fig. 1, using the input parameters for $c_e(0, 2)$ and $g_m(0, 2)$ quoted above. This reproduces the corresponding plot in the review [1] (see supplementary information there). The hyperfine splitting $(N + \frac{1}{2})c_e(v, N)$ at zero magnetic field in this case is approximately 105 MHz. Of course at the level of resolution of the plots, the effect of $g_m(v, N) \sim O(m_e/m_p)$ is not visible and the Zeeman energies are dominated by the electron spin term. This explains the form of the spectrum at large B , which splits into two sets of states with energies

rising (for $M_S = \frac{1}{2}$) or falling (for $M_S = -\frac{1}{2}$) linearly with B .⁴

III. BORN-OPPENHEIMER ANALYSIS WITH LORENTZ AND *CPT* VIOLATION

The dynamical analysis of the spectrum of the H_2^+ and $\bar{H}_2^-$ molecular ions is carried out in the framework of the Born-Oppenheimer approximation, extended here to include Lorentz and *CPT* violation. This was described in Paper I for the spin-independent SME couplings $c_{\mu\nu}$ and $a_{\mu\nu\lambda}$, and here we extend this to include also the spin-dependent couplings b_μ , $g_{\mu\nu\lambda}$, $d_{\mu\nu}$, and $H_{\mu\nu}$.

First recall the form of the nonrelativistic SME Hamiltonian for a single Dirac fermion, derived from the original QFT Lagrangian (1.1):

$$\begin{aligned} H_{\text{SME}} &= (A + 2B_k S^k) + (C_i + 2D_{ik} S^k) \frac{p^i}{m} \\ &\quad + (E_{ij} + 2F_{ijk} S^k) \frac{p^i p^j}{m^2}. \end{aligned} \quad (3.1)$$

We require only the even-parity operators, with coefficients [15–17]

$$\begin{aligned} A &= a_0 - mc_{00} + m^2 a_{000}, \\ B_k &= -b_k + md_{k0} + \frac{1}{2} \epsilon_{kmn} (H_{mn} - mg_{mn0}), \\ E_{ij} &= -m \left(c_{ij} + \frac{1}{2} c_{00} \delta_{ij} \right) + m^2 (3a_{0ij} + a_{000} \delta_{ij}), \\ F_{ijk} &= \frac{1}{2} \left[\frac{1}{2} (b_k \delta_{ij} - b_j \delta_{ik}) + m \left(d_{0j} + \frac{1}{2} d_{j0} \right) \delta_{ik} \right. \\ &\quad \left. - \frac{1}{4} \delta_{ik} \epsilon_{jmn} H_{mn} - m \epsilon_{ikm} \left(g_{m0j} + \frac{1}{2} g_{mj0} \right) \right] \\ &\quad + (i \leftrightarrow j), \end{aligned} \quad (3.2)$$

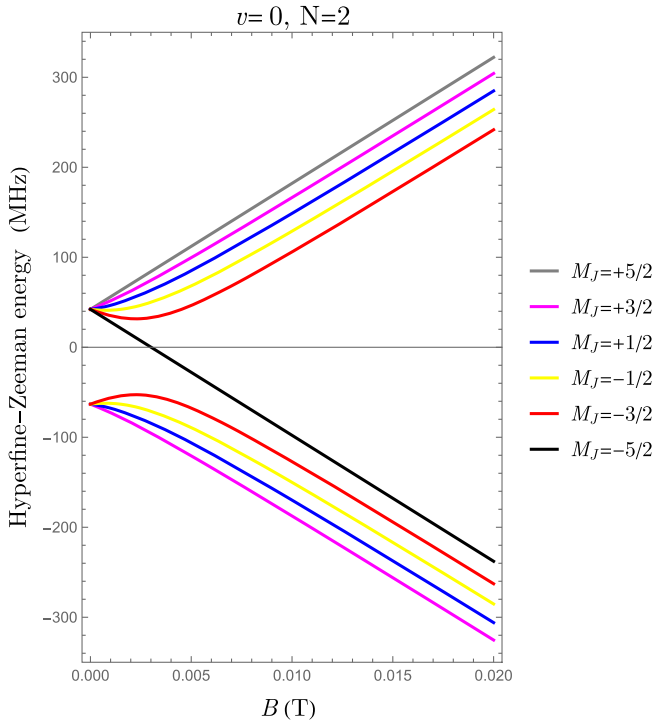


FIG. 1. Hyperfine-Zeeman energies for the rovibrational level $(v, N) = (0, 2)$. For general N , the eigenstates for given M_J are linear combinations of states with $J = N \pm \frac{1}{2}$ and are doubled, apart from the unmixed states $J = N + \frac{1}{2}, M_J = \pm(N + \frac{1}{2})$.

⁴It is interesting to contrast this with the corresponding hyperfine-Zeeman spectrum for the H atom with $L \neq 0$, for example the $2P$ states. This shows many similarities with the above analysis, except that for the atom the orbital angular momentum Zeeman interaction is not suppressed by $O(m_e/m_p)$ as here, resulting in a qualitatively different energy level diagram (see, for example, Refs. [12,23]).

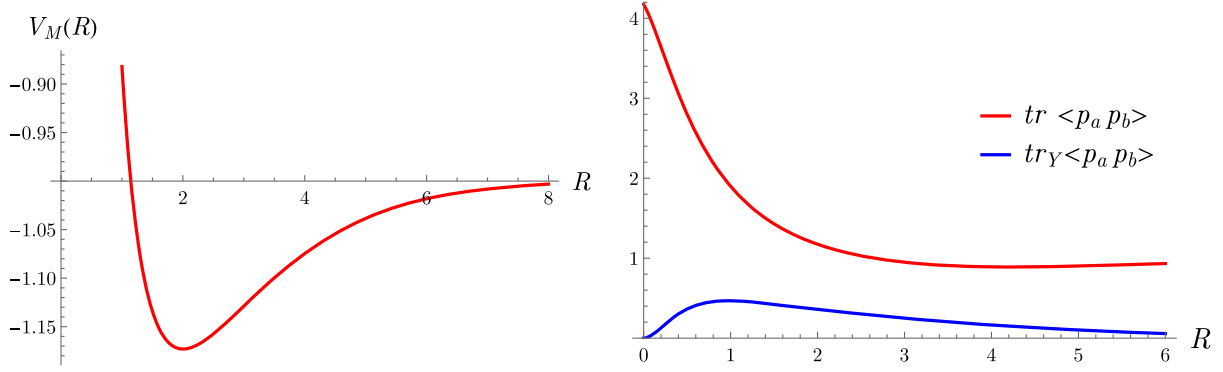


FIG. 2. The left-hand figure shows the internucleon potential $V_M(R)$ as a function of the bond length R . The equilibrium bond length is $R_0 = 2.003$ (in “atomic units,” see Paper I). The right-hand figure shows the momentum expectation values in the electron $1s\sigma_g$ ground state which determine the SME potential $V_{\text{SME}}^e(R)$.

where for later convenience we have explicitly symmetrized the F_{ijk} coupling on i, j . Note also that the overall constant term A is unobservable in spectroscopy.

The fundamental idea of the Born-Oppenheimer analysis is to separate the full Schrödinger equation for the molecular ion into two separate equations, the first describing the electron motion relative to the nucleon centre-of-momentum (CM) and the second describing the rovibrational motion of the nucleons. The energy eigenvalues of the electron Schrödinger equation depend on the internucleon separation R and feed back into the nucleon Schrödinger equation as a potential $V_M(R)$, which determines the rovibrational motion. $V_M(R)$ has the characteristic shape of a Morse potential, and a numerical determination is shown in Fig. 2, taken from Paper I.

The key step is to factorize the spatial part of the molecular wave function into nucleon and electron parts: $\Psi(\mathbf{R}, \mathbf{r}) = \Phi(\mathbf{R})\psi(\mathbf{r}; R)$. The spin operators are spectators at this stage, but the momentum dependence of the SME interactions is important. The effective electron Schrödinger equation is then,⁵

$$\left[-\frac{1}{2\hat{\mu}} \nabla_{\mathbf{r}}^2 + V_{\text{mol}}(R, r_{1e}, r_{2e}) + \frac{1}{m_e^2} (E_{ab}^e + F_{abk}^e S_k) p_a p_b + \frac{1}{2m_p^2} (E_{ab}^p + F_{abk}^p I_k) p_a p_b \right] \psi(\mathbf{r}; R) = E_e(\mathbf{R}) \psi(\mathbf{r}; R), \quad (3.3)$$

where we understand $\mathbf{p} \rightarrow -i\nabla_{\mathbf{r}}$. $V_{\text{mol}}(R, r_{1e}, r_{2e})$ is the electrostatic potential binding the molecule, and we assume the electron is in the $1s\sigma_g$ ground state. The electron

⁵The electron position relative to the nucleon CM is denoted by $\mathbf{r}$ with corresponding momentum $\mathbf{p} = \hat{\mu} \dot{\mathbf{r}}$, where $\hat{\mu} = 2m_e m_p / (m_e + m_p)$ is a reduced mass. The relative motion of the nucleons (protons/antiprotons in this case) is treated as that of a single particle at point $\mathbf{R}$ with momentum $\mathbf{P} = \mu \dot{\mathbf{R}}$ and reduced mass $\mu = m_p/2$.

momentum components p_a are defined in a frame, denoted MOL, which is fixed with respect to the molecular axis.⁶

As discussed in Paper I, the proton terms in the SME Hamiltonian acquire a dependence on $\mathbf{p}$ in this kinematics and so affect the energy levels in two ways—directly from the nucleon Schrödinger equation but also indirectly through their effect on the internucleon potential via (3.3), the latter with the same parametric dependence on m_e and m_p as in atomic hydrogen spectroscopy.

The eigenvalues define the internucleon potential,

$$E_e(\mathbf{R}) = V_M(R) + V_{\text{SME}}^e(\mathbf{R}; S_k) + V_{\text{SME}}^p(\mathbf{R}; I_k), \quad (3.4)$$

where the SME contributions depend on the expectation values $\langle p_a p_b \rangle$ of the electron momentum in the MOL frame. These have been calculated numerically in [10] and Paper I and are shown in Fig. 2. Inserting these back into the nucleon Schrödinger equation we have

$$\left[-\frac{1}{2\mu} \nabla_{\mathbf{R}}^2 + V_M(R) + V_{\text{SME}}^e(\mathbf{R}; S_k) + V_{\text{SME}}^p(\mathbf{R}; I_k) + 2B_k^e S_k + 2B_k^p I_k + \frac{2}{m_p^2} (E_{ij}^p + F_{ijk}^p I_k) P^i P^j \right] \times \Phi_{NM_N}(\mathbf{R}) |M_I M_S\rangle = E_{vNM_N M_I M_S} \Phi_{NM_N}(\mathbf{R}) |M_I M_S\rangle. \quad (3.5)$$

The final step is to separate the contributions and write the total energy eigenvalues as

⁶MOL frame components are indicated by indices $a, b, c, \dots$. The indices $i, j, k, \dots$ are used to specify the EXP frame, usually fixed with respect to the externally applied magnetic field, and in which the molecular axis rotates. For convenience we temporarily define the SME couplings E_{ab} etc. here with MOL frame components; the rotation between the MOL and EXP frames is discussed in Sec. IV. The spin operator components S_k, I_k are always given in the EXP frame.

$$E_{vNM_N M_I M_S} = \tilde{E}_{vNM_N M_I M_S} + \Delta E_{\text{SME}}^{eB} + \Delta E_{\text{SME}}^{pB} + \Delta E_{\text{SME}}^n, \quad (3.6)$$

where $\tilde{E}_{vNM_N M_I M_S}$ is found by setting $\Phi_{NM_N}(\mathbf{R}) = \frac{1}{R} \phi(R) Y_{NM}(\theta, \phi)$ in (3.5) and solving the rovibrational equation,

$$\left[-\frac{1}{2\mu} \frac{d^2}{dR^2} + \frac{1}{2\mu R^2} N(N+1) + V_M(R) + V_{\text{SME}}^e(R; S_k) + V_{\text{SME}}^p(R; I_k) \right] \phi(R) |M_I M_S\rangle = \tilde{E}_{vNM_N M_I M_S} \phi(R) |M_I M_S\rangle, \quad (3.7)$$

where

$$V_{\text{SME}}^e(R; S_k) = \langle vNM_N | V_{\text{SME}}^e(\mathbf{R}; S_k) | vNM_N \rangle, \quad (3.8)$$

together with

$$\Delta E_{\text{SME}}^{eB} = \langle vNM_N M_I M_S | 2B_k S_k | vNM_N M_I M_S \rangle, \quad (3.9)$$

and

$$\Delta E_{\text{SME}}^n = \frac{2}{m_p^2} \langle vNM_N M_I M_S | (E_{ij}^p + F_{ijk}^p I_k) \times P_i P_j | vNM_N M_I M_S \rangle, \quad (3.10)$$

with analogous expressions for $V_{\text{SME}}^p(R; I_k)$ and $\Delta E_{\text{SME}}^{pB}$.

$$\begin{aligned} E_{vNM_N} = & V_{\text{SME}}^e + (1 + \delta_{\text{SME}}^e + \delta_{\text{SME}}^n) \left(v + \frac{1}{2} \right) \omega_0 - (x_0 + x_{\text{SME}}^e + x_{\text{SME}}^n) \left(v + \frac{1}{2} \right)^2 \omega_0 \\ & + (B_0 + B_{\text{SME}}^e + B_{\text{SME}}^n) N(N+1) \omega_0 - (\alpha_0 + \alpha_{\text{SME}}^e + \alpha_{\text{SME}}^n) \left(v + \frac{1}{2} \right) N(N+1) \omega_0 \\ & - (D_0 + D_{\text{SME}}^e + D_{\text{SME}}^n) (N(N+1))^2 \omega_0 + \dots \end{aligned} \quad (3.13)$$

where ω_0 is the fundamental vibration frequency. Each coefficient of ω_0 is an expansion in powers of the small parameter $\lambda = 2/m_p \omega_0 R_0^2 \simeq 0.027$, with the leading terms in the coefficients x_0, B_0, α_0, D_0 being of order $\lambda, \lambda, \lambda^2, \lambda^3$ respectively. (Recall from Paper I that parametrically, $\lambda \sim \sqrt{\frac{m_e}{m_p}}$.)

In (3.13), we have defined $V_{\text{SME}}^e \equiv V_{\text{SME}}^e(R_0)$ where R_0 is the mean bond length, i.e. the minimum of the internucleon potential. The coefficients $\delta_{\text{SME}}^e, B_{\text{SME}}^e, \dots$ are given in terms of its derivatives at R_0 , e.g.

$$\begin{aligned} \delta_{\text{SME}}^e &= \frac{1}{2} \frac{1}{V_M''} \left[V_{\text{SME}}^{e''} - \frac{V_M'''}{V_M''} V_{\text{SME}}^{e'} \right], \\ B_{\text{SME}}^e &= \lambda \frac{1}{V_M''} \left[\frac{1}{R_0} V_{\text{SME}}^{e'} \right], \end{aligned} \quad (3.14)$$

In practice, we simplify this by for the most part considering Para- H_2^+ , in which case the nucleon spin $\mathbf{I}$ is zero. We also absorb the spin-independent proton coupling into $V_{\text{SME}}^e(R)$ by defining $\tilde{E}_{ij}^e = E_{ij}^e + \frac{1}{2} \frac{m_e^2}{m_p^2} E_{ij}^p$, leaving

$$V_{\text{SME}}^e(\mathbf{R}) = \frac{1}{m_e^2} (\tilde{E}_{ab}^e + F_{abk}^e S_k) \langle p_a p_b \rangle \quad (3.11)$$

and

$$V_{\text{SME}}^e(R) = \langle vNM_N M_S | V_{\text{SME}}^e(\mathbf{R}) | vNM_N M_S \rangle, \quad (3.12)$$

suppressing the spin labels.

In what follows, we evaluate (3.9), (3.10) and (3.11), (3.12) for Para- H_2^+ , initially in the basis states $|vNM_N M_S\rangle$, then in the hyperfine states $|vN J M_J\rangle$ described in Sec. II. Including the Zeeman as well as the hyperfine interaction, we find that the SME couplings give rise to spin and magnetic field-dependent corrections to the rovibrational energy levels, due to the mixing of states induced by the magnetic field.

A full description of how the SME-modified internucleon potential $V_M(R) + V_{\text{SME}}^e(R)$, together with the direct nucleon contribution ΔE_{SME}^n , determines the rovibrational energy levels E_{vNM_N} (for spin-independent SME couplings) was given in Paper I. It was shown there that they admit an expansion of the form

while the $\delta_{\text{SME}}^n, B_{\text{SME}}^n, \dots$ are determined by reducing (3.10) to a product of proton SME couplings and the rovibrational kinetic energy, then expanding the latter in powers of $(v + \frac{1}{2})$ and $N(N+1)$ as above.

Everything in this analysis now goes through exactly as before, where the expansion applies to each hyperfine-Zeeman eigenstate individually. The required $V_{\text{SME}}^e(R)$, ΔE_{SME}^n , and $\Delta E_{\text{SME}}^{eB}$ are evaluated in these hyperfine-Zeeman eigenstates in the following two sections.

IV. LORENTZ AND CPT VIOLATION IN THE H_2^+ AND $\tilde{\text{H}}_2^-$ SPECTRUM—SPIN-INDEPENDENT COUPLINGS

We begin in this section with the spin-independent SME couplings E_{ij} in (3.1). We restrict our discussion

to Para- H_2^+ for simplicity, the extension to Ortho- H_2^+ being straightforward in principle.

Following the Born-Oppenheimer analysis described in Paper I and Sec. III, the first step is to determine the potential $V_{\text{SME}}^e(\mathbf{R})$ by evaluating the expectation value of the SME Hamiltonian term,

$$H_{\text{SME}}^{eE} = \frac{1}{m_e^2} \tilde{E}_{ab} p_a p_b, \quad (4.1)$$

in the electron $1s\sigma_g$ ground state, where the couplings and momenta are in the MOL frame. Recall that the coupling here is $\tilde{E}_{ab}^e = E_{ab}^e + \frac{1}{2} \frac{m_e^2}{m_p^2} E_{ab}^p$ since the proton SME couplings also contribute to the electron Schrödinger equation. Using the cylindrical symmetry of the $1s\sigma_g$ wave function, the expectation values satisfy $\langle p_a p_b \rangle = 0$ for $a \neq b$, and $\langle p_x^2 \rangle = \langle p_y^2 \rangle$. It is then convenient to write $\langle p_a p_b \rangle$ in terms of the two independent expectation values as

$$\langle p_a p_b \rangle = \frac{1}{3} \text{tr} \langle p_a p_b \rangle \delta_{ab} + \frac{1}{6} \text{tr}_Y \langle p_a p_b \rangle Y_{ab}, \quad (4.2)$$

where

$$Y_{ab} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

and $\text{tr}_Y p_a p_b = p_x^2 + p_y^2 - 2p_z^2$. These expectation values have been evaluated numerically in [10] and Paper I and are shown here in Fig. 2.

