Periodic Trends of $\mathcal{P},\mathcal{T}$-violation in Linear Molecules

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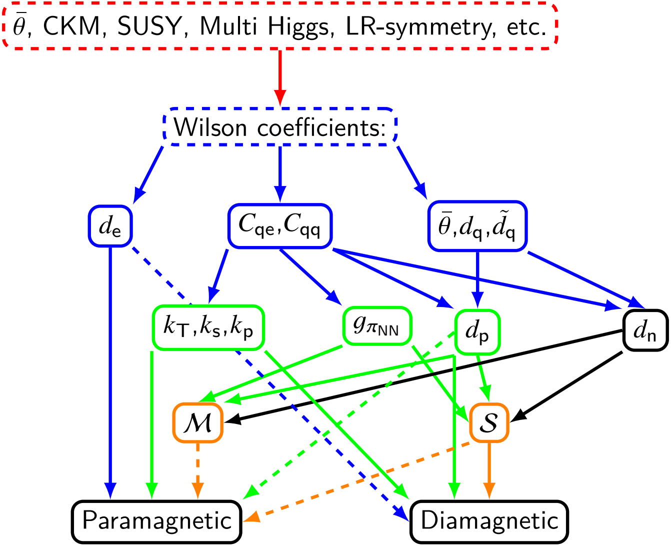
Sources of $\mathcal{P},\mathcal{T}$-Violation in Molecules



[1] M. Pospelov, A. Ritz, *Annals of Physics* **2005**, *318*, Special Issue, 119 –169, T. Chupp et al., *ArXiv e-prints* **2017**, *1710.02504*, [physics.atom–ph].

Effective $\mathcal{P},\mathcal{T}$-Odd Diatomic Hamiltonian

- Effective molecular electronic structure parameters W
- $\mathcal{P},\mathcal{T}$-odd parameters replaced by effective parameters (can depend on nuclear structure e.g. Schiff-moment $\mathcal{S}$)
- effective spin-rotational Hamiltonian

$$\begin{aligned}\hat{H}_{\mathrm{sr}_A} = \underbrace{\hat{D}\cdot\hat{\vec{S}}}_{\Omega}\left(W_{\mathrm{d}_A}d_{\mathrm{e}} + W_{\mathrm{s}_A}k_{\mathrm{s}}\right) + \underbrace{\hat{D}^T\cdot\hat{\mathbf{T}}_A\cdot\hat{\vec{S}}}_{\Theta_A}W_{\mathcal{M}_A}\tilde{\mathcal{M}}_A \\ + \underbrace{\hat{D}\cdot\hat{\vec{I}}_A}_{\mathcal{I}_A}\Big(W_{\mathrm{T}_A}k_{\mathrm{T}} + W_{\mathrm{p}_A}k_{\mathrm{p}} + W^{\mathrm{m}}_{\mathrm{s}_A}k_{\mathrm{s}} \\ + W_{\mathcal{S}_A}\mathcal{S}_A + (W_{\mathrm{m}_A} + W_{\mathcal{S}_A})d_{\mathrm{p}} + W^{\mathrm{m}}_{\mathrm{d}_A}d_{\mathrm{e}}\Big)\end{aligned}$$

[2] M. G. Kozlov, L. N. Labzowsky, *J. Phys. B* **1995**, *28*, 1933–1961.

Quasi-relativistic Calculation of Custom Properties

We want to . . .

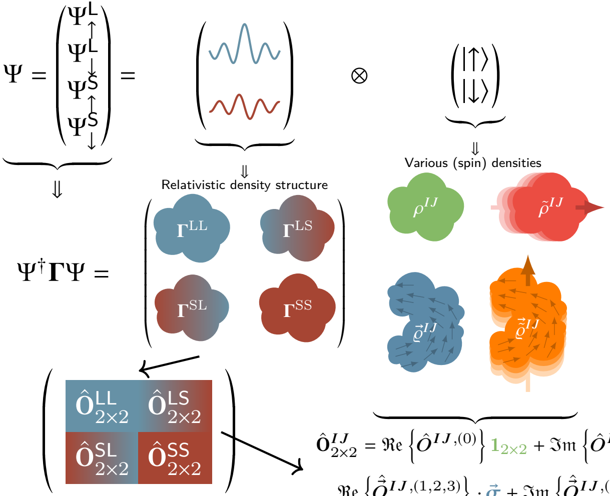
- determine general trends
- find models that help to design future experiments
- want to be able to study large number of molecules

