Formal Charges of Lewis Structures

In order to determine the best Lewis Structure, the formal charges of each element must be calculated, an ideal structure has an overall formal charge of 0 with each element having a formal charge of 0.

Formula for Formal Charges

Valence electrons - bonds - lone electrons

Draw the Lewis structure and determine the formal charges of each

H_2O CO_2 NH_4^+

Using the idea of formal charges, draw the resonance structures of CO_2 and determine which is the best.

Exceptions to the Octet Rule in Lewis structures

1) Species with odd number of electrons

-free radicals

example: NO (nitrogen monoxide)

2) Incomplete octets

-beryllium, aluminum, boron

Example: BH_3 (Borane, boron trihydride)

Example: BF_3 (boron triflouride)

3) Expanded Octet

-only elements with a minimum of n=3 can have expanded octets

Example: SF_6 (sulfur hexafluoride)

Example: SO_4^{2-} (sulfate)

You must look at the resonance structures and determine which has better formal charges.

Practice

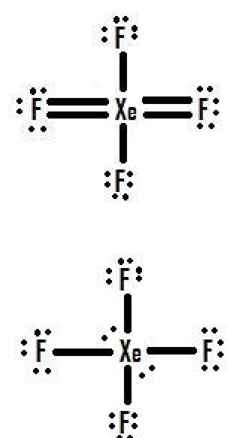
1) Draw the Lewis structure for the molecule I_3^-

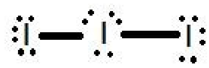
2) Draw the molecule ClF_3

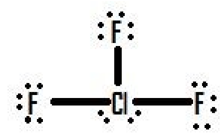
3) The central atom for an expanded octet must have an atomic number larger than what?

4) Draw the Lewis structure for NO_2

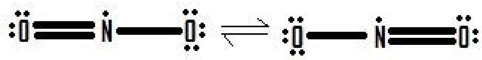
5) Which Lewis structure is more likely?

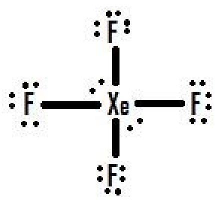


1) 

2) 

3) 10 (sodium or higher)

4) 

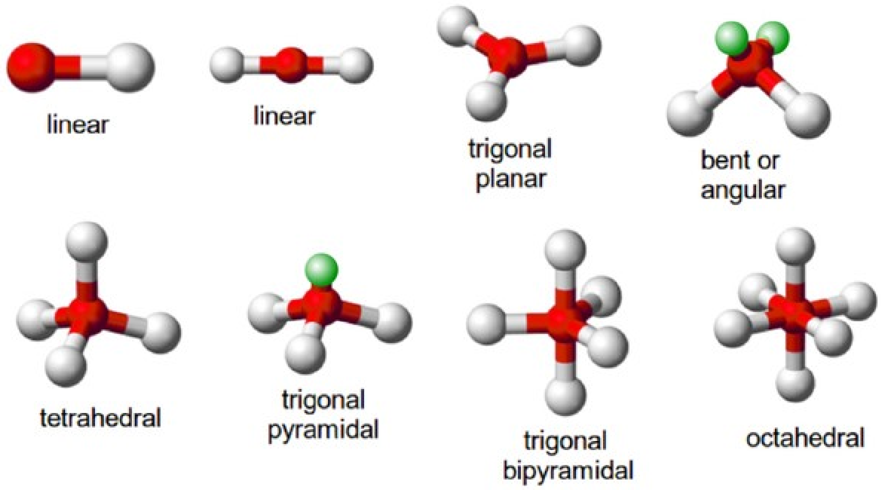
5) 

VSEPR Theory

Valence Shell Electron Pair Repulsion Theory

This is the theory that gives us molecular geometry. The general idea is atoms want to be as far from each other as they can, but lone electron pairs have a stronger repulsion than bonded atoms.

VSEPR Shapes



Molecule Type	Shape[12]	Electron arrangement†[12]	Geometry‡[12]	Examples
AX_2E_0	Linear			$BeCl_2$,[1] $HgCl_2$,[1] CO_2[11]
AX_2E_1	Bent			NO_2^-,[1] SO_2,[12] O_3,[1] CCl_2
AX_2E_2	Bent			H_2O,[12] OF_2[17]
AX_2E_3	Linear			XeF_2,[12] I_3^-,[18] $XeCl_2$
AX_3E_0	Trigonal planar			BF_3,[12] CO_3^{2-},[19] NO_3^-,[1] SO_3[11]
AX_3E_1	Trigonal pyramidal			NH_3,[12] PCl_3[20]
AX_3E_2	T-shaped			ClF_3,[12] BrF_3[21]
AX_4E_0	Tetrahedral			CH_4,[12] PO_4^{3-}, SO_4^{2-},[11] ClO_4^-,[1] XeO_4[22]
AX_4E_1	Seesaw (also called disphenoidal)			SF_4[12][23]
AX_4E_2	Square planar			XeF_4[12]
AX_5E_0	Trigonal bipyramidal			PCl_5[12]
AX_5E_1	Square pyramidal			ClF_5,[21] BrF_5,[12] $XeOF_4$[11]
AX_6E_0	Octahedral			SF_6,[12] WCl_6[24]

Bond angles

linear = 180^o

trigonal planar = 120^o

bent / angular = $<120^o$

H_20 is 104.5^o, SO_2 is 119^o

tetrahedral = 109.5^o

trigonal pyramidal = 107^o

trigonal bipyramidal = 90^o , 120^o , 180^o

octehdral = 90^o , 180^o

Polar Bonds

A type of covalent bond between two atoms in which electrons are shared unequally. Because of this, one end of the molecule has a slightly negative charge and the other a slightly positive charge.

Polar Bonds depend on geometric structure of the atom and the difference in electronegativity of the elements in the compounds.

Water is a polar molecule.

Is Carbon Dioxide a polar molecule?

Is hydrogen sulfide a polar molecule?

How about methane? (CH_4)