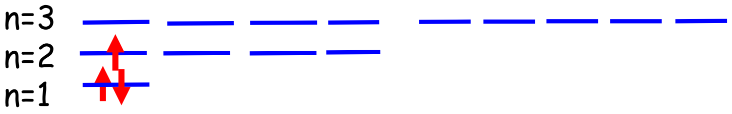
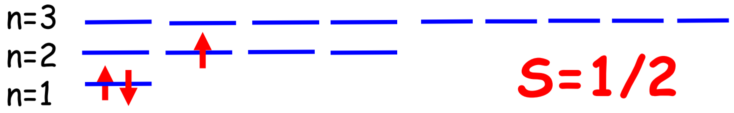
Rule: If there is a degeneracy between total **S=0** vs total **S=1**, the triplet has lower energy due to e-e repulsion.

But how do we order states if the degeneracy is between say ℓ=0 vs ℓ=1 for the same n? Example:

S=1/2
L=0

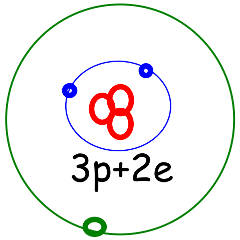


vs

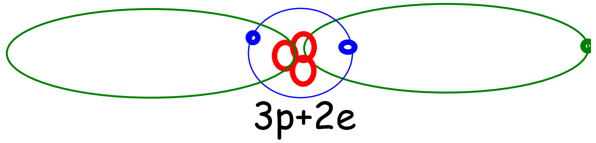


S=1/2
L=1

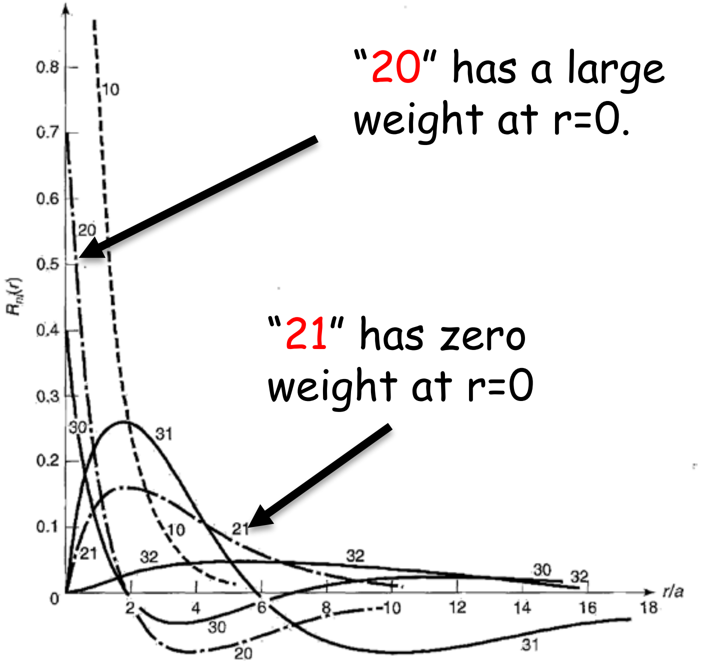
Rule: e-p attraction favors the lowest total "ℓ" between subshells (like s vs p) due to "screening" of p:



