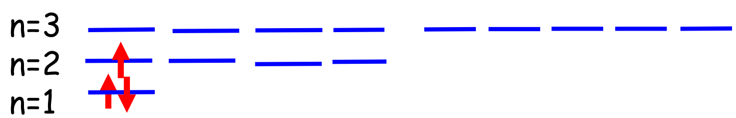
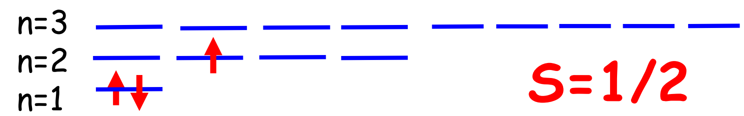
Hund's Rule: If there is a degeneracy between total S=0 vs total S=1, the triplet wins due to e-e repulsion.

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

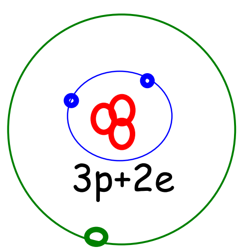


vs

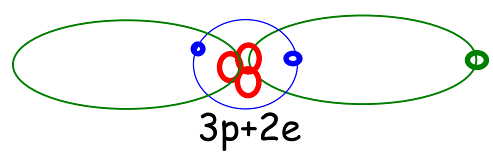


S=1/2
L=1

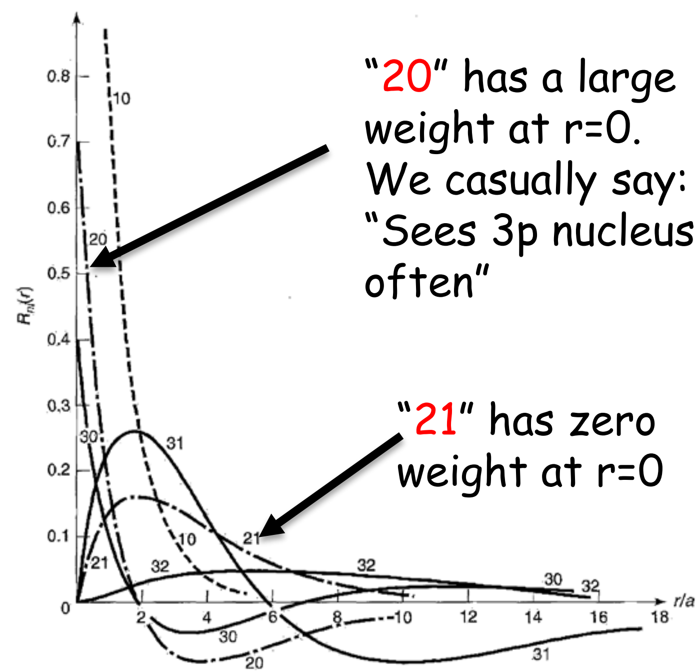
Rule: e-p attraction favors the lowest total "l" between subshells (like s vs p) due to "screening" of p:



