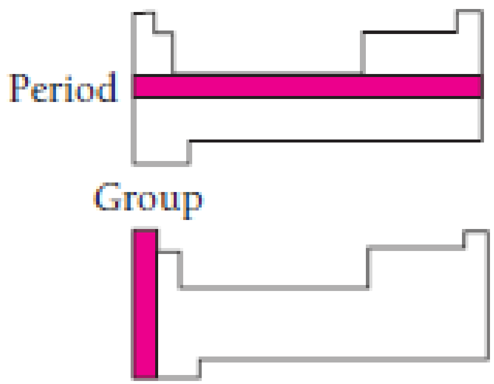
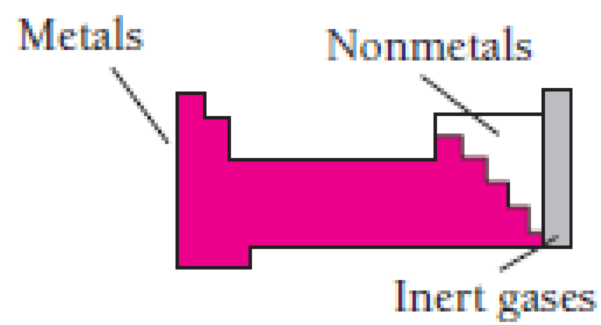
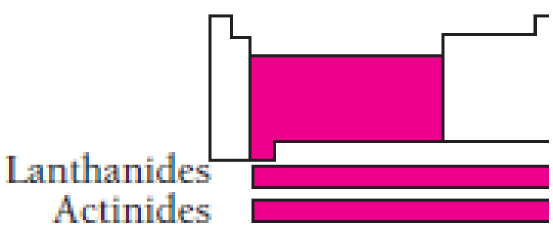
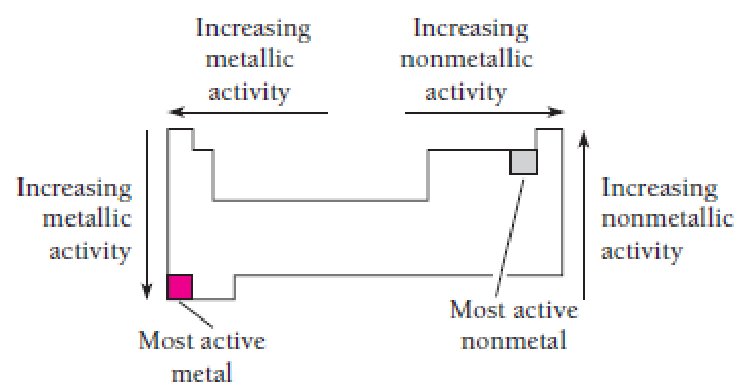
Periodic table: how electrons are organized.

✔ Periodic table: an arrangement of the elements according to atomic number in a series of rows such that elements with similar properties form vertical columns.









The Periodic Table of the Elements

The number above the symbol of each element is its atomic number, and the number below its name is its average atomic mass. The elements whose atomic masses are given in parentheses do not occur in nature but have been created in nuclear reactions. The atomic mass in such a case is the mass number of the most long-lived radioisotope of the element.

Elements with atomic numbers 110, 111, 112, 114, and 116 have also been created but not yet named.

