Chapter 8 - Electron Configurations and Periodicity

Section 1 – Writing Electron Configurations

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Introduction – Electron Configuration

In previous chapter we learned that electrons exist in atoms in specific locations and are always in motion – in the shell (orbit) and within the subshell (orbital).

In this chapter we will learn how to fill these electrons in atoms in two different ways:

- Electronic configuration (spdf notation): Here we fill electrons in the various sub shells according to given rules.
- Box configuration: In this case we show electrons as arrows and subshells as boxes and then fill out the electrons.

The Rules of Filling Electrons

There are three main rules for filling electrons in shells and subshells.

- Aufbau principle: building up the electronic configuration using ground state energies. Electrons and filled in the subshells according to energy levels of shells and subshells.
  - Fill the lowest energy electrons first, no matter which shell they belong to.
- Pauli's exclusion principle: No two electrons can have the same quantum numbers.
  - In one orbital/subshell (m_l number), the electrons should have opposite spin (magnetic spin numbers).
  - One orbital/subshell (m_l number) can have a maximum of 2 electrons.
- Hund's rule: Fill the electrons in the subshells singly first, then pair them up. (magnetic quantum number – m_l)
  - Electrons do not pair in degenerate orbitals (same energy orbitals) if an empty orbital is available.

The First Three Rows

Row 1

H	$1s^1$
He	$1s^2$

Here are the electron configurations in spdf notation, for the first 18 elements in the periodic table.
The shell number is written first, followed by subshell and then the number of electrons in that subshell, written as superscript.

Row 2

Li	$1s^2\ 2s^1$
Be	$1s^2\ 2s^2$
B	$1s^2\ 2s^2\ 2p^1$
C	$1s^2\ 2s^2\ 2p^2$
N	$1s^2\ 2s^2\ 2p^3$
O	$1s^2\ 2s^2\ 2p^4$
F	$1s^2\ 2s^2\ 2p^5$
Ne	$1s^2\ 2s^2\ 2p^6$

