Theoretical study of isotope shifts.

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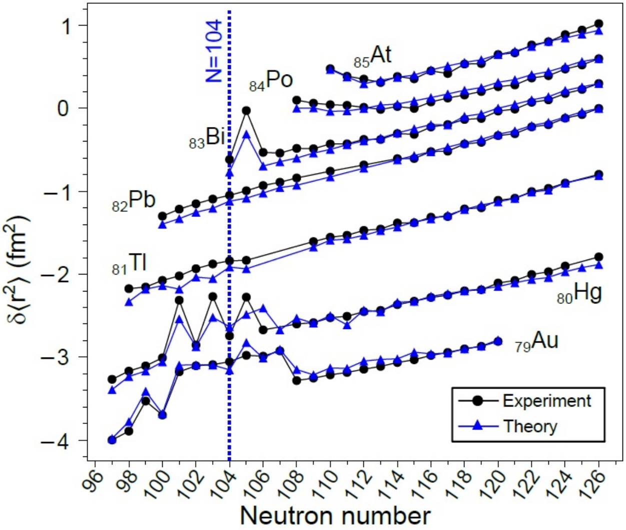
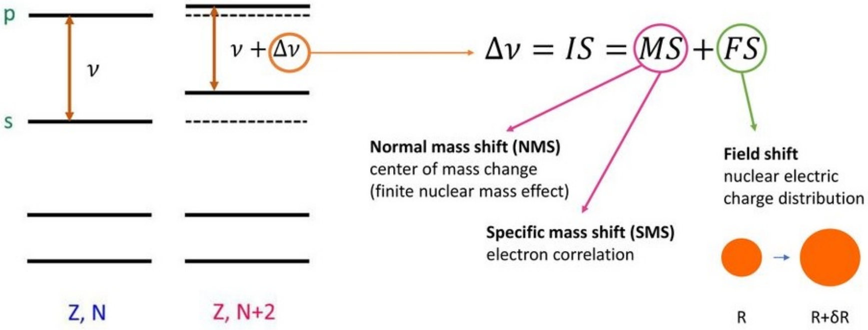
Comparison of experimental and calculated changes in mean-squared charge radii in the lead region



Isotope shift

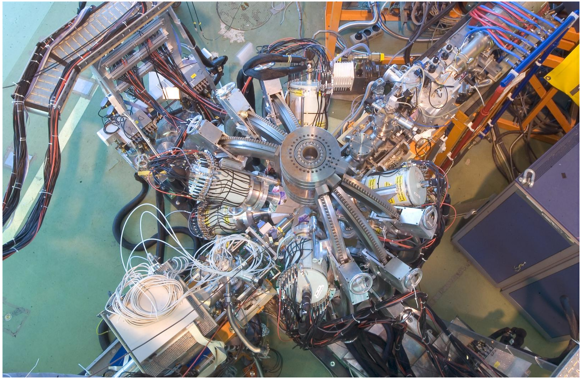


Slide from presentation of V. V. Flambaum, A. J. Geddes and A. V. Viatkina

Experimental facilities

IRIS (PNPI)

ISOLDE (CERN)



Isotope shift parametrization

$$\delta\nu^{M',M} = (k_{NMS} + k_{SMS})\left(\frac{1}{M'} - \frac{1}{M}\right) + F\delta\left\langle r^2\right\rangle.$$

$k_{NMS} = \nu_{exp}^{transition}/1822.888$ – normal mass shift

k_{SMS} – specific mass shift

$F = d\nu/d\left\langle r^2\right\rangle$ – field shift

Mass shift operator

$$H_{NMS} = \frac{1}{2M} \sum_i (\vec{p}_i^2 - \frac{\alpha Z}{r_i} \left[\vec{\alpha}_i + \frac{(\vec{\alpha}_i \cdot \vec{r}_i)\vec{r}_i}{r_i^2} \right] \cdot \vec{p}_i),$$

$$H_{SMS} = \frac{1}{2M} \sum_{i \neq k} (\vec{p}_i \cdot \vec{p}_k - \frac{\alpha Z}{r_i} \left[\vec{\alpha}_i + \frac{(\vec{\alpha}_i \cdot \vec{r}_i)\vec{r}_i}{r_i^2} \right] \cdot \vec{p}_k),$$

V. M. Shabaev, Theor. Math. Phys. 63, 588 (1985).
V. M. Shabaev, Sov. J. Nucl. Phys. 47, 69 (1988).
C. W. P. Palmer, J. Phys. B: At. Mol. Phys 20, 5987 (1987).

