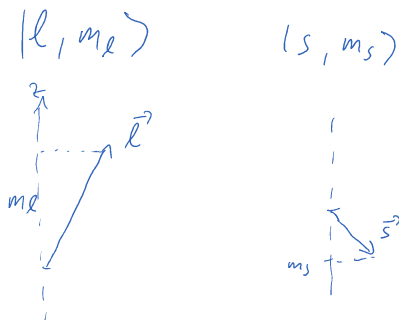


# Clebsch - Gordan coefficients

example  $sp_h - sp_h$  or  $sp_h - orbit$  interaction



$$\vec{j} = \vec{l} + \vec{s}$$

$$|l, m_l\rangle \otimes |s, m_s\rangle \equiv |l, m_l, s, m_s\rangle$$

$$n = 1, \dots, \infty$$

$$l = 0, \dots, n-1 \quad m_l = -l, \dots, l$$

$$s = \frac{1}{2} \quad m_s = -s, \dots, s$$

$$\rightarrow j = l \pm s \quad \text{but } j \geq 0 \quad m_j = -j, \dots, j$$

$$|l-s| \leq j \leq l+s$$

1  $sp_h$       2  $ndsp_h$

①  $\hat{=}$  2 s electrons in He

$$s_1 = \frac{1}{2} \quad s_2 = \frac{1}{2} \quad \text{singlett, triplett}$$

$$l = \frac{1}{2} \quad s = \frac{1}{2}$$

total  $sp_h$   $j = \frac{1}{2} \pm \frac{1}{2} = 0, 1$

①a  $j = 0 \Rightarrow m_j = 0 \quad m_j \in \{-j, \dots, j\}$

singlett

$$|j=0, m_j=0\rangle = \sum_{m_l+m_s=m_j} \langle m_l, m_s | j=0, m_j=0 \rangle |m_l, m_s\rangle$$

$$= \langle \uparrow, \downarrow | 0, 0 \rangle |\uparrow\downarrow\rangle + \langle \downarrow, \uparrow | 0, 0 \rangle |\downarrow\uparrow\rangle$$

$$= \frac{1}{\sqrt{2}} |\uparrow\downarrow\rangle - \frac{1}{\sqrt{2}} |\downarrow\uparrow\rangle$$

1b: Triplett

$$j = 1, m_j = \{-1, 0, 1\}$$

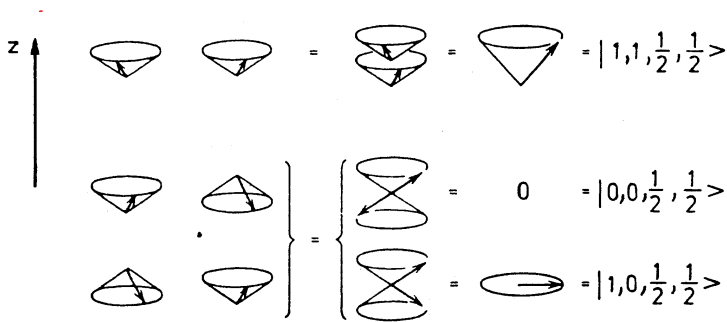
$$|j=1, m_j=1\rangle = \sum_{m_l, m_s} \langle m_l, m_s | j=1, m_j=1 \rangle |m_l, m_s\rangle$$

$$m_j = m_l + m_s \\ = \dots 1 \uparrow \uparrow \rangle$$

$$\frac{1}{2} \uparrow \uparrow \rangle + \frac{1}{2} \uparrow \uparrow \rangle = \uparrow \uparrow \rangle \quad j(j+1) \geq m_j$$

$$|j=1, m_j=-1\rangle \dots = 1 \downarrow \downarrow \rangle$$

$$|j=1, m_j=0\rangle = \frac{1}{\sqrt{2}} (\uparrow \downarrow) \oplus \frac{1}{\sqrt{2}} (\downarrow \uparrow)$$



44. Clebsch-Gordan coefficients 1

44. Clebsch-Gordan Coefficients, Spherical Harmonics, and d Functions

Note: A square-root sign is to be understood over every coefficient, e.g., for  $-8/15$  read  $-\sqrt{8/15}$ . Notation:  $\begin{matrix} j & j & \dots \\ m & m & \dots \end{matrix}$  Coefficients