We then have

$$V_{\text{SME}}^{eE}(\mathbf{R}) = \frac{1}{m_e^2} \left(\frac{1}{3} \text{tr} \langle p_a p_b \rangle \text{tr} \tilde{E}_{ab}^e + \frac{1}{6} \text{tr}_Y \langle p_a p_b \rangle \text{tr}_Y \tilde{E}_{ab}^e \right). \quad (4.3)$$

The next step is to reexpress the SME couplings in terms of their components $\tilde{E}_{ij}^e$ the EXP frame. With the rotation matrix R_{ai} introduced in Paper I,

$$R_{ai} = \begin{pmatrix} \cos \theta \cos \phi & \cos \theta \sin \phi & -\sin \theta \\ -\sin \phi & \cos \phi & 0 \\ \sin \theta \cos \phi & \sin \theta \sin \phi & \cos \theta \end{pmatrix}, \quad (4.4)$$

where (θ, ϕ) specify the orientation of the molecular axis in the EXP frame,

$$\tilde{E}_{ab}^e = R_{ai} \tilde{E}_{ij}^e R_{jb}^T. \quad (4.5)$$

It then follows immediately that $\text{tr} \tilde{E}_{ab}^e = \text{tr} \tilde{E}_{ij}^e$, while

$$\begin{aligned} \text{tr}_Y \tilde{E}_{ab}^e &= \text{tr} \tilde{E}_{ab}^e - 3 \tilde{E}_{zz}^e \\ &= \text{tr} \tilde{E}_{ij}^e - 3 \tilde{E}_{ij}^e R_{iz}^T R_{zj}. \end{aligned} \quad (4.6)$$

The product of rotation matrices can be expanded in terms of spherical harmonics as

$$R_{iz}^T R_{zj} = \frac{1}{3} \delta_{ij} + \sum_M C_{ij}^M Y_{2M}(\theta, \phi), \quad (4.7)$$

with known coefficients C_{ij}^M [9,17], so

$$\text{tr}_Y \tilde{E}_{ab}^e = -3 \sum_M C_{ij}^M Y_{2M}(\theta, \phi) \tilde{E}_{ij}^e. \quad (4.8)$$

Substituting back into (4.3) then gives the required expression for $V_{\text{SME}}^{eE}(\mathbf{R})$ in terms of the EXP frame SME couplings⁷:

$$\begin{aligned} V_{\text{SME}}^{eE}(\mathbf{R}) &= \frac{1}{m_e^2} \left(\frac{1}{3} \text{tr} \langle p_a p_b \rangle \text{tr} \tilde{E}_{ij}^e - \frac{1}{2} \text{tr}_Y \langle p_a p_b \rangle \right. \\ &\quad \left. \times \sum_M C_{ij}^M Y_{2M}(\theta, \phi) \tilde{E}_{ij}^e \right). \end{aligned} \quad (4.9)$$

To evaluate the matrix elements of $V_{\text{SME}}^{eE}(\mathbf{R})$ in the hyperfine states $|vN JM_J\rangle$ we use (2.4) to write

$$\begin{aligned} &\langle vN J' M_J' | Y_{2M}(\theta, \phi) | vN JM_J \rangle \\ &= \sum_{M_S} C_{NM_N, \frac{1}{2} M_S}^{J' M_J'} C_{NM_N, \frac{1}{2} M_S}^{J M_J} \langle vNM_N M_S | Y_{2M}(\theta, \phi) \\ &\quad \times | vNM_N M_S \rangle, \end{aligned} \quad (4.10)$$

where the matrix element is given by the Gaunt integral,

$$\begin{aligned} \langle vNM_N' M_S | Y_{2M}(\theta, \phi) | vNM_N M_S \rangle &= \int d\Omega Y_{NM_N'}^* Y_{2M} Y_{NM_N} \\ &= \sqrt{\frac{5}{4\pi}} C_{NM_N', 2M}^{NM_N'} C_{NM_N, 20}^{N0}. \end{aligned} \quad (4.11)$$

We now come to an important simplification. The hyperfine-Zeeman interactions in (2.1) and (2.2) commute

⁷Looking ahead to Sec. VI where we express our results in terms of SME couplings in a spherical tensor formalism, we can compare (4.9) and (4.14) directly with (6.17) and (6.18). The dictionary is

$$\sqrt{\frac{1}{4\pi}} \mathcal{V}_{200}^{\text{NR}} = -\frac{1}{3} \frac{1}{m^2} \text{tr} E_{ij}, \quad \sqrt{\frac{5}{4\pi}} \mathcal{V}_{220}^{\text{NR}} = \frac{1}{3} \frac{1}{m^2} \text{tr}_Y E_{ij},$$

the latter being a special case of $\mathcal{V}_{22m} = -\frac{1}{m^2} C_{ij}^m E_{ij}$. See Sec. VI for further discussion.

with J_z , so M_J is a good quantum number for their eigenstates. This is no longer the case when the SME Hamiltonian is included and in general (4.9) has matrix elements which are off-diagonal in M_J . However, since there are no corresponding matrix elements for $\langle H_{\text{HFS}} + H_Z \rangle$, when we extract the energy eigenvalues including the SME Hamiltonian, these off-diagonal matrix elements only contribute at second order in the SME couplings. Such $O(\text{SME})^2$ contributions to energy levels are universally neglected in the SME formalism.

It follows that we should only retain the matrix elements in (4.9) with $M'_N = M_N$, that is, with $M = 0$. In this case,

$$C_{ij}^0 = -\frac{1}{3} \sqrt{\frac{4\pi}{5}} Y_{ij}, \quad (4.12)$$

and the Clebsch-Gordan coefficients are

$$C_{NM_N, 20}^{NM_N} C_{N0, 20}^{N0} = \frac{N(N+1) - 3M_N^2}{(2N-1)(2N+3)} = c_{NM_N}, \quad (4.13)$$

in the notation of Paper I. So keeping only the terms in (4.9) which will contribute to energy levels at $O(\text{SME})$, we have

$$V_{\text{SME}}^{eE}(\mathbf{R}) = \frac{1}{m_e^2} \left(\frac{1}{3} \text{tr} \langle p_a p_b \rangle \text{tr} \tilde{E}_{ij}^e + \frac{1}{6} \sqrt{\frac{4\pi}{5}} \text{tr}_Y \langle p_a p_b \rangle \text{tr}_Y \tilde{E}_{ij}^e Y_{20}(\theta, \phi) \right), \quad (4.14)$$

and from (4.10) the matrix elements in the hyperfine states giving rise to the internucleon potential are therefore,⁸

$$\begin{aligned} V_{\text{SME}}^{eE}(R) &= \langle vNJ'M_J | V_{\text{SME}}^{eE}(\mathbf{R}) | vNJM_J \rangle \\ &= \sum_{M_S} C_{NM_N, \frac{1}{2}M_S}^{J'M_J} C_{NM_N, \frac{1}{2}M_S}^{JM_J} \frac{1}{m_e^2} \left(\frac{1}{3} \text{tr} \langle p_a p_b \rangle \text{tr} \tilde{E}_{ij}^e + \frac{1}{6} \text{tr}_Y \langle p_a p_b \rangle \text{tr}_Y \tilde{E}_{ij}^e c_{NM_N} \right). \end{aligned} \quad (4.15)$$

For the coefficient of $\text{tr} \tilde{E}_{ij}$, orthonormality of the Clebsch-Gordan coefficients implies these matrix elements are diagonal in J', J . However, the coefficient of $\text{tr}_Y \tilde{E}_{ij}$ has off-diagonal elements mixing $J = N \pm \frac{1}{2}$ states in the same way as $\langle H_{\text{HFS}} + H_Z \rangle$ in (2.14). The required sums over Clebsch-Gordan factors, weighted with c_{NM_N} , are given explicitly in Appendix B, Eq. (B5).

Adding (4.15) to $\langle vNJ'M_J | H_{\text{HFS}} + H_Z | vNJM_J \rangle$ from (2.14) now gives the full SME modification to the hyperfine-Zeeman energy levels. Calculating the eigenvalues of this combined matrix and, for simplicity, just quoting the results in the weak magnetic field limit, we find⁹

⁸We drop the implicit matrix element labels J', J, M_J on $V_{\text{SME}}^{eE}(R)$ here simply to avoid cluttering the notation.

⁹An elementary but useful algebraic result to quickly read off the $O(\text{SME})$ corrections to the hyperfine-Zeeman energy levels here and in Sec. V is found by first denoting

$$\langle H_{\text{HFS}} + H_Z \rangle = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B} & \mathbf{D} \end{pmatrix}, \quad V_{\text{SME}}^e(R) = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}.$$

Then adding these matrices and calculating the SME corrections $\Delta\lambda_{\text{SME}}^{\pm}$ to the eigenvalues gives, at $O(\text{SME})$,

$$\Delta\lambda_{\text{SME}}^{\pm} = \frac{1}{2}(\alpha + \delta) \pm \frac{1}{2} \frac{1}{\sqrt{(A-D)^2 + 4B^2}} ((A-D)(\alpha - \delta) + 2B(\beta + \gamma)).$$

In the case considered here, the off-diagonal element $\mathbf{B}$ is proportional to the magnetic field, so in the small-field regime where we can neglect terms of $O(B^2)$, we have the simple forms:

$$\Delta\lambda_{\text{SME}}^+ = \alpha + \frac{\mathbf{B}}{\mathbf{A} - \mathbf{D}}(\beta + \gamma), \quad \Delta\lambda_{\text{SME}}^- = \delta - \frac{\mathbf{B}}{\mathbf{A} - \mathbf{D}}(\beta + \gamma),$$

which are used to deduce (4.17) and (4.18) above. Usually $V_{\text{SME}}^e(R)$ here is symmetric so $\gamma = \beta$ but in Sec. V we encounter a case where it is Hermitian, $\gamma = \beta^*$. Also note that this method of calculating the eigenvalues gives the same result at $O(\text{SME})$ as evaluating the expectation values of the SME perturbation in the hyperfine-Zeeman eigenstates, without the need to explicitly calculate the corresponding mixing angles.

$$V_{\text{SME}\pm}^{eE}(R) = \frac{1}{m_e^2} \left(\frac{1}{3} \text{tr} \langle p_a p_b \rangle \text{tr} \tilde{E}_{ij}^e + \frac{1}{6} \text{tr}_Y \langle p_a p_b \rangle \text{tr}_Y \tilde{E}_{ij}^e \hat{c}_{NM_J}^\pm(B) \right), \quad (4.16)$$

with

$$\begin{aligned} \hat{c}_{NM_J}^+(B) &= \frac{1}{(2N+1)(2N+3)} \left[\left(N + \frac{1}{2} \right) \left(N + \frac{3}{2} \right) - 3M_J^2 \right], \\ &+ 24 \frac{[(N + \frac{1}{2})^2 - M_J^2]}{(2N+1)^3(2N-1)(2N+3)} \frac{1}{c_e(v, N)} (g_e + g_m(v, N)) \mu_B B M_J, \end{aligned} \quad (4.17)$$

and

$$\begin{aligned} \hat{c}_{NM_J}^-(B) &= \frac{1}{(2N-1)(2N+1)} \left[\left(N - \frac{1}{2} \right) \left(N + \frac{1}{2} \right) - 3M_J^2 \right] \\ &- 24 \frac{[(N + \frac{1}{2})^2 - M_J^2]}{(2N+1)^3(2N-1)(2N+3)} \frac{1}{c_e(v, N)} (g_e + g_m(v, N)) \mu_B B M_J, \end{aligned} \quad (4.18)$$

while for the unmixed states, the $\hat{c}_{NM_J}$ factor is independent of the magnetic field:

$$\hat{c}_{NM_J} = -\frac{N}{(2N+3)}. \quad (4.19)$$

Notice that the leading terms in $\hat{c}_{NM_J}^\pm$ can be written as $\frac{1}{4} \frac{1}{J(J+1)} [J(J+1) - 3M_J^2]$ with $J = N \pm \frac{1}{2}$ respectively.

This magnetic field dependence of the SME potential $V_{\text{SME}\pm}^{eE}(R)$ of course arises purely from the mixing of the states due to the hyperfine-Zeeman interactions. These terms are proportional to $\text{tr}_Y \tilde{E}_{ij}^e \mu_B B M_J$ but arise with a distinctive N dependence. While high-precision spectroscopy will use combinations of transitions with different ΔM_J to attempt to cancel the Zeeman effect [2,24], this SME-specific N dependence means these terms may still contribute even to otherwise Zeeman-free combinations of transitions. This important issue will be discussed in detail elsewhere.

For high magnetic fields, the hyperfine-Zeeman eigenstates just reduce to the $|vNM_N M_S\rangle$ states, for which the SME potential is simply

$$\begin{aligned} V_{\text{SME}\pm}^{eE}(R) &= \frac{1}{m_e^2} \left(\frac{1}{3} \text{tr} \langle p_a p_b \rangle \text{tr} \tilde{E}_{ij}^e \right. \\ &\left. + \frac{1}{6} \text{tr}_Y \langle p_a p_b \rangle \text{tr}_Y \tilde{E}_{ij}^e c_{NM_N} \right), \end{aligned} \quad (4.20)$$

with c_{NM_N} given in (4.13). This was the case analyzed in detail in Paper I.

The direct contribution of the proton SME couplings in the Born-Oppenheimer analysis is described in Paper I and,

while conceptually different, involves a similar calculation encompassing matrix elements in the mixed hyperfine-Zeeman states. In the notation introduced there, we require

$$\Delta E_{\text{SME}}^n = \frac{2}{m_p^2} E_{ij}^p \langle vN J' M_J | P_i P_j | vN J M_J \rangle, \quad (4.21)$$

where we resolve the relative motion of the protons to that of a single particle with momentum $\mathbf{P}$ and reduced mass $\mu = m_p/2$.

Here, we can expand the product of momenta in an analogous way to (4.7), that is [9,17]

$$P_i P_j = |\mathbf{P}|^2 \left(\frac{1}{3} \delta_{ij} + C_{ij}^M Y_{2M}(\theta, \phi) \right). \quad (4.22)$$

Then, since $K = |\mathbf{P}|^2/2\mu$ is the kinetic energy of the protons, and is independent of the spin state, we have

$$\begin{aligned} \Delta E_{\text{SME}}^n &= \frac{2}{m_p} \langle vN | K | vN \rangle \left(\frac{1}{3} \text{tr} E_{ij}^p + C_{ij}^M E_{ij}^p \right. \\ &\left. \times \langle vN J' M_J | Y_{2M}(\theta, \phi) | vN J M_J \rangle \right). \end{aligned} \quad (4.23)$$

The evaluation of the expectation value of the spherical harmonic, which physically is describing the dynamics of the orientation of the molecular axis in the relevant angular momentum state, now repeats the calculation following (4.10) above. We may again specialize to the case $M = 0$, and the c_{NM_J} factors are found in the same way. We therefore find, in the mixed hyperfine-Zeeman eigenstates,

$$\Delta E_{\text{SME}\pm}^n = \langle vN|K|vN\rangle \tilde{V}_{\text{SME}\pm}^n, \quad (4.24)$$

with

$$\tilde{V}_{\text{SME}\pm}^n = \frac{2}{3} \frac{1}{m_p} [\text{tr} E_{ij}^p - \text{tr}_Y E_{ij}^p \hat{c}_{NM_J}^\pm(B)], \quad (4.25)$$

with $\hat{c}_{NM_J}$ as in (4.19) for the unmixed states. For large applied magnetic fields, $\hat{c}_{NM_J}^\pm(B) \rightarrow c_{NM_N}$ as described above.

Finally, we can reexpress these results expressed in terms of E_{ij} with their equivalents with the spin-independent Lagrangian couplings $c_{\mu\nu}$ and $a_{\mu\nu\lambda}$. The dictionary, first in terms of the spherical tensor description, with $\mathcal{V}_{njm}^{\text{NR}} = c_{njm}^{\text{NR}} - a_{njm}^{\text{NR}}$, is

$$\begin{aligned} \text{tr} E_{ij} &= -3m^2 \frac{1}{\sqrt{4\pi}} (c_{200}^{\text{NR}} - a_{200}^{\text{NR}}), \\ \text{tr}_Y E_{ij} &= 3m^2 \sqrt{\frac{5}{4\pi}} (c_{220}^{\text{NR}} - a_{220}^{\text{NR}}). \end{aligned} \quad (4.26)$$

then with the original SME couplings in (1.1),

$$\begin{aligned} \frac{1}{\sqrt{4\pi}} c_{200}^{\text{NR}} &= \frac{1}{3m} \left(c_{ii} + \frac{3}{2} c_{00} \right) = \frac{5}{6m} c_{00}, \\ \frac{1}{\sqrt{4\pi}} a_{200}^{\text{NR}} &= a_{0ii} + a_{000}, \\ \sqrt{\frac{5}{4\pi}} c_{220}^{\text{NR}} &= -\frac{1}{3m} \text{tr}_Y c_{ij}, \quad \sqrt{\frac{5}{4\pi}} a_{220}^{\text{NR}} = -\text{tr}_Y a_{0ij}, \end{aligned} \quad (4.27)$$

since we may assume the spacetime trace of $c_{\mu\nu}$ vanishes (see [14]).

V. LORENTZ AND CPT VIOLATION IN THE H_2^+ AND $\bar{\text{H}}_2^-$ SPECTRUM—SPIN-DEPENDENT COUPLINGS

In this section, we extend the analysis of Lorentz and CPT violation in the H_2^+ spectrum to include the spin-

dependent couplings B_k and F_{ijk} in (3.1), corresponding to the couplings $b_\mu, g_{\mu\nu\lambda}, d_{\mu\nu}, H_{\mu\nu}$ in the fundamental SME Lagrangian (1.1).

We again focus on Para- H_2^+ as the simplest and most experimentally favored case, leaving comments on the extension to Ortho- H_2^+ until later. This means that the only spin dependence arises from the electron SME couplings B_k^e and F_{ijk}^e . The main technical task of this section is therefore to evaluate the contribution to the internucleon potential $V_{\text{SME}}^e(R)$ from the momentum-dependent F_{ijk}^e terms in (3.1).

