Theoretical study of ThO and HfF^+ for eEDM search experiments

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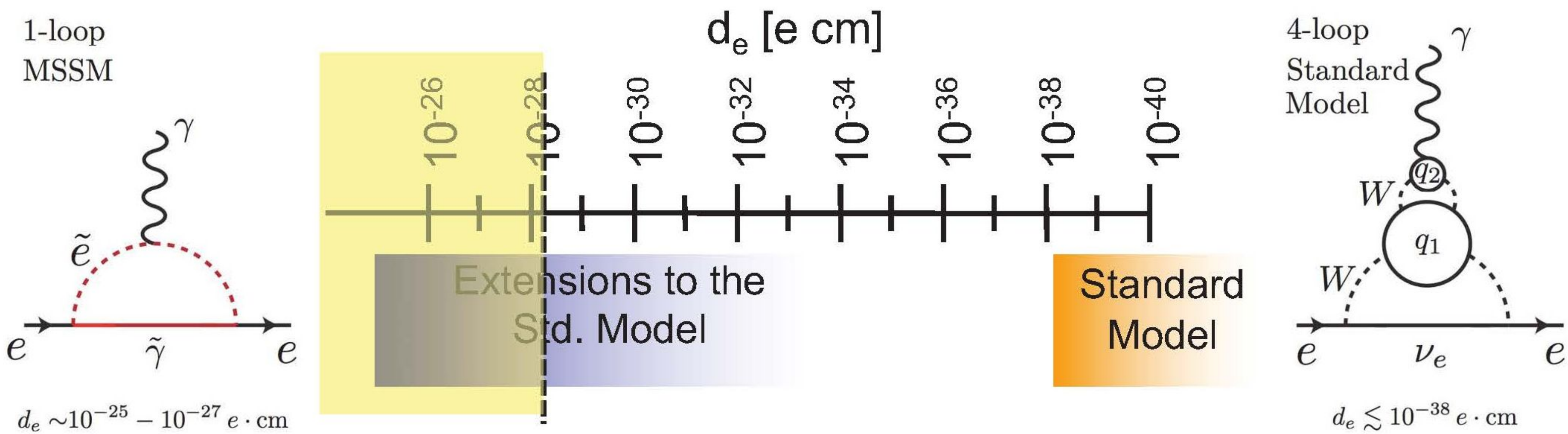
No experimental result contradicts to the standard model but it can not be considered as a complete theory of fundamental interactions:

- Standard Model does not supply any fundamental particles that are good dark matter candidates
- It does not explain dark energy
- According to the standard model, neutrinos are massless particles
- It has too many (19) empirical parameters known from experiment
- It does not explain Matter–antimatter asymmetry
- And others …

- The **Standard Model** doesn't contain enough CP violation
- Various **Extensions to the Standard Model** (such as supersymmetry) seek to add fixes by including new physics at higher energy scales
- New physics typically means larger **eEDM**



$|d_e| < 8.7 \times 10^{-29}$ e cm ACME [Science (2014)]

Tl-beam exp-t: **$|d_e| < 1.6\times10^{-27}$ e·cm**
[B. Regan et al., ***PRL*** **88,** 071805 **(2002)]**

YbF-beam exp-t: **$|d_e| < 1.05\times10^{-27}$ e·cm** **[**J. Hudson et al., ***Nature*** **473,** 493 **(2011)]**

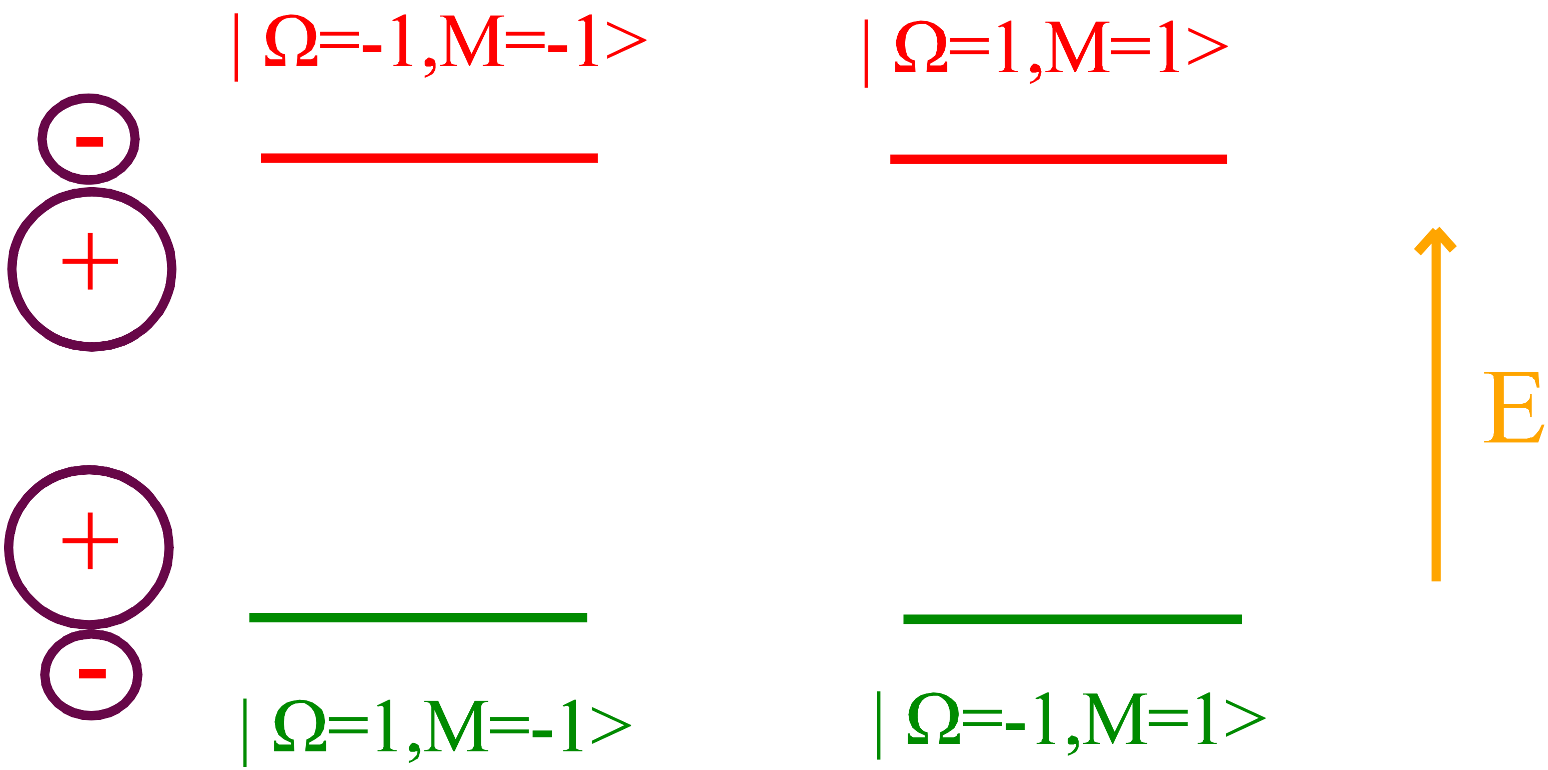
ThO-beam exp-t: **$|d_e| < 9\times10^{-29}$ e·cm** **[***ACME Collaboration***,** **Science 343,** 269 **(2014)]**

HfF^+-ion trap exp-t: **$|d_e| < 13.0\times10^{-29}$ e·cm**
[*Cornell & Ye group,* **PRL 119, 153001 (2017)]]**

ThO-beam exp-t: **$|d_e| < 1.1\times10^{-29}$ e·cm** **[***ACME Collaboration***,** **Nature 562,** 355 **(2018)]**

