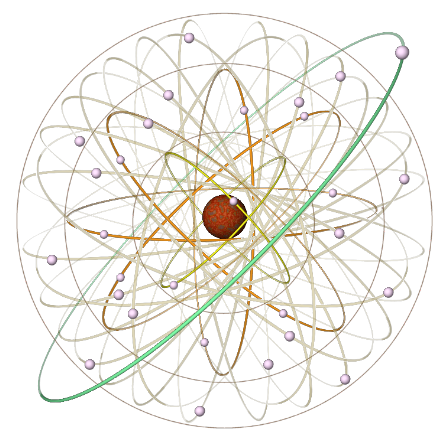
Ch08

Electron Configurations

We now understand the orbital structure of atoms.

Next we explore how electrons filling that structure change it.



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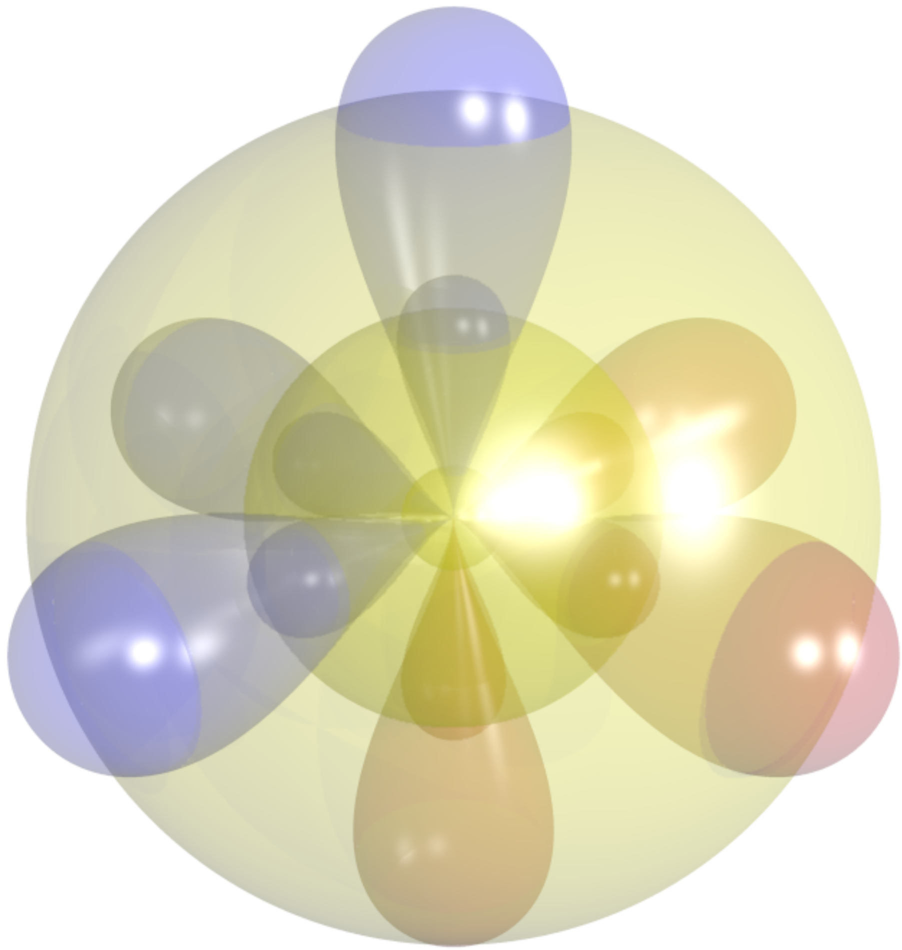
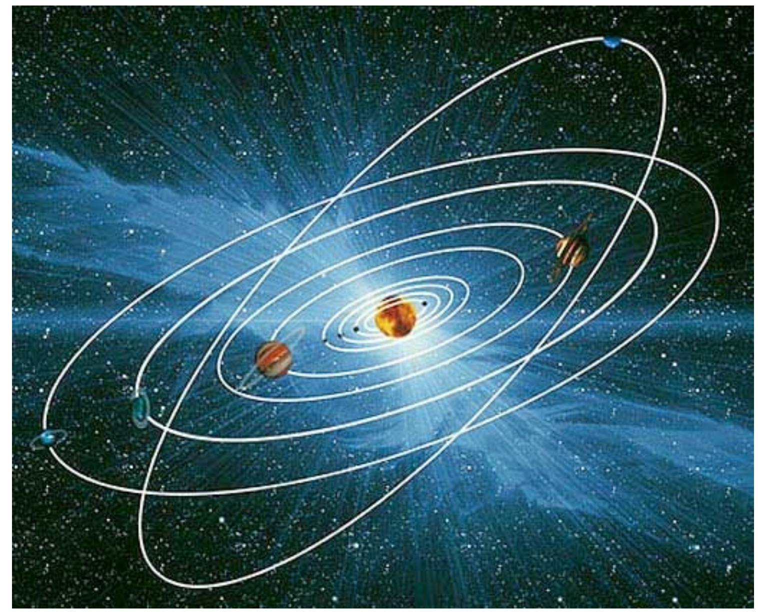
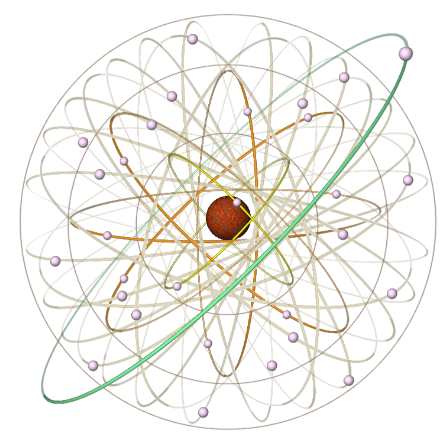


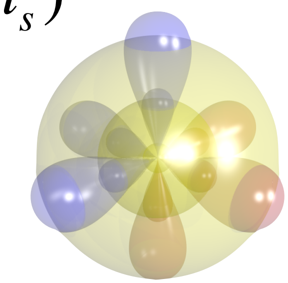


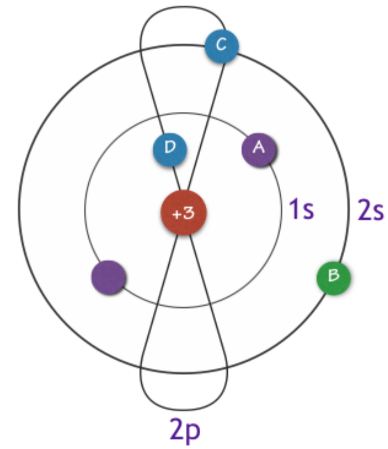


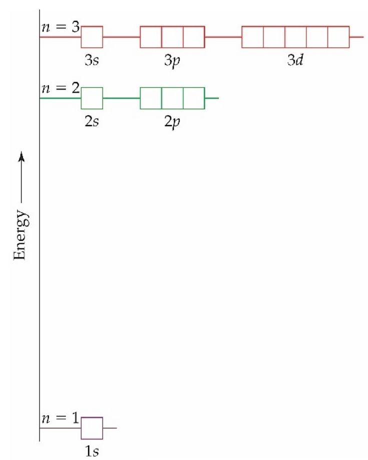
Putting Electrons into Orbitals

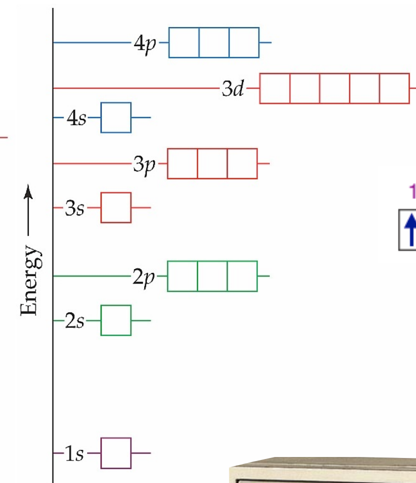
- Electron-Electron Interactions:
    - Electron Spin
    - Schrödinger Equation
        - The orbitals it defines
        - The energy of those orbitals
    - Orbital Splitting
        - Shielding & Penetration
    - Sub-level overlap
- Orbital Diagrams
    - Order of Sub-Levels
- Ground State Filling
    - Auf Bau Principle
    - Hund's Rule
    - Pauli Exclusion Principle
- Electron Shells
    - Valence Electrons
    - Core Electrons
- Electron Configuration notation
    - Compact notation
- Quantum Numbers
    - Describing Electron Positions

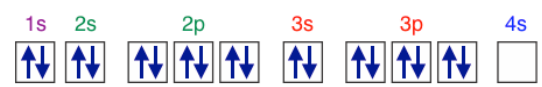
$$\Psi(n,l,m_l,m_s)$$

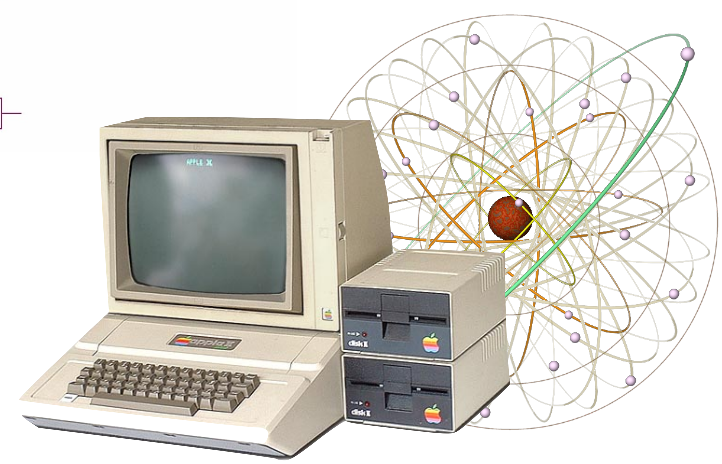






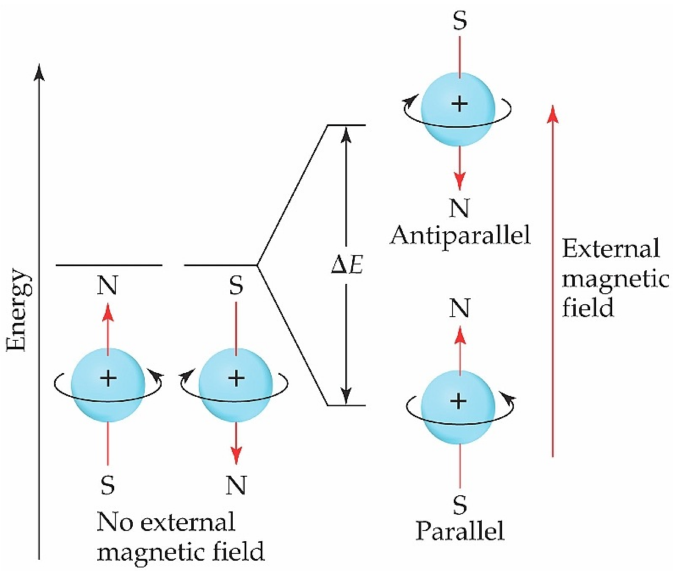


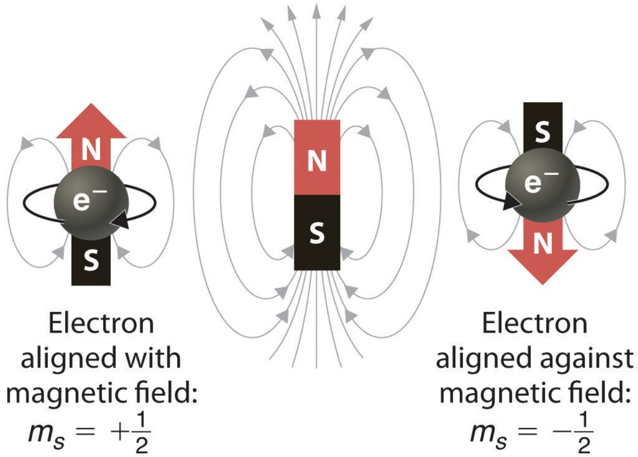




Electron Spin

- The Bohr Model predicts the line spectra of hydrogen perfectly.
- It's predictions for sodium or any multi-electron atom are close, but a little off.
- If we look closely at the line spectra of multi-electron atoms, we find lines split into two.
- Electrons are found to have a property called spin.
- Spin can be thought of as rotation relative to a magnetic pole.
  - Spin can be demonstrated by applying a magnetic fields, which increases electron splitting.
- There are only two kinds of spin, spin up (↑) and spin down (↓).
- Electrons with opposite spin have a small repulsion, they avoid each other but the repulsion is small enough that two electrons can occupy a single orbital.
- Electrons with the same spin have a huge repulsion, two electrons with the same spin do not occupy the same orbital.
- We say electrons are paired if they occupy the same orbital with opposite spin.
- We say an electrons is unpaired if it occupies an orbital by itself.





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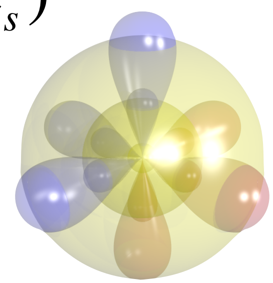
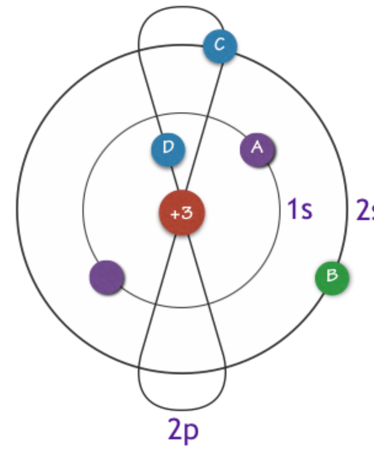
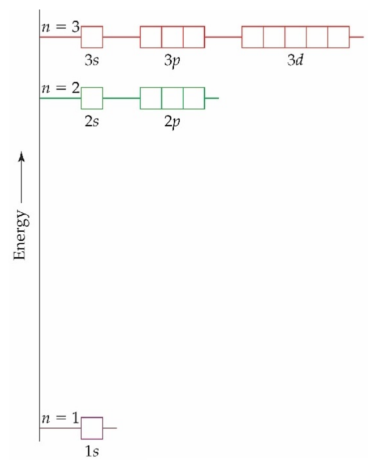
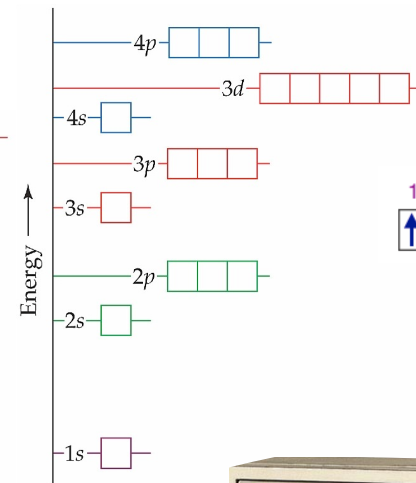
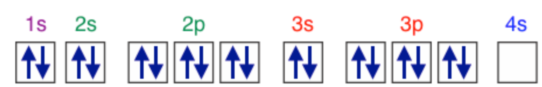
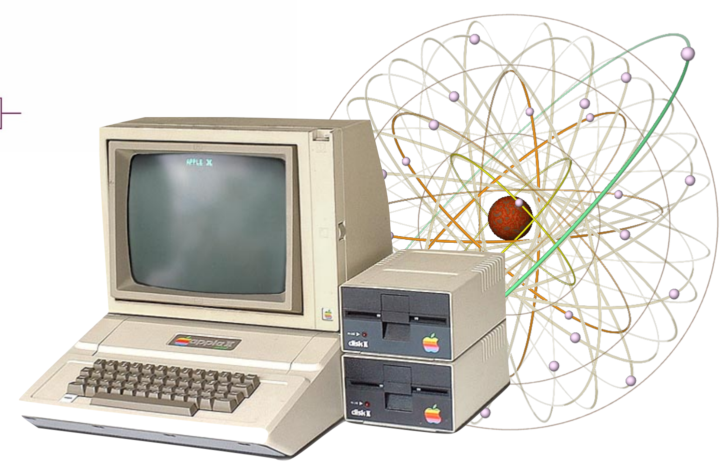












The Schrödinger Equation

- The Schrödinger equation $\Psi()$ describes the stable orbitals which can contain electrons inside the atom.
  - Think of them as buckets in which you can put electrons.
- The equation takes four variables which define the orbital.
  - n = 1, 2, 3, 4… (describes the size)
  - l = 0 … n-1 (describes the shape - we also uses letters s,p,d,f)
  - m_l = -l… 0… +l (describes the orientation)
  - m_s = +½ or -½ (describes the spin of the electron)

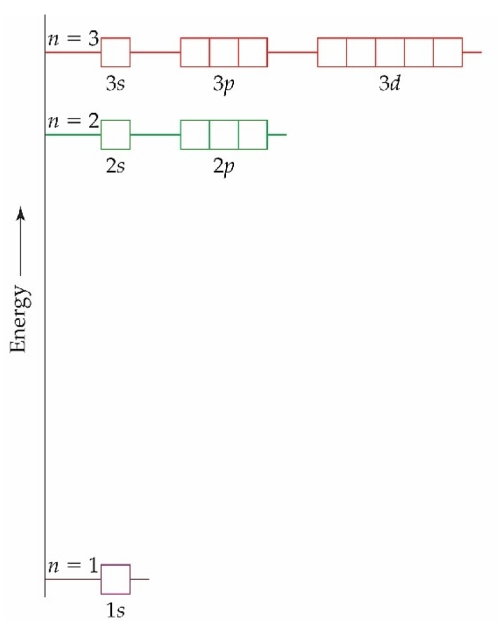
$$\Psi(n, l, m_l, m_s)$$

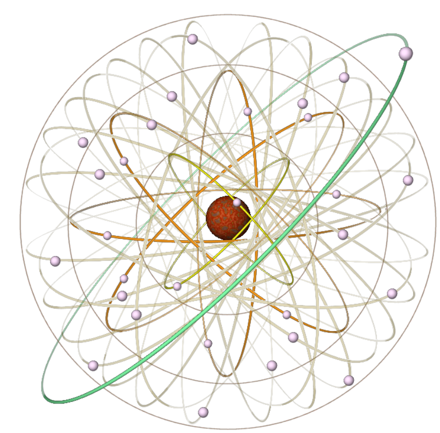
size

shape

orientation

spin





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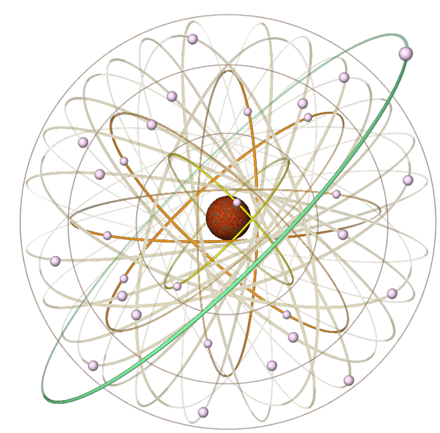

