

Announcements – Lecture XIII – Monday, June 10th

4th LAB : TUE, JUN 11th

EXAM II : FRI, JUN 14th, IN CLASS



8.3 Bond Properties

A: Bond Order, Bond Length, Bond Energy

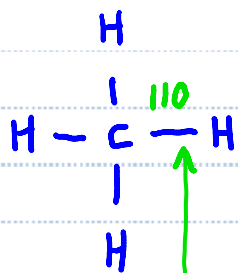
Average Single Bond Lengths (Picometers)

	H	C	N	O	F	Si	P	S	Cl	Br	I
H	74	110	98	94	92	145	138	132	127	142	161
C		154	147	143	141	194	187	181	176	191	210
N			140	136	134	187	180	174	169	184	203
O				132	130	183	176	170	165	180	199
F					128	181	174	168	163	178	197
Si						234	227	221	216	231	250
P							220	214	209	224	243
S								208	203	218	237
Cl									200	213	232
Br										228	247
I											266

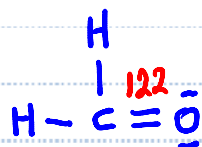
Average Multiple Bond Lengths (Picometers)

C = C	134	C ≡ C	121
C = N	127	C ≡ N	115
C = O	122	C ≡ O	113
N = O	115	N ≡ O	108

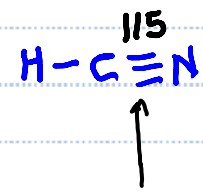
$$1 \text{ pm} = 1 \times 10^{-12} \text{ m}$$



Single bond
Bond Order = 1



Double bond
Bond Order = 2



Triple bond
Bond Order = 3

8.3 Bond Properties

A: Bond Order, Bond Length, Bond Energy

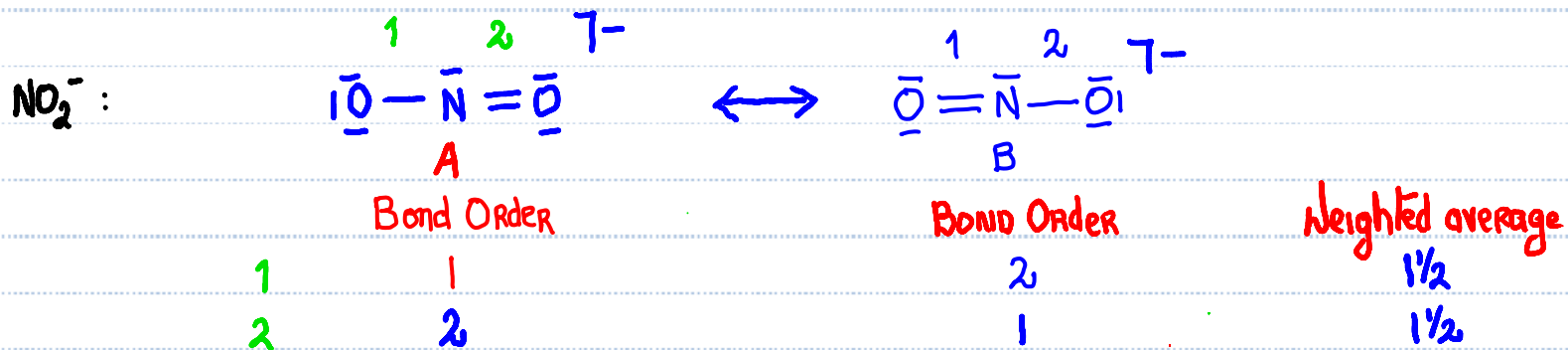
Average Single Bond Lengths (Picometers)

	H	C	N	O	F	Si	P	S	Cl	Br	I
H	74	110	98	94	92	145	138	132	127	142	161
C		154	147	143	141	194	187	181	176	191	210
N			140	136	134	187	180	174	169	184	203
O				132	130	183	176	170	165	180	199
F					128	181	174	168	163	178	197
Si						234	227	221	216	231	250
P							220	214	209	224	243
S								208	203	218	237
Cl									200	213	232
Br										228	247
I											266

Average Multiple Bond Lengths (Picometers)

C = C	134	C ≡ C	121
C = N	127	C ≡ N	115
C = O	122	C ≡ O	113
N = O	115	N ≡ O	108

$$1 \text{ pm} = 1 \times 10^{-12} \text{ m}$$



Expected N-O bond length : $> 115 \text{ pm}$ and $< 136 \text{ pm}$



8.3 Bond Properties

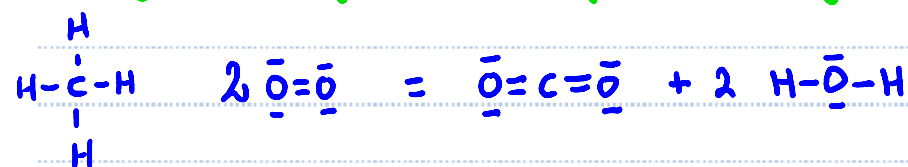
A: Bond Order, Bond Length, Bond Energy

Average Single Bond Energies (kJ per mole)

	H	C	N	O	F	Si	P	S	Cl	Br	I
H	436	414	389	464	569	293	318	339	431	368	297
C		347	293	351	439	289	264	259	330	276	238
N			159	201	272		209		201	243	
O				138	184	368	351		205		201
F					159	540	490	285	255	197	
Si						176	213	226	360	289	
P							213	230	331	272	213
S								213	251	213	
Cl									243	218	209
Br										192	180
I											151