Ground rotational level J=1 for diatomics with Ω=1

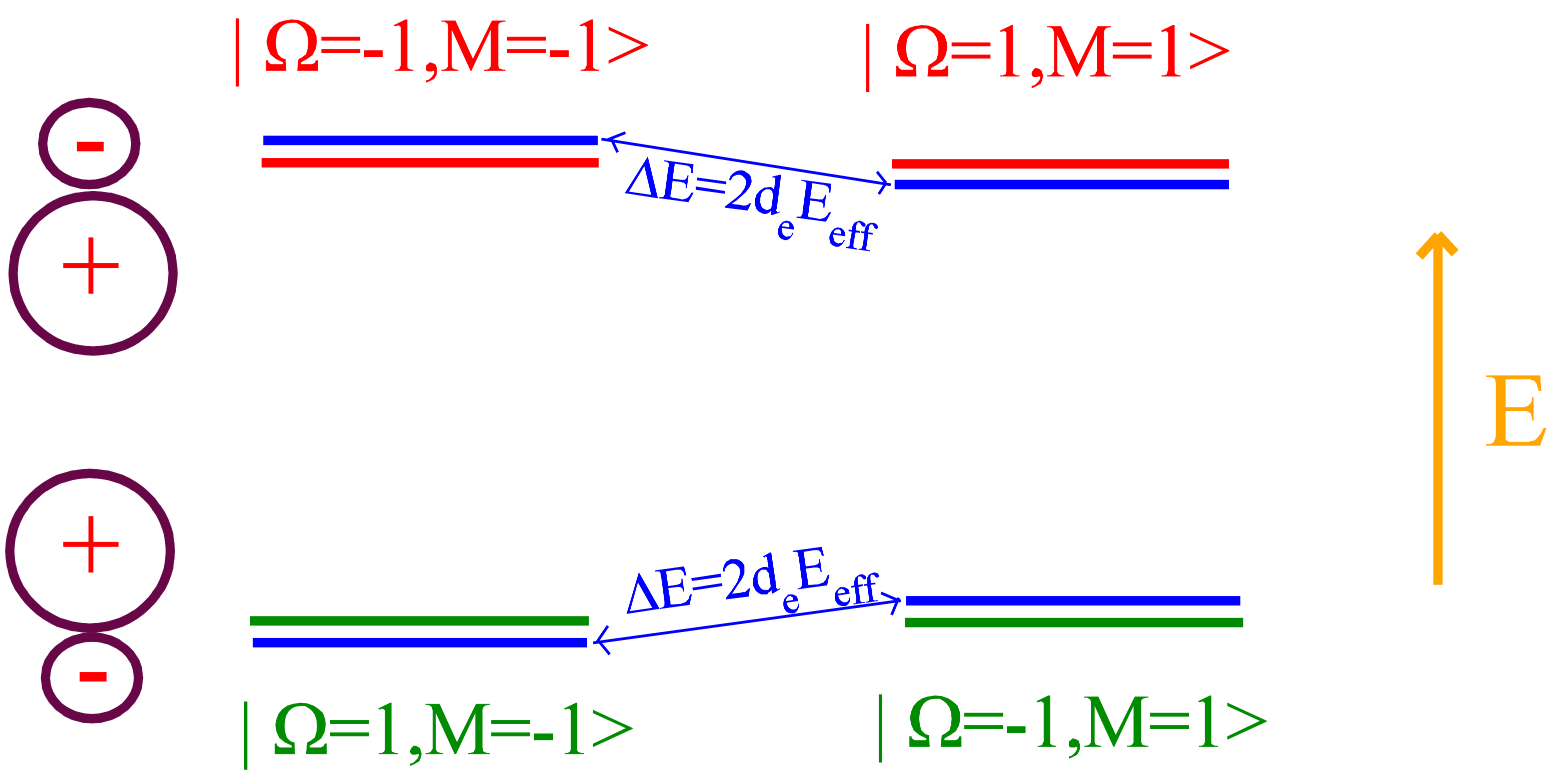
in the presence of Electric field



Ground rotational level J=1 for diatomics with Ω=1

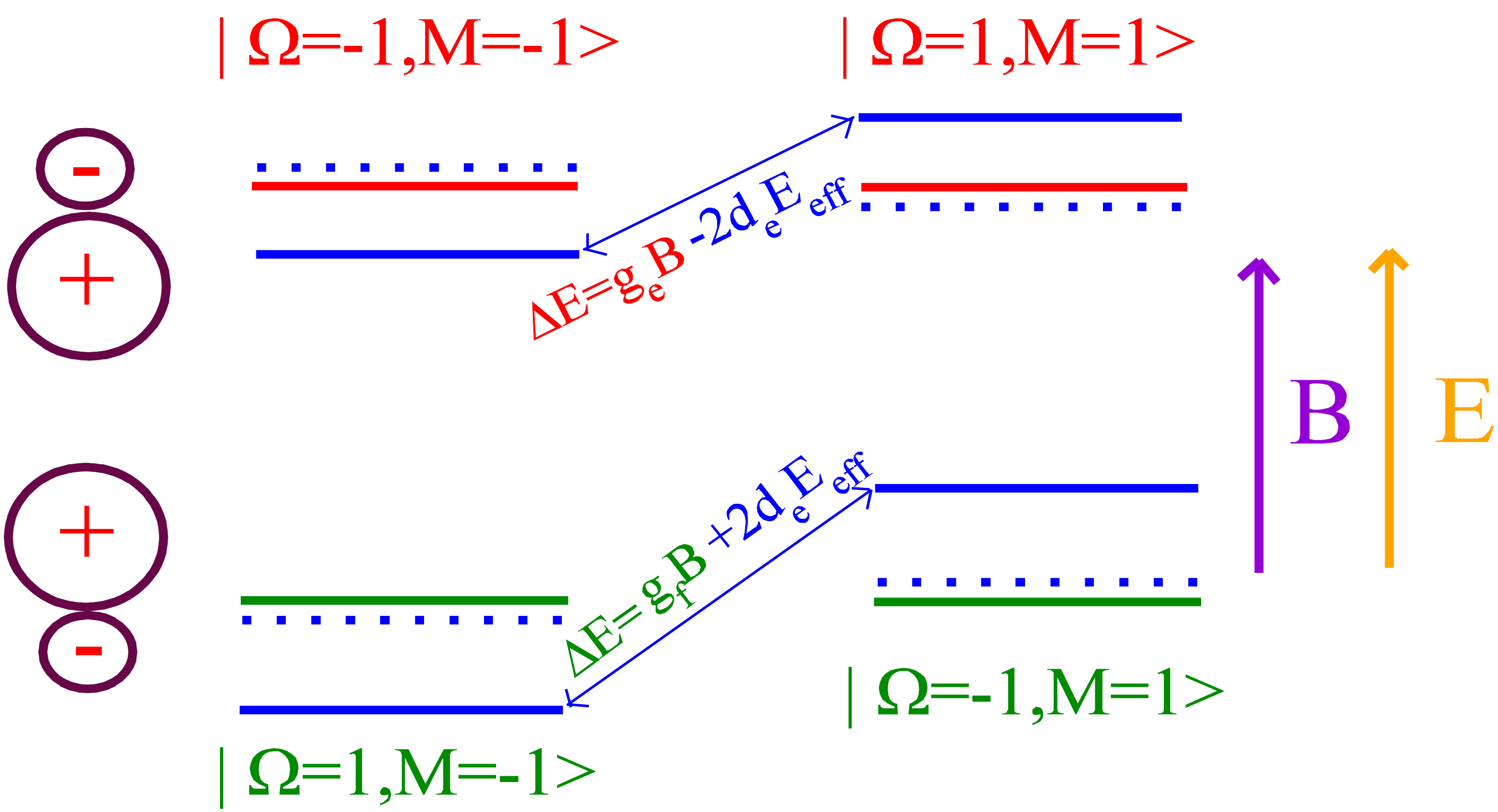
in the presence of Electric field

Blue lines are EDM shifts



Ground rotational level J=1 for diatomics with Ω=1
in the presence of Electric and Magnetic Fields

Blue lines are EDM and Zeeman shifts



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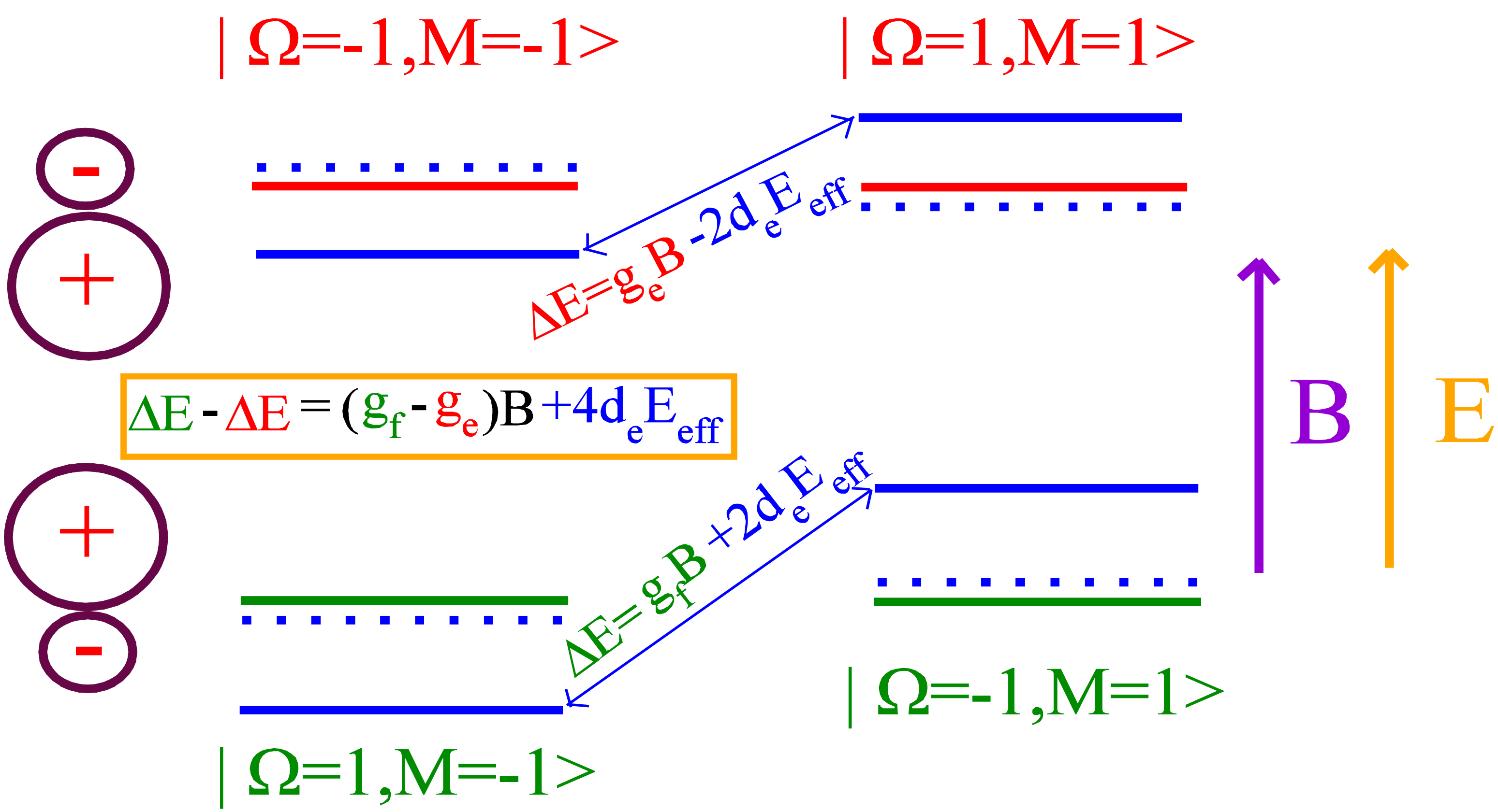

ThO, HfF^+ (and other molecules with similar electronic structure of the electron EDM sensitiv level) have additional possibility to suppress systematics due to the existence of closely-spaced levels of Ω-doublets.

g factors for $ThO\ ^3\Delta_1$

$$M_L = 2 \quad M_S = -1$$

$$g_L = 1 \quad g_S = 2.0023$$

$$g \sim g_L M_L + g_S M_S \approx 0$$

Off-diagonal matrix element

$$\frac{\left|\left\langle \Psi_1 \left| \hat{H}_{mag} \right| \Psi_2 \right\rangle \left\langle \Psi_2 \left| 2B\hat{\mathbf{J}} \cdot \hat{\mathbf{J}}_e \right| \Psi_1 \right\rangle\right|}{E_1 - E_2}$$

