VC210 Recitation Class 3

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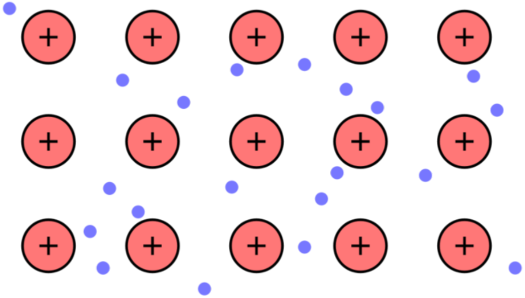
Contents

Metal Bond

metal-metal
positive ions in ”electron sea” (delocalized electrons)



Ionic Bond

- Metal (losing electrons)-nonmetal (gaining electrons)
- Electrostatic attraction between **all** the ions

Difference with covalent bond

- non-directional (没有方向性)
- unlimited number of atoms (没有饱和性)

Lattice energy

- What is lattice energy: the energy **released** when seperated ions bounded together.
- Higher lattice energy, stronger ionic bond, greater stability of crystal.

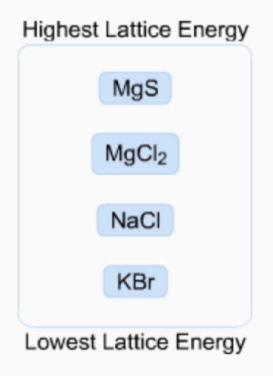
Two important problems

- How to compare the lattice energy of different ionic compounds?
- How to calculate lattice energy using Born-Harber Circulation? (in Thermodynamics)

Comparison of Lattice Energy

The **procedure** is as follows:

1. Compare the electric charge: charge $\uparrow$, lattice energy $\uparrow$.
2. Compare the radius of atom (when charge is same): radius $\uparrow$, lattice energy $\downarrow$.



Further explanations

For better understanding, here's the theretical formula of lattice energy:

$$L = \frac{N_A M Z_+ Z_- e^2}{4\pi\epsilon_0 r_0}(1 - \frac{1}{n})$$

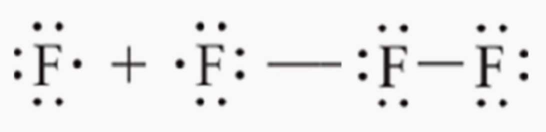
- r_0: average distance between two ions.
- Z_+ & Z_-: charge of ions. e.g. $MgCl_2$: Z_+=2, Z_-=1.
- M, n: constants, for **corrections (修正)**

Covalent Bond

- nonmetal-nonmetal
- sharing electrons

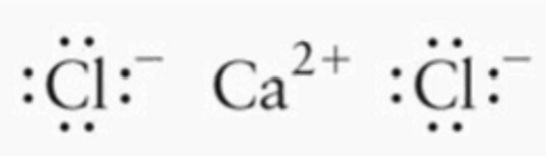
Octet Rule

Atoms tend to have nobel-gas configuration in valence shell.



Lewis Structure

1. Line: bonding pair (single bond: 1 line; double bond: 2 lines, etc.).
2. Dots: lone pairs of electrons (**Don't forget!!**).
3. For ionic bond: no lines (representing covalent bond); note electric charge.
4. Consistent with Octet Rule at most time.



Exercise 1

Draw the Lewis structure of the following compounds:

1. CH_2O
2. HOCl
3. NaBr

Hint: first connect all atoms with single bonds.

Resonance Structure

Based on Lewis structure

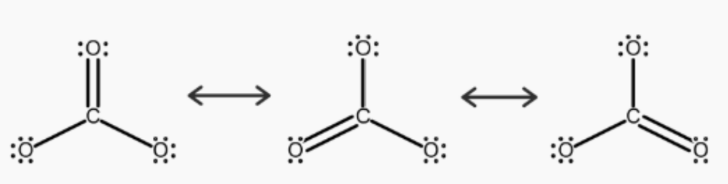
- Keep relative positions of atoms.
- Only change position of electrons.
- Number of paired and unpaired electrons unchanged.

That is to say, move the position of bonds&charges.

Example

${CO_3}^{2-}$

Exercises 2



Draw the resonance structure of the following compounds.

