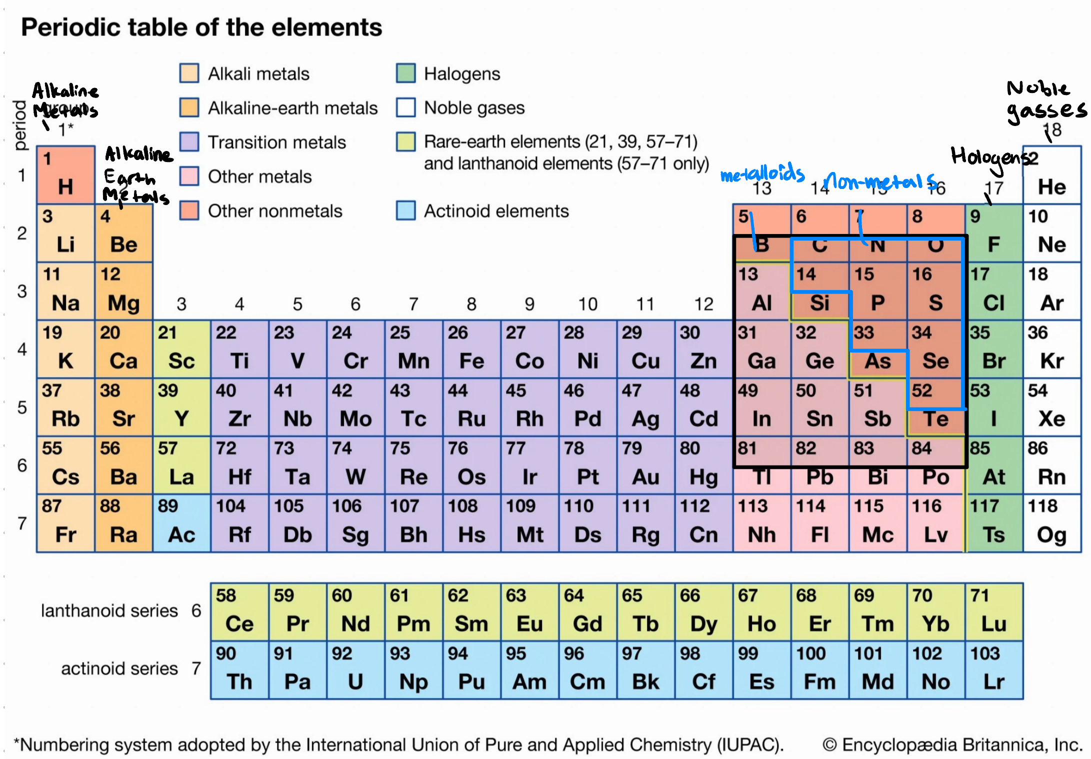
Atoms and Periodic Table



Atomic number

Charge on ion

Element symbol

Element name

Atomic mass

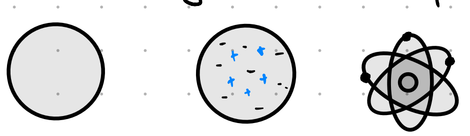
- 74 protons (atomic #)
- 68 electrons ($p^+ - e^- = q$)
- 110 neutrons ($p^+ + n^0$ = atomic mass)

Atomic Models

1809: Dalton had the first modern atomic model

1897: Thomson replaced it when electrons were discovered.
His plum pudding model shows uniform positive sphere with negative charges throughout.

1911: Rutherford replaced it when the gold-foil experiment showed there must be a tiny, massive nucleus. He proposed that electrons orbit in fixed, planetary orbits that can be anywhere in the sphere.

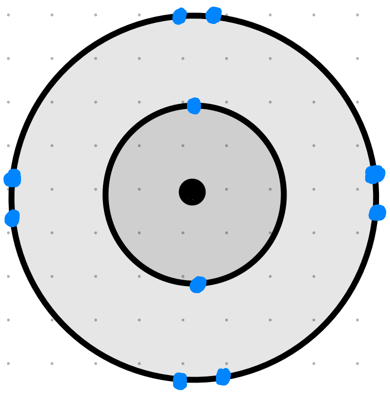


Dalton Thomson Rutherford

- Small, dense, positively charged nucleus
- Mostly empty space in atom.
- Electrons orbit the nucleus.

