Study of electric dipole amplitudes for alkali-like atoms and implications for atomic parity violation

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- Fairhall, BMR, Ginges, Phys. Rev. A **107**, 022813 (2023).
- BMR, Fairhall, Ginges, Phys. Rev. A **107**, 052812 (2023).
- Hamilton *et al.*, Phys. Rev. Applied **19**, 054059 (2023).

AIP Congress, Melbourne, 3 December 2024

High-precision study of E1 transitions

High-precision calculations

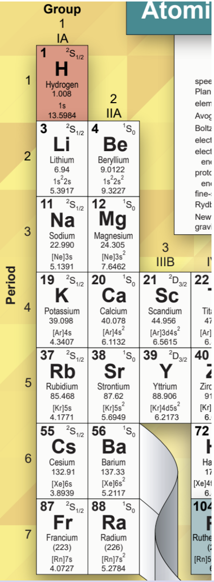
- E1 amplitudes for *s*, *p*, *d* transitions
- K, Ca^+, Rb, Sr^+, Cs, Ba^+, Fr, Ra^+ (and Li, Be^+, Na, Mg^+)
- 14 E1 transitions each – well over 100

High-precision calculations

- ∼50 high-precision experimental amplitudes
- Allows statistical analysis
- Test theory **and** test uncertainty method
- Important and often overlooked

Motivation

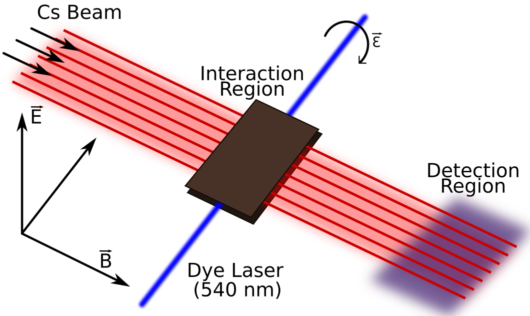
- Tests of atomic theory for atomic parity violation
- Development of atomic clocks



Motivation: PNC

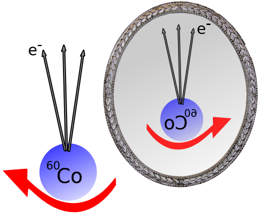
Atomic Parity Violation

- Weak (Z^0) perturbed E1 transition
- Test of electroweak theory
- Currently: theory-limited
- PNC – chasing $\sim$0.1% accuracy
- Need accurate calculations, AND:
- Crucial to confidently determine theoretical accuracy



Atomic Polarisabilities

- Atomic Clocks



All-orders calculations

Most others: Coupled cluster:

- Expand wavefunction to fixed (finite) order of excitations from reference
- Solve iteratively for expansion coefficients: all-orders (in Coulomb interaction)
- Highly accurate, computationally mostly, can be unstable (sensitive to basis, excitations)

Feynman technique:

- Dominating series of screening diagrams summed exactly to all-orders
- all-orders in screening + hole-particle (double, triple, quadupole etc. excitations)
- No basis required, instead integration over frequencies
- Highly accurate, highly computationally efficient

Prelim code available:

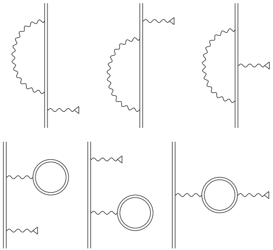
- AMPSCI: github.com/benroberts999/ampsci

• Dzuba, Flambaum, Silvestrov, Sushkov, Physics Letters A **131**, 461 (1988); Dzuba, Flambaum, Sushkov, Physics Letters A **140**, 493 (1989); Dzuba, Flambaum, Kraftmakher, Sushkov, Physics Letters A **142**, 373 (1989).

Surprising Result: Radiative QED Corrections

- **Radiative potential method**: Flambaum, Ginges, PRA**72**, 052115 (2005)

Several cases: QED *larger* than discrepancy between theory + experiment(!)

