

## HW Set #2

10

Higher  $IE_1$

A. Bi or Xe: Xe has the highest  $IE_1$ ,  
because it has a closed-shell configuration.

B. Se or Te: Se has a higher  $IE_1$ ,  
because its electrons are closer to its nucleus.

C. Rb or Y: Y will have a higher  $IE_1$ ,  
because Rb must only lose  $1e^-$  to obtain a  
noble gas configuration.

D. K or Ne: Ne will have a higher  $IE_1$ ,  
the electrons of K are much farther from its  
nucleus and K can easily lose one  $e^-$  to obtain  
a noble gas configuration.

14

Higher EA Table 3.2

A. Rb or Sr: Rb

B. I or Rn: I

C. Ba or Te: Te

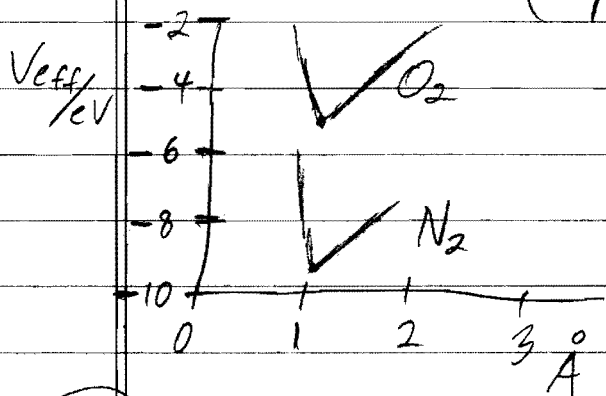
D. Bi or Cl: Cl

(18)  $N_2$  Bond length  $1.1 \text{ \AA}$  Energy:  $942 \text{ KJ/mol}$

$$942 \text{ KJ/mol} \left( \frac{0.010364 \text{ eV}}{1 \text{ KJ/mol}} \right) = 9.76 \text{ eV for } N_2$$

$O_2$  Bond length  $1.21 \text{ \AA}$  Energy  $495 \text{ KJ/mol}$

$$495 \text{ KJ/mol} \left( \frac{0.010364 \text{ eV}}{1 \text{ KJ/mol}} \right) = 5.13018 \text{ eV for } O_2$$



(22) # of  $e^-$  = valence and core

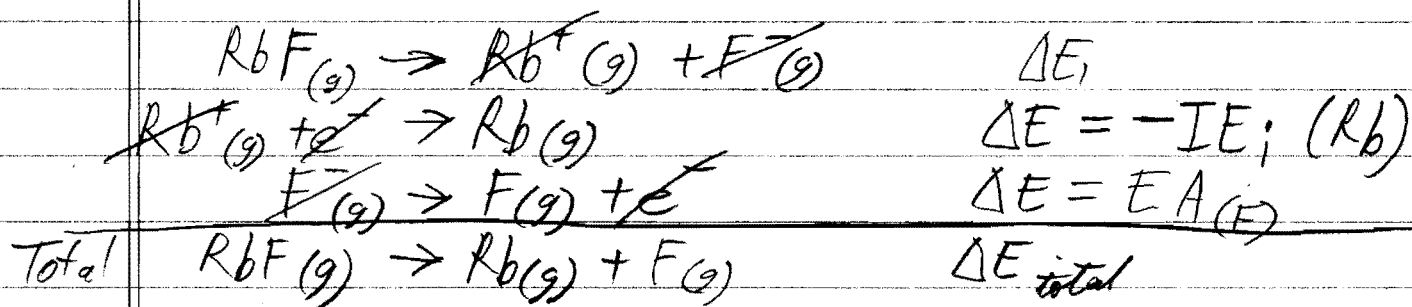
A.  $Ra^{+2}$ :  $86e^-$      $V=0e^-$      $C=86e^-$