Limitations: - constant movement of e^- would cause loss (radiation) of energy. But they don't.
- Losing energy would cause falling toward nucleus. But they don't.

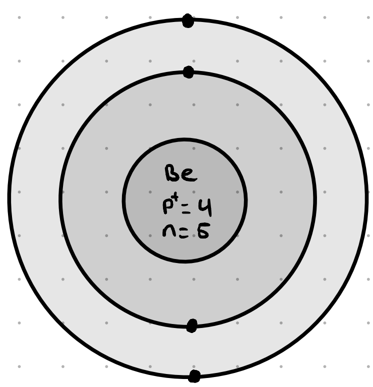
Bohr Model



- Electrons exist at specific, "quantized" energy levels. (at specific energy levels)
- They are stable unless external force / energy acts.
  - ↳ NO energy is emitted.
  - ↳ At "ground state", specific, quantized energy level.

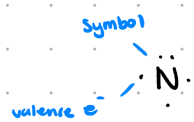
- If ray of light "excites" electron, it will raise it's energy level and move away from nucleus. It then comes down, which emits energy as photons at a specific wavelength percieved as color.

Bohr Rutherford Model



Beryllium

Lewis Structures



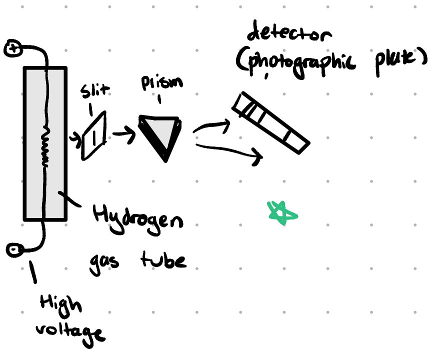
Nitrogen

- Quicker
- Only show symbol and valence e^-
- Shows how things bond

Quantum Mechanics

Quantum: A unit or "packet" of energy.

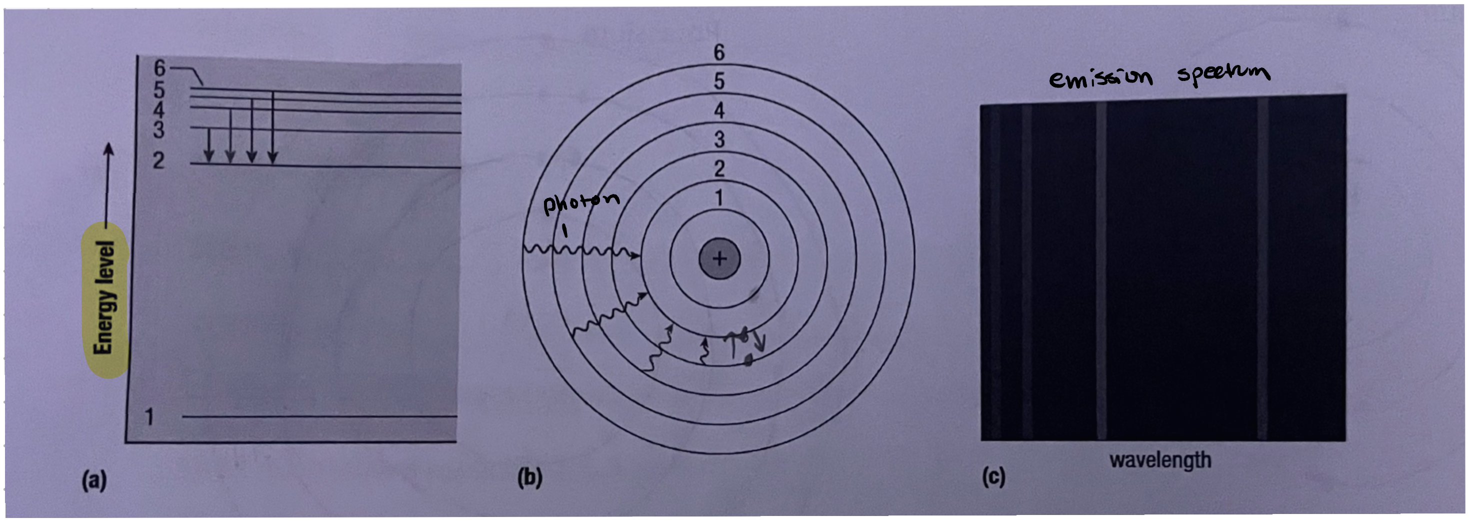
Photon: A unit of light energy.