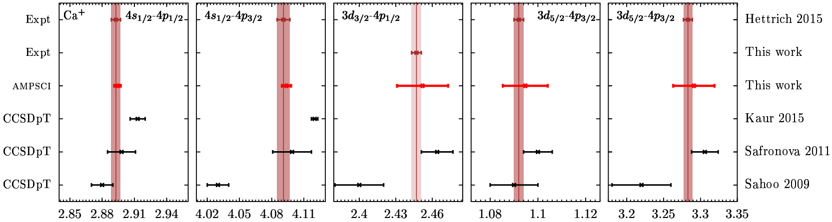


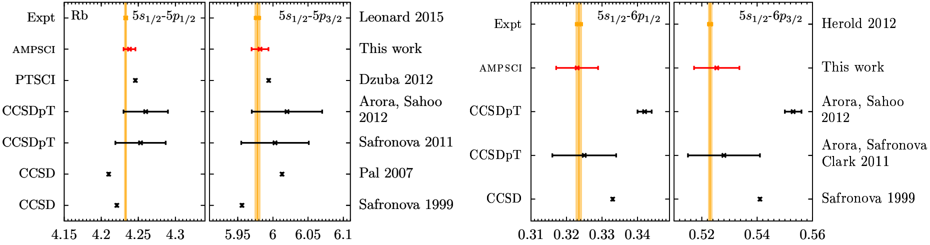
a	b	δ_{QED}	Theory	Expt.	Δ	$\Delta(\%)$
			Rb			
$5s_{1/2}$	$5p_{1/2}$	0.0019	4.2381	4.231(3)[1]	0.007	0.1
	$6p_{1/2}$	**-0.0012**	0.3232	0.3235(9)[2]	-0.0003	-0.1†
	$5p_{3/2}$	0.0027	5.9818	5.978(5)[1]	0.004	0.06†
	$6p_{3/2}$	-0.0015	0.5256	0.5230(8)[2]	0.0026	0.5
			Cs			
$6s_{1/2}$	$6p_{1/2}$	**0.0034**	4.5052	4.5057(16)[3]	-0.0005	-0.01†
	$7p_{1/2}$	**-0.0023**	0.2776	0.2781(4)[4]	-0.0005	-0.2
	$6p_{3/2}$	**0.0051**	6.3402	6.3398(22)[3]	0.0004	0.01†
	$7p_{3/2}$	**-0.0026**	0.5741	0.5742(6)[4]	-0.0001	-0.01†

- PhD student: Carter Fairhall – see poster

1. Volz, Schmoranzer, Phys. Scr. **T65**, 48 (1996). 2. Herold, Vaidya, Li, Rolston, Porto, Safronova Phys. Rev. Lett. **109**, 243003 (2012).
3. Toh, Damitz, Tanner, Johnson, Elliott Phys. Rev. Lett. **123**, 073002 (2019).
4. Damitz, Toh, Putney, Tanner, Elliott Phys. Rev. A **99**, 062510 (2019).

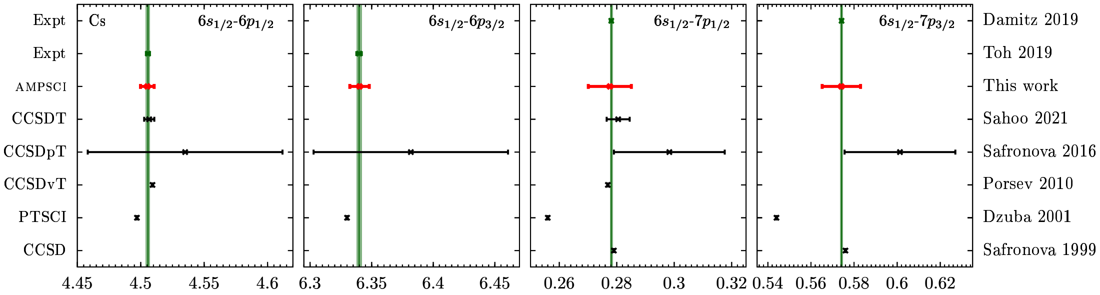
“Light” atoms: excellent agreement (no surprise)





Again, some theory strongly disagrees: highlights need to correct uncertainty analysis

