

# The isotope shift

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The isotope shift is the difference in the atomic state energies appearing for different isotopes of the same element. We present an inclusion of second-order perturbation theory for the specific mass (energy) shift. We also introduce an analysis of new *ab initio* calculations of isotope shifts in singly ionised calcium, by comparing them to recent empirical data, using King plot formalisms.

#### Atomic isotopes Atomic Hamiltonian Laboratory system

 $H(\vec{r}_0, \vec{r}_1, \vec{r}_2, \cdots, \vec{p}_0, \vec{p}_1, \vec{p}_2, \cdots) = \frac{p_0^2}{2M_A} + \sum_i \frac{p_i^2}{2m_e}$ 



 $\overrightarrow{r_1}$ 

## Second order theoretical specific mass shift results

<u>First order</u>

 $\delta E_{\rm SMS} = \frac{M_A}{(M_A + m_e)^2} \left\langle \sum_{i \neq i} \vec{p}_i \cdot \vec{p}_j \right\rangle$ 

Second order

$$+\sum_{i} V_{e-N}(\vec{r}_{i}-\vec{r}_{0}) + \frac{1}{2} \sum_{i\neq j} V_{e-e}(\vec{r}_{i}-\vec{r}_{j}).$$

Center of mass system  $H(\vec{\rho}_1, \vec{\rho}_2, \cdots, \vec{\pi}_1, \vec{\pi}_2, \cdots) = \sum_i \frac{\pi_i^2}{2\mu} + \sum_i V_{e-N}(\vec{\rho}_i) + \frac{1}{2} \sum_{i \neq j} V_{e-e}(\vec{\rho}_i - \vec{\rho}_j)$ +  $\frac{1}{M_A} \sum_{i \neq j} \vec{\pi}_i \cdot \vec{\pi}_j$ .

Different contributions to overall isotope shift Mass shifts :

Normal mass shift

$$E_{\mu} = \frac{\mu}{m_{e}} E_{\infty} \qquad \mu = \frac{m_{e} M_{n}}{m_{e} + M_{n}}$$
  
Specific mass shift  
$$H_{mpe} = -\frac{1}{M_{n}} \sum_{i=1}^{N} \sum_{j>i}^{N} \nabla_{\mathbf{r}_{i}} \cdot \nabla_{\mathbf{r}_{j}}$$
  
$$E_{mpe} = -\frac{1}{M_{n}} \left\langle \psi^{(0)} \left| \sum_{i=1}^{N} \sum_{j>i}^{N} \nabla_{\mathbf{r}_{i}} \cdot \nabla_{\mathbf{r}_{j}} \right| \psi^{(0)} \right\rangle$$

Ca+ and the

other

# Numerical shift

calculations

First order

Comparison between experimental values ([2]) and new calculation (this work) for DHF and RCC method, in GHz



$$\delta E_{SMS} = \left| \frac{M_A}{(M_A + m_e)^2} \left\langle \sum_{i \neq j} \vec{p_i} \cdot \vec{p_j} \right\rangle \right|$$

 $\vec{p}_i = \vec{\pi}_i + \frac{m_e}{M_T} \vec{P}$  $\vec{p}_0 = -\sum \vec{\pi}_i + \frac{M_A}{M_T} \vec{P}$ 

## The coupled cluster numerical method

 $\hat{T}_2 = \sum \hat{t}_i$  $\Psi = \Phi_0 + \hat{T}_2 \Phi_0 + \frac{1}{2!} \hat{T}_2^2 \Phi_0 + \frac{1}{3!} \hat{T}_2^3 \Phi_0 + \dots = e^{T_2} \Phi_0$ 

#### Field shift : $H_{\rm vol}(r_i \le r_{\rm n}) = \frac{Z}{2r_{\rm n}} \left( \frac{2r_{\rm n}}{r_i} + \frac{r_i^2}{r_{\rm n}^2} - 3 \right)$ $E_{\rm vol} = \langle \psi_{n00}(\mathbf{r}_i) | H_{\rm vol}(r_i) | \psi_{n00}(\mathbf{r}_i) \rangle$

### King plot approach

$$\mu_{(P,Q)}IS_{P,Q}^{a} = MS_{S,T}^{a} + \mu_{(P,Q)}FS_{P,Q}^{a}$$

$$\mu_{(P,Q)}IS_{P,Q}^{b} = MS_{S,T}^{b} + \mu_{(P,Q)}FS_{P,Q}^{b}$$

$$\mu_{(P,Q)} = \frac{(M_{S} - M_{T})(M_{P} + m)(M_{Q} + m)}{(M_{P} - M_{Q})(M_{S} + m)(M_{T} + m)}$$
King plot analysis of empirical data for the D1 - D2 transitions in Ca+

