Schiff-Moment and TPT-Ne Interactions in Mercury and Francium-Silver

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France

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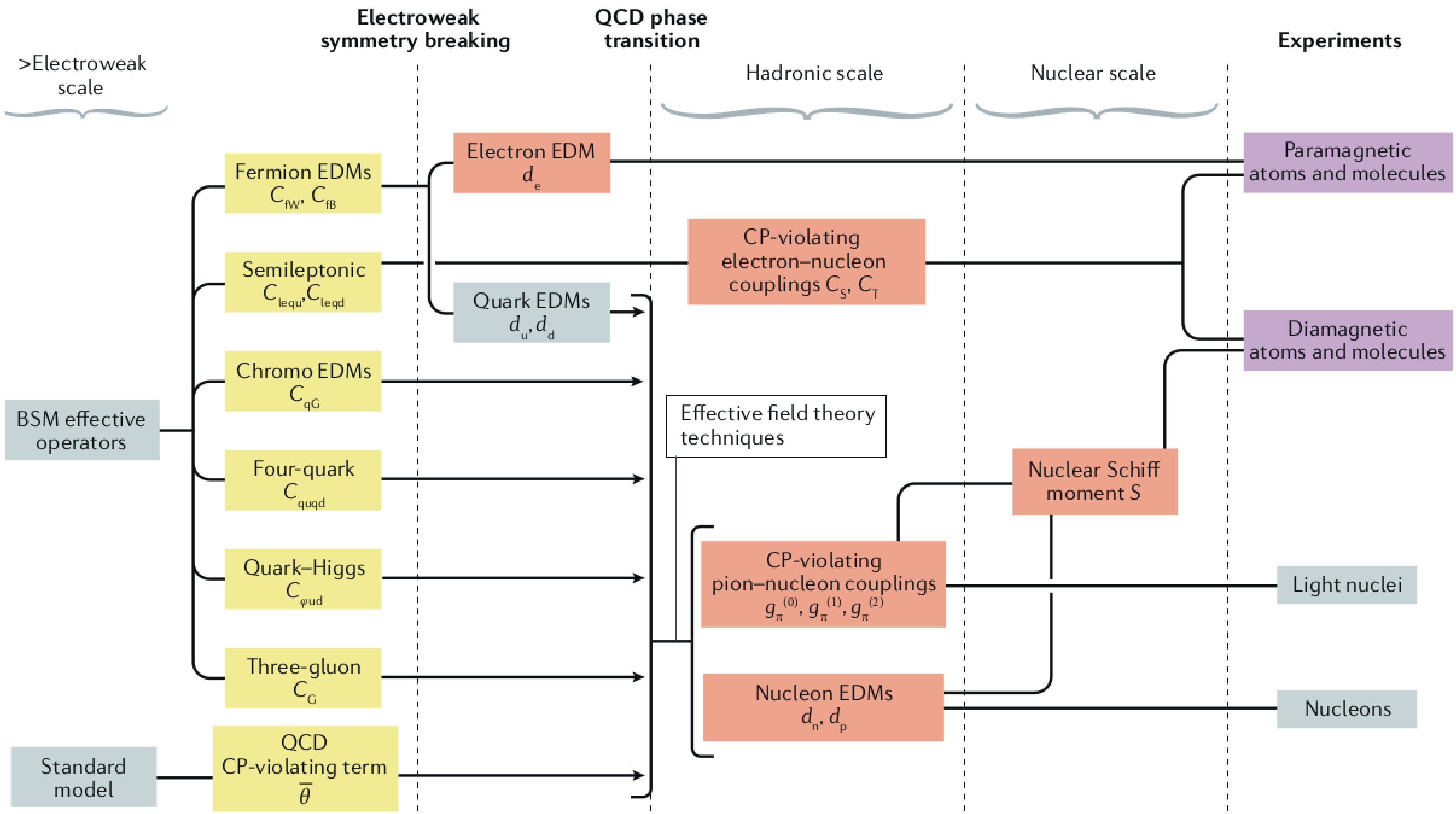
EDMs and their possible sources: An overview



W. Cairncross, J. Ye, *Nat. Rev. Phys.* **1** (2019) *510*

EDM Science

- Electron EDM interactions (HfF^+, ThO, Hg, Tl, TaO^+, RaAg et al.)

  T. F., D. DeMille, *New J. Phys.* **23** (2021) *113039*

  T. F., L. V. Skripnikov, *Symmetry* **12** (2020) *498*

  T. F., M. Jung, *J High Energy Phys. (JHEP)* **07** (2018) *012*

  T. F., *Phys. Rev. A* **96** (2017) *040502(R)*

  T. F., *Phys. Rev. A* **95** (2017) *022504*

  M. Denis, T. F., *J. Chem. Phys.* **145** (2016) *214307*

- Nuclear Schiff-moment interactions (Xe, Hg, TlF, FrAg et al.)

  A. Marc, M. Hubert, T. F., *Phys. Rev. A* **108** (2023) *062815*

  M. Hubert, T. F., *Phys. Rev. A* **106** (2022) *022817*

- Weak neutral current interactions (Xe, Hg, Ra, TlF, FrAg, CsAg)

  L. V. Skripnikov, T. F. (2026) *in preparation*

  A. Marc, T. F., *Eur. Phys. J. D* **79** (2025) *19*

  T. F., *Phys. Rev. A* **109** (2024) *022807*

  T. F., *Phys. Rev. A* **99** (2019) *012515*

- Nuclear MQM interactions (TaN, TaO^+, HfF^+, RaAg)

  T. F., M. K. Nayak, M. G. Kozlov, *Phys. Rev. A* **93** (2016) *012505*

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Current World Records

In the presence of a non-zero EDM d, the system's Hamiltonian is
$\hat{H} = -(\mu\mathbf{B} + d\mathbf{E}) \cdot \frac{\hat{\mathbf{J}}}{|J|}$

- **"Paramagnetic" systems**: Precession measurement on **HfF^+**
  JILA group; Ye, Cornell[1]
  measured $f = (-14.6 \pm 29.7)\ \mu\text{Hz} \Rightarrow |d_e| \leq 4.1 \times 10^{-30}\, e$ cm
- **"Diamagnetic" systems**: Precession measurement on **Hg**
  Seattle group; Heckel[2]
  measured $|d_{Hg}| \leq 7.4 \times 10^{-30}\, e$ cm
- **Neutron** (n) EDM experiment
  PSI, Switzerland[3]
  measured $|d_n| \leq 1.8 \times 10^{-26}\, e$ cm

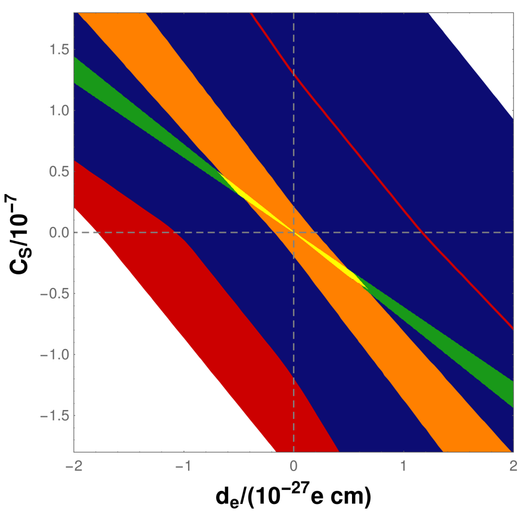
---

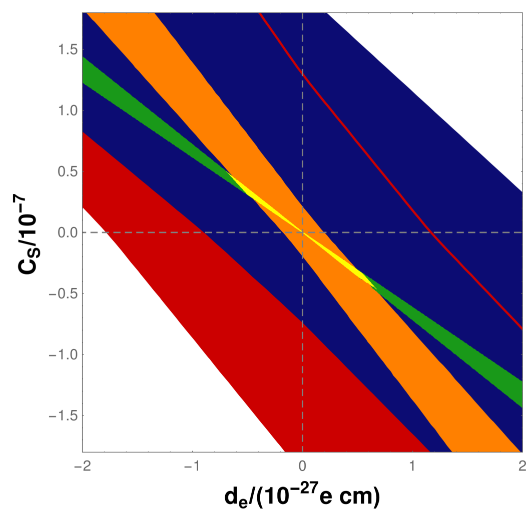
[1] T. S. Roussy, *et al.*, J. Ye, E. A. Cornell, Science **381** (2023) *46*
[2] B. Graner *et al.*, Phys Rev Lett **116** (2016) *161601*
[3] C. Abel *et al.*, Phys. Rev. Lett., **124** (2020) *081803*

The Tl EDM

T. F., L. V. Skripnikov, *Symmetry* **12** (2020) *498*

Work	α_{d_e}	$\alpha_{C_S}[10^{-18}e$ cm]
Flambaum (semi-empirical)	-500	
Johnson *et al.* (Norcross potential)	-562	
Mårtensson-Pendrill *et al.* (estimate)	-600 ± 200	7 ± 2
Liu *et al.*	$-585 \pm (30 - 60)$	
Dzuba *et al.*	-582 ± 20	7.0 ± 0.2
Nataraj *et al.* (CCSD(T))	-466 ± 10	
Sahoo *et al.* (CCSD(T))		4.06 ± 0.14
Porsev *et al.*	-573 ± 20	
This work CI	-539 ± 33	6.61 ± 0.4
This work CC	-559 ± 28	6.77 ± 0.34