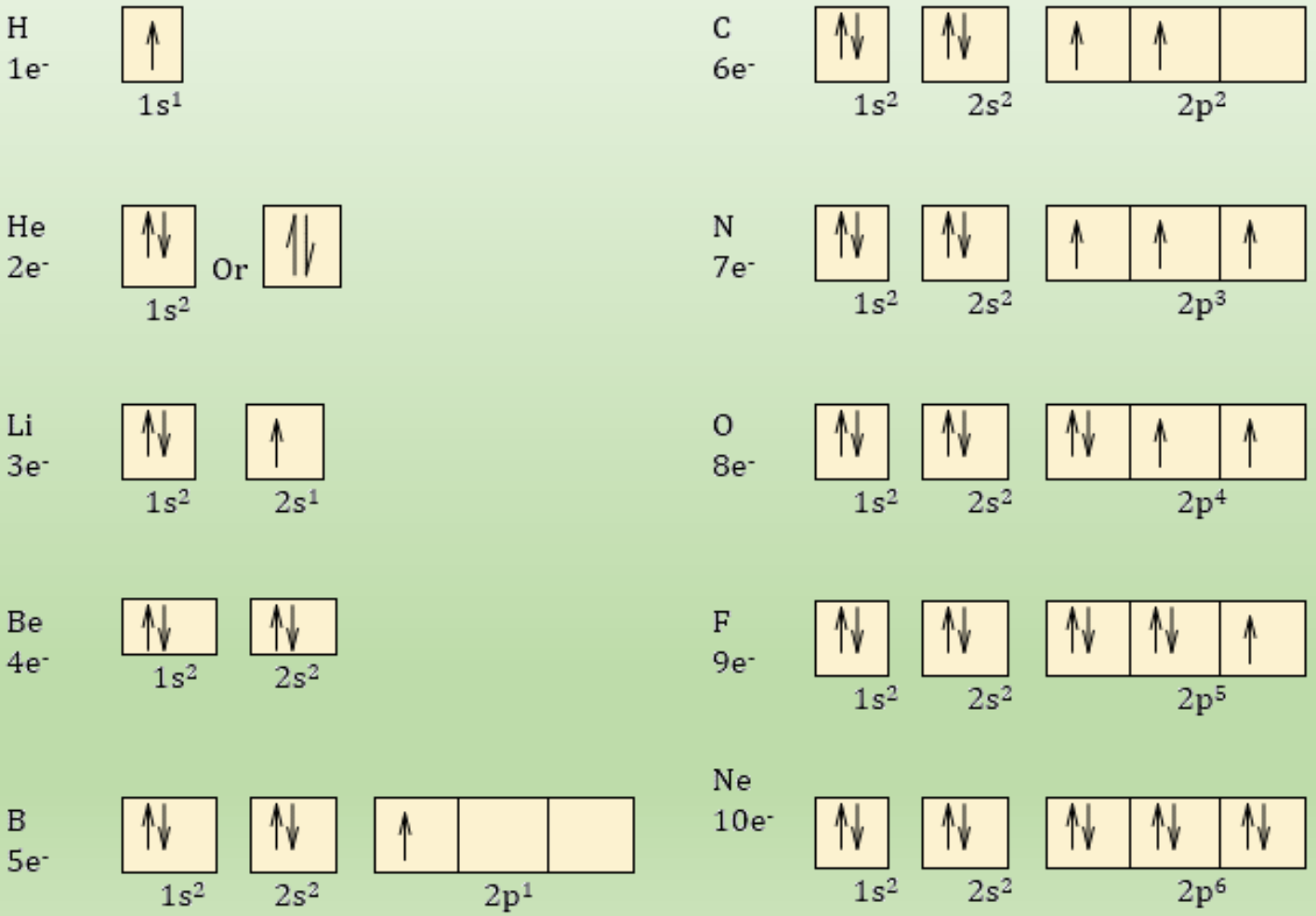
Row 3

Na	$1s^2\ 2s^2\ 2p^6\ 3s^1$
Mg	$1s^2\ 2s^2\ 2p^6\ 3s^2$
Al	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$
Si	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$
P	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3$
S	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^4$
Cl	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$
Ar	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$

Box Configuration

To fill the electrons in box, use full or half arrows to show electrons (as shown for He).

Electrons are filled singly first and then paired up in any orbital.



Rules for Writing Electron Configurations

The three rules for writing electron configurations are straightforward for the first 20 elements. After that, attention should be paid to Aufbau principle, which is that electrons should be in orbitals of lowest possible energy.

