$1\,eV = 1.6\times10^{-19}\,J$

$\mathcal{E} = -13.6(z-1)^2\left(\frac{1}{n_f^2}-\frac{1}{n_i^2}\right) = {hc}/{\lambda}$

$1\,W = 1\,J/s$

$1\,\text{Å} = 1\times10^{-10}\,m$

take it easy pal
you got this
it doesn't really matter
P-N-R!
Home in 24 hrs!

3.091 Final Notes

DELIA STEPHENS

Lewis Dot Structure

1. Connect atoms. Central atom least/less electronegative.
2. Determine total number of valence electrons.
3. Place bonding pair of e⁻ between adjacent atoms.
4. Add e⁻ to terminal pairs to form octet.
5. Add any remaining e⁻ to central atom.
6. If central atom < octet, use lone pair to make multiple bonds.
7. If too many, AH!

central atom ⟶ small electronegative

EXCEPTIONS

Hydrogen only needs one.

Be: 4, B: 6

- the larger the central atom ⟶ expanded octet ($n>3$)

Formal Charge

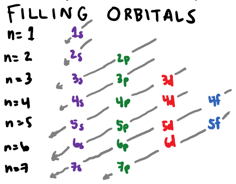
$\text{valence electrons} - \left(\text{nonbonding } e^- + \frac{\text{bonding } e^-}{2}\right)$

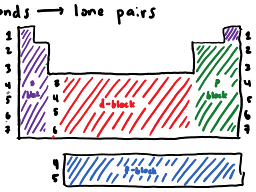
all available e⁻ — from Lewis structure

- resonant structure: change of location, eq. stability

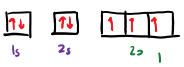
lone pairs ⟶ bonds, bonds ⟶ lone pairs

Filling Orbitals





N: 7 — prefers half or fully filled



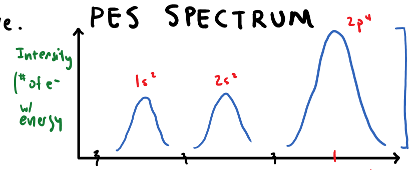
Bohr

- only 2e⁻ can occupy any given orbitals
- electrons closer in "shield" outer electrons, so outer electrons easier to ionize (rip off)

$\Delta\mathcal{E} = -13.6\,z^2\left(\frac{1}{n_f^2}-\frac{1}{n_i^2}\right)$ (in eV)

$\mathcal{E} = h\nu$ (light), $\mathcal{E} = \frac{hc}{\lambda}$ (Planck's, wavelength)

PES Spectrum



height determined by number of electrons in orbital

peak w/ lowest binding energy corresponds

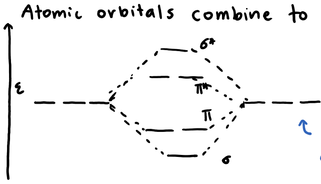
⟵ bigger binding energy

Quantum Numbers

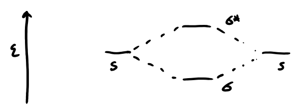
Number	Symbol	Values	Meaning
principal	n	1, 2, 3…	distance from nucleus (z)
angular	ℓ	0, 1, 2, …, n−1	0 = s, 1 = p, d, f
magnetic	m_ℓ	$-\ell, \ldots 0 \ldots \ell$	orientation ("block")
spin	m_s	$\frac{1}{2}, -\frac{1}{2}$	"up" or "down"

Orbitals

Atomic orbitals combine to make molecular orbitals



1. Valence electrons (only p ⟶ σ + π, s ⟶ σ)
2. Homonuclear or heteronuclear?
   ↑ orbitals of more electronegative atom have lower energy
3. Draw the diagram (different for s and p). If bonding s with p, some sort of hybridization will occur AND you won't have π (only p)
4. Fill in e⁻; lowest energy first



Bond order $= \frac{1}{2}(e^-$ in bonding − antibonding) Obey Hund's Rule.

If bond order > 0, then stable.

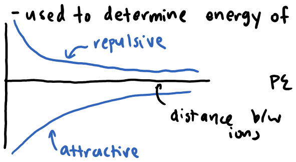
Unpaired electrons ⟶ paramagnetic

Bond Order ↑ Bond Length ↓ Bond Strength ↑

more electronegativity means less energetic

Lattice Energy

- used to determine energy of ionic bonds



$-k\frac{Q_1 Q_2}{r}$ = Coulomb's Energy

Bonds

ionic ⟶ atoms take from one another

covalent ⟶ atoms "share"

Δ electronegativity ⟶ type of bond

≥ 2: ionic

< 2: covalent

= 0: "purely covalent"

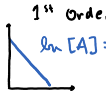
Reaction Rates

$aA + bB \longrightarrow cC + dD$

$-\frac{1}{a}\frac{d[A]}{dt} = -\frac{1}{b}\frac{d[B]}{dt} = \frac{1}{c}\frac{d[C]}{dt} + \frac{1}{d}\frac{d[D]}{dt}$

rate $= k[A]^M[B]^N$ — M and N determined experimentally.

