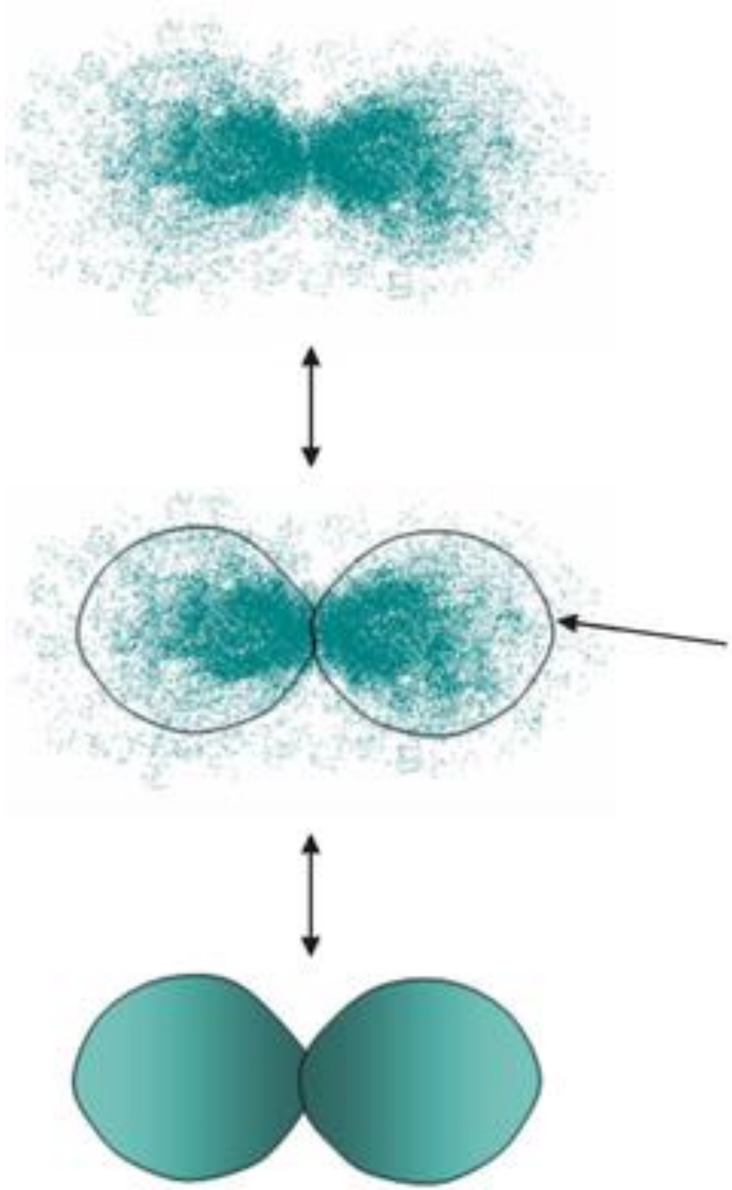
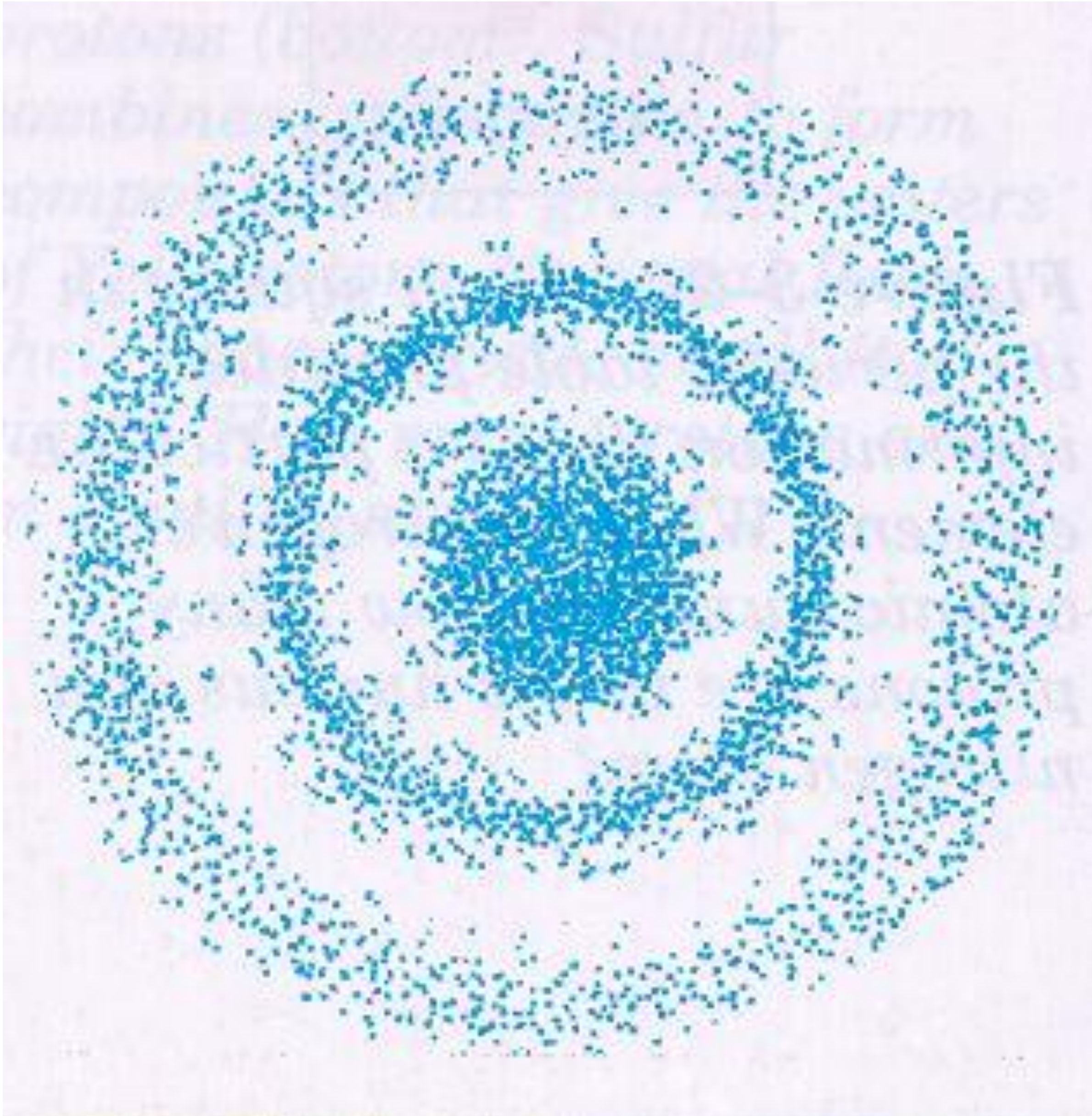
Electron Configurations