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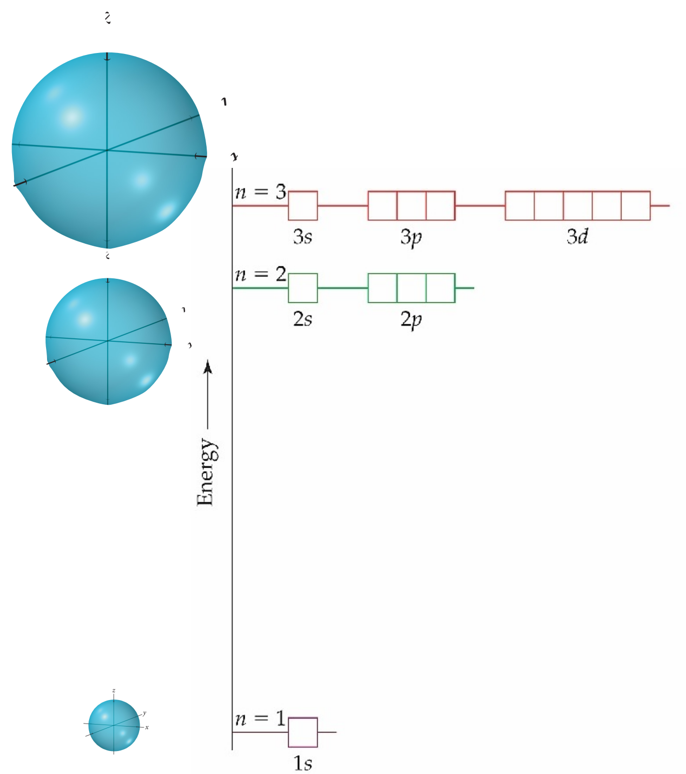

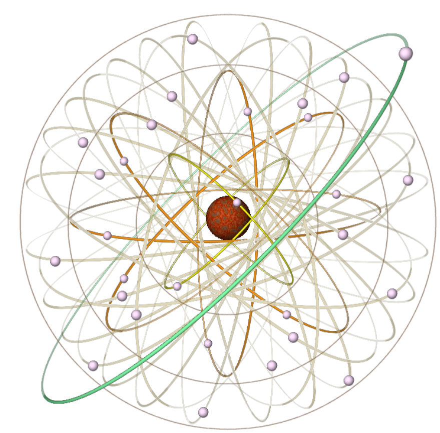

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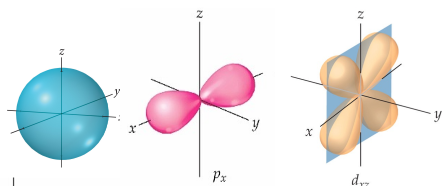
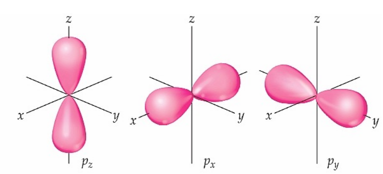
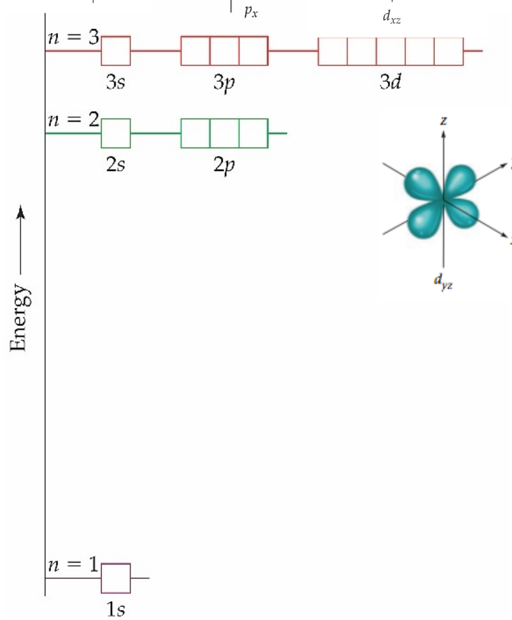
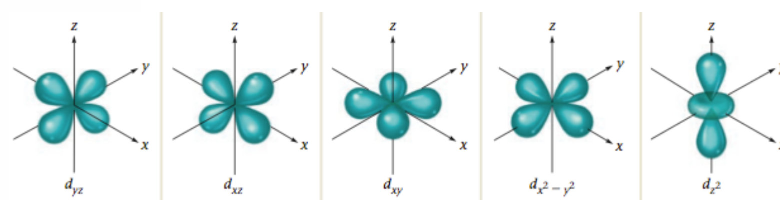
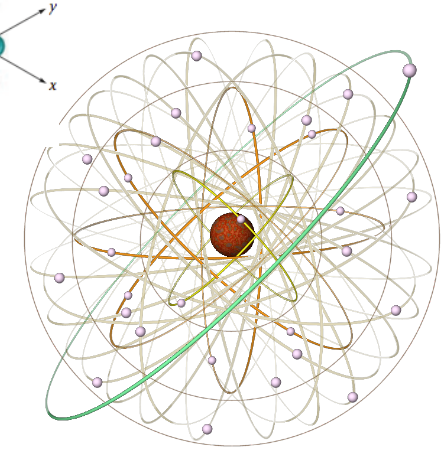
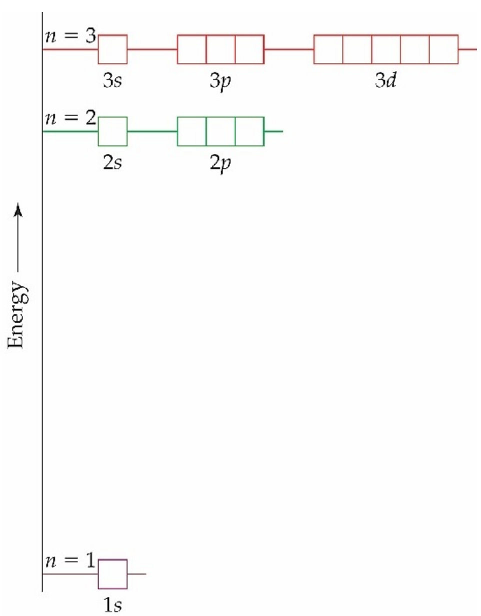


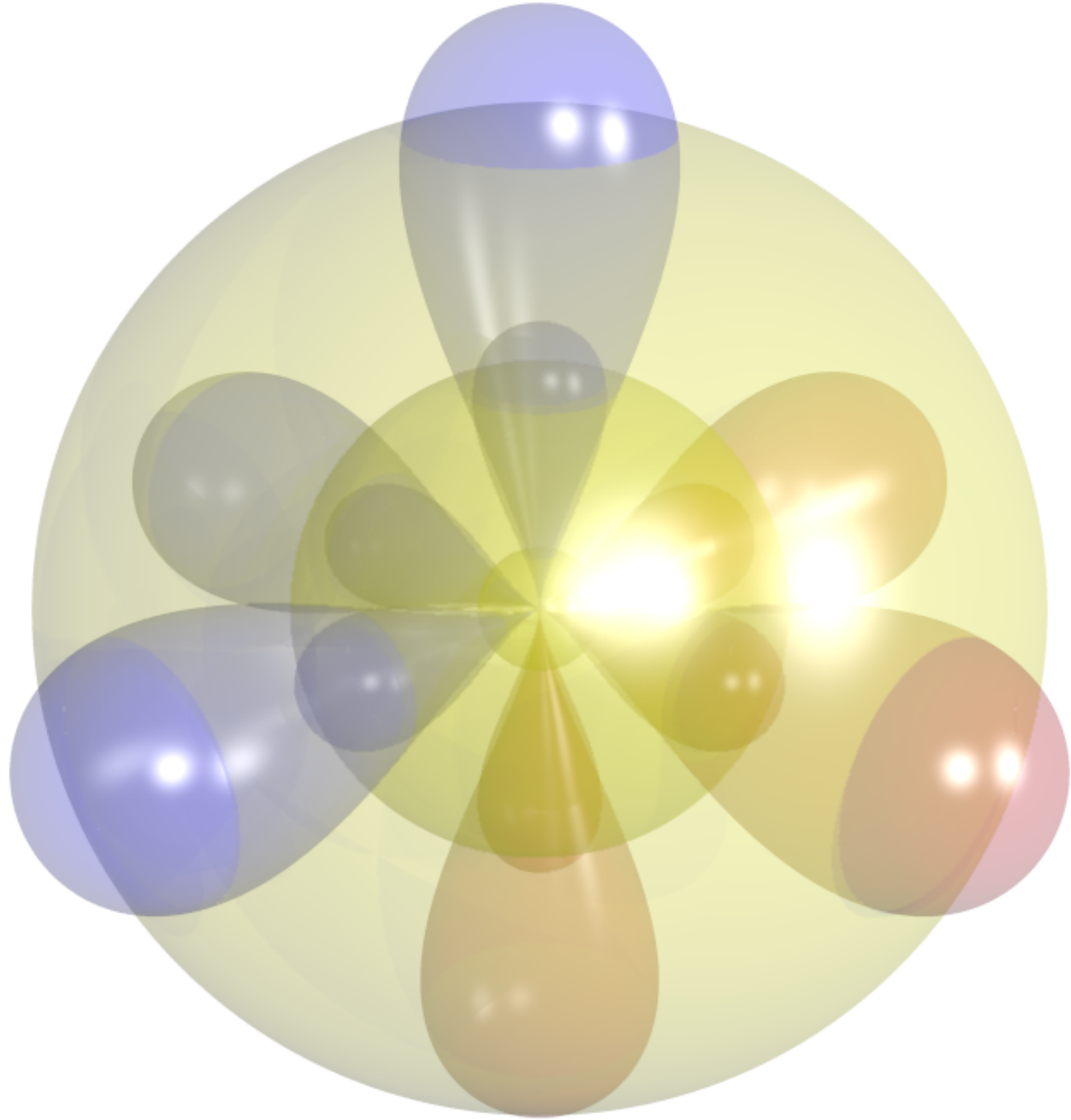









n = 3
3s
3p
3d
n = 2
2s
2p
Energy
n = 1
1s



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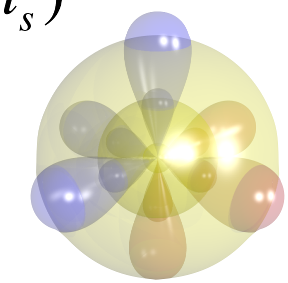
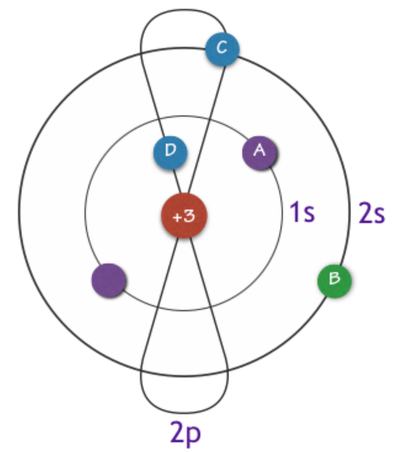
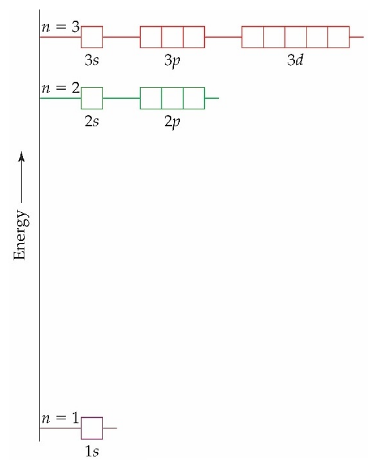
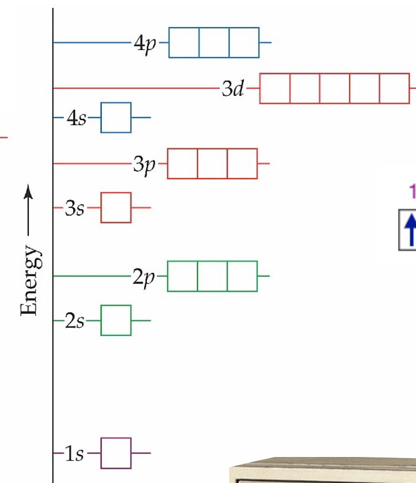
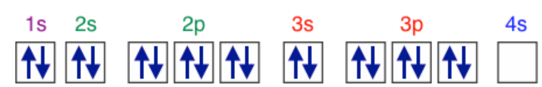
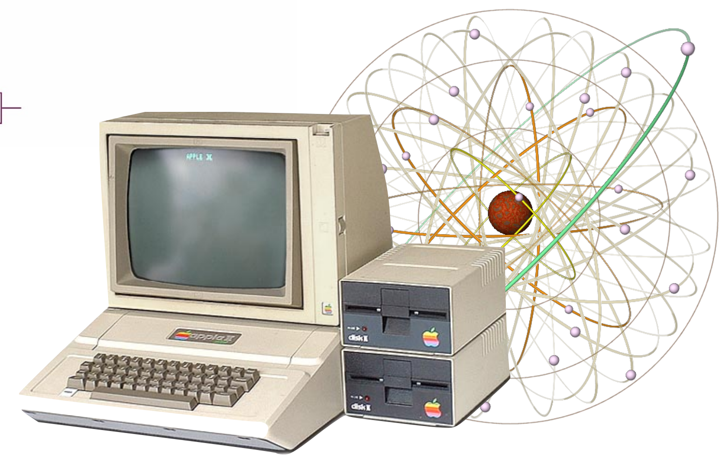








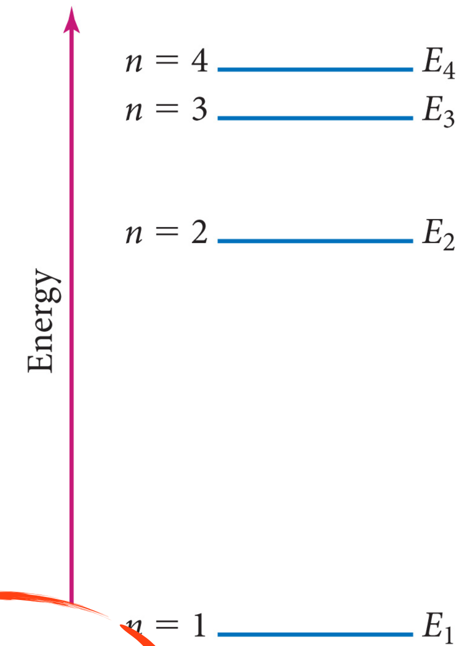




Orbital and Electron Energy

- Orbitals have energy that is reported as a negative number.
  - The energy represents the attraction between the nucleus and an electron in that orbital.
  - This is energy of position; potential energy.
  - It's represented as zero, when the electron is infinitely far away from the nucleus.
  - It becomes a larger number as the electron get's closer to the nucleus.
  - The energy of attraction is represented by Coulomb's law.
    - q is the electric charge
      - Negative for the electron
      - Positive for the nucleus
    - r is the distance between them

$$E = \frac{1}{4\pi\varepsilon_0} \times \frac{q_1 q_2}{r}$$

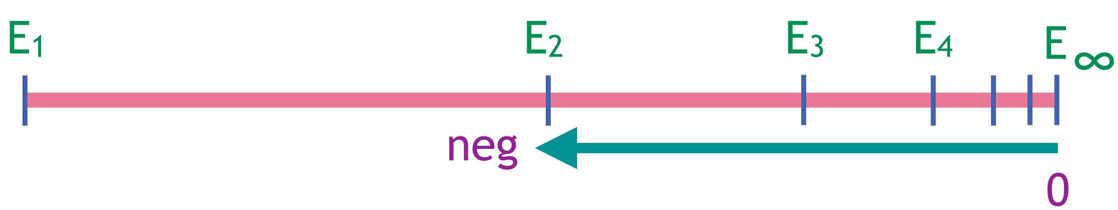


$$\hat{H}\psi = E\psi$$

$$E_{orbitals} = R_H \left[\frac{1}{n^2}\right]$$

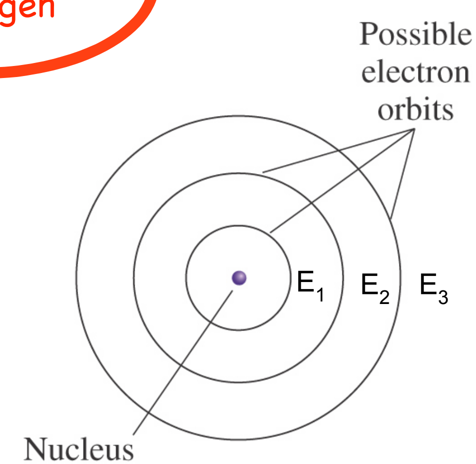
only for hydrogen

$$R_H = -2.18 \times 10^{-18} J$$



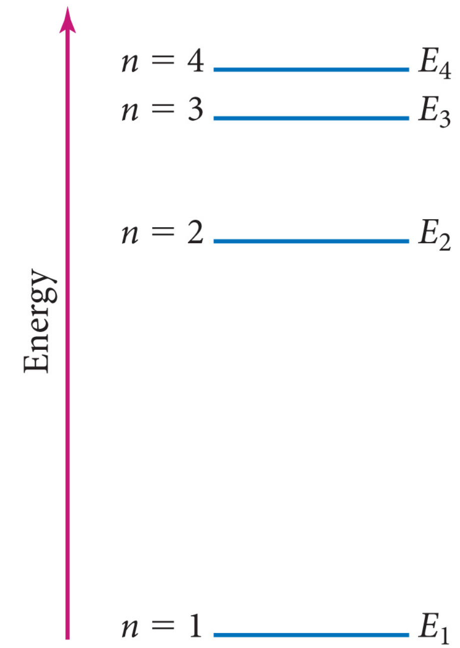
Larger negative number indicates how strong the nuclear attraction is at that position.

PE of the orbital



Orbital and Electron Energy

- Electrons have energy that is reported as a positive number.
  - The energy represents the motion of the electron.
    - Vibrations, rotations, etc
  - This is energy of motion; kinetic energy.
  - When an atom is radiated with e-m energy, the electron gains energy.
  - It gains energy as shown by Planck's Equation.



$$E_{photon} = h\nu = \left|\Delta E_{orbital}\right|$$

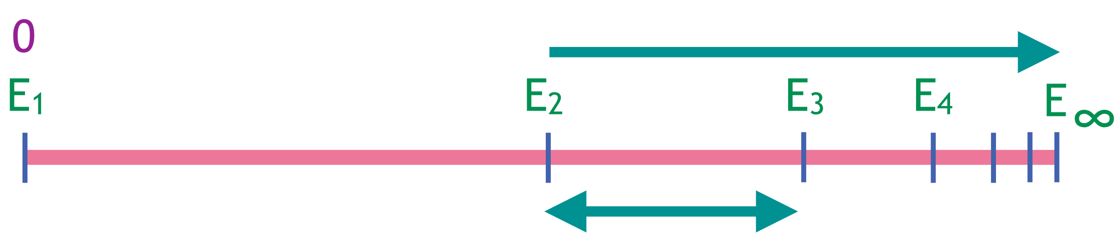
$$\Delta E = E_f - E_i$$

$$E_{orbitals} = R_H\left[\frac{1}{n^2}\right]$$

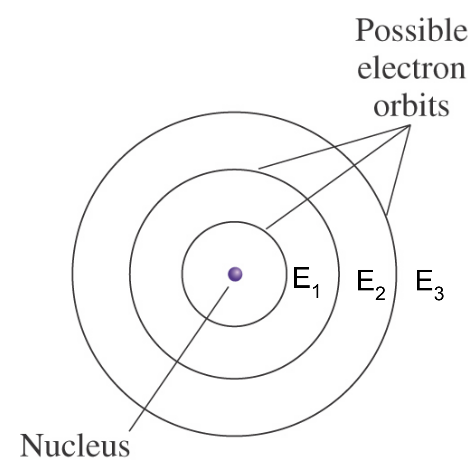
Larger positive number indicates

how much energy was put into the electron.