B.  $Br$ :  $35e^-$      $V=7e^-$      $C=28e^-$

C.  $Bi^{-2}$ :  $85e^-$      $V=7e^-$      $C=78e^-$

D.  $Ga^+$ :  $30e^-$      $V=2e^-$      $C=28e^-$

(26) RbF Bond length  $2.274 \times 10^{-10} \text{ m}$

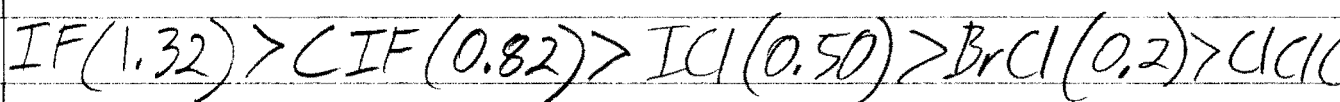


$$\Delta E_1 = \frac{e^2}{4\pi\epsilon_0 r} = \frac{(1.602 \times 10^{-19} \text{ C})^2 (6.022 \times 10^{23} \text{ mol}^{-1})}{4\pi(8.854 \times 10^{-12} \text{ C}^2 \text{ J}^{-1} \text{ m}^{-1})(2.274 \times 10^{-10} \text{ m})}$$

$$\Delta E_1 = 611 \times 10^3 \text{ J/mol}$$

$$\Delta E_{\text{total}} = \Delta E_1 - IE_1(\text{Rb}) + EAF = 611 - 403 + 328 = 536 \text{ kJ/mol}$$

(32) Most ionic to least ionic ranking.



(36)  $\left( \frac{0.2082 \text{ \AA}}{\text{debye}} \right) \left( \frac{\text{Dipole Moment}}{\text{Bond length \AA}} \right) = \% \text{ Char ionic}$