- When hydrogen atoms are exposed to energy, expected colors are observed as an emission spectrum.

- This happens because after e^-s jump to a different, higher energy level, they jump back down to ground state (more stable) and release energy as photons.

- If energy levels were not quantized, wavelengths would be emitted as a spectrum, shown as a rainbow.



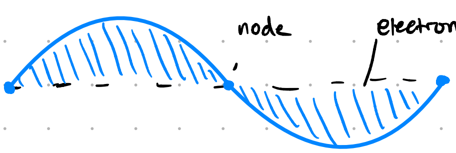
- The emission spectrum of hydrogen proved that electrons exist only at specific, discrete energy levels.

1^{st} energy level can hold: 2
2^{nd} : 8
3^{rd} : 18 electrons] Modelled by $2n^2$
4^{th} : 32

Electrons as Waves

1927: Schrodinger, de Broglie, and Heisenberg began looking at how electrons behave as waves instead of particles. Only a analogy.

- Compared electrons in orbitals as "standing waves" circular around the nucleus.



This model is consistent with the idea that only certain electron energies are allowed, because atoms are quantized. If $n = 4\frac{1}{3}$, for example, destructive interference occurs. e^- do not travel in circular orbits.

There are different orbitals for each energy level,

Heisenberg's uncertainty principle: Only the position or velocity of an electron can be known for certainty at a given time, not both. Therefore, electrons do not travel a fixed path, location is given as a probability distribution

Electron probability distribution: The probability of finding an electron at a given location is determined by it's wave function which also determines its orbital shape.

Electrons in the quantum mechanical model exist in 3 dimensions.

Quantum Numbers

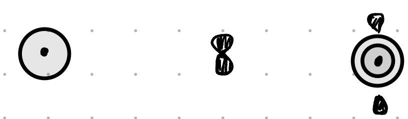
4 numbers representing a different, specific aspect about an electron's position.

n: Principle quantum number, $n > 0$
- Size and energy of an orbital.
- Maximum value of electrons in each orbital is $2n^2$.
- Period (row) of element on periodic table $= n$ value.

Ba: $n = 6$, Ne: $n = 2$

ℓ: Secondary quantum number
- Values from 0 to $n-1$: for $n=3$, $\ell = 0, 1, 2$
- ℓ represented as letters: $\{0, 1, 2, 3, 4\} = \{s\ p\ d\ f, g\}$
- Describes shape of orbital and number of orbitals?

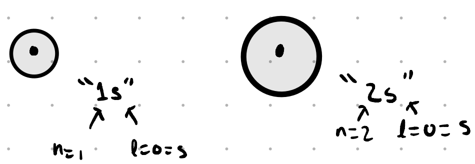
$\ell = 0$, s $\quad$ $\ell = 1$, p $\quad$ $\ell = 2$



m_ℓ: Magnetic quantum number
- Values from $-\ell$ to ℓ (including 0)
- For $\ell = 2$, $m\ell = -2, -1, 0, 1, 2$
- It describes the orientation of the orbital in space