$Y_0^0 = \sqrt{\frac{3}{4\pi}} \cos \theta$   
 $Y_1^0 = -\sqrt{\frac{3}{8\pi}} \sin \theta \cos \theta$   
 $Y_2^0 = \sqrt{\frac{5}{4\pi}} \left( \frac{3}{2} \cos^2 \theta - \frac{1}{2} \right)$   
 $Y_2^{\pm 1} = \frac{1}{4} \sqrt{\frac{15}{2\pi}} \sin^2 \theta e^{\pm 2i\phi}$

$Y_l^{-m} = (-1)^m Y_l^{m*}$   
 $d_{m,0}^l = \sqrt{\frac{4\pi}{2l+1}} Y_l^m e^{-im\phi}$

$(j_1 j_2 m_1 m_2 | j j m)$   
 $= (-1)^{j_1 - j_2 - m} (j_2 j_1 m_2 m_1 | j j m)$

②  $j_1 = 1, j_2 = 1$   
 $j = 0, 1, 2 \quad m_j = -2, -1, 0, 1, 2$

②a)  $|j=0, m_j=0\rangle = \frac{1}{\sqrt{3}} |m_{j1}=1, m_{j2}=-1\rangle$   
 $\rightarrow -\frac{1}{\sqrt{3}} |m_{j1}=0, m_{j2}=0\rangle$   
 $+ \frac{1}{\sqrt{3}} |m_{j1}=-1, m_{j2}=1\rangle$

②b)  $|j=1, m_j=1\rangle = \frac{1}{\sqrt{2}} |1, 0\rangle + \frac{1}{\sqrt{2}} |0, 1\rangle$

Many-electron atoms

$$\hat{L} = \sum_i \hbar \mathbf{p}_i \times \mathbf{r}_i - \sum_i \frac{e^2}{r_i} + \dots \rightarrow 1$$

Many - electron atoms

$$\hat{H} = \sum_{i=1}^Z \left( \frac{p_i^2}{2m_e} - \frac{Ze^2}{4\pi\epsilon_0 r_i} \right) + \underbrace{\sum_{i>j} \frac{e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_j|}}_{\text{difficult e-e repulsion}}$$

Pauli exclusion principle

↳ only  $2e^-$  in each subshell

$n=0, \dots$

each  $n$  state has  $n$  values of  $l: l=0, 1, \dots, n-1$

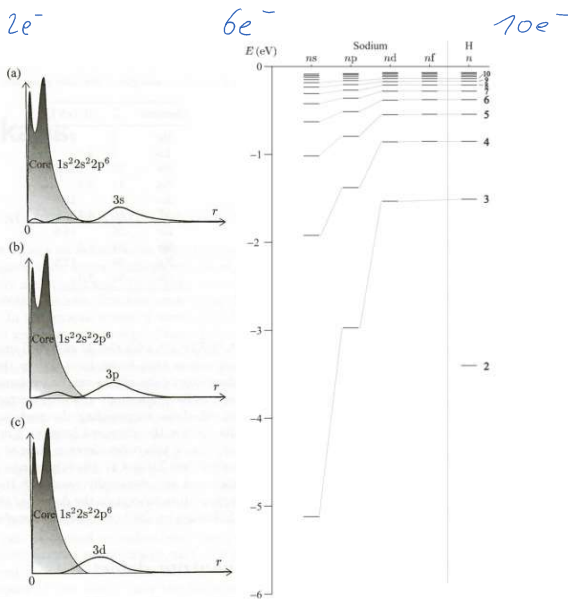
$l$   $(2l+1)$   $m_l: m_l = -l, \dots, l$

each  $(n, l)$  can hold  $2 \times (2l+1)$

↑  
Pauli ↑↓

E ↑	K L M N	4s	$\frac{K}{19} \frac{Ca}{20}$											Zn 30	
		3s	$\frac{Na}{11} \frac{Mg}{12}$	3p	$\frac{Al}{13} \frac{Si}{14} \frac{P}{15} \frac{S}{16} \frac{Cl}{17} \frac{Ar}{18}$	3d	$\frac{Sc}{21} \frac{Ti}{22} \dots$								
		2s	$\frac{Li}{3} \frac{Be}{4}$	2p	$\frac{B}{5} \frac{C}{6} \frac{N}{7} \frac{O}{8} \frac{F}{9} \frac{Ne}{10}$										
		1s	$\frac{H}{1} \frac{He}{2}$												
		$2(2l+1)$	$2e^-$											$6e^-$	$10e^-$