ThO electronic structure

Th: [Rn] $6d^2 7s^2$

O: [$1s^2$] $2s^2 2p^4$

[core] [valence]

ThO valence (4e) configuration:

$\sigma_1^2 \sigma_2^2$ ($^1\Sigma^+$)

$\sigma_1^2 \sigma_2^1 \delta^1$ (**$^3\Delta_1$(5317 cm^{-1})**, **$^3\Delta_2$(6128 cm^{-1})**, $^3\Delta_3$, $^1\Delta_2$)

$\sigma_1^2 \sigma_2^1 \pi^1$ ($^3\Pi_2$, $^3\Pi_1$, **$^3\Pi_{0^+}$(10601 cm^{-1})**, **$^3\Pi_{0^-}$(10233 cm^{-1})**, $^1\Pi_1$)

- $\sigma_1 \approx 2p_z$(O)
- $\sigma_2 \approx 7s$(Th)
- $\delta, \pi \approx 6d$(Th)

g factors for ThO (in units 10^{-3})

Calculation (E_{ext}=0)			**Exper. (ACME)**
J	**g**	**g**	**g**
1	**-4.144**	**-4.400**	**-4.40(5)**
2	**-1.381**	**-2.618**	**-2.7(1)**
3	**-0.691**	**-2.173**	**-2.4(2)**

1.A.N. Petrov, L.V. Skripnikov, A.V. Titov, N.R. Hutzler, P.W. Hess, B.R. O'Leary, B. Spaun, D. DeMille, G. Gabrielse, and J.M. Doyle, *Zeeman interaction in ThO* $H^3\Delta_1$ *for the electron electric-dipole-moment search*, Phys.Rev.A 89, 062505 (2014)

g factors for ThO (in units 10^{-3})

Calculation (E_{ext}=0)					**Exper. (ACME)**
J	**g**	**g_e**	**g_f**	**g**	**g**
1	**-4.144**	**-4.409**	**-4.391**	**-4.400**	**-4.40(5)**
2	**-1.381**	**-2.628**	**-2.609**	**-2.618**	**-2.7(1)**
3	**-0.691**	**-2.182**	**-2.164**	**-2.173**	**-2.4(2)**

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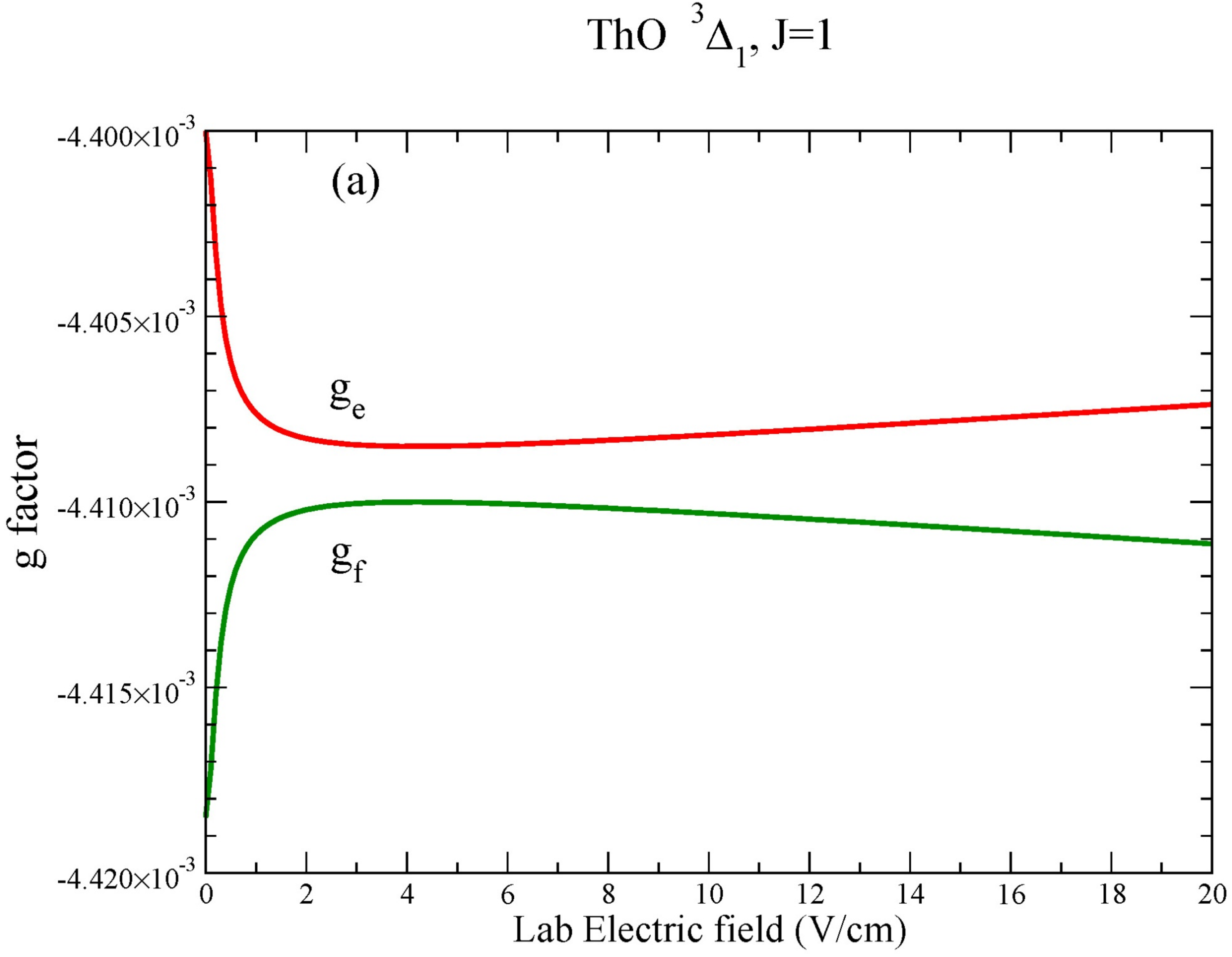
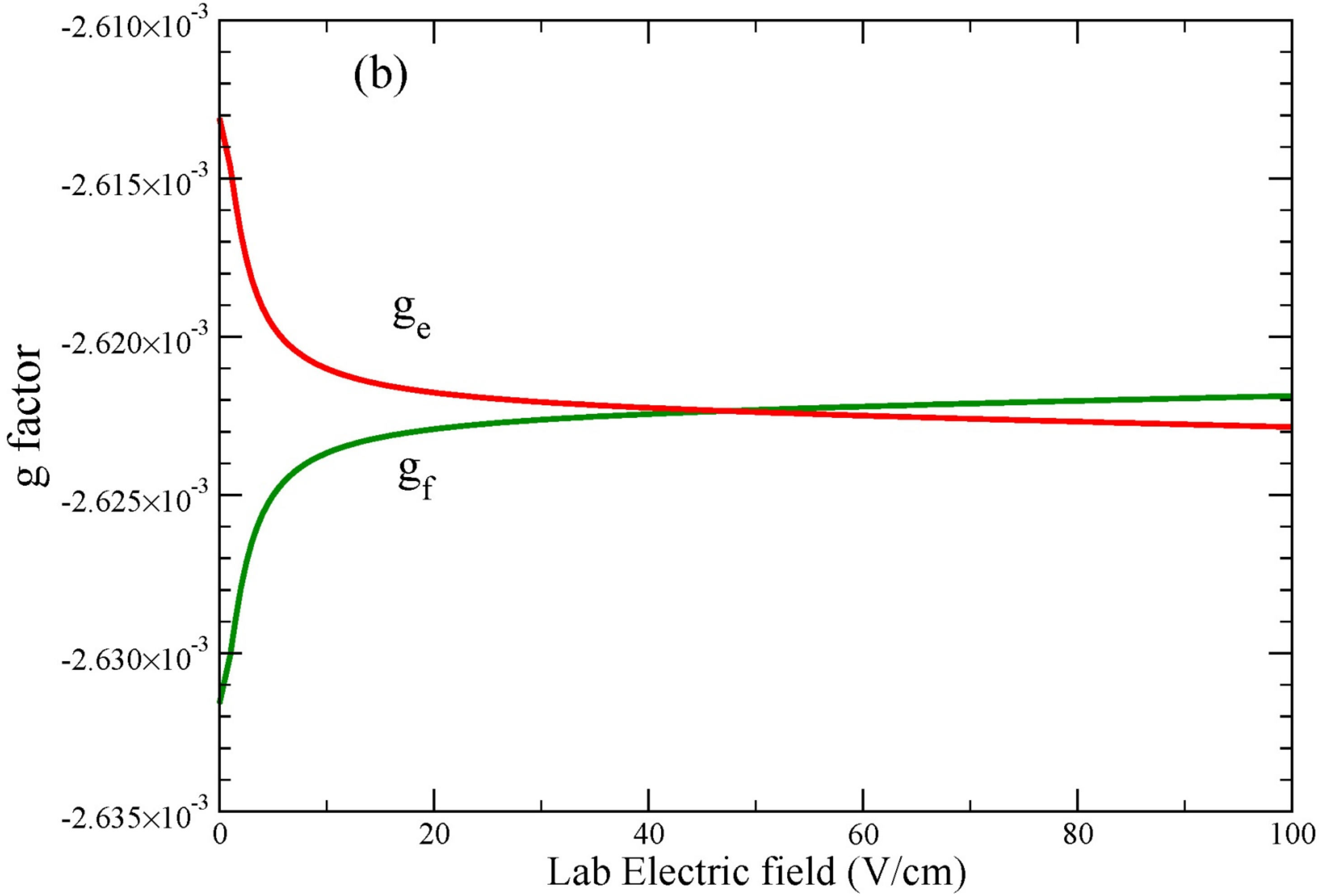


ThO $^3\Delta_1$, J=1
(a)
g_e
g_f
g factor
-4.400×10^-3
-4.405×10^-3
-4.410×10^-3
-4.415×10^-3
-4.420×10^-3
0
2
4
6
8
10
12
14
16
18
20
Lab Electric field (V/cm)

ThO $^3\Delta_1$, J=2, $|M_J|$=1



We find that the *g*-factor difference between doublets is smaller in *J* = 2 than in *J* = 1 and reaches zero at an experimentally accessible electric field. This means that the *H,J* = 2 state should be even more robust against a number of systematic errors compared to *H,J* = 1.