KE of the electron



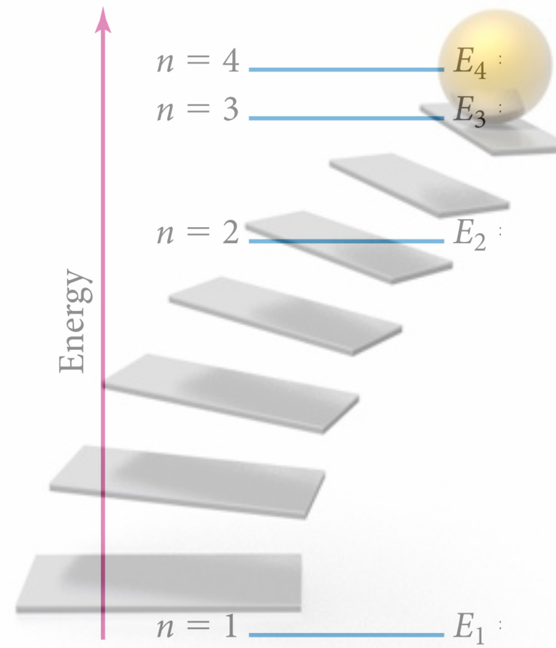
$$\Delta E = R_H\left[\frac{1}{n_f^{\,2}} - \frac{1}{n_i^{\,2}}\right]$$



Orbital and Electron Energy

- The electron can only exist in the positions defined by the Schrödinger equation. (n=1, n=2, n=3, etc).
- If the electron gains enough energy it can offset the pull of the nucleus.
- When the kinetic energy of the particle is equal but opposite to the potential energy of the orbital. The electron will settle into that orbital.
- More energy, drives it to a higher orbital.
- Less energy, causes it to fall into a lower orbital.

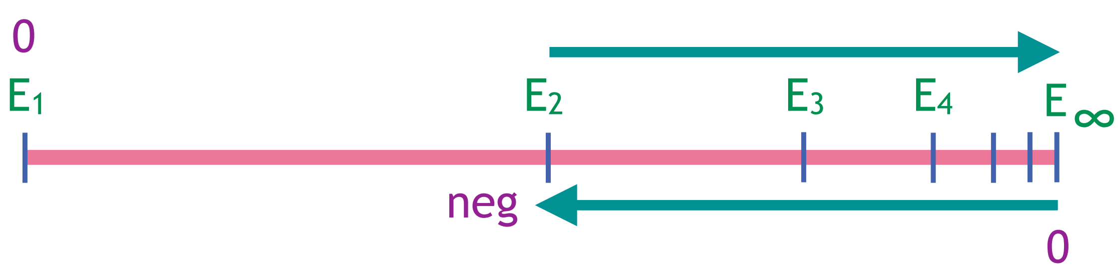
$$E_{electron} = -E_{orbital}$$



Larger positive number indicates

how much energy was put into the electron.

KE of the electron



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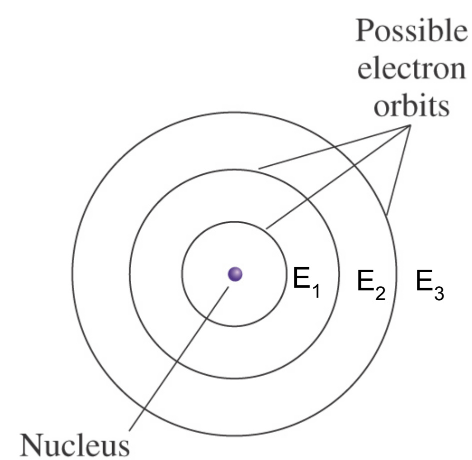
PE of the orbital



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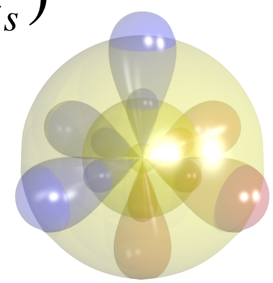

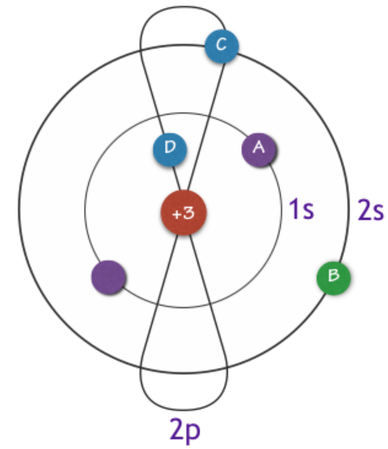

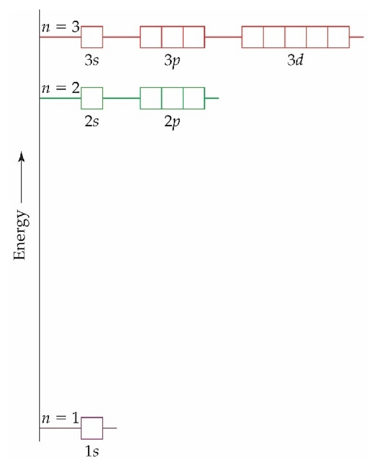

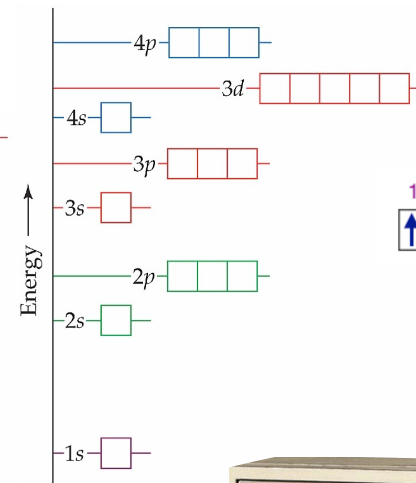

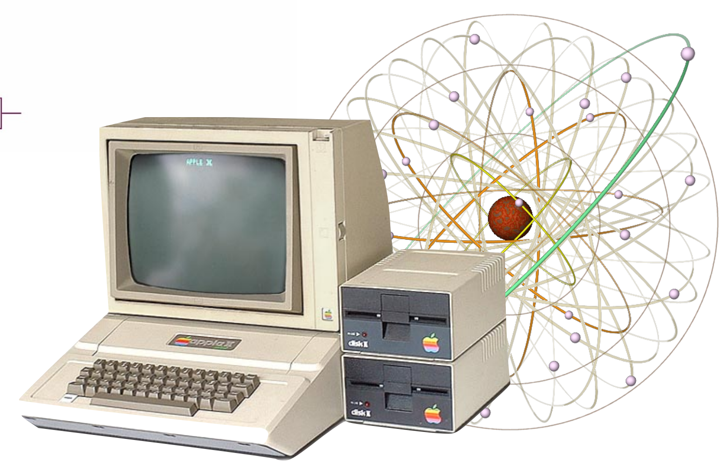

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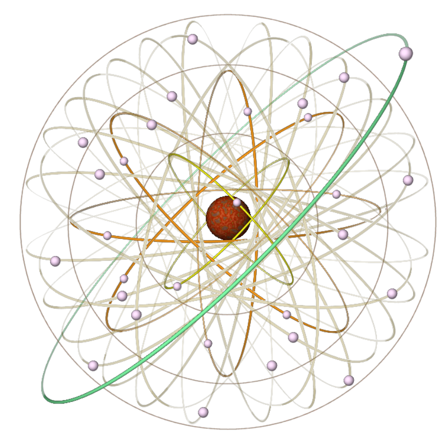
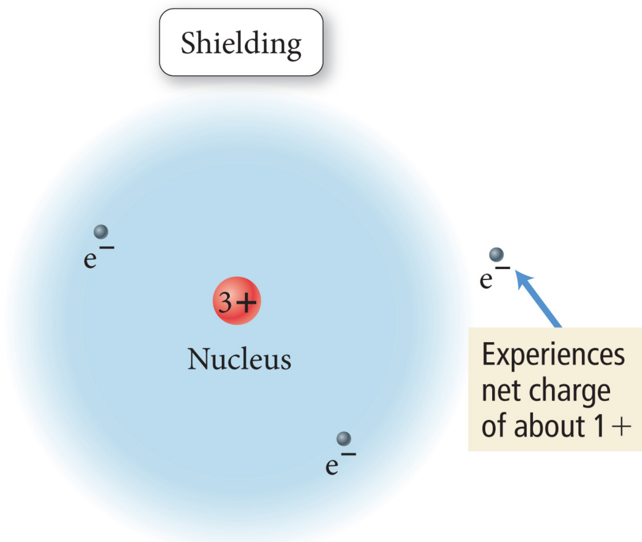
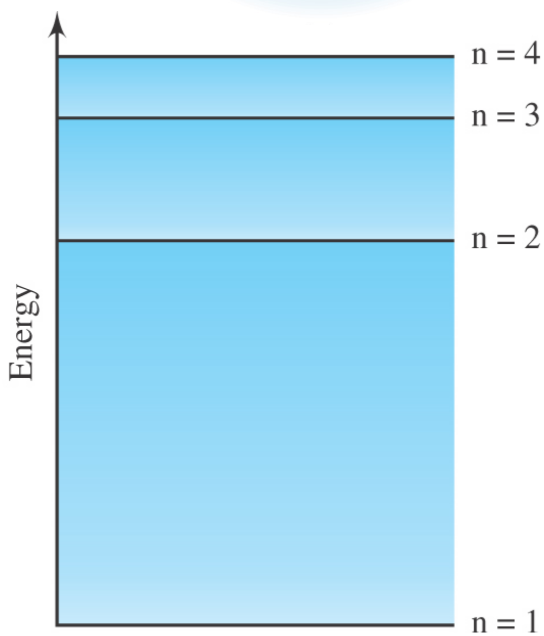


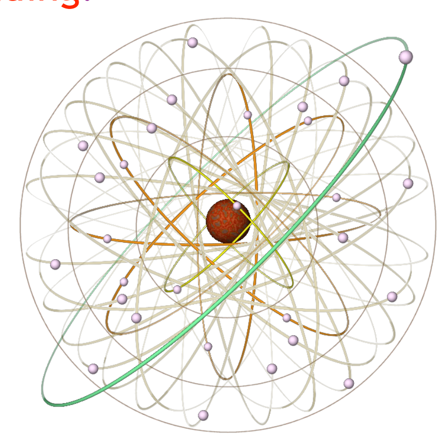
Electron Shielding & Penetration



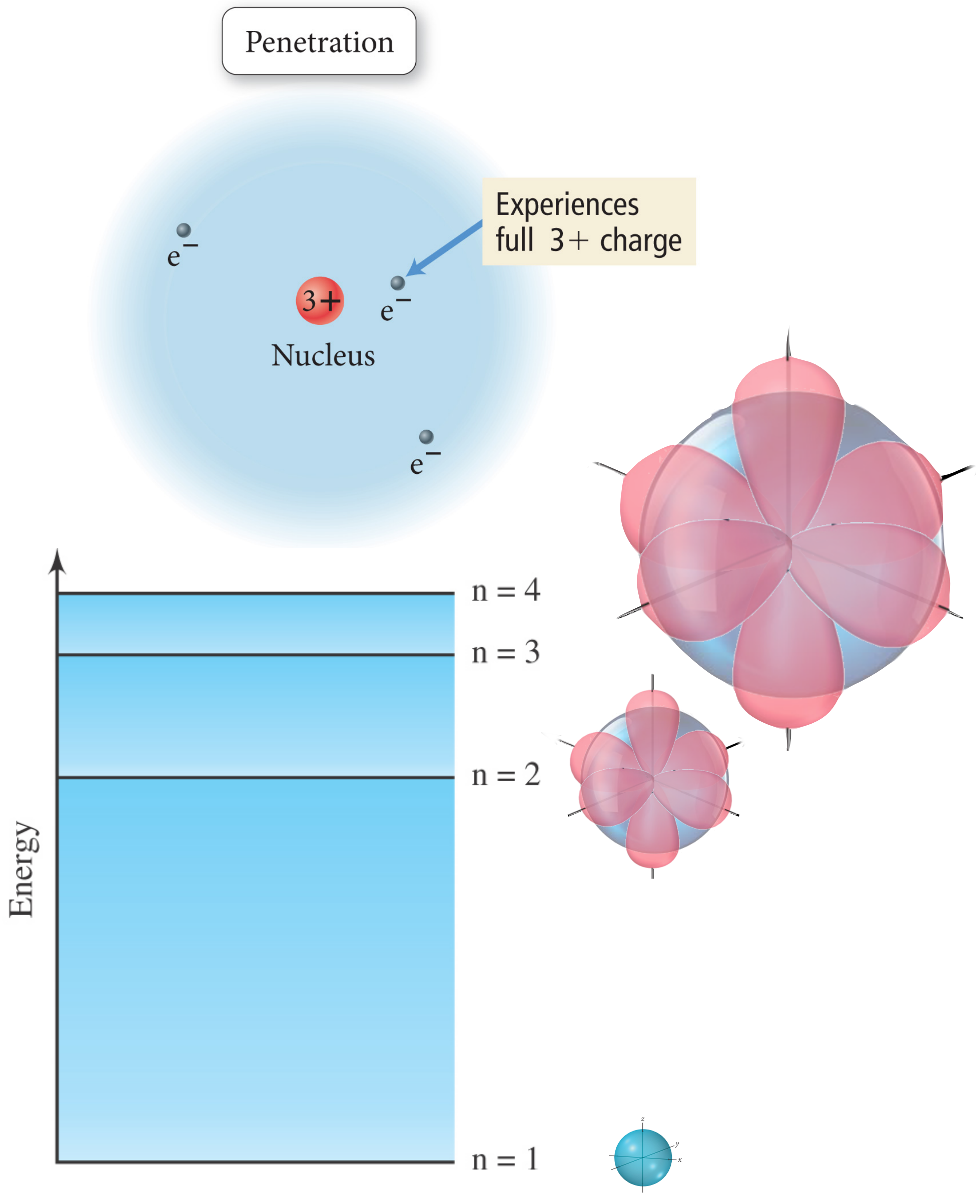


- In a multi-electron atom, each electron sees a different nuclear charge.
- Electrons farther away from the nucleus, see a reduced nuclear charge.
  - Electrons between the outer electron and the nucleus cancel out part of the nuclear charge.
  - An electron on the outer shell is held with a smaller charge.
  - The charge it sees is called the effective nuclear charge.
  - The electron has more energy than it would have if it were held more tightly by the atom.
  - This effect is called electron shielding.

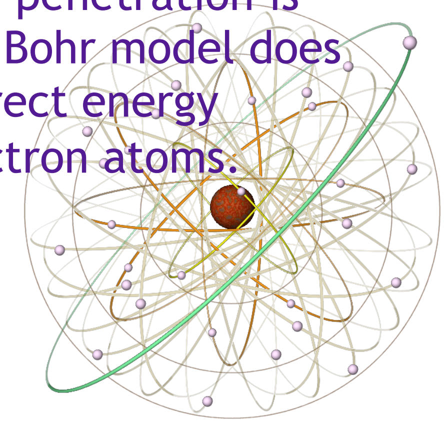
$$E = \frac{1}{4\pi\varepsilon_0} \times \frac{q_1 q_2}{r}$$



Electron Shielding & Penetration



- In a multi-electron atom, each electron sees a different nuclear charge.
- If the electron moves closer to the nucleus, electron shielding is reduced.
- The electron is said to have penetrated the electron shell that is causing the shielding.
- The electron now sees a greater effective nuclear charge than it saw in it’s previous position.
- Electron shielding & penetration is one reason why the Bohr model does not provide the correct energy levels for multi-electron atoms.



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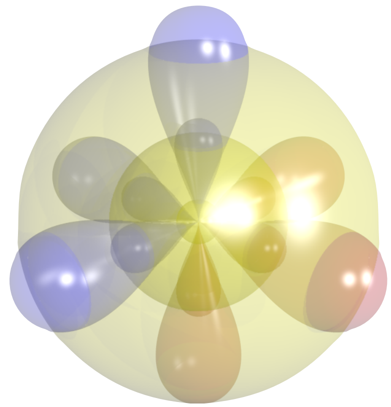

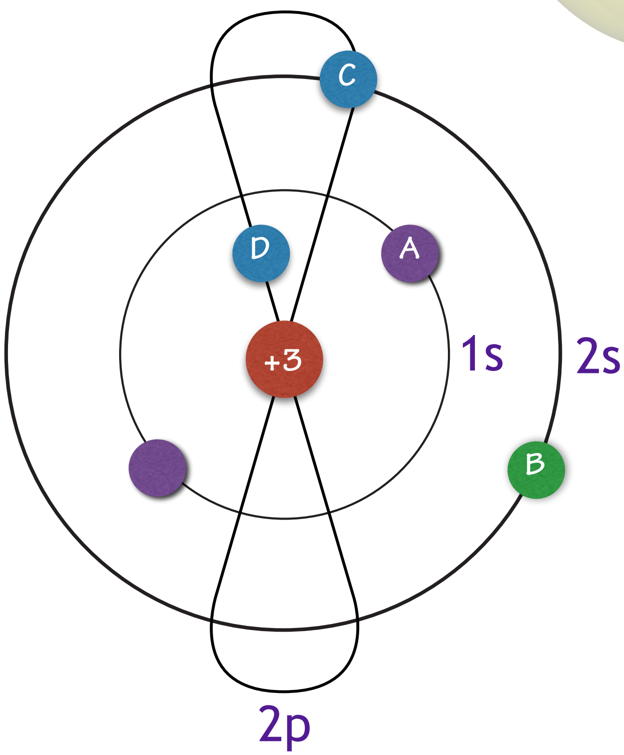

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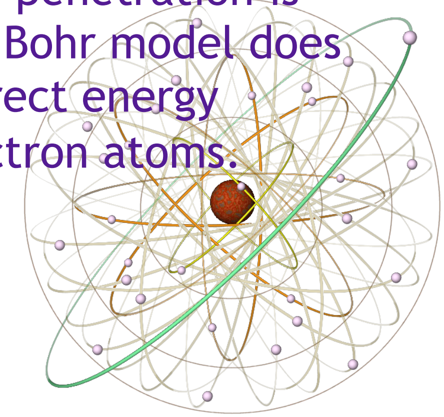