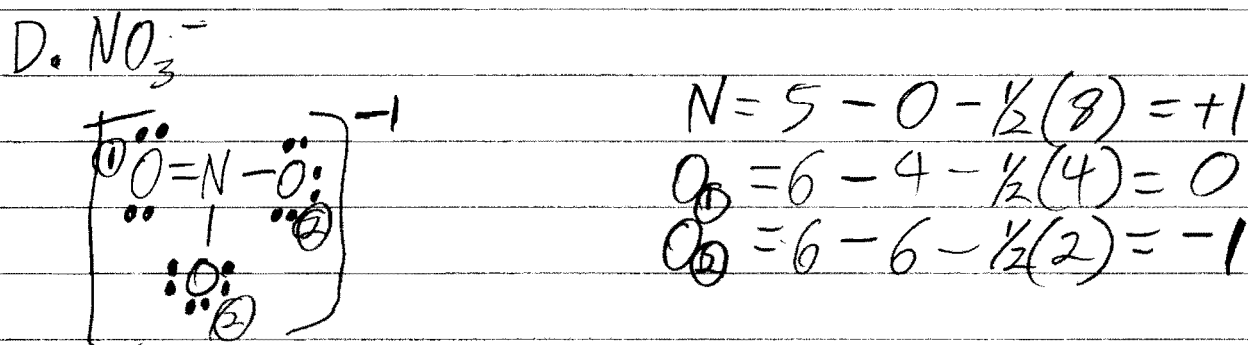
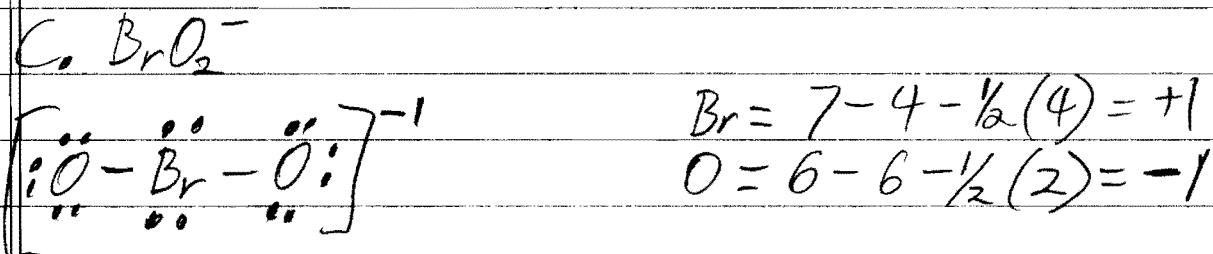
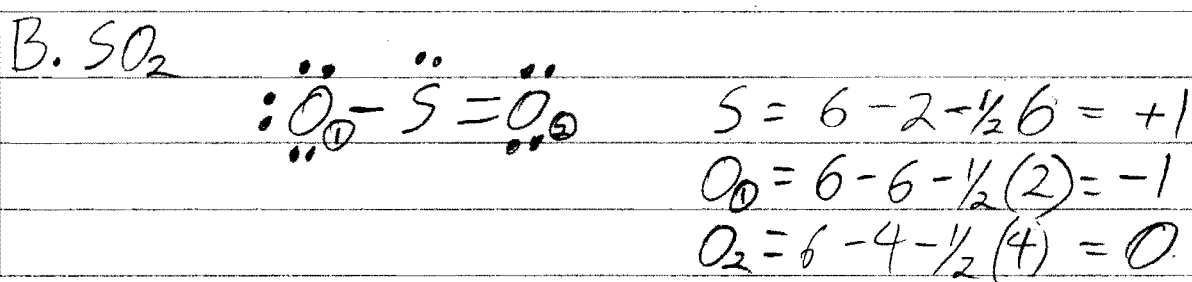
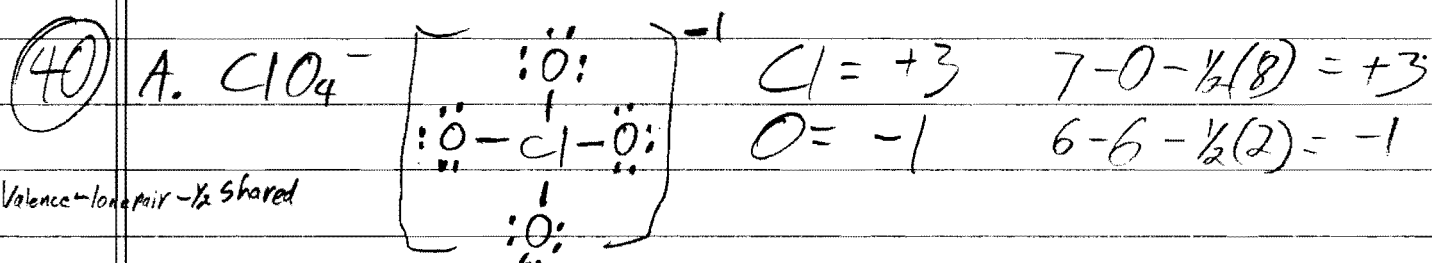
$$\text{OH} = \left( \frac{0.2082 \text{ \AA}}{0.980 \text{ \AA}} \right) \left( \frac{1.66 \text{ D}}{\text{D}} \right) = 0.353 \quad 35.3\% \text{ for OH}$$