1st order



$\ln[A] = \ln[A_0] + kt$ (slope = −k)

2nd order

$\frac{1}{[A]} = \frac{1}{[A_0]} + kt$

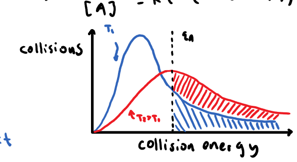
$Q = \frac{[C]^c[D]^d}{[A]^a[B]^b}$

if equilibrium, $Q = K_{eq}$

$Q > K_{eq}$ ⟶ reactants

$Q < K_{eq}$ ⟶ products

$\ln\frac{[A_0]}{[A]} = kt$ (1st order), $[A] = \frac{1}{2}[A_0]$. Solve for T



increasing temperature increases number of collisions, increasing rate

$r = k = Ae^{-E_a/k_bT}$

- catalysts reduce activation energy by providing "alternate path"

Acids and Bases

acids: H⁺ (donates protons), bases: OH⁻ (accepts protons)

$pH = -\log_{10}[H^+]$

strong acid + weak base — pH < 7

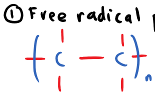
weak acid + strong base — pH > 7

weak acid + weak base — < 7 $K_a > K_B$; = 7 $K_A = K_B$; > 7 $K_A < K_B$

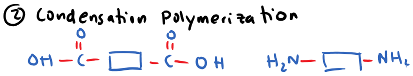
acids + bases ⟶ salt + water

Polymerization

1. Free radical polymerization



2. Condensation Polymerization



take OH from one and H from the other — COOH + NH₂, OH + H

more surface area ⟶ more polarizable, higher melting temp (bulkier side groups)

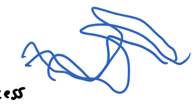
more crystalline ⟶ higher MP

the stronger the bonds, the higher the MP!

Types of Polymers

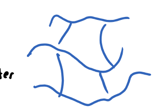
THERMOPLASTIC

- no cross-linking
- vdW and H bonds
- can re-heat and reprocess
- most linear and slightly branched polymers



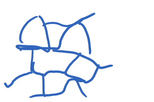
ELASTOMER

- light cross-linking
- returns to original shape after stress
- must be above T_g



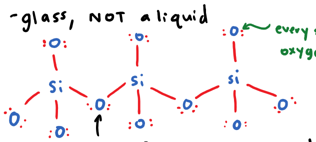
THERMOSET

- highly crosslinked
- solidifies irreversibly when heated
- rigid



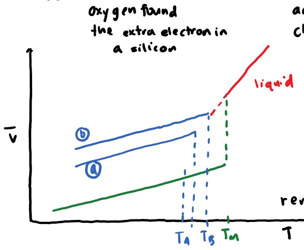
Amorphous Solids

- glass, NOT a liquid



= a chain of silicate groups

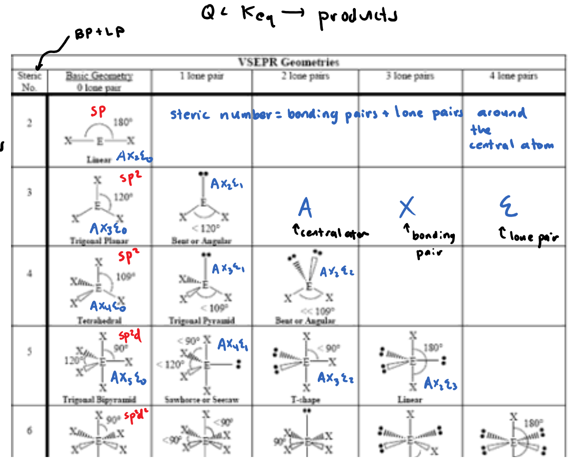
adding fewer oxygens causes chainscission and breaks bonds (network modifier)



B: 1. Faster cooling rate
2. Fewer network modifiers
3. More viscous

remember, O has a charge of 2⁻

Strengthen glass:



O-Chem Naming

1. Count # carbons in longest chain/chain w/ double bond.

   1: meth, 2: eth, 3: pro, 4: but, >4: Latin

2. Calculate bond order

   single: one, double: one, triple: yne

Fick's First Law

$J = -D\frac{d}{dx}$ — change in concentration per unit distance; D — diffusion const.; J — flux

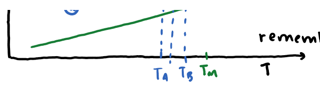
More Acids and Bases

$pH = -\log_{10}[H^+]$ $pH + pOH = pK_w$

$pOH = -\log_{10}[OH^-]$

$K_A \cdot K_B = K_w$

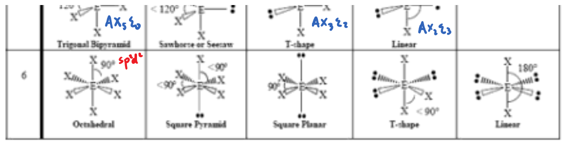
$K_w = 10^{-14}$



remember, O has a charge of 2⁻

Strengthen glass:

1. Temper (cool outside faster than inside)
2. Ion exchange



can use VSEPR to determine if a molecule polar or nonpolar

$pH = -\log_{10}[H^+]$

$pOH = -\log_{10}[OH^-]$

$K_A \cdot K_B = K_w$

$K_w = 10^{-14}$

$pK_A = -\log_{10} K_A$

$pK_A + pK_B = pK_w = 14$

$pH + pOH = 14$

$pH + pOH = pK_w$