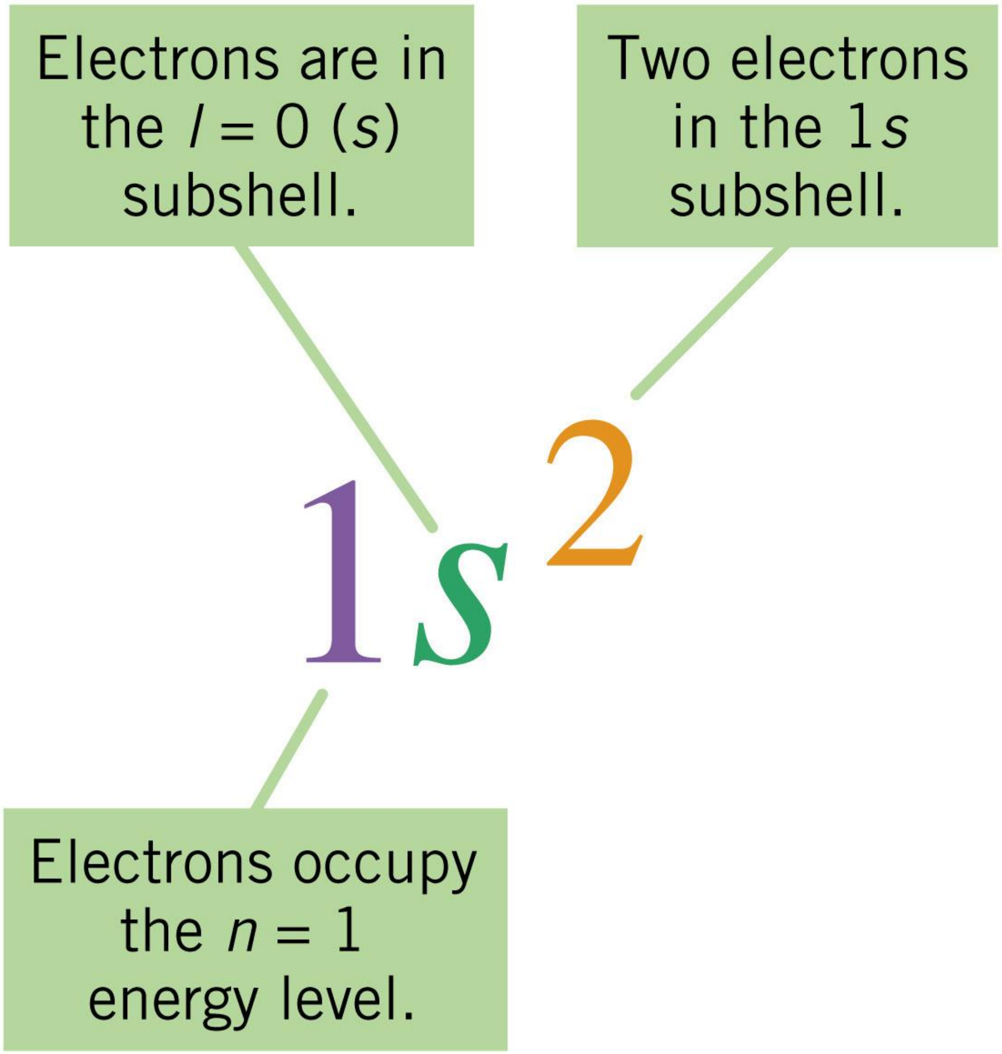
And Orbital Diagrams


the electron density in an electron wave
90% of the electron density is inside the two lobes drawn on the electron wave
these balloons represent the region of space which contains 90% of the electron density for this particular electron wave