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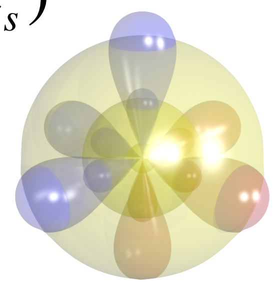
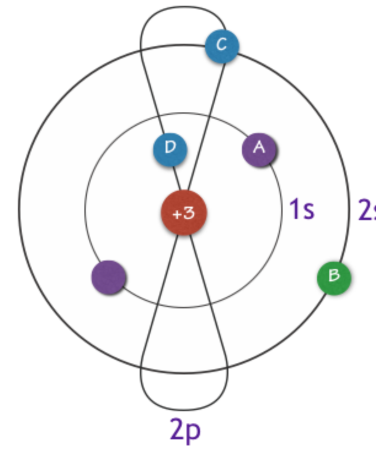
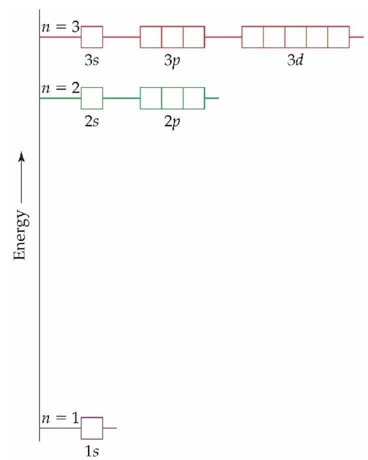
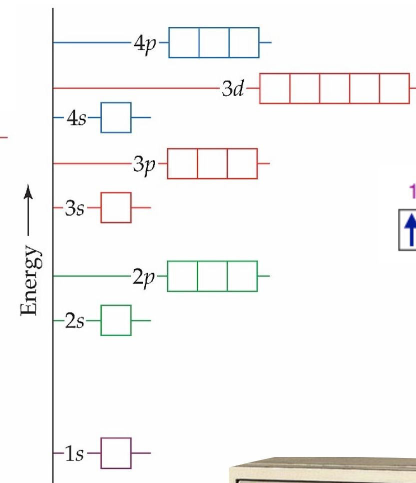
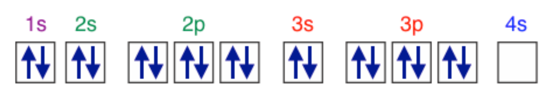
$$\Psi(n,l,m_l,m_s)$$

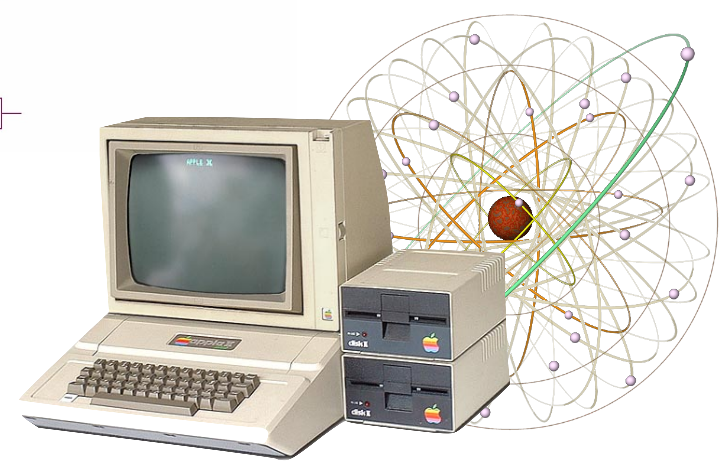






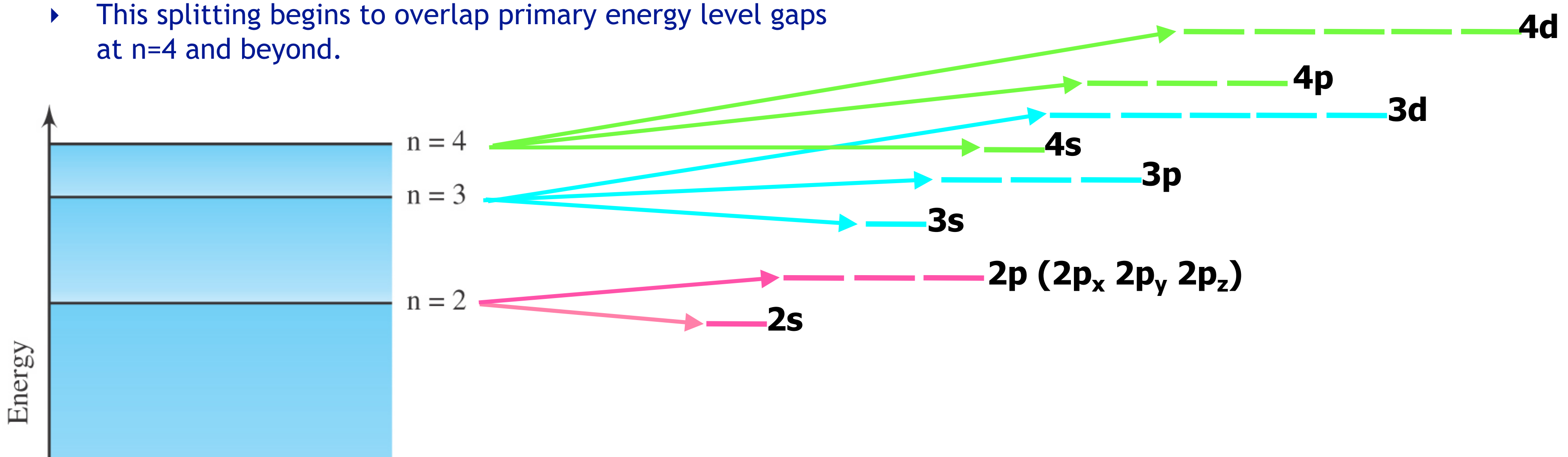


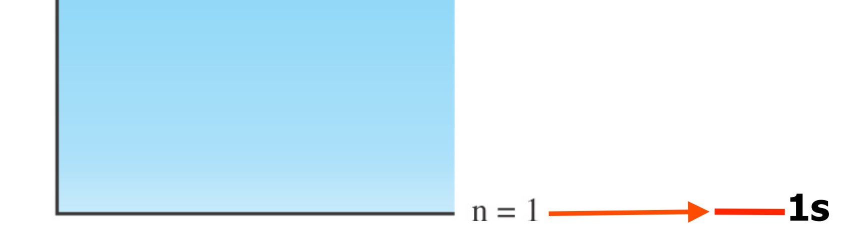


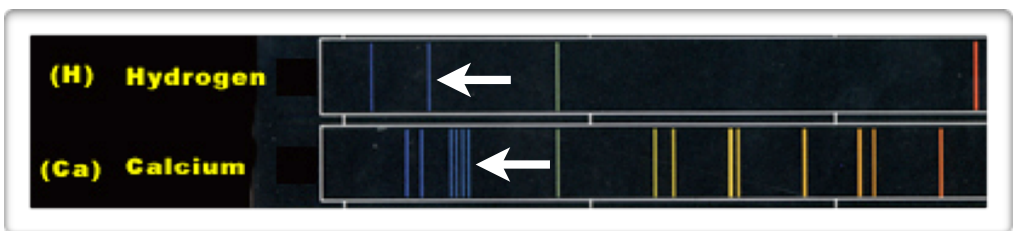


Orbital Splitting

- The Bohr Model predicts the line spectra of hydrogen perfectly.
- It's predictions for sodium or any multi-electron atom are close, but a little off.
- One of the consequence of the wave mechanic analysis of the atom, is the existence of sub-levels (s, p, d, f, etc).
- When we put more than one electron into an atom, electron interactions cause the sub-levels to split.
- This corresponds to complexity we see in the line spectra of many electron atoms.
- With a primary level, the sub-levels have increasing energy according to the sequence s, p, d, f.
- All orbitals of the same sub-level are degenerate. Degenerate means having the same energy.
- This splitting begins to overlap primary energy level gaps at n=4 and beyond.







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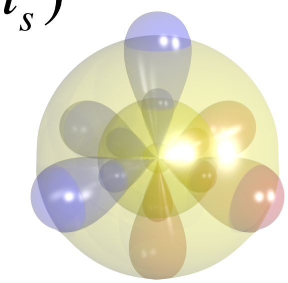
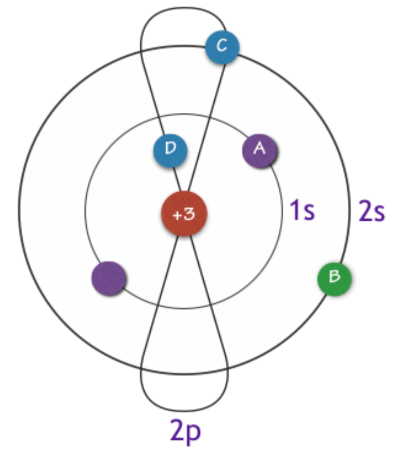
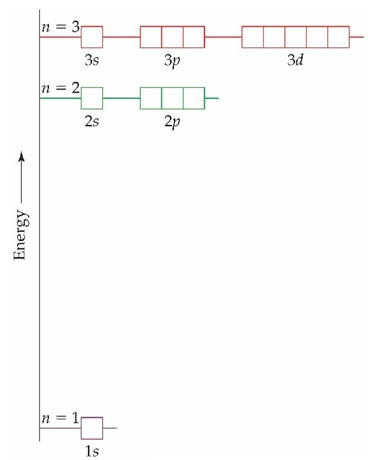
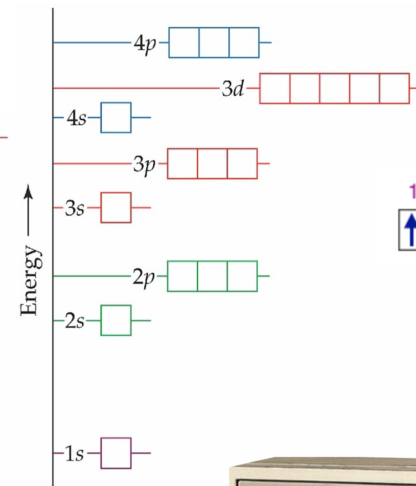
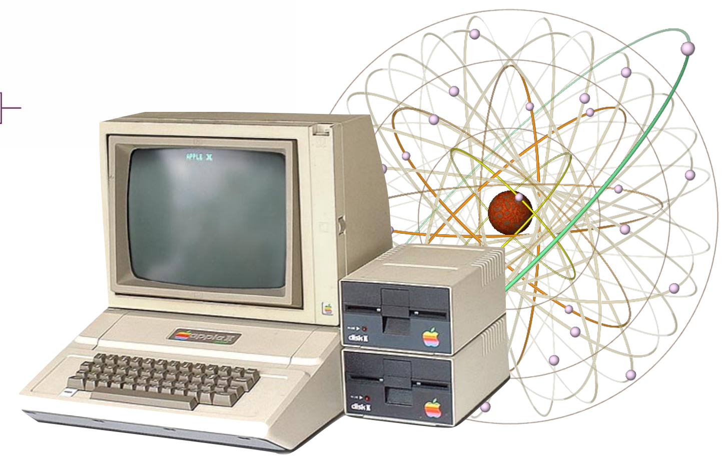




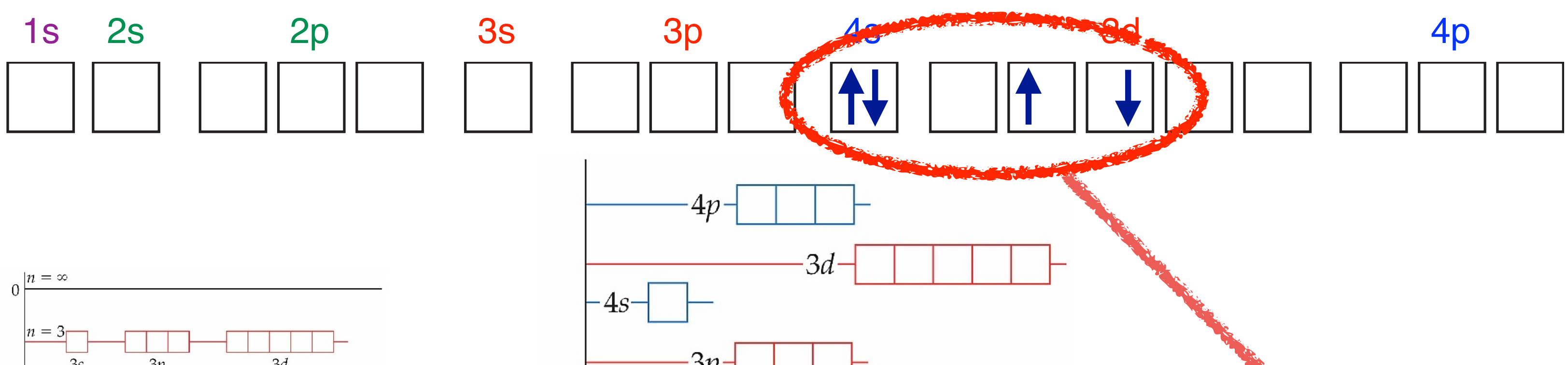


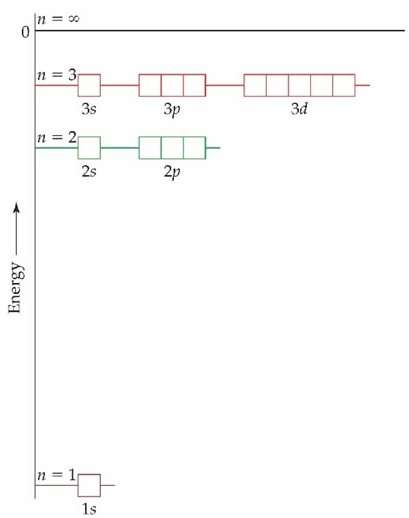


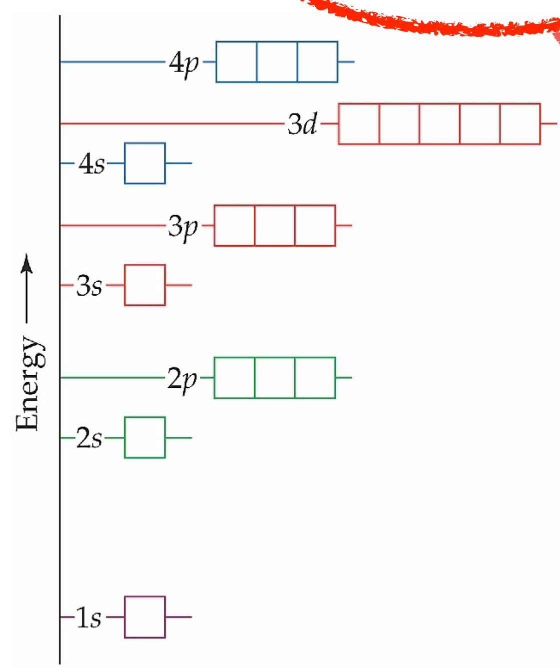


Orbital Diagrams

- Orbital diagrams order the position of orbitals according to increasing energy.
- Electrons can and do populate these orbitals in endless combinations.
- Changing the configuration of electrons in an atom, changes it's chemical properties. Like a computer program.
- Many important chemical reactions are initiated by exciting electrons from one configuration to another.
- We call the lowest energy electron configuration of an atom it's ground state. It's the rest state of the atom.
- There are rules that will help you locate the ground state of any neutral atom or ion.







The position of electrons are indicated with an arrow.
The arrow is drawn pointing up for electrons a spin up, and down for those with a spin down.

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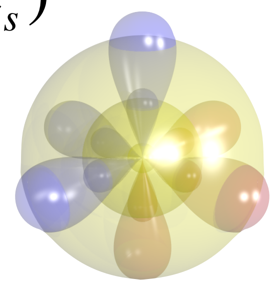
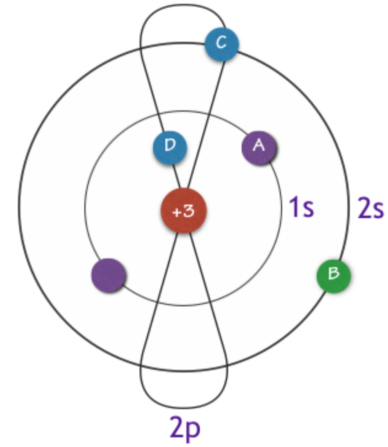
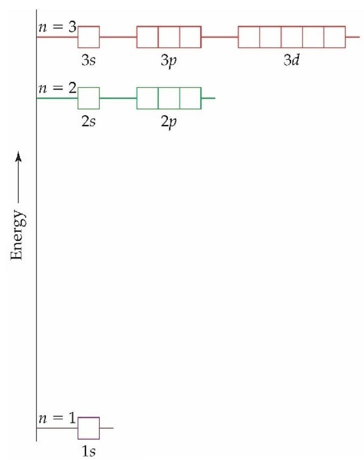
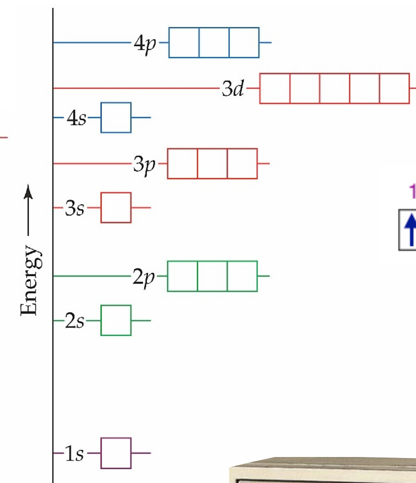
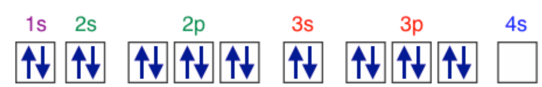
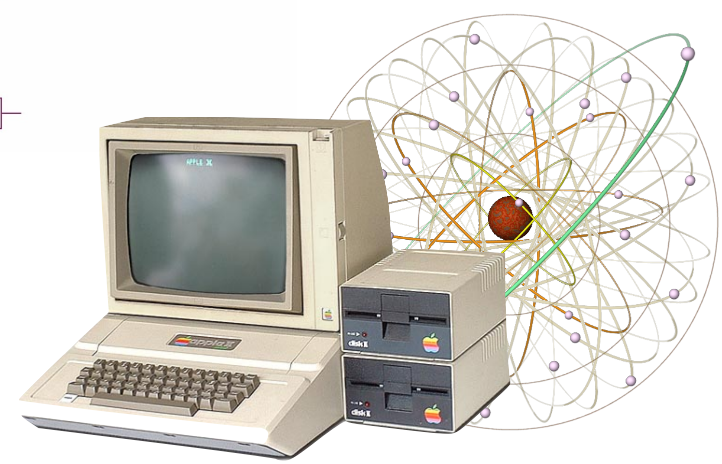