1. O_3
2. $NO_3{}^-$

Formal Charge

$$Formal\ Charge = V - \left(L + \frac{1}{2}B\right)$$

- V -- number of valence electrons
- L -- number of lone-pair electrons
- B -- number of bonding electrons

Caution

The structure with lowest formal charge on each atoms is the most stable form. But sometimes it's not that case!

Figure out the most stable structure

- Lower formal charge.
- More symmetrical structure.
- Atom with higher electronegativity has negative formal charge.

Exercise 3

1. Draw the resonance structures of NNO and HCNO. Find the most stable form.

Exception of Octet Rule

Summary:

1. Molecule with 1 unpaired electron.
2. More than 8 electrons in valence shell. e.g. S, P, Cl, etc.
3. Less than 8 electrons in valence shell. e.g. B

Expanded valence shell

If an atom has more than 8 electrons in valence shell,

- it is Period 3 or above, so d-orbital can be used.
- the radius should be large enough to hold more bonds.

Exercise 4

Draw the Lewis structure of:

- PCl_5
- ${SO_4}^{2-}$
- BF_3

B is special!

Bond Strength

Determinant factors:

1. Bond order: bond order ↑, bond strength ↑.
   - single bond: 1; double bond: 2; triple bond:3.
2. Bond length: bond length ↓, bond strength ↑.
   - Bond length=distance between two atoms, so the radius of atoms ↑, bond length ↑.

Calculating bond order

$$\text{B.O.} = \frac{\textit{number of bonds}}{\textit{number of bonding pairs}}$$

Exercise 5

(From the slides of Prof. Sun)Write the bond order of:

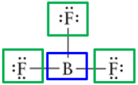
- CO_2
- ${CO_3}^{2-}$

Remember: the bond order in a resonance structure need to **take the average**.

VSEPR

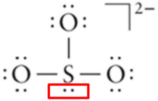
1. Draw the Lewis structure. Find the formula:

   The generic formula "AX_nE_m"
   "A" represent a central atom,
   "X" a bonded electron region
   "E" a lone pair electron region



Boron trifluoride, BF_3

AX_3

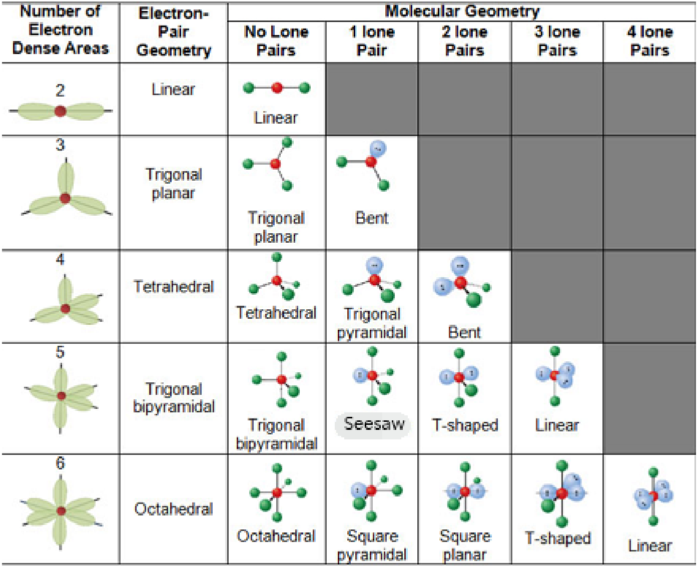


AX_3E

Bonding pair: electrons in covalence bond
Nonbonding pair (lone pair): electrons located on one atom

2. Find the corresponding molecular shape on your cheating paper.

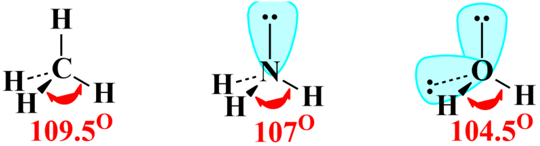
VSEPR table



Number of Electron Dense Areas	Electron-Pair Geometry	Molecular Geometry				
		No Lone Pairs	1 lone Pair	2 lone Pairs	3 lone Pairs	4 lone Pairs
2	Linear	Linear				
3	Trigonal planar	Trigonal planar	Bent			
4	Tetrahedral	Tetrahedral	Trigonal pyramidal	Bent		
5	Trigonal bipyramidal	Trigonal bipyramidal	Seesaw	T-shaped	Linear	
6	Octahedral	Octahedral	Square pyramidal	Square planar	T-shaped	Linear