$\Rightarrow$ We do not need to be very exact:

- Quasi-relativistic calculations with ZORA/HF and DFT
- Transformation of operators into ZORA-picture needed
- Needs implementation of a lot of non-standard operators

Quasi-relativistic Calculation of Custom Properties

Customized One-Electron Properties via Density Functions



$$\hat{\mathbf{O}}^{IJ}_{2\times2} = \Re\mathfrak{e}\left\{\hat{O}^{IJ,(0)}\right\}\mathbf{1}_{2\times2} + \Im\mathfrak{m}\left\{\hat{O}^{IJ,(0)}\right\}\iota\mathbf{1}_{2\times2} + \Re\mathfrak{e}\left\{\hat{\vec{O}}^{IJ,(1,2,3)}\right\}\cdot\vec{\sigma} + \Im\mathfrak{m}\left\{\hat{\vec{O}}^{IJ,(1,2,3)}\right\}\cdot\iota\vec{\sigma}$$

- Approximate wave function in zeroth order regular approximation (ZORA)

$$\Psi^{\mathrm{L}} \approx \Psi^{\mathrm{ZORA}}; \quad \Psi^{\mathrm{S}} \approx \frac{c}{2c^2 - \tilde{V}} \vec{\boldsymbol{\sigma}} \cdot \hat{\vec{p}} \Psi^{\mathrm{ZORA}} = c\omega \vec{\boldsymbol{\sigma}} \cdot \hat{\vec{p}} \Psi^{\mathrm{ZORA}}$$

- Evaluation of one-electron density functions in a set of basis functions $\{\chi\}$:

$$\boldsymbol{\Gamma}_i^{IJ}(\vec{r}, \vec{r}\,') = \sum_{\mu\nu}^{N_{\mathrm{basis}}} \left\langle \mathbf{C}_{i\mu\nu}(\boldsymbol{\Xi}), \boldsymbol{\mathcal{X}}_{\mu\nu}(\vec{r}, \vec{r}\,') \right\rangle, \ \boldsymbol{\Xi} = 1_{2\times 2}, \iota 1_{2\times 2}, \vec{\boldsymbol{\sigma}}, \iota\vec{\boldsymbol{\sigma}}$$

IJ / tensor	LL	LS	SL	SS
$\mathbf{C}_{i\mu\nu}$	$C_{i\mu}^{\dagger} \boldsymbol{\Xi} C_{i\nu}$	$C_{i\mu}^{\dagger} \boldsymbol{\Xi} \left(\iota \vec{\boldsymbol{\sigma}} C_{i\nu}\right)$	$\left(C_{i\mu}^{\dagger} \iota \vec{\boldsymbol{\sigma}}\right) \boldsymbol{\Xi} C_{i\nu}$	$\left(C_{i\mu}^{\dagger} \vec{\boldsymbol{\sigma}}\right) \boldsymbol{\Xi} \left(\vec{\boldsymbol{\sigma}} C_{i\nu}\right)$
$\boldsymbol{\mathcal{X}}_{\mu\nu}$	$\chi_\mu \chi_\nu'$	$-c\left(\chi_\mu \omega' \vec{\nabla}' \chi_\nu'\right)$	$c\left(\chi_\mu \vec{\nabla} \omega \chi_\nu'\right)$	$c^2\left(\chi_\mu \vec{\nabla} \omega \omega' \vec{\nabla}' \chi_\nu'\right)$

- All *16* $\mathbf{C}_{i\mu\nu}$ can be reduced to , , , .