A. SME B_k^e couplings

First though, we consider the momentum-independent term,

$$H_{\text{SME}}^{eB} = 2B_k^e S_k = 2B_3^e S_3 + (B_+^e S_- + B_-^e S_+), \quad (5.1)$$

in the SME Hamiltonian. Clearly this just gives a direct addition $\Delta E_{\text{SME}}^{eB}$ to the energy in the hyperfine states, where

$$\Delta E_{\text{SME}}^{eB} = 2B_k^e \langle vNJ'M_J | S_k | vNJM_J \rangle. \quad (5.2)$$

As always, to evaluate these matrix elements we first expand the hyperfine states in terms of the basis states $|vNM_N M_S\rangle$ as in (2.4). It is then clear that the operators $S_\pm^e$ only contribute to matrix elements with $\Delta M_J \neq 0$ and so, by the argument following (4.11), only give corrections to the energy levels at $O(\text{SME})^2$. The SME couplings $B_\pm^e$ can therefore be neglected. This leaves only the matrix elements of S_3 to be evaluated, which we have already found in (2.6) [see also (B4)]. Indeed, no new calculations are required here. The SME term $B_k^e S_3$ acts entirely analogously to a background magnetic field and the required results may be read off immediately from Sec. II.

We therefore find

$$\Delta E_{\text{SME}}^{eB} = 2B_3^e \frac{1}{2N+1} \begin{pmatrix} M_J & -\sqrt{\left(N+\frac{1}{2}\right)^2 - M_J^2} \\ -\sqrt{\left(N+\frac{1}{2}\right)^2 - M_J^2} & -M_J \end{pmatrix} \quad (5.3)$$

for the mixed $J', J = N \pm \frac{1}{2}$ sector. Determining the corresponding eigenvalues, we find in the low magnetic field regime,

$$\begin{aligned} \Delta E_{\text{SME}\pm}^{eB} = & \pm 2B_3^e \frac{1}{2N+1} M_J \\ & \pm 8B_3^e \frac{1}{(2N+1)^3} \left[\left(N + \frac{1}{2}\right)^2 - M_J^2 \right] \\ & \times \frac{1}{c_e(v, N)} (g_e + g_m(v, N)) \mu_B B, \end{aligned} \quad (5.4)$$

to $O(\mu_B B/c_e)$. For the unmixed states with $J = N + \frac{1}{2}$, $M_J = \pm(N + \frac{1}{2})$ we have simply $\Delta E_{\text{SME}}^{eB} = \pm B_3^e$ with no $O(\mu_B B/c_e)$ correction.

In the large magnetic field limit, the eigenstates are $|vNM_N M_S\rangle$ and we have

$$\Delta E_{\text{SME}}^{eB} = 2B_3^e M_S. \quad (5.5)$$

In this case there is no $O(c_e/\mu_B B)$ correction since, restricting to states with fixed M_J , the matrix elements

of H_{SME}^{eB} are diagonal in the $|vNM_N M_S\rangle$ basis (see footnote 9).

B. SME F_{ijk}^e couplings

Now consider the spin and momentum-dependent terms in the SME Hamiltonian,

$$H_{\text{SME}}^{eF} = 2 \frac{1}{m_e^2} F_{ijk}^e p_i p_j S_k = 2 \frac{1}{m_e^2} F_{abk}^e p_a p_b S_k, \quad (5.6)$$

where we reexpress the electron momenta in the MOL frame in which their expectation values are evaluated (see Fig. 2).

In this case, we first need to calculate $V_{\text{SME}}^{eF}(\mathbf{R})$, extending the corresponding expression (4.3) for the spin-independent couplings. Here,

$$V_{\text{SME}}^{eF}(\mathbf{R}) = 2 \frac{1}{m_e^2} \left(\frac{1}{3} \text{tr} \langle p_a p_b \rangle \text{tr} F_{abk}^e + \frac{1}{6} \text{tr}_Y \langle p_a p_b \rangle \text{tr}_Y F_{abk}^e \right) S_k \quad (5.7)$$

where the traces act only on the first two indices of F_{abk}^e . Following the analysis in Sec. IV, we relate these MOL frame components to those in the EXP frame by

$$\text{tr}_Y F_{abk}^e = -3 \sum_M C_{ij}^M Y_{2M}(\theta, \phi) F_{ijk}^e, \quad (5.8)$$

while of course $\text{tr} F_{abk}^e = \text{tr} F_{ijk}^e$, giving

$$V_{\text{SME}}^{eF}(\mathbf{R}) = 2 \frac{1}{m_e^2} \left(\frac{1}{3} \text{tr} \langle p_a p_b \rangle \text{tr} F_{ijk}^e - \frac{1}{2} \text{tr}_Y \langle p_a p_b \rangle \sum_M C_{ij}^M Y_{2M}(\theta, \phi) F_{ijk}^e \right) S_k. \quad (5.9)$$

Then, with C_{ij}^0 from (4.12) and

$$C_{ij}^{\pm 1} = \mp \sqrt{\frac{2\pi}{15}} (\delta_{i\mp} \delta_{j3} + \delta_{i3} \delta_{j\mp}), \quad (5.10)$$

and keeping only the $M = 0, \pm 1$ contributions as explained below, we have

$$\begin{aligned} V_{\text{SME}}^{eF}(\mathbf{R}) = & \frac{1}{m_e^2} \left[\frac{2}{3} \text{tr} \langle p_a p_b \rangle \text{tr} F_{ij3}^e S_3 + \frac{1}{3} \sqrt{\frac{4\pi}{5}} \text{tr}_Y \langle p_a p_b \rangle \text{tr}_Y F_{ij3}^e Y_{20}(\theta, \phi) S_3 \right. \\ & \left. + \sqrt{\frac{1}{6}} \sqrt{\frac{4\pi}{5}} \text{tr}_Y \langle p_a p_b \rangle (F_{-3+}^e Y_{21}(\theta, \phi) S_- + F_{+3-}^e Y_{2-1}(\theta, \phi) S_+) \right]. \end{aligned} \quad (5.11)$$

The next step is to determine the contribution to the internucleon potential $V_{\text{SME}}^{eF}(\mathbf{R})$ by taking the matrix elements of (5.11). We evaluate first in the $|vNM_N M_S\rangle$ basis states, then extend to the hyperfine states $|vNJM_J\rangle$ using Clebsch-Gordan coefficients as usual.

The coefficient of $\text{tr} \langle p_a p_b \rangle$ is straightforward since we only need the matrix elements of S_k , so this is carried out as above for B_k^e , with only $\text{tr} F_{ij3}^e$ contributing at $O(\text{SME})$ because of the $\Delta M_J = 0$ criterion.

For the coefficient of $\text{tr}_Y \langle p_a p_b \rangle$ we need the matrix elements of $Y_{2M}(\theta, \phi)$, which are given by the Gaunt integral in (4.11). Here, however, due to the presence of the spin operator in (5.11), we must also take into account contributions with $M \neq 0$. Consider these in turn:

(i) $M = 0$: In this case,

$$\langle vNM'_N M'_S | Y_{20}(\theta, \phi) S_k | vNM_N M_S \rangle = \sqrt{\frac{5}{4\pi}} c_{NM_N} M_S, \quad (5.12)$$

since $M'_N = M_N$ and then $\Delta M_J = 0$ requires $M'_S = M_S$, so only S_3 contributes. So here, we need only

$$\langle vNM_N M_S | Y_{20}(\theta, \phi) S_3 | vNM_N M_S \rangle C_{ij}^0 F_{ij3}^e = -\frac{1}{3} c_{NM_N} M_S \text{tr}_Y F_{ij3}^e. \quad (5.13)$$

(ii) $M = \pm 1$: Here, $M'_N = M_N \pm 1$, so we require $M'_S = M_S \mp 1$ to maintain $\Delta M_J = 0$. We therefore have contributions from the raising and lowering spin operators $S_{\pm}$. For the matrix elements, we need

$$\langle vNM_N \pm 1 M_S \mp 1 | Y_{2\pm 1}(\theta, \phi) | vNM_N M_S \rangle = \sqrt{\frac{5}{4\pi}} C_{NM_N, 2\pm 1}^{N(M_N \pm 1)} C_{N0, 20}^{N0}. \quad (5.14)$$

Evaluating the Clebsch-Gordan coefficients using (B7), we find

$$\langle vNM_N \pm 1 M_S \mp 1 | Y_{2\pm 1}(\theta, \phi) | vNM_N M_S \rangle C_{ij}^{\pm 1} F_{ij\pm}^e = -\frac{1}{(2N-1)(2N+3)} \left[\left(N + \frac{1}{2} \right)^2 - M_J^2 \right] M_J F_{\mp 3\pm}. \quad (5.15)$$

Evidently there is no contribution from $M = 2$ given the constraint $\Delta M_J = 0$.

Putting all this together, the matrix elements $\hat{V}_{\text{SME}}^{eF}(R)$ expressed in an $|vNM_J M_S\rangle$ basis with fixed M_J , with $M_S = \pm \frac{1}{2}$ rows and columns, are

$$\hat{V}_{\text{SME}}^{eF}(R) = \frac{1}{3} \frac{1}{m_e^2} \text{tr} \langle p_a p_b \rangle \text{tr} F_{ij3} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \frac{1}{m_e^2} \text{tr}_Y \langle p_a p_b \rangle \begin{pmatrix} \frac{1}{6} c_{N(M_J - \frac{1}{2})} \text{tr}_Y F_{ij3}^e & \frac{\sqrt{(N+\frac{1}{2})^2 - M_J^2}}{(2N-1)(2N+3)} M_J F_{+3-} \\ \frac{\sqrt{(N+\frac{1}{2})^2 - M_J^2}}{(2N-1)(2N+3)} M_J F_{-3+} & -\frac{1}{6} c_{N(M_J + \frac{1}{2})} \text{tr}_Y F_{ij3}^e \end{pmatrix}. \quad (5.16)$$

For the unmixed states with $M_J = \pm(N + \frac{1}{2})$, the off-diagonal elements vanish and both $c_{N(M_J \mp \frac{1}{2})}$ coefficients reduce to c_{NM_N} .

The next step is to evaluate $V_{\text{SME}}^{eF}(R)$ in the hyperfine basis $|vNJM_J\rangle$, as required for the weak magnetic field regime. Here, analogously to (4.15) for the spin-independent couplings, we need

$$V_{\text{SME}}^{eF}(R) = \sum_{M'_S, M_S} C_{N(M_J - M'_S), \frac{1}{2} M'_S}^{J' M_J} C_{N(M_J - M_S), \frac{1}{2} M_S}^{J M_J} \hat{V}_{\text{SME}}^{eF}(R), \quad (5.17)$$

with $\hat{V}_{\text{SME}}^{eF}(R)$ in (5.16). Notice that the presence of off-diagonal terms in (5.16) means that for these terms we have to sum over M_S and M'_S .

We now need the sums over Clebsch-Gordan coefficients weighted by the appropriate factors in (5.16). These are given in Appendix B. For the $\text{tr} F_{ij3}^e$ term, we just need the weight factor M_S as in (B4), while for $\text{tr}_Y F_{ij3}^e$ we need the combined weight factor $c_{N(M_J - M_S)} M_S$ which is given in (B6). This leaves the coefficients of F_{+3-}^e and F_{-3+}^e . In this case we simply need a single M'_S, M_S term, and using the Clebsch-Gordan coefficients in (2.5) and Appendix B, we readily find

$$C_{N(M_J + \frac{1}{2}), \frac{1}{2} - \frac{1}{2}}^{J' M_J} C_{N(M_J - \frac{1}{2}), \frac{1}{2} \frac{1}{2}}^{J M_J} = \frac{1}{(2N+1)} \begin{pmatrix} \sqrt{(N + \frac{1}{2})^2 - M_J^2} & -(N + \frac{1}{2} - M_J) \\ (N + \frac{1}{2} + M_J) & \sqrt{(N + \frac{1}{2})^2 - M_J^2} \end{pmatrix} \quad (5.18)$$

for $J', J = N \pm \frac{1}{2}$. This determines the coefficient of F_{-3+}^e , while the transpose matrix gives the coefficient for F_{+3-}^e .

The simplest presentation of the full result is to express $V_{\text{SME}}^{eF}(R)$ as a matrix for fixed M_J with $J', J = N \pm \frac{1}{2}$ as

$$V_{\text{SME}}^{eF}(R) = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}, \quad (5.19)$$

with $\gamma = \beta^*$, where

$$\begin{aligned} \alpha = & \frac{2}{3} \frac{1}{m_e^2} \text{tr} \langle p_a p_b \rangle \text{tr} F_{ij3}^e \frac{1}{2N+1} M_J \\ & + \frac{1}{m_e^2} \text{tr}_Y \langle p_a p_b \rangle \left[\frac{1}{3} \text{tr}_Y F_{ij3}^e \frac{1}{(2N+1)(2N-1)(2N+3)} \left(N^2 + 4N + \frac{3}{4} - 3M_J^2 \right) M_J \right. \\ & \left. + (F_{+3-}^e + F_{-3+}^e) \frac{1}{(2N+1)(2N-1)(2N+3)} \left[\left(N + \frac{1}{2} \right)^2 - M_J^2 \right] M_J \right], \end{aligned} \quad (5.20)$$

and

$$\begin{aligned} \delta = & -\frac{2}{3} \frac{1}{m_e^2} \text{tr} \langle p_a p_b \rangle \text{tr} F_{ij3}^e \frac{1}{2N+1} M_J \\ & - \frac{1}{m_e^2} \text{tr}_Y \langle p_a p_b \rangle \left[\frac{1}{3} \text{tr}_Y F_{ij3}^e \frac{1}{(2N+1)(2N-1)(2N+3)} \left(N^2 - 2N - \frac{9}{4} - 3M_J^2 \right) M_J \right. \\ & \left. + (F_{+3-}^e + F_{-3+}^e) \frac{1}{(2N+1)(2N-1)(2N+3)} \left[\left(N + \frac{1}{2} \right)^2 - M_J^2 \right] M_J \right], \end{aligned} \quad (5.21)$$

while,

$$\begin{aligned} \text{Re} \beta = & \sqrt{\left(N + \frac{1}{2} \right)^2 - M_J^2} \left(-\frac{2}{3} \frac{1}{m_e^2} \text{tr} \langle p_a p_b \rangle \text{tr} F_{ij3}^e \frac{1}{2N+1} \right. \\ & + \frac{1}{m_e^2} \text{tr}_Y \langle p_a p_b \rangle \left[-\frac{1}{3} \text{tr}_Y F_{ij3}^e \frac{1}{(2N+1)(2N-1)(2N+3)} \left(N^2 + N - \frac{3}{4} - 3M_J^2 \right) \right. \\ & \left. \left. + (F_{+3-}^e + F_{-3+}^e) \frac{1}{(2N+1)(2N-1)(2N+3)} M_J^2 \right] \right). \end{aligned} \quad (5.22)$$

The expectation values in the hyperfine-Zeeman energy eigenstates are read off by applying footnote 9 and we find

$$V_{\text{SME}+}^{eF}(R) = \alpha - 4\text{Re}\beta \frac{1}{(2N+1)^2} \sqrt{\left(N + \frac{1}{2} \right)^2 - M_J^2} \frac{1}{c_e(v, N)} (g_e + g_M(v, N)) \mu_B B, \quad (5.23)$$

and

$$V_{\text{SME}-}^{eF}(R) = \delta + 4\text{Re}\beta \frac{1}{(2N+1)^2} \sqrt{\left(N + \frac{1}{2} \right)^2 - M_J^2} \frac{1}{c_e(v, N)} (g_e + g_M(v, N)) \mu_B B. \quad (5.24)$$

For the unmixed states, there is no dependence on F_{+3-}^e and F_{-3+}^e , and no subleading term of $O(B/c_e)$, and we simply have

$$V_{\text{SME}}^{eF}(R) = \pm \frac{1}{3} \frac{1}{m_e^2} \text{tr} \langle p_a p_b \rangle \text{tr} F_{ij3}^e \mp \frac{1}{6} \frac{1}{m_e^2} \text{tr}_Y \langle p_a p_b \rangle \text{tr}_Y F_{ij3}^e \frac{N}{2N+3}, \quad (5.25)$$

for $M_J = \pm(N + \frac{1}{2})$ respectively. In fact, the final factor has a direct interpretation as c_{NN} since, from (4.13), $c_{NM=N} = N/(2N+3)$. The reason for this becomes clear in the large field limit, (5.29).

These expressions certainly appear complicated in this level of generality. However, in the following sub-section, we show how they simplify remarkably in the case of the minimal SME, due to the relations (5.34), (5.35) amongst the F_{ijk}^e couplings.

In the large magnetic field limit, we may again exploit the fact that the eigenstates of the hyperfine-Zeeman Hamiltonian are $|vNM_JM_S\rangle$ to calculate the leading and

subleading (in $c_e/\mu_B B$) corrections to $V_{\text{SME}}^{eF}(R)$. Here, we have already evaluated $\hat{V}_{\text{SME}}^{eF}(R)$ in these states, so it is straightforward to read off the large- B limit.