	Ca	aisotopes	>
Etat	DHF method R	CC method	
Field Shift	constant (MHz/fr	m²)	
4s	-215,697	-261,921	
4p 1/2	-0,417	20,238	
4p 3/2	-0,0000104	20,627	Isotope shift
Normal Mass	Shift constant (GI	Iz.amu)	calculations done
4s	2383,856	1556,449	
4p 1/2	1619,66	1139,921	using DHF and RCC
4p 3/2	1611,921	1138,666	
			method
Specific Mass	Shift constant (GI	Hz.amu)	
4s	-926,112	-152,95	
4p 1/2	-501,109	-163,504	
4p 3/2	-492,553	-158,492	
		ſ	
<sup>35</sup> C; <sup>36</sup> C;	<sup>37</sup> C; <sup>38</sup> C; <sup>39,</sup>	C: <sup>40</sup> C <sup>41</sup> Ca	42C:43C:44C:45C:46C:47C:48C*
<sup>5</sup> C; <sup>36</sup> C; Di	<sup>37</sup> C; <sup>38</sup> C; <sup>39,</sup> fference in	C: $4^{\circ}$ C: $4$	alcium <sup>acto</sup>
<sup>15</sup> C; <sup>36</sup> C; Di sp	<sup>37</sup> C; <sup>38</sup> C; <sup>39</sup> fference in pectrums of	C $4^{\circ}$ C $4^{\circ}$ Ca, $4^{7}$ Ca,	And <sup>51</sup> Ca
5 <mark>5C;36C;</mark> Di sp	<sup>37</sup> C; <sup>38</sup> C; <sup>39</sup> fference in pectrums of	C $4^{\circ}$ C $4^{\circ}$ C $4^{\circ}$ Ca, $4^{7}$ Ca,	e structure
5 <b>C:</b> 36C: Di Sp 60	$37Ci^{38}Ci^{39}$	C $4^{9}$ Ca, $4^{7}$ C	<b>alcium</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contraction</b> <b>Contractio</b>
5 <mark>5C; 36C;</mark> Di Sp فقع 20	37C: 38C: 39	C $4^{9}$ Ca, $4^{7}$ C	e structure
5C; 36C; Di Sp 60 9100	$37Ci^{38}Ci^{39}$	C $4^{\circ}$ C $4^{\circ}$ C	alcium <sup>42</sup> Cl <sup>43</sup> Cl <sup>44</sup> Cl <sup>45</sup> Cl <sup>46</sup> Cl <sup>47</sup> Cl <sup>48</sup> Cl <sup>48</sup> Cl <sup>44</sup> Cl <sup>45</sup> Cl <sup>46</sup> Cl <sup>47</sup> Cl <sup>48</sup>
5C; 36C; Di SD 60 40 20 100	$37Ci^{38Ci^{39}}$	C: $4^{\circ}$ C (1C: hyperfin of $4^{9}$ Ca, $4^{7}$ C	alcium action of the structure ta and <sup>51</sup> Ca
5C: 36C: Di SP 60 40 50 50	$37Ci^{38}Ci^{39}$	C $4^{\circ}$ C $4^{\circ}$ C	<b>alcium</b> <b>Conscience of Conscience of Consc</b>









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spectroscopy.	This is a manifestation of the isotope shift.	

**References** 

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ı	56 Ba barium 6s <sup>2</sup>	<b>Ba</b> barium lanthanides		72 Hf hafnium 5d <sup>2</sup> 6s <sup>2</sup>	Hf 73 Ta tantalum s <sup>2</sup> 5d <sup>3</sup> 6s <sup>2</sup>		<b>V</b> ssten <sup>2</sup> <b>75</b> <b>F</b> rhe 5d <sup>5</sup> 6	Re 05 nium 05 s <sup>2</sup> 5d <sup>6</sup> 6	Ds nium s <sup>2</sup>	77 78 Ir 91 iridium 91a 5d <sup>7</sup> 6s <sup>2</sup> 5d <sup>9</sup> 6		t A num gg 5d10 6	ald s 5	30 Hg mercury 5d <sup>10</sup> 6s <sup>2</sup>	81 T thall 6p	1 ium 82 6p <sup>2</sup>	Pb ead	B3 Bi bismuth 5p3	84 Polor 6p <sup>4</sup>	o nium	At astatine	86 Rn radon 6p <sup>6</sup>	
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