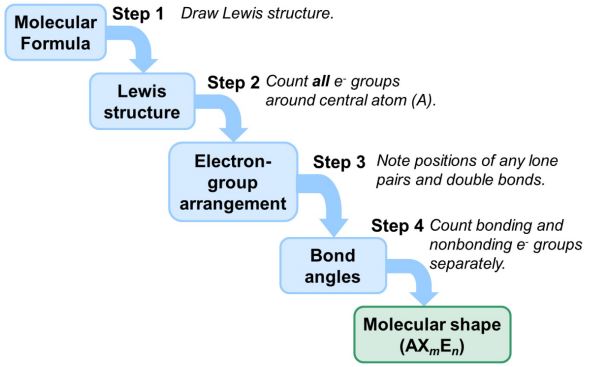
Applying VSEPR Theory

The shape of a molecule can be determined from a *correctly drawn* lewis structure:



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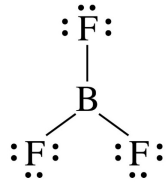
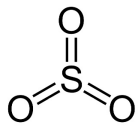
Examples of Molecular Shapes



3 EGG trigonal planar MS trigonal planar



3 trigonal planar trig. pla.

bond angle(s), hybridization, MS, EGG

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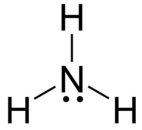
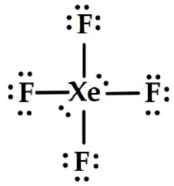
Examples of Molecular Shapes



4 EGG tetra MS trig. pyr.



6 octahedral Square planar

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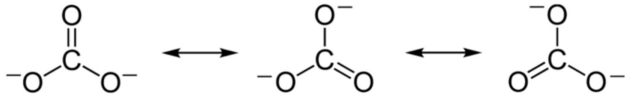
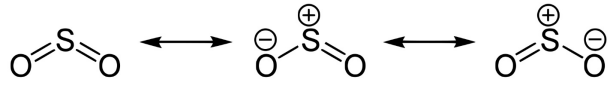
Resonance Structures

Resonance structures are a way of describing delocalized electrons within certain molecules or polyatomic ions where the bonding cannot be expressed by one single Lewis formula.



Example: SO_2



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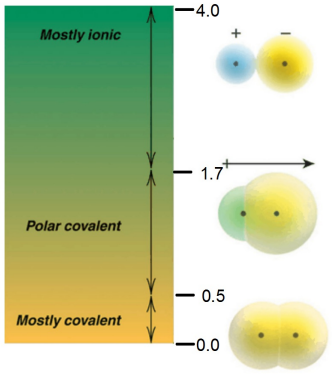
Electronegativity Difference Scale

Bond Polarity

ΔEN	IONIC CHARACTER
>1.7	Mostly ionic
0.4-1.7	Polar covalent
<0.4	Mostly covalent
0	Nonpolar covalent

ΔEN

Boundary ranges for classifying ionic character of chemical bonds.



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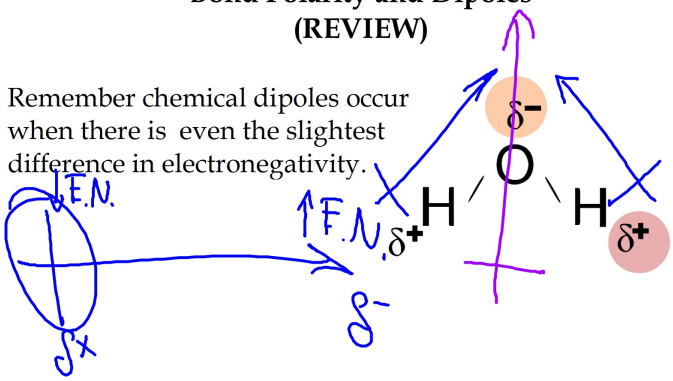
Bond Polarity and Dipoles (REVIEW)

Remember chemical dipoles occur when there is even the slightest difference in electronegativity.