First we evaluate the matrix elements $\langle H_{\text{HFS}} + H_Z \rangle$ in these states, which we use as $\begin{pmatrix} A & B \\ B & D \end{pmatrix}$ in the method of footnote 9:

$$\begin{aligned} & \langle vNM_JM'_S | H_{\text{HFS}} + H_Z | vNM_JM_S \rangle \\ &= \begin{pmatrix} \frac{1}{2}c_e\left(M_J - \frac{1}{2}\right) + \left(\frac{1}{2}g_e - g_m\left(M_J - \frac{1}{2}\right)\right)\mu_B B & \frac{1}{2}c_e\sqrt{\left(N + \frac{1}{2}\right)^2 - M_J^2} \\ \frac{1}{2}c_e\sqrt{\left(N + \frac{1}{2}\right)^2 - M_J^2} & -\frac{1}{2}c_e\left(M_J + \frac{1}{2}\right) - \left(\frac{1}{2}g_e + g_m\left(M_J + \frac{1}{2}\right)\right)\mu_B B \end{pmatrix} \end{aligned} \quad (5.26)$$

The expectation values of the internucleon potential in the hyperfine-Zeeman eigenstates are then found from footnote 9 as

$$\begin{aligned} V_{\text{SME}+}^{eF}(R) &= \frac{1}{3} \frac{1}{m_e^2} \text{tr}\langle p_a p_b \rangle \text{tr} F_{ij3}^e + \frac{1}{m_e^2} \text{tr}_Y \langle p_a p_b \rangle \left[\frac{1}{6} c_{N(M_J - \frac{1}{2})} \text{tr}_Y F_{ij3}^e \right. \\ &\quad \left. + \frac{1}{2} \frac{c_e}{(g_e + g_m)\mu_B B} (F_{+3-}^e + F_{-3+}^e) \frac{[(N + \frac{1}{2})^2 - M_J^2]}{(2N - 1)(2N + 3)} M_J \right] \end{aligned} \quad (5.27)$$

and

$$\begin{aligned} V_{\text{SME}-}^{eF}(R) &= -\frac{1}{3} \frac{1}{m_e^2} \text{tr}\langle p_a p_b \rangle \text{tr} F_{ij3}^e - \frac{1}{m_e^2} \text{tr}_Y \langle p_a p_b \rangle \left[\frac{1}{6} c_{N(M_J + \frac{1}{2})} \text{tr}_Y F_{ij3}^e \right. \\ &\quad \left. + \frac{1}{2} \frac{c_e}{(g_e + g_m)\mu_B B} (F_{+3-}^e + F_{-3+}^e) \frac{[(N + \frac{1}{2})^2 - M_J^2]}{(2N - 1)(2N + 3)} M_J \right]. \end{aligned} \quad (5.28)$$

The $O(c_e/\mu_B B)$ term depends solely on the mixing of states and is proportional to the off-diagonal term in $\hat{V}_{\text{SME}}(R)$ in the $|vNM_JM_S\rangle$ basis.

The unmixed states in this basis have $M_J = \pm(N + \frac{1}{2})$, $M_S = \pm\frac{1}{2}$, and as usual the mixing factor $[(N + \frac{1}{2})^2 - M_J^2]$ vanishes. This leaves simply

$$\begin{aligned} V_{\text{SME}}^{eF}(R) &= \pm \frac{1}{3} \frac{1}{m_e^2} \text{tr}\langle p_a p_b \rangle \text{tr} F_{ij3}^e \\ &\quad \mp \frac{1}{6} \frac{1}{m_e^2} \text{tr}_Y \langle p_a p_b \rangle c_{NN} \text{tr}_Y F_{ij3}^e, \end{aligned} \quad (5.29)$$

with no $O(c_e/\mu_B B)$ correction. Notice that the factor $c_{NN} = N/(2N + 3)$, and so $V_{\text{SME}}^{eF}(R)$ here and in (5.25) are the same for the unmixed states, as they must be since the states are identical, irrespective of whether they are expressed in the $|vNJM_J\rangle$ or $|v, NM_JM_S\rangle$ basis.

This completes the derivation of the contributions of the spin-dependent SME couplings to the internucleon potential $V_{\text{SME}}^e(R)$, in both the large and small magnetic field regimes including subleading corrections of $O(\mu_B B/c_e)$ and $O(c_e/\mu_B B)$ respectively.

C. Minimal SME

We now reexpress these combinations B_3 , $\text{tr} F_{ij3}$, $\text{tr}_Y F_{ij3}$, and $(F_{+3-} + F_{-3+})$ of the spin-dependent SME couplings more directly in terms of the b_μ , $g_{\mu\nu\lambda}$, $d_{\mu\nu}$, and $H_{\mu\nu}$ appearing in the QFT Lagrangian (1.1).

It is convenient to define the following frequently occurring combinations of the CPT odd and CPT even couplings for which experimental bounds are known [18]. In fact this also reveals some interesting further simplification.

We now restrict to the minimal SME, with B_k and F_{ijk} defined in (3.1). First define

$$\begin{aligned}\tilde{b}_i &= \left(b_i + \frac{1}{2}m\epsilon_{ijk}g_{jk0}\right) - \left(md_{i0} + \frac{1}{2}\epsilon_{ijk}H_{jk}\right), \\ \tilde{b}_i^* &= \left(b_i + \frac{1}{2}m\epsilon_{ijk}g_{jk0}\right) + \left(md_{i0} + \frac{1}{2}\epsilon_{ijk}H_{jk}\right),\end{aligned}\quad (5.30)$$

and

$$\begin{aligned}\tilde{g}_{Di} &= -b_i + m\epsilon_{ijk}\left(g_{j0k} + \frac{1}{2}g_{jk0}\right), \\ \tilde{d}_i &= m\left(d_{0i} + \frac{1}{2}d_{i0}\right) - \frac{1}{4}\epsilon_{ijk}H_{jk}.\end{aligned}\quad (5.31)$$

In particular, the couplings arising here in the calculation of $V_{\text{SME}}^e(R)$ are

$$\begin{aligned}\tilde{b}_3 &= (b_3 + mg_{120}) - (md_{30} + H_{12}), \\ \tilde{g}_{D3} &= -b_3 + m(g_{102} - g_{201} + g_{120}), \\ \tilde{d}_3 &= m\left(d_{03} + \frac{1}{2}d_{30}\right) - \frac{1}{2}H_{12}.\end{aligned}\quad (5.32)$$

A straightforward calculation from the SME Hamiltonian (3.1) and (3.2) now shows that the following very simple relations hold in the minimal SME:

$$B_3 = -\tilde{b}_3, \quad (5.33)$$

and

$$\begin{aligned}\text{tr}F_{ij3} &= -\tilde{g}_{D3} + \tilde{d}_3, \\ \text{tr}_Y F_{ij3} &= -\tilde{g}_{D3} - 2\tilde{d}_3,\end{aligned}\quad (5.34)$$

while

$$(F_{+3-} + F_{-3+}) = \tilde{g}_{D3} + 2\tilde{d}_3. \quad (5.35)$$

This shows that in the minimal SME, the momentum and spin-dependent contributions to $V_{\text{SME}}^e(R)$ depend on just *two* independent couplings, the *CPT* odd $\tilde{g}_{D3}$ and *CPT* even $\tilde{d}_3$, in two distinct combinations.

This raises an interesting point. In principle, we can use the different N dependence of the coefficients of the terms in $V_{\text{SME}}^e(R)$ (see $f_{NM_J}^\pm$ and $f_{NM_J}^{Y\pm}$ below) to extract $\text{tr}F_{ij3}^e$ and $\text{tr}_Y F_{ij3}^e$ from combinations of transition energies, as described in Paper I and here in Sec. VII. But then according to (5.34), we would determine $\tilde{g}_{D3}$ and $\tilde{d}_3$ *independently*. A nonzero value of $\tilde{g}_{D3}$ would indicate *CPT* violation, deduced from the spectrum of the pure matter ion H_2^+ .

However, this conclusion may simply be an artifact of restricting to the minimal SME. In Sec. VI, the equivalent analysis would lead us to an independent determination of the two spherical tensor couplings, $\mathcal{T}_{210}^{\text{NR}(OB)} = g_{210}^{\text{NR}(OB)} - H_{210}^{\text{NR}(OB)}$ and $\mathcal{T}_{210}^{\text{NR}(1B)} = g_{210}^{\text{NR}(1B)} - H_{210}^{\text{NR}(1B)}$, as identified

in (6.20). So then we would not be able to conclude whether or not one of the g_{210}^{NR} couplings was nonzero and so whether or not *CPT* was violated. The issue arises because for this particular measurement, the minimal SME has only half the relevant number of couplings as are permitted in general. This special case arises because of the two zeroes in the dictionary in (6.24) and (6.25), which we have no obvious reason to expect to persist in higher order. In such cases, we must apply the minimal SME with caution.

In fact, this is a common feature of effective field theories in general, where unless a sufficiently complete number of operators are included in the low-energy theory, spurious predictions will follow from its use. It is the logic, for example, behind the inclusion here of the nonminimal *CPT* odd operator with coupling $a_{\mu\nu\lambda}$.

The individual terms F_{+3-} and F_{-3+} are given by

$$\begin{aligned}F_{+3-} &= \frac{1}{2}\tilde{g}_{D3} - \frac{i}{2}m\text{tr}_Y g_{i0j} + \tilde{d}_3, \\ F_{-3+} &= \frac{1}{2}\tilde{g}_{D3} + \frac{i}{2}m\text{tr}_Y g_{i0j} + \tilde{d}_3,\end{aligned}\quad (5.36)$$

where of course the imaginary part proportional to $\text{tr}_Y g_{i0j}$ cancels in the sum, which controls the physical energy levels.

The couplings $|\tilde{g}_{Di}|$ and $|\tilde{d}_i|$ are constrained by several experiments, notably spin-precession and clock comparison experiments, with already very stringent bounds of $O(10^{-22} \text{ GeV})$ [18]. For $|\tilde{b}_i|$, even tighter bounds of up to 10^{-24} GeV are quoted in [18]. Weaker bounds may be deduced from atomic hydrogen and antihydrogen spectroscopy, from nS - $n'P$ or D and ground-state hyperfine transitions respectively.

For completeness, we also record here some further results which are useful in the comparison of the SME Hamiltonian written in terms of these Cartesian tensor couplings and their equivalent expression as spherical tensors. The relations with spherical tensors are discussed in Sec. VI B.

In particular, we find

$$\begin{aligned}B_\pm &= -(b_\pm \mp img_{\pm 30}) + (md_{\pm 0} \mp iH_{\pm 3}), \\ \text{tr}F_{ij\pm} &= -\tilde{g}_{D\pm} + \tilde{d}_\pm, \\ \text{tr}_Y F_{ij\pm} &= \frac{1}{2}\tilde{g}_{D\pm} + \tilde{d}_\pm \mp 3im(g_{\pm 03} + g_{30\pm}).\end{aligned}\quad (5.37)$$

As indicated earlier, we can now use the minimal SME relation $(F_{+3-}^e + F_{-3+}^e) = \text{tr}_Y F_{ijk}^e$ from (5.34) and (5.35) to simplify our earlier expressions (5.19)–(5.24) for $V_{\text{SME}}^e(R)$.

In this case, remarkable cancellations occur between the two terms in the coefficient of $\text{tr}_Y \langle p_a p_b \rangle$. Re-expressing α , δ , and β in terms of the couplings $\tilde{g}_{D3}$ and $\tilde{d}_3$, we now find simply

$$\alpha = \frac{1}{3} \frac{1}{m_e^2} \text{tr} \langle p_a p_b \rangle (-\tilde{g}_{D3} + \tilde{d}_3) \frac{2}{2N+1} M_J + \frac{1}{6} \frac{1}{m_e^2} \text{tr}_Y \langle p_a p_b \rangle (\tilde{g}_{D3} + 2\tilde{d}_3) \frac{2N}{(2N+1)(2N+3)} M_J, \quad (5.38)$$

and

$$\delta = -\frac{1}{3} \frac{1}{m_e^2} \text{tr} \langle p_a p_b \rangle (-\tilde{g}_{D3} + \tilde{d}_3) \frac{2}{2N+1} M_J - \frac{1}{6} \frac{1}{m_e^2} \text{tr}_Y \langle p_a p_b \rangle (\tilde{g}_{D3} + 2\tilde{d}_3) \frac{2(N+1)}{(2N-1)(2N+1)} M_J, \quad (5.39)$$

while

$$\begin{aligned} \text{Re}\beta &= \frac{1}{3} \frac{1}{m_e^2} \text{tr} \langle p_a p_b \rangle (-\tilde{g}_{D3} + \tilde{d}_3) \frac{(-2)}{2N+1} \sqrt{\left(N + \frac{1}{2}\right)^2 - M_J^2} \\ &\quad - \frac{1}{6} \frac{1}{m_e^2} \text{tr}_Y \langle p_a p_b \rangle (\tilde{g}_{D3} + 2\tilde{d}_3) \frac{1}{2(2N+1)} \sqrt{\left(N + \frac{1}{2}\right)^2 - M_J^2}. \end{aligned} \quad (5.40)$$

Notice that the diagonal terms α and δ are proportional to M_J , whereas the off-diagonal term instead has the common factor $\sqrt{\left(N + \frac{1}{2}\right)^2 - M_J^2}$ [compare (2.6)], which vanishes for the unmixed states where $M_J = \pm(N + \frac{1}{2})$.

We can now write (5.23)–(5.25) in a particularly compact form analogous to (4.16)–(4.19):

$$V_{\text{SME}\pm}^{eF}(R) = \frac{1}{3} \frac{1}{m_e^2} \text{tr} \langle p_a p_b \rangle (-\tilde{g}_{D3} + \tilde{d}_3) f_{NM_J}^{\pm}(B) + \frac{1}{6} \frac{1}{m_e^2} \text{tr}_Y \langle p_a p_b \rangle (\tilde{g}_{D3} + 2\tilde{d}_3) f_{NM_J}^{Y\pm}(B), \quad (5.41)$$

where

$$\begin{aligned} f_{NM_J}^{+} &= \frac{2}{2N+1} M_J + \frac{8}{(2N+1)^3} \left[\left(N + \frac{1}{2}\right)^2 - M_J^2 \right] \frac{1}{c_e(v, N)} (g_e + g_m(v, N)) \mu_B B, \\ f_{NM_J}^{Y+} &= \frac{2N}{(2N+1)(2N+3)} M_J - \frac{2}{(2N+1)^3} \left[\left(N + \frac{1}{2}\right)^2 - M_J^2 \right] \frac{1}{c_e(v, N)} (g_e + g_m(v, N)) \mu_B B, \end{aligned} \quad (5.42)$$

and

$$\begin{aligned} f_{NM_J}^{-} &= -\frac{2}{2N+1} M_J - \frac{8}{(2N+1)^3} \left[\left(N + \frac{1}{2}\right)^2 - M_J^2 \right] \frac{1}{c_e(v, N)} (g_e + g_m(v, N)) \mu_B B, \\ f_{NM_J}^{Y-} &= -\frac{2(N+1)}{(2N-1)(2N+1)} M_J + \frac{2}{(2N+1)^3} \left[\left(N + \frac{1}{2}\right)^2 - M_J^2 \right] \frac{1}{c_e(v, N)} (g_e + g_m(v, N)) \mu_B B, \end{aligned} \quad (5.43)$$

while for the unmixed states, we simply write $V_{\text{SME}}^{eF}(R)$ as in (5.41) with

$$f_{NM_J} = \pm 1, \quad f_{NM_J}^Y = \pm \frac{N}{2N+3}. \quad (5.44)$$

We return to these expressions in Sec. VII where we show how, together with the analysis of Paper I, they immediately give the SME contributions to the hyperfine-Zeeman energy levels E_{vNJM_J} , including mixing.

VI. THE SME SPHERICAL TENSOR COUPLING FORMALISM

The SME Hamiltonian and associated parameter constraints may alternatively be described in terms of the spherical tensor representation of the Lorentz and *CPT* couplings most widely used in the analysis of spectroscopy in this theory. This has a number of virtues, notably allowing a compact description of higher-dimensional

operators in the extension beyond the minimal SME. However, it also necessarily obscures the immediate relation with the couplings as they appear in the QFT Lagrangian. In order to make contact with the extensive body of literature on the SME using this formalism, in this section we show how our results for the molecular ion spectrum may be rewritten in the spherical tensor form and give a detailed dictionary between the Cartesian and spherical tensor couplings.

The nonrelativistic SME Hamiltonian in the spherical tensor formalism is presented in a very general form including higher-dimensional operators in [15] and we use this extensively in what follows. In that work, however, the initial Hamiltonian is written with the couplings defined

in what in our context we are calling the MOL frame, but with the spin operators in a “helicity frame” HEL with z axis aligned with the electron momentum. The first task is therefore to find the SME Hamiltonian for the electron with both the spin operators and couplings expressed in the MOL frame. This construction is described in Appendix A. We distinguish the couplings in the MOL frame with circumflex accents, e.g. $\hat{V}_{njm}^{\text{NR}}$.

We find the following result, (A18), for the SME Hamiltonian H_{SME} in the MOL frame, which in the Born-Oppenheimer analysis is incorporated in the electron Schrödinger equation leading to the potential $V_{\text{SME}}^e(\mathbf{R})$:

$$H_{\text{SME}} = -\sqrt{\frac{1}{4\pi}} \left[\hat{V}_{000}^{\text{NR}} + \text{tr} p_a p_b \hat{V}_{200}^{\text{NR}} - \sqrt{5} \frac{1}{2} \text{tr}_Y p_a p_b \hat{V}_{220}^{\text{NR}} + \sqrt{3} \hat{\sigma}_s \delta_{sm} \hat{T}_{01m}^{\text{NR(0B)}} + \sqrt{3} \hat{\sigma}_s \left(\frac{1}{3} \text{tr} p_a p_b \delta_{sm} + \frac{1}{6} \text{tr}_Y p_a p_b Y_{sm} \right) \hat{T}_{21m}^{\text{NR(0B)}} \right. \\ \left. + \sqrt{3} \hat{\sigma}_s \left(\frac{2}{3} \text{tr} p_a p_b \delta_{sm} - \frac{1}{6} \text{tr}_Y p_a p_b Y_{sm} \right) \hat{T}_{21m}^{\text{NR(1B)}} + \sqrt{5} \frac{1}{2} \text{tr}_Y p_a p_b \hat{\sigma}_s T_{sm} i \hat{T}_{22m}^{\text{NR(1E)}} \right]. \quad (6.1)$$

Recall that here we have omitted the $\hat{T}_{23m}^{\text{NR(0B)}}$ and $\hat{T}_{23m}^{\text{NR(1B)}}$ terms since these couplings correspond to higher-dimensional operators not present in the minimal SME, which is our primary focus here. We have also kept only the electron momentum factors $\text{tr} p_a p_b$ and $\text{tr}_Y p_a p_b$ which give nonvanishing expectation values in the molecular ion $1s\sigma_g$ state.

A. SME Hamiltonian H_{SME} in the EXP frame

As discussed earlier, spectroscopic measurements are made in the EXP frame of reference with the quantization axis aligned with the externally applied magnetic field. In this frame, the molecule rotates and vibrates and is described, for Para- H_2^+ , by the states $|vNJM_J\rangle$ or $|vNM_N M_J\rangle$ as described in Sec. II. The electron spin quantum number M_S is referred to the 3-axis in the EXP frame, while $\mathbf{N}$ is the total molecular orbital angular momentum in this frame. We therefore need to transform the SME Hamiltonian (6.1) from the MOL frame to the EXP frame in order to evaluate $V_{\text{SME}}^e(\mathbf{R})$.