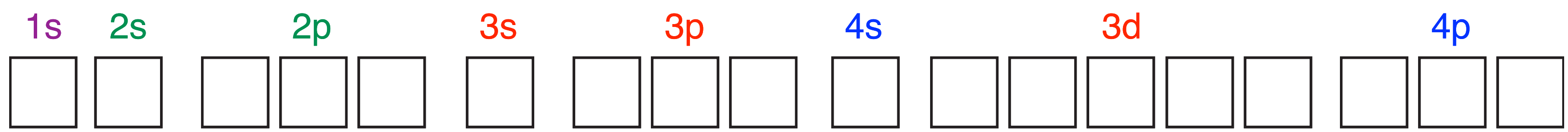




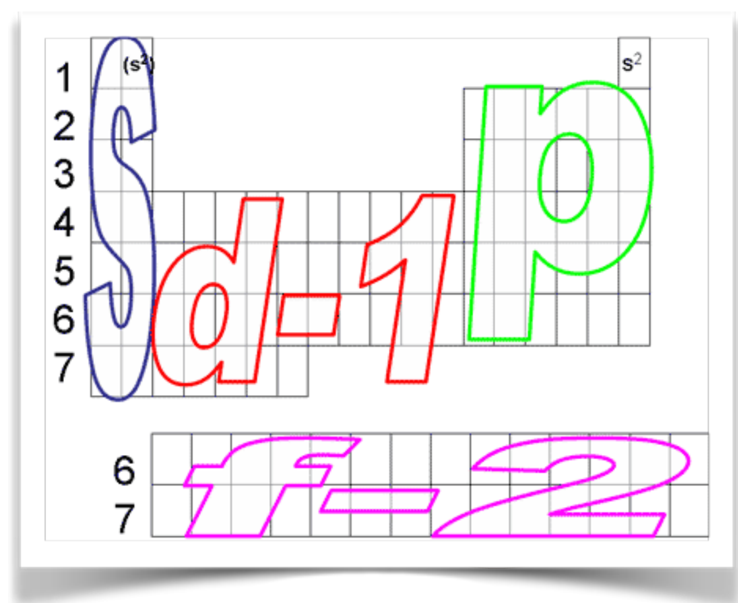




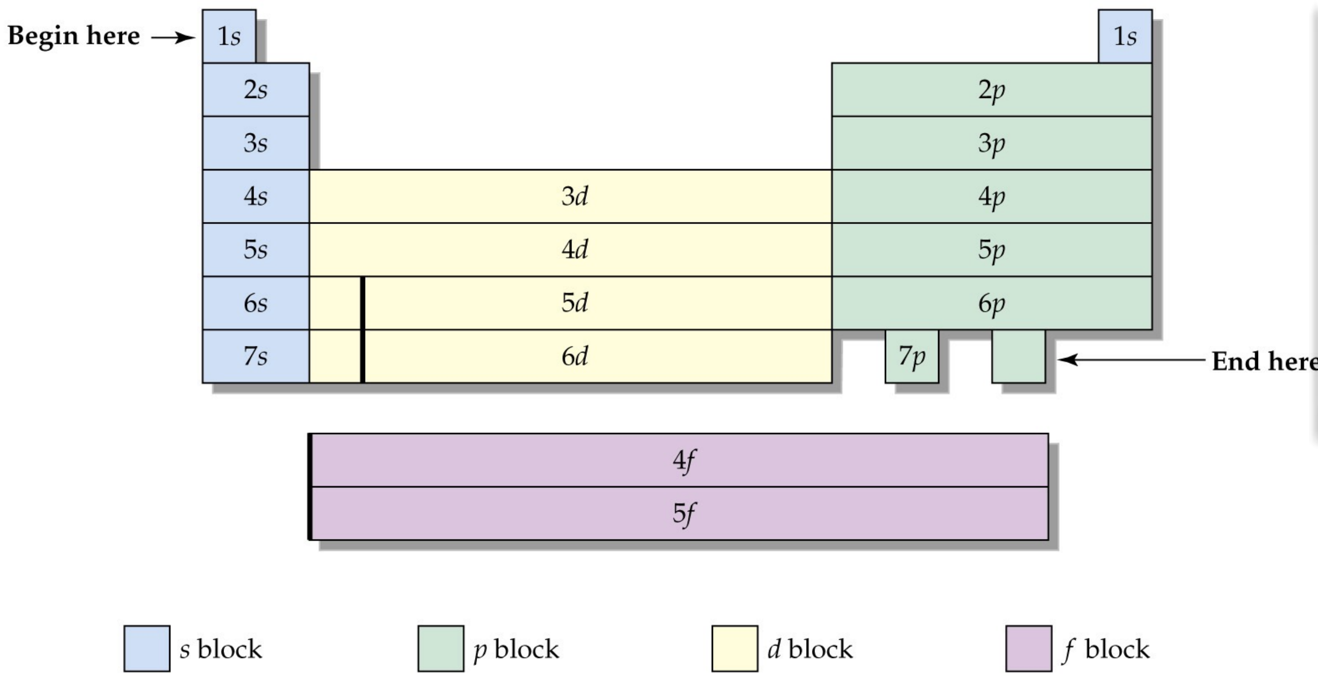
The Ground State

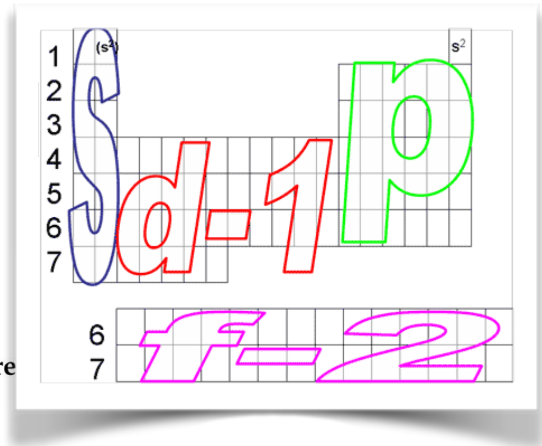


- Any combination of electrons in orbitals is theoretically possible.
- In chemistry, we will sometimes put extra energy into an atom to trigger a chemical reaction.
  - Atoms with extra energy form higher energy configurations of electrons called excited states.
- Most configurations are unstable and not useful.
- The most useful configuration to know is the ground state.
- The ground state configuration of electrons is the lowest energy arrangement of electrons around a nucleus.
- Atoms will relax to the ground state in the absence

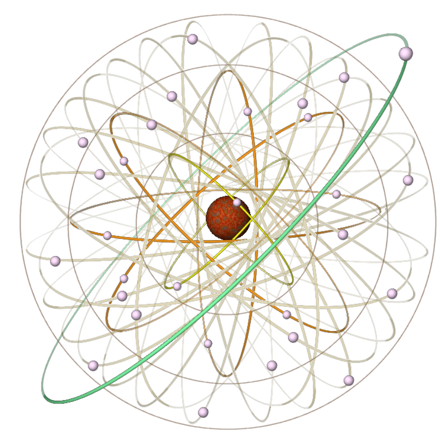


Orbital Diagrams





- The periodic table is a useful tool for drawing orbital diagrams.
  - It helps you find the number of electrons for any given atom.
  - Each period will tell you the n value of the box.
  - Each block of the periodic table will tell you l value.



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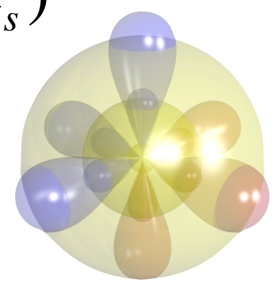

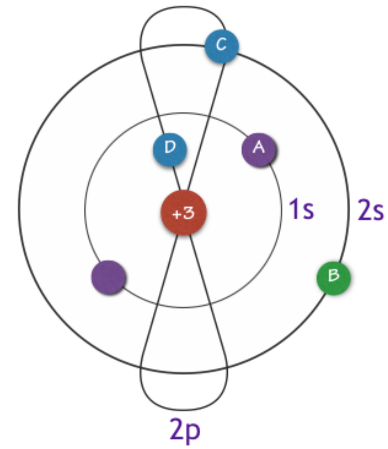

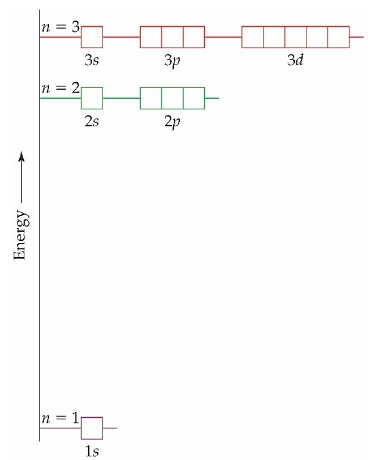

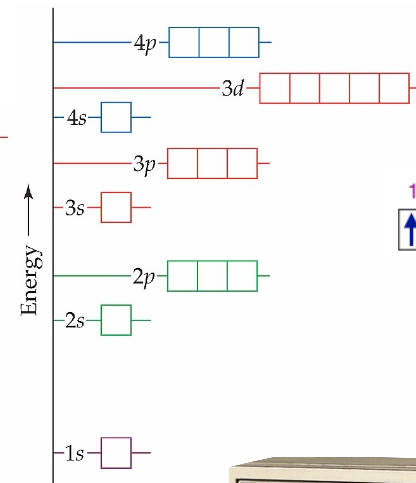

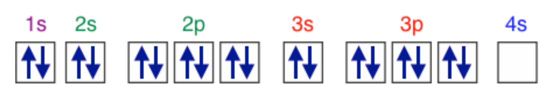

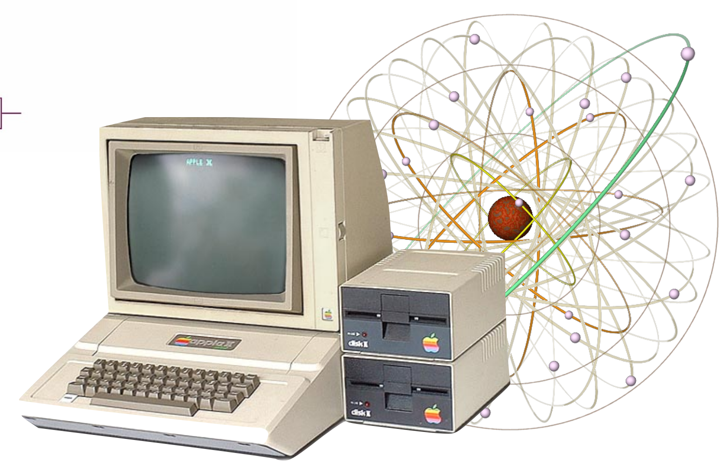

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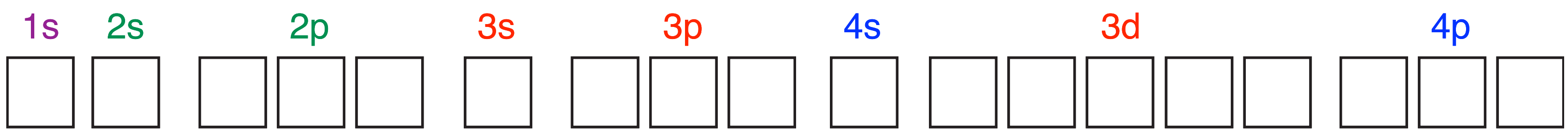

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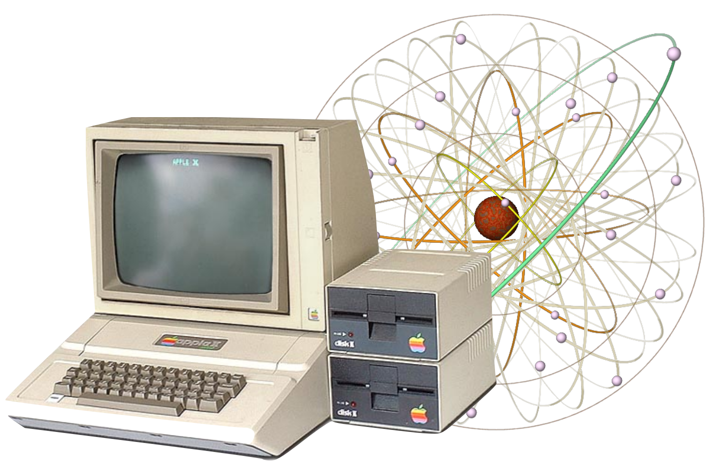

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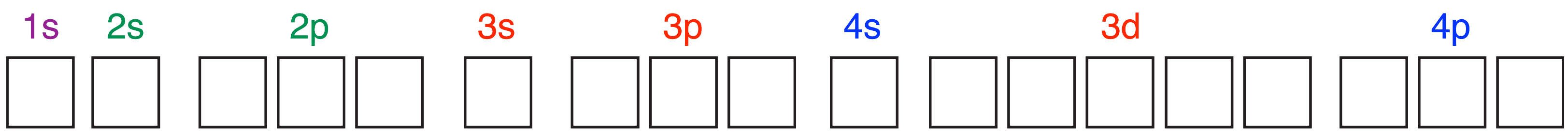

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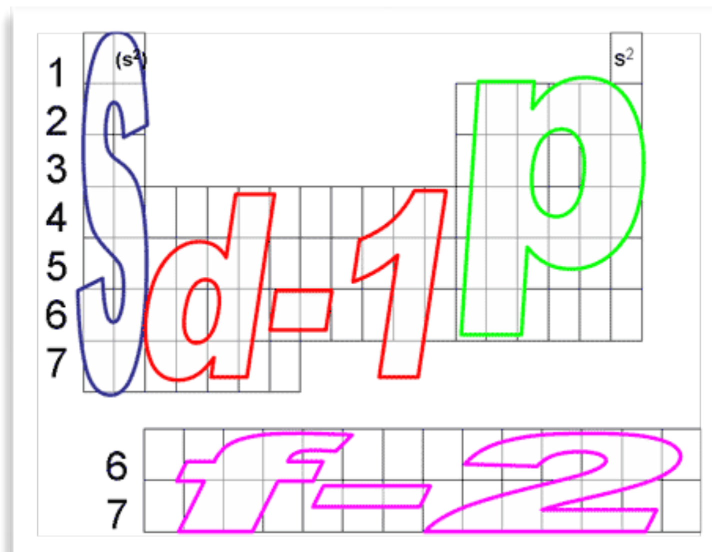

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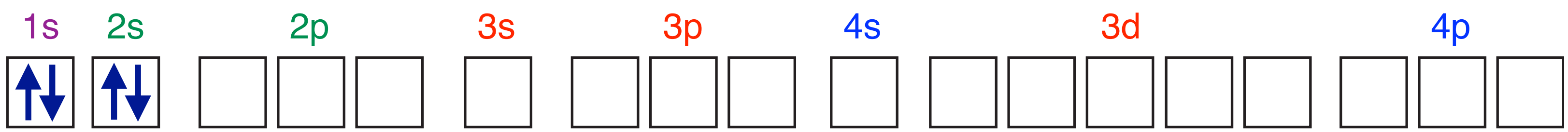

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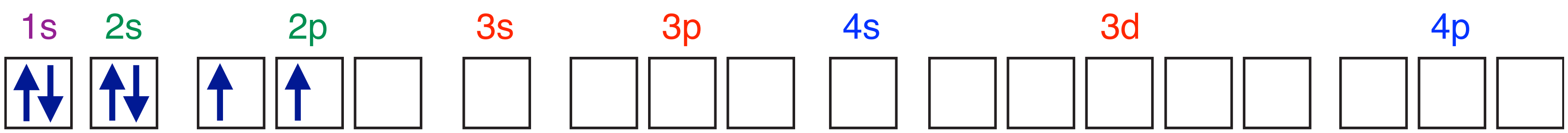
Be (4 electrons)

	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	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112	113	114	115	116		118

57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No

Metals
Metalloids
Nonmetals

Orbital Diagrams



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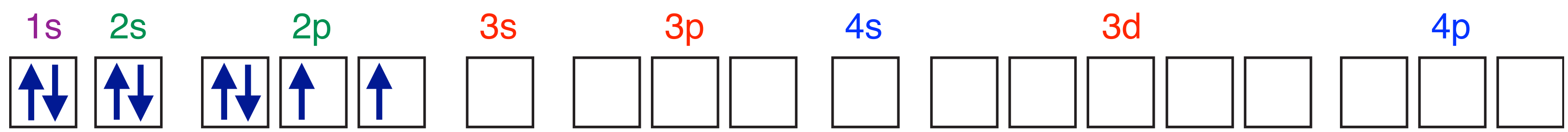
C (6 electrons)

	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	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112	113	114	115	116		118

57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No

Metals
Metalloids
Nonmetals

Orbital Diagrams



- Rules for filling orbitals to create the ground state configuration:
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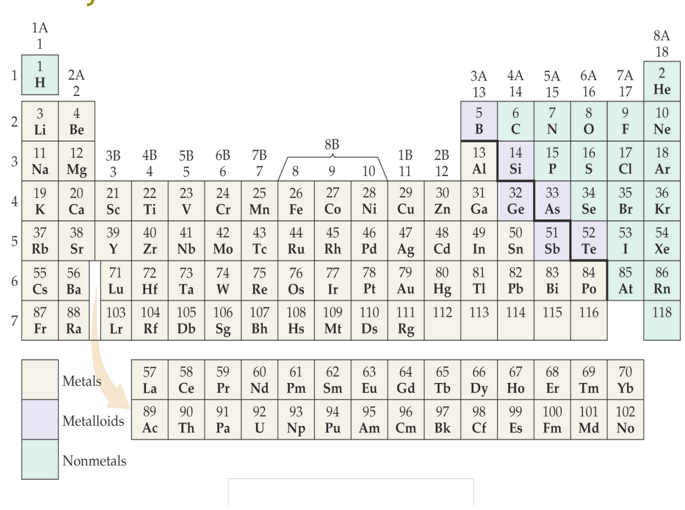
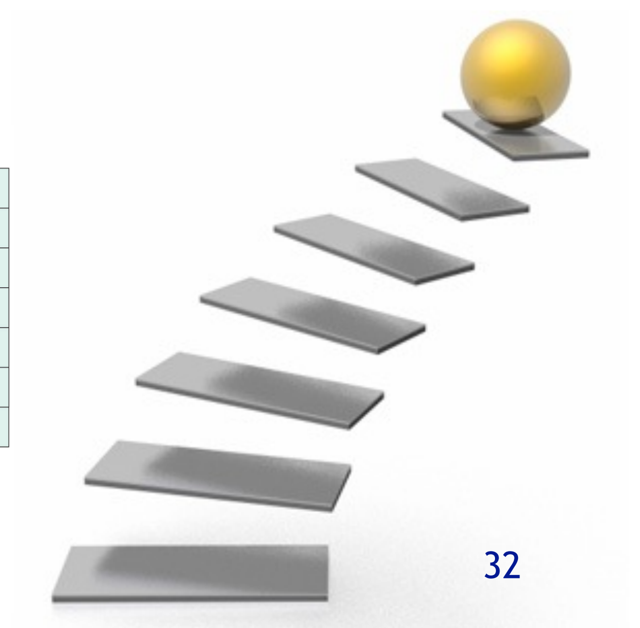
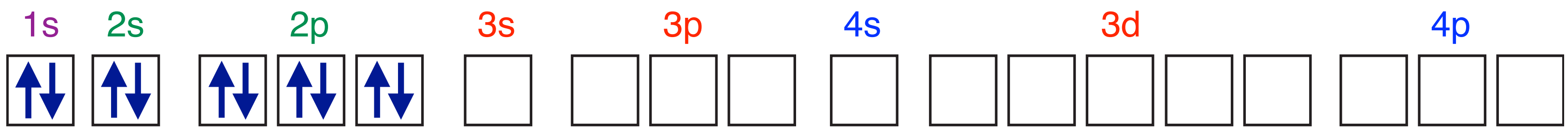
O (8 electrons)