The Hg EDM

T. Chupp, P. Fierlinger, M. J. Ramsey-Musolf, J. T. Singh, *Rev. Mod. Phys.* **91 (2019)** *015001*

TABLE IV. Coefficients for P-odd and T-odd parameter contributions to EDMs for diamagnetic systems and the neutron. The second line for each entry is the reasonable range for each coefficient. The $\partial d^{\mathrm{exp}}/\partial d_e$ and $\partial d^{\mathrm{exp}}/\partial C_S$ are from Ginges and Flambaum (2004) and are based on Mårtensson-Pendrill (1985) and Mårtensson-Pendrill and Öster (1987) for ^{129}Xe and ^{199}Hg. Also see Fleig and Jung (2018) for ^{199}Hg. The $\partial d^{\mathrm{exp}}/\partial d_e$ and $\partial d^{\mathrm{exp}}/\partial C_S$ for TlF are compiled by Cho, Sangster, and Hinds (1991). The $\partial d^{\mathrm{exp}}/\partial C_T^{(0)}$ are adjusted for the unpaired neutron in ^{129}Xe, ^{199}Hg, and ^{225}Ra using k_T from Ginges and Flambaum (2004) and is consistent with Sahoo (2017). For ^{225}Ra $\partial d^{\mathrm{exp}}/\partial C_T^{(0)}$ is from Dzuba, Flambaum, and Porsev (2009) and Singh and Sahoo (2015a). The $\bar{g}_\pi^{(0)}$, $\bar{g}_\pi^{(1)}$, and $\bar{d}_n^{sr}$ coefficients for atoms and molecules are based on data provided in Table V; the range for ^{225}Ra corresponds to $0 \le s_n \le 2$ fm^2. For TlF, the unpaired neutron is replaced by an unpaired proton and the "best value" assumes $\bar{d}_p^{sr} = -\bar{d}_n^{sr}$, i.e., mostly isovector in analogy to the anomalous magnetic moment, while the range is defined by $|\bar{d}_p^{sr}| \le |\bar{d}_n^{sr}|$.

System	$\partial d^{\mathrm{exp}}/\partial d_e$	$\partial d^{\mathrm{exp}}/\partial C_S$ (e cm)	$\partial d^{\mathrm{exp}}/\partial C_T^{(0)}$ (e cm)	$\partial d^{\mathrm{exp}}/\partial \bar{g}_\pi^{(0)}$ (e cm)	$\partial d^{\mathrm{exp}}/\partial \bar{g}_\pi^{(1)}$ (e cm)	$\partial d^{\mathrm{exp}}/\partial \bar{d}_n^{sr}$
Neutron				1.5×10^{-14}	1.4×10^{-16}	1
^{129}Xe	−0.0008	-4.4×10^{-23}	-6.1×10^{-21}	-0.4×10^{-19}	-2.2×10^{-19}	1.7×10^{-5}
		−4.4 − (−5.6)	−6.1 − (−9.1)	−23.4 − (1.8)	−19 − (−1.1)	1.7–2.4
^{199}Hg	−0.014	-5.9×10^{-22}	3.0×10^{-20}	-11.8×10^{-18}	0	-5.3×10^{-4}
	−0.014 − 0.012		3.0–9.0	−38 − (−9.9)	$(-4.9 - 1.6) \times 10^{-17}$	−7.7 − (−5.2)
^{225}Ra			5.3×10^{-20}	1.7×10^{-15}	-6.9×10^{-15}	
			5.3–10.0	6.9–0.9	−27.5 − (−3.8)	$(-1.6 - 0) \times 10^{-3}$
TlF	81	2.9×10^{-18}	2.7×10^{-16}	1.9×10^{-14}	-1.6×10^{-13}	0.46
				0.5–2		−0.5 − 0.5

The Hg EDM

Literature results

Source	Method	α_{C_T} $\left[10^{-20}\ \langle\Sigma\rangle_{\text{Hg}}\ e\text{cm}\right]$
Mårtensson-Pendrill [4]	HF	-6.0
Dzuba *et al.* [5]	CI+MBPT	-5.1
Latha *et al.* [6]		-4.3
Singh *et al.* [7]	CCSD$_p$T	-4.3
Sahoo *et al.* [8]	RNCCSD	-3.3
T. F. [9]	GAS-CI	-5.0

[4] A.-M. Mårtensson-Pendrill, *Phys. Rev. Lett.* **54** (1985) *1153*

[5] V. A. Dzuba, V. V. Flambaum, S. G. Porsev, *Phys. Rev. A* **80** (2009) *032120*

[6] K. V. P. Latha, D. Angom, B. P. Das, D. Mukherjee, *Phys. Rev. Lett.* **103** (2009) *083001*

[7] Y. Singh and B. K. Sahoo, *Phys. Rev. A* **91** (2015) *030501(R)*

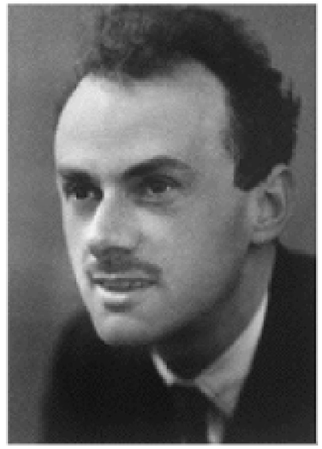
[8] B. K. Sahoo, B. P. Das, *Phys. Rev. Lett.* **120** (2018) *203001*

[9] T. F., *Phys. Rev. A* **99** (2019) *012515*
updated in K. Gaul, R. Berger, *JHEP* **08** (2024) *100*

Methods / Packages

P rogram
• for
A tomic
• and
M olecular

D irect
I terative
R elativistic
A ll-electron
C alculations



diracprogram.org

KR-CI module

T. F., H.J.Å. Jensen, J. Olsen, L. Visscher, *J Chem Phys* **124** (2006) *104106*
S. Knecht, H.J.Å. Jensen, T. F., *J Chem Phys* **132** (2010) *014108*

www.MRCC.hu

Atomic EDM

in terms of underlying symmetry breaking

Electric dipole moment of an atom:[10]

$d_a := -\lim_{E_{\text{ext}}\to 0}\left[\frac{\partial(\Delta\varepsilon_{\not P\not T})}{\partial E_{\text{ext}}}\right]$ $\Delta\varepsilon_{\not P\not T}$ is **some** P,T-odd energy shift.

Sources are particle EDMs, nuclear MQM, nuclear Schiff moment, $\mathcal{T}$-odd contribution to weak interaction etc.

For some Hamiltonian $\hat{H}_{\not P\not T} = C_{\not C\not P}\hat{O}_{\not P\not T}$, we then have

$$d_a = -\lim_{E_{\text{ext}}\to 0}\frac{\partial}{\partial E_{\text{ext}}}C_{\not C\not P}\left\langle \hat{O}_{\not P\not T}\right\rangle_{\psi(E_{\text{ext}})}$$

Defining a general interaction constant as $\alpha_{\not P\not T} := \frac{d_a}{C_{\not C\not P}}$ the linear-regime atomic interaction constant is then:

$$\alpha_{\not P\not T} = -\lim_{E_{\text{ext}}\to 0}\frac{\left\langle \hat{O}_{\not P\not T}\right\rangle_{\psi(E_{\text{ext}})}}{E_{\text{ext}}} \approx \alpha_{\not P\not T}(\text{lin}) = -\frac{\left\langle \hat{O}_{\not P\not T}\right\rangle_{\psi(E_{\text{ext}})}}{E_{\text{ext}}}$$

with finite but very small E_{ext}.