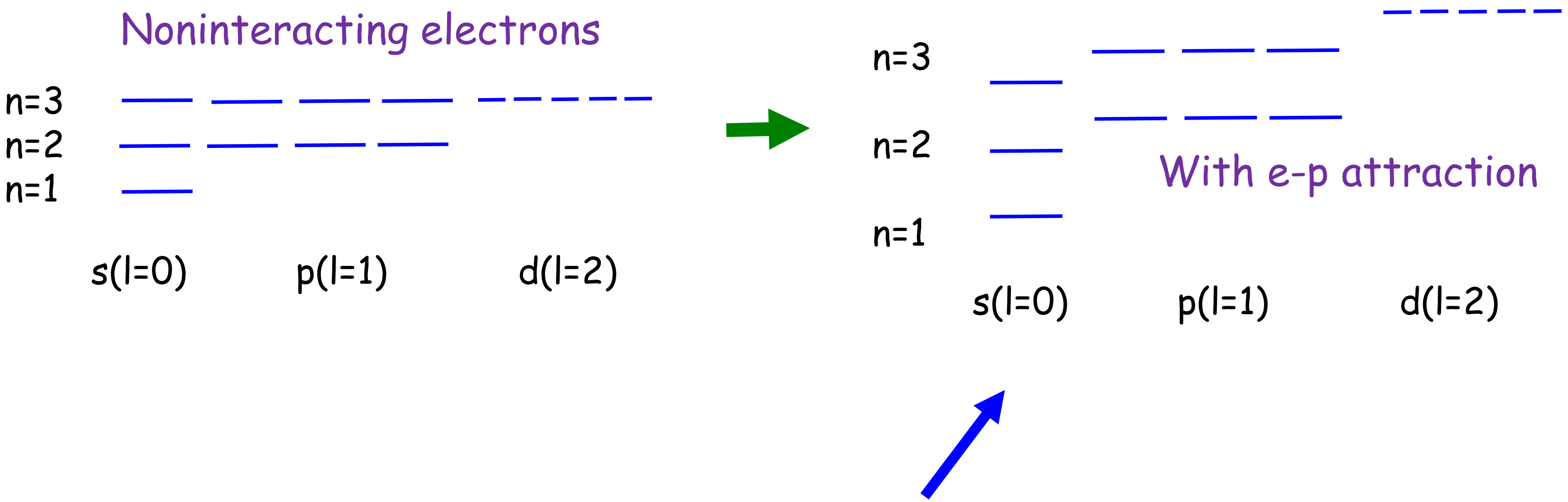
"Green 20" electron is close to nucleus i.e. lower energy. See wave function.