The transformations under the rotation from MOL to EXP of the spin operators and SME couplings written as spherical tensors are described by Wigner matrices as follows:

$$\begin{aligned} \hat{\sigma}_{s'} &= \sigma_s d_{ss'}^1(\theta) e^{-is\phi}, \\ \hat{V}_{njm'} &= \mathcal{V}_{njm} d_{mm'}^j(\theta) e^{im\phi}, \\ \hat{T}_{njm'} &= \mathcal{T}_{njm} d_{mm'}^j(\theta) e^{im\phi}, \end{aligned} \quad (6.2)$$

where (θ, ϕ) are the standard spherical polar angles specifying the orientation of the molecular axis in the EXP frame.

It will be useful to record here some general properties of Wigner matrices which are used extensively below. They are defined in terms of angular momentum states $|jm\rangle$ by

$$d_{m'm}(\theta) = \langle jm' | e^{-i\theta J_z} | jm \rangle, \quad (6.3)$$

and are related to the spherical harmonics by

$$Y_{jm}(\theta, \phi) = \sqrt{\frac{2j+1}{4\pi}} d_{m0}^j(\theta) e^{im\phi}. \quad (6.4)$$

They satisfy orthonormality relations,

$$\sum_k d_{m'k}^j d_{mk}^j = \delta_{m'm}, \quad (6.5)$$

and satisfy the useful identities,

$$d_{mm'}^j = (-1)^{m'-m} d_{mm'}^j = d_{-m, -m'}^j. \quad (6.6)$$

As reducible representations of the rotation group, products of the $d_{m'm}^j(\theta)$ may be expanded in terms of a sum of irreducible representations using Clebsch-Gordan coefficients,

$$d_{s'm'}^{j'}(\theta) d_{sm}^j(\theta) = \sum_J C_{j's',js}^{J(s'+s)} C_{j'm',jm}^{J(m+m')} d_{s'+s, m'+m}^J(\theta), \quad (6.7)$$

with the sum over $J = |j' - j|, \dots, (j' + j)$.

First, consider the spin-independent couplings in (6.1). $\hat{V}_{000}^{\text{NR}}$ and $\hat{V}_{200}^{\text{NR}}$ are invariant under the rotation (6.2), while $\hat{V}_{220}^{\text{NR}} = \mathcal{V}_{22m}^{\text{NR}} d_{m0}^2 e^{im\phi}$. So using (6.4) to reexpress in terms

of spherical harmonics, and replacing the electron momentum factors with their expectation values, we find the contribution of the spin-independent couplings to the potential $V_{\text{SME}}^e(\mathbf{R})$:

$$V_{\text{SME}}^{e\mathcal{V}}(\mathbf{R}) = -\sqrt{\frac{1}{4\pi}}(\mathcal{V}_{000}^{\text{NR}} + \text{tr}\langle p_a p_b \rangle \mathcal{V}_{200}^{\text{NR}}) + \frac{1}{2} \text{tr}_Y \langle p_a p_b \rangle Y_{2m}(\theta, \phi) \mathcal{V}_{22m}^{\text{NR}}. \quad (6.8)$$

For the spin-dependent terms, those where the spin and coupling indices are contracted with δ_{sm} are clearly invariant, since in that case both transform with Wigner matrices with $j = 1$ and we can use the orthonormality relation (6.5). The main technical problem is therefore to transform the terms of the form $\hat{\sigma}_s \mathbf{Y}_{sm} \hat{\mathcal{T}}_{2jm}^{\text{NR}}$ and $\hat{\sigma}_s \mathbf{T}_{sm} \hat{\mathcal{T}}_{2jm}^{\text{NR}}$ in (6.1) to the EXP frame.

First, we may write, for example,

$$\hat{\sigma}_s \mathbf{Y}_{sm} \hat{\mathcal{T}}_{21m}^{\text{NR}(0B)} = \hat{\sigma}_m \hat{\mathcal{T}}_{21m}^{\text{NR}(0B)} - 3\hat{\sigma}_0 \hat{\mathcal{T}}_{210}^{\text{NR}(0B)}, \quad (6.9)$$

where the first term is invariant. For the second term, using the product formula (6.7) and reexpressing in terms of spherical harmonics, we find

$$\begin{aligned} \hat{\sigma}_0 \hat{\mathcal{T}}_{210}^{\text{NR}(0B)} &= \sigma_s (e^{-is\phi} d_{s0}^1(\theta) d_{m0}^1(\theta) e^{im\phi}) \mathcal{T}_{21m}^{\text{NR}(0B)} \\ &= \sigma_s \left((-1)^s \sum_{J=0,1,2} \sqrt{\frac{4\pi}{2J+1}} C_{10,10}^{J0} C_{1-s,1m}^{JM} Y_{JM}(\theta, \phi) \right) \mathcal{T}_{21m}^{\text{NR}(0B)}, \end{aligned} \quad (6.10)$$

with $M = -s + m$. Here, we have used the identity $d_{s0}^1 = (-1)^s d_{-s,0}^1$ to recast the Wigner matrix product in a convenient form to simplify the subsequent calculation. Then, since the Clebsch-Gordan coefficient $C_{10,10}^{10} = 0$, only $J = 0$ and $J = 2$ contribute to the sum in (6.10). The $J = 0$ contribution precisely cancels the first term on the right-hand side of (6.9) leaving simply

$$\hat{\sigma}_s \mathbf{Y}_{sm} \hat{\mathcal{T}}_{21m}^{\text{NR}(0B)} = -3\sqrt{\frac{4\pi}{5}} \sqrt{\frac{2}{3}} \sigma_s \left((-1)^s \sum_M C_{1-s,1m}^{2M} Y_{2M}(\theta, \phi) \right) \mathcal{T}_{21m}^{\text{NR}(0B)}, \quad (6.11)$$

where we have displayed the sum over $M = -2, \dots, 2$ (which is anyway implicit in the sums over s, m) simply for clarity. Substituting back into $\hat{H}_{\text{SME}}$, we therefore find the contribution of the (0B) and (1B) couplings with $j = 1$ to $V_{\text{SME}}^e(\mathbf{R})$ as

$$\begin{aligned} V_{\text{SME}}^{e(0B),(1B)} &= -\sqrt{\frac{3}{4\pi}} \left[\sigma_m \mathcal{T}_{01m}^{\text{NR}(0B)} + \frac{1}{3} \text{tr}\langle p_a p_b \rangle \sigma_m (\mathcal{T}_{21m}^{\text{NR}(0B)} + 2\mathcal{T}_{21m}^{\text{NR}(1B)}) \right] \\ &\quad - \sqrt{\frac{1}{10}} \text{tr}_Y \langle p_a p_b \rangle \sigma_s \left((-1)^s \sum_M C_{1-s,1m}^{2M} Y_{2M}(\theta, \phi) \right) (\mathcal{T}_{21m}^{\text{NR}(0B)} - \mathcal{T}_{21m}^{\text{NR}(1B)}). \end{aligned} \quad (6.12)$$

Next consider the $\mathcal{T}_{22m}^{\text{NR}(1E)}$ couplings. Here, we need to evaluate directly:

$$\hat{\sigma}_s \mathbf{T}_{sm} i \hat{\mathcal{T}}_{22m}^{\text{NR}(1E)} = \sigma_s e^{-is\phi} (-1)^{s-1} (d_{-s,-1}^1 d_{m,1}^2 - d_{-s,1}^1 d_{m,-1}^2) e^{im\phi} i \mathcal{T}_{22m}^{\text{NR}(1E)}, \quad (6.13)$$

where we again use a Wigner matrix identity, $d_{s,1}^1 = (-1)^{s-1} d_{-s,-1}^1$, to put the product into a convenient form to reexpress in spherical harmonics. Then,

$$(d_{-s,-1}^1 d_{m,1}^2 - d_{-s,1}^1 d_{m,-1}^2) = \sum_{J=1,2,3} C_{1-s,2m}^{J(-s+m)} (C_{1-1,21}^{J0} - C_{11,2-1}^{J0}) d_{(-s+m),0}^J, \quad (6.14)$$

and explicitly evaluating the Clebsch-Gordan coefficients in brackets shows that again only $J = 2$ gives a nonvanishing contribution, leaving

$$\hat{\sigma}_s \mathbf{T}_{sm} i \hat{\mathcal{T}}_{22m}^{\text{NR}(1E)} = \sqrt{2} \sqrt{\frac{4\pi}{5}} \sigma_s \left((-1)^s \sum_M C_{1-s,2m}^{2M} Y_{2M}(\theta, \phi) \right) i \mathcal{T}_{22m}^{\text{NR}(1E)}. \quad (6.15)$$

The contribution of the $(1E)$ couplings to $V_{\text{SME}}^e(\mathbf{R})$ is therefore

$$V_{\text{SME}}^{e(1E)} = -\frac{1}{\sqrt{2}} \text{tr}_Y \langle p_a p_b \rangle \sigma_s \left((-1)^s \sum_M C_{1-s,2m}^{2M} Y_{2M}(\theta, \phi) \right) iT_{22m}^{\text{NR}(1E)}. \quad (6.16)$$

This completes the transformation of the SME Hamiltonian from the MOL frame to the required expression in terms of EXP frame spins and couplings. The expectation values of the electron momenta $\langle p_a p_b \rangle$ remain of course evaluated in the MOL frame. Finally, therefore, collecting the results (6.8), (6.12), and (6.16), we can write the full contribution to the potential $V_{\text{SME}}^e(\mathbf{R})$ as

$$\begin{aligned} V_{\text{SME}}^e(\mathbf{R}) = & -\sqrt{\frac{1}{4\pi}} (\mathcal{V}_{000}^{\text{NR}} + \text{tr} \langle p_a p_b \rangle \mathcal{V}_{200}^{\text{NR}}) + \frac{1}{2} \text{tr}_Y \langle p_a p_b \rangle Y_{2m}(\theta, \phi) \mathcal{V}_{22m}^{\text{NR}} \\ & - \sqrt{\frac{3}{4\pi}} \left[\sigma_m \mathcal{T}_{01m}^{\text{NR}(0B)} + \frac{1}{3} \text{tr} \langle p_a p_b \rangle \sigma_m (\mathcal{T}_{21m}^{\text{NR}(0B)} + 2\mathcal{T}_{21m}^{\text{NR}(1B)}) \right] \\ & + \sqrt{\frac{1}{10}} \text{tr}_Y \langle p_a p_b \rangle \sigma_s \left((-1)^s \sum_M C_{1-s,1m}^{2M} Y_{2M}(\theta, \phi) \right) (\mathcal{T}_{21m}^{\text{NR}(0B)} - \mathcal{T}_{21m}^{\text{NR}(1B)}) \\ & - \sqrt{\frac{1}{2}} \text{tr}_Y \langle p_a p_b \rangle \sigma_s \left((-1)^s \sum_M C_{1-s,2m}^{2M} Y_{2M}(\theta, \phi) \right) iT_{22m}^{\text{NR}(1E)}. \end{aligned} \quad (6.17)$$

As we have already seen for the spin-independent couplings in Paper I, and here in Secs. IV and V, the contributions proportional to $\text{tr}_Y \langle p_a p_b \rangle$ involve a nontrivial dependence on the spherical harmonics $Y_{2M}(\theta, \phi)$, which capture the orientation of the molecular axis in the EXP frame.

Now, as discussed in Secs. IV and V, the next step in the Born-Oppenheimer analysis is to evaluate $V_{\text{SME}}^e(\mathbf{R})$ in the hyperfine states $|vNJM_J\rangle$ to yield the modified internucleon potential itself, $V_{\text{SME}}^e(R)$. These states are linear combinations of the states $|vNM_N M_S\rangle$ in which the expectation values of the spin operators in (6.17) are calculated. In general, this involves many contributions, but at this point we may use the simplification introduced in Sec. V.

As we saw there, the hyperfine and Zeeman interactions do not mix states with different M_J . Any terms in $V_{\text{SME}}^e(\mathbf{R})$ with matrix elements between states with $\Delta M_J \neq 0$ therefore give

rise to off-diagonal entries which are purely of $O(\text{SME})$ and therefore contribute only at $O(\text{SME})^2$ to the energy eigenvalues. These terms should therefore be neglected.

In the present formalism, the requirement $\Delta M_J = \Delta M_N + \Delta M_S = 0$ implies that $M + s = 0$ in (6.17), restricting the spherical harmonics that can contribute at $O(\text{SME})$. Then, since the Clebsch-Gordan coefficients impose $M = -s + m$, we see that only the SME couplings with $m = 0$ contribute at $O(\text{SME})$. This enormously simplifies the application of (6.17).

The required Clebsch-Gordan coefficients in (6.17) with $m = 0$, $M = -s$ are $(-1)^s C_{1-s,10}^{2-s} = -\sqrt{\frac{1}{2}}, -\sqrt{\frac{1}{2}}, \sqrt{\frac{2}{3}}$ and $(-1)^s C_{1-s,20}^{2-s} = -\sqrt{\frac{1}{2}}, \sqrt{\frac{1}{2}}, 0$ for the spin index $s = 1, -1, 0$ respectively. Keeping only these terms, (6.17) reduces to

$$\begin{aligned} V_{\text{SME}}^e(\mathbf{R}) = & -\sqrt{\frac{1}{4\pi}} (\mathcal{V}_{000}^{\text{NR}} + \text{tr} \langle p_a p_b \rangle \mathcal{V}_{200}^{\text{NR}}) + \frac{1}{2} \text{tr}_Y \langle p_a p_b \rangle Y_{20}(\theta, \phi) \mathcal{V}_{220}^{\text{NR}} \\ & - \sqrt{\frac{3}{4\pi}} \left[\sigma_0 \mathcal{T}_{010}^{\text{NR}(0B)} + \frac{1}{3} \text{tr} \langle p_a p_b \rangle \sigma_0 (\mathcal{T}_{210}^{\text{NR}(0B)} + 2\mathcal{T}_{210}^{\text{NR}(1B)}) \right] \\ & + \sqrt{\frac{1}{15}} \text{tr}_Y \langle p_a p_b \rangle \sigma_0 (\mathcal{T}_{210}^{\text{NR}(0B)} - \mathcal{T}_{210}^{\text{NR}(1B)}) Y_{20}(\theta, \phi) \\ & - \frac{1}{2} \sqrt{\frac{1}{5}} \text{tr}_Y \langle p_a p_b \rangle [\sigma_1 (\mathcal{T}_{210}^{\text{NR}(0B)} - \mathcal{T}_{210}^{\text{NR}(1B)}) - \sqrt{5} i \mathcal{T}_{220}^{\text{NR}(1E)}] Y_{2,-1}(\theta, \phi) \\ & + \sigma_{-1} (\mathcal{T}_{210}^{\text{NR}(0B)} - \mathcal{T}_{210}^{\text{NR}(1B)} + \sqrt{5} i \mathcal{T}_{220}^{\text{NR}(1E)}) Y_{2,1}(\theta, \phi). \end{aligned} \quad (6.18)$$

This expression for $V_{\text{SME}}^e(\mathbf{R})$ in terms of the spherical tensor couplings may now be compared directly with our original forms (4.14), (5.1), and (5.11). We see that they coincide precisely, given the identifications:

$$\frac{1}{m^2} \text{tr} E_{ij} = -3 \sqrt{\frac{1}{4\pi}} \mathcal{V}_{200}^{\text{NR}}, \quad \frac{1}{m^2} \text{tr}_Y E_{ij} = 3 \sqrt{\frac{5}{4\pi}} \mathcal{V}_{220}^{\text{NR}}, \quad (6.19)$$

and also $A = -\sqrt{\frac{1}{4\pi}} \mathcal{V}_{000}^{\text{NR}}$ (though this is unobservable), and for the spin-dependent couplings,

$$\begin{aligned} B_3 &= -\sqrt{\frac{3}{4\pi}} \mathcal{T}_{010}^{\text{NR}(0B)}, \\ \frac{1}{m^2} \text{tr} F_{ij3} &= -\sqrt{\frac{3}{4\pi}} (\mathcal{T}_{210}^{\text{NR}(0B)} + 2\mathcal{T}_{210}^{\text{NR}(1B)}), \\ \frac{1}{m^2} \text{tr}_Y F_{ij3} &= 2\sqrt{\frac{3}{4\pi}} (\mathcal{T}_{210}^{\text{NR}(0B)} - \mathcal{T}_{210}^{\text{NR}(1B)}), \\ \frac{1}{m^2} F_{-3+} &= -\sqrt{\frac{3}{4\pi}} (\mathcal{T}_{210}^{\text{NR}(0B)} - \mathcal{T}_{210}^{\text{NR}(1B)} - \sqrt{5}i\mathcal{T}_{220}^{\text{NR}(1E)}), \\ \frac{1}{m^2} F_{+3-} &= -\sqrt{\frac{3}{4\pi}} (\mathcal{T}_{210}^{\text{NR}(0B)} - \mathcal{T}_{210}^{\text{NR}(1B)} + \sqrt{5}i\mathcal{T}_{220}^{\text{NR}(1E)}). \end{aligned} \quad (6.20)$$

B. Minimal SME—equivalence with Lagrangian couplings

We can verify these identifications in the minimal SME by expressing the spherical tensor couplings in terms of those in the original SME Lagrangian and comparing with the equivalent formulas for E_{ij} , B_k , and F_{ijk} in Secs. IV and V.

First, for the spin-independent terms

$$\mathcal{V}_{njm}^{\text{NR}} = c_{njm}^{\text{NR}} - a_{njm}^{\text{NR}}, \quad (6.21)$$

and we can check the equivalence directly with the results already stated in (4.26) and (4.27).

For the spin-dependent terms, the tensor operators $\mathcal{T}_{njm}^{\text{NR}}$ are defined in terms of CPT odd, g_{njm}^{NR} , and CPT even, H_{njm}^{NR} , operators,

$$\mathcal{T}_{njm}^{\text{NR}} = g_{njm}^{\text{NR}} - H_{njm}^{\text{NR}}, \quad (6.22)$$

for each of the types (0B), (1B), and (1E). The required expressions for the g_{njm}^{NR} and H_{njm}^{NR} couplings in terms of b_μ , $g_{\mu\lambda}$, $d_{\mu\nu}$, and $H_{\mu\nu}$ are given in [15], but in many cases require significant calculation to extract the results we need since the minimal SME identifications in [15] are quoted in terms of dual couplings and related to the spherical tensors

before taking the nonrelativistic limit (indicated by the subscript NR here) which mixes couplings with different values of n .