Na



Foot, Atomic Physics

Foot, Atomic Physics

Fig. 4.2 The energies of the s, p, d and f configurations in sodium. The energy levels of hydrogen are marked on the right for comparison. The guidelines link configurations with the same  $n$  to show how the energies become closer to the hydrogenic values as  $l$  increases, i.e. the quantum defects decrease so that  $\delta_l \approx 0$  for  $l$ -electrons (and for the configurations with  $l > 3$  that have not been drawn).

energetically favourable to occupy 4s shell before the 3d shell

→ chemical properties

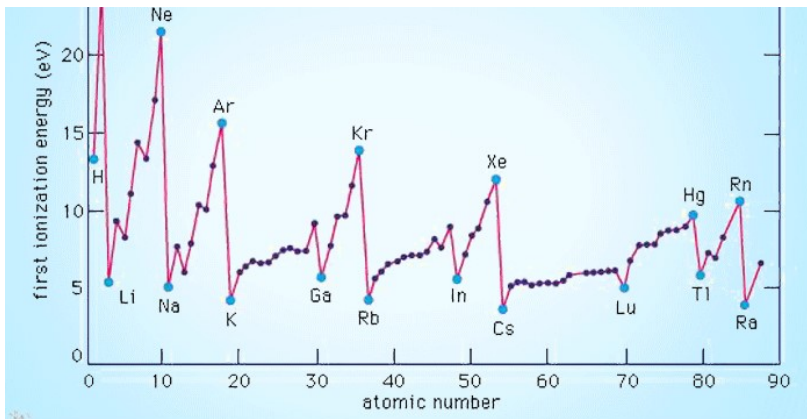
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H 1,008	Atomic # Symbol Name Weight																2 He 4,002602
2 Li 6,94	3 Be 9,012182	C Fest Nichtmetalle Halbmetalle Metalle Alkalimetalle Erdalkalimetalle Lanthanoide Actinoide Übergangsmetalle Post-transition metals										6 B 10,81	7 C 12,011	8 N 14,007	9 O 15,999	10 F 18,998	11 Ne 20,1797
4 K 39,0983	5 Ca 40,078	6 Sc 44,955912	7 Ti 47,88	8 V 50,9415	9 Cr 51,9961	10 Mn 54,938	11 Fe 55,845	12 Co 58,933	13 Ni 58,6934	14 Cu 63,546	15 Zn 65,38	16 Ga 69,723	17 Ge 72,63	18 As 74,921	19 Se 78,971	20 Br 79,904	21 Kr 83,798
6 Rb 85,4678	7 Sr 87,62	8 Y 88,90584	9 Zr 91,224	10 Nb 92,90638	11 Mo 95,94	12 Tc 98,90625	13 Ru 101,07	14 Rh 101,07	15 Pd 106,3675	16 Ag 107,8682	17 Cd 112,4114	18 In 114,818	19 Sn 118,710	20 Sb 121,757	21 Te 127,603	22 I 126,90544	23 Xe 131,29
8 Cs 132,90545196	9 Ba 137,327	10 La 138,90487	11 Hf 178,49	12 Ta 180,94788	13 W 183,84	14 Re 186,207	15 Os 190,23	16 Ir 192,222	17 Pt 195,084	18 Au 196,966569	19 Hg 200,59	20 Tl 204,38	21 Pb 207,2	22 Bi 208,98038	23 Po 209	24 At 210	25 Rn 222
7 Fr 223	8 Ra 226	9 Ac 227	10 Th 232,0375	11 Pa 231,03688	12 U 238,02891	13 Np 237	14 Pu 244	15 Am 243	16 Cm 247	17 Bk 247	18 Cf 251	19 Es 252	20 Fm 257	21 Md 258	22 No 259	23 Lr 260	

Für Elemente, die keine stabilen Isotope aufweisen, ist die Massenzahl des Isotops mit der höchsten Halbwertszeit angegeben.