g factors difference g_e-g_f for ThO (in units 10^{-6})

J	Calculation	Exper. (ACME)
1 (E_{ext}=36 V/cm)	**-3.1**	**-2.9(0.7)**
1 (E_{ext}=141 V/cm)	**-12.1**	**-11.3(2)**
2 (E_{ext}=106 V/cm)	**+0.50**	**+0.32(22)**

1.A.N. Petrov, L.V. Skripnikov, A.V. Titov, N.R. Hutzler, P.W. Hess, B.R. O'Leary, B. Spaun, D. DeMille, G. Gabrielse, and J.M. Doyle, *Zeeman interaction in ThO* $H^3\Delta_1$ *for the electron electric-dipole-moment search*, Phys.Rev.A 89, 062505 (2014)

g factors for HfF^+ (in units 10^{-3})

J	Calculation[1]	Exper.
1(E_{ext}=11.6 V/cm)	**-2.97**	**+3.06(10)** [2] **-3.06(10)** [3]

1. A.N. Petrov, L. V. Skripnikov, and A. V. Titov, *Zeeman interaction in the $^3\Delta_1$ state of HfF^+ to search for the electron electric dipole moment*, Phys.Rev.A, 96, 022508 (2017)
2. H. Loh, K. C. Cossel, M. C. Grau, K.-K. Ni, E. R. Meyer J. L. Bohn, J. Ye, and E. A. Cornell, Science 342, 1220 (2013)
3. W. B. Cairncross, D. N. Gresh, M. Grau, K. C. Cossel, T. S. Roussy, Y. Ni, Y. Zhou, J. Ye, and E. A. Cornell, arXiv:1704.07928. (2017)

g factors difference g_e-g_f for HfF^+ (in units 10^{-6})

J	Calculation[1]	Exper.
1(E_{ext}=11.6 V/cm)	**+3.4**	**+10(20)** [2] **-10(20)** [3]

1. A.N. Petrov, L. V. Skripnikov, and A. V. Titov, *Zeeman interaction in the $^3\Delta_1$ state of HfF^+ to search for the electron electric dipole moment*, Phys.Rev.A, 96, 022508 (2017)
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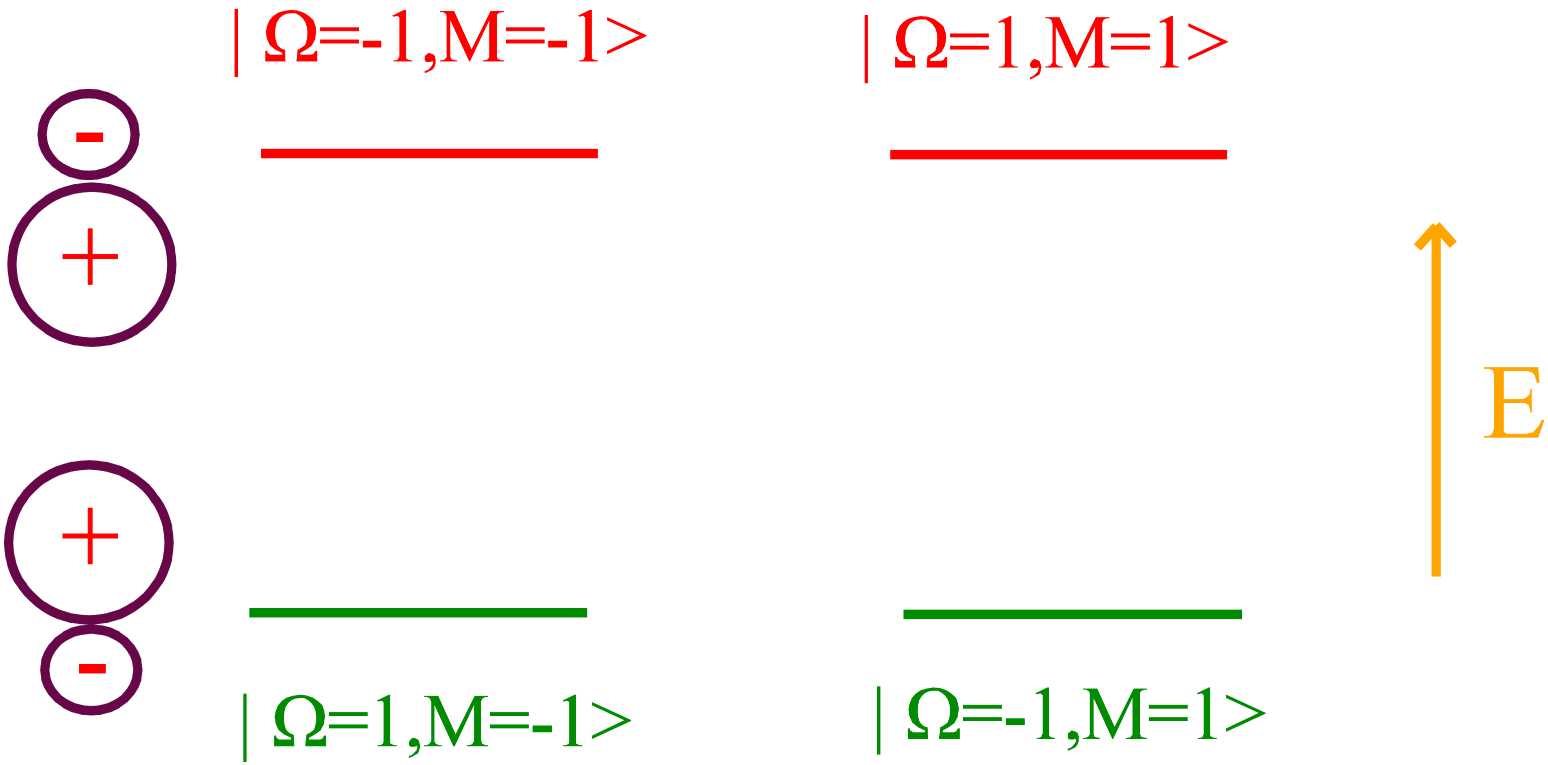
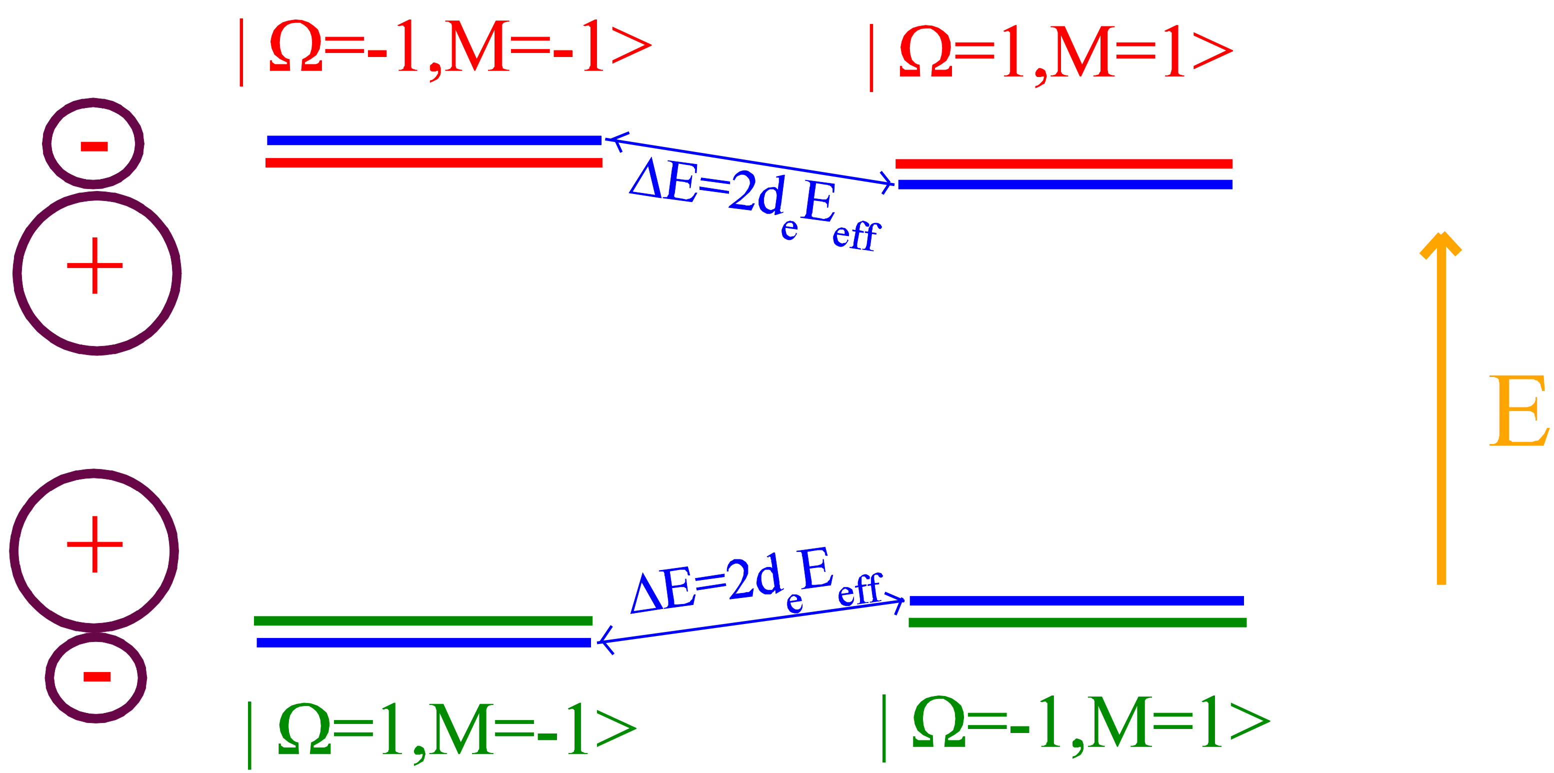