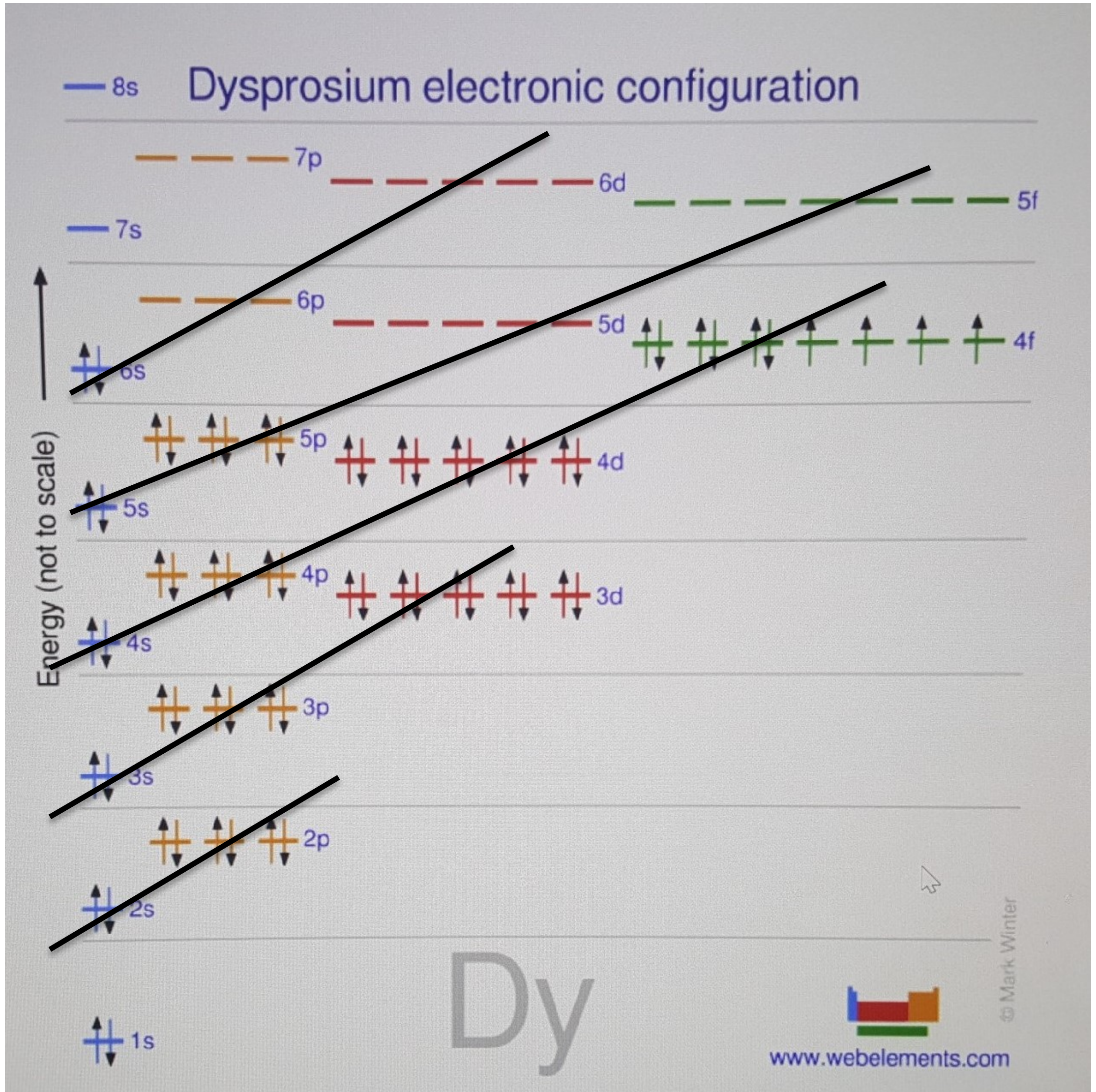
"Green 21" electron is further from nucleus than green 20 electron (screening), see wave function.