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[10] E.D. Commins, *Adv. Mol. Opt. Phys.* **40** (1999) *1*

Atomic and Molecular Correlated Wavefunctions[11]

Hamiltonians

- Dirac-Coulomb Hamiltonian + external electric field (atoms)

$$\hat{H}^{\text{Dirac-Coulomb}} + \hat{H}^{\text{Int-Dipole}} = \sum_{i}^{n} \left[c\,\boldsymbol{\alpha}_i \cdot \mathbf{p}_i + \beta_i c^2 - \frac{Z}{r_i} \mathbb{1}_4 \right] + \sum_{i,j>j}^{n} \frac{1}{r_{ij}} \mathbb{1}_4 + \sum_{i}^{n} \mathbf{r}_i \cdot \mathbf{E}_{\text{ext}}\, \mathbb{1}_4$$

- Dirac-Coulomb Hamiltonian operator (molecules)

$$\hat{H}^{DC} = \sum_{i}^{n} \left[c\,\boldsymbol{\alpha}_i \cdot \mathbf{p}_i + \beta_i c^2 - \sum_{A}^{N} \frac{Z}{r_{iA}} \mathbb{1}_4 \right] + \sum_{i,j>i}^{n} \frac{1}{r_{ij}} \mathbb{1}_4 + \sum_{A,B>A}^{N} V_{AB}$$

- Dirac-Coulomb-Gaunt[12] Hamiltonian operator (molecules)

$$\hat{H}^{DCG} = \sum_{i}^{n} \left[c\,\boldsymbol{\alpha}_i \cdot \mathbf{p}_i + \beta_i c^2 - \sum_{A}^{N} \frac{Z}{r_{iA}} \mathbb{1}_4 \right] + \sum_{i,j>i}^{n} \left(\frac{1}{r_{ij}} \mathbb{1}_4 - \frac{1}{2} \frac{\vec{\alpha}_i \vec{\alpha}_j}{r_{ij}} \right) + \sum_{A,B>A}^{N} V_{AB}$$

---

[11] T. F., H.J.Å. Jensen, J. Olsen, L. Visscher, *J Chem Phys* **124** (2006) *104106*
S. Knecht, H.J.Å. Jensen, T. F., *J Chem Phys* **132** (2010) *014108*
[12] A. Marc, T.F., in preparation

Calculation of Properties Including $\mathcal{P}$,$\mathcal{T}$-Violating Effects[13]

Using String-Based CI Techniques

Solve CI problem $\Rightarrow \psi_k^{(0)}$; expectation value over relativistic Configuration Interaction wavefunction

$$\left\langle \hat{O} \right\rangle_{\psi_k^{(0)}} = \sum_{I,J=1}^{\dim\mathcal{F}^{\mathrm{t}}(\mathrm{M,n})} c_{kI}^* c_{kJ} \left\langle \, | (\mathcal{S}\overline{\mathcal{T}})_I^\dagger \left| \hat{O} \right| (\mathcal{S}\overline{\mathcal{T}})_J \, | \, \right\rangle$$

Property operator $\hat{O}$ in basis of Kramers-paired atomic/molecular spinors

$$\hat{O} = \sum_{i,j=1}^{P_u} o_{ij}\, a_i^\dagger a_j + \sum_{i=1}^{P_u} \sum_{j=P_u+1}^{P} o_{i\overline{j}}\, a_i^\dagger a_{\overline{j}} + \sum_{i=P_u+1}^{P} \sum_{j=1}^{P_u} o_{\overline{i}j}\, a_{\overline{i}}^\dagger a_j + \sum_{i,j=P_u+1}^{P} o_{\overline{i}\overline{j}}\, a_{\overline{i}}^\dagger a_{\overline{j}}$$

First-term contribution to expectation value

$$O(\Psi_k)_1 = \sum_{I,J=1}^{\dim\mathcal{F}^{\mathrm{t}}(\mathrm{M,n})} c_{kI}^* c_{kJ} \sum_{i,j=1}^{P_u} o_{ij}$$
$$\left\langle \, | \prod_{p=1}^{N_p} \prod_{\overline{p}=N_p+1}^{N_p+N_{\overline{p}}} a_{\overline{p}} a_p\, a_i^\dagger a_j \prod_{q=1}^{N_p} \prod_{\overline{q}=N_p+1}^{N_p+N_{\overline{p}}} a_q^\dagger a_{\overline{q}}^\dagger \, | \, \right\rangle$$

[13] S. Knecht, Dissertation, HHU Düsseldorf (2009)
T. F., M.K. Nayak, *Phys Rev A* **88** (2013) *032514*

Search for Semi-Hadronic-Source EDM: TPT-Ne Interaction

Hg atom; Dirac-Coulomb Hartree-Fock

Atomic interaction constant[15] as implemented into KRCI/DIRAC[16]

$$\alpha_{C_T} := \frac{\Delta\varepsilon_{C_T}}{C_T\, E_{\text{ext}}} = \frac{G_F\sqrt{2}\,\langle\Sigma\rangle_A}{E_{\text{ext}}} \left\langle \imath \sum_{j=1}^{n} \left(\gamma_3\right)_j\, \rho(\mathbf{r}_j) \right\rangle_{\psi(E_{\text{ext}})}$$

Model	α_{C_T} $\left[10^{-20}\ \langle\Sigma\rangle_{\text{Hg}}\ e\text{cm}\right]$	$\Delta\%$	$C_{\text{Hg}_{6s^2}}$	dim.
QZ/DCHF [17]	**−5.980**	**0.0**	**1.0**	**1**
Mårtensson-Pendrill [14] (RPA)	−6.0	0.0		
Dzuba *et al.* [18] (RPA)	−5.9	0.0		
Dzuba *et al.* [18] (CI+MBPT)	−5.1	13.6		

[14] A.-M. Mårtensson-Pendrill, *Phys. Rev. Lett.* **54** (1985) *1153*

[15] E. A. Hinds, C. E. Loving, and P. G. H. Sandars, *J. Phys. B, At. Mol. Phys.* **1** (1968) *499*
T.F., *Phys. Rev. A* **99** (2019) *012515*

[16] S. Knecht and H. J. Aa. Jensen, T.F., *J. Chem. Phys.* **132** (2010) *014108*
T. Saue *et al.*, *J. Chem. Phys.* **152** (2020) *204104*

[17] L. V. Skripnikov, T. F., (2026) *unpublished*

[18] V. A. Dzuba, V. V. Flambaum, S. G. Porsev, *Phys. Rev. A* **80** (2009) *032120*

Search for Semi-Hadronic-Source EDM: TPT-Ne Interaction

Hg atom; shell effects

$$\alpha_{C_T} := \frac{\Delta\varepsilon_{C_T}}{C_T\, E_{\text{ext}}} = \frac{G_F\sqrt{2}\,\langle\Sigma\rangle_A}{E_{\text{ext}}} \left\langle \imath \sum_{j=1}^{n} \left(\gamma_3\right)_j \, \rho(\mathbf{r}_j) \right\rangle_{\psi(E_{\text{ext}})}$$

Model [17]	α_{C_T} $\left[10^{-20}\ \langle\Sigma\rangle_{\text{Hg}}\ e\text{cm}\right]$	$\Delta\%$	$C_{\text{Hg}_{6s^2}}$	dim.
QZ/DCHF	-5.980	$0.$	1.0	1
QZ/SD2/8au	**−5.271**	**11.9**	**0.981**	**2,474**
Dzuba *et al.* [18] (RPA)	-5.9	$0.$		
Dzuba *et al.* [18] (CI+MBPT)	-5.1	13.6		

- Partial removal of electron density from most strongly $s-p$-mixed shell ($6s$)

[17] L. V. Skripnikov, T. F., (2026) *unpublished*

[18] V. A. Dzuba, V. V. Flambaum, S. G. Porsev, *Phys. Rev. A* **80** (2009) *032120*

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QZ/SD2/8au	-5.271	11.9	0.981	$2,474$
QZ/SD12/8au	**−5.329**	**−1.0**	**0.958**	**131,111**
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- Net removal of electron density from non-contributing shells (d, f, ...)

[17] L. V. Skripnikov, T. F., (2026) *unpublished*

[18] V. A. Dzuba, V. V. Flambaum, S. G. Porsev, *Phys. Rev. A* **80** (2009) *032120*

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QZ/SD20/8au	**−5.240**	**1.5**	**0.955**	**390,929**
Dzuba *et al.* [18] (RPA)	-5.9	$0.$		
Dzuba *et al.* [18] (CI+MBPT)	-5.1	13.6		

- Partial removal of electron density from directly contributing shells ($5s$, $5p$)

[17] L. V. Skripnikov, T. F., (2026) *unpublished*

[18] V. A. Dzuba, V. V. Flambaum, S. G. Porsev, *Phys. Rev. A* **80** (2009) *032120*

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QZ/SD20/8au	-5.240	1.5	0.955	390,929
QZ/SD34/8au	**−5.307**	**−1.1**	**0.955**	**1,046,374**
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Dzuba *et al.* [18] (CI+MBPT)	-5.1	13.6		

- Net removal of electron density from non-contributing shells (d, f, ...)