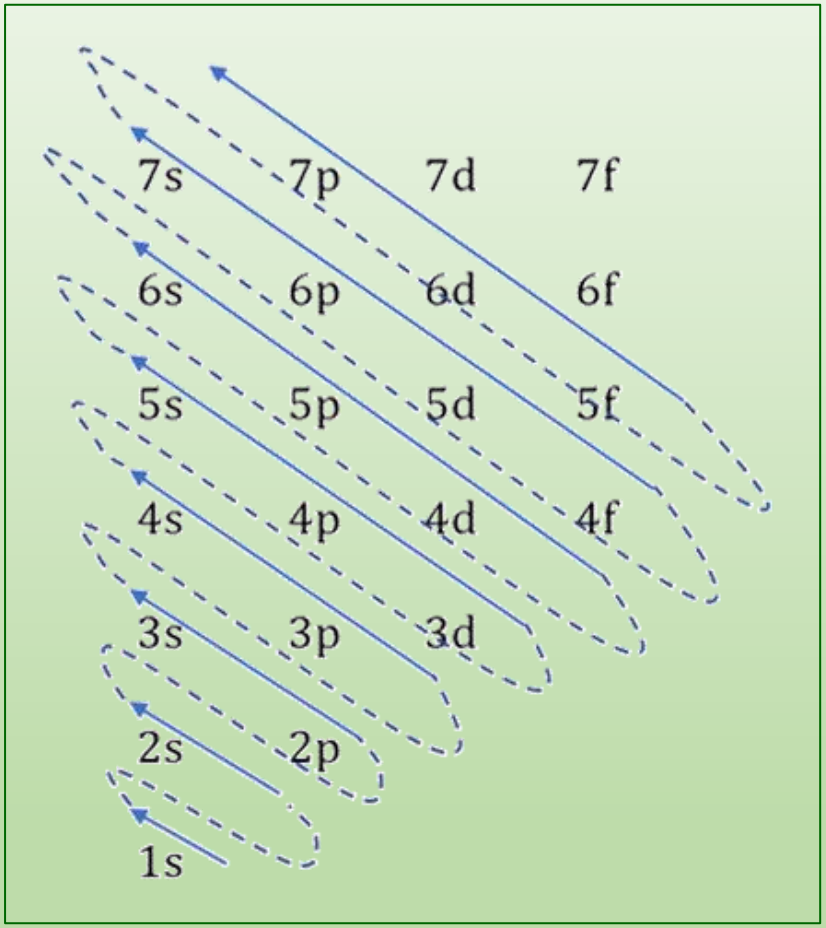
To understand this, the diagram on the right can help to see how energy levels are lower in orbitals that have higher shell number – e.g. 4s is lower in energy than 3d and 4p is higher than 3d.

- Orbitals fill in the following order:

  1s 2*s* 2*p* 3*s* 3*p* 4*s* 3*d* 4*p* 5*s* 4*d* 5*p* 6*s*

  or as shown on the right.

  (*Follow the arrow*)



Use the Periodic Table

IA	IIA											IIIA	IVA	VA	VIA	VIIA	VIIIA
1 H 1.008																	2 He 4.003
3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 15.99	9 F 18.99	10 Ne 20.18
11 Na 22.98	12 Mg 24.31	IIIB	IVB	VB	VIB	VIIB		VIIIB		IB	IIB	13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
19 K 39.1	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 51.99	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.63	33 As 74.92	34 Se 78.96	35 Br 79.9	36 Kr 83.8
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc 98.81	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
55 Cs 132.9	56 Ba 137.3	57 La 138.9	72 Hf 178.5	73 Ta 180.9	74 W 183.8	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.1	79 Au 197	80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209	84 Po [209]	85 At [210]	86 Rn [222]
87 Fr 223	88 Ra 226	89 Ac 227	104 Rf [267]	105 Db [268]	106 Sg [271]	107 Bh [267]	108 Hs [277]	109 Mt [276]	110 Ds [281]	111 Rg [272]	112 Cn [285]	113 Nh [266]	114 Fl [289]	115 Mc [289]	116 Lv [293]	117 Ts [294]	118 Og [294]

Patterns in Filling Electrons

When filling out electrons of the same group a pattern emerges.