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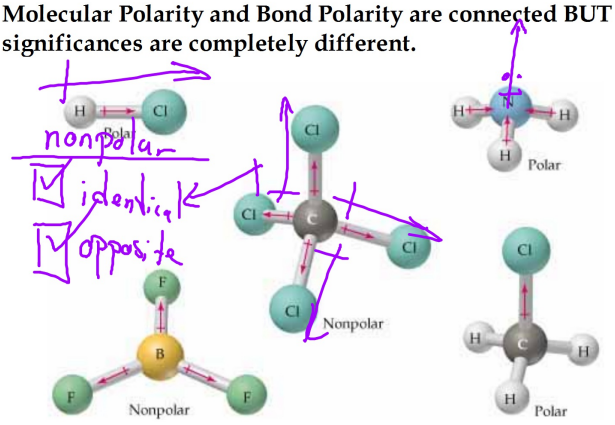
Molecular Polarity

Molecular Polarity and Bond Polarity are connected BUT their significances are completely different.



equal and opposite = nonpolar

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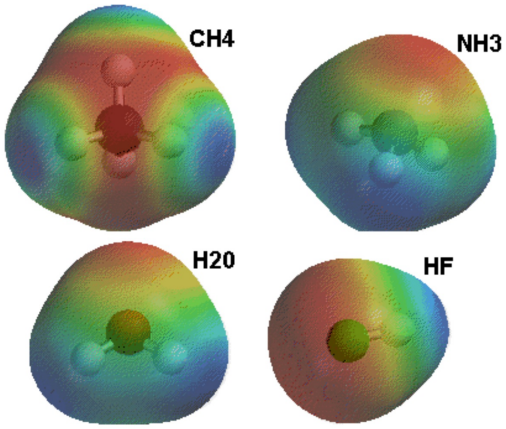
Electron Density Maps



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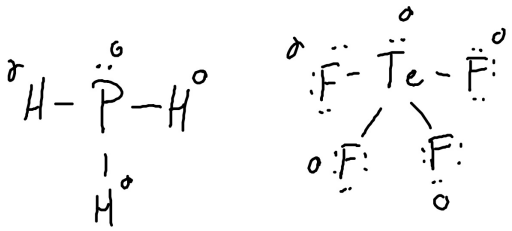
Molecular Polarity Examples

CCl_4 PH_3 TeF_4



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Intermolecular Forces

Definition: the forces that hold molecules together.

Intra- vs. intermolecular forces:

- Intra "inward"
  - Examples: ionic, covalent, metallic
- Inter "outward"
  - Examples: Hydrogen bonding, dipole-dipole, van der Waals.

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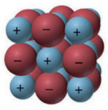
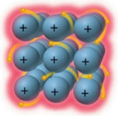
Table 12.2 Comparison of Bonding and Nonbonding (Intermolecular) Forces

Force	Model	Basis of Attraction	Energy (kJ/mol)	Example
Bonding				
Ionic		Cation–anion	400–4000	NaCl
Covalent		Nuclei–shared e^- pair	150–1100	H—H
Metallic		Cations–delocalized electrons	75–1000	Fe

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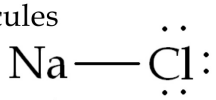
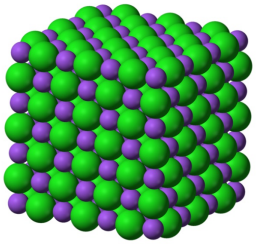
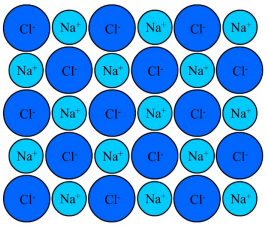
Intermolecular Forces

IMFs dominate covalent molecules



Intermolecular forces are weaker than intramolecular forces.





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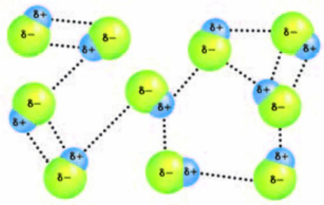
Dipole – Dipole Forces

- Permanent dipoles
- Attraction between polar molecules
- Stronger than London Dispersion



What is a dipole?

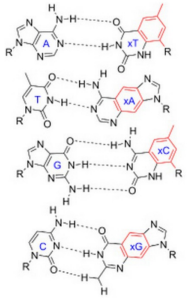
polar + polar

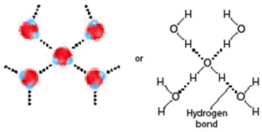
Hydrogen bonding

Occurs when hydrogen is bonded to fluorine, oxygen, nitrogen, and sulfur.

FON(S)

The strongest of the IMFs





- Has many applications in biological systems.
- Cohesion and adhesion
- Protein stabilization

*It is not really a bond. It is an **interaction** between molecules.*

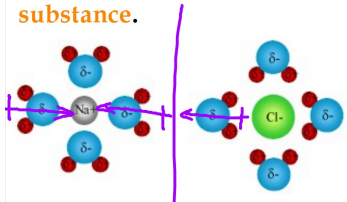
Intra vs. Inter-molecular forces

intermolecular force

intramolecular force

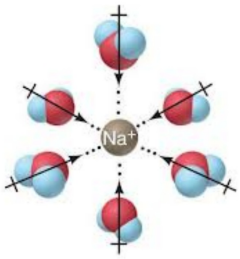
Ion - Dipole Forces

Occurs when an ionic substance is dissolved in a polar substance.



