19F-CHEM20A-1 Exam 1

TOTAL POINTS

98 / 100

QUESTION 1

1 17 pts

1.1 1a **7 / 7**

✓ **+ 7 pts Correct**

+ **4 pts** Correct balanced equation

+ **3 pts** Correct equation to calculate mass of nitrogen

- **2 pts** Calculation or units error

+ **0 pts** Incorrect

1.2 1b **7 / 7**

✓ **+ 7 pts Correct**

+ **1 pts** H2 correct

+ **3 pts** N2 correct

+ **3 pts** NH3 correct

+ **0 pts** Incorrect

1.3 1c **3 / 3**

✓ **+ 3 pts Correct**

+ **1 pts** H2 correct

+ **1 pts** N2 correct

+ **1 pts** NH3 correct

+ **0 pts** Incorrect

QUESTION 2

2 30 pts

2.1 2a **10 / 10**

✓ **+ 10 pts Correct**

+ **5 pts** $$F_A=F_{Ae}-F_{AB}$$

+ **5 pts** Used correct equation to calculate $$F_A$$, with correct q and r values

- **3 pts** incorrect numerical answer or algebraic expression for $$F_A$$

2.2 2b **10 / 10**

✓ **+ 10 pts Correct**

+ **5 pts** $$F_B=F_{Be}-F_{BA}$$

+ **5 pts** Used correct equation to calculate $$F_B$$, with correct q and r values

- **3 pts** incorrect numerical answer or algebraic expression for $$F_A$$

2.3 2c **10 / 10**

✓ **+ 10 pts Correct**

+ **7 pts** Correct interpretation of the overall direction of the forces

+ **3 pts** Bonding electron

+ **0 pts** Wrong

QUESTION 3

3 23 pts

3.1 3a **7 / 7**

✓ **+ 7 pts Correct**

+ **4 pts** Correct Zeff for H

+ **3 pts** Correct Value of IE for H (14.4 eV)

- **2 pts** Math or unit error or incorrect final answer

- **2 pts** Negative value for IE

+ **3 pts** Used correct formula for IE

+ **0 pts** Click here to replace this description.

3.2 3b **8 / 8**

✓ **+ 8 pts Correct**

+ **4 pts** Correct Zeff for N

+ **4 pts** Correct IE for N (43.2 eV)

- **2 pts** Math or unit error or incorrect final answer

- **2 pts** Negative value for IE

+ **4 pts** Used correct formula for IE

- **2 pts** Carried over incorrect IE from part a

+ **0 pts** Click here to replace this description.

3.3 3c **8 / 8**

✓ **+ 8 pts Correct**

+ 4 pts Correct Zeff for Al

+ 4 pts Correct IE for Al (28.8 eV)

- 2 pts Math or unit error or incorrect final answer

- 2 pts Negative value for IE

+ 4 pts Used correct formula for IE

- 2 pts Carried over incorrect IE from part a

+ 0 pts Blank

QUESTION 4

4 30 pts

4.1 4a **10 / 10**

✓ **+ 10 pts Correct**

+ 5 pts Y is more electronegative or X is more electropositive. Must show reasoning

+ 5 pts X is the positively-charged ion

+ 3 pts X is positively-charged, insufficient or no reason given.

+ 7 pts Determines that X is positively-charged considering only EA or IE without considering both together

+ 3 pts Incorrect, partial credit given

+ 0 pts No attempt

4.2 4b **18 / 20**

✓ **+ 20 pts Correct**

+ 3 pts Using the BE equation

+ 5 pts Use IE of X (with positive value) in BE equation

+ 5 pts Use EA of Y (with positive value) in BE equation

+ 7 pts Calculate V(r) term correctly including the partial charges

+ 17 pts All correct except application of partial charges

✓ **- 2 pts Math or unit error**

1. (17 pts) The Haber-Bosch process is used to produce commercial ammonia. The process reacts molecular hydrogen (H_2) with molecular nitrogen (N_2) to produce ammonia (NH_3).
   a. What mass of nitrogen, in grams, is required to produce 1 kg of ammonia?
   b. Draw Lewis dot structures for molecular hydrogen, molecular nitrogen and ammonia.
   c. Determine the shapes of molecular hydrogen, molecular nitrogen, and ammonia.