Ground rotational level J=1 for diatomics with Ω=1

in the presence of Electric field

Blue lines are EDM shifts



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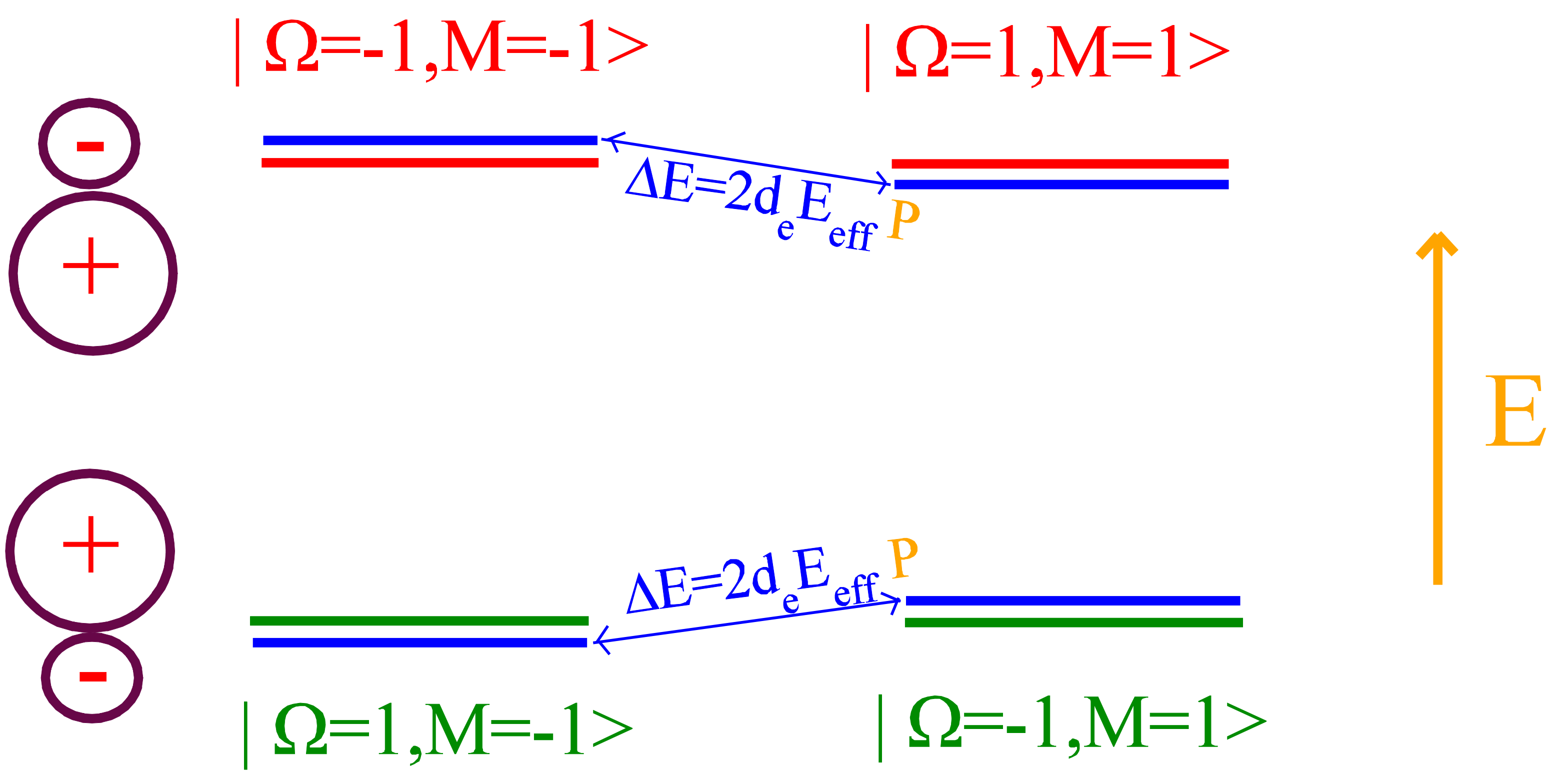
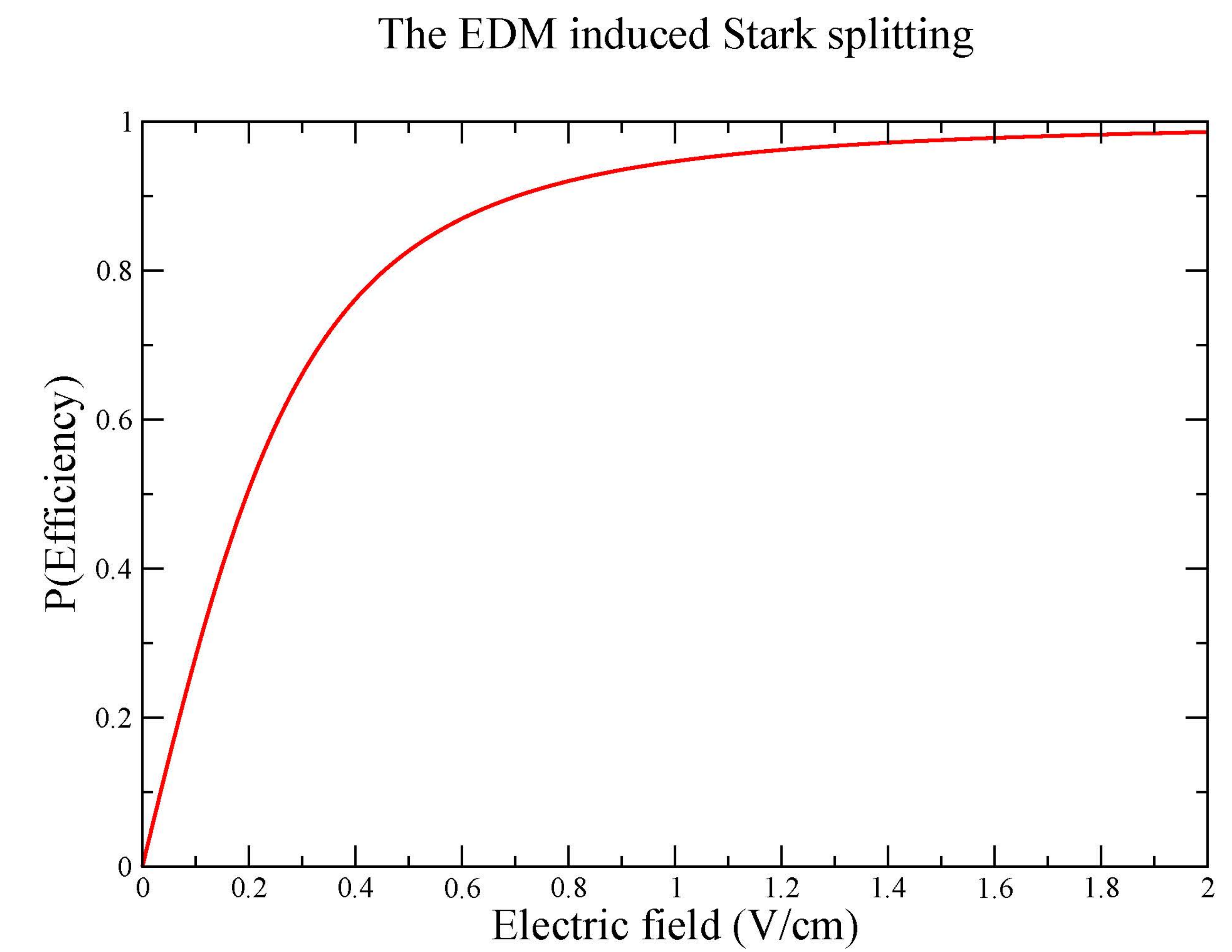
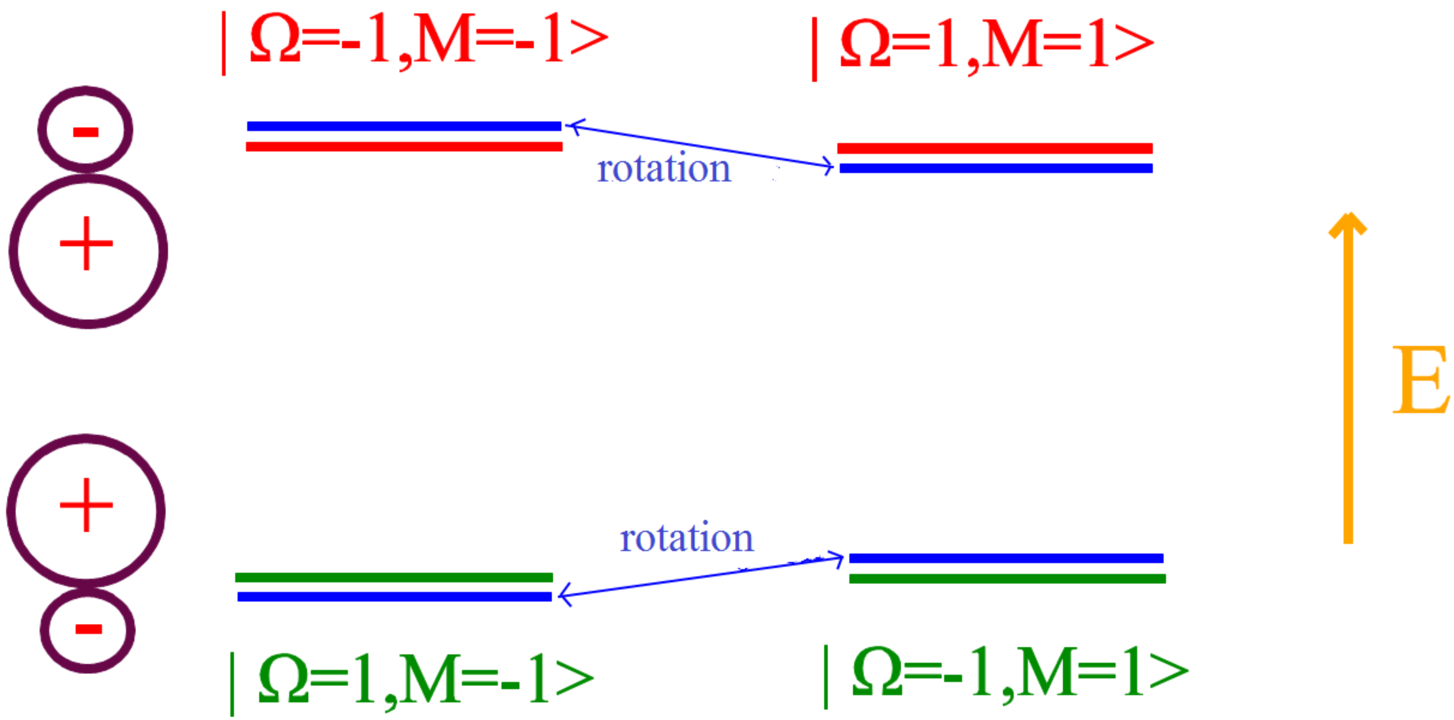