S orbitals - spherical so only 1 orientation

$n=1$	$n=2$
$\ell=0$	$\ell = \boxed{0}, 1$ ← s
$m\ell=0$	$m\ell=0$

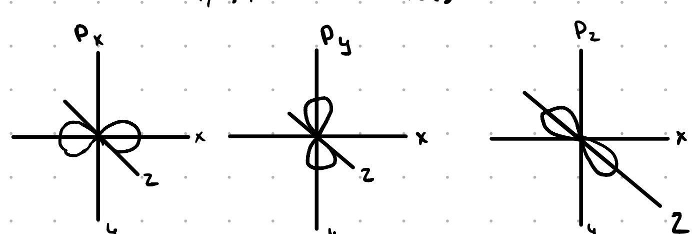


P orbitals

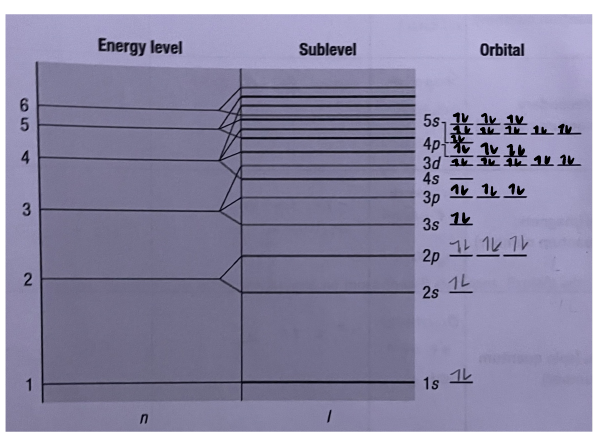
$n = 2$

$\ell = 0, \boxed{1}$ ← p

$m\ell = -1, 0, 1$ → 3 orientations



n	ℓ	nℓ	m_ℓ	num orbitals	num e^- in energy level
1	0	1s	0	1	2
2	0	2s	0	1	8
	1	2p	-1,0,1	3	↓
3	0	3s	0	1	18
	1	3p	-1,0,1	3	
	2	3d	-2,-1,0,1,2	5	↓
4	0	4s	0	1	32
	1	4p	-1,0,1	3	
	2	4d	-2,-1,0,1,2	5	↓
	3	4f	-3,-2,-1,0,1,2,3	7	



- At higher energy levels, the subshells overlap.

m_s: Spin quantum number

- Accounts for magnetism observed in certain elements
- Represents "spin state" of electron: $+\frac{1}{2}$ or $-\frac{1}{2}$, representing opposite spin directions.
- Describes orientation of spin of e^-

2p: ↑↓ ↑↓ ↑↓

1s: ↑↓

Quantum Number	Describes	Rules	Example
n (Principle quantum #)	Size + energy of orbitals	n = period of element	n = 3 for Na (Sodium)
ℓ (Secondary quantum #)	Shape of orbitals	From 0 to n−1	For n = 3 ℓ = 0, 1, 2 s p d
m_ℓ (Magnetic quantum #)	Orientation of orbital in space	From $-\ell$ to $-\ell$ including 0	For $\ell = 2$ $m_\ell = -3, -2, -1, 0, 1, 2, 3$
m_s (Spin quantum #)	Orientation of spin of electron	$-\frac{1}{2}$ or $+\frac{1}{2}$	Always $-\frac{1}{2}$ or $\frac{1}{2}$

Practice Questions

1. Which of the following sets of quantum number are not allowed? If it's not allowed, state why.

a) n=3, l=2, m_l = 2

$n = \boxed{3}$
$l = 0, 1, \boxed{2}$
$m_l = -2, -1, 0, 1, \boxed{2}$

b) n=4, l=3, m_l=4

$n = \boxed{4}$
$l = 0, 1, 2, \boxed{3}$
$m_l = -3, -2, -1, 0, 1, 2, 3$ 4

c) n=0, l=0, m_l=0

$n > 0$

d) n=2, l=-1, m_l=1

$n = \boxed{2}$
$l = 0, 1$ -1

e) n=1, l=1, m_l=2

$n = \boxed{1}$
$l = 0, \boxed{1}$
$m_l = -1, 0, 1$ 2

2. The second energy shell (n=2) in an atom can hold no more than 8 electrons. Explain why.

where $n = 2$, $l = 0, 1$

0 is s
which hold
$2e^-$: ↿⇂

1 is p
which have 3 orientations: -1, 0, 1
each hold $2e^-$
$2 \cdot 3 = 6$

In total $6 + 2 = 8e^-$ capacity for all orbitals in second energy shell

Also, rule $2n^2$ checks out.
$= 2(2)^2$
$= 2(4)$
$= 8$

3. List all the possible quantum numbers for an electron in the

a) 2s orbital

b) 6s orbital

c) 3p orbital

a) 2s
$n = 2$ $l = 0$

where $n = 2$
$l = 0, 1$

$m_l = 0$
$= -1, 0, 1$

$m_s = -\frac{1}{2}, \frac{1}{2}$

b) 6s
$n = 6$ $l = 0$

where $n = 6$
$l = 0, 1, 2, 3, 4, 5$

$m_l = 0$
$= -1, 0, 1$
$= -2, -1, 0, 1, 2$
$= -3, -2, -1, 0, 1, 2, 3$
$= -4, -3, -2, -1, 0, 1, 2, 3, 4$
$= -5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5$

$m_s = -\frac{1}{2}, \frac{1}{2}$

c) 3p
$n = 3$ $l = 1$

where $n = 3$
$l = 0, 1, 2$

$m_l = 0$
$= -1, 0, 1$
$= -2, -1, 0, 1, 2$

$m_s = -\frac{1}{2}, \frac{1}{2}$

Electron Configurations

Pauli Exclusion Principle: No 2 electrons can have the same four quantum numbers.