Orbital Diagrams



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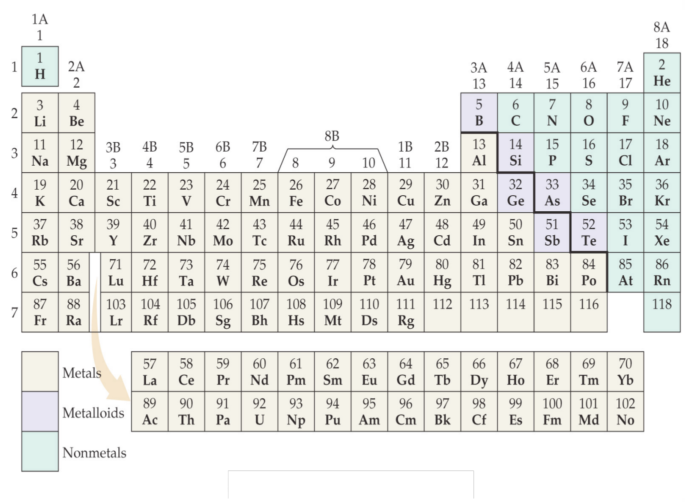
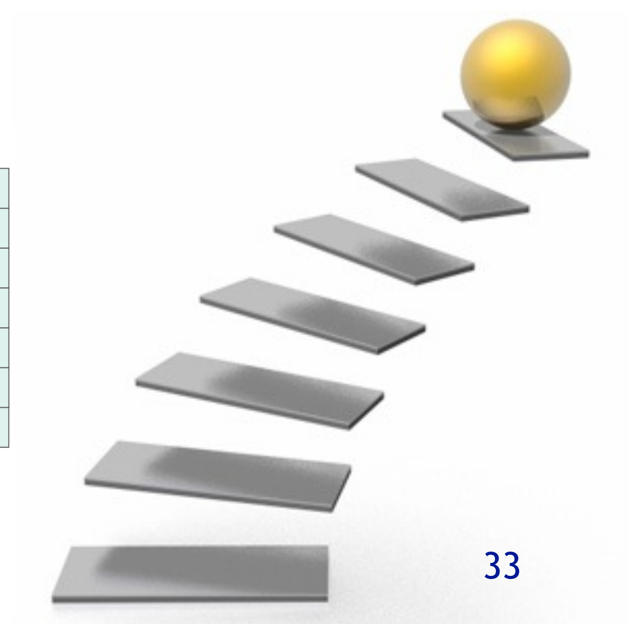
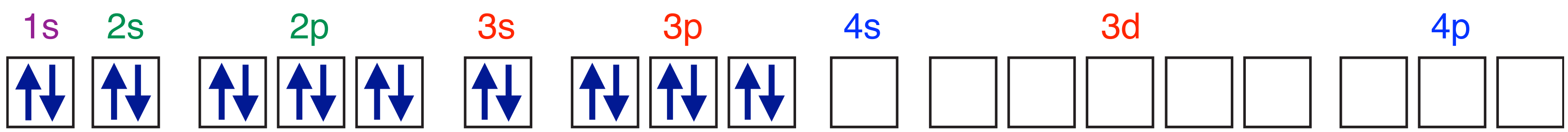
Ne (10 electrons)





Orbital Diagrams



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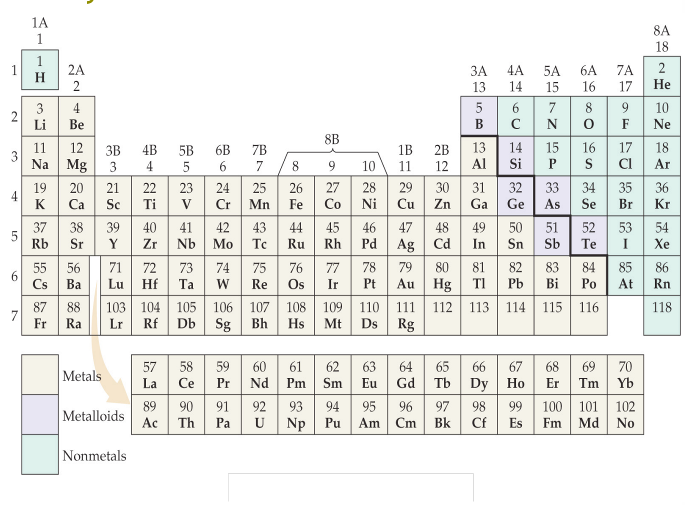
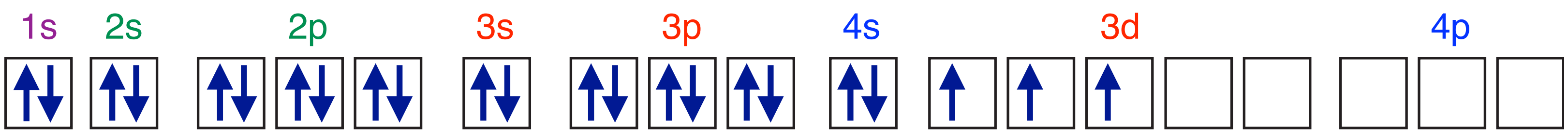
P^{3-}

(15 protons;

18 electrons)



Orbital Diagrams



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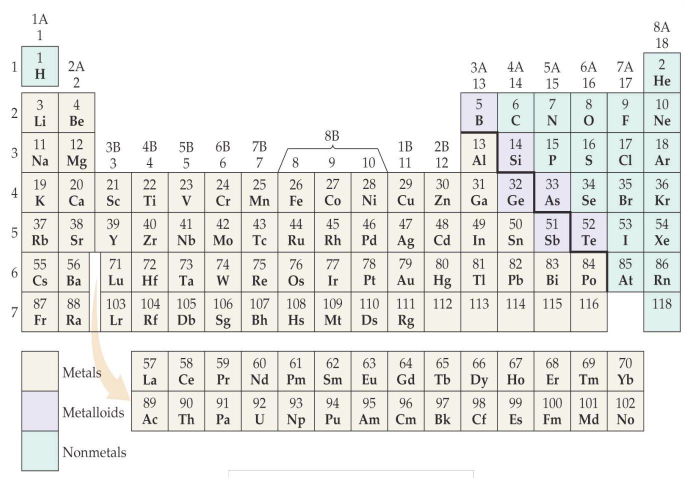
V (23 electrons)



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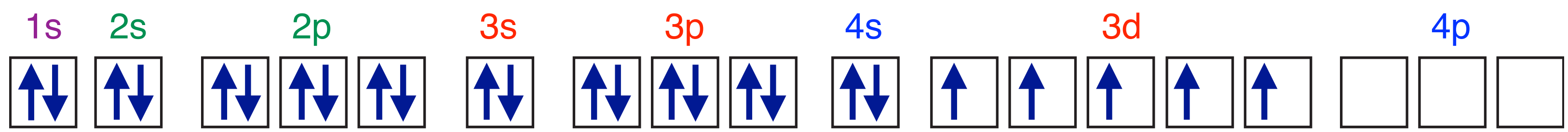

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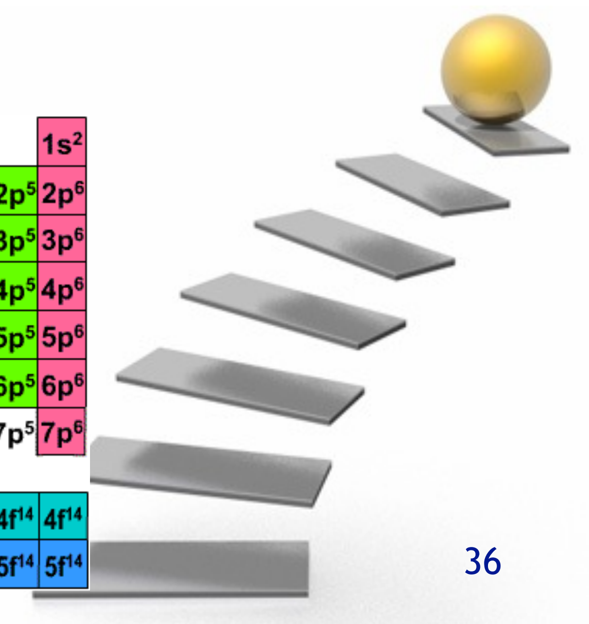
    - Pauli Exclusion Principle: states their spins must be paired when you do.

Cr (24 electrons)



Ch08

Putting Electrons into Orbitals

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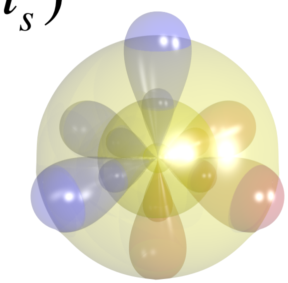
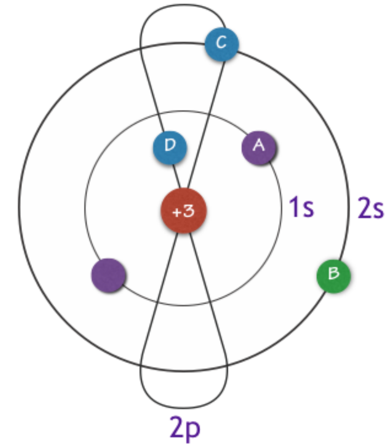
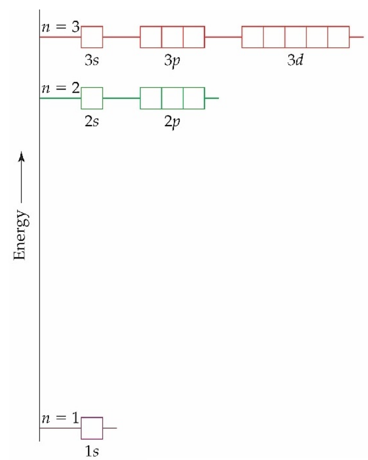
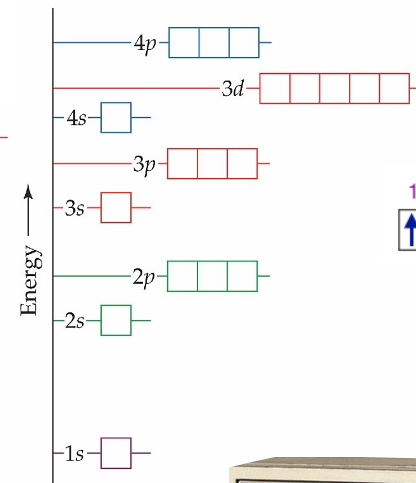
  - Core Electrons
- Electron Configuration notation
  - Compact notation
- Quantum Numbers
  - Describing Electron Positions

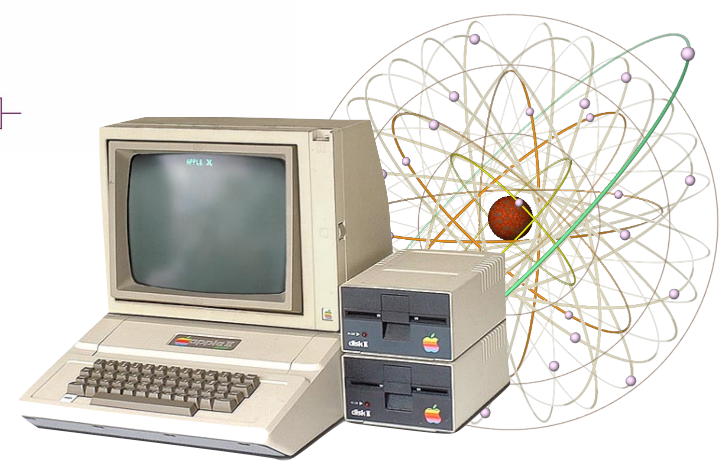
$$\Psi(n, l, m_l, m_s)$$



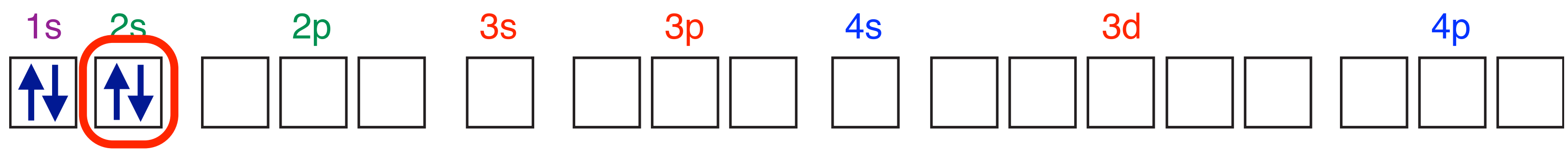




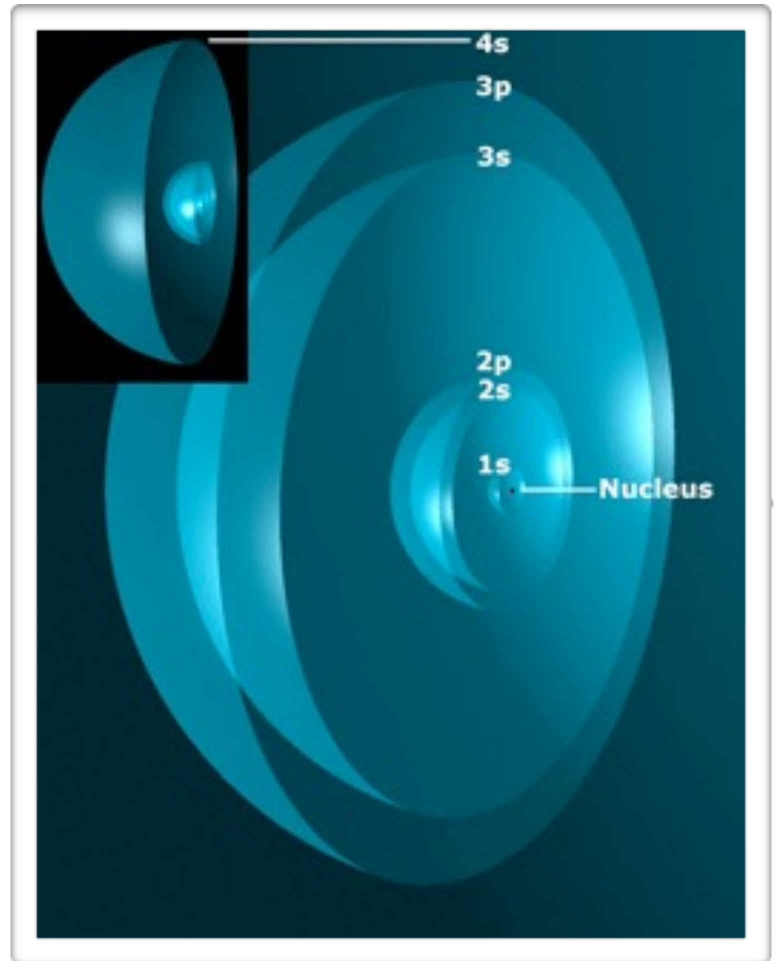




Orbital Shells

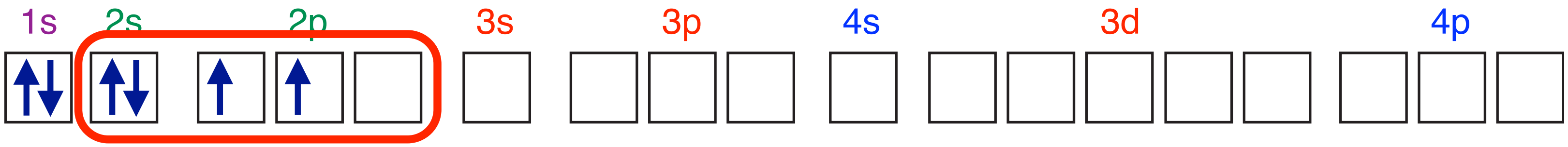


- The principle quantum number corresponds to the shell:
  - All sub-levels that share that number are part of that shell.
  - The shell with the greatest quantum number is valence shell.
    - The valence shell is the outermost layer of the atom.
    - Other atoms interact with the valence shell.
    - There are always 1-8 electrons in the valence shell.
  - All other shells (if any) contain the core electrons.



Be (4 electrons)

Orbital Shells



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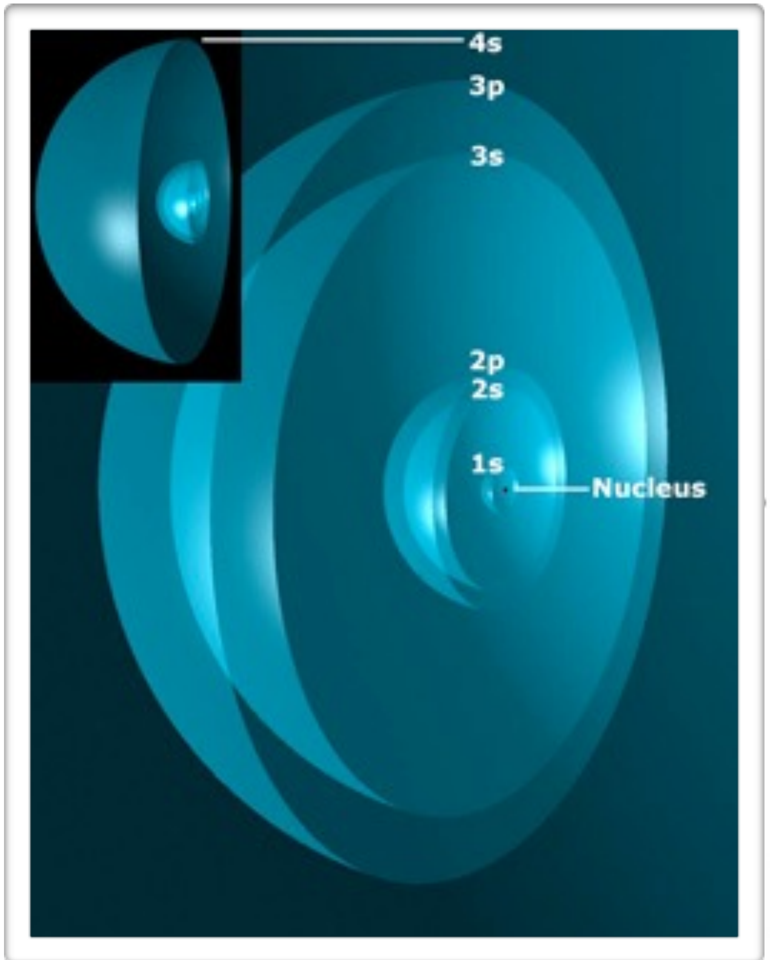
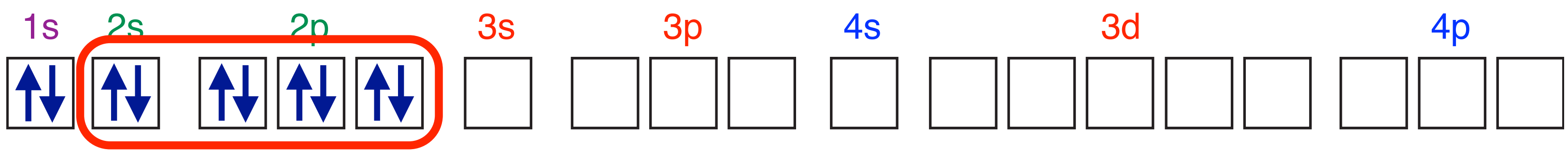