The Effect of Non-bonding Pair

The repulsion between electron pairs:
Non-bonding&non-bonding>non-bonding&bonding>bonding&bonding
This will cause the change of bond angle:



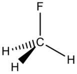
Polarity

How to figure whether a molecule is polar or non-polar:

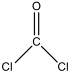
1. Are there **polar bonds**? If a molecule only has non-polar bonds, it must be non-polar.
2. Is the **molecule shape symmetric**? Asymmetric: must be polar.
3. Judge if the dipole can cancel each other out.

Exercise 6

(From Prof. Sun's slides) Predict the polarity of following molecules.



A.



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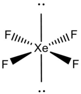
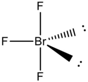
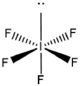


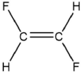
C.



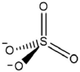
D.



B.



C.



D.

Valence Bond Theory

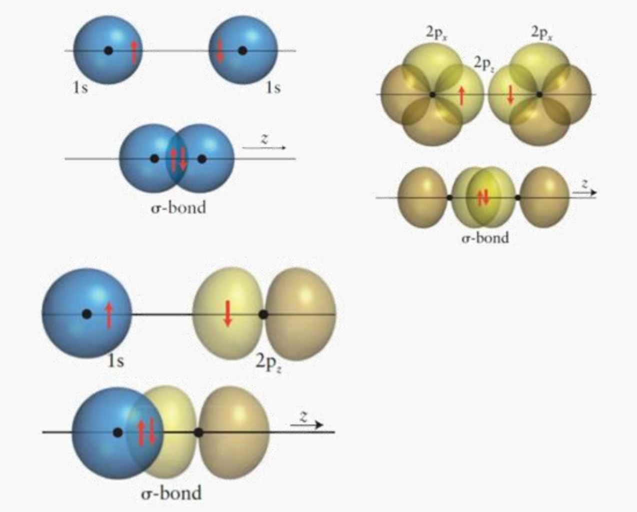
How bonds form: two valence orbitals of two atoms overlap, so two electrons of opposite spin in the orbitals overlap.

Caution

Pay attention to the connection with Quantum mechanics (wave functions, electron clouds, etc.)

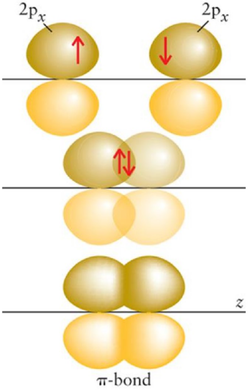
Head-to-head

Forming σ-**bond**.



Side-by-side

Forming π-**bond**.



Bond strength in VB

- Single bond: 1 σ-bond
- Double bond: 1 σ-bond & 1 π-bond
- Triple bond: 1 σ-bond & 2 π-bond

Overlap $\uparrow$, bond strength $\uparrow$ $\quad \Longrightarrow$ σ-bond is stronger than π-bond.

Hybrization

1. Find the type of hybrization.
   - Remember in VSEPR, formula: AX_nE_m.
   - k=m+n

$$
\begin{aligned}
sp&: k = 2 \\
sp^2&: k = 3 \\
sp^3&: k = 4 \\
sp^3d&: k = 5 \\
sp^3d^2&: k = 6
\end{aligned}
$$

2. Check the table to find the molecular shape.

Types of hybridization	**Geometry**
sp hybridisation	Linear
sp^2 hybridisation	Triangular planar
sp^3 hybridisation	Tetrahedral
dsp^2 hybridisation	Square planar
dsp^3 hybridisation	Trigonal bipyramidal
d^2sp^3 hybridisation	Octahedral
d^3sp^3 hybridisation	Pentagonal bipyramidal

End

Thanks for your attendance.
Get prepare for your Quiz 1! Start early or stay up late!