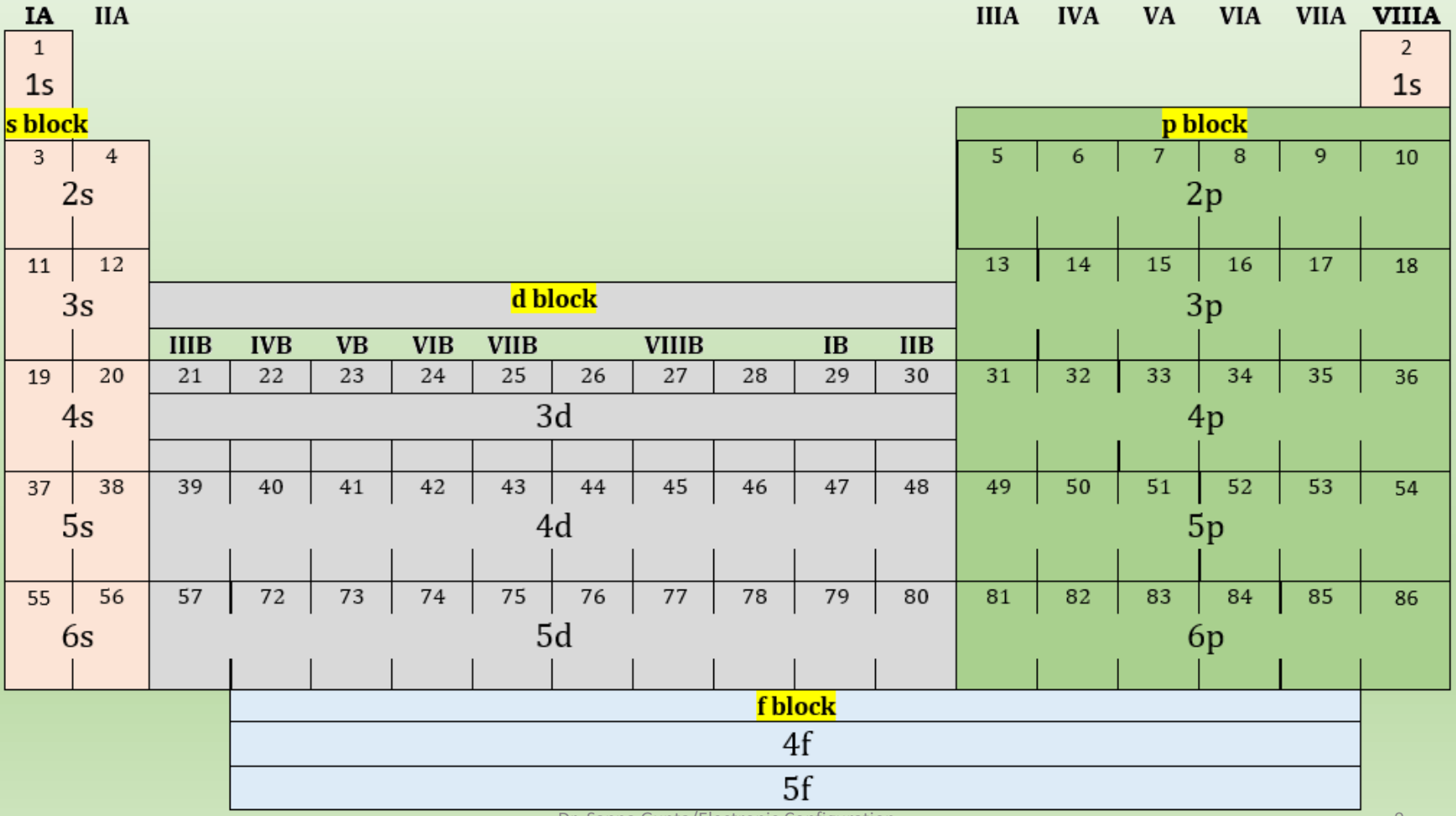
Group I $_{1}H$: $1s^1$ $_{3}Li$: $1s^2\ 2s^1$ $_{11}Na$: $1s^2\ 2s^2\ 2p^6\ 3s^1$	Group II $_{4}Be$: $1s^2\ 2s^2$ $_{12}Mg$: $1s^2\ 2s^2\ 2p^6\ 3s^2$
Group IV $_{6}C$: $1s^2\ 2s^2\ 2p^4$ $_{14}Si$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 2p^4$	Group VII $_{9}F$: $1s^2\ 2s^2\ 2p^5$ $_{17}Cl$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$

As we can see all group I element configuration ends in s^1, group II in s^2, group IV in p^4 and group VII in p^5. This patterns helps us to view the periodic table as different blocks depending on what subshell is filled last, s, p, d or f.

The other quick information one can get from the periodic table is the identity of the last electron filled, which shell and which orbital. See the next couple slides for more on this.