For the spin-dependent $\mathcal{T}_{010}^{\text{NR}}$ couplings, we need

$$\begin{aligned} \sqrt{\frac{3}{4\pi}} g_{010}^{\text{NR}(0B)} &= \sqrt{\frac{3}{4\pi}} g_{010}^{\text{NR}(1B)} = \frac{1}{2} (\tilde{b}_3 + \tilde{b}_3^*) = b_3 + m g_{120}, \\ \sqrt{\frac{3}{4\pi}} H_{010}^{\text{NR}(0B)} &= \sqrt{\frac{3}{4\pi}} H_{010}^{\text{NR}(1B)} = -\frac{1}{2} (\tilde{b}_3 - \tilde{b}_3^*) = m d_{30} + H_{12}, \end{aligned} \quad (6.23)$$

consistent with the identification $B_3 = -\tilde{b}_3$ in Sec. V C.

Next, we have the $\mathcal{T}_{210}^{\text{NR}}$ relations familiar from applications in atomic spectroscopy:

$$\sqrt{\frac{3}{4\pi}} g_{210}^{\text{NR}(0B)} = 0, \quad \sqrt{\frac{3}{4\pi}} g_{210}^{\text{NR}(1B)} = \frac{1}{2} \frac{1}{m^2} \tilde{g}_{D3}, \quad (6.24)$$

and

$$\sqrt{\frac{3}{4\pi}} H_{210}^{\text{NR}(0B)} = \frac{1}{m^2} \tilde{d}_3, \quad \sqrt{\frac{3}{4\pi}} H_{210}^{\text{NR}(1B)} = 0, \quad (6.25)$$

which together with (5.34) confirms the identifications above for $\text{tr} F_{ij3}$ and $\text{tr}_Y F_{ij3}$. The identity (5.35) for the sum $(F_{+3-} + F_{-3+})$ also follows.

For the individual relations for F_{+3-} and F_{-3+} in (6.20), we also need the $\mathcal{T}_{220}^{\text{NR}(1E)}$ coupling. In this case, only $g_{220}^{\text{NR}(1E)}$ contributes in the minimal SME, and we find¹⁰

$$i g_{220}^{\text{NR}(1E)} = \sqrt{\frac{\pi}{15}} i \text{tr}_Y g_{i0j}, \quad (6.26)$$

where the trace is over i, j , in agreement with (5.36). This completes the necessary identifications to establish the equivalence of $V_{\text{SME}}^e(\mathbf{R})$ in the spherical and Cartesian tensor frameworks.

It is also interesting to verify directly the equivalence of the SME Hamiltonians in the MOL frame. For this, we need to extend the above results to include those with index $m \neq 1$. In particular, we need to verify the identities (A20) given the expressions for $B_\pm$, $\text{tr} F_{ij\pm}$, and $\text{tr}_Y F_{ij\pm}$ in (5.37).

¹⁰There is a subtlety here since reading off the equivalent result from [15], where results are quoted in terms of the four-dimensional duals $\tilde{g}^{\mu\nu\lambda}$, there is an apparent discrepancy proportional to $\text{tr} g_{i0j}$. However, this can be reexpressed as $(\tilde{g}^{123} + \tilde{g}^{231} + \tilde{g}^{312})$ which is omitted in [15] as being unobservable.

First, for $\mathcal{T}_{01\pm1}^{\text{NR}}$, we have

$$\begin{aligned}\sqrt{\frac{3}{4\pi}}g_{01\pm1}^{\text{NR}(0B)} &= \sqrt{\frac{3}{4\pi}}g_{01\pm1}^{\text{NR}(1B)} = \mp\sqrt{\frac{1}{2}}(b_{\mp} \pm img_{\mp30}), \\ \sqrt{\frac{3}{4\pi}}H_{01\pm1}^{\text{NR}(0B)} &= \sqrt{\frac{3}{4\pi}}H_{01\pm1}^{\text{NR}(1B)} = \mp\sqrt{\frac{1}{2}}(md_{\mp0} \pm iH_{\mp3}),\end{aligned}\quad (6.27)$$

which confirms the required relation for $B_{\pm}$.

Next, we find

$$\begin{aligned}\sqrt{\frac{3}{4\pi}}g_{21\pm1}^{\text{NR}(1B)} &= \mp\frac{1}{2\sqrt{2}}\frac{1}{m^2}\tilde{g}_{D\mp}, \\ \sqrt{\frac{3}{4\pi}}H_{21\pm1}^{\text{NR}(0B)} &= \mp\frac{1}{\sqrt{2}}\frac{1}{m^2}\tilde{d}_{\mp},\end{aligned}\quad (6.28)$$

as the natural generalisations of (6.25), noting that the vanishing of $g_{21m}^{\text{NR}(0B)}$ and $H_{21m}^{\text{NR}(1B)}$ holds in the minimal SME for all index m . Then,

$$\sqrt{\frac{5}{4\pi}}ig_{22\pm1}^{\text{NR}(1E)} = \pm\frac{1}{2\sqrt{2}}\frac{i}{m}(g_{\mp03} + g_{30\mp}).\quad (6.29)$$

This closes the loop establishing the consistency of (A20) with the expressions (5.37) for $\text{tr}F_{ij\pm}$ and $\text{tr}_Y F_{ij\pm}$.

VII. ROVIBRATIONAL SPECTRUM OF H_2^+ AND $\tilde{\text{H}}_2^-$

In this final section, we use the analysis of Paper I to translate the results of Secs. IV and V for the internucleon potentials $V_{\text{SME}}^{eE}(R)$ and $V_{\text{SME}}^{eF}(R)$, and ΔE_{SME}^n , into explicit expressions for the rovibrational energies in the hyperfine-Zeeman states. We also comment briefly on how these results may influence an experimental programme of testing Lorentz and CPT symmetry in high-precision spectroscopy with H_2^+ and $\tilde{\text{H}}_2^-$. Further details will be presented elsewhere.

Restricting for clarity just to the leading terms in $(v + \frac{1}{2})$ and $N(N+1)$ in the expansion (3.13), we consider here the rovibrational energies,

$$\begin{aligned}E_{vNJM_J} &= \mathcal{E}_{\text{SME}}^e + (1 + \delta_{\text{SME}}^e + \delta_{\text{SME}}^n)\left(v + \frac{1}{2}\right)\omega_0 \\ &\quad + (B_0 + B_{\text{SME}}^e + B_{\text{SME}}^n)N(N+1)\omega_0 + \dots\end{aligned}\quad (7.1)$$

for Para- H_2^+ . The other terms in (3.13) may be read off immediately from Paper I given the results below.

The first term in (7.1) is defined as

$$\mathcal{E}_{\text{SME}}^e = \Delta E_{\text{SME}}^B + V_{\text{SME}}^{eE} + V_{\text{SME}}^{eF},\quad (7.2)$$

where $V_{\text{SME}}^{eE} \equiv V_{\text{SME}}^{eE}(R_0)$ is evaluated from (4.16). Similarly for V_{SME}^{eF} . To determine the coefficients of ω_0 , we first need the relations

$$\begin{aligned}\delta_{\text{SME}}^e &= \frac{1}{2}\frac{1}{V_M'''}\left[V_{\text{SME}}^{e''} - \frac{V_M'''}{V_M''}V_{\text{SME}}^{e'}\right], \\ B_{\text{SME}}^e &= \lambda\frac{1}{V_M'''}\left[\frac{1}{R_0}V_{\text{SME}}^{e'}\right] + \dots,\end{aligned}\quad (7.3)$$

where the derivatives are evaluated at the mean bond length R_0 . Also,

$$\delta_{\text{SME}}^n = \frac{1}{2}\tilde{V}_{\text{SME}}^n, \quad B_{\text{SME}}^n = B_0\tilde{V}_{\text{SME}}^n,\quad (7.4)$$

with $B_0 = \lambda/2$, where recall $\lambda \simeq 0.027$ is a small parameter governing the hierarchy of terms in the expansion of E_{vNJM_J} , and $\tilde{V}_{\text{SME}}^n$ is given in (4.25).

$V_{\text{SME}}^e(R)$ depends on the electron expectation values $\text{tr}\langle p_a p_b \rangle$ and $\text{tr}_Y\langle p_a p_b \rangle$. Numerical values for these and $V_M(R)$ and their derivatives were given in [10] and Paper I using a simple ansatz (which may be arbitrarily improved as necessary) for the $1s\sigma_g$ wave function. Using these results, it was shown in Paper I how to write δ_{SME}^e and B_{SME}^e (and the higher-order terms) directly in terms of the coefficients of $\text{tr}\langle p_a p_b \rangle$ and $\text{tr}_Y\langle p_a p_b \rangle$.

To extract the rovibrational energies from the internucleon potential $V_{\text{SME}\pm}^{eE}(R)$, we simply have to adapt these results for the hyperfine-Zeeman eigenstates, based on (4.16),

$$\begin{aligned}V_{\text{SME}\pm}^{eE}(R) &= \frac{1}{3}\frac{1}{m_e^2}\text{tr}\langle p_a p_b \rangle\text{tr}\tilde{E}_{ij}^e \\ &\quad + \frac{1}{6}\frac{1}{m_e^2}\text{tr}_Y\langle p_a p_b \rangle\text{tr}_Y\tilde{E}_{ij}^e\hat{c}_{NM_J}^{\pm}(B).\end{aligned}\quad (7.5)$$

We find¹¹

$$\begin{aligned}V_{\text{SME}}^{eE} &= \left[0.782\frac{1}{m_e}\text{tr}\tilde{E}_{ij}^e - 0.120\hat{c}_{NM_J}^{\pm}\frac{1}{m_e}\text{tr}_Y\tilde{E}_{ij}^e\right], \\ \delta_{\text{SME}}^{eE} &= \left[-1.000\frac{1}{m_e}\text{tr}\tilde{E}_{ij}^e + 0.272\hat{c}_{NM_J}^{\pm}\frac{1}{m_e}\text{tr}_Y\tilde{E}_{ij}^e\right], \\ B_{\text{SME}}^{eE} &= \lambda\left[-0.666\frac{1}{m_e}\text{tr}\tilde{E}_{ij}^e + 0.112\hat{c}_{NM_J}^{\pm}\frac{1}{m_e}\text{tr}_Y\tilde{E}_{ij}^e\right],\end{aligned}\quad (7.6)$$

¹¹Recall that in the atomic units used here, the energy E_{vNJM_J} is expressed in units of the Rydberg constant, $R_H \simeq 13.6$ eV. The vibration angular frequency is $\omega_0 = 0.020$. The SME coupling combinations $\frac{1}{m_e}\text{tr}\tilde{E}_{ij}^e$ etc. are dimensionless. In spectroscopic units where $\hbar = 1$, 1 eV = 2.418×10^{14} Hz = 8065.5 cm⁻¹. See Paper I for details.

using the appropriate $\hat{c}_{NM_J}^\pm(B)$ from (4.17) and (4.18) for the mixed states with $J = N \pm \frac{1}{2}$, and an identical result with $\hat{c}_{NM_J}$ from (4.19) for the unmixed states, with $J = N + \frac{1}{2}, M_J = \pm(N + \frac{1}{2})$. Recall that the couplings are written in spherical tensor form as

$$\begin{aligned} \frac{1}{m} \text{tr} \tilde{E}_{ij} &= -3m \frac{1}{\sqrt{4\pi}} (\tilde{c}_{200}^{\text{NR}} - \tilde{a}_{200}^{\text{NR}}), \\ \frac{1}{m} \text{tr}_Y \tilde{E}_{ij} &= 3m \sqrt{\frac{5}{4\pi}} (\tilde{c}_{220}^{\text{NR}} - \tilde{a}_{220}^{\text{NR}}), \end{aligned} \quad (7.7)$$

and we maintain the notation where $\tilde{E}_{ij}^e$ contains both electron and proton couplings, implying $\tilde{c}_{200}^{\text{NR}e} = c_{200}^{\text{NR}e} + \frac{1}{2} c_{200}^{\text{NR}p}$, etc.

Similarly, from (4.25),

$$\begin{aligned} \delta_{\text{SME}}^n E &= 0.333 \left[\frac{1}{m_p} \text{tr} E_{ij}^p - \hat{c}_{NM_J}^\pm(B) \frac{1}{m_p} \text{tr}_Y E_{ij}^p \right], \\ B_{\text{SME}}^n E &= 0.333 \lambda \left[\frac{1}{m_p} \text{tr} E_{ij}^p - \hat{c}_{NM_J}^\pm(B) \frac{1}{m_p} \text{tr}_Y E_{ij}^p \right], \end{aligned} \quad (7.8)$$

with $\hat{c}_{NM_J}^\pm(B)$ and $\hat{c}_{NM_J}$ for the respective hyperfine-Zeeman eigenstates.

Next, for the F_{ijk}^e couplings, recall from (5.41) that in the minimal SME where $(F_{+3-} + F_{-3+}) = -\text{tr}_Y F_{ijk}$, we can write $V_{\text{SME}}^{eF}(R)$ in the form

$$\begin{aligned} V_{\text{SME}\pm}^{eF}(R) &= \frac{1}{3} \frac{1}{m_e^2} \text{tr} \langle p_a p_b \rangle \text{tr} F_{ij3}^e f_{NM_J}^\pm(B) \\ &\quad - \frac{1}{6} \frac{1}{m_e^2} \text{tr}_Y \langle p_a p_b \rangle \text{tr}_Y F_{ij3}^e f_{NM_J}^{Y\pm}(B), \end{aligned} \quad (7.9)$$

for the mixed states with $J = N \pm \frac{1}{2}$, where the $f_{NM_J}^\pm(B)$ and $f_{NM_J}^{Y\pm}$ are given in (5.42) and (5.43), with a similar expression for the two unmixed states with f_{NM_J} from (5.44). This now has a perfectly analogous form to $V_{\text{SME}}^E(R)$ in (7.5), with different coefficients f_{NM_J} and $f_{NM_J}^Y$ replacing the $\hat{c}_{NM_J}$. Notice that in this case both the $\text{tr} \langle p_a p_b \rangle$ and $\text{tr}_Y \langle p_a p_b \rangle$ terms have nontrivial coefficients.

The corresponding expressions for the rovibrational energies are then simply read off:

$$\begin{aligned} V_{\text{SME}}^{eF} &= \left[0.782 f_{NM_J}^\pm(B) \frac{1}{m_e} \text{tr} F_{ij3}^e - 0.120 f_{NM_J}^{Y\pm}(B) \frac{1}{m_e} \text{tr}_Y F_{ij3}^e \right], \\ \delta_{\text{SME}}^{eF} &= \left[-1.000 f_{NM_J}^\pm(B) \frac{1}{m_e} \text{tr} F_{ij3}^e - 0.272 f_{NM_J}^{Y\pm}(B) \frac{1}{m_e} \text{tr}_Y F_{ij3}^e \right], \\ B_{\text{SME}}^{eF} &= \lambda \left[-0.666 f_{NM_J}^\pm(B) \frac{1}{m_e} \text{tr} F_{ij3}^e - 0.112 f_{NM_J}^{Y\pm}(B) \frac{1}{m_e} \text{tr}_Y F_{ij3}^e \right] \end{aligned} \quad (7.10)$$

for the mixed states, and similarly with f_{NM_J} and $f_{NM_J}^Y$ for the unmixed states. Here, the couplings are [see (5.34), (6.24), and (6.25)],

$$\begin{aligned} \frac{1}{m_e} \text{tr} F_{ij3}^e &= \frac{1}{m_e} (-\tilde{g}_{D3} + \tilde{d}_3), \\ \frac{1}{m_e} \text{tr}_Y F_{ij3}^e &= -\frac{1}{m_e} (\tilde{g}_{D3} + 2\tilde{d}_3), \end{aligned} \quad (7.11)$$

with

$$\frac{1}{m_e} \tilde{g}_{D3} = 2m_e \sqrt{\frac{3}{4\pi}} g_{210}^{\text{NR}(1B)}, \quad \frac{1}{m_e} \tilde{d}_3 = m_e \sqrt{\frac{3}{4\pi}} H_{210}^{\text{NR}(0B)}. \quad (7.12)$$

Many of the important implications for H_2^+ and H_2^- rovibrational spectroscopy are encoded in the precise form of the various coefficients $\hat{c}_{NM_J}^\pm$, $f_{NM_J}^\pm$, and $f_{NM_J}^{Y\pm}$ determining the energies E_{vNJM_J} through (7.6), (7.8), and (7.10). It

is therefore useful to collect these coefficients together here, in both the zero and high magnetic field limits.

First, at zero B , and for the states $J = N \pm \frac{1}{2}$,

$$\begin{aligned} \hat{c}_{NM_J}^+ &= \frac{1}{(2N+1)(2N+3)} \left[\left(N + \frac{1}{2}\right) \left(N + \frac{3}{2}\right) - 3M_J^2 \right], \\ \hat{c}_{NM_J}^- &= \frac{1}{(2N-1)(2N+1)} \left[\left(N - \frac{1}{2}\right) \left(N + \frac{1}{2}\right) - 3M_J^2 \right]. \end{aligned} \quad (7.13)$$

The value $\hat{c}_{NM_J}$ for the unmixed states, $J = N + \frac{1}{2}$, $M_J = \pm(N + \frac{1}{2})$ is read off from the first of these,

$$\hat{c}_{NM_J} = -\frac{N}{2N+3}. \quad (7.14)$$

For the coefficients of the spin-dependent couplings, we have

$$\begin{aligned}
f_{NM_J}^+ &= \frac{2}{2N+1} M_J, & f_{NM_J}^{Y+} &= \frac{2N}{(2N+1)(2N+3)} M_J, \\
f_{NM_J}^- &= -\frac{2}{2N+1} M_J, & f_{NM_J}^{Y-} &= -\frac{2(N+1)}{(2N-1)(2N+1)} M_J,
\end{aligned} \tag{7.15}$$

for the states $J = N \pm \frac{1}{2}$, reducing to

$$f_{NM_J} = \pm 1, \quad f_{NM_J}^Y = \pm \frac{N}{2N+3}, \tag{7.16}$$

for the unmixed states with $M_J = \pm(N + \frac{1}{2})$.

In the large B limit, the states are labeled by $M_N = M_J - M_S$ and M_S . The corresponding coefficients are

$$c_{NM_N} = \frac{1}{(2N-1)(2N+3)} [N(N+1) - 3M_N^2] \tag{7.17}$$

and

$$f_{NM_N}^\pm = \pm 1, \quad f_{NM_N}^{Y\pm} = \pm c_{NM_N} \tag{7.18}$$

for the states with $M_S = \pm \frac{1}{2}$.