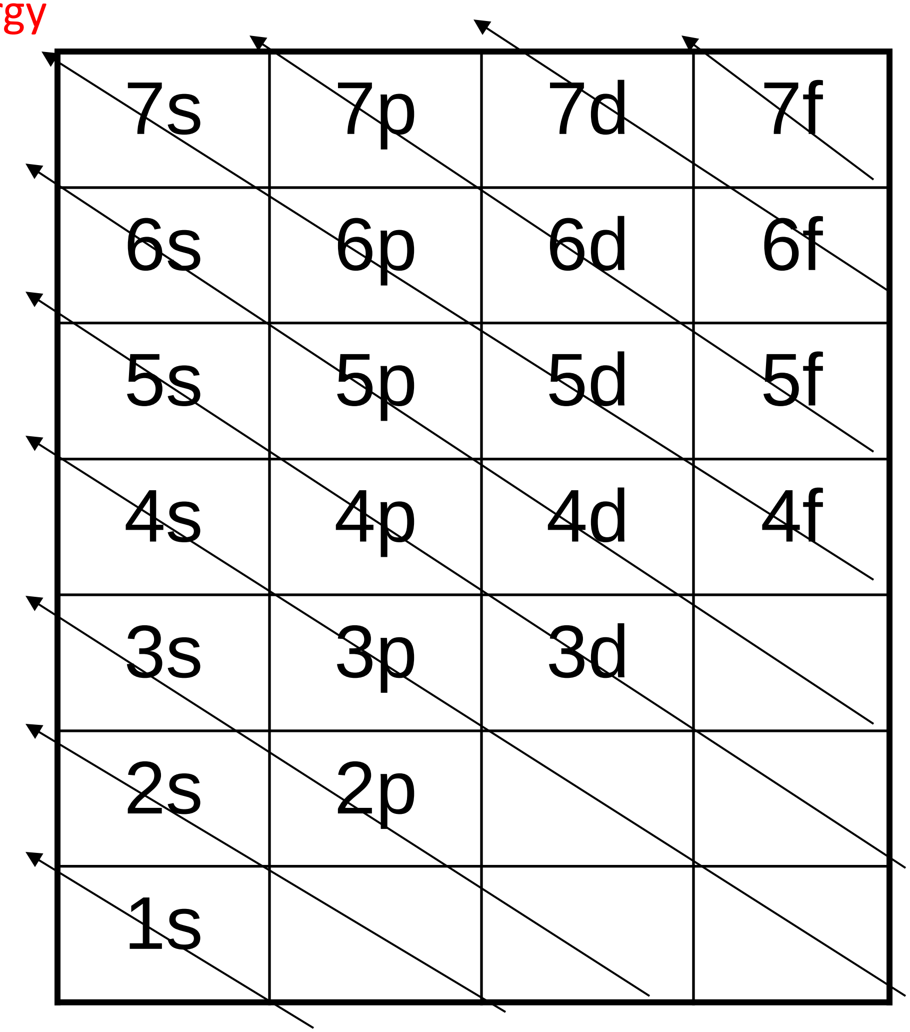


Principles for Filling Orbitals

- Writing electron configurations –



Aufbau principle

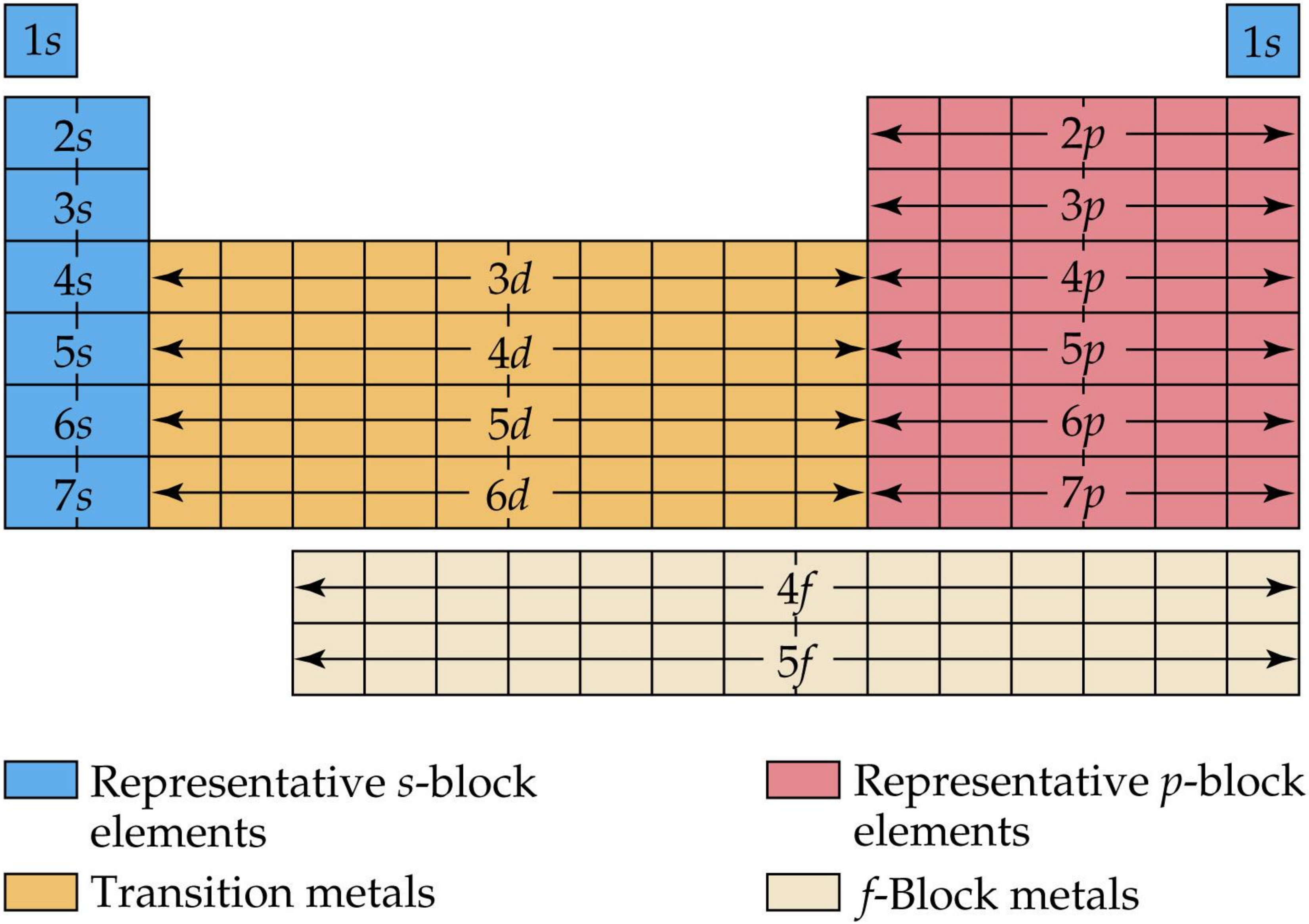


- Electrons are added one at a time to the lowest energy levels available until all the electrons have been accounted for –
- 2 electrons per orbital

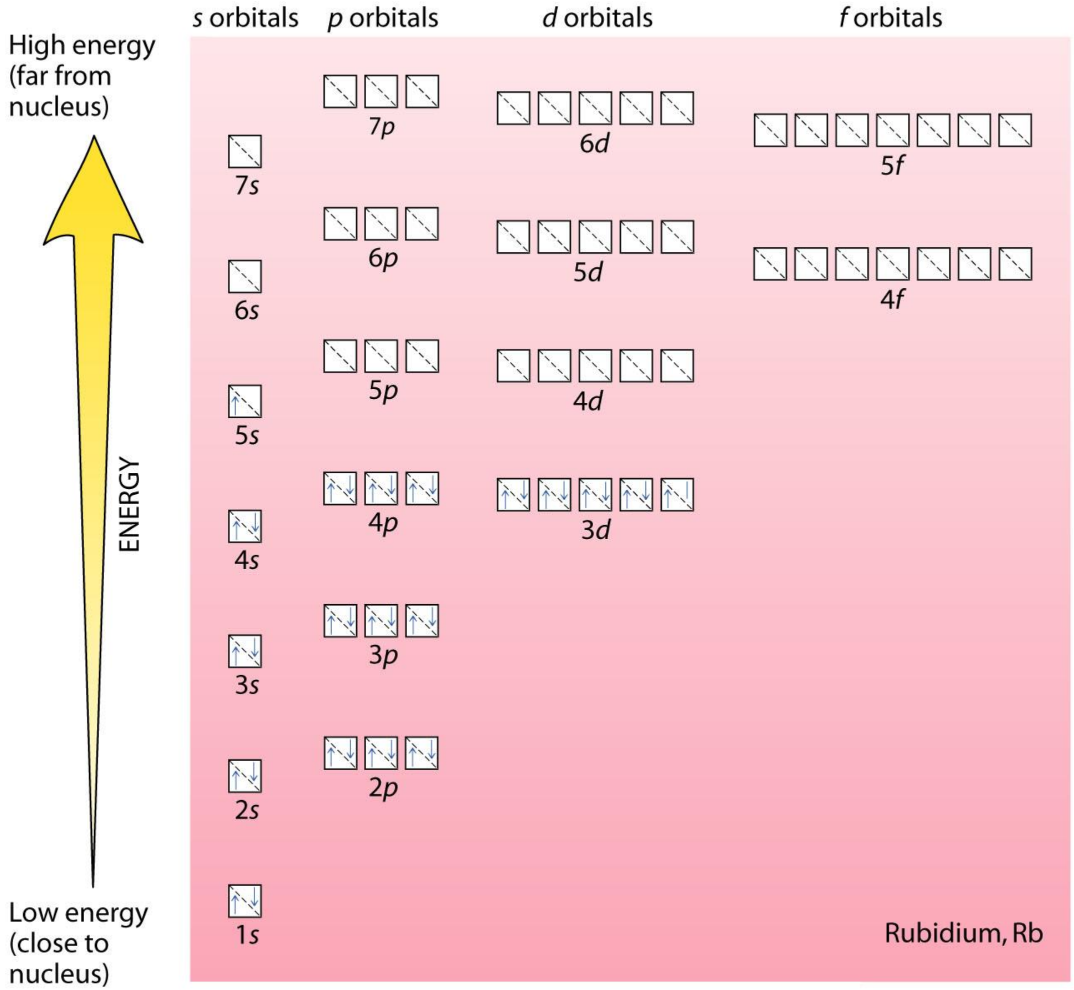
Carbon: $1s^2\ 2s^2\ 2p^2$

(up to 6 electrons can fit in a psublevel, 2 in each of 3 orbitals)

The Periodic Table and Predicted Orbital Configurations



Another way to show an Aufbau diagram:



Two Other Rules for Filling Orbitals:

- **Pauli Exclusion Principle** - Electrons must have opposite spins to occupy the same orbital.
- **Hund's Rule**: Orbitals must be filled in a way that gives the maximum number of unpaired electrons.
  – By placing electrons in different orbitals, electron-electron repulsions are minimized.