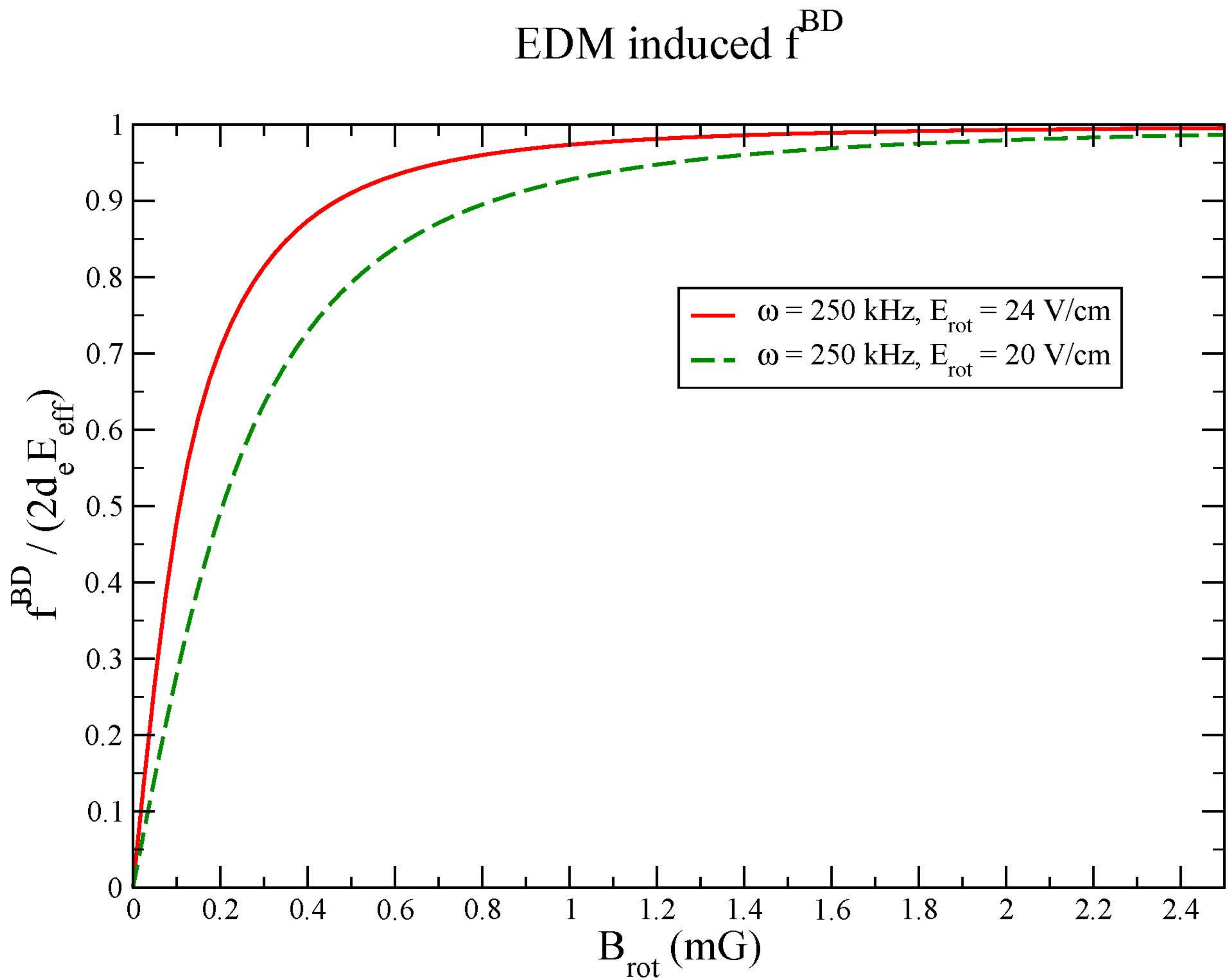

The EDM induced Stark splitting
P(Efficiency)
Electric field (V/cm)
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2

Ground rotational level J=1 for diatomics with Ω=1

in the presence of Electric field

Blue lines are rotation shifts





EDM induced f^BD
f^BD / (2d_e E_eff)
B_rot (mG)
ω = 250 kHz, E_rot = 24 V/cm
ω = 250 kHz, E_rot = 20 V/cm
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
2.2
2.4

HfF^+:

E_{eff}=22.5 GV/cm [A. N. Petrov, N. S. Mosyagin, T. A. Isaev, and A. V. Titov, PRA 76, 030501R (2007), Timo Fleig and Malaya K. Nayak Phys. Rev. A 88, 032514 (2013) L.V. Skripnikov JCP 147, 021101 (2017)]

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E_{rot}= 24 V/cm ⇨ E_{eff}=22.2 GV/cm

E_{rot}= 20 V/cm ⇨ E_{eff}=21.3 GV/cm

Effect	Correction	Uncertainty
Non-reversing $\mathcal{B}_{\text{rot}}$	-1	5
Geometric phases		4
Axial secular motion		2
Rotation-odd $\mathcal{E}_{\text{rot}}$		14
Doublet population background		195
Total systematic	-1	195
Statistical		868
Total uncertainty		890

$$f^{BD} = 0.10 \pm 0.87_{\text{stat}} \pm 0.20_{\text{syst}} \text{ mHz}.$$

$$d_e = (0.9 \pm 7.7_{\text{stat}} \pm 1.7_{\text{syst}}) \times 10^{-29}\, e\,\text{cm},$$

$$|d_e| < 1.3 \times 10^{-28}\, e\,\text{cm} \quad (90\%\ \text{confidence}).$$

William B. Cairncross, Daniel N. Gresh, Matt Grau, Kevin C. Cossel, Tanya S. Roussy, Yiqi Ni, Yan Zhou, Jun Ye, and Eric A. Cornell, PRL 119, 153001 (2017)

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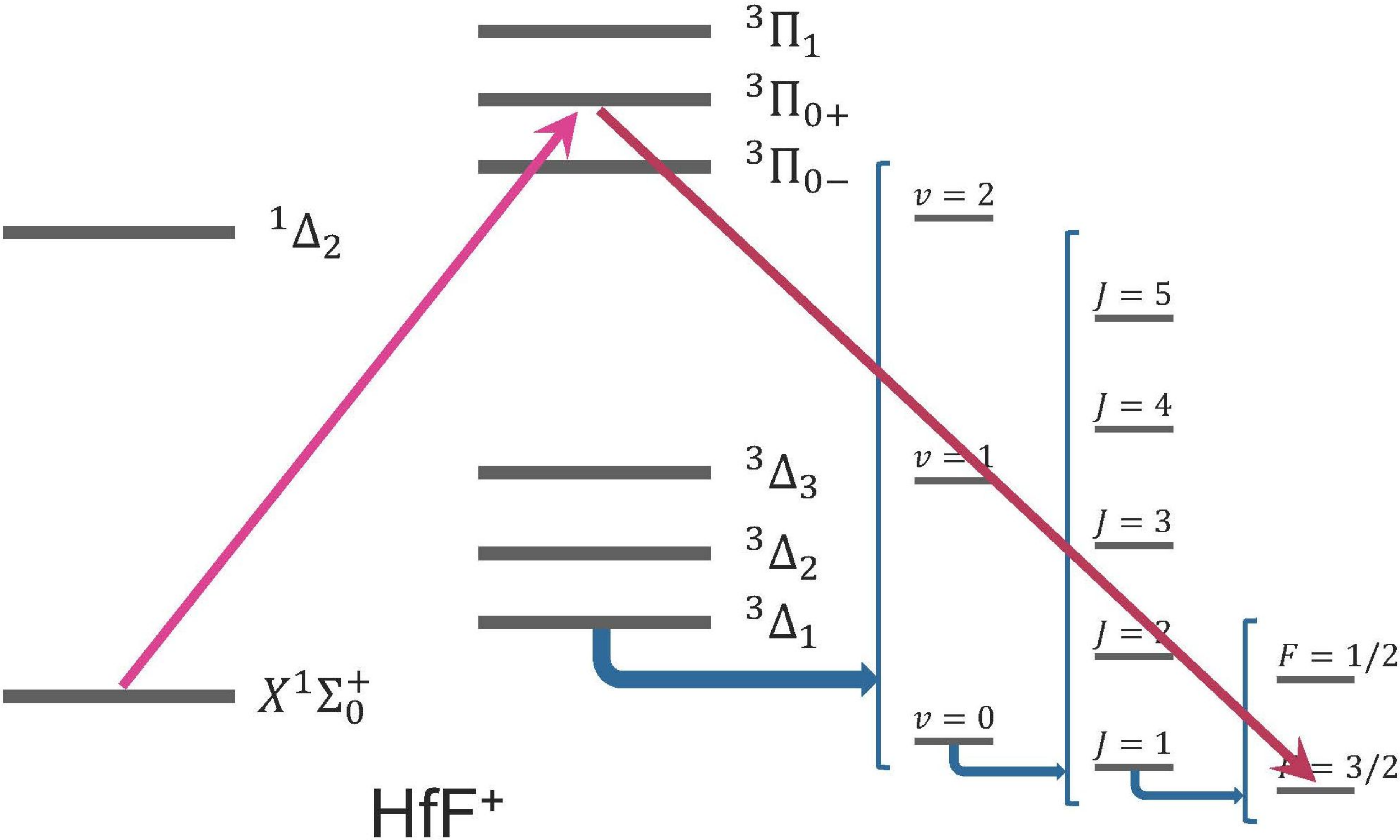
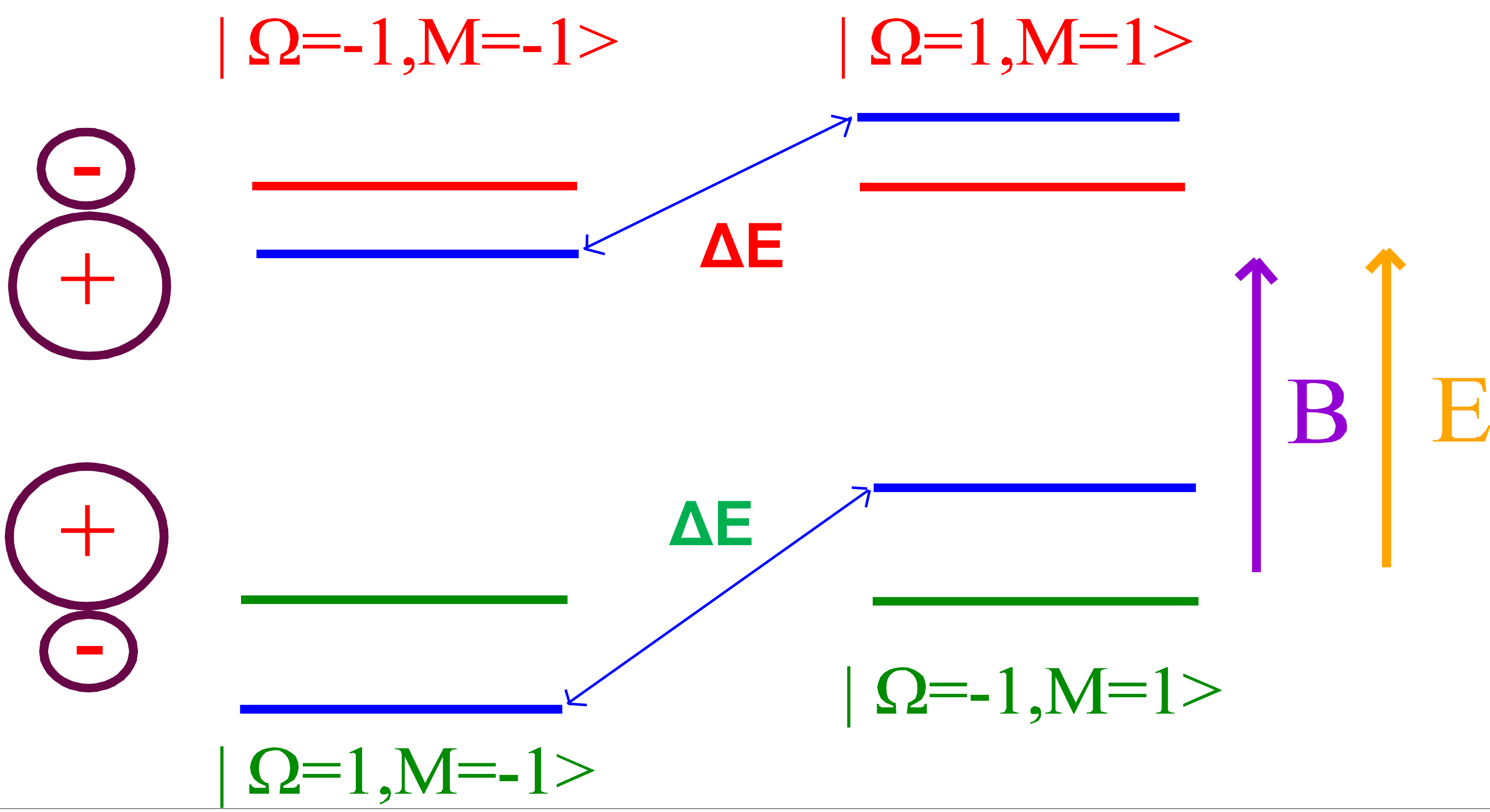