Results: Cs

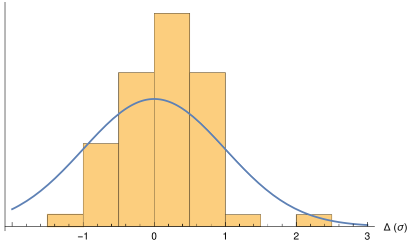


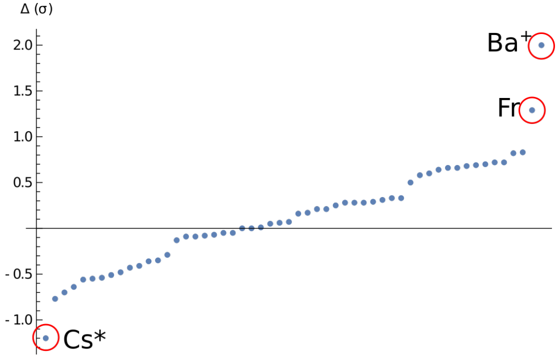
- Most precise experiment is for Cs:
- Excellent agreement between theory and experiment for 6*s*-*np*
- Even for extremely small (6s-7p), small due to cancellations

Results: Overview

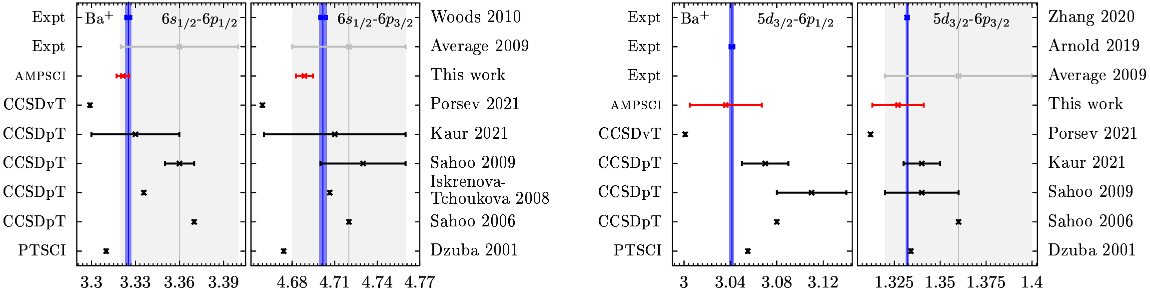
Compared with 46 high-precision experiment

- All but 2 (or 3) within 1σ
  - Combined theory+experiment errors
  - Dominated by theory (mostly)
- Better than statistically expected
  - Conservative uncertainties!
- $\approx$ Half within experimental uncertainties!
  - Require experimental improvements





Ba^+



- Largely agree, though large spread in theory – some disagree very significantly
  - Highlights importance of robust theory uncertainty estimate
- Largest disagreement: $6s$-$6p_{3/2}$ (2σ)
- While single 2σ in ~ 46 cases is expected, we think this may be experimental issue

Ba^+: Ratio

Also 2σ tension in ratio

$$\frac{|\langle 6s||d||6p_{3/2}\rangle|}{|\langle 6s||d||6p_{1/2}\rangle|} = \begin{cases} 1.4116(2) & \text{Theory} \\ 1.4140(12) & \text{Expt. [Woods \textit{et al}, PRA (2010)].} \end{cases} \tag{1}$$

c.f. Rb (for example) – Ba^+ difference is 100x larger!

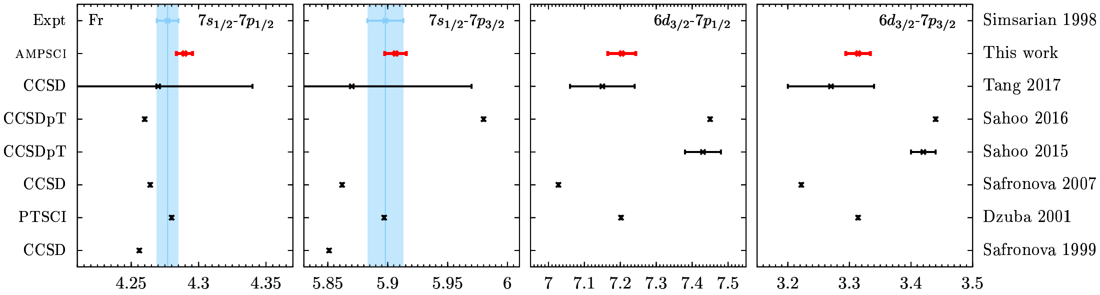
$$\frac{|\langle 5s||d||5p_{3/2}\rangle|}{|\langle 5s||d||5p_{1/2}\rangle|} = \begin{cases} 1.41141(9) & \text{Theory} \\ 1.41144(1) & \text{Expt. [Leonard \textit{et al}, PRA (2015)].} \end{cases} \tag{2}$$