Isotope shift in Au

Calculated values of the normal, k_{NMS}, specific, k_{SMS}, total, k_{Total}, mass shift constants (in GHz·a.m.u.) and field shift constants F (in GHz/fm^2) for transition $6s_{1/2} - 6p_{1/2}$ of Au atom

	k_{NMS}	k_{SMS}	k_{Total}	F
79e-CCSD(T)	723	221	944	-41.9
19e-CCSDT - 19e-CCSD(T)	-125	-37	-161	+1.0
19e-CCSDT(Q) - 19e-CCSDT	-4	-31	-35	+0.5
Basis set correction	–	-28	-28	–
Gaunt	+5	-22	-17	+0.3
Total	600(40)	103(93)	703(101)	-40.1(11)

Paper accepted by Phys. Rev. Lett.!

Comparison with previous results

Field shift constants F (in GHz/fm^2) for transition $6s_{1/2} - 6p_{1/2}$ of Au

This work	-40.1(11)
SCDF [1]	-41.5
MCDF [1]	-39.6

Normal, k_{NMS}, specific, k_{SMS} and total, k_{Total}, mass shift constants (in GHz·a.m.u.) for transition $6s_{1/2} - 6p_{1/2}$ of Au

This work	600(40)	103(93)	703(101)
Exp	615	-	-
SE [2]	-	-	799(553)

[1] Rosén, A., Fricke, B., & Torbohm, G. (1984). Volume isotope shifts in low lying transitions of Au I. Zeitschrift für Physik A Atoms and Nuclei, 316(2), 157-16.
[2] Angeli, I., & Marinova, K. P. (2013). Table of experimental nuclear ground state charge radii: An update. Atomic Data and Nuclear Data Tables, 99(1), 69-95.

Isotope shift in Al

Calculated values of the normal, k_{NMS}, specific, k_{SMS}, total, k_{Total}, mass shift constants (in GHz·a.m.u.) and field shift constants F (in MHz/fm^2) for transition $3s^23p\ ^2P_{1/2} \rightarrow 3s^24s\ ^2S_{1/2}$ of Al atom

	k_{NMS}	k_{SMS}	k_{Total}	F
13e-CCSDT	-415.45	653.41	237.96	76.95
CCSDT(Q) - CCSDT	+0.01	−0.10	−0.08	−0.01
Basis set correction, +s, p, d	−0.35	+0.04	−0.31	+0.03
Basis set correction, +hm	−0.40	+0.48	+0.08	+0.02
Gaunt	+0.63	−0.88	−0.25	−0.10
Nuclear charge model	–	–	–	+0.04
Total	-415.55	652.94	237.39	76.92

Isotope shift in Al

Calculated values of the normal, k_{NMS}, specific, k_{SMS}, total, k_{Total}, mass shift constants (in GHz·a.m.u.) and field shift constants F (in MHz/fm^2) for transition $3s^2 3p\ ^2P_{3/2} \rightarrow 3s^2 4s\ ^2S_{1/2}$ of Al atom

	k_{NMS}	k_{SMS}	k_{Total}	F
13e-CCSDT	-414.38	654.47	240.10	76.85
CCSDT(Q) - CCSDT	−0.01	−0.57	−0.58	−0.01
Basis set correction, +s, p, d	−0.35	+0.04	−0.32	+0.02
Basis set correction, +hm	−0.41	+0.48	+0.07	+0.02
Gaunt	+0.02	−0.48	−0.46	−0.08
Nuclear charge model	–	–	–	+0.04
Total	-415.13	653.94	238.81	76.83

Calculated values of mass shift constants (in GHz·a.m.u.) and field shift constants F (in MHz/fm^2) of Al atom

	K_{Total}	F
$3s^23p\ ^2P_{1/2} \rightarrow 3s^24s\ ^2S_{1/2}$		
Our results	237(1.3)	76.92(12)
Ref. [3]	240(5)	76.5(20)
$3s^23p\ ^2P_{3/2} \rightarrow 3s^24s\ ^2S_{1/2}$		
Our results	239(1)	76.83(11)
Ref. [3]	243(4)	76.2(22)

[3] Filippin, L., Beerwerth, R., Ekman, J., Fritzsche, S., Godefroid, M., Jonsson, P. (2016). Multiconfiguration calculations of electronic isotope shift factors in Al I. Physical Review A, 94(6), 062508.

Thank you for attention!