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QZ/SD34/8au	-5.307	-1.1	0.955	$1,046,374$
QZ/SD44/8au	**−5.340**	**−0.6**	**0.955**	**1,770,973**
Dzuba *et al.* [18] (RPA)	-5.9	$0.$		
Dzuba *et al.* [18] (CI+MBPT)	-5.1	13.6		

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Search for Semi-Hadronic-Source EDM: TPT-Ne Interaction

Hg atom; higher-rank correlations

$$\alpha_{C_T} := \frac{\Delta\varepsilon_{C_T}}{C_T\, E_{\text{ext}}} = \frac{G_F\sqrt{2}\,\langle\Sigma\rangle_A}{E_{\text{ext}}} \left\langle \imath \sum_{j=1}^{n} \left(\gamma_3\right)_j\, \rho(\mathbf{r}_j) \right\rangle_{\psi(E_{\text{ext}})}$$

Model [17]	α_{C_T} $\left[10^{-20}\ \langle\Sigma\rangle_{\text{Hg}}\ e\text{cm}\right]$	Δ%	$C_{\text{Hg}_{6s^2}}$	dim.
QZ/DCHF	-5.980	0.	1.0	1
QZ/SD12/8au	**−5.329**	**10.9**	**0.958**	**131,111**
Dzuba *et al.* [18] (RPA)	-5.9	0.		
Dzuba *et al.* [18] (CI+MBPT)	-5.1	13.6		

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QZ/SDT10_SDTQ12/8au	**−4.555**	**5.5**	**0.939**	**1,192,109,441**
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QZ/SD10_SDT12/15au	**−4.911**	**−0.1**	**0.953**	**23,359,445**
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QZ/SD10_SDT12/20au	**−4.915**	**−0.1**	**0.953**	**32,027,149**
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QZ/SD10_SDT12/40au	**−4.916**	**−0.0**	**0.953**	**40,795,699**
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QZ/SD10_SDT12/100au	**-4.916**	**-0.0**	**0.953**	**61,989,103**
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QZ/DCHF	-5.980	$0.$	1.0	1
QZ/SD20/8au	-5.240	12.4	0.955	$390,929$
QZ/SD20/10au	-5.342	-1.7		$604,983$
QZ/SD20/15au	-5.337	0.1		$655,433$
QZ/SD20/20au	**−5.348**	**−0.2**		**806,331**
Dzuba *et al.* [18] (RPA)	-5.9	$0.$		
Dzuba *et al.* [18] (CI+MBPT)	-5.1	13.6		

[17] L. V. Skripnikov, T. F., (2026) *unpublished*

[18] V. A. Dzuba, V. V. Flambaum, S. G. Porsev, *Phys. Rev. A* **80** (2009) *032120*

Search for Semi-Hadronic-Source EDM: TPT-Ne Interaction

Hg atom; inner shells and cutoff

$$\alpha_{C_T} := \frac{\Delta\varepsilon_{C_T}}{C_T\, E_{\text{ext}}} = \frac{G_F\sqrt{2}\,\langle\Sigma\rangle_A}{E_{\text{ext}}} \left\langle \imath \sum_{j=1}^{n} (\gamma_3)_j\, \rho(\mathbf{r}_j) \right\rangle_{\psi(E_{\text{ext}})}$$

Model [17]	α_{C_T} $\left[10^{-20}\ \langle\Sigma\rangle_{\text{Hg}}\ e\text{cm}\right]$	$\Delta\%$	$C_{\text{Hg}_{6s^2}}$	dim.
QZ/DCHF	-5.980	$0.$	1.0	1
QZ/SD20/8au	-5.240	12.4	0.955	$390,929$
QZ/SD20/10au	-5.342	-1.7		$604,983$
QZ/SD20/15au	-5.337	0.1		$655,433$
QZ/SD20/20au	-5.348	-0.2		$806,331$
QZ/SD20/40au	**−5.352**	**−0.1**		**951,795**
Dzuba *et al.* [18] (RPA)	-5.9	$0.$		
Dzuba *et al.* [18] (CI+MBPT)	-5.1	13.6		

[17] L. V. Skripnikov, T. F., (2026) *unpublished*

[18] V. A. Dzuba, V. V. Flambaum, S. G. Porsev, *Phys. Rev. A* **80** (2009) *032120*

Search for Semi-Hadronic-Source EDM: TPT-Ne Interaction

^{199}Hg

$$\alpha_{C_T} := \frac{\Delta\varepsilon_{C_T}}{C_T\, E_{\text{ext}}} = \frac{G_F\sqrt{2}\,\langle\Sigma\rangle_A}{E_{\text{ext}}} \left\langle \imath \sum_{j=1}^{n} (\gamma_3)_j\, \rho(\mathbf{r}_j) \right\rangle_{\psi(E_{\text{ext}})}$$

Model [19]	α_{C_T} $\left[10^{-20}\,\langle\Sigma\rangle_{\text{Hg}}\ e\text{cm}\right]$	$\Delta\%$ corr.
T. F. DCHF	-5.98	
Skripnikov DCHF	-5.98	
T. F. CI current best	-4.13	31
Skripnikov CC current best	-3.83	36
Dzuba *et al.* [20] (RPA)	-5.9	
Dzuba *et al.* [20] (CI+MBPT)	-5.1	13.6
Singh *et al.* [21] CCSD$_p$T	-4.3	
Sahoo *et al.* [22] RNCCSD	-3.3	

[19] L. V. Skripnikov, T. F. (2026) *unpublished*

[20] V. A. Dzuba, V. V. Flambaum, S. G. Porsev, *Phys. Rev. A* **80** (2009) *032120*

[21] Y. Singh and B. K. Sahoo, *Phys. Rev. A* **91** (2015) *030501(R)*

[22] B. K. Sahoo, B. P. Das, *Phys. Rev. Lett.* **120** (2018) *203001*

Search for Hadron-Source EDM: Schiff-Moment Interaction

^{199}Hg atom

Atomic interaction constant[23] as implemented into KRCI/DIRAC[24]

$$\alpha_{\text{SM}} := \frac{\Delta\varepsilon_{\text{SM}}}{S_z\, E_{\text{ext}}} = \frac{-\frac{3}{B}\left\langle \sum\limits_{j=1}^{n} \hat{z}_j\, \rho(\mathbf{r}_j) \right\rangle_{\psi(E_{\text{ext}})}}{E_{\text{ext}}}$$

Model	$\alpha_{\text{SM}}\ \left[10^{-17}\frac{e\text{cm}}{e\text{fm}^3}\right]$	$\lvert\Delta\%\rvert$ corr.
Fleig DCHF	-2.89	
Skripnikov DCHF	-2.90	
Fleig CI current best	-2.26	21.8%
Skripnikov CC current best	-1.88	35.2%
Dzuba *et al.* [25] (RPA, 2009)	-3.0	
Dzuba *et al.* [25] (CI+MBPT, 2009)	-2.6	13.3%

[23] V. A. Dzuba, V. V. Flambaum, J. S. M. Ginges, and M. G. Kozlov, *Phys. Rev. A* **66** (2002) *021111*
M. Hubert, T.F., *Phys. Rev. A* **106** (2022) *022817*
[24] S. Knecht and H. J. Aa. Jensen, T.F., *J. Chem. Phys.* **132** (2010) *014108*
T. Saue *et al.*, *J. Chem. Phys.* **152** (2020) *204104*
[25] V. A. Dzuba, V. V. Flambaum, S. G. Porsev, *Phys. Rev. A* **80** (2009) *032120*

EDM Science

- Electron EDM interactions (HfF^+, ThO, Hg, Tl, TaO^+, RaAg et al.)

  T. F., D. DeMille, *New J. Phys.* **23** (2021) *113039*

  T. F., L. V. Skripnikov, *Symmetry* **12** (2020) *498*

  T. F., M. Jung, *J High Energy Phys. (JHEP)* **07** (2018) *012*

  T. F., *Phys. Rev. A* **96** (2017) *040502(R)*

  T. F., *Phys. Rev. A* **95** (2017) *022504*

  M. Denis, T. F., *J. Chem. Phys.* **145** (2016) *214307*

- Nuclear Schiff-moment interactions (Xe, Hg, TlF, FrAg et al.)

  A. Marc, M. Hubert, T. F., *Phys. Rev. A* **108** (2023) *062815*

  M. Hubert, T. F., *Phys. Rev. A* **106** (2022) *022817*

- Weak neutral current interactions (Xe, Hg, Ra, TlF, FrAg, CsAg)

  L. V. Skripnikov, T. F. (2026) *in preparation*

  A. Marc, T. F., *Eur. Phys. J. D* **79** (2025) *19*

  T. F., *Phys. Rev. A* **109** (2024) *022807*

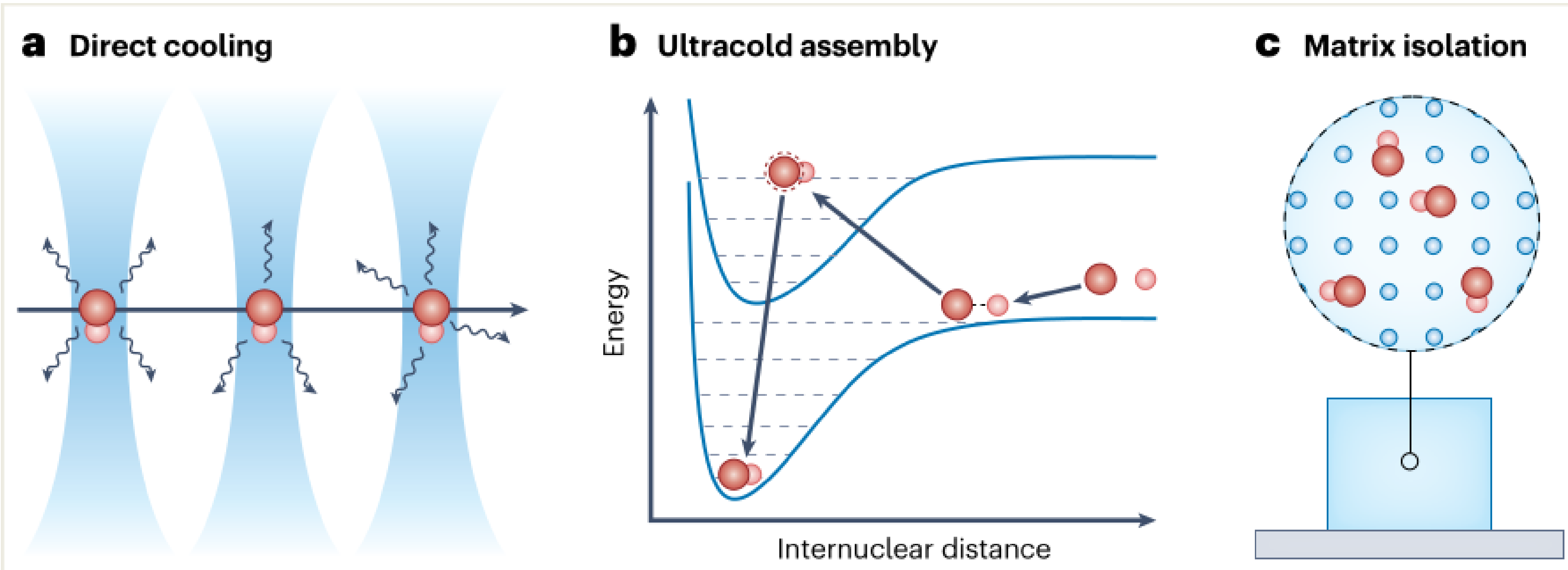
  T. F., *Phys. Rev. A* **99** (2019) *012515*