Correlations cancel. Non-rel limit: $\sqrt{2} = 1.41421$

Other theory*:

- 1.4109(2) – Iskrenova-Tchoukova *et al.* (2008)
- *1.412 – Dzuba* et al. *(2001)*
- *1.40 – Sahoo* et al. *(2006)*
- *1.411 – Kaur* et al. *(2021),*
- *1.412 – Porsev* et al. *(2021)*

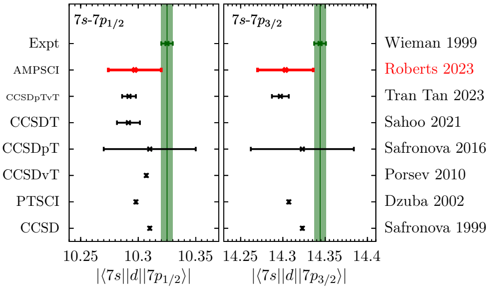
Fr



- Other discrepancy: Fr $7s$-$7p_{1/2}$ - 1.2σ – within expectations
- Large spread in theory values, limited experiment
- Based on comparison for other systems: expect ours to be most accurate

Important case: Cs $7s$–$7p$

- Extracted from $6s - 7s$ stark shift [1]
- 0.5% theory vs. Experiment
  - Leads directly to 0.5% shift in $E_{\rm PNC}$
  - Nearly 2x claimed $E_{\rm PNC}$ uncertainty from *single term*
- Problem for uncertainty 0.3% / goal of 0.1%!



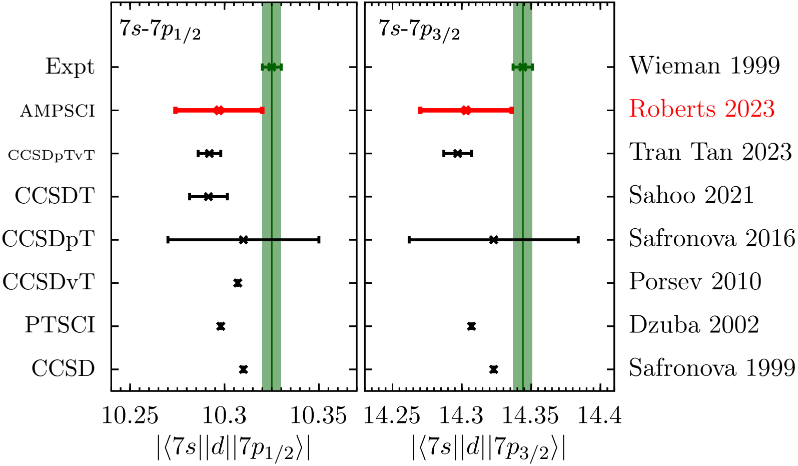
1. Bennett, J. L. Roberts, Wieman, PRA**59**, R16(R) (1999)
2. Toh, Damitz, Tanner, Johnson, Elliott PRL**123**, 073002 '19
3. Safronova, Johnson, Derevianko, PRA**60**, 4476 (1999)

$$E_{\rm PNC} = \frac{\langle 7s|d_z|6p_{1/2}\rangle\langle 6p_{1/2}|h_{\rm W}|6s\rangle}{E_{6s}-E_{6p_{1/2}}} + \frac{\langle 7s|h_{\rm W}|6p_{1/2}\rangle\langle 6p_{1/2}|d_z|6s\rangle}{E_{7s}-E_{6p_{1/2}}} + \frac{\langle 7s|d_z|7p_{1/2}\rangle\langle 7p_{1/2}|h_{\rm W}|6s\rangle}{E_{6s}-E_{7p_{1/2}}} + \ldots$$