The Periodic Table Divided in Blocks

Last subshell for Group I will is always s^1, Group II always in s^2, hence group I and II is referred to "s block". Groups III to VIII are the "p block" as those elements fill the p subshell which can have 6 electrons. I have also written the **n** quantum number to show how each row indicates the shell number.



Two Considerations After n=3

Aufbau Principle: Energy of orbitals is not linear after 3rd shell. Here are things to watch out for when filling out the 3rd shell and above.

- Fill s in the higher n number before starting d. Fill the 4s before 3d because of energy consideration. Same goes for 5s before 4d.
- This gets more complicated when we get to filling f orbitals because f starts in the fourth shell but does not start filling until after 6s!

The chart on the previous slide showed the order in which to fill the electrons. The other way is to follow the periodic table as it is and remember that the transition metals will have one lower n number than the start of that row.

Transition Metals: In transition metals there are 10 electrons in d orbital and the consideration here is of stability. You will always fill s completely before d for two columns below:

- Chromium (4th column in transition metals) and elements below:
  Should be $4s^2, 3d^4$; But is $\mathbf{4s^1, 3d^5}$ (for Mo: $5s^1, 4d^5$)
- Copper (9th column in transition metals) and the elements below:
  Should be $4s^2\ 3d^9$; But is $\mathbf{4s^1, 3d^{10}}$ (for Ag: $5s^2, 4d^{10}$)

This is to make the d configuration more stable.

Use the Periodic Table

IA	IIA											IIIA	IVA	VA	VIA	VIIA	VIIIA
1 H 1.008																	2 He 4.003
3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 15.99	9 F 18.99	10 Ne 20.18
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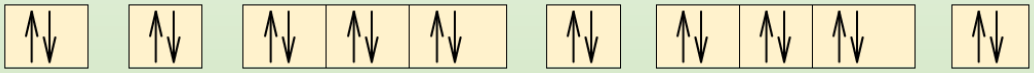
More Electron Configurations

Using all the rules and information we have learned, now we can fill electrons for elements with higher number electrons.

Calcium = 20 electrons; spdf notation: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$

Box notation:



Iron = 26 electrons; spdf notation: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$

Box notation:

Bromine = 35 electrons; spdf notation: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^5$

Box notation:

Electronic Configuration of Periodic Table

If you look in each of elements in the periodic table below, I have shown how the electrons are filled in the last shell of that element, e.g. the last shell filled in bromine is 4, so the last electrons filled are $4s^2\ 4p^5$. You can clearly see the trend in how electrons are filled in a row and in each group.

IA	IIA										IIIA	IVA	VA	VIA	VIIA	VIIIA
1 H $1s^1$																2 He $1s^2$
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 $2s^22p^6$
11 Na $3s^1$	12 Mg $3s^2$	IIIB	IVB	VB	VIB	VIIB		VIIIB		IB	IIB	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 $3s^23p^6$
19 K $4s^1$	20 Ca $4s^2$	21 Sc $4s^23d^1$	22 Ti $4s^23d^2$	23 V $4s^23d^3$	24 Cr $4s^13d^5$	25 Mn $4s^23d^5$	26 Fe $4s^23d^6$	27 Co $4s^23d^7$	28 Ni $4s^23d^8$	29 Cu $4s^13d^{10}$	30 Zn $4s^23d^{10}$	31 Ga $4s^24p^1$	32 Ge $4s^24p^2$	33 As $4s^24p^3$	34 Se $4s^24p^4$	35 Br $4s^24p^5$	36 Kr $4s^24p^6$
37 Rb $5s^1$	38 Sr $5s^2$	39 Y $5s^24d^1$	40 Zr $5s^24d^2$	41 Nb $5s^24d^3$	42 Mo $5s^14d^5$	43 Tc $5s^24d^5$	44 Ru $5s^24d^6$	45 Rh $5s^24d^7$	46 Pd $5s^24d^8$	47 Ag $5s^14d^{10}$	48 Cd $5s^24d^{10}$	49 In $5s^25p^1$	50 Sn $5s^25p^2$	51 Sb $5s^25p^3$	52 Te $5s^25p^4$	53 I $5s^25p^5$	54 Xe $5s^25p^6$
55 Cs $6s^1$	56 Ba $6s^2$	57 La $6s^25d^1$	72 Hf $6s^25d^2$	73 Ta $6s^25d^3$	74 W $6s^15d^5$	75 Re $6s^25d^5$	76 Os $6s^25d^6$	77 Ir $6s^25d^7$	78 Pt $6s^25d^8$	79 Au $6s^15d^{10}$	80 Hg $6s^25d^{10}$	81 Tl $6s^26p^1$	82 Pb $6s^26p^2$	83 Bi $6s^26p^3$	84 Po $6s^26p^4$	85 At $6s^26p^5$	86 Rn $6s^26p^6$