- Nuclear MQM interactions (TaN, TaO^+, HfF^+, RaAg)

  T. F., M. K. Nayak, M. G. Kozlov, *Phys. Rev. A* **93** (2016) *012505*

EDM Search with Assembled Ultracold Molecules

D. DeMille, N. R. Hutzler, A. M. Rey, T. Zelevinsky, *Nat. Phys.* **20** (2024) *741*



FrAg J. Kłos, H. Li, E. Tiesinga, S. Kotochigova, *New J. Phys.* **24** (2022) *025005*

RaAg T. F., D. DeMille, *New J. Phys.* **23** (2021) *113039*

Search for Hadron-Source EDM: Francium-Silver (FrAg)

Schiff moment in terms of QCD $\overline{\theta}$ and π-meson–nucleon CP-violating interaction constants[26]

$$S\left({}^{223}\text{Fr}\right) \approx \left(-4.16 g\bar{g}_0 + 20.64 g\bar{g}_1 - 11.04 g\bar{g}_2\right)\, e\text{fm}^3$$
$$S\left({}^{205}\text{Tl}\right) \approx \left(0.13\, g\bar{g}_0 - 0.004\, g\bar{g}_1 - 0.27\, g\bar{g}_2\right)\, e\text{fm}^3$$
$$S\left({}^{225}\text{Ra}\right) \approx \left(-2.6\, g\bar{g}_0 + 12.9\, g\bar{g}_1 - 6.9\, g\bar{g}_2\right)\, e\text{fm}^3$$

$$S\left({}^{223}\text{Fr}\right) \approx -1.6\,\overline{\theta} e\ \text{fm}^3$$
$$S\left({}^{205}\text{Tl}\right) \approx 0.02\,\overline{\theta} e\text{fm}^3$$
$$S\left({}^{225}\text{Ra}\right) \approx -\overline{\theta} e\text{fm}^3$$

^{223}Fr orders of magnitude more sensitive than ^{205}Tl

[26] V. V. Flambaum, V. A. Dzuba, and H. B. Tran Tan, *Phys. Rev. A* **101** (2020) *042501*
V. A. Dzuba, V. V. Flambaum, *Phys. Rev. A* **101** (2020) *042504*

Search for Hadron-Source EDM: Francium-Silver (FrAg)

Atomic Basis Sets / Hartree-Fock Theory

Molecular Schiff-moment interaction Hamiltonian[27]

$$W_{\mathrm{SM}}(A) := \frac{\Delta\varepsilon_{\mathrm{SM}}(A)}{S_z(A)} = -\frac{3}{B}\left\langle \sum_{j=1}^{n} \hat{z}_j\, \rho_A(\mathbf{r}_j) \right\rangle_{\psi}$$

as implemented into KRCI/DIRAC[28]

	CsLi ($R_e = 6.927$ a.u.)		FrAg ($R_e = 6.190$ a.u.)	
Basis	$\varepsilon_{\mathrm{DCHF}}$ [a.u.]	W_{SM} [a.u.]	$\varepsilon_{\mathrm{DCHF}}$ [a.u.]	W_{SM} [a.u.]
cvDZ	-7794.1925854	-10110	-29622.7980959	5946
cvTZ	-7794.2033064	-2849	-29622.8345496	28173
cvQZ	-7794.2038442	2098	-29622.8362766	29451
cvQZ+	-7794.2038394	2887	-29622.8354238	31350

[27] V. A. Dzuba, V. V. Flambaum, J. S. M. Ginges, and M. G. Kozlov, *Phys. Rev. A* **66** (2002) *021111*

[28] M. Hubert, T.F., *Phys. Rev. A* **106** (2022) *022817*

Search for Hadron-Source EDM: Francium-Silver (FrAg)

Electron Correlation Effects

Basis/cutoff	ε_{CI} [a.u.]	W_{SM} [a.u.]
cvQZ+/DCHF	-29622.8354238	31350
cvQZ+/SD2_2au	-29622.8604657	30359
cvQZ+/SD2_5au	-29622.8605445	30355
cvQZ+/SD2_8au	-29622.8605500	30360
cvQZ+/SD10_8au	-29623.0196812	29980
cvQZ+/SDT10_8au	-29623.0260848	29909
cvQZ+/SD12_8au	-29623.1920759	30711
cvQZ+/SD20_8au	-29623.3371101	30127
cvQZ+/SD36_5au	-29623.7102434	30333
cvQZ+/SD36_8au	-29623.8379481	30239

- SD36 model includes Fr($7s, 6p, 6s, 5d$) and Ag($5s, 4d, 4p$) shells
- Excitations out of Fr(s, p) shells diminish W_{SM}.
- Excitations out of other shells increase W_{SM}.

Search for Hadron-Source EDM: Francium-Silver (FrAg)

Comparison with other $^1\Sigma_0$ molecules

	Z (heavy)	EA (light) [eV]	W_{SM} [a.u.] (at respective R_e)
CsAg	55	1.304	3530[29]
FrLi	87	0.618	24414[29]
FrAg	87	1.304	30168 ± 2504[29]
TlF	81	3.401	39967 ± 3600[30]
			37192[31]
			40539[32]

- Cs $\longrightarrow$ Fr order of magnitude gain
- Li $\longrightarrow$ Ag substantial gain
- TlF benefits from huge EA(F)

[29] A. Marc, M. Hubert, T. F., *Phys. Rev. A* **108** (2023) *062815*

[30] M. Hubert, T.F., *Phys. Rev. A* **106** (2022) *022817*

[31] L. V. Skripnikov, N. S. Mosyagin, A. V. Titov, and V. V. Flambaum, *Phys. Chem. Chem. Phys.* **22** (2020) *18374*

[32] V. V. Flambaum, V. A. Dzuba, and H. B. Tran Tan, *Phys. Rev. A* **101** (2020) *042501*
A. N. Petrov, N. S. Mosyagin, T. A. Isaev, A. V. Titov, V. F. Ezhov, E. Eliav, and U. Kaldor, *Phys. Rev. Lett.* **88** (2002) *073001*

Search for Hadron-Source EDM: Francium-Silver (FrAg)

Atomic Basis Sets / Hartree-Fock Theory

Molecular TPT-Ne interaction Hamiltonian[33]

$$W_T(A) = \sqrt{2} G_F \langle \Sigma \rangle_A \left\langle \psi^{(0)} \left| \imath \sum_{j=1}^{n} (\gamma_3)_j \, \rho_A(\mathbf{r}_j) \right| \psi^{(0)} \right\rangle$$

as implemented into KRCI/DIRAC[34]

Basis/model	ε_{CI} [a.u.]	$W_T(\text{Fr})$ $[10^{-13} \langle \Sigma \rangle_A$ a.u.]
cvDZ/DCHF	-29622.8235344	4.109
cvTZ/DCHF	-29622.8356809	4.148
cvQZ/DCHF	-29622.8363746	4.150
cvQZ+/DCHF	-29622.8354238	4.151

[33] E. A. Hinds, C. E. Loving, and P. G. H. Sandars, *J. Phys. B, At. Mol. Phys.* **1** (1968) *499*

[34] T.F., *Phys. Rev. A* **109** (2024) *022807*

Search for Hadron-Source EDM: Francium-Silver (FrAg)

Correlation Effects

$$W_T(A) = \sqrt{2} G_F \langle\Sigma\rangle_A \left\langle \psi^{(0)} \left| \imath \sum_{j=1}^{n} (\gamma_3)_j \, \rho_A(\mathbf{r}_j) \right| \psi^{(0)} \right\rangle$$