$$\approx -1.91 + 1.49 + 1.35 + \mathcal{O}(10^{-1})$$

- **Any shift in this ME leads directly to shift in $E_{\rm PNC}$**

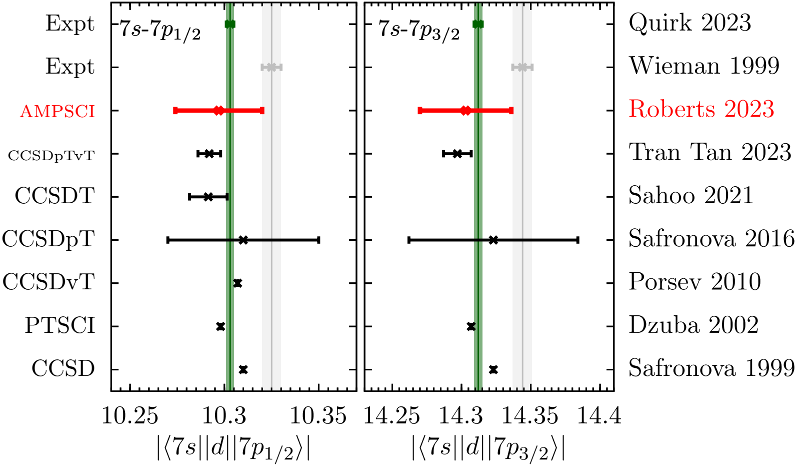
Important case: Cs $7s$–$7p$: New measurement



New measurement

- Elliot group, Purdue
- 5σ shift
- *After our calculations*

Important case: Cs $7s$–$7p$: New measurement



New measurement

- Elliot group, Purdue
- 5σ shift
- *After our calculations*

- Back in perfect agreement
- Other theory: still too small error bars?

- Quirk *et al.*, Phys. Rev. Lett. **132**, 233201 (2024)

Summary

High-precision calculations

- E1 amplitudes for *s*, *p*, *d* transitions
- K, Ca^+, Rb, Sr^+, Cs, Ba^+, Fr, Ra^+

Uncertainty

- Compare to 46 high-precision experimental amplitudes
- Better than expected agreement: conservative uncertainty
- Half lie *within experimental errors*
- Many at 0.1% level or better: demonstrate robust uncertainty method

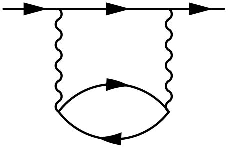
- Fairhall, BMR, Ginges, Phys. Rev. A **107**, 022813 (2023).
- BMR, Fairhall, Ginges, Phys. Rev. A **107**, 052812 (2023).
- Hamilton *et al.*, Phys. Rev. Applied **19**, 054059 (2023).

- AMPSCI: github.com/benroberts999/ampsci

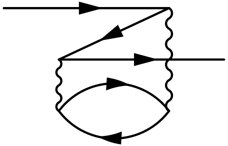
Extra

Outline of method

Goldstone:

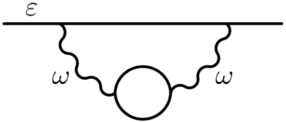


$$\sum_{amn} \frac{g_{vamn} g_{nmav}}{\varepsilon_v + \varepsilon_a - \varepsilon_m - \varepsilon_n}$$



$$\sum_{abn} \frac{g_{vnba} g_{banv}}{\varepsilon_v + \varepsilon_n - \varepsilon_a - \varepsilon_b}$$

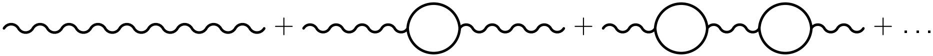
Feynman:



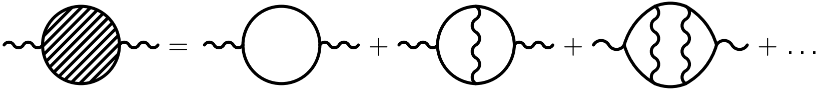
$$\int \frac{d\omega}{2\pi} G(\varepsilon + \omega) Q \Pi(\omega) Q$$

• Dzuba, Flambaum, Silvestrov, Sushkov, Physics Letters A **131**, 461 (1988); Dzuba, Flambaum, Sushkov, Physics Letters A **140**, 493 (1989); Dzuba, Flambaum, Kraftmakher, Sushkov, Physics Letters A **142**, 373 (1989).