- An one-electron operator can be defined by a generic tensor function:

$$\mathbf{\Omega}^{IJ}(\vec{r}) = \hat{s}\hat{\vec{v}} \circ \hat{\partial}(\vec{r}' \vee \vec{r})\mathbf{\Gamma}^{IJ}(\vec{r}, \vec{r}')\Big|_{\vec{r}'=\vec{r}}, \tag{1}$$

with $\vec{r}' \vee \vec{r}$ meaning $\vec{r}$ or $\vec{r}'$

- Evaluation of expectation values on a grid:

$$\left\langle \hat{\mathbf{O}}^{IJ}_{2\times 2} \right\rangle = \Re\mathrm{e} \left\{ \int \mathrm{d}\vec{r} \;\; \mathbf{\Omega}^{IJ}(\vec{r}) \right\} \tag{2}$$

- The following building blocks define the operator:
  - Non-differential **scalar operator** $\hat{s}$,
  - **vector operator** $\vec{v} = \tilde{\vec{r}}_A \vee 1, \; \tilde{\vec{r}}_A = (\vec{r} - \vec{r}_A)$ contracted with the (derivative) density tensor as $\circ = \otimes \vee \cdot \vee \times$
  - **differential operator** $\hat{\partial}(\vec{r}) = \vec{\nabla}\otimes, \vec{\nabla}\cdot, \vec{\nabla}\times, \vec{\nabla}\cdot\vec{\nabla}\otimes, \vec{\nabla}\otimes\vec{\nabla}\cdot, \vec{\nabla}\otimes\vec{\nabla}\times, \vec{\nabla}\times\vec{\nabla}\times$; $\hat{\partial}(\vec{r}')$ analogue

Diamagnetic Molecules

- Electronic structure enhancement of nuclear Schiff moment:

$$W_{\mathcal{S}_A} = \frac{\left\langle \Psi_{\mathrm{e}} \middle| \mathcal{S} \hat{\vec{I}}_A \cdot \vec{\mathcal{E}}_A(\vec{r}) \Theta(\vec{r}_{\mathrm{nuc}} - \vec{r}) \middle| \Psi_{\mathrm{e}} \right\rangle}{\mathcal{I}_A \mathcal{S} r_{\mathrm{nuc}}^2} = \frac{\Re\mathfrak{e}\left\{ \int \mathrm{d}\vec{r}\ \frac{\Theta(\vec{r}_{\mathrm{nuc}} - \vec{r})(z - z_A)}{|\vec{r}_A|^3} \left(\rho^{\mathrm{LL}}(\vec{r}) + \rho^{\mathrm{SS}}(\vec{r}) \right) \right\}}{r_{\mathrm{nuc}}^2} \tag{3}$$

- Electronic structure enhancement of the proton electric dipole moment:

$$W_{\mathrm{m}_A} = \frac{\left\langle \Psi_{\mathrm{e}} \middle| 2 \left(\frac{1}{2 M_A c} + \frac{\mu_A}{2 Z_A c} \right) d_{\mathrm{p}} \frac{1}{|\vec{r}_A|^3} \hat{\vec{I}}_A \cdot \vec{\alpha} \times \vec{\ell}_A \middle| \Psi_{\mathrm{e}} \right\rangle}{\mathcal{I}_A d_{\mathrm{p}}}$$

$$= 2 \left(\frac{1}{2 M_A c} + \frac{\mu_A}{2 Z_A c} \right) \Re\mathfrak{e} \left\{ \int \mathrm{d}\vec{r}\ \frac{1}{|\vec{r}_A|^3} \left[\left(\vec{r}_A \times \vec{\nabla} \right) \times \left(\vec{\varrho}^{\mathrm{LS}}(\vec{r}', \vec{r}) + \vec{\varrho}^{\mathrm{SL}}(\vec{r}', \vec{r}) \right) \right]_{\vec{r}' = \vec{r}} \right\} \tag{4}$$