Basis/model	ε_{CI} [a.u.]	$W_T(\text{Fr})$ $[10^{-13} \langle\Sigma\rangle_A$ a.u.]
cvQZ/DCHF	-29622.8363746	4.150
cvQZ/SD2_8a.u.	-29622.8615002	**4.013**
cvQZ/SD10_3a.u.	-29623.0079474	4.041
cvQZ/SD10_cc	-29623.0157765	4.013
cvQZ/SD10_8a.u.	-29623.0206732	4.015
cvQZ/SD10_11.5a.u.	-29623.0210675	4.013
cvQZ/SD8_SDT10_3a.u.	-29623.0100912	4.045
cvQZ/SD8_SDTQ10_3a.u.	-29623.0171368	**3.941**
cvQZ/SD8_SDT10_cc	-29623.0179520	4.021
cvQZ/SD12_8a.u.	-29623.1930035	4.050
cvQZ/SD20_8a.u.	-29623.3380747	4.007
cvQZ/SD36_8a.u.	-29623.8389564	4.018

Search for Hadron-Source EDM: Francium-Silver (FrAg)

Sensitivity Ratios [35]

$$\tilde{M} := \frac{W_{\mathsf{SM}}(A)}{W_T(A)} = \frac{-\frac{3}{B}\left\langle \sum_{j=1}^{n} \hat{z}_j\, \rho_A(\mathbf{r}_j)\right\rangle_\psi}{\sqrt{2} G_F \langle\Sigma\rangle_A \left\langle \psi^{(0)} \middle| \imath \sum_{j=1}^{n} (\gamma_3)_j\, \rho_A(\mathbf{r}_j) \middle| \psi^{(0)} \right\rangle}$$

System	W_{SM} [a.u.]	W_T $[10^{-13}\,\langle\Sigma\rangle_A$ a.u.]	$\tilde{M}$ $[10^{13}\,\langle\Sigma\rangle_A^{-1}$ a.u.]	I_A	M $[10^{13}$ a.u.]
^{223}FrAg	30168	3.93	7676	3/2	5117
^{133}CsAg	3529.6	0.374	9437	7/2	2697
^{205}TlF	40539 [36]	6.25 [37]	6486	1/2	12972

[35] A. Marc, T. F., *Eur. J. Phys. D* **79** *(2025) 19*

[36] O. Grasdijk *et al.*, *Quantum Sci. Technol.* **6** *(2021) 044007*

[37] T. F., *Phys. Rev. A* **109** *(2024) 022807*

Schiff-Moment, TPT-Ne Interactions and Method Development

Mickaël Hubert, Lecturer

Schiff-moment interaction implementation

Basis sets

Aurélien Marc

Schiff-moment interaction calculations in molecules

TPT-Ne interaction calculations in molecules

DCG-GASCI

Thanks for your attention !

EDM Science

- Electron EDM interactions (HfF^+, ThO, Hg, Tl, TaO^+, RaAg et al.)

  T. F., D. DeMille, *New J. Phys.* **23** (2021) *113039*

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  T. F., *Phys. Rev. A* **95** (2017) *022504*

  M. Denis, T. F., *J. Chem. Phys.* **145** (2016) *214307*

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  M. Hubert, T. F., *Phys. Rev. A* **106** (2022) *022817*

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  T. F., *Phys. Rev. A* **109** (2024) *022807*

  T. F., *Phys. Rev. A* **99** (2019) *012515*

- Nuclear MQM interactions (TaN, TaO^+, HfF^+, RaAg)

  T. F., M. K. Nayak, M. G. Kozlov, *Phys. Rev. A* **93** (2016) *012505*

Towards Ultracold DLT EDM Measurement[35]

Picking the cherry

Target atom:

Z(Ra) $= 88$ α_D(Ra) $= 246 \pm 4$ a.u.[36]

Polarizing partner:

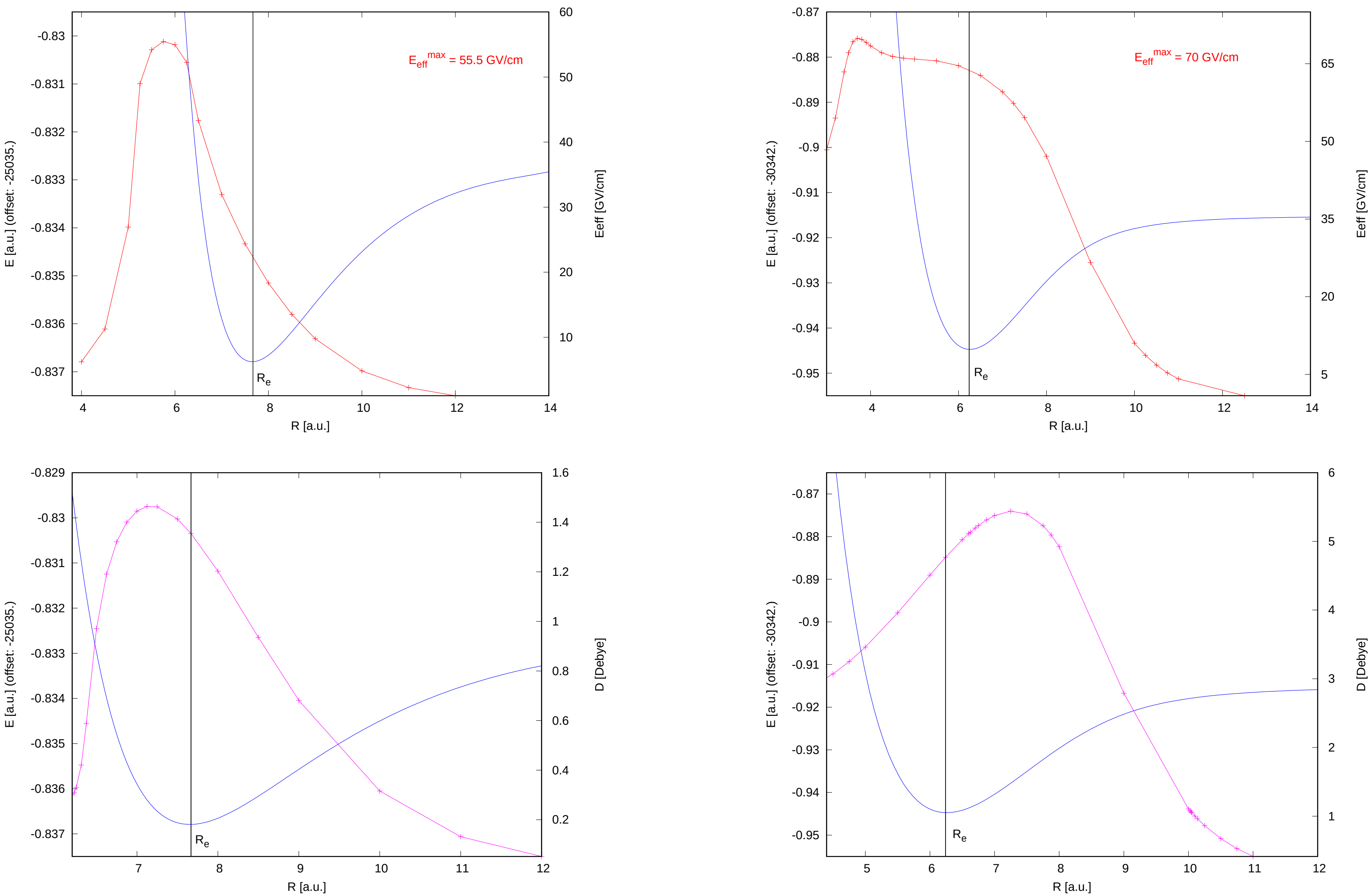
Alkali(-like) atoms: Li, Na, K, Rb, Cs, Fr; Cu, Ag, Au

	R_e [a.u.]	B_e [cm^{-1}]	D[Debye]	EA [eV]	E_{eff} $\left[\frac{\text{GV}}{\text{cm}}\right]$	W_S [kHz]	E_{pol} $\left[\frac{\text{kV}}{\text{cm}}\right]$
RaLi	7.668	0.151	1.36	0.618	22.2	-59.5	13.3
RaNa	8.703	0.038	0.51	0.548	12.0	-32.2	8.90
RaK	10.37	0.017	0.39	0.501	5.44	-14.6	5.18
RaRb	10.75	0.008	0.36	0.486	5.01	-13.6	2.75
RaCs	11.25	0.006	0.46	0.472	4.52	-12.6	1.48
RaFr	11.26	0.004	0.24	0.486	3.44	-12.4	2.06
RaCu	6.050	0.033	**4.30**	**1.236**	67.0	-180.6	0.92
RaAg	6.241	0.021	**4.76**	**1.304**	**63.9**	**-175.1**	0.53
RaAu	5.836	0.017	**5.71**	**2.309**	50.4	-166.4	0.36