To complete the contributions to $\mathcal{E}_{\text{SME}}^e$ in (7.2), we also add the simple SME spin contribution $\Delta E_{\text{SME}}^{eB}$ given by (5.4), or (5.5) in the high magnetic field limit, which is proportional to the coupling $\tilde{b}_3^e$. At zero B , this is simply

$$\Delta E_{\text{SME}}^{eB} = \mp \tilde{b}_3^e \frac{2}{2N+1} M_J, \tag{7.19}$$

for $J = N \pm \frac{1}{2}$, reducing to $\pm \tilde{b}_3^e$ for the unmixed states, while in the large B limit,

$$\Delta E_{\text{SME}}^{eB} = -2\tilde{b}_3^e M_S. \tag{7.20}$$

In Paper I, we discussed how the N , and M_J , dependence of the coefficients $\hat{c}_{NM_J}$ allow the spin-independent couplings to be individually determined from a relatively small number of rovibrational transitions. The results above show how this can be extended to the spin-dependent couplings $\tilde{b}_3$, $\tilde{g}_{D3}$, and $\tilde{d}_3$ when transitions between hyperfine states identified by J, M_J , as in Fig. 1, as well as v, N are isolated. Already, in [2], the rovibrational transitions between $|vNJ\rangle = |10\frac{1}{2}\rangle$ and $|32\frac{3}{2}\rangle$ or $|32\frac{5}{2}\rangle$ have recently been studied. The specific N dependence of the coefficients $f_{NM_J}^\pm$ and $f_{NM_J}^{Y\pm}$ is important in disentangling the individual SME couplings from measurements of several rovibrational transitions. Our results also describe the dependence on the SME couplings of transitions between hyperfine states with the same rovibrational quantum numbers v, N [1,25].

In the quest for high precision, one experimental strategy is to combine transitions so that the linear Zeeman effects

proportional to M_J cancel. This has been extended to subleading effects including the quadratic Zeeman and electric quadrupole shifts in the comprehensive paper [24]. A concern might be that in canceling the Zeeman contributions we may also lose sensitivity to the spin-dependent SME couplings. However, the N and M_J dependence of the $f_{NM_J}^\pm$ and $f_{NM_J}^{Y\pm}$ coefficients ensures that suitably chosen transitions will remain sensitive to most of the SME couplings even when the Zeeman and subleading contributions are systematically canceled. Further details will be presented elsewhere.

Throughout this paper we have carefully included the interplay of the SME couplings with a background magnetic field. The additional flexibility afforded by knowing the dependence of the rovibrational energies on the magnetic field, encoded here in the B dependence of the coefficients $f_{NM_J}^\pm(B)$ and $f_{NM_J}^{Y\pm}(B)$ in (5.42) and (5.43), should also prove useful in isolating potential Lorentz and *CPT* violating effects from higher-order systematics and Zeeman and QED effects.

In addition, it is probable that spectroscopy with $\bar{\text{H}}_2^-$ will require confinement in a trap with a magnetic field well into our high- B regime. Direct comparisons could therefore require performing H_2^+ spectroscopy in similar fields.

One of the most promising opportunities for an early discovery of Lorentz violation would be the observation of annual variations of the transition frequencies in H_2^+ . It is worth commenting in this context that the expected precision of rovibrational spectroscopy on the H_2^+ molecular ion will far exceed that of current high-order QED calculations, so Lorentz and *CPT* tests will require comparisons of different spectroscopic measurements rather than a simple theory/experiment comparison on a single transition.

In Paper I we gave an explicit formula for the annual variations implied by the spin-independent couplings c_{200}^{NR} and a_{200}^{NR} . In particular, it was shown how the variations are sensitive to different components of the fundamental SME couplings than appear in the basic transition frequencies themselves, though suppressed by $O(10^{-4})$ (the ratio of Earth's orbital velocity to the speed of light). The same analysis can be applied to the spin-dependent couplings $\tilde{b}_3$, $\tilde{g}_{D3}$, and $\tilde{d}_3$, with added complexity due their nonisotropic nature. In Appendix C we give a brief outline of some of the extra features needed to generalize the discussion of annual variations to the spin-dependent couplings considered here.

A key point in Paper I was the observation that the dependence of the rovibrational energies on the proton SME couplings arising from the direct contribution ΔE_{SME}^n is enhanced by $O(m_p/m_e)$ relative to the contribution from the internucleon potential $V_{\text{SME}}^e(R)$. The latter gives the same parametric dependence as occurs in atomic spectroscopy with H and $\bar{\text{H}}$. This gives rovibrational spectroscopy of the molecular ion a potential $O(10^3)$ increased sensitivity to *CPT* violation in the proton sector given comparable experimental measurement precisions.

However, to achieve this sensitivity gain for the spin-dependent proton couplings, we need the analog of ΔE_{SME}^n which would arise from the term proportional to $F_{ijk}^p I_k$ in the SME Hamiltonian, i.e. depending on the nucleon spin. This of course implies performing rovibrational spectroscopy with Ortho- H_2^+ . It is straightforward to extend all our results to Ortho- H_2^+ with no further issues of principle, simply involving the extra complexity associated with the Clebsch-Gordan analysis required to describe mixing amongst the $|vNFJM_J\rangle$ hyperfine states.

In summary, the richness and extremely high precision of the spectrum of rovibrational transitions make an experimental program of H_2^+ , and in future $\bar{\text{H}}_2^-$, spectroscopy ideal for testing fundamental symmetries such as Lorentz and CPT invariance. The detailed results presented here should help to guide this program and ensure that the experimentally selected rovibrational transitions maintain maximum sensitivity to potential Lorentz and CPT violating effects, wherever they may occur.

ACKNOWLEDGMENTS

I am grateful to Stefan Eriksson for many helpful discussions in the course of this work and to the Higgs Centre for Theoretical Physics at the University of Edinburgh for hospitality.

DATA AVAILABILITY

No data were created or analyzed in this study.

APPENDIX A: SME HAMILTONIAN $\hat{H}_{\text{SME}}$ IN THE MOL FRAME

The SME Hamiltonian for a single Dirac particle is given in terms of spherical tensor couplings in Ref. [15], in a formalism which systematically includes higher-dimensional operators. With particle momentum $\mathbf{p}$ with respect to the fixed frame in which the spherical tensor couplings are defined, the nonrelativistic Hamiltonian is

$$H_{\text{SME}} = -\sum_{njm} |\mathbf{p}|^n Y_{jm}(\hat{\mathbf{p}}) \mathcal{V}_{njm}^{\text{NR}} - \sigma^r \sum_{njm} |\mathbf{p}|^n Y_{jm}(\hat{\mathbf{p}}) T_{njm}^{\text{NR}(OB)} + \sigma^\pm \sum_{njm} |\mathbf{p}|^n Y_{jm}(\hat{\mathbf{p}}) (\pm T_{njm}^{\text{NR}(1B)} + iT_{njm}^{\text{NR}(1E)}), \quad (\text{A1})$$

with

$$\mathcal{V}_{njm}^{\text{NR}} = c_{njm}^{\text{NR}} - a_{njm}^{\text{NR}}, \quad (\text{A2})$$

and

$$T_{njm}^{\text{NR}(OB)} = g_{njm}^{\text{NR}(OB)} - H_{njm}^{\text{NR}(OB)}, \quad (\text{A3})$$

and similarly for the (1B)- and (1E)-type couplings. For further details and the motivation for (A1), see Ref. [15].

For our purposes, we first consider this to be the Hamiltonian for the electron, with the fixed frame identified as the MOL frame with whose z axis is aligned with the molecular axis. The electron momentum $\mathbf{p}$, with components p_a , has direction $\hat{\mathbf{p}}$ specified by spherical polar angles (θ, ϕ) in the MOL frame.

In (A1), the Pauli spin operators $\sigma^r, \sigma^\pm$ are defined in the “helicity” frame (HEL) whose z axis is chosen to lie along the direction $\hat{\mathbf{p}}$ of the electron momentum. The first step in adapting (A1) to our problem is therefore to transform these spin operators to the MOL frame so the SME Hamiltonian is written consistently in a single frame. As in the main text, we identify the spin operators and couplings in the MOL frame with a circumflex accent, to distinguish from their components in the EXP frame used later.

First, we need an explicit expression for the spin-weighted spherical harmonics ${}_s Y_{jm}(\hat{\mathbf{p}})$ in (A1) in terms of the Wigner matrices $d_{sm}^j(\theta)$ introduced in the text, viz.

$${}_s Y_{jm}(\theta, \phi) = \sqrt{\frac{2j+1}{4\pi}} (-1)^m d_{-sm}^j(\theta) e^{im\phi}. \quad (\text{A4})$$

Then, writing $\sigma^r, \sigma^\pm$ in standard spherical tensor notation σ_m ($m = 1, -1, 0$) in the HEL frame, we have $\sigma^+ = \sigma_{m=-1}^{\text{HEL}}$, $\sigma^- = -\sigma_{m=1}^{\text{HEL}}$ and $\sigma^r = \sigma_{m=0}^{\text{HEL}}$ according to the definitions in [15]. Rotating these spin operators from the HEL to the MOL frame using the Wigner matrices, as described in the main text,

$$\sigma_{s'}^{\text{HEL}} = \hat{\sigma}_s d_{ss'}^1(\theta) e^{-is\phi}, \quad (\text{A5})$$

and using the identity $d_{m'm}^j = (-1)^{m'-m} d_{mm'}^j$ to reorganize indices, we find the SME Hamiltonian with all quantities in the MOL frame:

$$\hat{H}_{\text{SME}} = -\sum_{njm} |\mathbf{p}|^n \sqrt{\frac{2j+1}{4\pi}} \left[e^{im\phi} d_{m0}^j \hat{\mathcal{V}}_{njm}^{\text{NR}} + e^{i(m-s)\phi} (\hat{\sigma}_s d_{s0}^1 d_{m0}^j \hat{T}_{njm}^{\text{NR}(OB)} + \hat{\sigma}_s (d_{s,-1}^1 d_{m,-1}^j + d_{s1}^1 d_{m1}^j) \hat{T}_{njm}^{\text{NR}(1B)} + \hat{\sigma}_s (d_{s,-1}^1 d_{m,-1}^j - d_{s1}^1 d_{m1}^j) i \hat{T}_{njm}^{\text{NR}(1E)}) \right]. \quad (\text{A6})$$

The spherical tensor couplings are subject to a number of constraints on the allowed values of (n, j, m) which follow from their fundamental definition and the subsequent nonrelativistic expansion of the Hamiltonian in powers of $|\mathbf{p}|^n$, together with some identities which hold for low values of n and j .

Consider first the contribution to (A6) independent of momentum, so $n = 0$. Here, the index j is restricted to $j = 0$ for $\hat{\mathcal{V}}_{0jm}^{\text{NR}}$ and $j = 1$ for $\hat{T}_{0jm}^{\text{NR}(OB)} = \hat{T}_{01m}^{\text{NR}(1B)}$. There is

no corresponding (1E) coupling with $n = 0$. Using orthonormality of the Wigner matrices [see (6.5)] and $d_{00}^0 = \sqrt{4\pi}Y_{00} = 1$, the Hamiltonian simplifies to

$$\hat{H}_{\text{SME}}|_{p^2=0} = -\sqrt{\frac{1}{4\pi}}\hat{\mathcal{V}}_{000}^{\text{NR}} - \sqrt{\frac{3}{4\pi}}\hat{\sigma}_m\hat{\mathcal{T}}_{01m}^{\text{NR}(0B)}, \quad (\text{A7})$$

where as always a sum over the index m is assumed.

$$\begin{aligned} \hat{H}_{\text{SME}}|_{p^2} = & -\sqrt{\frac{1}{4\pi}}|\mathbf{p}|^2 \sum_m \left[\hat{\mathcal{V}}_{200}^{\text{NR}} + \sqrt{5}e^{im\phi}d_{m0}^2\hat{\mathcal{V}}_{22m}^{\text{NR}} \right. \\ & + e^{i(m-s)\phi}\hat{\sigma}_s(\sqrt{3}d_{s0}^1d_{m0}^1\hat{\mathcal{T}}_{21m}^{\text{NR}(0B)} + \sqrt{7}d_{s0}^1d_{m0}^3\hat{\mathcal{T}}_{23m}^{\text{NR}(0B)} \\ & + \sqrt{3}(d_{s,-1}^1d_{m,-1}^1 + d_{s1}^1d_{m1}^1)\hat{\mathcal{T}}_{21m}^{\text{NR}(1B)} + \sqrt{7}(d_{s,-1}^1d_{m,-1}^3 + d_{s1}^1d_{m1}^3)\hat{\mathcal{T}}_{23m}^{\text{NR}(1B)} \\ & \left. + \sqrt{5}(d_{s,-1}^1d_{m,-1}^2 - d_{s1}^1d_{m1}^2)i\hat{\mathcal{T}}_{22m}^{\text{NR}(1E)} \right]. \end{aligned} \quad (\text{A8})$$

Evidently, the SME Hamiltonian in this full generality is complicated, with many couplings and angle-dependent coefficients. At this point, therefore, we specialize to the case of the molecular ion. The first major simplification is to impose cylindrical symmetry, which requires the expectation values $\langle p_a p_b \rangle = 0$ for $a \neq b$, and $\langle p_x^2 \rangle = \langle p_y^2 \rangle$.

Then, for example, the coefficient of $\hat{\mathcal{V}}_{220}^{\text{NR}}$ is $|\mathbf{p}|^2 d_{00}^2 = -\frac{1}{2}|\mathbf{p}|^2(1 - 3\cos^2\theta) = -\frac{1}{2}\text{tr}_Y p_a p_b$. Examination of the $m \neq 0$ contributions shows that they give vanishing expectation values, e.g. $|\mathbf{p}|^2 d_{20}^2 e^{2i\phi} = \frac{\sqrt{6}}{4}|\mathbf{p}|^2 \sin^2\theta e^{2i\phi} = (p_x + ip_y)^2 \rightarrow 0$. The $O(|\mathbf{p}|^2)$ Hamiltonian for the spin-independent couplings therefore reduces to

$$\hat{H}_{\text{SME}}^{\mathcal{V}}|_{p^2} = -\sqrt{\frac{1}{4\pi}}\text{tr}_Y p_a p_b \hat{\mathcal{V}}_{200}^{\text{NR}} + \frac{1}{2}\sqrt{\frac{5}{4\pi}}\text{tr}_Y p_a p_b \hat{\mathcal{V}}_{220}^{\text{NR}} + \dots \quad (\text{A9})$$

where $+\dots$ indicate terms with zero expectation value for the molecular ion with the electron in the $1s\sigma_g$ ground state.

For the (0B) and (1B) couplings we need the products of Wigner matrices, which are evaluated in terms of Clebsch-Gordan coefficients using the formula (6.7) in the main text. It is convenient here to first use the identity $d_{s0}^j = (-1)^s d_{-s0}^j$, then evaluate

$$d_{-s0}^1 d_{m0}^j = \sum_{J=|j-1|}^{j+1} C_{10,10}^{J0} C_{1-s,1m}^{J(-s+m)} d_{(-s+m)0}^J. \quad (\text{A10})$$

For $j = 1$ only $J = 0, 2$ are allowed, since $C_{10,10}^{10} = 0$, and again keeping only terms with nonvanishing expectation values when combined with $|\mathbf{p}|^2$, leaves

Next, consider the $O(|\mathbf{p}|^2)$ contribution. Here, for $n = 2$, the permitted values for the spherical tensor couplings are $j = 2, 0$ for $\hat{\mathcal{V}}_{2jm}^{\text{NR}}$, $j = 3, 1$ for $\hat{\mathcal{T}}_{2jm}^{\text{NR}(0B)}$ and $\hat{\mathcal{T}}_{2jm}^{\text{NR}(1B)}$, and $j = 2, 0$ for $\hat{\mathcal{T}}_{2jm}^{\text{NR}(1E)}$. So in general we have

$$d_{-s0}^1 d_{m0}^1 = -\sqrt{\frac{1}{3}}C_{1-s,1m}^{00}d_{00}^0 + \sqrt{\frac{2}{3}}C_{1-s,1m}^{20}d_{00}^2 + \dots \quad (\text{A11})$$

Evaluating the Clebsch-Gordan coefficients then gives

$$(-1)^s d_{-s0}^1 d_{m0}^1 = \frac{1}{3}\delta_{sm}d_{00}^0 - \sqrt{\frac{2}{3}}\sqrt{\frac{1}{6}}Y_{sm}d_{00}^2 + \dots \quad (\text{A12})$$

with

$$Y_{sm} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.$$

Finally, substituting back into the SME Hamiltonian, we find the contribution of the (0B) couplings with $j = 1$ as

$$\begin{aligned} \hat{H}_{\text{SME}}^{\mathcal{T}(0B)}|_{p^2} = & \sqrt{\frac{3}{4\pi}}\hat{\sigma}_s \left(\frac{1}{3}\text{tr}_Y p_a p_b \delta_{sm} + \frac{1}{6}\text{tr}_Y p_a p_b Y_{sm} \right) \\ & \times \hat{\mathcal{T}}_{21m}^{\text{NR}(0B)} + \dots \end{aligned} \quad (\text{A13})$$

The same product of Wigner matrices, when combined with orthonormality, is sufficient to evaluate the coefficient of the $\hat{\mathcal{T}}_{21m}^{\text{NR}(1B)}$ couplings as well. For those with $j = 3$, the same method can in principle be carried through, but since these couplings do not arise in the minimal SME since their associated Lorentz and CPT violating operators are of higher dimension, we do not make further use of them here.