- Tensor-Pseudotensor nucleon-electron current interaction:

$$W_{\mathrm{T}_A} = \frac{\left\langle \Psi_{\mathrm{e}} \middle| \frac{G_{\mathrm{F}}}{\sqrt{2}} k_{\mathrm{T}} \mathrm{i} \hat{\vec{I}}_A \cdot \vec{\gamma} \rho_{\mathrm{nuc},A} \middle| \Psi_{\mathrm{e}} \right\rangle}{\mathcal{I}_A k_{\mathrm{T}}} = \sqrt{2} G_{\mathrm{F}} \Re\mathfrak{e} \left\{ \int \mathrm{d}\vec{r}\ \rho_{\mathrm{nuc}}(\vec{r}) \left(\vec{\varrho}^{\mathrm{LS}}(\vec{r}) - \vec{\varrho}^{\mathrm{SL}}(\vec{r}) \right) \right\} \tag{5}$$

[3] I. B. Khriplovich, S. K. Lamoreaux, *CP Violation without Strangeness*, Springer, Berlin, **1997**, E. A. Hinds, P. G. H. Sandars, *Phys. Rev. A* **1980**, *21*, 471–479.

Method	$W_{\mathrm{T}}/h\mathrm{Hz}$	$W_{\mathrm{m}}/\frac{h10^{18}\ \mathrm{Hz}}{e\cdot\mathrm{cm}}$	$W_{\mathcal{S}}/a_0^4$
GHF-ZORA	4681	-2.36	8701
GKS-ZORA/B3LYP	3433	-1.56	6203
DHF[4]	4632	-2.39	8747
GRECP/RCC-SD[5]	-	-2.02	7635
DF[6]	-	-2.73	7738

[4] H. M. Quiney et al., *Phys. Rev. A* **1998**, *57*, 920–944.

[5] A. N. Petrov et al., *Phys. Rev. Lett.* **2002**, *88*, 073001.

[6] F. A. Parpia, *Journal of Physics B: Atomic Molecular and Optical Physics* **1997**, *30*, 3983.

Diamagnetic Molecules

How good is ZORA for TlF

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- Excellent agreement between ZORA and DHF

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- Excellent agreement between ZORA and DHF
- Correlation effects a bit overestimated with DFT/B3LYP

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Paramagnetic Molecules

- Scalar-Pseudoscalar nucleon-electron current interaction:

$$W_{\mathrm{s}_A} = \frac{\left\langle \Psi_{\mathrm{e}} \left| \frac{G_{\mathrm{F}}}{\sqrt{2}} k_{\mathrm{s}} \mathrm{i}\boldsymbol{\gamma}^0\boldsymbol{\gamma}^5 \rho_{\mathrm{nuc},A} \right| \Psi_{\mathrm{e}} \right\rangle}{\Omega k_{\mathrm{s}}} = \frac{G_{\mathrm{F}} \Re\mathrm{e} \left\{ \int \mathrm{d}\vec{r}\ \rho_{\mathrm{nuc}}(\vec{r}) \left(\tilde{\rho}^{\mathrm{LS}}(\vec{r}) - \tilde{\rho}^{\mathrm{SL}}(\vec{r}) \right) \right\}}{\sqrt{2}\Omega} \tag{6}$$

- Electronic structure enhancement of the eEDM:

$$W_{\mathrm{d}} = \frac{\left\langle \Psi_{\mathrm{e}} \left| \frac{2c\,d_{\mathrm{e}}}{e\hbar} \mathrm{i}\boldsymbol{\gamma}^0\boldsymbol{\gamma}^5 \hat{\vec{p}}^2 \right| \Psi_{\mathrm{e}} \right\rangle}{\Omega d_{\mathrm{e}}} = \frac{-2c \Re\mathrm{e} \left\{ \int \mathrm{d}\vec{r}\ \left(\vec{\nabla}^2 \tilde{\rho}^{\mathrm{LS}}(\vec{r}', \vec{r}) - \vec{\nabla}^2 \tilde{\rho}^{\mathrm{SL}}(\vec{r}', \vec{r}) \right)_{\vec{r}'=\vec{r}} \right\}}{e\Omega} \tag{7}$$