[35] T. F., D. DeMille, *New J. Phys.* **23** (2021) *113039*

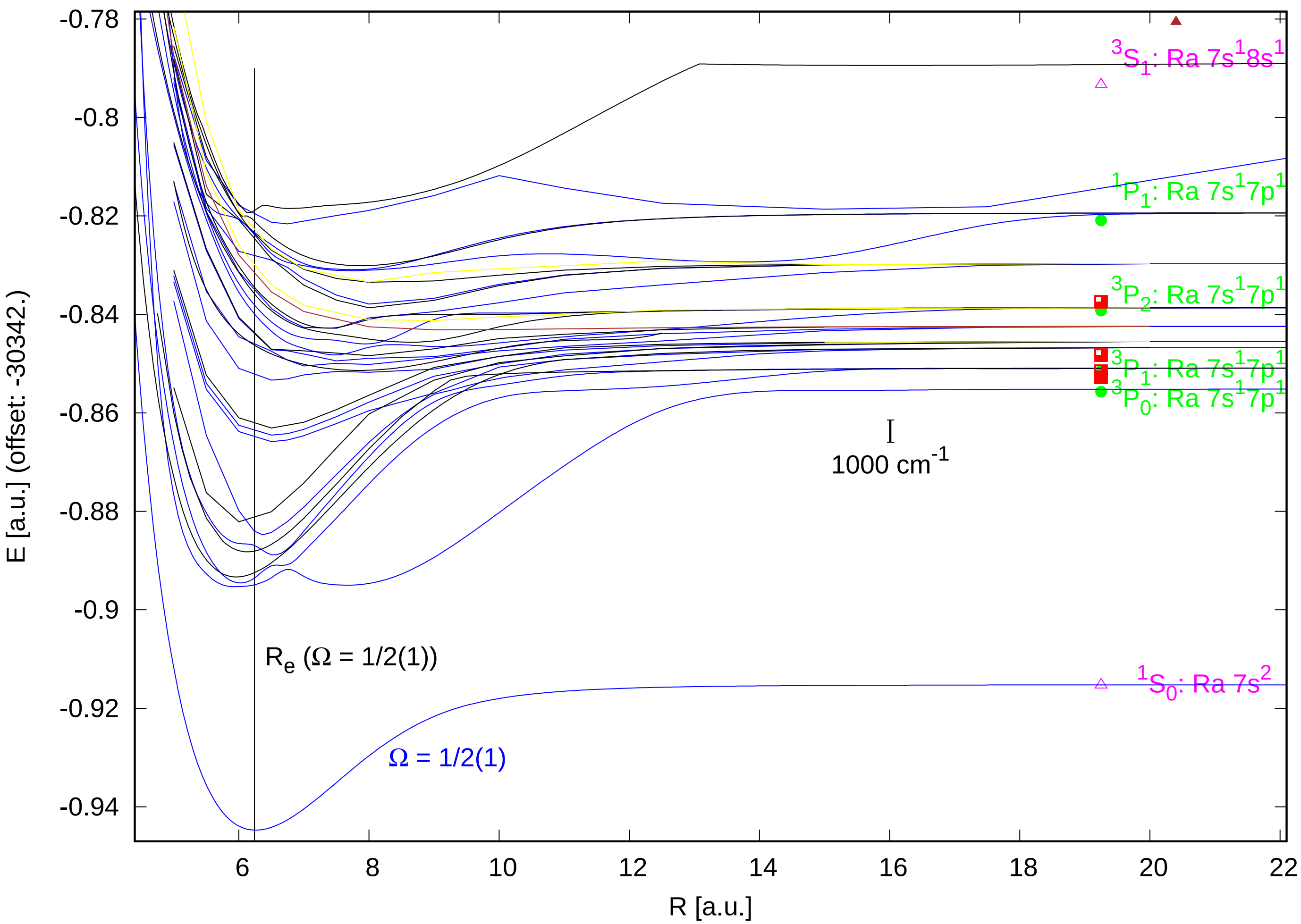
[36] P. Schwerdtfeger, J. K. Nagle, *Mol. Phys.* **117** (2019) *1200*

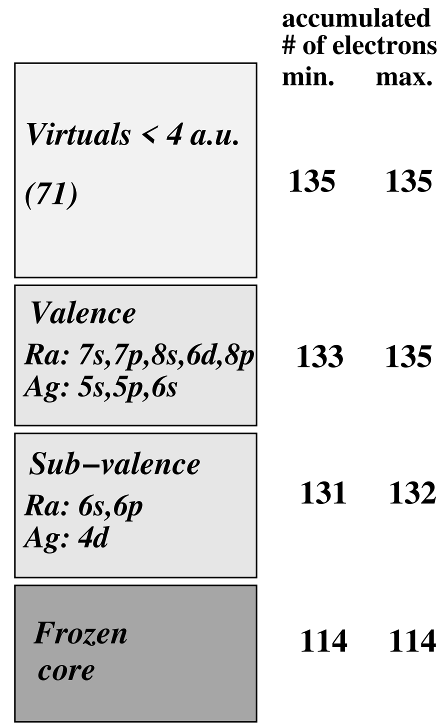
RaLi vs. RaAg[37]



[37] T. F., D. DeMille, *New J. Phys.* **23** (2021) *113039*

1) RaAg: Complete Spectrum up to $T \approx 5$ eV (TZ basis)





$D_e(1/2(1)) \approx 0.83$ eV

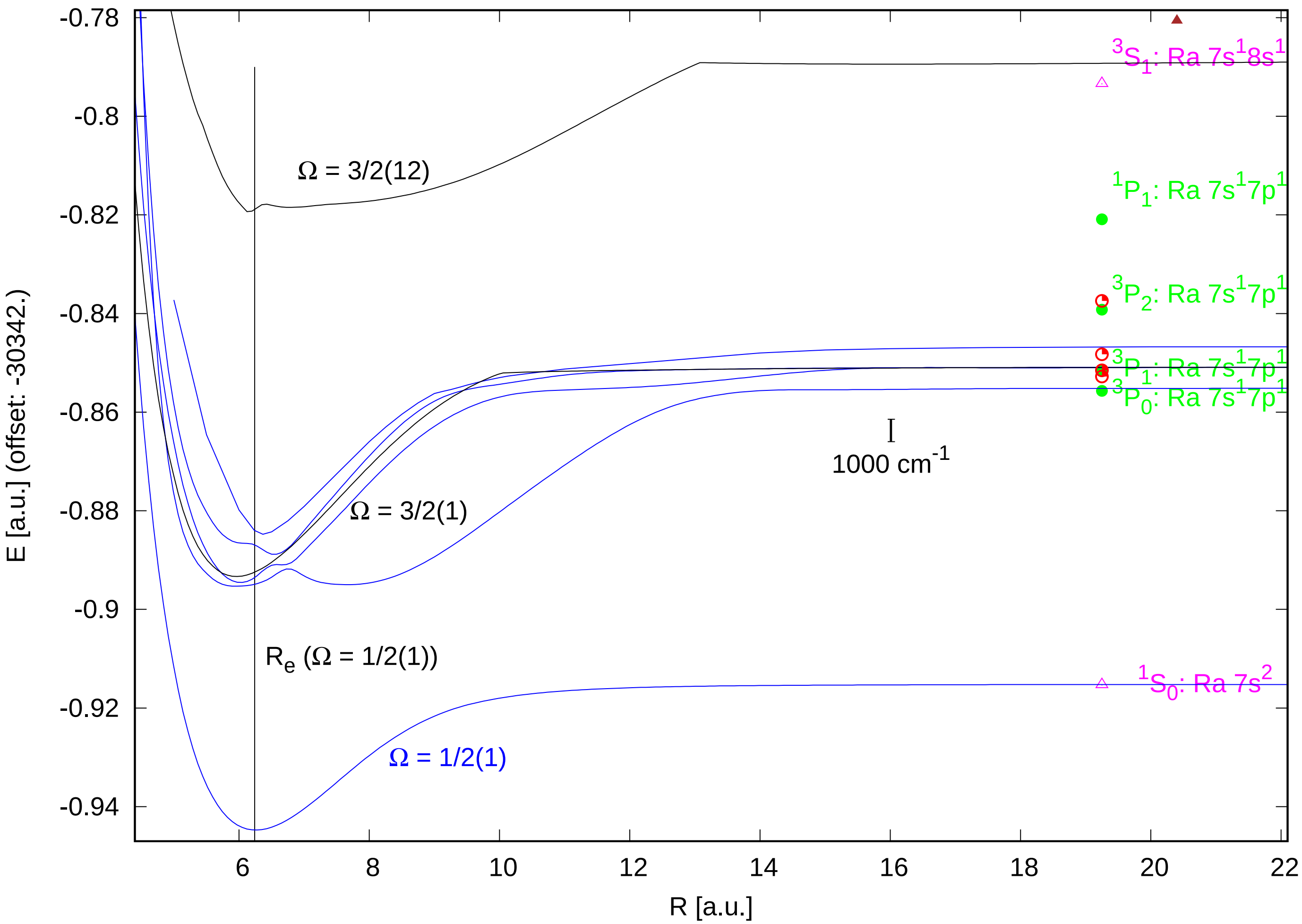
$D_e(\text{KRb}) \approx 0.52$ eV[26]

$D_e(\text{YbRb}) \approx 0.11$ eV[27]

[26] S. Kasahara, C. Fujiwara, N. Okada, H. Katô, M. Baba, *J. Chem. Phys.* **111** (1999) *8857*