s – block **p – block** **d - block**

Filling out electrons in Using the PT

Iodine

53 (I) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^5$

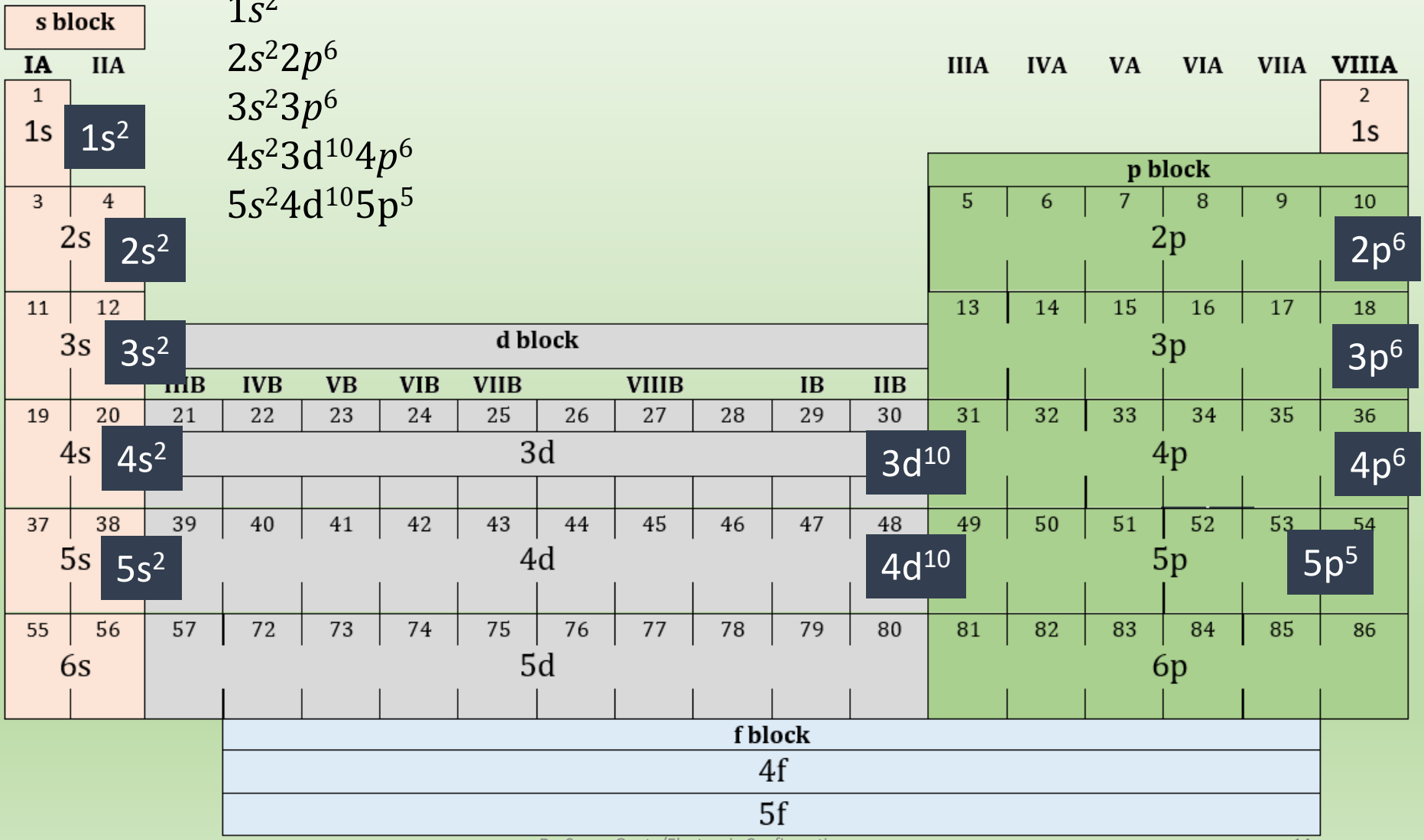
$1s^2$

$2s^2 2p^6$

$3s^2 3p^6$

$4s^2 3d^{10} 4p^6$

$5s^2 4d^{10} 5p^5$



Solved Problem: Identifying errors in spdf notation

Which of the following electron configurations are allowed and which are not allowed? If they are not allowed, explain why? And if possible, which rule is being violated.

a. $1s^2 2s^1 2p^3$

b. $1s^2 2s^2 2p^8$

c. $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{11}$

a. Not allowed; Fill s before starting p. Aufbau principle

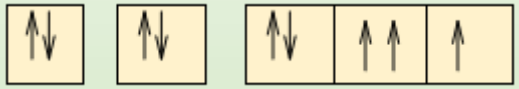
b. p^8 is not allowed. p can have only 6 e-. Pauli's exclusion principle.

c. Fill s before d and also d^{11} is not allowed because d has only 10 e- so fill it to 9 e (which also should be $s^1 d^{10}$). Aufbau principle.

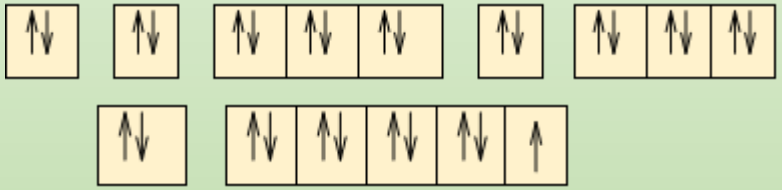