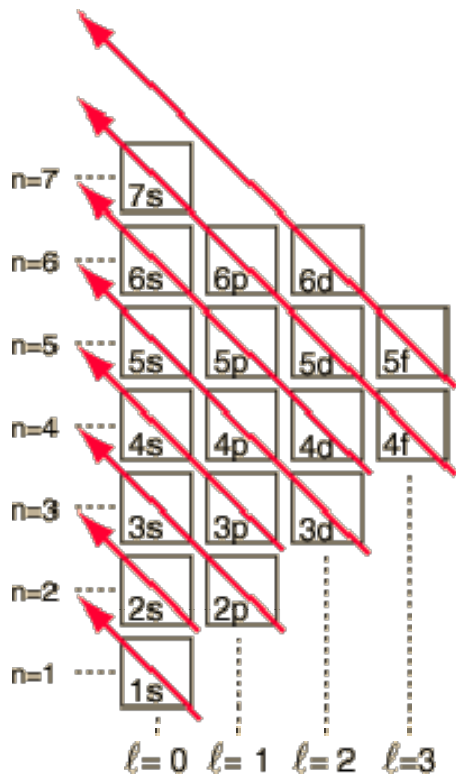
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Alkalis

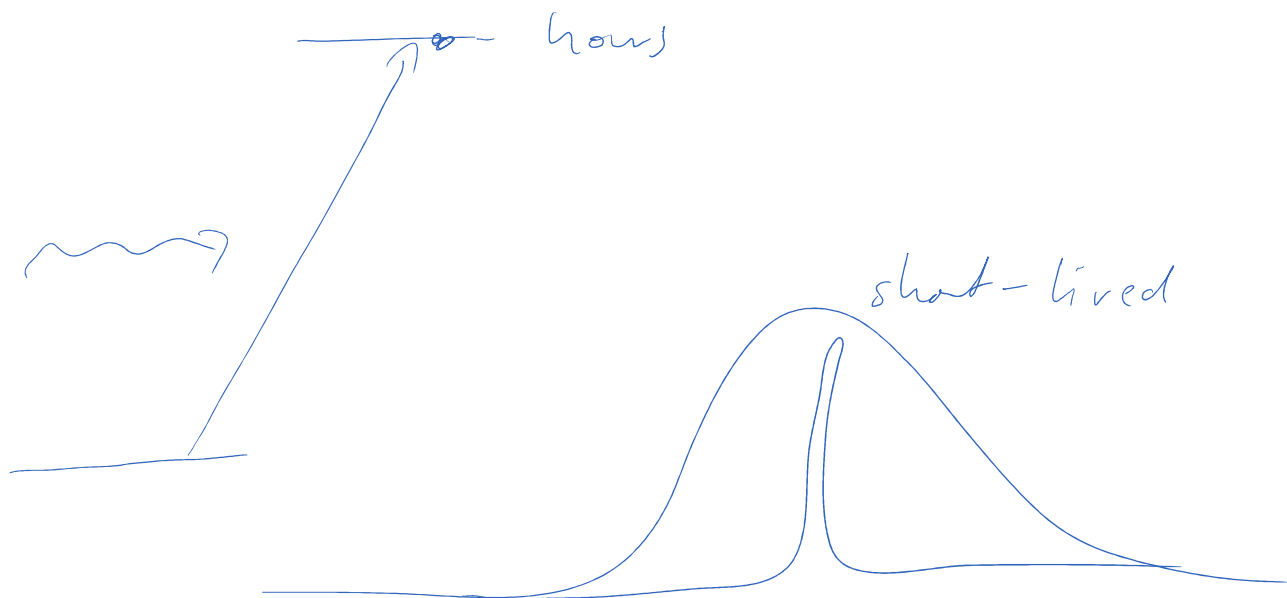
<http://www.ptable.com/>



## THE IONIZATION ENERGY OF THE GROUP 1 ELEMENTS



Lars van der Wense MPD, LITU



$^{229}\text{Th}$   $\Delta E \approx 8\text{eV}$