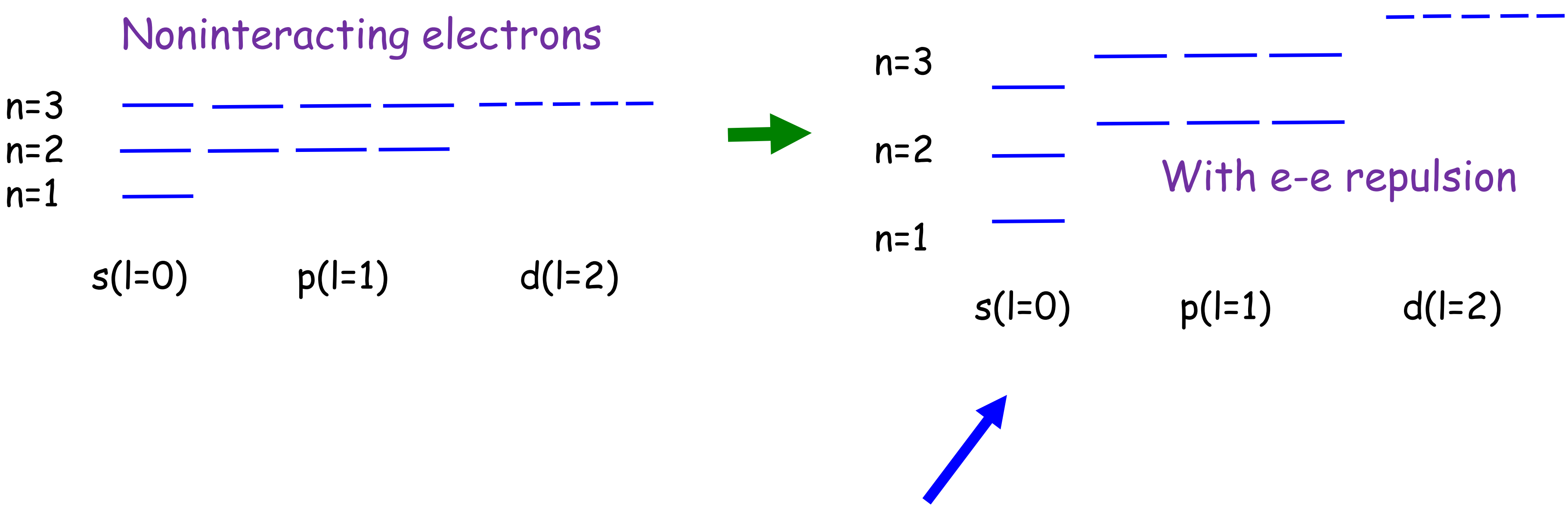
Sees the nuclear 3p often



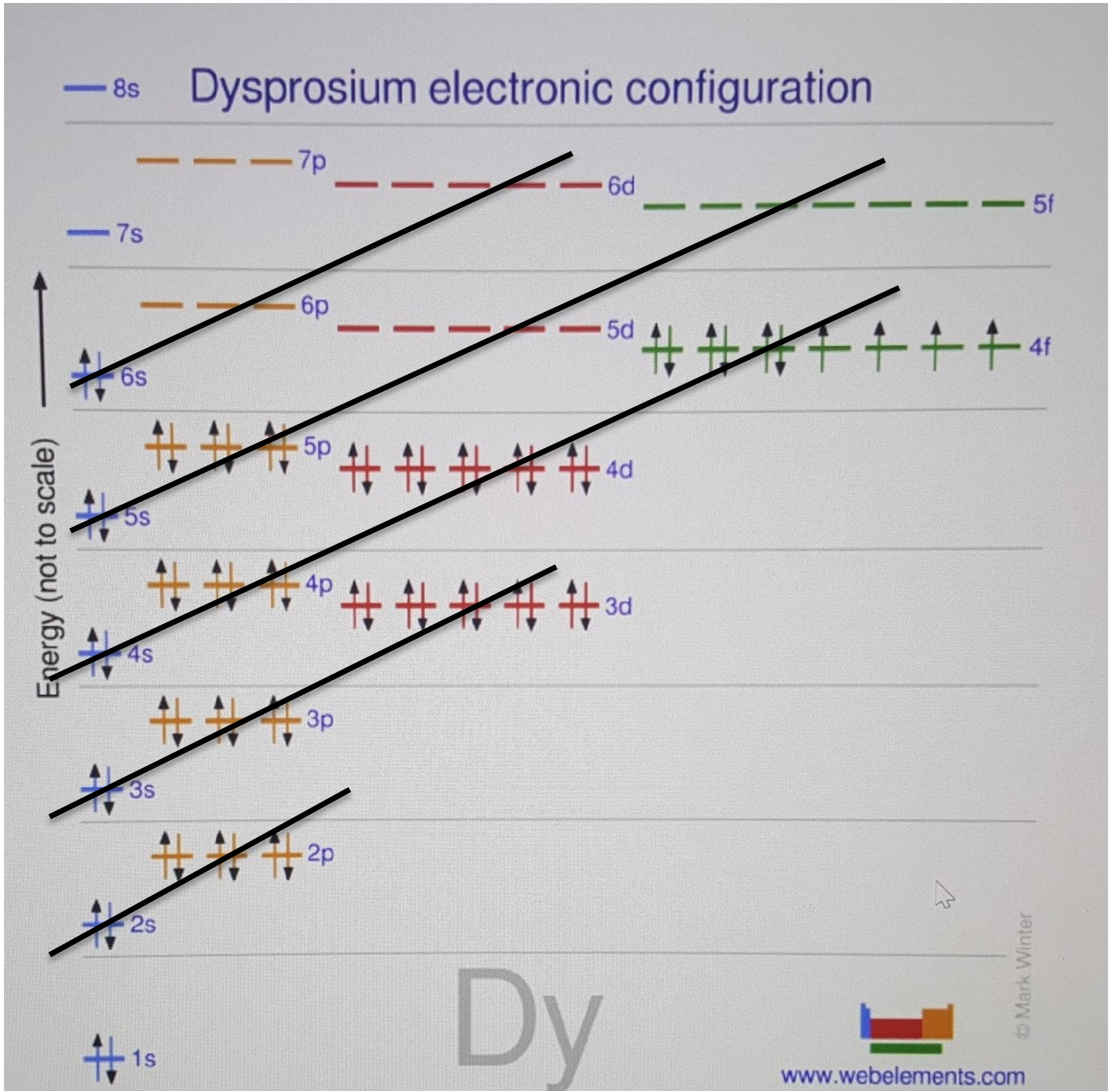
Sees a net central charge 3p+2e often (screening)