C (6 electrons)

Orbital Shells



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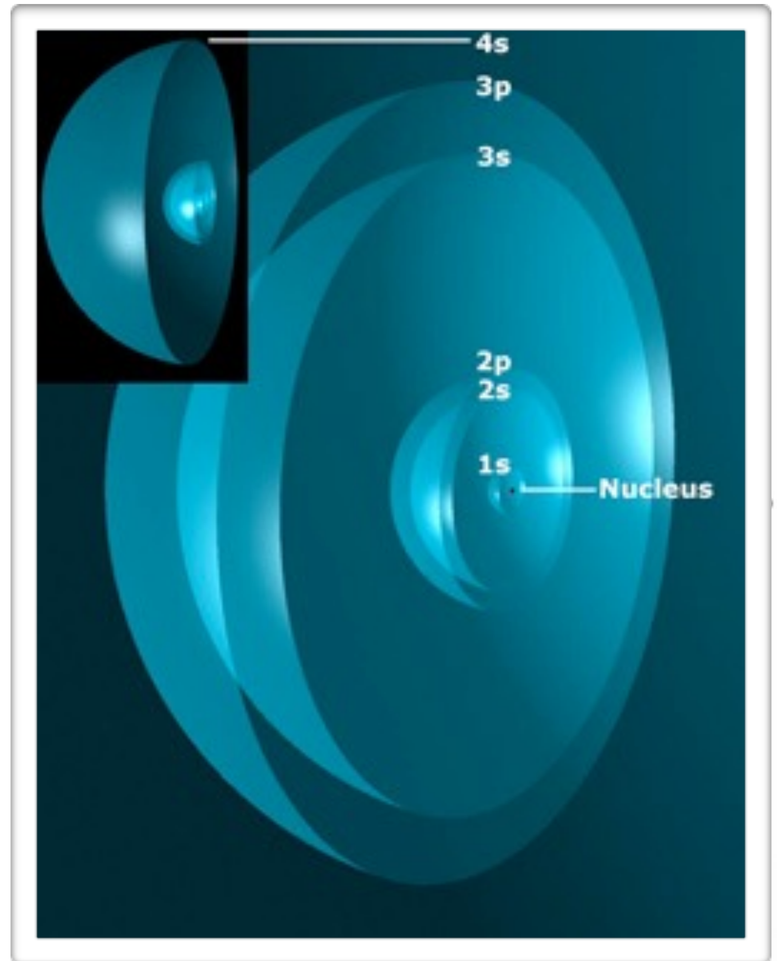
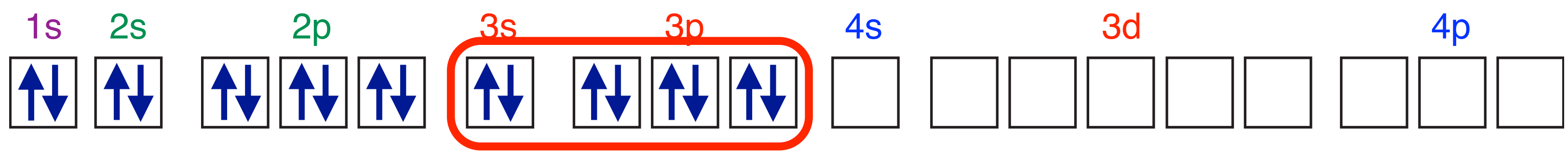


Ne (10 electrons)

Orbital Shells



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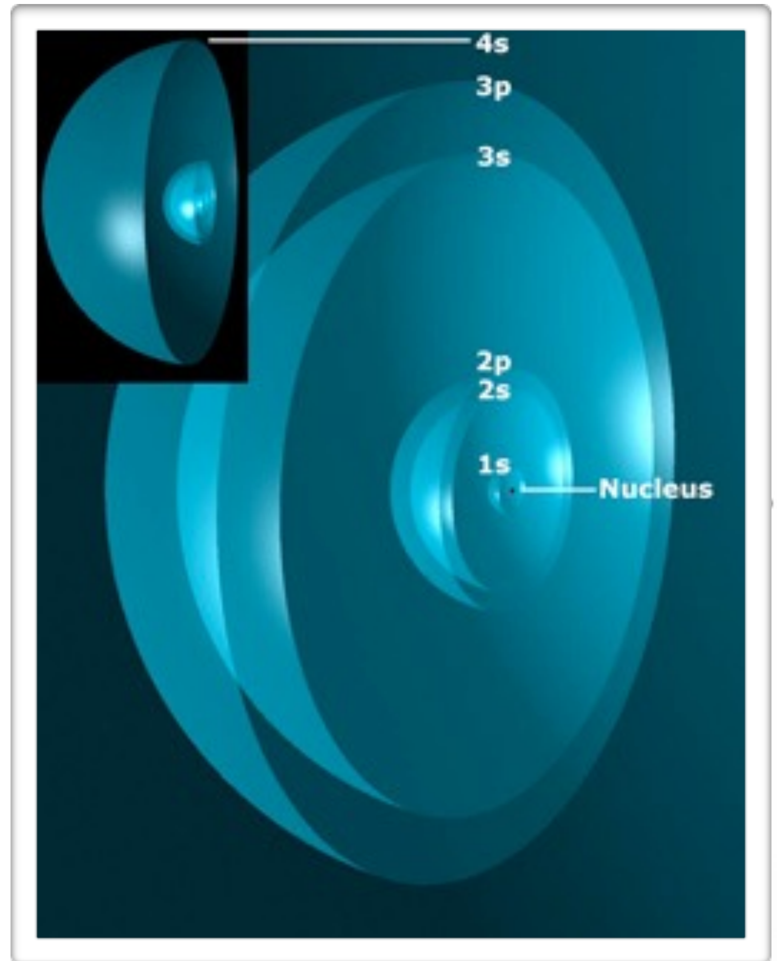
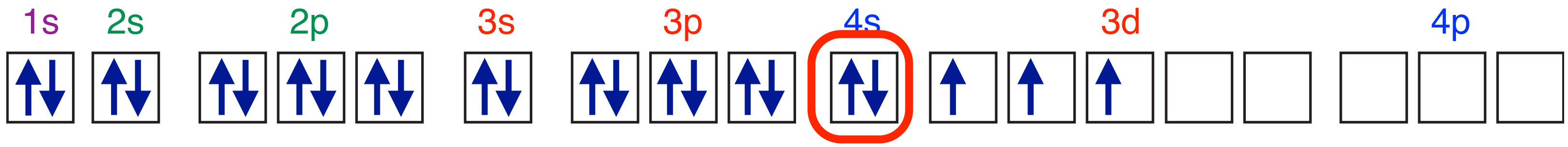


P^{3-} (15 protons; 18 electrons)

Orbital Shells



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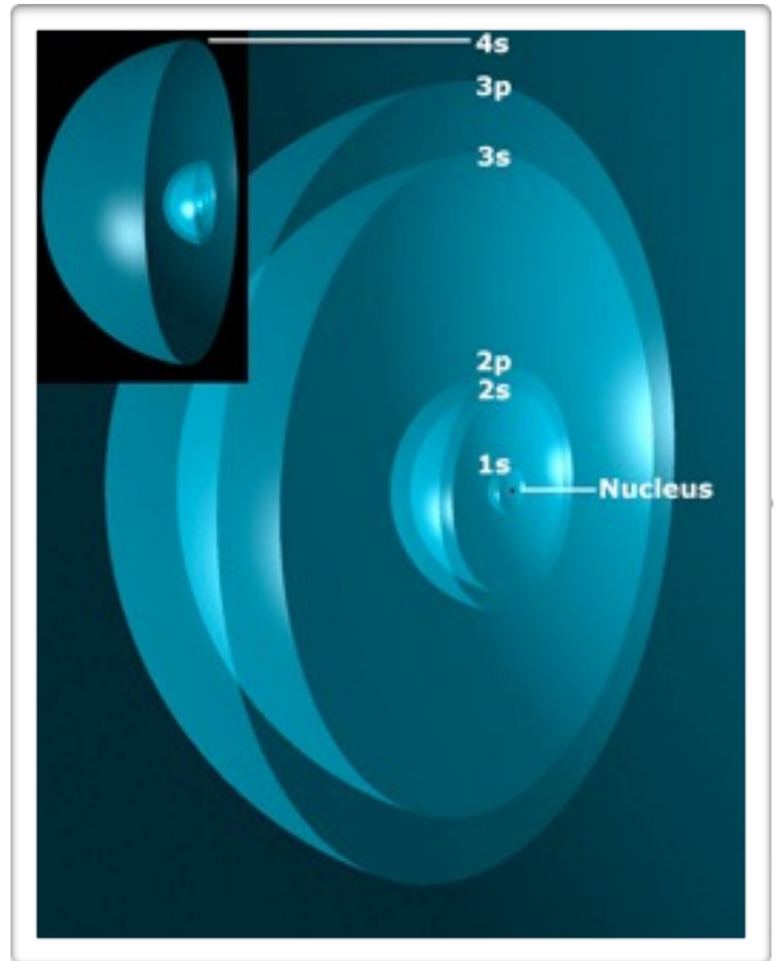
V (23 electrons)



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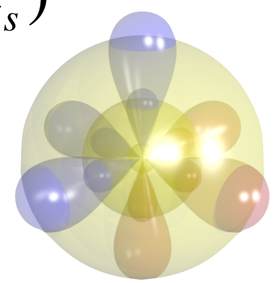
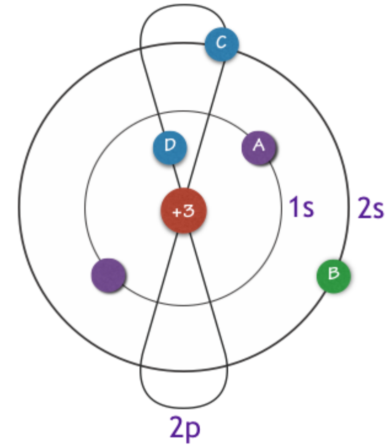
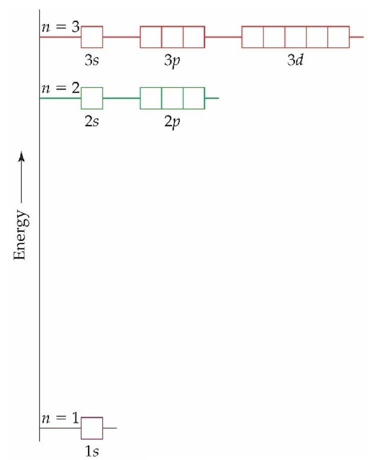
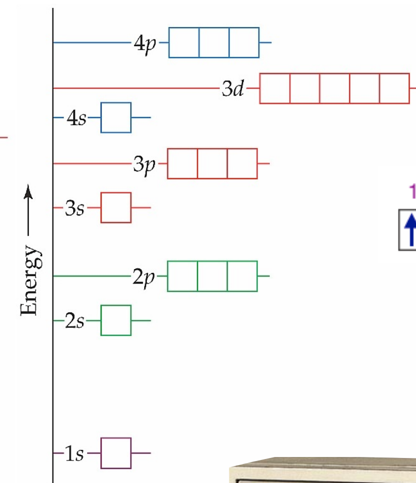
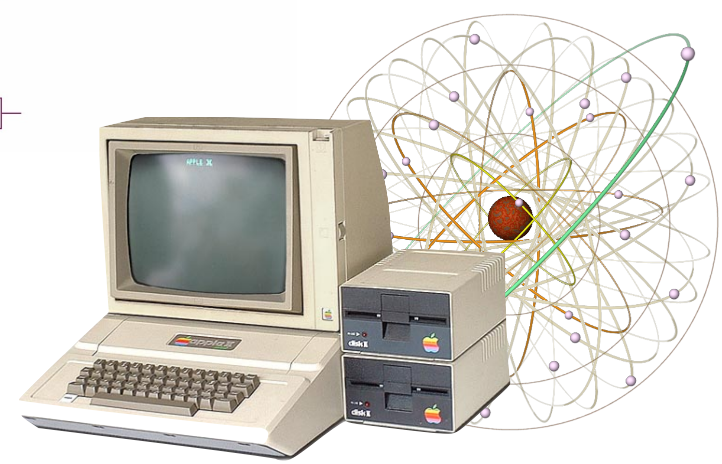
$$\Psi(n,l,m_l,m_s)$$



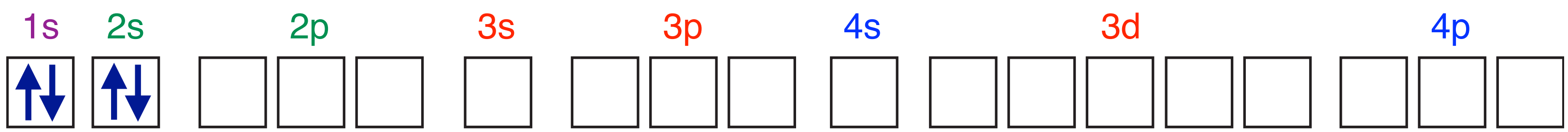








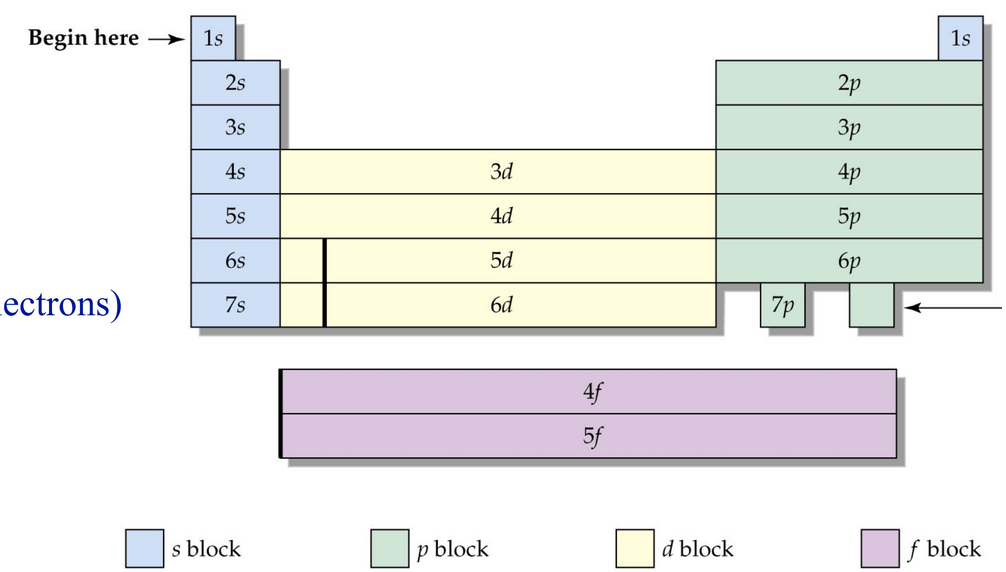
Electron Configuration Notation



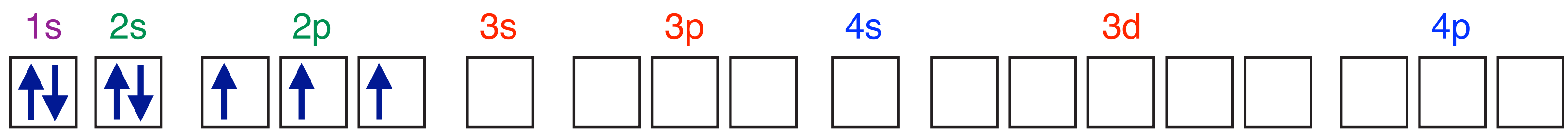
$$1s^2 2s^2$$

- Electron Configuration notation is a compact description of the electron distribution in an orbital diagram.
- Each occupied sub-shell is listed in order of increasing energy.
- A superscript denotes the number of electrons in that sub-shell.

Be (4 electrons)



Electron Configuration Notation



$$1s^2 2s^2 2p^3$$

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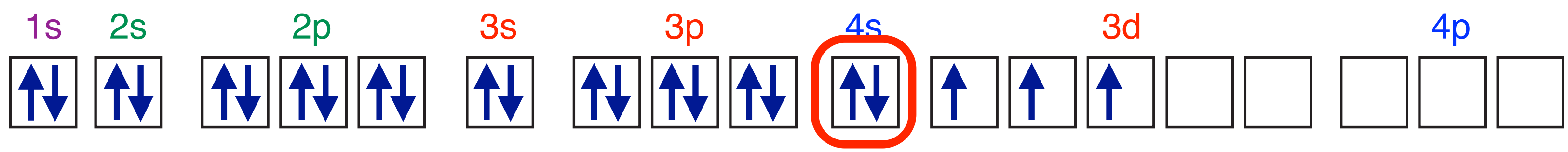
N (7 electrons)

Electron Configuration Notation



$$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^3 \qquad [Ar]4s^2 3d^3$$

- Electron Configuration notation is a compact description of the electron distribution in an orbital diagram.
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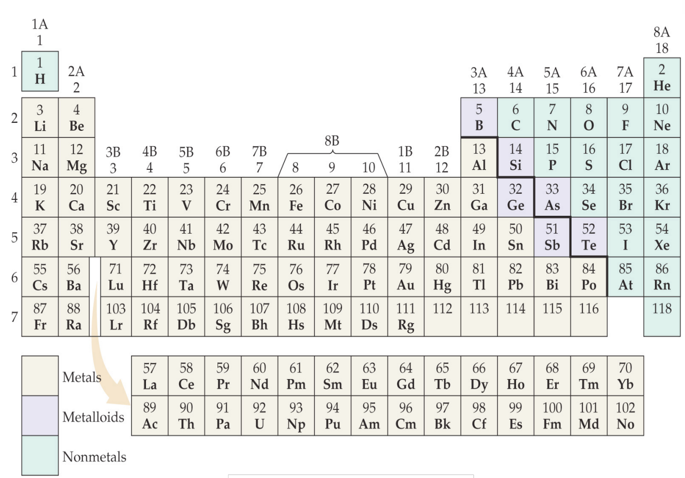
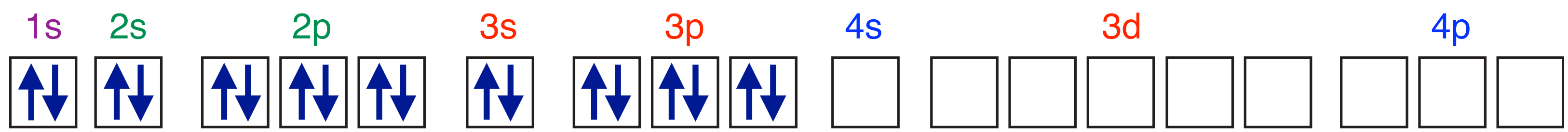
- Compact electron configuration replaces the core electrons with the corresponding nobel gas symbol.