- Electronic structure enhancement of the NMQM:

$$W_{\mathcal{M}_A} = \frac{\left\langle \Psi_{\mathrm{e}} \left| -\tilde{\mathcal{M}} \frac{3}{2|\vec{r}_A|^5} \left(\vec{r}_A^T \cdot \hat{\mathbf{T}}_A \cdot (\vec{\boldsymbol{\alpha}} \times \vec{r}_A) + (\vec{\boldsymbol{\alpha}} \times \vec{r}_A)^T \cdot \hat{\mathbf{T}}_A \cdot \vec{r}_A \right) \right| \Psi_{\mathrm{e}} \right\rangle}{\Theta_A \tilde{\mathcal{M}}}$$

$$= \frac{3 \Re\mathrm{e} \left\{ \int \mathrm{d}\vec{r}\ \frac{z - z_A}{|\vec{r}_A|^5} \left[\vec{r}_A \times \left(\vec{\varrho}^{\mathrm{LS}}(\vec{r}) + \vec{\varrho}^{\mathrm{SL}}(\vec{r}) \right) \right]_z \right\}}{\Omega} \tag{8}$$

[7] I. B. Khriplovich, S. K. Lamoreaux, *CP Violation without Strangeness*, Springer, Berlin, **1997**, A. Mårtensson-Pendrill, P Öster, *Phys. Scr.* **1987**, *36*, 444–452.

Paramagnetic Molecules

^{223}RaF as probe for the full parameter space

- ^{223}Ra has nuclear spin $^3/_2$ and thus could have NMQM

Method	$W_\mathrm{T}/h\mathrm{Hz}$	$W_\mathrm{m}/\frac{h10^{18}\ \mathrm{Hz}}{e\cdot\mathrm{cm}}$	$W_\mathcal{S}/a_0^4$
GHF-ZORA	-1812	-1.01	-4119
GKS-ZORA/B3LYP	-1661	-0.88	-3736
GRECP/FSCC[8]	-	-	-4260

Method	$W_\mathrm{s}/h\mathrm{kHz}$	$W_\mathrm{d}/\frac{h10^{24}\ \mathrm{Hz}}{e\cdot\mathrm{cm}}$	$W_\mathcal{M}/\frac{h10^{33}\ \mathrm{Hz}}{e\cdot\mathrm{cm}^2}$
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[8] A. D. Kudashov et al., *Phys. Rev. A* **2014**, *90*, 052513.
[9] S. Sasmal et al., *Phys. Rev. A* **2016**, *93*, 062506.
[10] V. V. Flambaum et al., *Phys. Rev. Lett.* **2014**, *113*, 103003.

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- Diamagnetic $\mathcal{P},\mathcal{T}$-odd effects enhanced half as strong as in TlF

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- Diamagnetic $\mathcal{P},\mathcal{T}$-odd effects enhanced half as strong as in TlF
- Electronic NMQM effect larger than predicted for YbF or ThO[10]

[8] A. D. Kudashov et al., *Phys. Rev. A* **2014**, *90*, 052513.

[9] S. Sasmal et al., *Phys. Rev. A* **2016**, *93*, 062506.

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Periodic Trends in Paramagnetic Molecules

Periodic Trends in Paramagnetic Molecules

Coverage region in d_e-k_s parameter space

$$h\begin{pmatrix}\nu_1\\ \nu_2\end{pmatrix} = \Omega\underbrace{\begin{pmatrix}W_{\mathrm{d},1} & W_{\mathrm{s},1}\\ W_{\mathrm{d},2} & W_{\mathrm{s},2}\end{pmatrix}}_{\mathbf{C}}\begin{pmatrix}d_\mathrm{e}\\ k_\mathrm{s}\end{pmatrix} \tag{9}$$