Average Multiple Bond Energies (kJ per mole)

N = N	418	C = C	611
N ≡ N	946	C ≡ C	837
N = O	590	C = O	803 <i>In CO₂ Only</i>
C ≡ N	891	C = O	745
O = O	498	C ≡ O	1075



Σ Bonds broken - Σ Bonds formed

$$4(\text{C-H}) + 2(\text{O=O}) - \{ 2(\text{C=O}) + 4(\text{O-H}) \}$$

$$4(414) + 2(498) - \{ 2(803) + 4(464) \}$$

$$1656 + 996 - \{ 1606 + 1856 \}$$

$$2652 - 3462$$

$$- 810 \text{ kJ.mol}^{-1}$$



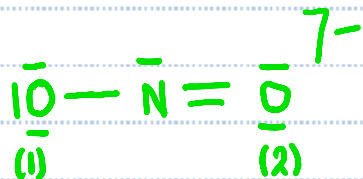
Exothermic ... gives off heat

8.4 Electron Distribution in Molecules

A: Formal Charge Vs Oxidation Numbers – Oxidation Numbers

Electron book-keeping where electrons in a bond are considered to belong solely to the most electronegative atom in the bond ... very useful in electrochemistry.

Oxidation Number = Group Number - Lone Pair electrons - Bond Pair electrons

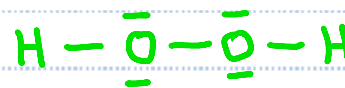


O: More electronegative than N

$$\text{O1: } 6 - 6 - 2 = -2$$

$$\text{N: } 5 - 2 - 0 = +3$$

$$\text{O2: } 6 - 4 - 4 = -2$$



O: More electronegative than H

$$\text{H: } 1 - 0 - 0 = +1$$

$$\text{O: } 6 - 4 - (2+1) = -1$$

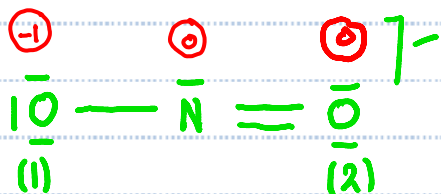
8.4 Electron Distribution in Molecules

A: Formal Charge Vs Oxidation Numbers – Formal Charge

Formal Charge, an electron book-keeping system where the electrons in a bond are considered to be equally shared between the atoms forming the bond.

$$\text{FORMAL CHARGE} = \text{Group Number} - \text{Lone Pair Electrons} - \frac{1}{2} \text{Bond Pair electrons}$$

NO_2^- :



$$\text{O}_1: 6 - 6 - \frac{1}{2}(2) = -1$$

$$\text{N}: 5 - 2 - \frac{1}{2}(6) = 0$$

$$\text{O}_2: 6 - 4 - \frac{1}{2}(4) = 0$$

a) Sum of the formal charges in a molecule must equal the charge on the molecule.

b) Ideally like to see the smallest charge separation possible.

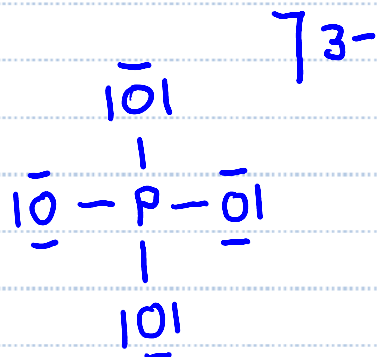
c) Like to see negative formal charges on the most electronegative atom(s).

8.4 Electron Distribution in Molecules

C: Resonance Structures, Formal Charge – Refining Structures

PO_4^{3-} (Octet Rule)

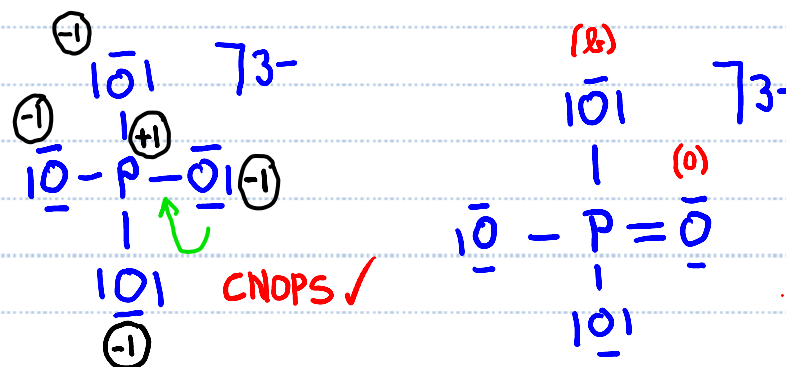
$$\begin{array}{r} \text{P: } 5 \\ \text{O: } 4 \times 6 \\ 3^-: \quad 3 \\ \hline 32 \\ 4 \times \text{BP: } -8 \\ \hline 24 \end{array}$$



FORMAL CHARGE CHECK?

$$\begin{array}{l} \text{O: } 6 - 6 - \frac{1}{2}(2) = -1 \\ \text{P: } 5 - 0 - \frac{1}{2}(8) = +1 \end{array}$$

PO_4^{3-} (Minimal Formal Charge)



FORMAL CHARGE CHECK?

$$\begin{array}{l} \text{O}^{(a)}: 6 - 4 - \frac{1}{2}(4) = 0 \\ \text{O}^{(b)}: 6 - 6 - \frac{1}{2}(2) = -1 \\ \text{P}: 5 - 0 - \frac{1}{2}(10) = 0 \end{array}$$

How about Resonance Structures? ✓