Using Hund's Rule and the Pauli Exclusion Principle

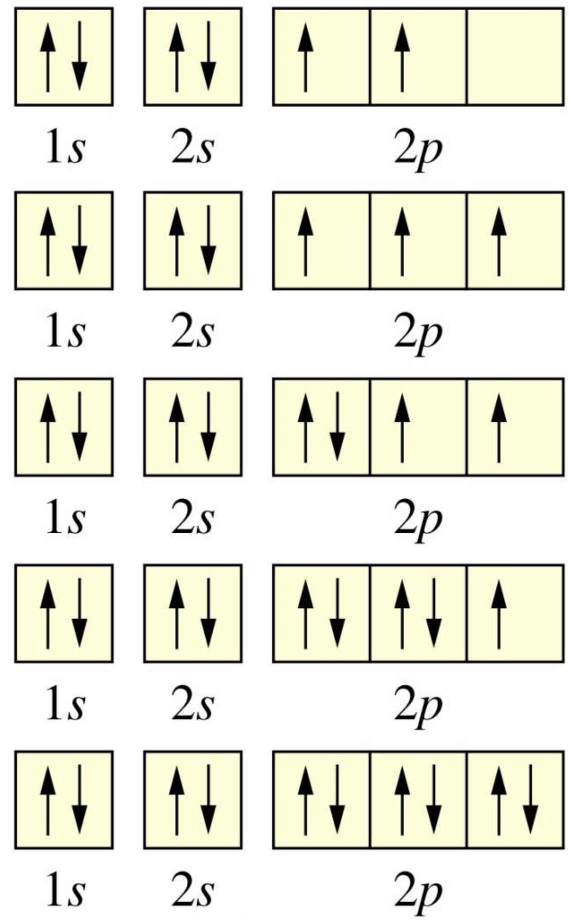
(Z = 6) C $1s^2 2s^2 2p^2$

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

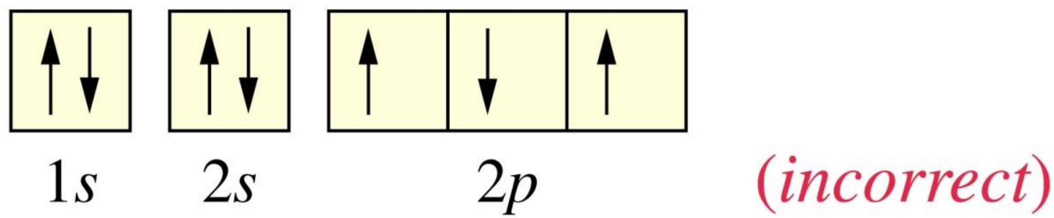
(Z = 8) O $1s^2 2s^2 2p^4$