Group / Period	1	2											3	4	5	6	7	8
1	1 H Hydrogen 1.008																	2 He Helium 4.003
2	3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.81	6 C Carbon 12.01	7 N Nitrogen 14.01	8 O Oxygen 16.00	9 F Fluorine 19.00	10 Ne Neon 20.18
3	11 Na Sodium 22.99	12 Mg Magnesium 24.31											13 Al Aluminium 26.98	14 Si Silicon 28.09	15 P Phosphorus 30.97	16 S Sulfur 32.07	17 Cl Chlorine 35.45	18 Ar Argon 39.95
4	19 K Potassium 39.10	20 Ca Calcium 40.08	21 Sc Scandium 44.96	22 Ti Titanium 47.88	23 V Vanadium 50.94	24 Cr Chromium 52.00	25 Mn Manganese 54.94	26 Fe Iron 55.8	27 Co Cobalt 58.93	28 Ni Nickel 58.69	29 Cu Copper 63.55	30 Zn Zinc 65.39	31 Ga Gallium 69.72	32 Ge Germanium 72.59	33 As Arsenic 74.92	34 Se Selenium 78.96	35 Br Bromine 79.90	36 Kr Krypton 83.80
5	37 Rb Rubidium 85.47	38 Sr Strontium 87.62	39 Y Yttrium 88.91	40 Zr Zirconium 91.22	41 Nb Niobium 92.91	42 Mo Molybdenum 95.94	43 Tc Technetium (98)	44 Ru Ruthenium 101.1	45 Rh Rhodium 102.9	46 Pd Palladium 106.4	47 Ag Silver 107.9	48 Cd Cadmium 112.4	49 In Indium 114.8	50 Sn Tin 118.7	51 Sb Antimony 121.9	52 Te Tellurium 127.6	53 I Iodine 126.9	54 Xe Xenon 131.8
6	55 Cs Cesium 132.9	56 Ba Barium 137.3		72 Hf Hafnium 178.5	73 Ta Tantalum 180.9	74 W Tungsten 183.9	75 Re Rhenium 186.2	76 Os Osmium 190.2	77 Ir Iridium 192.2	78 Pt Platinum 195.1	79 Au Gold 197.0	80 Hg Mercury 200.6	81 Tl Thallium 204.4	82 Pb Lead 207.2	83 Bi Bismuth 209.0	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
7	87 Fr Francium (223)	88 Ra Radium 226.0		104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (263)	107 Ns Nielsbohrium (262)	108 Hs Hassium (264)	109 Mt Meitnerium (266)									

Transition metals

Alkali metals

Halogens Inert gases

Lanthanides (rare earths)

57 La Lanthanum 138.9	58 Ce Cerium 140.1	59 Pr Praseodymium 140.9	60 Nd Neodymium 144.2	61 Pm Promethium (145)	62 Sm Samarium 150.4	63 Eu Europium 152.0	64 Gd Gadolinium 157.3	65 Tb Terbium 158.9	66 Dy Dysprosium 162.5	67 Ho Holmium 184.9	68 Er Erbium 167.3	69 Tm Thulium 168.9	70 Yb Ytterbium 173.0	71 Lu Lutetium 175.0
89 Ac Actinium (227)	90 Th Thorium 232.0	91 Pa Protactinium 231.0	92 U Uranium 238.0	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (260)	102 No Nobelium (259)	103 Lw Lawrencium (262)

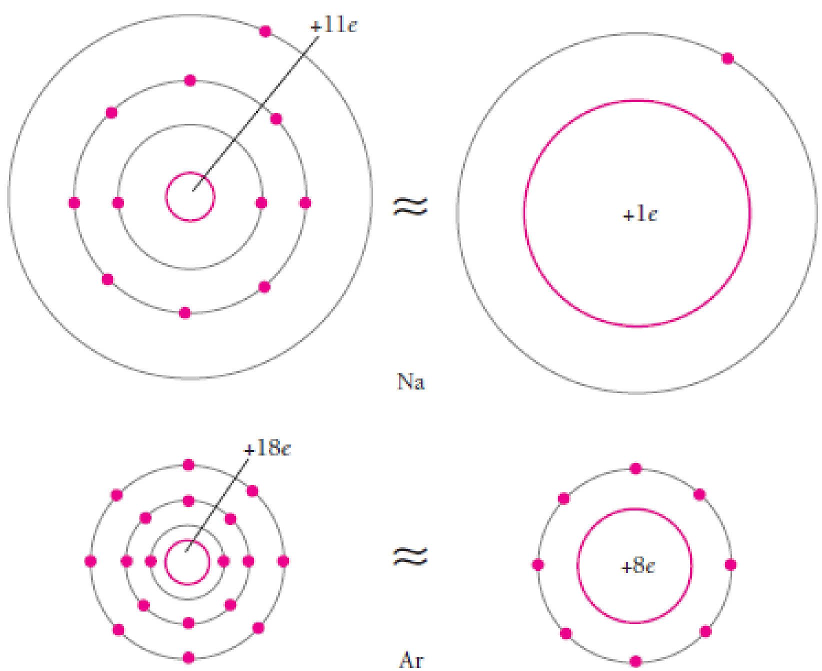
Actinides

Mean field in an atom

✔ A system of particles is stable when its total energy is the minimum.