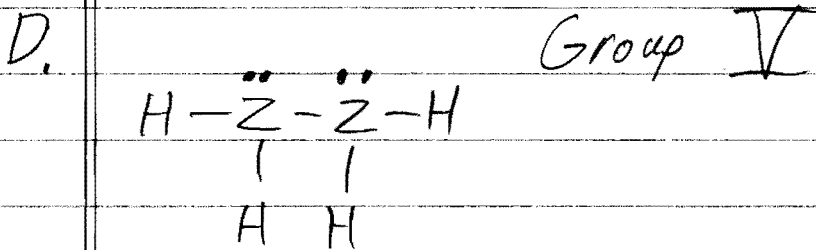
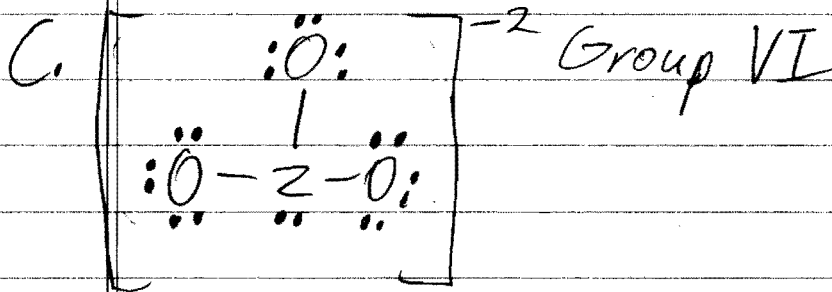
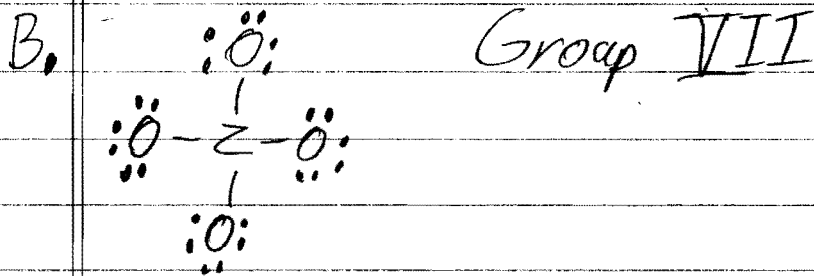
$$\text{CH} = \left( \frac{0.2082 \text{ \AA}}{\text{D}} \right) \left( \frac{1.66 \text{ D}}{1.131 \text{ \AA}} \right) = 0.269 \quad 26.9\% \text{ for CH}$$

36 Continued

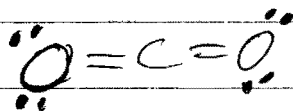
$$CN = \left( \frac{0.2082 \text{ \AA}}{D} \right) \left( \frac{1.45 D}{1.175 \text{ \AA}} \right) = 0.257 \quad 25.7\% \text{ for CN}$$

$$C_2 = \left( \frac{0.2082 \text{ \AA}}{D} \right) \left( \frac{0}{1.246 \text{ \AA}} \right) = 0\% \text{ for CN}$$

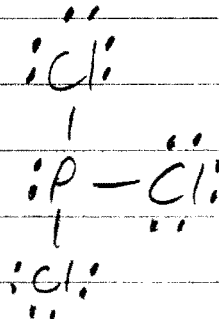




B. Carbon Dioxide



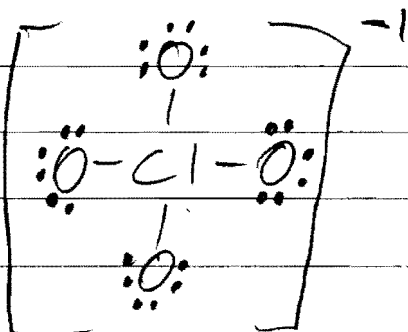
C. Phosphorus trichloride



(46)

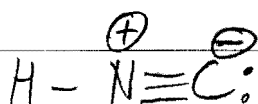
Continued

D. perchlorate

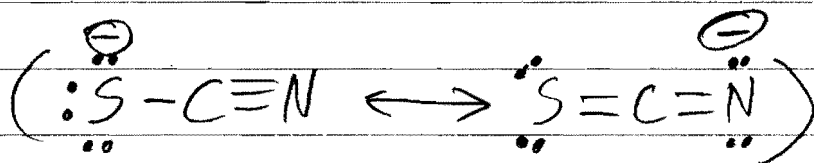


(52)