Solved Problem: Identifying errors in box configuration

Which of the following electron configurations are allowed and which are not allowed? If they are not allowed, explain why and give the correct answer.

a. Fluorine



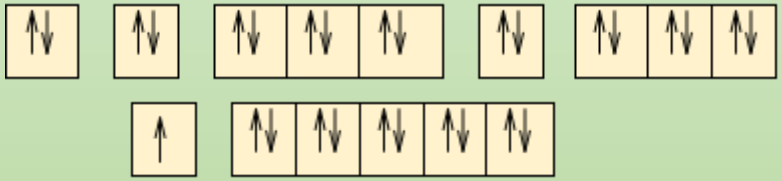
b. Copper



c. Sulfur

a. Fluorine has 9 electrons, so count it okay. It should have 5 electrons in the p orbital. Also, two electrons cannot have the same quantum numbers i.e. going in the same direction.

b. Copper has 29 electrons, so total count is okay, but d orbital needs to fill first before s in this case to make d electrons more stable.



c. Sulfur has 16 electrons, so total count is okay, and p should have 4 electrons, but any orbital cannot have more than 2 electrons.

Key Words

- Spdf and box configurations
- Pauli exclusion principle
- Hund's rule
- Aufbau principle
- Exceptions in filling out electrons after 3^{rd} shell and in d orbital.