The Aufbau Principle: Atoms are "built up" by adding electrons that fill lower energy levels first.

5s 5p 5d 5f
4s 4p 4d 4f
3s 3p 3d
2s 2p
1s

ie: 1s, 2s, 2p, 3s, 3p, 3d, etc

Hund's Rule: If 2 or more degenerate (same energy level) orbitals are available, one electron goes into each until all of them are half full before pairing up.

2p: $\frac{\uparrow}{p_x}$ $\frac{\uparrow}{p_y}$ $\frac{\uparrow}{p_z}$ $\xrightarrow{\text{then}}$ $\frac{\uparrow\downarrow}{p_x}$ $\frac{\uparrow\downarrow}{p_y}$ $\frac{\uparrow\downarrow}{p_z}$

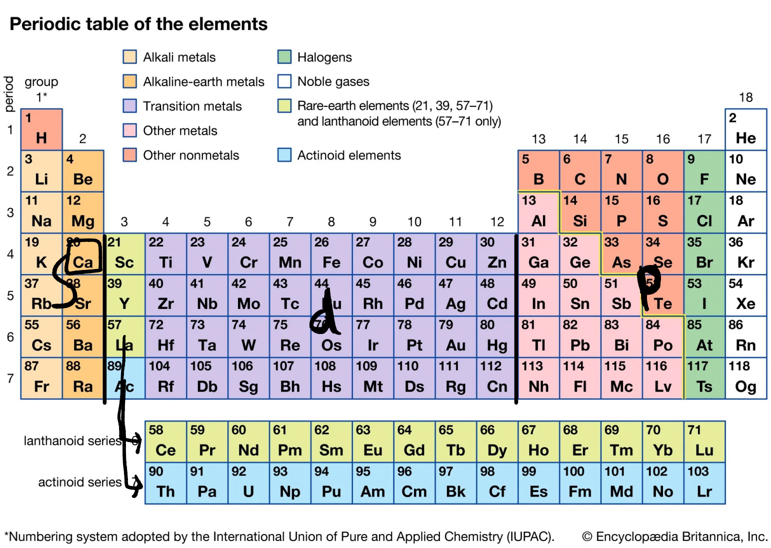
Energy-level diagrams:

- Slow to set up

2p: ↑ ↑ ↑
2s: ↑↓
1s: ↑↓

Nitrogen (N)

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



Ca: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$

or

$[Ar] 4s^2$

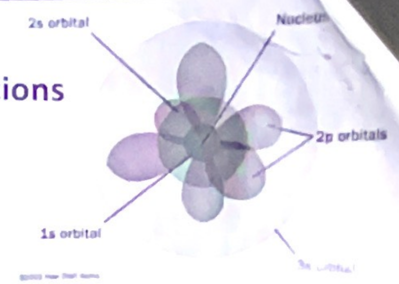
↳ Previous noble gas

Exceptions:

Copper (Cu): $3d^9 4s^2 \rightarrow 3d^{10} 4s^1$
Chromium (Cr): $3d^4 4s^2 \rightarrow 3d^5 4s^1$

→ More preferable to fill all 3d up half or full than fill 4s up to 2.

3d: $\underline{\uparrow}$ $\underline{\uparrow}$ $\underline{\uparrow}$ $\underline{\uparrow}$ $\underline{\uparrow}$



Homework: Quantum Model and Electron Configurations

1. What does it mean when we say an electron's energy is *quantized*?

there are discrete energy levels wherein electrons assume a ground state.

2. How do emission spectra prove this idea?

Electron emission spectrum for hydrogen shows as a few wavelengths instead of a spectrum or rainbow proving quantized energy levels in hydrogen atom.

3. How does representing electrons as "standing waves" help model this idea?

electrons exist within a probabilistic distribution which can be analogized with a standing wave where the area between nodes is comparable to orbitals.