$^3\Pi_1$
$^3\Pi_{0+}$
$^3\Pi_{0-}$
$^1\Delta_2$
$^3\Delta_3$
$^3\Delta_2$
$^3\Delta_1$
$X^1\Sigma_0^+$
HfF⁺
$v = 2$
$v = 0$
$J = 5$
$J = 4$
$J = 3$
$J = 1$
$F = 1/2$

Ground rotational level J=1 for diatomics with Ω=1
in the presence of Electric and Magnetic Fields



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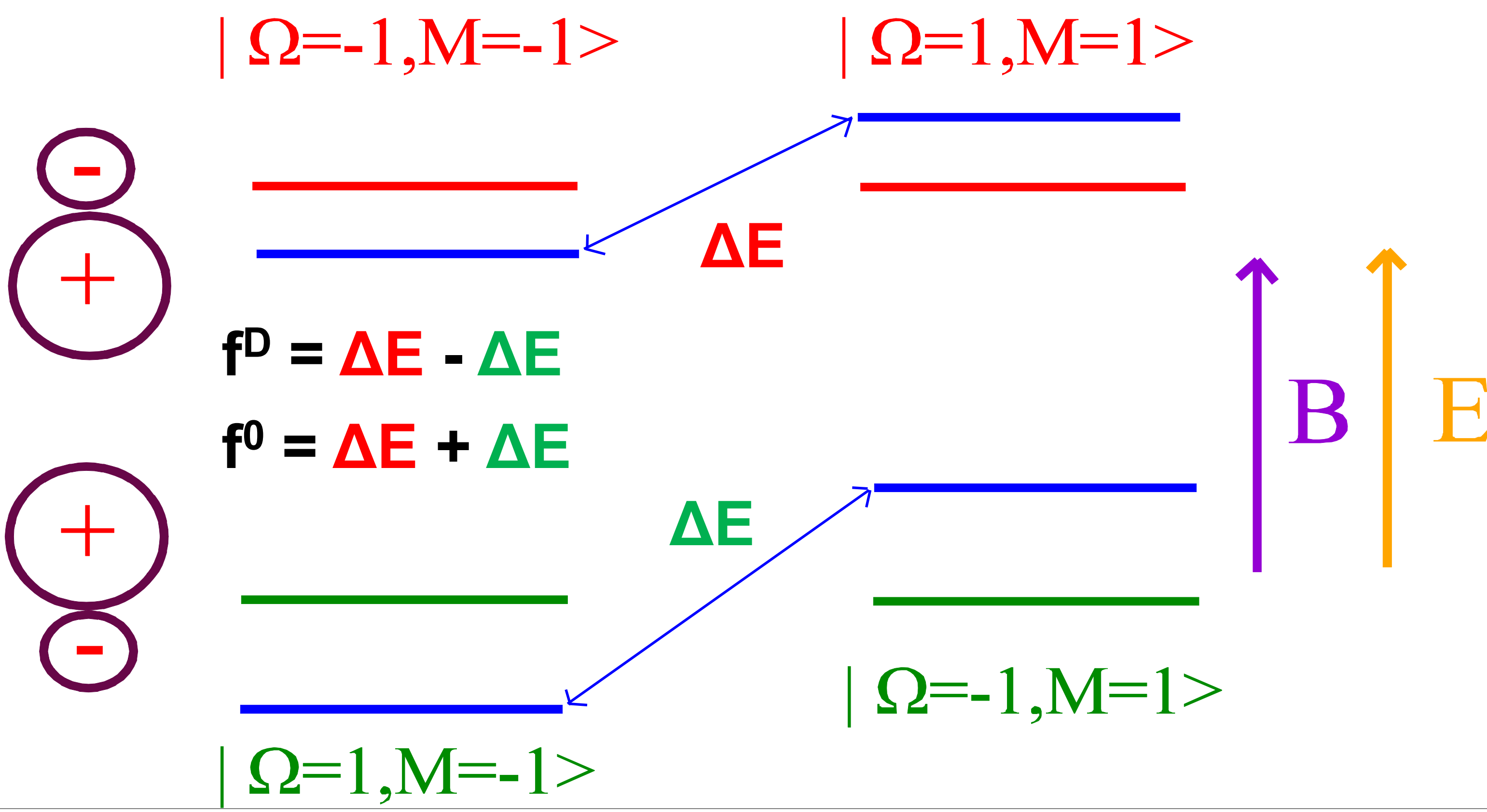

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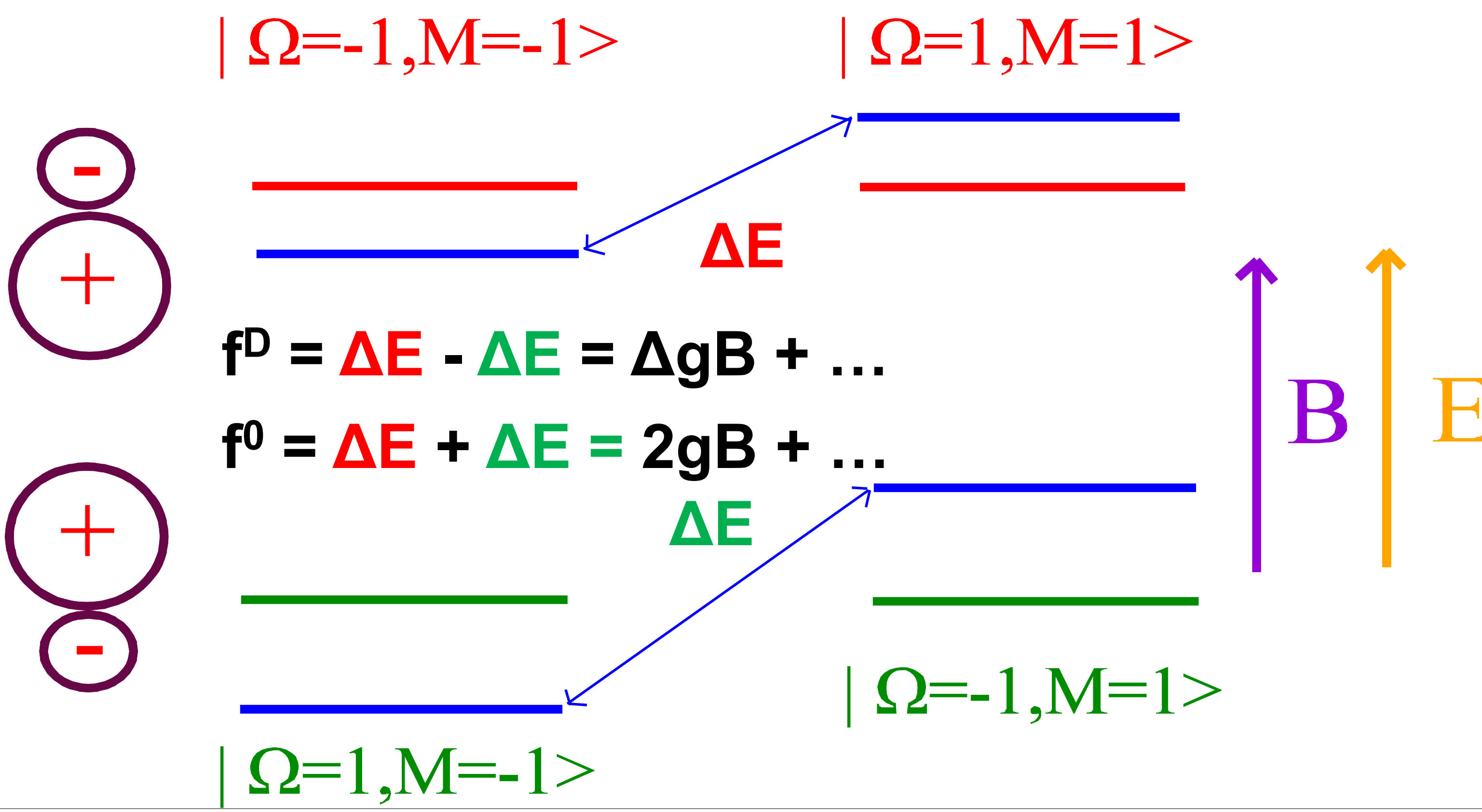