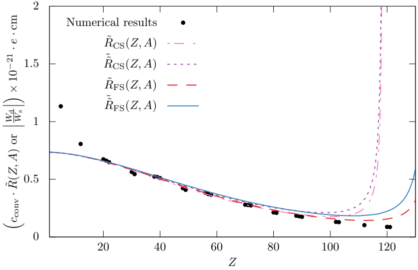
$$\begin{aligned} f_\mathrm{e}(x_\mathrm{d}, x_\mathrm{s}) = {} & \left(\frac{W_{\mathrm{d},1}^2}{u^2(\nu_1)} + \frac{W_{\mathrm{d},2}^2}{u^2(\nu_2)}\right)x_\mathrm{d}^2 + 2\left(\frac{W_{\mathrm{d},1}^2}{u^2(\nu_1)}\frac{W_{\mathrm{s},1}}{W_{\mathrm{d},1}} + \frac{W_{\mathrm{d},2}^2}{u^2(\nu_2)}\frac{W_{\mathrm{s},2}}{W_{\mathrm{d},2}}\right)x_\mathrm{d}x_\mathrm{s} \\ & + \left(\frac{W_{\mathrm{d},1}^2}{u^2(\nu_1)}\left(\frac{W_{\mathrm{s},1}}{W_{\mathrm{d},1}}\right)^2 + \frac{W_{\mathrm{d},2}^2}{u^2(\nu_2)}\left(\frac{W_{\mathrm{s},2}}{W_{\mathrm{d},2}}\right)^2\right)x_\mathrm{s}^2 \end{aligned} \tag{10}$$

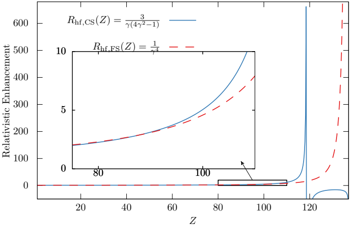
$$A_\mathrm{ellipse} = \frac{2h^2k_p^2\pi}{\sqrt{\frac{\partial^2 f_\mathrm{e}(x_\mathrm{d},x_\mathrm{s})}{\partial x_\mathrm{s}^2}\frac{\partial^2 f_\mathrm{e}(x_\mathrm{d},x_\mathrm{s})}{\partial x_\mathrm{d}^2} - \left(\frac{\partial^2 f_\mathrm{e}(x_\mathrm{d},x_\mathrm{s})}{\partial x_\mathrm{d}\partial x_\mathrm{s}}\right)^2}} = \boxed{\frac{h^2k_p^2\pi|u(\nu_1)u(\nu_2)|}{\left|W_{\mathrm{d},1}W_{\mathrm{d},2}\right|\left|\frac{W_{\mathrm{s},1}}{W_{\mathrm{d},1}} - \frac{W_{\mathrm{s},2}}{W_{\mathrm{d},2}}\right|}} \tag{11}$$

[11] K. Gaul et al., *ArXiv e-prints* **2018**, *1805.05494*, [physics.chem–ph].

Periodic Trends in Paramagnetic Molecules

Model for $\mathcal{P}, \mathcal{T}$-odd ratio





$$\tilde{R}_{\mathrm{CS}}(Z, A) = \frac{6}{\gamma\left(4\gamma^2 - 1\right)(\gamma + 1) \cdot f(Z) R(Z, A)}$$

$$\tilde{\tilde{R}}_{\mathrm{CS}}(Z, A) = \frac{3}{\gamma^2\left(4\gamma^2 - 1\right) \cdot R(Z, A)}$$

$$\tilde{R}_{\mathrm{FS}}(Z, A) = \frac{2}{\gamma^4(\gamma + 1) \cdot R(Z, A) f(Z)}$$

$$\tilde{\tilde{R}}_{\mathrm{FS}}(Z, A) = \frac{1}{\gamma^5 \cdot R(Z, A)}$$

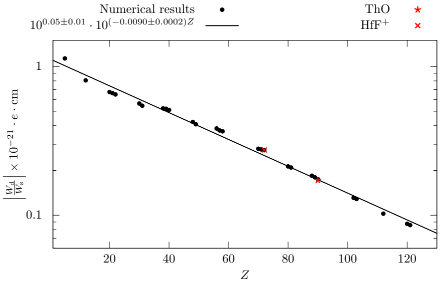
$$\gamma = \sqrt{\left(j + \frac{1}{2}\right)^2 - (\alpha Z)^2}$$