This leaves the (1E) couplings. Here, since the products involve Wigner matrices with different j , the orthonormality trick which simplifies the coefficient of the $\mathcal{T}_{21m}^{\text{NR}(1B)}$ is not available and we must evaluate directly:

$$(d_{s,-1}^1 d_{m,-1}^2 - d_{s1}^1 d_{m1}^2) = \sum_{J=2,3} (C_{1-1,2-1}^{J-2} C_{1s,2m}^{J(s+m)} d_{(s+m)-2}^J - C_{11,21}^{J2} C_{1s,2m}^{J(s+m)} d_{(s+m)2}^J) \quad (\text{A14})$$

the sum being over $J = 2, 3$ only since $J = 1$ has a vanishing Clebsch-Gordan coefficient. The $J = 2$ term contributes

$$\sqrt{\frac{1}{3}} C_{1s,2m}^{2(s+m)} (d_{(s+m),-2}^2 + d_{(s+m)2}^2) = -\frac{1}{6} (1 + \cos^2 \theta) \mathbf{T}_{sm}, \quad (\text{A15})$$

restricting to $s = m$ by cylindrical symmetry, while after some remarkable simplification of the Wigner matrices, the $J = 3$ term gives

$$\sqrt{\frac{2}{3}} C_{1s,2m}^{3(s+m)} (d_{(s+m),-2}^3 - d_{(s+m)2}^3) = -\frac{2}{3} (1 - 2 \cos^2 \theta) \mathbf{T}_{sm}, \quad (\text{A16})$$

with

$$\mathbf{T}_{sm} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Combining the $J = 2$ and $J = 3$ contributions and evaluating with the momentum factor, we find they once again conspire to give the familiar $\text{tr}_Y p_a p_b$ combination, leaving the $(1E)$ contribution to the SME Hamiltonian,

$$\hat{H}_{\text{SME}}^{\mathcal{T}(1E)}|_{p^2} = -\sqrt{\frac{5}{4\pi}} \frac{1}{2} \text{tr}_Y p_a p_b \hat{\sigma}_s \mathbf{T}_{sm} i \hat{\mathcal{T}}_{22m}^{\text{NR}(1E)} + \dots \quad (\text{A17})$$

Finally, putting everything together, and keeping only the momentum factors that have nonvanishing expectation values given the cylindrical symmetry of the molecular ion, we find the following compact expression for the SME Hamiltonian with all quantities expressed in the MOL frame:

$$\begin{aligned} \hat{H}_{\text{SME}} = & -\sqrt{\frac{1}{4\pi}} \left[\hat{\mathcal{V}}_{000}^{\text{NR}} + \text{tr}_Y p_a p_b \hat{\mathcal{V}}_{200}^{\text{NR}} - \sqrt{5} \frac{1}{2} \text{tr}_Y p_a p_b \hat{\mathcal{V}}_{220}^{\text{NR}} \right. \\ & + \sqrt{3} \hat{\sigma}_s \delta_{sm} \hat{\mathcal{T}}_{01m}^{\text{NR}(0B)} + \sqrt{3} \hat{\sigma}_s \left(\frac{1}{3} \text{tr}_Y p_a p_b \delta_{sm} + \frac{1}{6} \text{tr}_Y p_a p_b \mathbf{Y}_{sm} \right) \hat{\mathcal{T}}_{21m}^{\text{NR}(0B)} \\ & \left. + \sqrt{3} \hat{\sigma}_s \left(\frac{2}{3} \text{tr}_Y p_a p_b \delta_{sm} - \frac{1}{6} \text{tr}_Y p_a p_b \mathbf{Y}_{sm} \right) \hat{\mathcal{T}}_{21m}^{\text{NR}(1B)} + \sqrt{5} \frac{1}{2} \text{tr}_Y p_a p_b \hat{\sigma}_s \mathbf{T}_{sm} i \hat{\mathcal{T}}_{22m}^{\text{NR}(1E)} \right]. \quad (\text{A18}) \end{aligned}$$

Recall we have also omitted the $\hat{\mathcal{T}}_{23m}^{\text{NR}(0B)}$ and $\hat{\mathcal{T}}_{23m}^{\text{NR}(1B)}$ couplings which do not occur in the minimal SME.

We can compare this with the equivalent expression for $\hat{H}_{\text{SME}}$ written directly from the original SME Lagrangian (1.1). With all quantities defined in the MOL frame, and imposing the same cylindrical symmetry constraints on the momentum as in (A18), the spin-dependent terms are

$$\hat{H}_{\text{SME}} = \hat{B}_c \hat{\sigma}_c + \frac{1}{m^2} \left[\frac{1}{3} \text{tr}_Y p_a p_b \text{tr} \hat{F}_{abc} \hat{\sigma}_c + \frac{1}{6} \text{tr}_Y p_a p_b \text{tr}_Y \hat{F}_{abc} \hat{\sigma}_c \right]. \quad (\text{A19})$$

Comparing (A18) and (A19), we see that they are equivalent provided the following identities hold, in addition to those already quoted at the end of Sec. VIA:

$$\begin{aligned}
\frac{1}{\sqrt{2}}\hat{B}_{\pm} &= \mp \sqrt{\frac{3}{4\pi}}\hat{T}_{0\mp 1}^{\text{NR}(0B)}, \\
\frac{1}{\sqrt{2}}\frac{1}{m^2}\text{tr}\hat{F}_{ab\pm} &= \mp \sqrt{\frac{3}{4\pi}}(\hat{T}_{21\mp 1}^{\text{NR}(0B)} + 2\hat{T}_{21\mp 1}^{\text{NR}(1B)}), \\
\frac{1}{\sqrt{2}}\frac{1}{m^2}\text{tr}_Y\hat{F}_{ab\pm} &= \mp \sqrt{\frac{3}{4\pi}}(\hat{T}_{21\mp 1}^{\text{NR}(0B)} - \hat{T}_{21\mp 1}^{\text{NR}(1B)}) + \sqrt{\frac{5}{4\pi}}3i\hat{T}_{22\mp 1}^{\text{NR}(1E)}.
\end{aligned} \tag{A20}$$

We verify these relations explicitly in the minimal SME in Sec. [VIB](#).

APPENDIX B: CLEBSCH-GORDAN RELATIONS

We collect here a number of relations for weighted sums over Clebsch-Gordan coefficients which are used in the main text in transforming results to the Para- H_2^+ hyperfine states $|vNJM_J\rangle$. First recall the relation between the basis states,

$$|vNJM_J\rangle = \sum_{M_S} C_{NM_N, \frac{1}{2}M_S}^{JM_J} |vNM_N M_S\rangle, \tag{B1}$$

with $M_N = M_J - M_S$, where for $J = N \pm \frac{1}{2}$ we have the explicit forms:

$$\begin{aligned}
C_{NM_J \mp \frac{1}{2}, \frac{1}{2} \pm \frac{1}{2}}^{N + \frac{1}{2} M_J} &= \frac{1}{\sqrt{2N+1}} \sqrt{N + \frac{1}{2} \pm M_J}, \\
C_{NM_J \mp \frac{1}{2}, \frac{1}{2} \pm \frac{1}{2}}^{N - \frac{1}{2} M_J} &= \mp \frac{1}{\sqrt{2N+1}} \sqrt{N + \frac{1}{2} \mp M_J}.
\end{aligned} \tag{B2}$$

First, for the unweighted sums, with M_J fixed and $J', J = N \pm \frac{1}{2}$, we can explicitly verify

$$\sum_{M_S} C_{N(M_J - M_S), \frac{1}{2}M_S}^{J'M_J} C_{N(M_J - M_S), \frac{1}{2}M_S}^{JM_J} = \delta_{J'J}, \tag{B3}$$

which follows from the general orthonormality property of Clebsch-Gordan coefficients.

Next we need the corresponding sums weighted by the spin quantum number M_S :

$$\begin{aligned}
\sum_{M_S} (C_{N(M_J - M_S), \frac{1}{2}M_S}^{N + \frac{1}{2} M_J})^2 M_S &= \frac{1}{2N+1} M_J, \\
\sum_{M_S} (C_{N(M_J - M_S), \frac{1}{2}M_S}^{N - \frac{1}{2} M_J})^2 M_S &= -\frac{1}{2N+1} M_J, \\
\sum_{M_S} C_{N(M_J - M_S), \frac{1}{2}M_S}^{N + \frac{1}{2} M_J} C_{N(M_J - M_S), \frac{1}{2}M_S}^{N - \frac{1}{2} M_J} M_S &= -\frac{1}{2N+1} \sqrt{\left(N + \frac{1}{2}\right)^2 - M_J^2},
\end{aligned} \tag{B4}$$

which are required to determine the hyperfine-Zeeman energies and the effect of the SME coupling B_3^e in Secs. [II](#) and [V](#).

For the analysis in Sec. [IV](#) with the spin-independent couplings E_{ij} , we need these sums with the weight factor c_{NM_N} , defined below. Here,

$$\begin{aligned}
\sum_{M_S} (C_{N(M_J-M_S), \frac{1}{2}M_S}^{N+\frac{1}{2}M_J})^2 c_{N(M_J-M_S)} &= \frac{1}{(2N+1)(2N+3)} \left[\left(N+\frac{1}{2}\right) \left(N+\frac{3}{2}\right) - 3M_J^2 \right], \\
\sum_{M_S} (C_{N(M_J-M_S), \frac{1}{2}M_S}^{N-\frac{1}{2}M_J})^2 c_{N(M_J-M_S)} &= \frac{1}{(2N-1)(2N+1)} \left[\left(N-\frac{1}{2}\right) \left(N+\frac{1}{2}\right) - 3M_J^2 \right], \\
\sum_{M_S} C_{N(M_J-M_S), \frac{1}{2}M_S}^{N+\frac{1}{2}M_J} C_{N(M_J-M_S), \frac{1}{2}M_S}^{N-\frac{1}{2}M_J} c_{N(M_J-M_S)} &= -6 \frac{1}{(2N-1)(2N+1)(2N+3)} \left[\left(N+\frac{1}{2}\right)^2 - M_J^2 \right]^{\frac{1}{2}} M_J. \quad (\text{B5})
\end{aligned}$$

Finally, for the momentum and spin-dependent couplings F_{ijk} considered in Sec. V, we need the corresponding sums with both c_{NM_N} and M_S as weight factors. In this case,

$$\begin{aligned}
\sum_{M_S} (C_{N(M_J-M_S), \frac{1}{2}M_S}^{N+\frac{1}{2}M_J})^2 c_{N(M_J-M_S)} M_S &= \frac{1}{(2N+1)(2N-1)(2N+3)} \left[N^2 + 4N + \frac{3}{4} - 3M_J^2 \right] M_J, \\
\sum_{M_S} (C_{N(M_J-M_S), \frac{1}{2}M_S}^{N-\frac{1}{2}M_J})^2 c_{N(M_J-M_S)} M_S &= -\frac{1}{(2N+1)(2N-1)(2N+3)} \left[N^2 - 2N - \frac{9}{4} - 3M_J^2 \right] M_J, \\
\sum_{M_S} C_{N(M_J-M_S), \frac{1}{2}M_S}^{N+\frac{1}{2}M_J} C_{N(M_J-M_S), \frac{1}{2}M_S}^{N-\frac{1}{2}M_J} c_{N(M_J-M_S)} M_S &= -\frac{\sqrt{(N+\frac{1}{2})^2 - M_J^2}}{(2N-1)(2N+1)(2N+3)} \left[N^2 + N - \frac{3}{4} - 3M_J^2 \right]. \quad (\text{B6})
\end{aligned}$$

We also include here some other Clebsch-Gordan coefficients used in the evaluation of matrix elements of the spherical harmonics in Secs. IV and V:

$$\begin{aligned}
C_{N0,20}^{N0} &= -\left(\frac{N(N+1)}{(2N-1)(2N+3)} \right)^{\frac{1}{2}}, \\
C_{NM_N,20}^{NM_N} &= -\left(\frac{1}{N(N+1)(2N-1)(2N+3)} \right)^{\frac{1}{2}} (N(N+1) - 3M_N^2), \\
C_{NM_N,2\pm 1}^{N(M_N\pm 1)} &= -\sqrt{\frac{3}{2}} \left(\frac{1}{N(N+1)(2N-1)(2N+3)} \right)^{\frac{1}{2}} ((N+1 \pm M_N)(N \mp M_N))^{\frac{1}{2}} (1 \pm 2M_N), \quad (\text{B7})
\end{aligned}$$

from which we find

$$c_{NM_N} = C_{NM_N,20}^{NM_N} C_{N0,20}^{N0} = \frac{N(N+1) - 3M_N^2}{(2N-1)(2N+3)}, \quad (\text{B8})$$

which enters extensively in the calculations in Paper I, and here in Secs. IV and V.

APPENDIX C: ANNUAL VARIATIONS AND SPIN-DEPENDENT COUPLINGS

To compare the constraints on the Lorentz violating SME couplings from different experiments, it is necessary to refer them to a standard reference frame, generally taken to be a solar-centered, or SUN, frame [11,18]. A useful intermediary is provided by a standard laboratory, LAB, frame with fixed orientation relative to Earth. In order to study annual variations, we therefore need to rotate our results from the EXP frame first to the LAB and then to the

SUN frames. We then perform a Lorentz boost to describe Earth's orbital motion around the Sun.

In the special case of the isotropic spin-independent couplings c_{200}^{NR} and a_{200}^{NR} , since they are invariant under rotations our results hold directly in the SUN frame, with

$$\begin{aligned}
\sqrt{\frac{1}{4\pi}} c_{200}^{\text{NR}} &= \frac{1}{3m} \left(c_{KK} + \frac{3}{2} c_{TT} \right) = \frac{5}{6m} c_{TT}, \\
\sqrt{\frac{1}{4\pi}} a_{200}^{\text{NR}} &= (a_{TKK} + a_{TTT}), \quad (\text{C1})
\end{aligned}$$

where we have again used the vanishing of the spacetime trace of the $c_{\mu\nu}$ couplings [14].

The Lorentz boost depends on Earth's orbital velocity $\mathbf{v}_{\oplus}$, given in SUN frame coordinates by

$$\mathbf{v}_{\oplus} = v_{\oplus} (\sin \Omega_{\oplus} T \mathbf{e}_X - \cos \Omega_{\oplus} T (\cos \eta \mathbf{e}_Y + \sin \eta \mathbf{e}_Z)), \quad (\text{C2})$$

where $\Omega_\oplus$ is the orbital frequency and the tilt angle $\eta = 23.4^\circ$ is the angle between Earth's equator and orbital plane.

To first order in $v_\oplus$, which is of $O(10^{-4})$, the boosts are simply

$$\delta_\oplus c_{TT} = 2v_\oplus^J c_{JT}, \quad \delta_\oplus a_{TTT} = 3v_\oplus^J a_{JTT}, \quad \delta_\oplus a_{TKK} = v_\oplus^J (a_{JKK} + 2a_{JTT}), \quad (C3)$$

from which we find the annual variation,

$$\begin{aligned} \frac{1}{\sqrt{4\pi}} \delta_\oplus (c_{200}^{\text{NR}} - a_{200}^{\text{NR}}) = & v_\oplus \sin \Omega_\oplus T \left(\frac{5}{3m} c_{XT} - 5a_{XTT} - a_{XKK} \right) - v_\oplus \cos \Omega_\oplus T \left(\cos \eta \left(\frac{5}{3m} c_{YT} - 5a_{YTT} - a_{YKK} \right) \right. \\ & \left. + \sin \eta \left(\frac{5}{3m} c_{ZT} - 5a_{ZTT} - a_{ZKK} \right) \right), \end{aligned} \quad (C4)$$

which implies the corresponding variation in the rovibrational transition frequencies. Note that these variations are governed by the components c_{JT} , a_{JTT} , and a_{JKK} of the SME Lagrangian couplings, different from those in the transition frequencies themselves.

To generalize this to the spin-dependent couplings in the combinations $\tilde{b}_3$, $\tilde{g}_{D3}$, and $\tilde{d}_3$, we need to rotate from the EXP to the SUN frame. A significant simplification is to consider only sidereal averages,¹² in which case we can show that the required rotation has nonvanishing components only for $J = 3$, for example,

$$\tilde{b}_3 = \mathcal{R}_{3J} \tilde{b}_J = \mathcal{R}_{3Z} \tilde{b}_Z. \quad (C5)$$

Here, $\mathcal{R}_{3Z} = -\cos \theta \sin \beta \sin \chi + \cos \beta \cos \chi$, where θ , β describe the orientation of the EXP frame relative to LAB

¹²In fact it is precisely these sidereal (daily) variations which [19] proposes to identify in order to constrain the SME couplings. If we retain the sidereal variations in (C5), we can show

$$\begin{aligned} \tilde{b}_3 = & [\cos \theta \sin \beta \cos \chi + \cos \beta \sin \chi] (\tilde{b}_X \cos \omega_\oplus T_\oplus + \tilde{b}_Y \sin \omega_\oplus T_\oplus) \\ & + [\sin \theta \sin \beta] (-\tilde{b}_X \sin \omega_\oplus T_\oplus + \tilde{b}_Y \cos \omega_\oplus T_\oplus) \\ & + [-\cos \theta \sin \beta \sin \chi + \cos \beta \cos \chi] \tilde{b}_Z, \end{aligned}$$

where $\omega_\oplus$ is the sidereal angular frequency and $T_\oplus$ is a local sidereal time. Identical results hold for $\tilde{g}_{D3}$ and $\tilde{d}_3$. Isolating the coefficients of $\cos \omega_\oplus T_\oplus$ and $\sin \omega_\oplus T_\oplus$ therefore enables constraints to be set on all three components, $\tilde{b}_X$ and $\tilde{b}_Y$ as well as $\tilde{b}_Z$.

(i.e. the direction of the applied magnetic field) and χ is the colatitude of the laboratory. For a horizontal magnetic field, $\beta = \pi/2$. The same rotation also holds for $\tilde{g}_{D3}$ and $\tilde{d}_3$.

The annual variations are then determined by the Lorentz boosts of the individual couplings in $\tilde{b}_Z$, $\tilde{g}_{D3}$, and $\tilde{d}_3$. For example, for b_Z itself we have

$$\delta_\oplus b_Z = v_\oplus \cos \Omega_\oplus T \sin \eta b_T. \quad (C6)$$

The variations of the higher-tensor couplings are defined in the same way, with

$$\begin{aligned} \delta_\oplus b_Z &= v_\oplus^Z b_T, \\ \delta_\oplus d_{TZ} &= v_\oplus^J d_{JZ} + v_\oplus^Z d_{TT}, \\ \delta_\oplus H_{XY} &= v_\oplus^X H_{TY} + v_\oplus^Y H_{XT}, \\ \delta_\oplus g_{XYT} &= v_\oplus^X g_{TYT} + v_\oplus^Y g_{XTT} + v_\oplus^J g_{XYJ}, \end{aligned} \quad (C7)$$

and so on for the remaining components, including the nonisotropic spin-independent couplings, $\sqrt{\frac{5}{4\pi}} c_{220}^{\text{NR}} = -\frac{1}{3m} \text{tr}_Y c_{JK}$ and $\sqrt{\frac{5}{4\pi}} a_{220}^{\text{NR}} = -\text{tr}_Y a_{TJK}$.

Evidently, combining all these terms to determine the annual variation of a particular rovibrational transition frequency from the energy levels quoted in Sec. VII gives a very complicated mix of couplings in the coefficients of $\cos \Omega_\oplus T$ and $\sin \Omega_\oplus T$. Nevertheless, the search for annual variations represents one of the more promising routes to uncovering a signal for Lorentz and CPT violation in H_2^+ and $\bar{\text{H}}_2^-$ molecular ion spectroscopy.

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