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

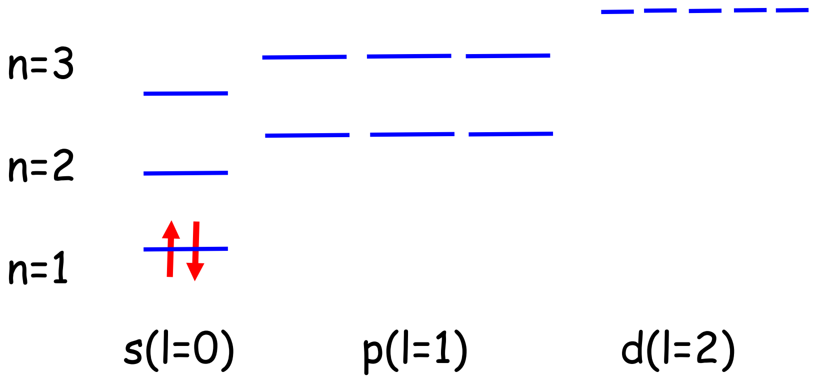


This is the order we have to use to construct the periodic table from now on.

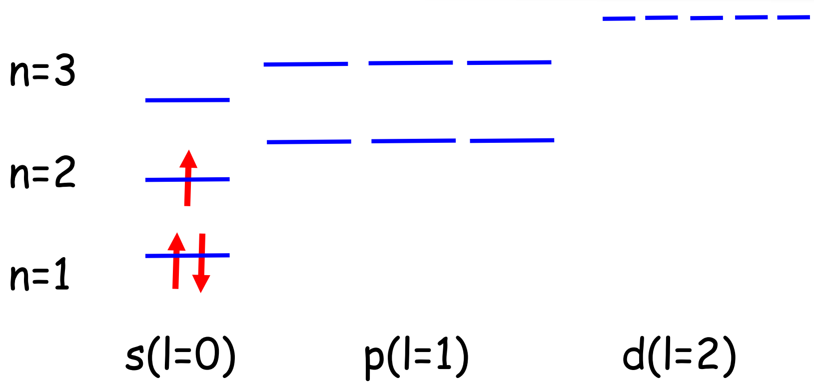


Schematic electronic configuration of dysprosium.

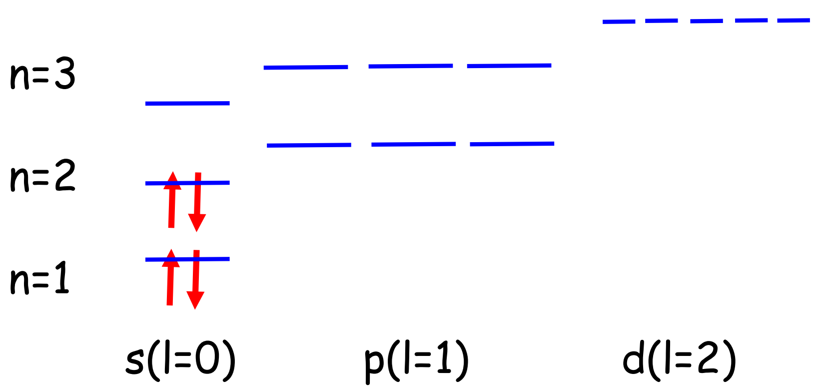
5.2.2 Periodic table *(ground states only)*