✔ Only one electron can exist in any particular quatntum state in an atom.

Consider each electron as if it exists in a mean field,



Quantum numbers

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r) Y_\ell^m(\theta,\phi)$$

$n = 1, 2, 3, \cdots$

$\ell = 0, 1, 2, \cdots (n-1)$

$m = 0, \pm 1, \pm 2, \pm 3 \cdots, \pm \ell$

Quantum numbers:

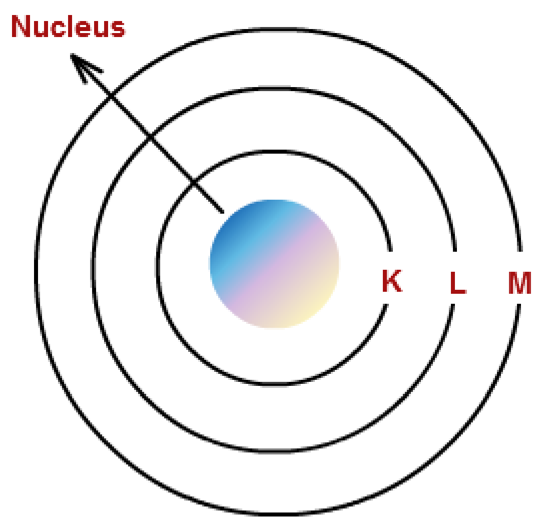
✔ **Principal quantum number: n=1, 2, 3,…**
: Principal energy level of the electron

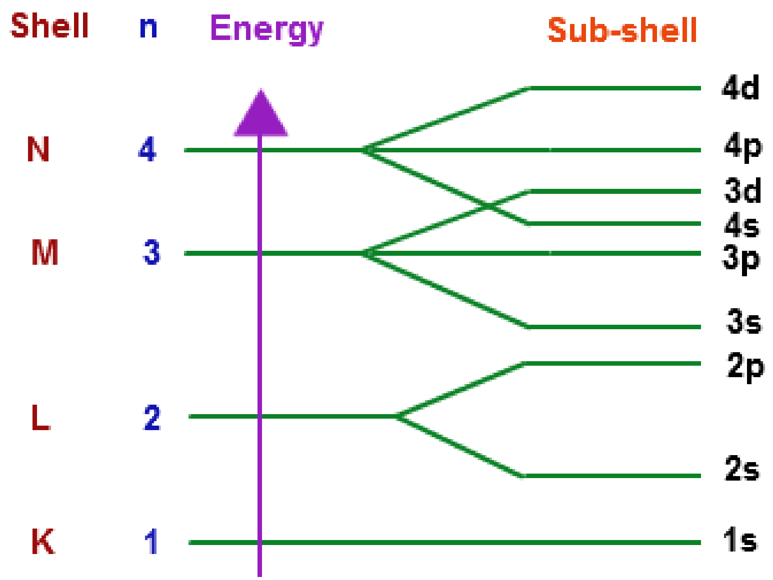
✔ **Orbital quantum number: ℓ=0, 1, 2, … , (n-1)**
: Values of the angular momentum of the electron

✔ **Magnetic quantum number: m_ℓ=0, ±1, ± 2, … , ±ℓ**
: Possible properties of an electron in a magnetic field

✔ **Spin quantum number: m_s= -1/2, +1/2**
: Possible spin vectors or orientations of an electron in a magnetic field