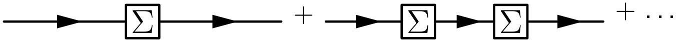
Screening + Hole-particle + chaining



$$Q^{\mathrm{scr.}}(\omega) = Q + Q(-i\Pi Q) + +Q(-i\Pi Q)^2 + \dots$$
$$= Q\left[1 + i\Pi(\omega)\right]^{-1}$$



$$V_0^a = y_{aa}^0(r) - \sum_{k=2}^{\mathrm{even}} \frac{|\langle a||C^k||a\rangle|^2}{(2j_a+1)^2} y_{aa}^k(r)$$



$$(H + \Sigma(\varepsilon) - \varepsilon)\,\phi = 0$$

Estimate higher-order diagrams + uncertainty

Re-scale Σ to match experimental energies:

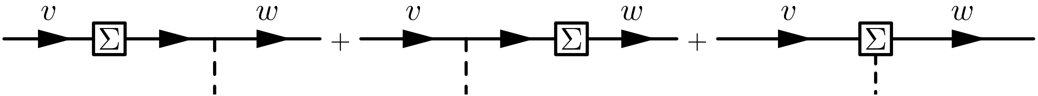
$$\Sigma \to \lambda\Sigma$$

- $\lambda \approx 1$
- Enter at $\sim 0.05\%$ level (for *s*-*p*)
- $\sim 0.5\%$ level (for *p*-*d*)
- Must account for QED, Breit (no double-counting)

Estimate uncertainty:

- Compare $\lambda\Sigma^{(2)}$, $\Sigma^{(\infty)}$, $\lambda\Sigma^{(\infty)}$
- $\sim$30% From Breit, QED, SR+Norm
- Uncertainty: always larger than $\delta\lambda$ semi-empirical correction

SR + Norm (non-Brueckner)



Structure Radiation:

- Non-separable Σ and h_{external}
- $< 1\%$

Normalisation:

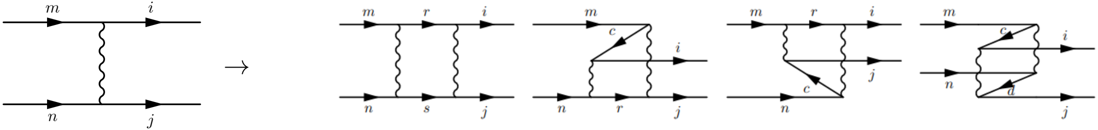
- Change in normalisation of many-body states

- Goldstone technique (direct diagram calculation)
- Only computationally intensive part (still $\sim$ minutes)
- Easily saturate basis

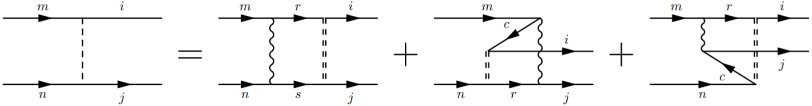
Johnson, Idrees, Sapirstein, PRA**35**, 3218 (1987); Dzuba, Flambaum, Silvestrov, Sushkov, J. Phys. B **20**, 1399 (1987)

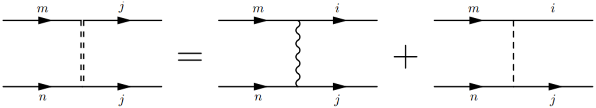
Missing: ladder diagrams

Lowest (third) order:



All orders:





Similar to: Dzuba, PRA **78**, 042502 (2008)

Ladder diagrams [preliminary]

Table: Ab initio calculations of ionization energies (cm^{-1}) for the lowest states of Cs.

Level	RHF	$\delta\Sigma^{(2)}$	$\delta\Sigma^{(\infty)}$	Breit	QED	Final	Expt.	$\Delta(\%)$
$6s_{1/2}$	27954	4458	-998	2.8	-21.5	31395	31406	-0.04%
$6p_{1/2}$	18791	1747	-294	-7.4	1.1	20236	20228	0.04%
$6p_{3/2}$	18389	1550	-258	-0.7	0.1	19680	19674	0.03%
$5d_{3/2}$	14138	3424	-458	25.8	5.6	17136	16907	1%
$5d_{5/2}$	14163	3240	-402	30.3	4.7	17035	16810	1%

Table: Ladder corrections to the lowest *d*-state energies of Cs, showing the lowest (third-order) $\delta L^{(3)}$ and subsequent all-order $\delta L^{(\infty)}$ corrections (including chaining). The column Σ is the all-orders correlation potential result including Breit and QED

Level	Expt.	Σ	$\Delta(\%)$	$\delta L^{(3)}$	$\delta L^{(\infty)}$	Total	$\Delta(\%)$
$5d_{3/2}$	16907	17136	1%	-173	-60	16903	-0.03%
$5d_{5/2}$	16810	17035	1%	-175	-64	16796	-0.08%

Similar to: Dzuba, PRA **78**, 042502 (2008)