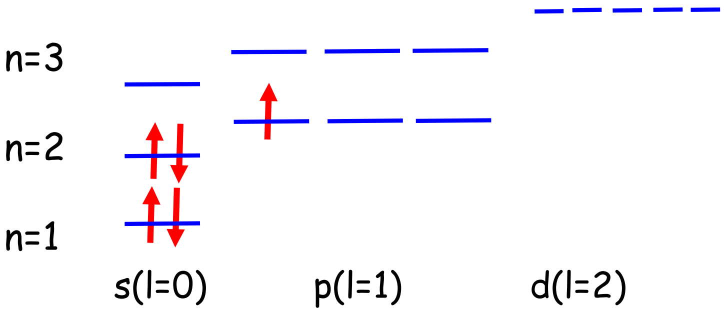
Z=2 He $(1s)^2$ **S=0**



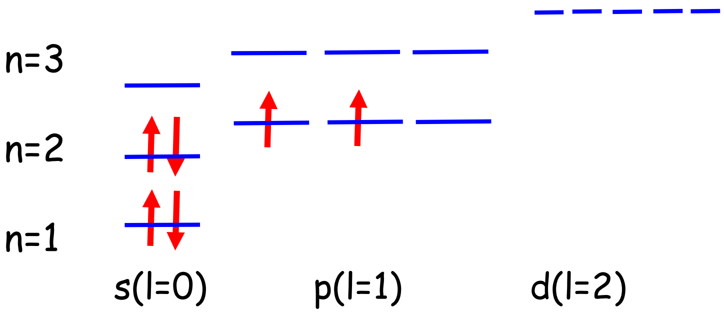
Z=3 Li $(1s)^2(2s)$ **S=1/2**



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

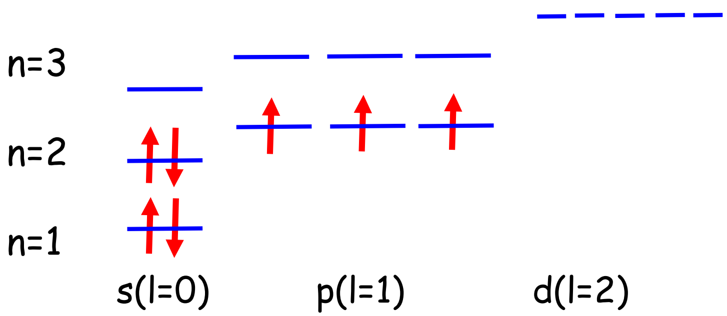


Z=5 B $(1s)^2(2s)^2(2p)$ **S=1/2**



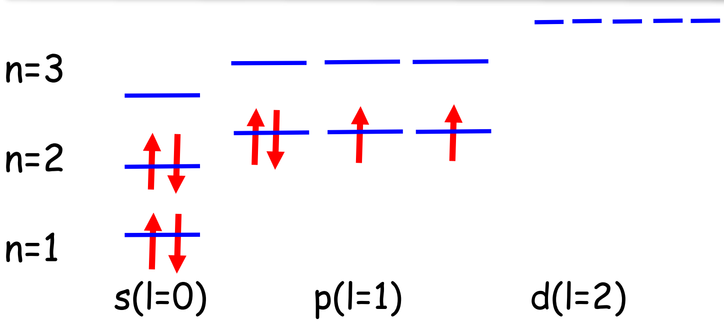
Z=6 C $(1s)^2 (2s)^2(2p)^2$ **S=1**

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



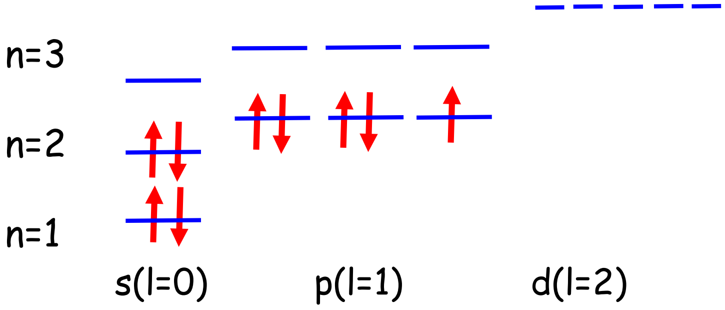
Z=7 N $(1s)^2(2s)^2(2p)^3$ **S=3/2**

Hund's rule (e-e repulsion)