Also, if n isn't a whole number, destructive interference occurs as n must be a whole number in atoms

4. What is the most electrons that can fit within a...

a) one individual orbital? (one m_l) 2

b) A p sublevel? ("p orbitals") 6

c) A d sublevel? ("d orbitals") 10

$3s^2\ 3p^6\ 3d^x = 2(3)^2$

$x+8 = 18$

$= 10$

5. Write the *full* electron configurations for

a) magnesium

Mg: $1s^2\ 2s^2\ 2p^6\ 3s^2$

b) sodium ion (Na^+)

Na: $1s^2\ 2s^2\ 2p^6\ \cancel{3s}$

c) chromium

Cr: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1\ 4p^5$

d) lanthanum (atomic number 57)

: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^6\ 6s^2\ 4f$

6. Write the *shorthand* electron configurations for

a) aluminum

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

b) bromine

$[Ar]\ 4s^2\ 3d^{10}\ 4p^5$

c) copper

$[Ar]\ 4s^1\ 4d^{10}$

d) tungsten (atomic number 74)

$[Xe]\ 6s^2\ 4f^{14}\ 5d^4$

Bonding

Ionic bond: - Electrons are given / taken (transferred)
- Between a non-metal and a metal

Covalent bond: - Electrons are shared
- Between a non-metal and a non-metal

Electronegativity: Ability of an atom to attract shared electrons to itself.
Greater ΔEN creates more ionic bond character.

Lewis' Theory of bonding

- Atoms and ions are stable when they have full valence shell.
- Electrons are most stable when paired
- The goal of bonding is to become isoelectronic with noble gases (get a full valence shell)
  ↳ Same # of electrons.

H_2

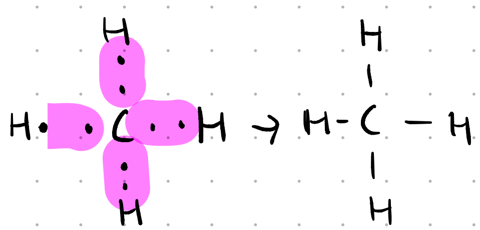
H· ·H → H – H

F_2

:F· ·F: → :F – F:

Lewis Dot Diagrams

CH_4

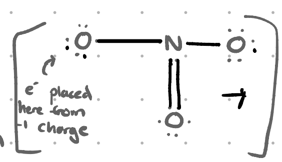


- Add valence electrons up to check after
- Central atom
  - Lowest quantity usually
  - Least electronegative atom
  - not hydrogen
- Write FC to check work.
- Bonds to fulfil octet / duet rule
- Past atomic # 15, octet can be overfilled
- Boron can be underfilled

Formal charge of atom: Valence electrons - # of bonds - lone electrons
↳ Will be 0 for neutral molecules

NO_3^-

$5 + 3(6)$
$= 23 + 1$ ↳ Because -1 charge means extra electron
$= 24$

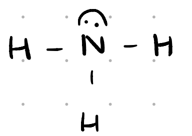
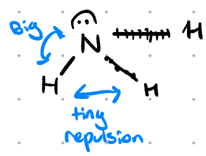


Resonance structures
↳ Double bond could be to any oxygen atom.
Can make three different, identical versions.

FC - verify
O: 6 - 1 - 6 = -1
O: 6 - 1 - 6 = -1
N: 5 - 4 - 0 = 1
-1
matches charge -1

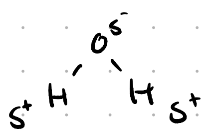
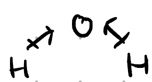
VSEPR Theory

- Helps predict 3D shape of molecules and bond angles.
- Stands for Valence Shell Electron Pair Repulsion
- Lone pairs and bonds consist of electrons that repel each other and affect bond angles.
- Bond pairs repel each other the least. Lone pairs repel each other the most.

 ← lewis | VSEPR → 

Polarity

- The individual bond or the molecule as a whole.
- When a bond is polar, electrons are not shared equally.
- When a molecule is polar, overall, the electrons are closer to one part than another.
- Symmetry can affect the polarity of a molecule.
- Molecules can have polar bonds and be non-polar

 or  ← The arrow points to more electronegative atom
Size of arrow matters.

polar: water, ethanol, ammonia
non-polar: CO_2, oils, fats, octane, CH_4

- Polarity affects miscibility, melting point, and boiling point. Other properties too.