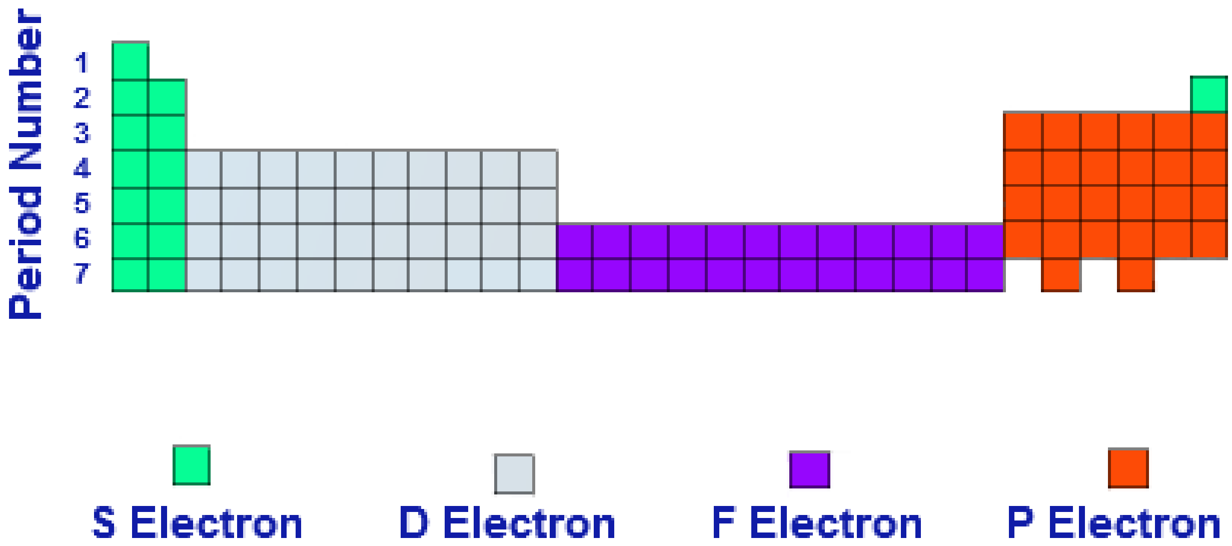
Shells and subshells of electrons





- ✔ Shells split into subshells labelled s, p, d and f.
- ✔ Within each sub shell, there are a number of possible Orbitals ($2\ell+1$). The energy values of the orbitals in a sub shell are normally degenerate.
- ✔ These energy levels are then described by the quantum number m which can have values from $-\ell$ to $+\ell$.
- ✔ Each electron has a spin quantum number s.

Periodic table with quantum numbers



✔ Each electron in an atom is described by a set of four quantum numbers.
✔ n represents the period of the periodic table while also noting that the d and f electrons have n quantum numbers that are 1 and 2 units less than the period in which they are found.
✔ Next the l quantum number represents various "blocks" within the periodic table similar to the periodic table shown below.

Energy term

C atom: α spin and β spin

C: $(1s)^2(2s)^2(2p)^2$ $(2p)^2$: Open shell

$2p_+$, $2p_0$, $2p_-$: How two electrons are located?

Coupling of n electrons:

$$L = \ell_1 + \ell_2 + \cdots \ell_n, \quad S = s_1 + s_2 + \cdots s_n$$

Total angular momentum: $J = L + S$

$$J = |L - S|, |L - S| + 1, |L - S| + 2, \cdots, L + S$$

# of J values: $L \geq S \Rightarrow 2S + 1$ $S \geq L \Rightarrow 2L + 1$

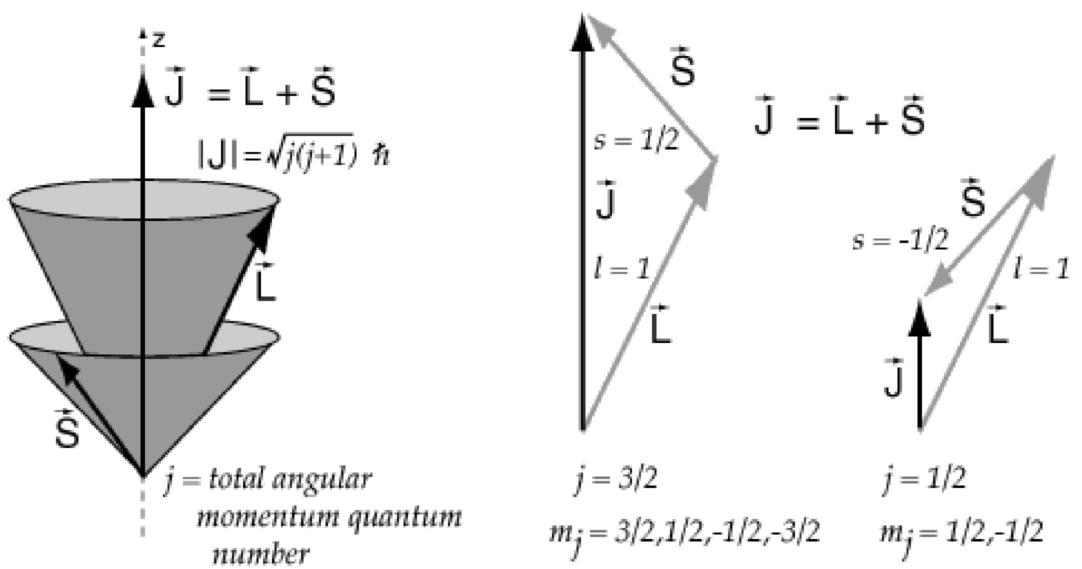
Term: ${}^{2S+1}L_J$

$L = 0, \quad 1, \quad 2, \quad 3, \quad \cdots$

S P D F

Russel-Saunders or L-S coupling

1. The orbital angular momenta of the individual electrons add to form a resultant orbital angular momentum L.
2. Likewise, the individual spin angular momenta are presumed to couple to produce a resultant spin angular momentum S.
3. Then L and S combine to form the total angular momentum.



How to deduce terms?

$(2p)^2$ $\ell_1=1$; $\ell_2=1$ $m_1=1, 0, -1$; $m_2=1, 0, -1$

$\ell_1=1$

m_1	1	0	-1	m_2
	2	1	0	1
	1	0	-1	0
	0	-1	-2	-1

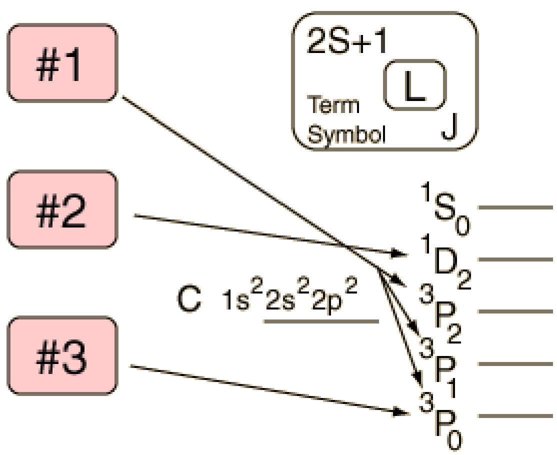
$\ell_2=1$

Hund's rule

1. The term with maximum multiplicity lies lowest in energy. (Spin-spin interaction)

2. For a given multiplicity, the term with the largest value of L lies lowest in energy. (Orbit-orbit interaction)

3. For atoms with less than half-filled shells, the level with the lowest value of J lies lowest in energy. When the shell is more than half full, the opposite rule holds (highest J lies lowest).
   (Spin-orbit interaction)



About Hund's rule #1

Consider two one-electron orbitals a and b, a: ε_a b: ε_b

Electron configuration (a) (b)

Spin: anti-parallel → singlet
Spin: parallel → triplet

If $\varepsilon_a = \varepsilon_b$: Degenerated states

If $\varepsilon_a < \varepsilon_b$

$$^1\psi = \frac{1}{\sqrt{2}}\{a(1)b(2) + b(1)a(2)\} \qquad ^3\psi = \frac{1}{\sqrt{2}}\{a(1)b(2) - b(1)a(2)\}$$

$$\hat{H} = \hat{h}(1) + \hat{h}(2) + \frac{1}{r_{12}}, \quad \hat{h}(i) = -\frac{1}{2}\nabla^2 - \frac{1}{r_i} \quad (i = 1, 2)$$

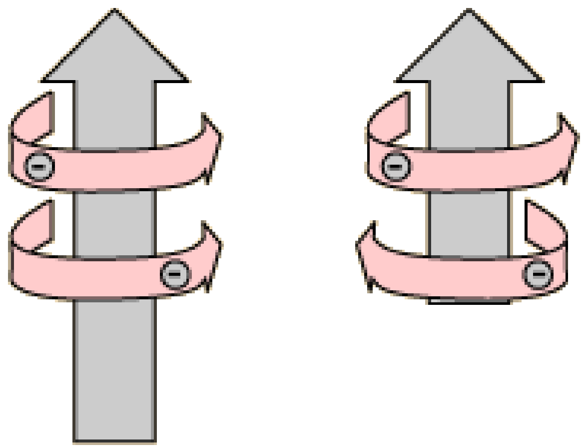
$$^1E = h_{aa} + h_{bb} + J_{ab} + K_{ab}, \quad ^3E = h_{aa} + h_{bb} + J_{ab} - K_{ab}$$

$$J_{ab} = \left\langle a(1)b(2)\left|\frac{1}{r_{12}}\right|a(1)b(2)\right\rangle = J_{ba}, \quad K_{ab} = \left\langle a(1)b(2)\left|\frac{1}{r_{12}}\right|b(1)a(2)\right\rangle = K_{ba}$$

About Hund's rule #2

For a given multiplicity, the term with the largest value of L lies lowest in energy.