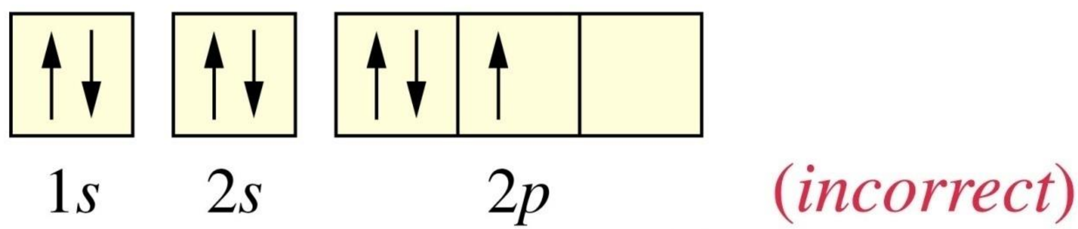
(Z = 9) F $1s^2 2s^2 2p^5$

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

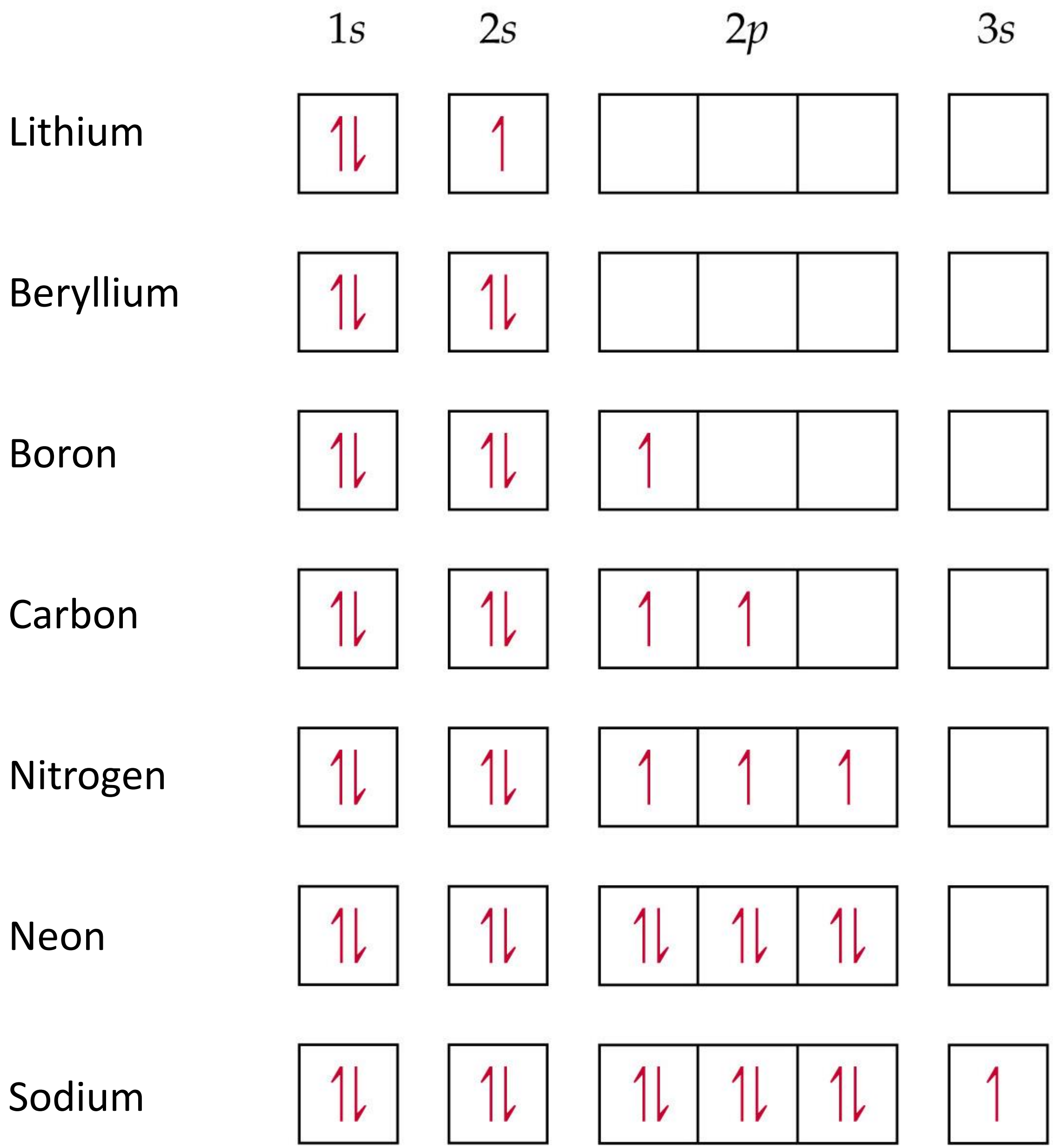


2 mistakes

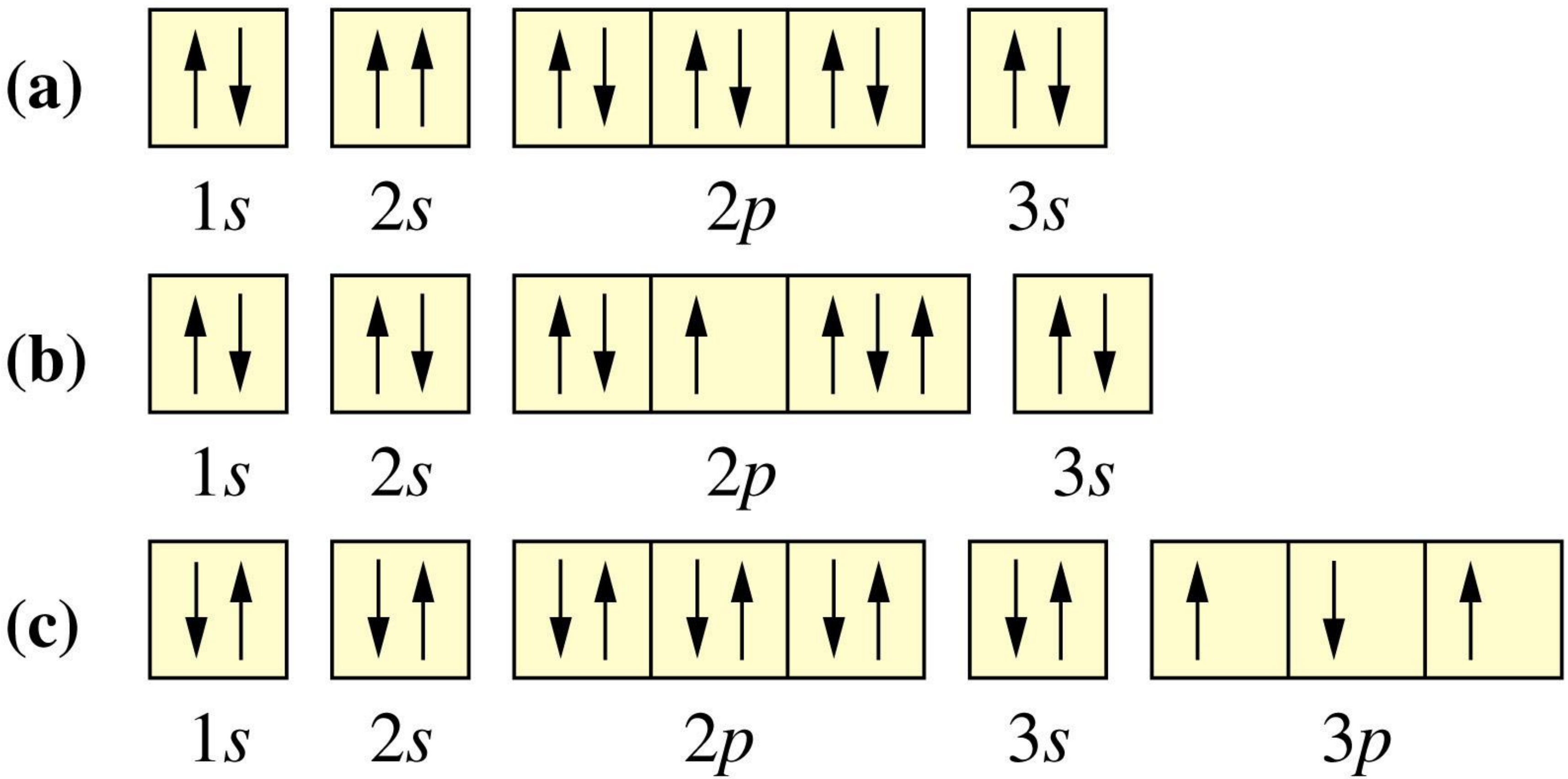




Orbital Diagrams



What is wrong with these?