ΔEN (Change in electronegativity):

<0.5 → Non-polar (covalent)
0.5-1.7 → Polar (covalent)
>1.7 → Ionic

- EN values tend to increase ↑ and → in periodic table.
  - Halogens really want one more e^- to fill valence shell.
  - Lots of positive charge in nucleus with little electron shielding.

<u>H and O</u>

$\Delta EN = EN_O - EN_H$
$= 3.44 - 2.20$
$= 1.24$ ∴ polar

H_2O shape:

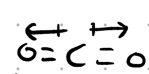
- 4 e^- pairs
- 2 lone pairs
∴ bent
↓
polar

<u>C and O</u>

$\Delta EN = EN_O - EN_C$
$= 3.44 - 2.55$
$= 0.89$ ∴ polar

CO_2 shape

- 2 e^- pairs
- 0 lone pairs
∴ linear
↓
non-polar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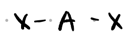
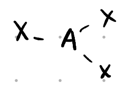
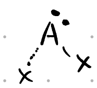
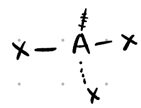
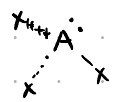
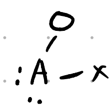
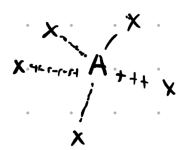
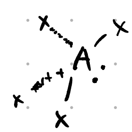
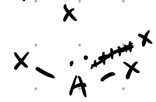
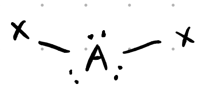
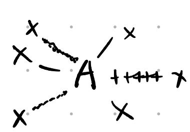
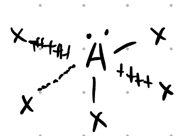
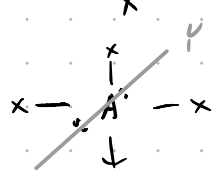
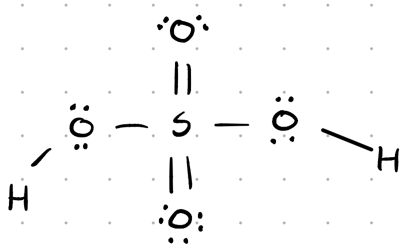
Death Chart (VSEPR theory Chart)

ē pairs	Lone pairs	Name	angles	shape
2	0	Linear	180°	
3	0	Trigonal Planar	120°	
↓	1	Bent	<120°	
4	0	Tetrahedral	109.5°	
↓	1	Trigonal Pyramidal	<109.5°	
↓	2	Bent	<109.5°	
5	0	Trigonal Bipyramidal	120° 90.0° 180°	
↓	1	Seesaw	<90° <120°	
↓	2	T-Shaped	<90° <180°	
↓	3	Linear	<180°	
6	0	Octahedral	90°	
↓	1	Square Pyramid	<90°	
↓	2	Square Planar	<90°	

H_2SO_4 valence e: $6 + 4(6) + 2(1) = 32 e^-$ - multiple of 8 → no lone e^-



$FC_S = 6 - \text{Bonds} - \text{lone } e^-$

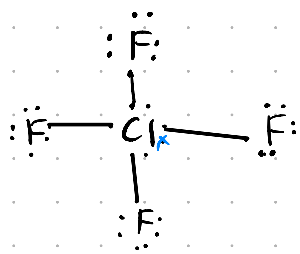
$= 6 - B - 0$

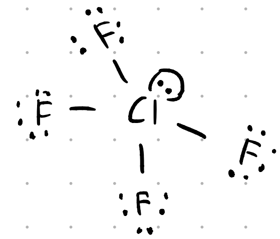
$B = 6$

ClF_4^{+} $Ve^- = 7(1) + 4(7)$

$= 7 + 28 - 1$

$= 34$





FC

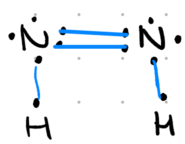
F: $7 - 1 - 6 = 0$

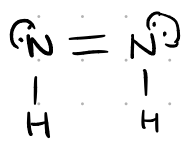
Cl: $7 - 4 - 2 = 1$

1

N_2H_2 $Ve^- = 2(1) + 5(2)$

$= 12$





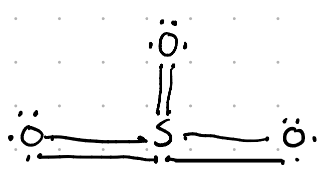
FC

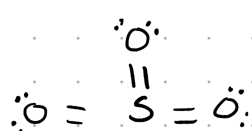
N: $5 - 3 - 2 = 0$

H: $1 - 1 = 0$

$\boxed{0}$

Predict shape : SO_3 (sulfur trioxide)