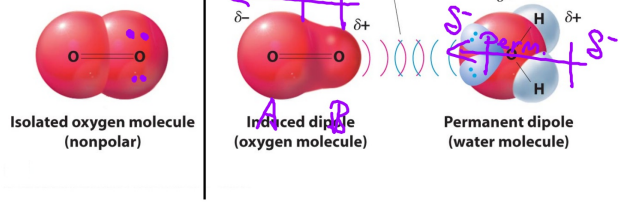
Examples:

1. NaCl in H_2O
2. $MgCl_2$ in NH_3
3. KBr in $TeBr_4$



Induced Dipole Interactions

Two varieties: (1) dipole - induced dipole
(2) ion - induced dipole



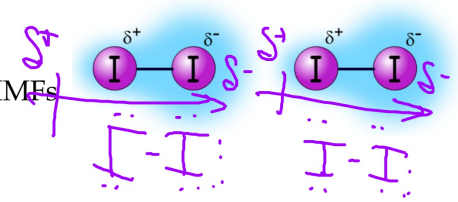
What would an ion-induced dipole interaction look like?

London Dispersion Forces

(van der waals forces)

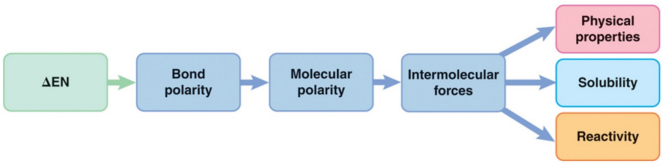
Weak attraction between the opposite ends of different molecules

Weakest of all IMFs



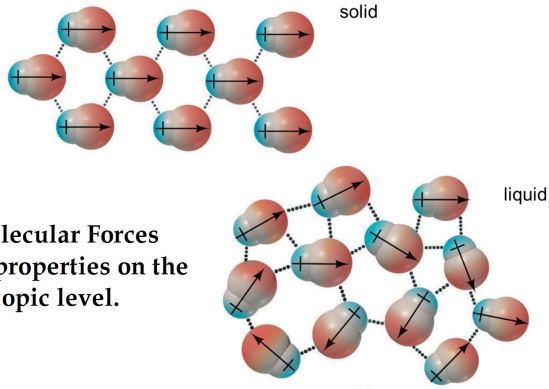
Occurs between all molecules

The Significance of IMFs



Map indicating the connection between electronegativity and the chemical and physical characteristics of substances.

The Significance of IMFs



Intermolecular Forces dictate properties on the macroscopic level.

Table 12.2 Comparison of Bonding and Nonbonding (Intermolecular) Forces

Nonbonding (Intermolecular)			
Ion-dipole	Ion charge–dipole charge	40–600	$Na^+ \cdots O$ (H, H)
H bond	$\delta^- \; \delta^+ \; \delta^-$ $-A-H \cdots :B-$ Polar bond to H–dipole charge (high EN of N, O, F)	10–40	$:\ddot{O}-H \cdots :\ddot{O}-H$ (H, H)
Dipole-dipole	Dipole charges	5–25	$I-Cl \cdots I-Cl$
Ion–induced dipole	Ion charge–polarizable e^- cloud	3–15	$Fe^{2+} \cdots O_2$
Dipole–induced dipole	Dipole charge–polarizable e^- cloud	2–10	$H-Cl \cdots Cl-Cl$
Dispersion (London)	Polarizable e^- clouds	0.05–40	$F-F \cdots F-F$

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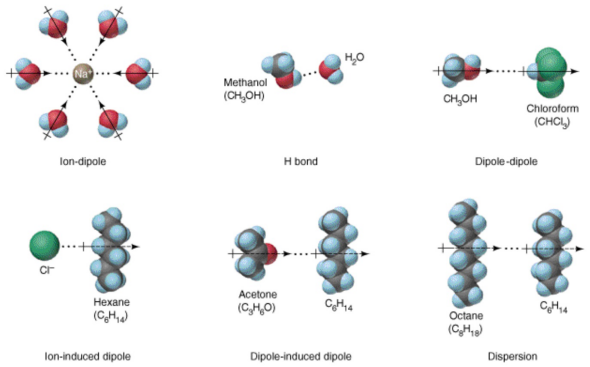
Summary of Intermolecular Forces



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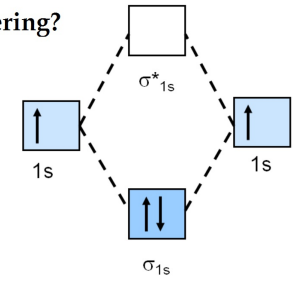
Molecular Orbital Theory

Which question are we answering?