Abbreviated Electron Configurations

- Highlights Valence electrons
- The preceding noble gas symbol in brackets followed by the rest of the configuration.

For Example:

Sodium [Ne] $3s^1$

Fluorine [He} $2s^2$ $2p^5$

Electronic Classification

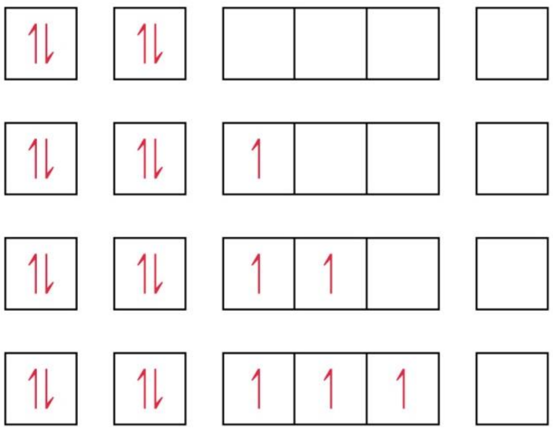
- ***Core e$^-$***: complete the previously filled noble gas
- ***Valence e$^-$***: are in the highest energy level outside the noble gas core. Involved in bonding.
- ***Pseudo-valence e-*** : are outside the noble gas core in lower energy levels
  - contribute to shielding
  - occasionally take part in bonding

Patterns in Electron Configurations

Atomic number	Symbol	Electron configuration
1	H	$1s^1$
2	He	$1s^2$
3	Li	$[He]2s^1$
4	Be	$[He]2s^2$
5	B	$[He]2s^22p^1$
6	C	$[He]2s^22p^2$
7	N	$[He]2s^22p^3$
8	O	$[He]2s^22p^4$
9	F	$[He]2s^22p^5$
10	Ne	$[He]2s^22p^6$
11	Na	$[Ne]3s^1$
12	Mg	$[Ne]3s^2$
13	Al	$[Ne]3s^23p^1$
14	Si	$[Ne]3s^23p^2$
15	P	$[Ne]3s^23p^3$
16	S	$[Ne]3s^23p^4$
17	Cl	$[Ne]3s^23p^5$
18	Ar	$[Ne]3s^23p^6$
19	K	$[Ar]4s^1$
20	Ca	$[Ar]4s^2$
21	Sc	$[Ar]4s^23d^1$
22	Ti	$[Ar]4s^23d^2$
23	V	$[Ar]4s^23d^3$
24	Cr	$[Ar]4s^23d^5$
25	Mn	$[Ar]4s^23d^5$
26	Fe	$[Ar]4s^23d^6$
27	Co	$[Ar]4s^23d^7$
28	Ni	$[Ar]4s^23d^8$
29	Cu	$[Ar]4s^23d^{10}$
30	Zn	$[Ar]4s^23d^{10}$
31	Ga	$[Ar]4s^23d^{10}4p^1$
32	Ge	$[Ar]4s^23d^{10}4p^2$
33	As	$[Ar]4s^23d^{10}4p^3$
34	Se	$[Ar]4s^23d^{10}4p^4$
35	Br	$[Ar]4s^23d^{10}4p^5$
36	Kr	$[Ar]4s^23d^{10}4p^6$
37	Rb	$[Kr]5s^1$
38	Sr	$[Kr]5s^2$
39	Y	$[Kr]5s^24d^1$
40	Zr	$[Kr]5s^24d^2$
41	Nb	$[Kr]5s^14d^4$
42	Mo	$[Kr]5s^14d^5$
43	Tc	$[Kr]5s^24d^5$
44	Ru	$[Kr]5s^14d^7$
45	Rh	$[Kr]5s^14d^8$
46	Pd	$[Kr]4d^{10}$
47	Ag	$[Kr]5s^14d^{10}$
48	Cd	$[Kr]5s^24d^{10}$
49	In	$[Kr]5s^14d^{10}5p^1$
50	Sn	$[Kr]5s^14d^{10}5p^2$
51	Sb	$[Kr]5s^14d^{10}5p^3$
52	Te	$[Kr]5s^14d^{10}5p^4$
53	I	$[Kr]5s^14d^{10}5p^5$

Unpaired Electrons

- Unpaired electrons are important.
- If an element has unpaired electrons, it is paramagnetic and attracts a magnet.
- If an element has no unpaired electrons it is diamagnetic and does not attract a magnet.



Exceptions to the electronic configurations

Following the rules for Cr, Cu, Ag, and Au using noble gas notation we expect the following:

Element	Expected	Experimental
Cr	[Ar] $3d^4\ 4s^2$	[Ar] $3d^5\ 4s^1$
Cu	[Ar] $3d^9\ 4s^2$	[Ar] $3d^{10}\ 4s^1$
Ag	[Kr] $4d^9\ 5s^2$	[Kr] $4d^{10}\ 5s^1$
Au	[Xe] $5d^9\ 6s^2$	[Xe] $5d^{10}\ 6s^1$