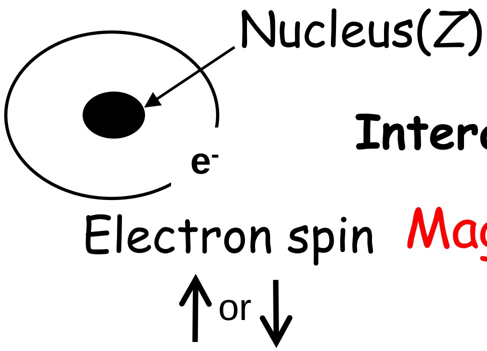
High L values:	Low L values:
Electrons orbiting the same direction to add to L values.	Electrons orbiting the opposite direction to reduce L values.



✔ Electrons meet less often than when they orbit in opposite directions. Hence their repulsion is less on average when L is large.

About Hund's rule #3

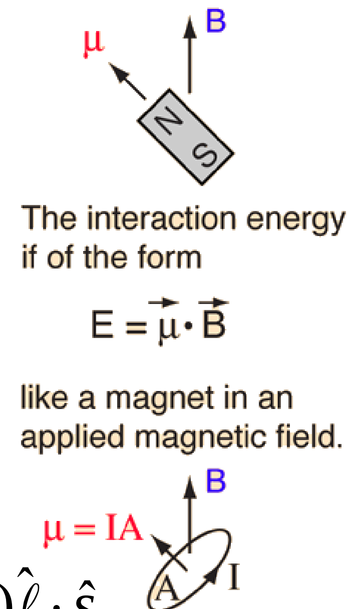
Heavy atom effect: Spin-orbit coupling

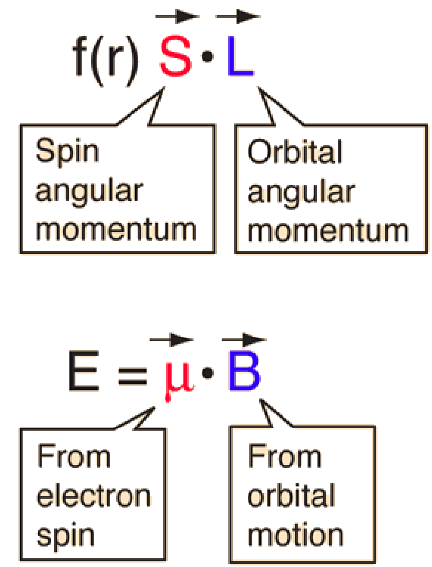


Field: Ze/r

Interaction

Magnetic dipole moment





$$\mathbf{B}_n = \frac{Ze\mu_0}{4\pi r^3 m_e}\cdot\ell \qquad \mu_s = -\frac{e}{m}\mathbf{s}$$

$$\hat{\mathbf{H}}_{\mathbf{SO}} = -\frac{1}{2}\mathbf{B}_n\cdot\mu_s = \frac{Ze^2}{8\pi\varepsilon_0 m_e^2 c^2 r^3}\hat{\ell}\cdot\hat{s} = \xi(r)\hat{\ell}\cdot\hat{s}$$

$$\hat{\mathbf{H}}_{\mathbf{SO}} = \sum_i^I \xi_i(r_i)\hat{\ell}_i\cdot\hat{s}_i \qquad \langle\psi_{n,\ell,m}|\xi(r)|\psi_{n,\ell,m}\rangle = \frac{e^2}{2m_e^2c^2a_0^3}\frac{Z^4}{n^3\ell(\ell+1)\left(\ell+\frac{1}{2}\right)}$$

The scalar product **S**·**L** is negative if the spin and orbital angular momentum are in opposite directions. Since the coefficient of **S**·**L** is positive, lower J is lower in energy.