HfF^+ electronic structure

Hf: [Xe4f^{14}] 5d^{2}6s^2

F: [1s^2] 2s^{2}2p^5

[core] [valence]

HfF^+ valence (4e) configuration:

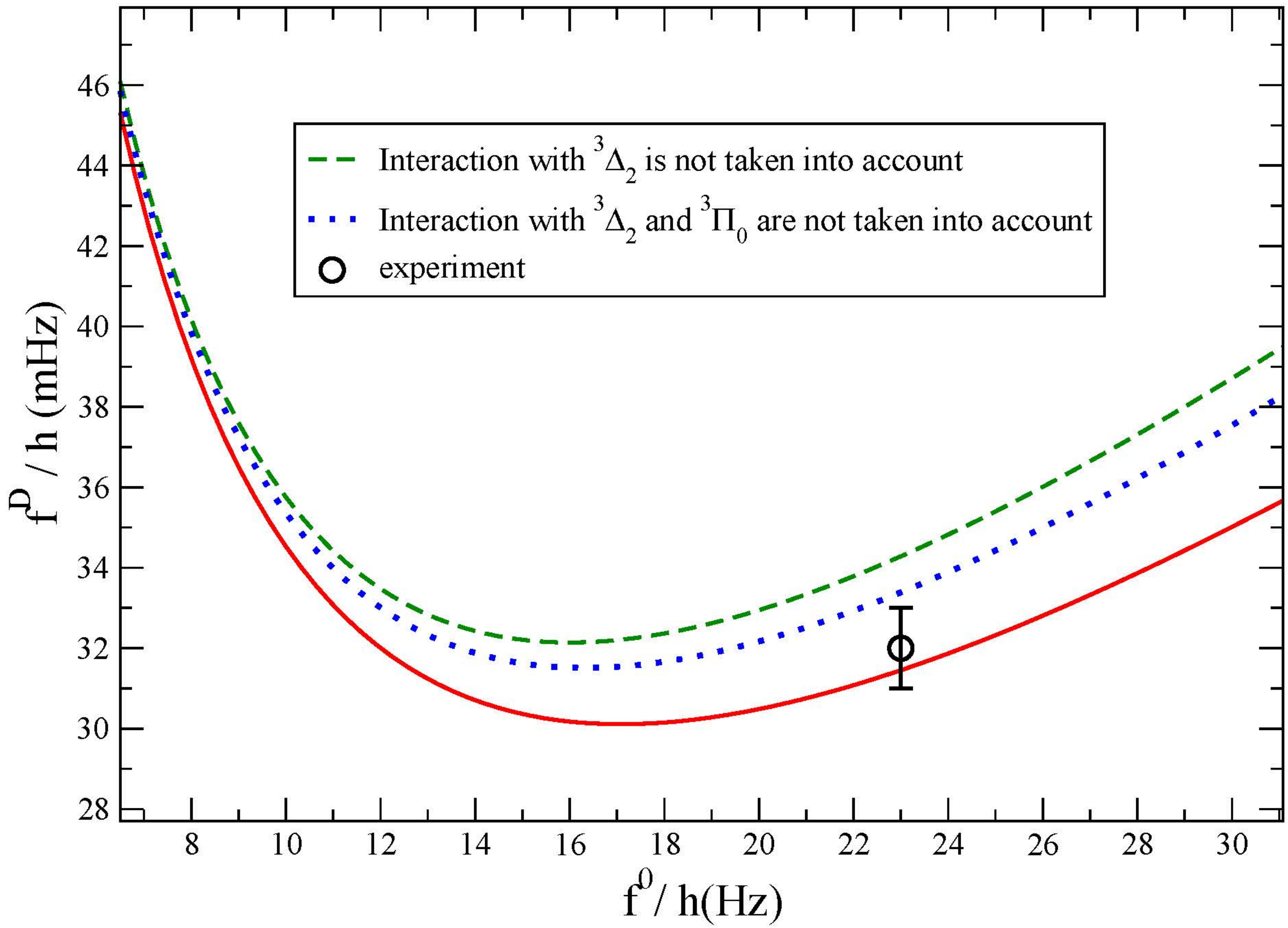
$\sigma_1^2\sigma_2^2$ ($^1\Sigma^+$)

$\sigma_1^2\sigma_2^1\delta^1$ ($^3\Delta_1$(977 cm^{-1}), $^3\Delta_2$(2149 cm^{-1}), $^3\Delta_3$, $^1\Delta_2$)

$\sigma_1^2\sigma_2^1\pi^1$ ($^3\Pi_2$, $^3\Pi_1$, $^3\Pi_{0^+}$(10402 cm^{-1}), $^3\Pi_{0^-}$(10213 cm^{-1}), $^1\Pi_1$)

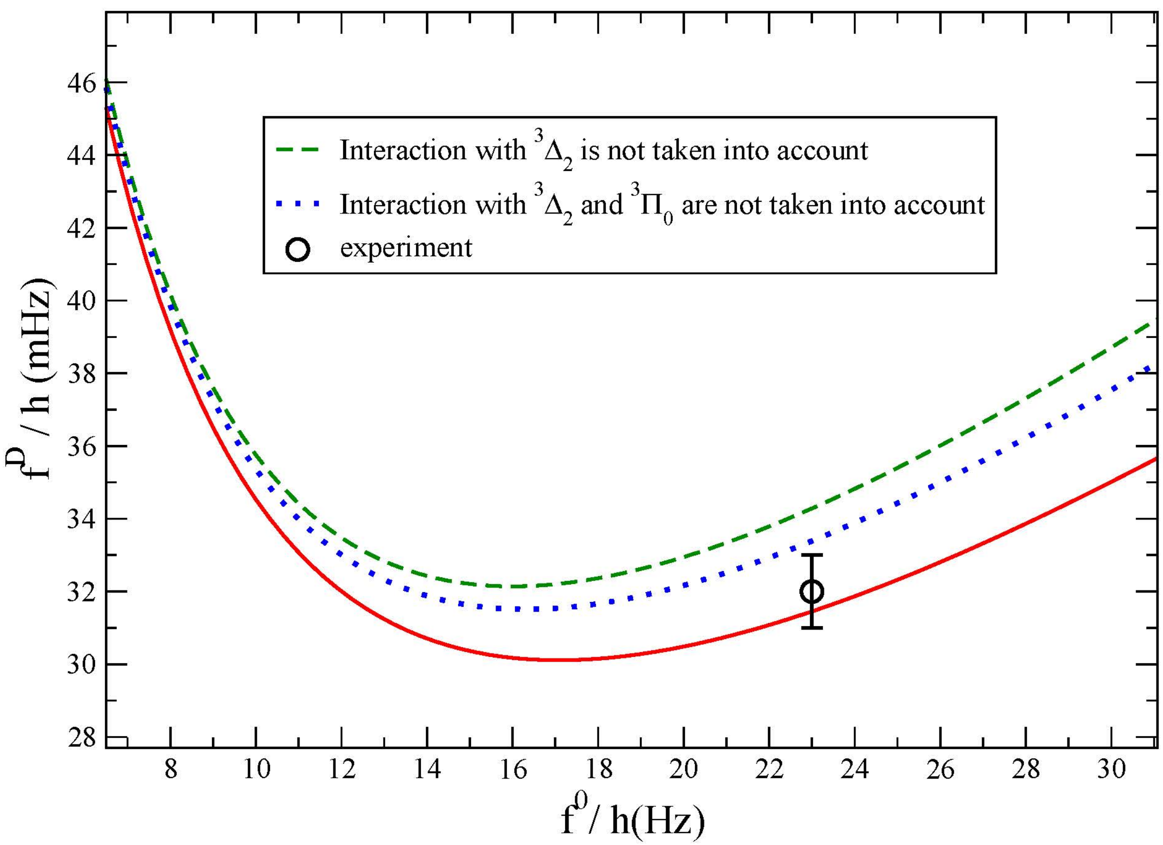
- $\sigma_1 \approx 2p_z$(F)
- $\sigma_2 \approx 6s$(Hf)
- $\delta, \pi \approx 5d$(Hf)

Calculated f^D & f^0



A.N. Petrov, Phys.Rev.A, 97, 052504 (2018)

Calculated f^D & f^0



Theoretical study of systematic effects in the HfF^+-ion experiment to search for the electron electric dipole moment in **[A.N. Petrov, Phys.Rev.A, 97, 052504 (2018) (red curve)]** goes beyond the theoretical study of systematic effects presented in **[PRL 119, 153001 (2017)]** (**blue curve**). The agreement between experimental and theoretical values of $\mathbf{f^D}$ reached in the present work indicates that systematic effects in the experiment can be reduced significantly, thus confirming the prospects of HfF+ for the electron electric dipole moment search.

Thank you!