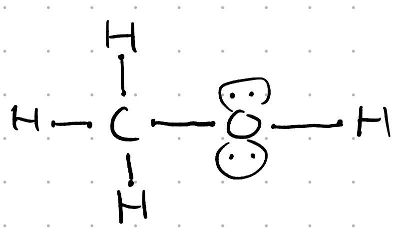
3 electron pairs

0 lone electrons

trigonal planar

120°

Predict shape CH_3OH



FC

H: $1 - 1 = 0$

C: $4 - 4 = 0$

O: $6 - 2 - 4 = 0$

0 ✓

Shape:

For C: $4 e^-$ pair, 0 lp) tetrahedral

O: 2 lp, $4 e^-$p) Bent

H: 1e pair, 0 le (109.5°

Intermolecular Forces

1. Hydrogen Bonding (Strongest)

- Hydrogen atom (with polarity) in a molecule is attracted to an electromagnetic atom (F, O, or N) in a different molecule.
- Example: water - high BP as result.

2. Dipole-dipole interactions (Strong)

- When polar molecules line up with each other so that their opposite partial charges (dipoles) are next to each other.
- Requires polar molecules

3. London Dispersion Forces (weak)

- Attraction forces caused by random unequal distributions of electrons. Causes temporary dipole.
- More strongly affects molecules with large number of electrons (large molecules).
- Does not require dipole / polarity. Requires electrons.

H_2O intermolecular forces:
- H-bonding (O)
- D-d interactions (polar)
- LDF (e^-s)
(all)

$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$:
- LDF only (e^-s)
- No dipole for d-d interactions.
- NO F, O, N for h-bonding.

Solids

Crystaline solids:
- metallic
- ionic
- covalent network
- molecular

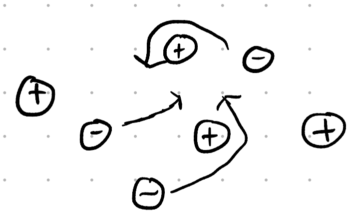
Ionic Crystals:

- Formed between metal and non-metal ions.
- Arranged into a crystal lattice solid.
- Arranged by alternating positive and negative ions.
- Brittle, hard, high melting point, conducts electricity when dissolved in water.
- Properties reflect that ionic bonds are strong

Metallic Crystals:

- Held together by electronic interactions and free-moving electrons.
- Different metallic crystals have very different properties

Electron Sea Theory: A theory that electrons in a metallic crystal move freely around positively charged nuclei.



- Sheen: Valence electrons that absorb and emit light.
- Malleability: The electron sea allows atoms to slide over each other.
- Electrical conductivity: Mobile valence electrons can produce an electric current (need source)
- Hardness: The electron sea surrounding the positive nuclei produces strong electrostatic attractions that hold nuclei together.

Molecular Crystals:

- Solid composed of individual molecules held together by inter-molecular forces (IMF) of attraction.
- Lower melting points and less hard than ionic crystals due to IMF.
- It is an electrical non-conductor due to being composed of neutral molecules - no free flowing electrons.

Covalent Network Crystals:

- Covalent bonds in an interwoven network creating crystal.
- Typically very high melting point and extreme hardness due to atoms interlocking.
- Not good conductors because no free-flowing electrons occupied in covalent bonds.

Diamond vs graphite:

- Diamond is tetrahedral (4 bonds)
- Graphite is stacks of layered sheets (3 bonds)

- Diamond is stronger because each molecule is interlinked in all directions. The bonds are covalent and more tightly sealed.

- Many covalent network crystals involve carbon and silicon. They both have the same number of valence electrons and same periodic table group.

Overview / Review

Type	Particles Involved	Force of Attraction	BP	Conductivity	Physical Properties	Example
Ionic	Ions	Ionic bonds	High	In solution	Brittle + hard	NaCl
Metallic	Metals	Electrostatic interactions	High-ish	High	Malleable Shiny	Cu
Molecular	Molecules	IMF	Low	Low	Soft	CO_2 (s)
Covalent Network	Non-metals	Covalent bonds	High	Low	Many have C and Si	diamond