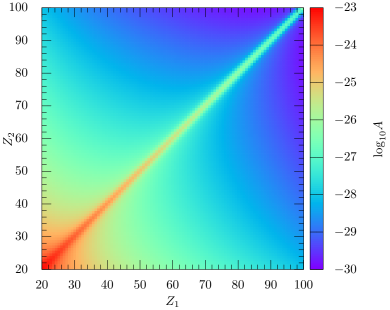
$$R(Z, A) = \frac{4}{\Gamma^2(2\gamma + 1)}\left(2 Z r_{\mathrm{nuc}}/a_0\right)^{2\gamma - 2}$$

$$f(Z) = \frac{1 - 0.56\alpha^2 Z^2}{\left(1 - 0.283\alpha^2 Z^2\right)^2}$$

[11] K. Gaul et al., *ArXiv e-prints* **2018**, *1805.05494*, [physics.chem–ph].
[12] V. A. Dzuba et al., *Phys. Rev. A* **2011**, *84*, 052108.

$$\log_{10}\left\{\left|\frac{W_\mathrm{d}}{W_\mathrm{s}}\right| \times 10^{-21}\ e\cdot\mathrm{cm}\right\} = q\cdot Z + p \tag{12}$$





$$A \sim \left(\left|W_{\mathrm{d},1}W_{\mathrm{d},2}\right| 0.89\cdot\left|1.0210^{Z_1} - 1.0210^{Z_2}\right| \times 10^{-21}\ e\cdot\mathrm{cm}\right)^{-1} \tag{13}$$

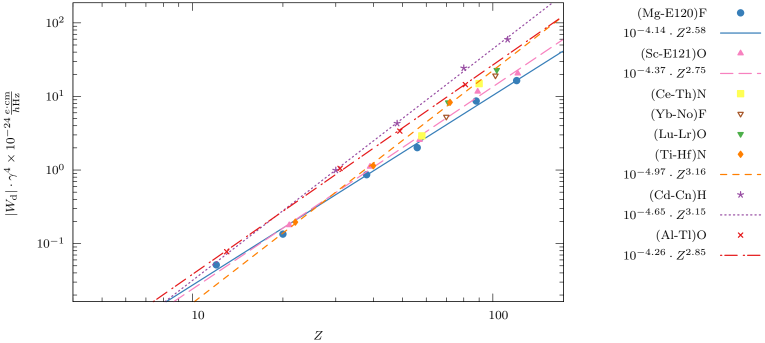
[11] K. Gaul et al., *ArXiv e-prints* **2018**, *1805.05494*, [physics.chem–ph].

[12] T. Fleig, *Phys. Rev. A* **2017**, *96*, 040502.

Periodic Trends in Paramagnetic Molecules

Chemical influence on scaling behavior

$$\log_{10}\left\{|W_\mathrm{d}|\gamma^4 \times 10^{-24}\,\frac{e\cdot\mathrm{cm}}{h\mathrm{Hz}}\right\} = b_{\mathrm{d,FS}} + \log_{10}\left\{Z^{a_{\mathrm{d,FS}}}\right\}$$



$$\frac{k_p^2\pi|u(\nu_1)u(\nu_2)|}{10^{b_{\mathrm{d},1}+b_{\mathrm{d},2}}\,\dfrac{Z_1^{a_{\mathrm{d},1}}Z_2^{a_{\mathrm{d},2}}}{\gamma^8}\;0.89\cdot\left|1.0210^{Z_1}-1.0210^{Z_2}\right|\times10^{27}\;\frac{\mathrm{Hz}^2}{e\cdot\mathrm{cm}}}$$

[11] K. Gaul et al., *ArXiv e-prints* **2018**, *1805.05494*, [physics.chem–ph].