Then, because of the effect in the previous page that distinguishes between cases l=0, l=1, l=2, etc. there is a split of accidentally "degenerate" orbitals:

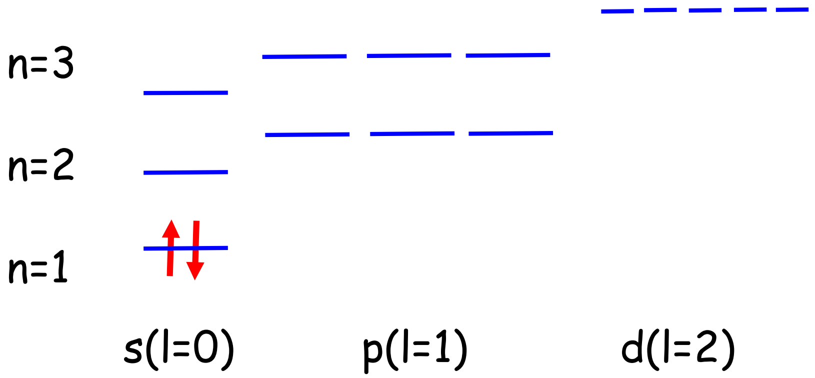


This is the energy order we have to use in order to construct the periodic table from now on.

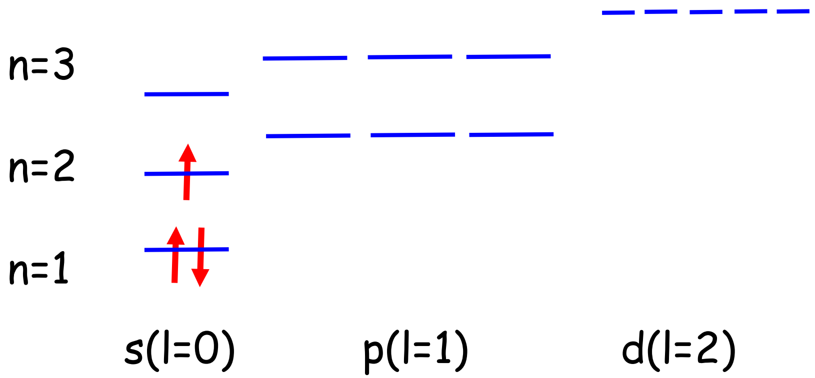


Schematic electronic configuration of dysprosium.