VSEPR: molecular shape

VB: orbital overlap



What about magnetism and spectral properties?

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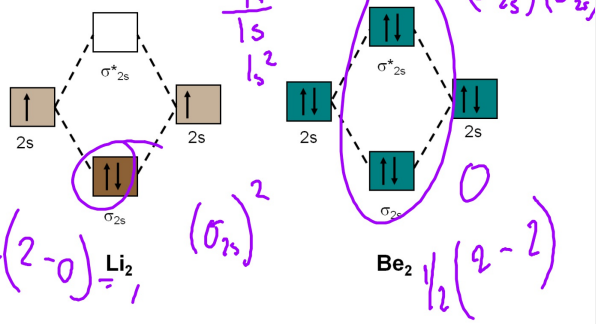
Molecular Orbital Theory Applications

$BO = \frac{1}{2}(BE - ABE)$

Used to predict the existence and/or stability of a substance through the calculation of the bond order.



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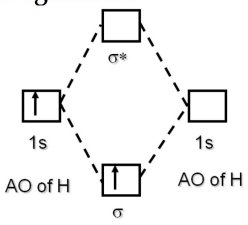
MO Examples

Use MO diagrams to find bond orders and predict whether H_2^+ and H_2^- exist. If either exists, write its electron configuration.

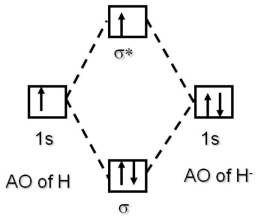


MO of H_2^+

BO = ½(1 - 0)

BO = ½

EXISTS



MO of H_2^-

BO = ½(2 - 1)

BO = ½

EXISTS

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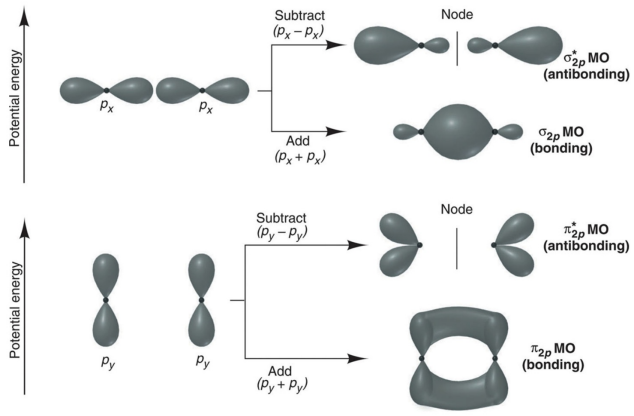

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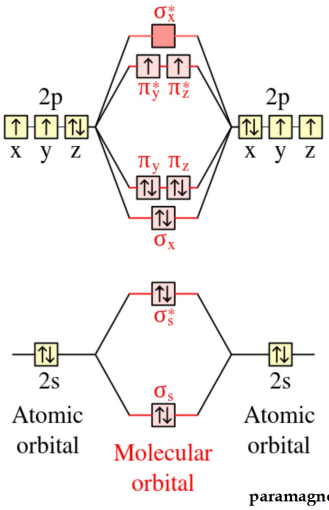

paramagnetism / diamagnetism

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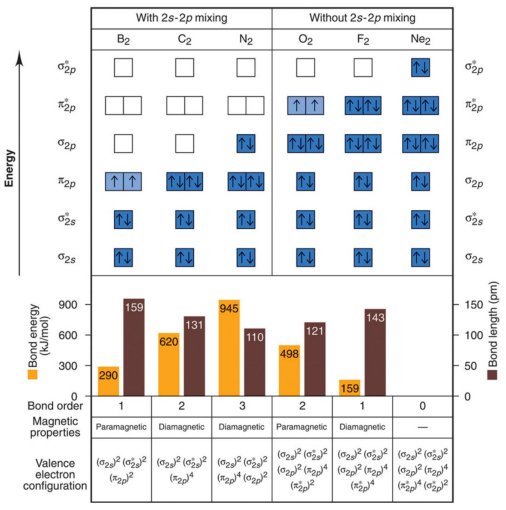

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