V (23 electrons)



Electron Configuration Notation



$1s^2 2s^2 2p^6 3s^2 3p^6$ $[Ne]3s^2 3p^6$

- Electron Configuration notation is a compact description of the electron distribution in an orbital diagram.
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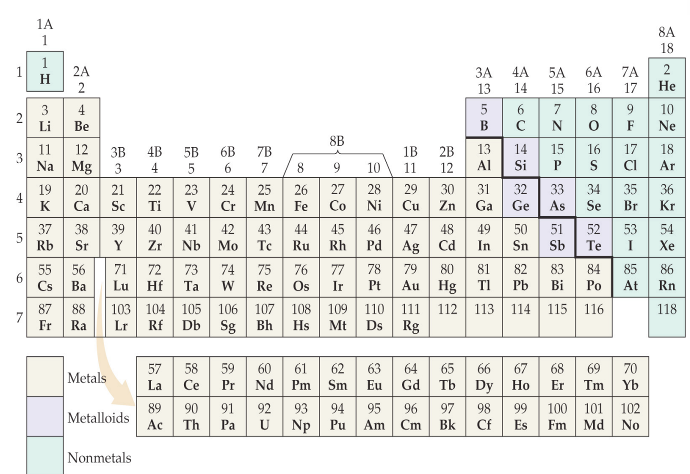
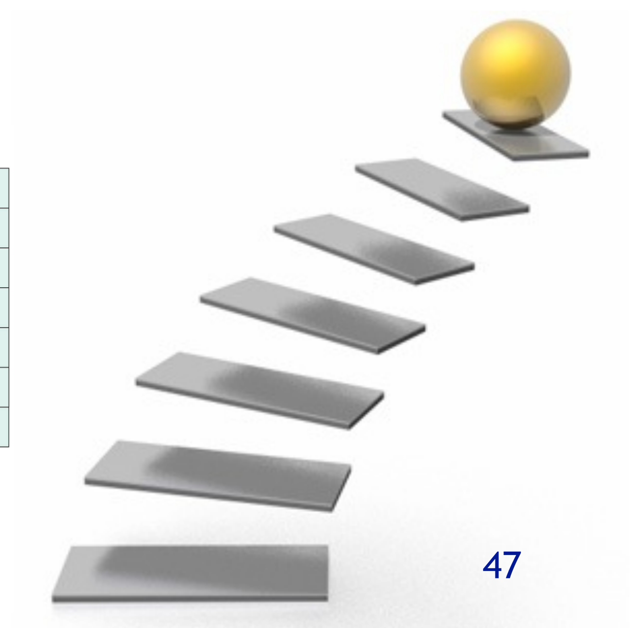
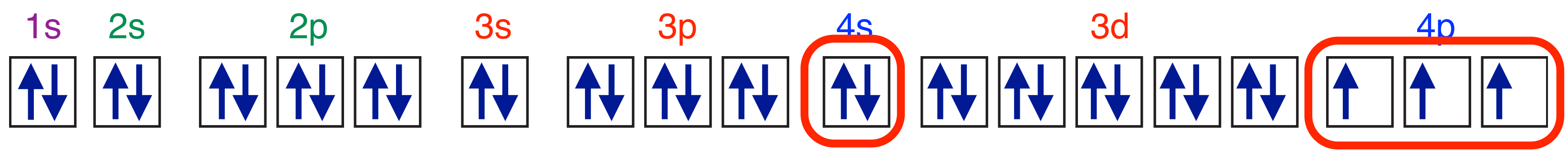
Ar (18 electrons)





Electron Configuration Notation



$$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^3 \qquad [Ar]4s^2 3d^{10} 4p^3$$

- Electron Configuration notation is a compact description of the electron distribution in an orbital diagram.
- Each occupied sub-shell is listed in order of increasing energy.
- A superscript denotes the number of electrons in that sub-shell.
- Compact electron configuration replaces most of the core electrons with the corresponding nobel gas symbol.

As (33 electrons)

	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	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112	113	114	115	116		118
				57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	
				89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	

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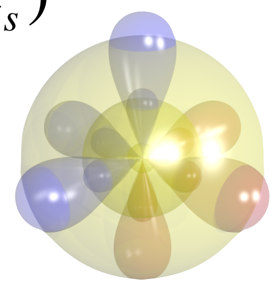
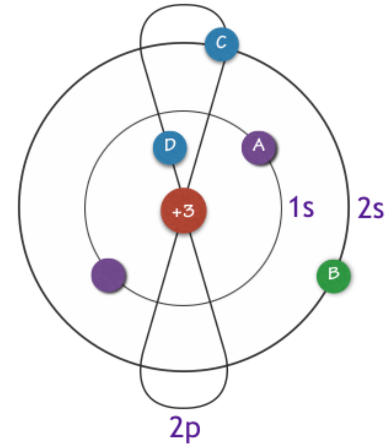
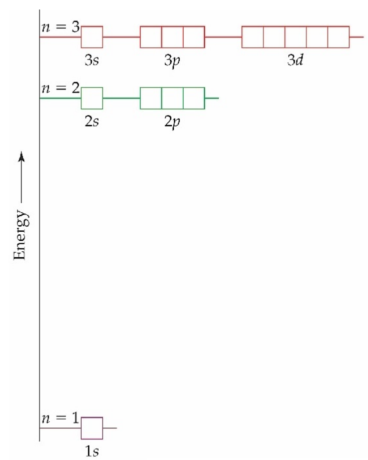
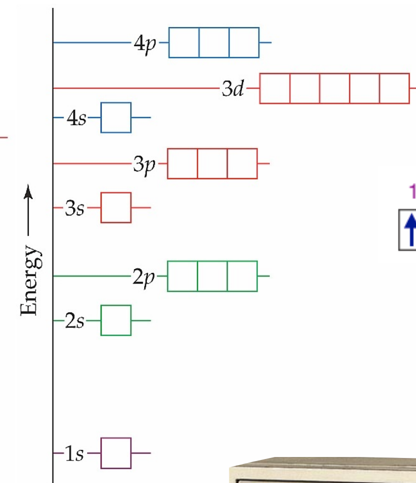
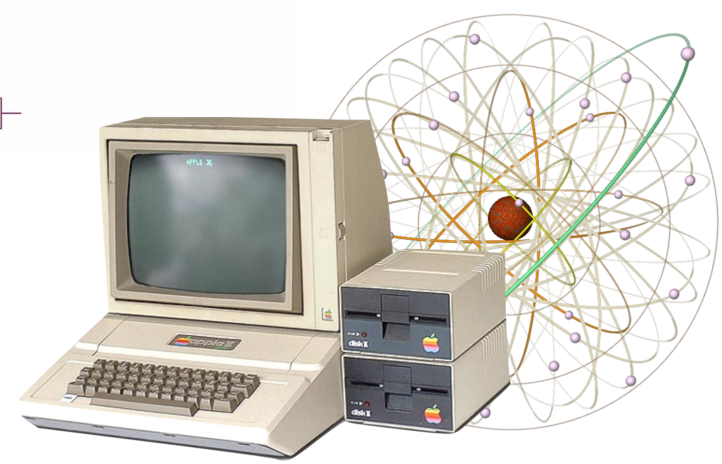


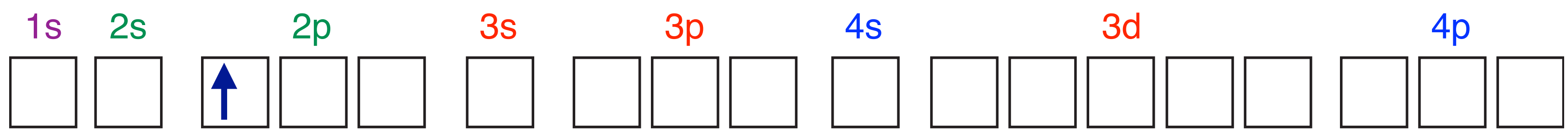






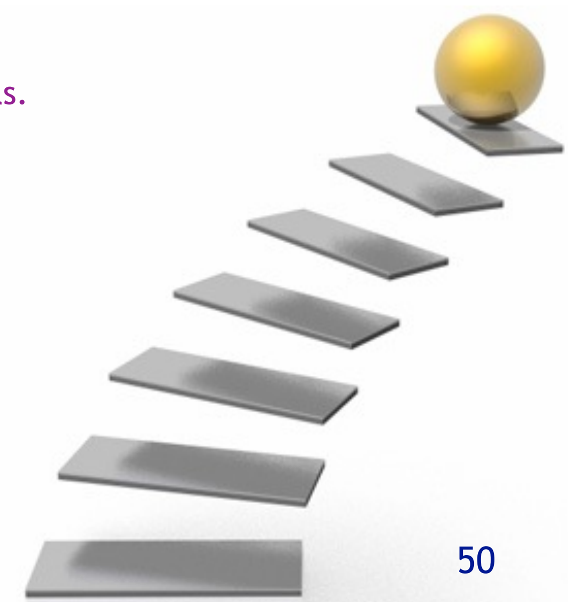


Quantum Numbers

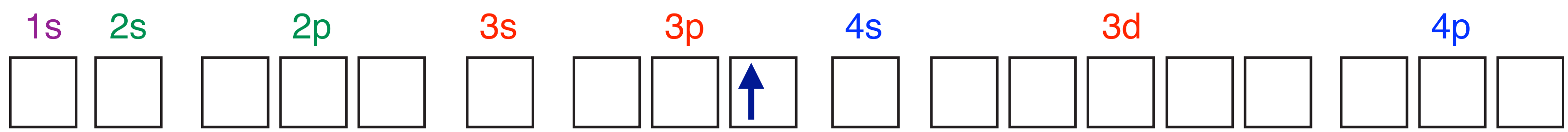


$$n = 2; l = 1; m_l = -1; m_s = +½$$

- The position of any electron position can be described by four numbers.
  - n is the principle quantum number, it corresponds to the shell.
  - l is the angular quantum number, it corresponds to the sub-shell.
    - l < n eg, if n =3 l = 0, 1, or 2
    - 0 = s; 1 = p; 2 = d; 3 = f
  - m_l is the magnetic quantum number, it's used to differentiate degenerate sub-shells.
    - m_l has values that run from -l ... +l; eg if l=3 m_l = -2, -1, 0, 1, 2
  - m_s is the spin quantum number, it's either +½ (spin up) or -½ (spin down)



Quantum Numbers



$$n = 3;\ l = 1;\ m_l = +1;\ m_s = +\tfrac{1}{2}$$

- The position of any electron position can be described by four numbers.
  - n is the principle quantum number, it corresponds to the shell.
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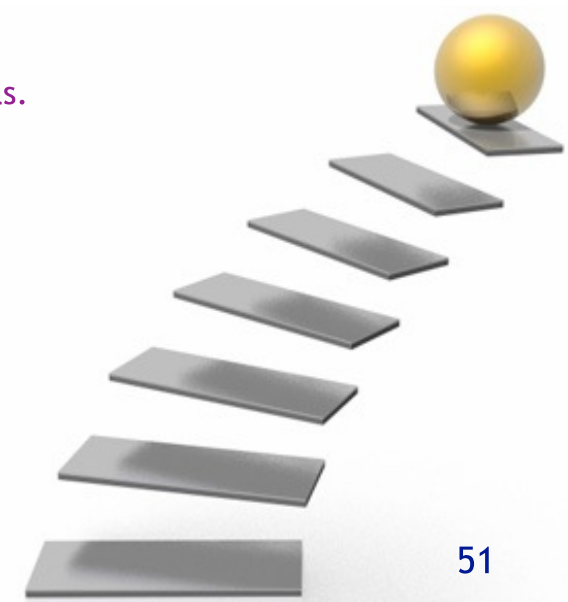
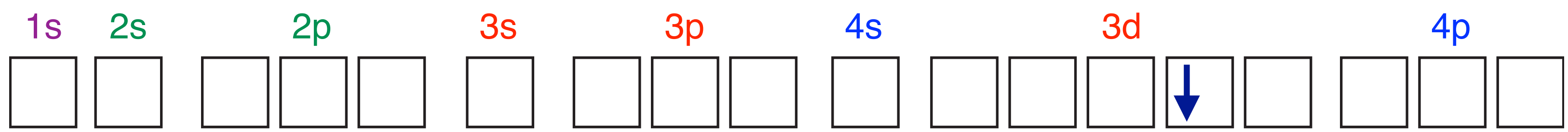
  - m_s is the spin quantum number, it's either $+\tfrac{1}{2}$ (spin up) or $-\tfrac{1}{2}$ (spin down)



Quantum Numbers



$$n = 3;\ l = 2;\ m_l = +1;\ m_s = -\tfrac{1}{2}$$

- The position of any electron position can be described by four numbers.
  - n is the principle quantum number, it corresponds to the shell.
  - l is the angular quantum number, it corresponds to the sub-shell.
    - $l < n$ eg, if $n = 3$ $l = 0, 1,$ or 2
    - 0 = s; 1 = p; 2 = d; 3 = f
  - m_l is the magnetic quantum number, it's used to differentiate degenerate sub-shells.
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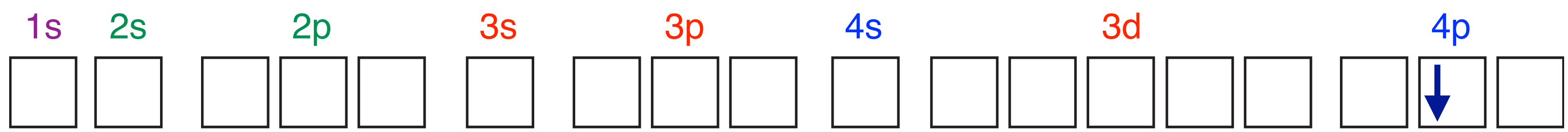
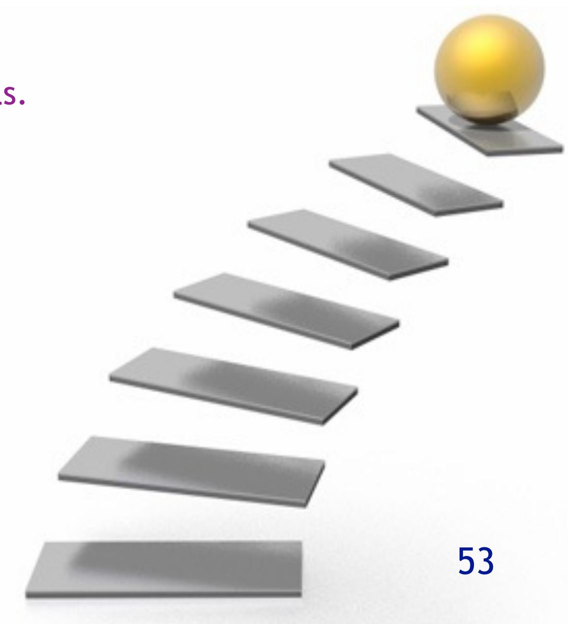
Quantum Numbers



$$n = 4;\ l = 1;\ m_l = 0;\ m_s = -\tfrac{1}{2}$$

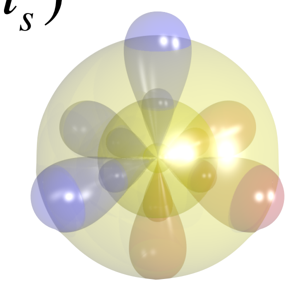
- The position of any electron position can be described by four numbers.
  - n is the principle quantum number, it corresponds to the shell.
  - l is the angular quantum number, it corresponds to the sub-shell.
    - $l < n$ eg, if $n = 3$ $l = 0, 1,$ or 2
    - $0 = s;\ 1 = p;\ 2 = d;\ 3 = f$
  - m_l is the magnetic quantum number, it's used to differentiate degenerate sub-shells.
    - m_l has values that run from $-l \ldots +l$; eg if $l=3$ $m_l = -2, -1, 0, 1, 2$
  - m_s is the spin quantum number, it's either $+\frac{1}{2}$ (spin up) or $-\frac{1}{2}$ (spin down)

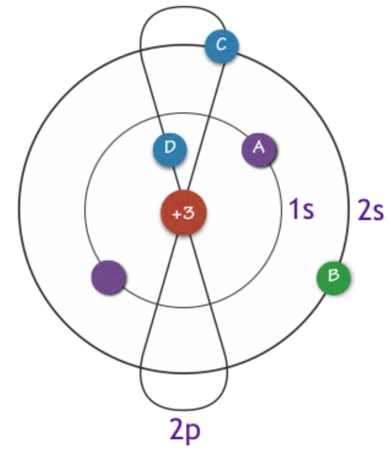


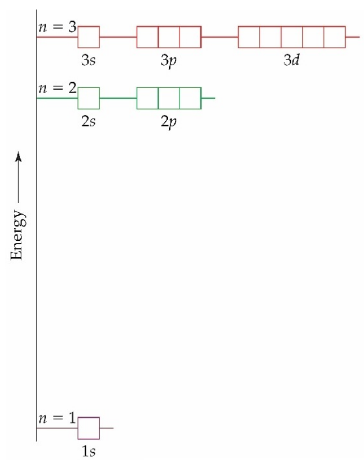
Putting Electrons into Orbitals

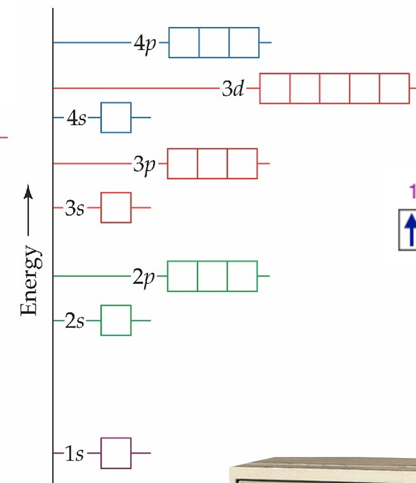
- Electron-Electron Interactions:
  - Electron Spin
  - Schrödinger Equation
    - The orbitals it defines
    - The energy of those orbitals
  - Orbital Splitting
    - Shielding & Penetration
  - Sub-level overlap
- Orbital Diagrams
  - Order of Sub-Levels
- Ground State Filling
  - Auf Bau Principle
  - Hund's Rule
  - Pauli Exclusion Principle
- Electron Shells
  - Valence Electrons
  - Core Electrons
- Electron Configuration notation
  - Compact notation
- Quantum Numbers
  - Describing Electron Positions

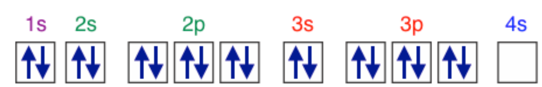
$$\Psi(n,l,m_l,m_s)$$

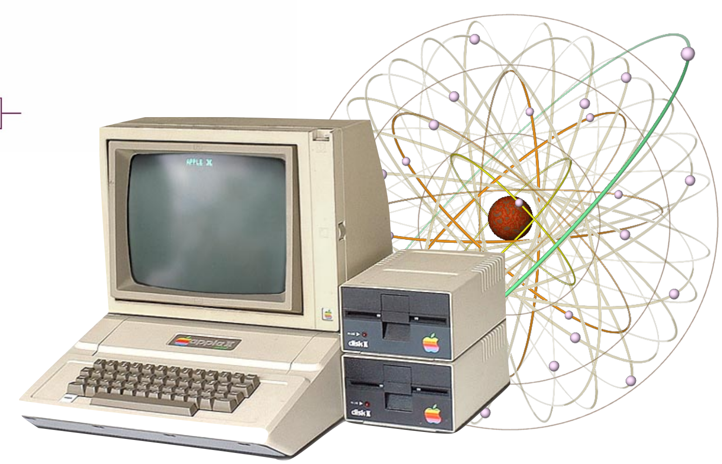












Questions?