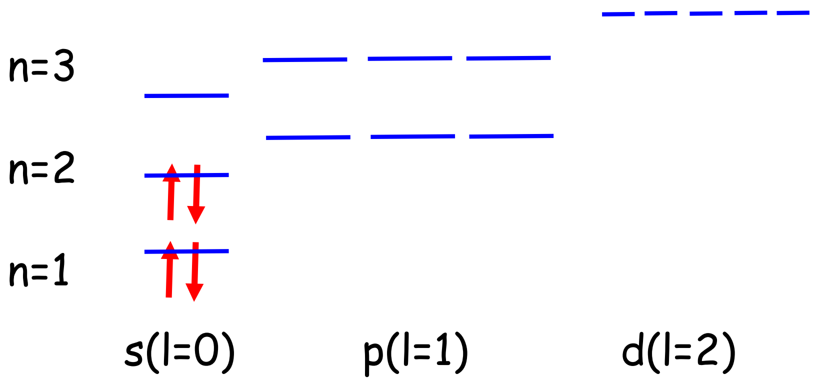
5.2.2 Periodic table (ground states only)



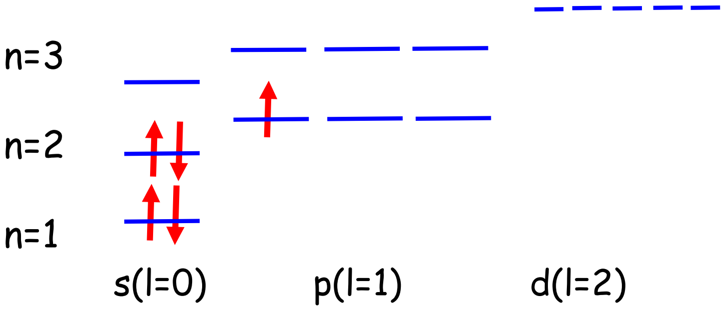
$Z=2$ He $(1s)^2$ **S=0**



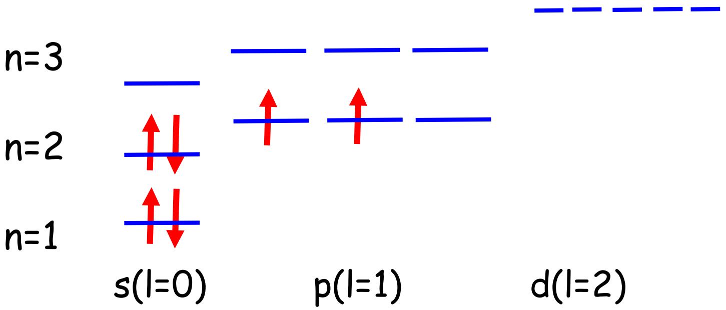
$Z=3$ Li $(1s)^2(2s)$ **S=1/2**



$Z=4$ Be $(1s)^2(2s)^2$ **S=0**

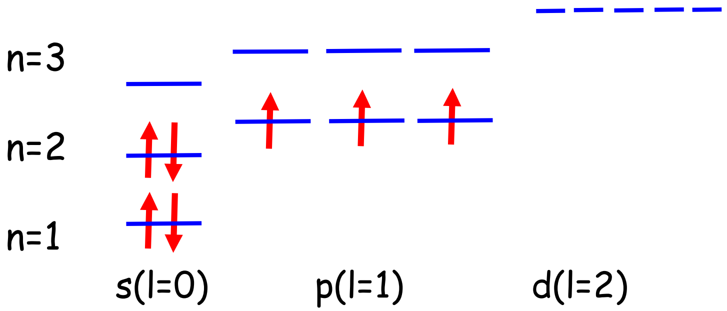


Z=5 B $(1s)^2(2s)^2(2p)$ **S=1/2**



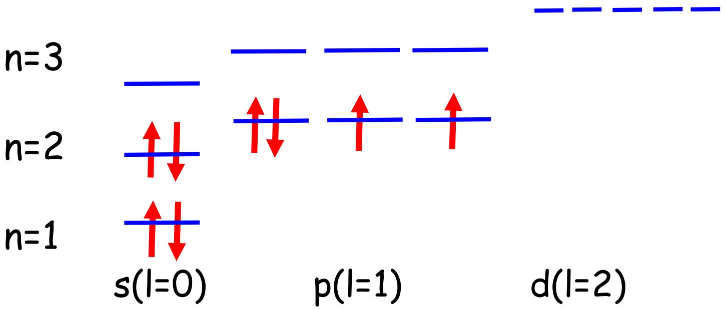
Z=6 C $(1s)^2\,(2s)^2(2p)^2$ **S=1**

Hund's rule (e-e repulsion, as we learned for He)



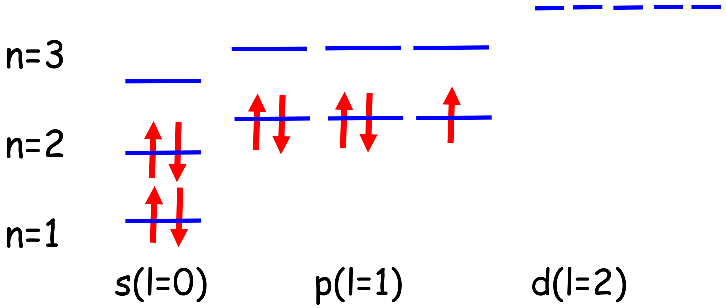
Z=7 N $(1s)^2(2s)^2(2p)^3$ **S=3/2**

Hund's rule (e-e repulsion)

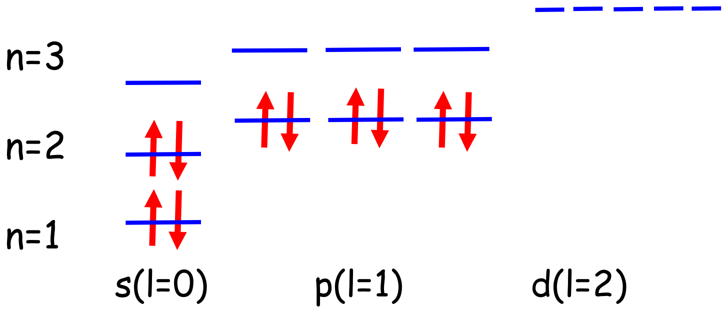


Z=8 O $(1s)^2(2s)^2(2p)^4$ **S=1**

Hund's rule (e-e repulsion)