Tl isotopes radii

A	I	$\delta\langle r^2\rangle$, fm^2 [4, 5]	$\delta\langle r^2\rangle$, fm^2
208g	5	0.183(13){13}	0.1919(130){38}[a]
207g	1/2	0.1048(2){70}	0.1100(2){22}[b]
205g	1/2	0	0
204g	2	−0.0635(71){40}	−0.0667(74){13}[c]
203g	1/2	−0.10321(2){700}	−0.10840(3){220}[d]
202g	2	−0.1834(71){130}	−0.1926(74){38}[c]
201g	1/2	−0.2077(9){150}	−0.2182(9){43}[e]
200g	2	−0.2979(71){210}	−0.3129(74){62}[c]
199g	1/2	−0.3116(71){220}	−0.3275(74){65}[c]
198g	2	−0.4035(71){290}	−0.4239(74){84}[f]
198m	7	−0.3804(71){270}	−0.3998(74){80}[g]
197g	1/2	−0.4119(71){290}	−0.4330(74){86}[f]
197m	9/2	−0.272(26){19}	−0.2871(270){75}[h]
196g	2	−0.4795(5){340}	−0.5036(5){100}[i]
196m	7	−0.4544(6){320}	−0.4773(6){95}[i]

Tl isotopes radii

A	I	$\delta\langle r^2\rangle$, fm^2 [4, 5]	$\delta\langle r^2\rangle$, fm^2
195g	1/2	$-0.4820(71)\{340\}$	$-0.5068(75)\{100\}^i$
195m	9/2	$-0.324(11)\{23\}$	$-0.3419(120)\{90\}^h$
194g	2	$-0.5551(39)\{50\}$	$-0.5831(5)\{120\}^i$
194m	7	$-0.5481(5)\{380\}$	$-0.5759(5)\{110\}^i$
193g	1/2	$-0.5716(11)\{400\}$	$-0.6007(12)\{120\}^e$
193m	9/2	$-0.4111(10)\{290\}$	$-0.4329(11)\{87\}^e$
192g	2	$-0.6296(4)\{440\}$	$-0.6616(4)\{130\}^i$
192m	7	$-0.6358(6)\{450\}$	$-0.6681(6)\{130\}^i$
191g	1/2	$-0.6544(7)\{460\}$	$-0.6878(7)\{140\}^i$
191m	9/2	$-0.4899(6)\{340\}$	$-0.5158(6)\{100\}^i$
190g	2	$-0.7063(4)\{490\}$	$-0.7424(4)\{150\}^i$
190m	7	$-0.7223(5)\{510\}$	$-0.7591(5)\{150\}^i$
189m	9/2	$-0.5543(41)\{390\}$	$-0.5837(43)\{120\}^e$
188m	7	$-0.8134(5)\{570\}$	$-0.8549(5)\{170\}^i$
187m	9/2	$-0.616(31)\{43\}$	$-0.650(32)\{17\}^h$

Tl isotopes radii

A	I	$\delta\langle r^2\rangle$, fm^2 [4, 5]	$\delta\langle r^2\rangle$, fm^2
186m1	7	$-0.9324(15)\{650\}$	$-0.9799(15)\{200\}^k$
186m2	10	$-0.719(23)\{50\}$	$-0.758(24)\{20\}^h$
185g	1/2	$-0.938(41)\{66\}$	$-0.987(43)\{25\}^h$
185m	9/2	$-0.731(29)\{51\}$	$-0.770(30)\{20\}^h$
184m1	2	$-0.979(32)\{69\}$	$-1.031(32)\{27\}^l$
184m2	7	$-0.976(24)\{68\}$	$-1.027(26)\{27\}^l$
184m3	10	$-0.777(20)\{54\}$	$-0.820(23)\{21\}^l$
183g	1/2	$-1.033(15)\{72\}$	$-1.086(17)\{28\}^l$
183m	9/2	$-0.775(15)\{54\}$	$-0.818(17)\{22\}^l$
182m1	4	$-1.120(18)\{78\}$	$-1.179(19)\{30\}^l$
182m2	7	$-1.123(30)\{78\}$	$-1.182(33)\{30\}^l$
181	1/2	$-1.174(16)\{82\}$	$-1.236(17)\{32\}^l$
180	4	$-1.254(22)\{88\}$	$-1.319(24)\{34\}^l$
179	1/2	$-1.274(29)\{89\}$	$-1.340(31)\{35\}^l$

Tl isotopes radii

[4] A. E. Barzakh et al. Changes in the mean square charge radii and magnetic moments of neutron deficient Tl isotopes.
In: Phys. Rev. C 88 (2 Aug. 2013), p.024315.
doi: 10.1103/PhysRevC.88.024315.
url: https://link.aps.org/doi/10.1103/PhysRevC.88.024315
[5] A. E. Barzakh et al. Changes in mean squared charge radii and magnetic moments of 179-184Tl measured by in source laser spectroscopy. In: Phys. Rev. C 95 (1 Jan. 2017), p. 014324. doi: 10.1103/PhysRevC.95.014324. url: https://link.aps.org/doi/10.1103/PhysRevC.