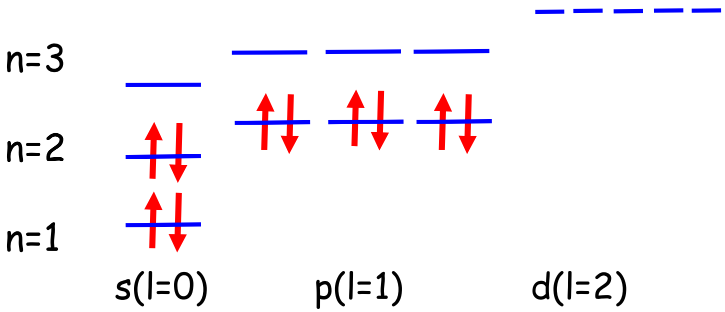


Z=8 O $(1s)^2(2s)^2(2p)^4$ **S=1**

Hund's rule (e-e repulsion)

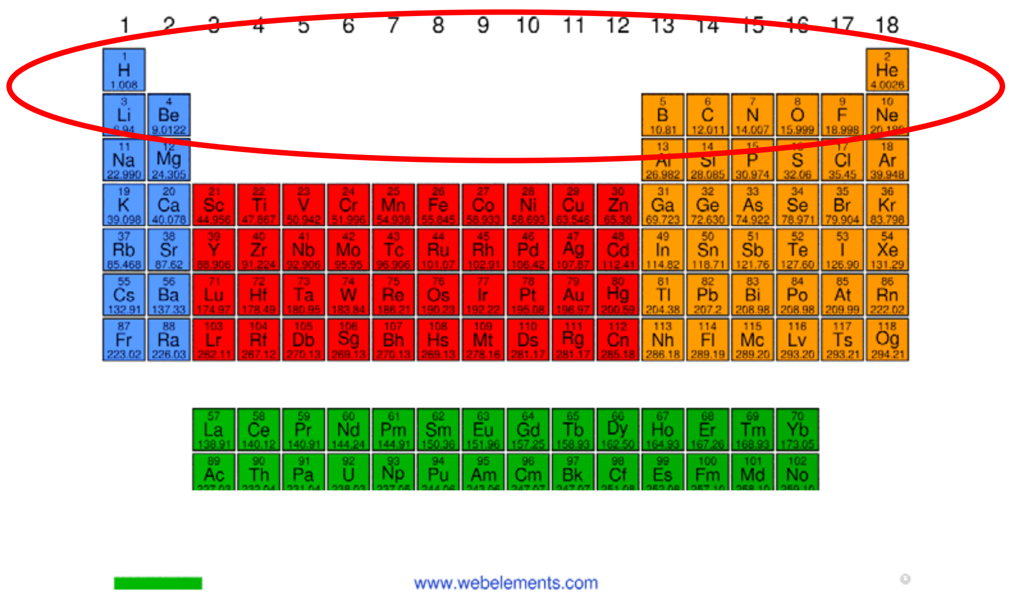


$Z=9$ F $(1s)^2(2s)^2(2p)^5$ **S=1/2**

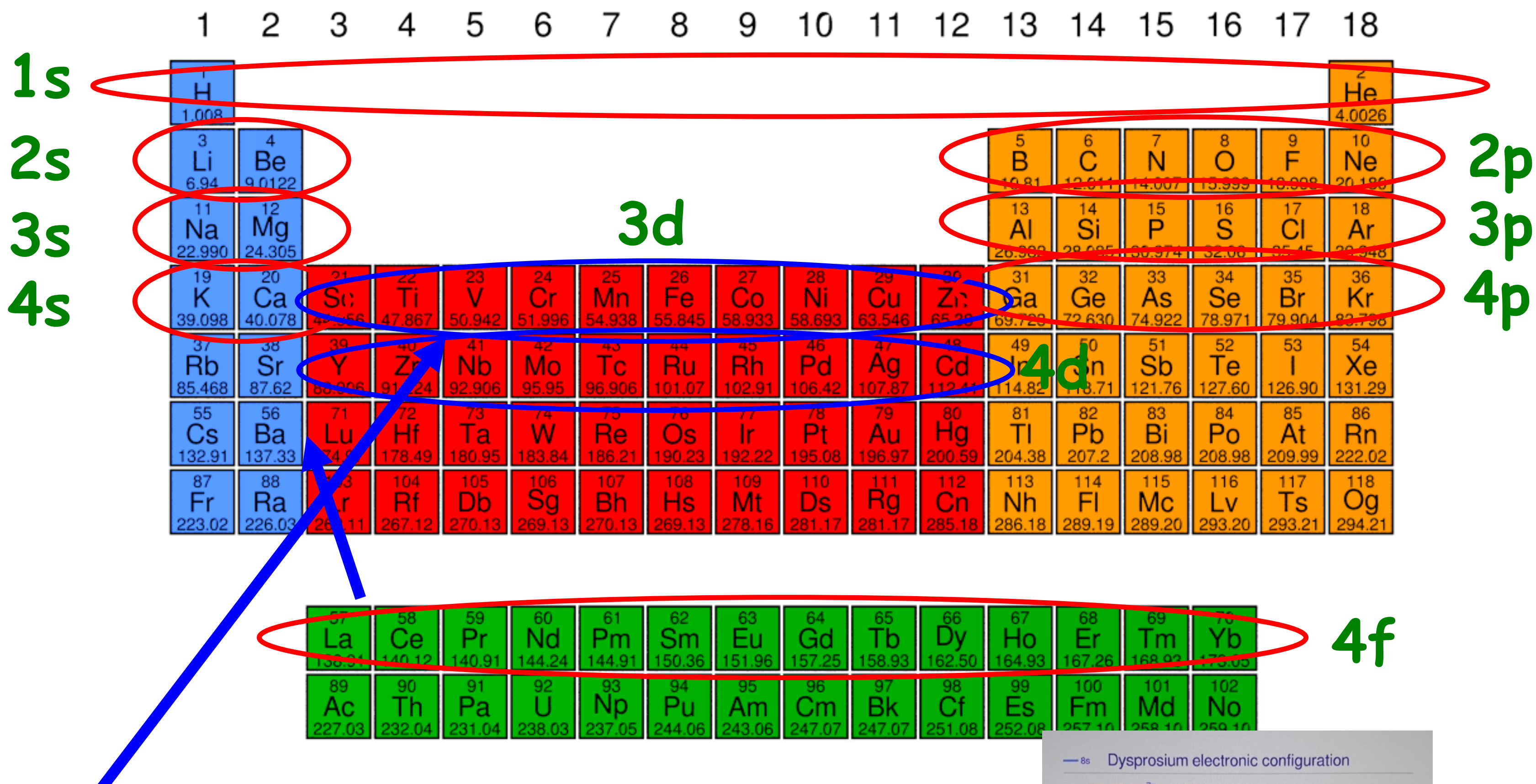


$Z=10$ Ne $(1s)^2(2s)^2(2p)^6$ **S=0**

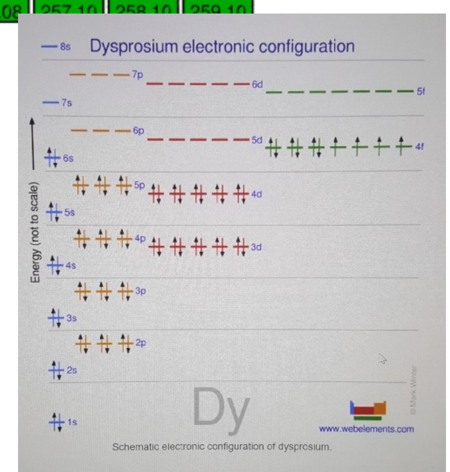
Noble gas



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 subshell, 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.

Problem 1 will involve the diagonalization of a 2x2 matrix in the context of a spin in a magnetic field