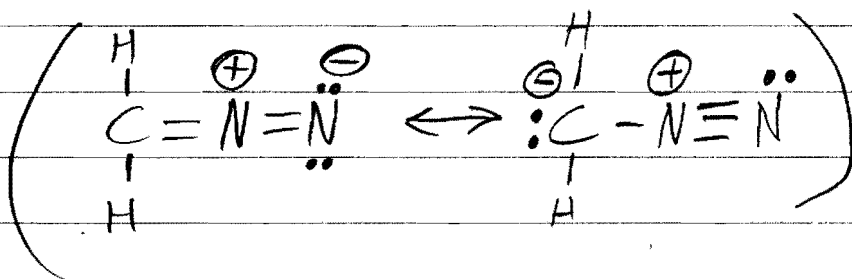
A. HNC



B. SCN<sup>-</sup>

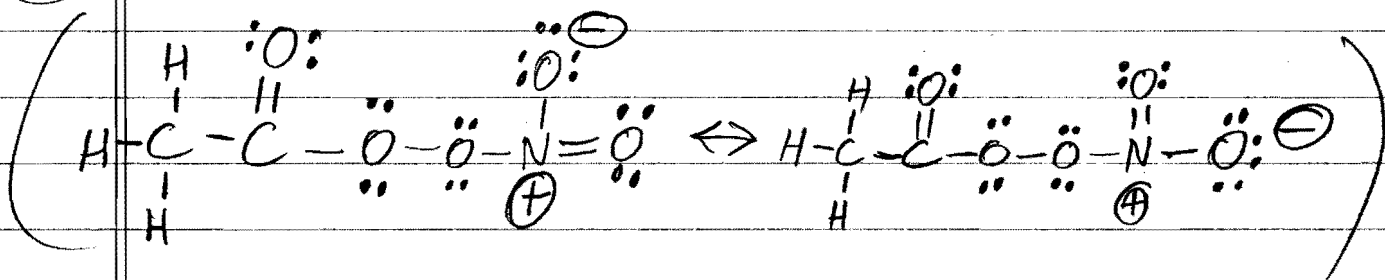


C. H<sub>2</sub>CNN



(56)

CH<sub>3</sub>COONO<sub>2</sub>



# Other Problems

## 1. Mulliken scale Electronegativity

$$EN \propto \frac{1}{2} (IE_1 + EA)$$

$$\text{Oxygen} = \frac{1}{2} \left( \overset{IE_1}{1.31 \times 10^6 \frac{\text{J}}{\text{mol}}} + \overset{EA}{141 \times 10^3 \frac{\text{J}}{\text{mol}}} \right) = 725,500 \frac{\text{J}}{\text{mol}}$$

$$\text{Sodium} = \frac{1}{2} \left( 0.5 \times 10^6 \frac{\text{J}}{\text{mol}} + 53 \times 10^3 \frac{\text{J}}{\text{mol}} \right) = 276,500 \frac{\text{J}}{\text{mol}}$$

$$\frac{O}{Na} = \frac{725,500}{276,500} = 2.62$$

The  $IE_1$  is the major contributor to the EN. Oxygen is just over 2.5x more electronegative than Na.

$$IE_1 \frac{O}{Na} = \frac{1.31 \times 10^6}{0.5 \times 10^6} = 2.62$$

$$EA \frac{O}{Na} = \frac{141}{53} = 2.66$$

$$2. \quad \begin{aligned} IE_2 \text{ of Na} &= 4.65 \\ IE_1 \text{ of Ne} &= 2.08 \end{aligned}$$

Both atoms have the same # of  $e^-$  so both atoms have equal shielding. The one extra proton in Na gives it a much larger effective charge than Ne. This causes Na to hold  $e^-$  more "tightly" than Ne.

③ HBr bond length = 1.424 Å Moment = 0.828 D

Partial charges of H and Br in units of electron charge.

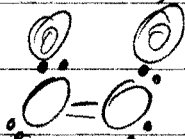
$$\mu = 0.828 \text{ D} \quad R = 1.424 \text{ \AA}$$

$$\mu(\text{D}) = [R(\text{\AA}) / 0.2082 \text{ \AA}]$$

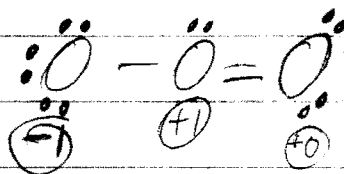
$$\frac{0.828 \text{ D}}{1.424 \text{ \AA} / 0.2082 \text{ \AA}} = \delta$$

$$\delta = 0.121 = 12.1\%$$

④ Which has a stronger O-O bond? O<sub>2</sub> or O<sub>3</sub>



$$0 = 6 - 4 - \frac{1}{2}(4) = 0$$



O<sub>2</sub> = stronger

With resonance this acts as 1.5 bonds

This acts as a double bond.