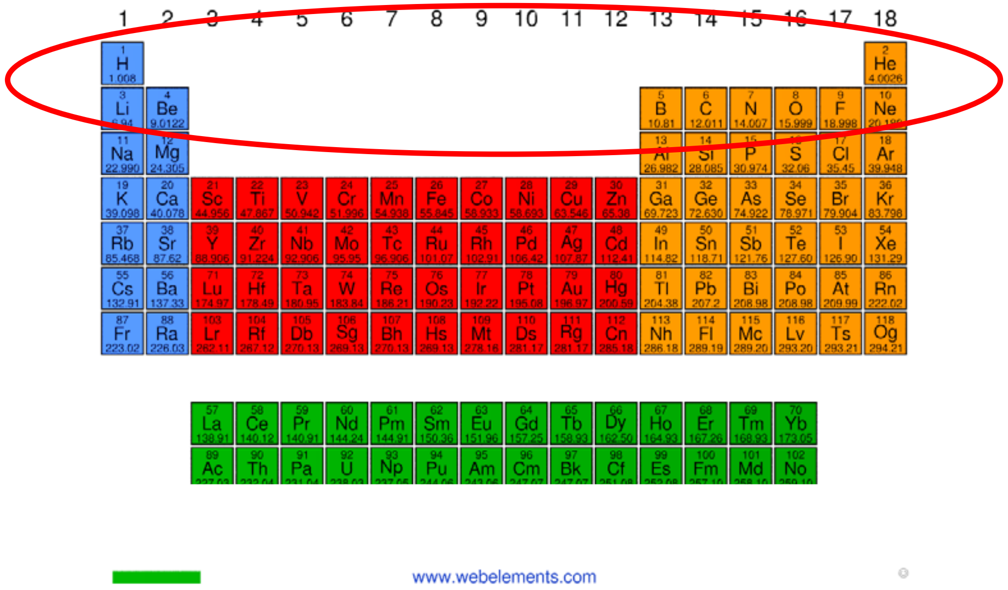


Z=9 F $(1s)^2(2s)^2(2p)^5$ **S=1/2**

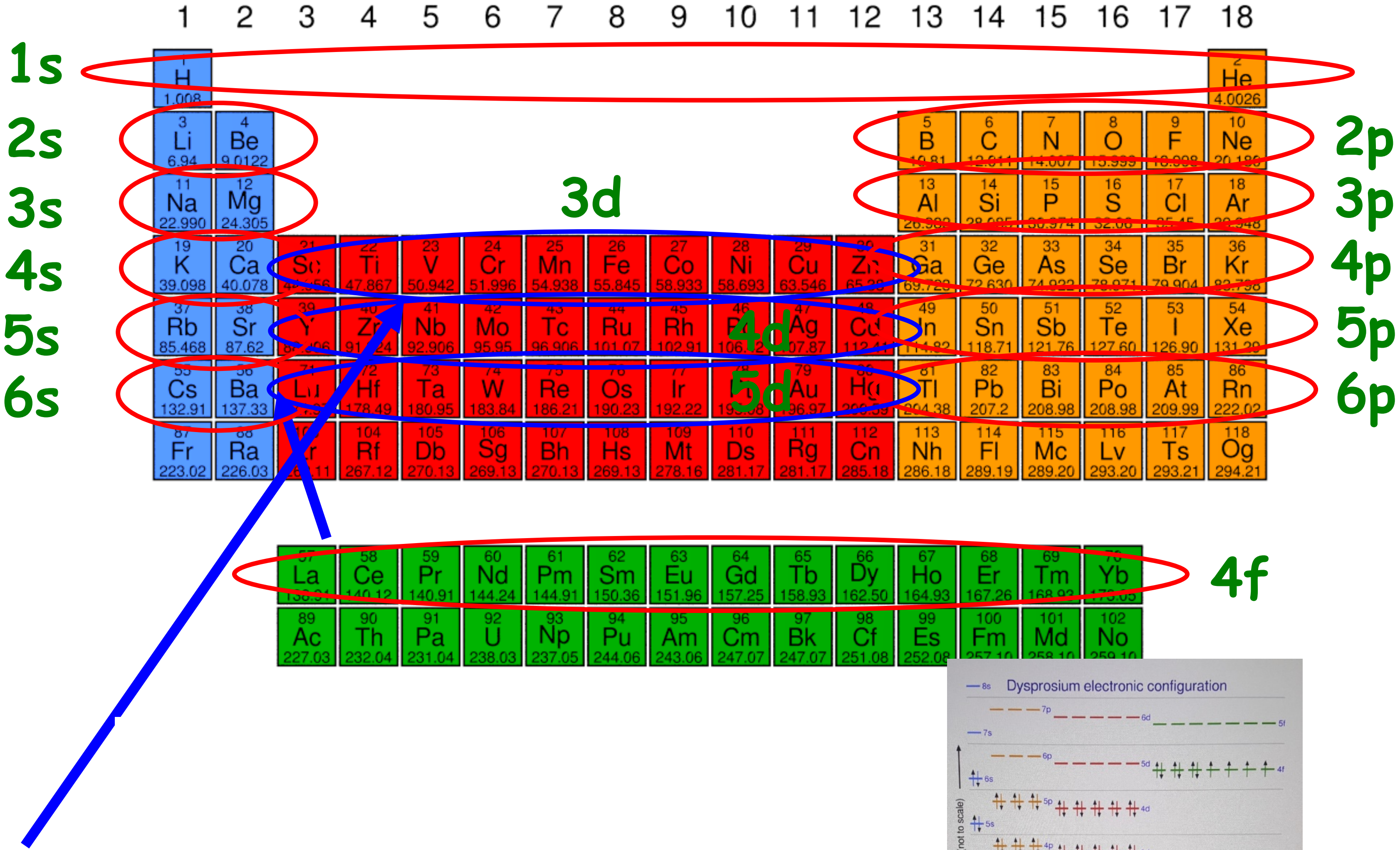


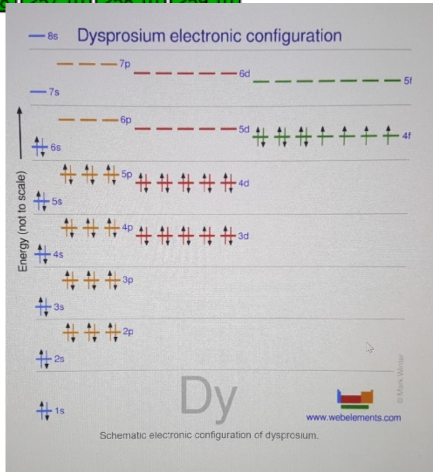
Z=10 Ne $(1s)^2(2s)^2(2p)^6$ **S=0**

Noble gas



Think for a few seconds what we achieved: ***the periodic table of Mendeleev***





Anomaly: in the split s vs p vs d,
3d ends up having more energy than 4s

Z	Element	Configuration	S	
1	H	$(1s)$	1/2	$^2S_{1/2}$
2	He	$(1s)^2$	0	$^1S_0$
3	Li	$(He)(2s)$	1/2	$^2S_{1/2}$
4	Be	$(He)(2s)^2$	0	$^1S_0$
5	B	$(He)(2s)^2(2p)$	1/2	$^2P_{1/2}$
6	C	$(He)(2s)^2(2p)^2$	1	$^3P_0$
7	N	$(He)(2s)^2(2p)^3$	3/2	$^4S_{3/2}$
8	O	$(He)(2s)^2(2p)^4$	1	$^3P_2$
9	F	$(He)(2s)^2(2p)^5$	1/2	$^2P_{3/2}$
10	Ne	$(He)(2s)^2(2p)^6$	0	$^1S_0$
11	Na	$(Ne)(3s)$	1/2	$^2S_{1/2}$
12	Mg	$(Ne)(3s)^2$	0	$^1S_0$
13	Al	$(Ne)(3s)^2(3p)$	1/2	$^2P_{1/2}$
14	Si	$(Ne)(3s)^2(3p)^2$	1	$^3P_0$
15	P	$(Ne)(3s)^2(3p)^3$	3/2	$^4S_{3/2}$
16	S	$(Ne)(3s)^2(3p)^4$	1	$^3P_2$
17	Cl	$(Ne)(3s)^2(3p)^5$	1/2	$^2P_{3/2}$
18	Ar	$(Ne)(3s)^2(3p)^6$	0	$^1S_0$

$^{2S+1}L_J$

All 3 numbers are TOTAL

In each subsell, like 2p, the state with max S total, wins. **Example**: N has 2S+1=4 i.e. S=3/2 due to e-e repulsion.

About L: "S" means L=0, "P" means L=1, "D" means L=2,…, but now L is "total L".

J, the total angular momentum, could be L+S, …. ,|L-S| depending on small energy differences.

The "Hund's rules" for L and J are more chaotic, with many exceptions. Just read about them in the book if you like …

Up to this point is what you need to know for Test 1.

One problem will surely involve the diagonalization of a 2x2 matrix in the context of a spin in a magnetic field.