Core	1A 1	2A 2	3B 3	4B 4	5B 5	6B 6	7B 7	8B 8	8B 9	8B 10	1B 11	2B 12	3A 13	4A 14	5A 15	6A 16	7A 17	8A 18
	1 **H** $1s^1$																	2 **He** $1s^2$
[He]	3 **Li** $2s^1$	4 **Be** $2s^2$											5 **B** $2s^22p^1$	6 **C** $2s^22p^2$	7 **N** $2s^22p^3$	8 **O** $2s^22p^4$	9 **F** $2s^22p^5$	10 **Ne** $2s^22p^6$
[Ne]	11 **Na** $3s^1$	12 **Mg** $3s^2$											13 **Al** $3s^23p^1$	14 **Si** $3s^23p^2$	15 **P** $3s^23p^3$	16 **S** $3s^23p^4$	17 **Cl** $3s^23p^5$	18 **Ar** $3s^23p^6$
[Ar]	19 **K** $4s^1$	20 **Ca** $4s^2$	21 **Sc** $3d^14s^2$	22 **Ti** $3d^24s^2$	23 **V** $3d^34s^2$	24 **Cr** $3d^54s^1$	25 **Mn** $3d^54s^2$	26 **Fe** $3d^64s^2$	27 **Co** $3d^74s^2$	28 **Ni** $3d^84s^2$	29 **Cu** $3d^{10}4s^1$	30 **Zn** $3d^{10}4s^2$	31 **Ga** $3d^{10}4s^2 4p^1$	32 **Ge** $3d^{10}4s^2 4p^2$	33 **As** $3d^{10}4s^2 4p^3$	34 **Se** $3d^{10}4s^2 4p^4$	35 **Br** $3d^{10}4s^2 4p^5$	36 **Kr** $3d^{10}4s^2 4p^6$
[Kr]	37 **Rb** $5s^1$	38 **Sr** $5s^2$	39 **Y** $4d^15s^2$	40 **Zr** $4d^25s^2$	41 **Nb** $4d^35s^2$	42 **Mo** $4d^55s^1$	43 **Tc** $4d^55s^2$	44 **Ru** $4d^75s^1$	45 **Rh** $4d^85s^1$	46 **Pd** $4d^{10}$	47 **Ag** $4d^{10}5s^1$	48 **Cd** $4d^{10}5s^2$	49 **In** $4d^{10}5s^2 5p^1$	50 **Sn** $4d^{10}5s^2 5p^2$	51 **Sb** $4d^{10}5s^2 5p^3$	52 **Te** $4d^{10}5s^2 5p^4$	53 **I** $4d^{10}5s^2 5p^5$	54 **Xe** $4d^{10}5s^2 5p^6$
[Xe]	55 **Cs** $6s^1$	56 **Ba** $6s^2$	71 **Lu** $4f^{14}5d^1 6s^2$	72 **Hf** $4f^{14}5d^2 6s^2$	73 **Ta** $4f^{14}5d^3 6s^2$	74 **W** $4f^{14}5d^4 6s^2$	75 **Re** $4f^{14}5d^5 6s^2$	76 **Os** $4f^{14}5d^6 6s^2$	77 **Ir** $4f^{14}5d^7 6s^2$	78 **Pt** $4f^{14}5d^9 6s^1$	79 **Au** $4f^{14}5d^{10} 6s^1$	80 **Hg** $4f^{14}5d^{10} 6s^2$	81 **Tl** $4f^{14}5d^{10} 6s^26p^1$	82 **Pb** $4f^{14}5d^{10} 6s^26p^2$	83 **Bi** $4f^{14}5d^{10} 6s^26p^3$	84 **Po** $4f^{14}5d^{10} 6s^26p^4$	85 **At** $4f^{14}5d^{10} 6s^26p^5$	86 **Rn** $4f^{14}5d^{10} 6s^26p^6$
[Rn]	87 **Fr** $7s^1$	88 **Ra** $7s^2$	103 **Lr** $5f^{14}6d^1 7s^2$	104 **Rf** $5f^{14}6d^2 7s^2$	105 **Db** $5f^{14}6d^3 7s^2$	106 **Sg** $5f^{14}6d^4 7s^2$	107 **Bh** $5f^{14}6d^5 7s^2$	108 **Hs** $5f^{14}6d^6 7s^2$	109 **Mt** $5f^{14}6d^7 7s^2$	110	111	112		114		116		

Core	Series														
[Xe]	Lanthanide series	57 **La** $5d^16s^2$	58 **Ce** $4f^15d^1 6s^2$	59 **Pr** $4f^36s^2$	60 **Nd** $4f^46s^2$	61 **Pm** $4f^56s^2$	62 **Sm** $4f^66s^2$	63 **Eu** $4f^76s^2$	64 **Gd** $4f^75d^1 6s^2$	65 **Tb** $4f^96s^2$	66 **Dy** $4f^{10}6s^2$	67 **Ho** $4f^{11}6s^2$	68 **Er** $4f^{12}6s^2$	69 **Tm** $4f^{13}6s^2$	70 **Yb** $4f^{14}6s^2$
[Rn]	Actinide series	89 **Ac** $6d^17s^2$	90 **Th** $6d^27s^2$	91 **Pa** $5f^26d^1 7s^2$	92 **U** $5f^36d^1 7s^2$	93 **Np** $5f^46d^1 7s^2$	94 **Pu** $5f^67s^2$	95 **Am** $5f^77s^2$	96 **Cm** $5f^76d^1 7s^2$	97 **Bk** $5f^97s^2$	98 **Cf** $5f^{10}7s^2$	99 **Es** $5f^{11}7s^2$	100 **Fm** $5f^{12}7s^2$	101 **Md** $5f^{13}7s^2$	102 **No** $5f^{14}7s^2$

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