Laser-Coolable Linear Polyatomic Molecules: MOH

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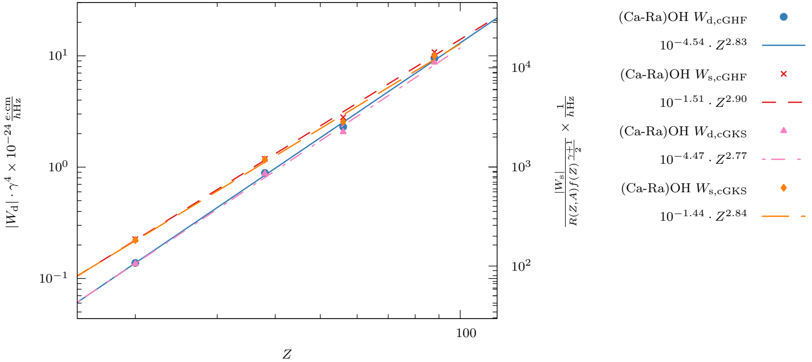
Enhancement of d_e and k_s



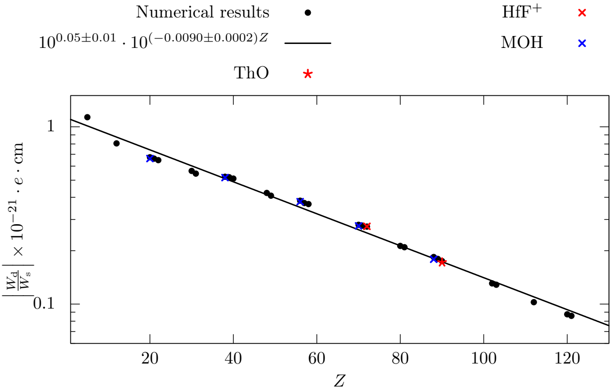
Molecule	$W_\mathrm{s}\,\frac{1}{h\cdot\mathrm{Hz}}$	$W_\mathrm{d}\,\frac{e\cdot\mathrm{cm}}{10^{24}\cdot h\cdot\mathrm{Hz}}$
CaOH	-2.18×10^{2}	-1.44×10^{-1}
SrOH	-2.00×10^{3}	-1.04
BaOH	-8.79×10^{3}	-3.32
RaOH	-1.53×10^{5}	-2.75×10^{1}
YbOH	-4.12×10^{4}	-1.14×10^{1}

- As expected very similar to MF
- Large enhancement factors: for RaOH and YbOH
- Promising candidates for search for eEDM due to experimental advantages

[12] T. A. Isaev, R. Berger, *Phys. Rev. Lett.* **2016**, *116*, 063006, I. Kozyryev, N. R. Hutzler, *Phys. Rev. Lett.* **2017**, *119*, 133002.
[13] K. Gaul, R. Berger, *ArXiv e-prints* **2018**, *arXiv:1811.05749*, [physics.chem–ph].

Laser-Coolable Linear Polyatomic Molecules: MOH

Complementarity with respect to diatomics



$\Rightarrow$ No **new** information on parameter space

$\longrightarrow$ Exploring more complex polyatomic molecules.

$\longrightarrow$ Exploiting diamagnetic systems (see[14])

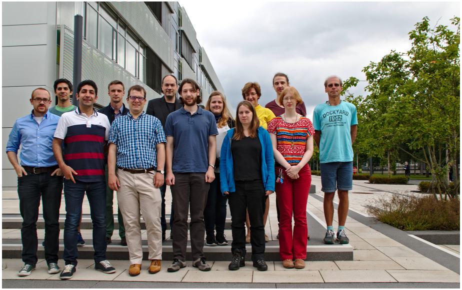
[14] T. Fleig, M. Jung, *Journal of High Energy Physics* **2018**, *2018*, 12.

Conclusion

- Method for quasi-relativistic calculation of arbitrary $\mathcal{P},\mathcal{T}$-odd operators
- ZORA performs well in calculation of "diamagnetic" properties
- Chemical enhanced $\mathcal{P},\mathcal{T}$-odd effects in diatomic radicals of group 4 and 12
- Simple equation for determination of coverage region in parameter space of d_e and k_s for paramagnetic molecules
- Similar information on d_e-k_s-parameter space from MOH as from MF
- MOH promising candidates for future experiments due to experimental advantages and large enhancement factors

- More complex polyatomic molecules
- Studying advantages of diamagnetic molecules
- Second order properties like enhancement of d_e and k_s in diamagnetic molecules

Acknowledgments



Thanks to the Organizers!

Thank You for Your Attention!