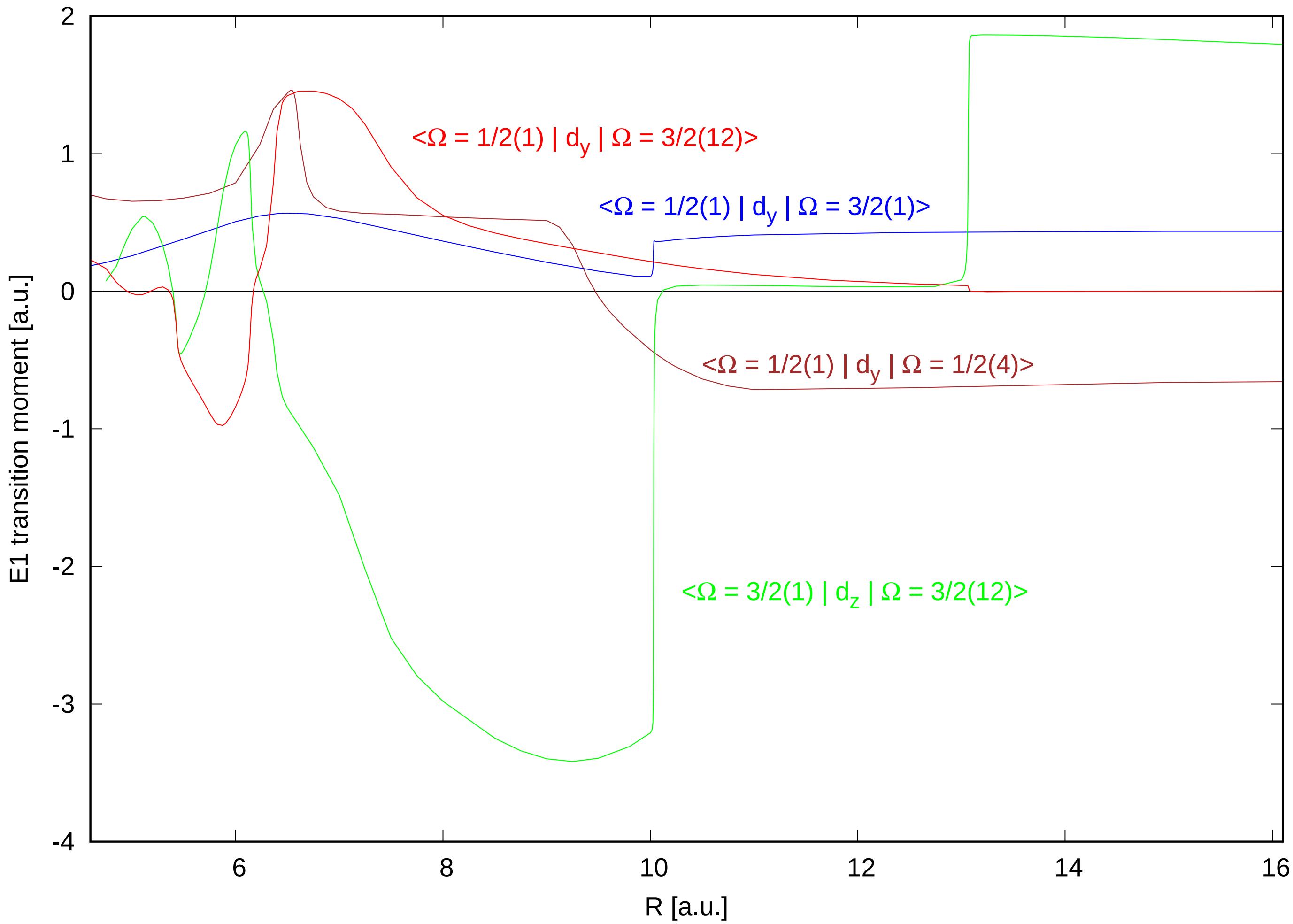
[27] L. K. Sørensen, S. Knecht, T. F., C. M. Marian, *J. Phys. Chem A* **113** (2009) *12607*

1) RaAg: Relevant States $T \approx 5$ eV (TZ basis)



	accumulated # of electrons min.	max.
Virtuals < 4 a.u. (71)	135	135
Valence Ra: 7s,7p,8s,6d,8p; Ag: 5s,5p,6s	133	135
Sub−valence Ra: 6s,6p; Ag: 4d	131	132
Frozen core	114	114

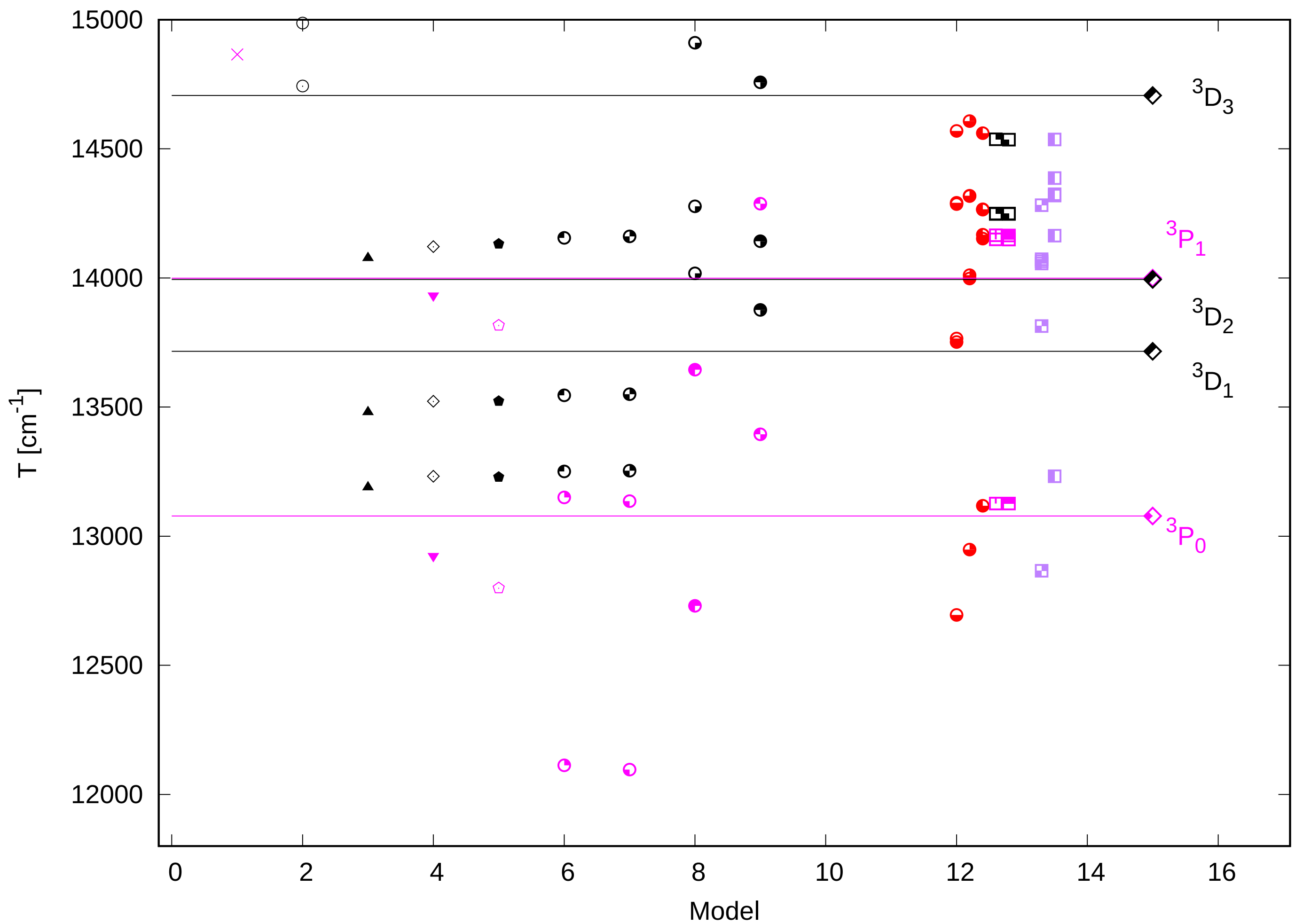
1) RaAg[40]: E1 TDM $d_{XY}(R) = \left\langle \Psi_X \middle| \sum_j q_j \, \hat{\mathbf{r}}_j \middle| \Psi_Y \right\rangle (R)$



Then: $d_{v,v'} = \int_R \psi_{vX}(R) \, d_{XY}(R) \, \psi_{v'Y}(R) dR$

[40] T. Fleig, O. Grasdijk, D. DeMille (2024)

2) RaAg: Limited Spectrum up to $T \approx 3$ eV (QZ basis)



	accumulated # of electrons min.	max.
Virtuals < 4 a.u. (141)	135	135
Ra: 7p,8s,6d,8p,9s Ag: 5p,6s	133	135
Ra: 7s Ag: 5s	132	135
Ra: 6s,6p	130	132
Ag: 4d	123	124
Frozen core	114	114

4: SD8_8s6d9s7d7p8pSDT_SD10

9: SD8_8s6d9s7d7p8pSDTQ_SD10

12: RaAg (SDT)

13: RaAg (SDTQ)