$H_2 + N_2 \rightarrow NH_3$

balanced: $3H_2 + N_2 \Rightarrow 2NH_3$

a) 1 kg NH_3 = 1000 g NH_3

from the balanced chemical equation, a reaction with 1 mol N_2 yields 2 mol $2NH_3$

$$\Rightarrow m_{N_2} = 1000\,g\,NH_3 \left(\frac{1\text{ mol }NH_3}{(14+3(1))\,g}\right)\left(\frac{1\text{ mol }N_2}{2\text{ mol }NH_3}\right)\left(\frac{2(14)\text{ g }N_2}{1\text{ mol }N_2}\right)$$

$$= \boxed{823.5\text{ g }N_2}$$

b) molecular hydrogen: $H - H$

molecular nitrogen: $:N \equiv N:$

amonia: $H - \ddot{N} - H$ with H bonded below N

c) molecular hydrogen - linear

molecular nitrogen - linear

amonia - trigonal pyramidal

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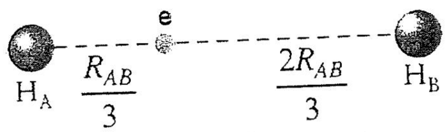
2. (30 pts) Consider the simple molecule H_2^+, with its electron positioned along the internuclear axis, a distance $\frac{R_{AB}}{3}$ from proton A (as shown below), where $R_{AB} = 1.1\text{Å}$ is the distance between the two nuclei. Determine whether this is a bonding electron. Please show your reasoning.



$\hat{z} \rightarrow$

using $\hat{z}$ points from proton A to proton B

force on proton A:

$$\vec{F}_{BA} = \left|\frac{q_1 q_2}{4\pi\varepsilon_0 R_{AB}^2}\right| \underbrace{(-\hat{z})}_{\text{away from proton B}} = \left|\frac{e(e)}{4\pi\varepsilon_0 (1.1\text{Å})^2}\right|(-\hat{z}) = \left|\frac{(1.602\times10^{-19}\,C)^2}{4\pi(8.85\times10^{-12}\frac{C^2}{Jm})(1.1\times10^{-10}\,m)^2}\right|(-\hat{z})$$

force by B on A

$$= 1.9072\times10^{-8}\,N\,(-\hat{z})$$

$$\vec{F}_{eA} = \left|\frac{q_1 q_2}{4\pi\varepsilon_0 (\frac{R_{AB}}{3})^2}\right| \underbrace{(\hat{z})}_{\text{towards electron}} = \left|\frac{e(-e)}{4\pi\varepsilon_0 (\frac{R_{AB}}{9}^2)}\right|(\hat{z}) = \frac{(1.602\times10^{-19}\,C)^2}{4\pi(8.85\times10^{-12}\frac{C^2}{Jm})(\frac{1.1\times10^{-10}\,m}{a})} \quad \hat{z}$$

force by electron on A

$$= 1.716\times10^{-7}\,N\,(\hat{z})$$

$$\vec{F}_A = \vec{F}_{BA} + \vec{F}_{eA} = 1.52\times10^{-7}\,N\,(\hat{z}) \quad \text{(to the right)}$$

similarly, for proton B, the net force is:

by symmetry, $|\vec{F}_{AB}| = |\vec{F}_{BA}|$ but they are antiparallel

$$\vec{F}_B = \vec{F}_{AB} + \vec{F}_{eB}$$

$$= -\vec{F}_{BA} + \left|\frac{(-e)(e)}{4\pi\varepsilon_0 (\frac{2}{3}(1.1\text{Å}))^2}\right|(-\hat{z}) = (1.9072\times10^{-8}\,N)(\hat{z}) + (4.29\times10^{-8}\,N)(-\hat{z}$$

$$= 2.38\times10^{-8}\,(-\hat{z}) \quad \text{(to the left)}$$

$\boxed{\text{the electron is a bonding electron since it attracts the protons together more strongly than they repel each other.}}$

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using $1\,J = \frac{1}{1.602\times10^{-19}}\,eV$

3. (23 pts) Using the simple model

$$Z_{eff} = Z - (\#e's\,lower\,n\,shells) - \frac{1}{2}(\#e's\,same\,n\,shell)$$ for many-electron atoms, calculate the first ionization energies of H, N and Al, in eV, assuming the bound electron is 1 Å away from the nucleus.

H: $Z_{eff} = 1 - 0 - \frac{1}{2}(0) = 1$

$$IE_1(H) = V_\infty - V_{1\text{Å}} = 0 - \frac{Z_{eff}e(-e)}{4\pi\varepsilon_0(1\text{Å})^2} = \frac{e^2}{4\pi(8.85\times10^{-12}\frac{C^2}{Jm})(10^{-10}m)}$$

$$= \frac{(1.602\times10^{-19})^2\,C^2}{4\pi(8.85\times10^{-12}\frac{C^2}{Jm})(10^{-10}m)} = \boxed{14.4\ eV}$$

N: $Z_{eff} = 7 - 2 - \frac{1}{2}(4) = 3$

$$IE_1(N) = V_\infty - V_{1\text{Å}} = 0 - \frac{Z_{eff}(e)(-e)}{4\pi\varepsilon_0(1\text{Å})} = \frac{3(1.602\times10^{-19}\,C)^2}{4\pi(8.85\times10^{-12}\frac{C^2}{Jm})(10^{-10}m)}$$

$$= \boxed{43.2\ eV}$$

Al: $Z_{eff} = 13 - 10 - \frac{1}{2}(2) = 2$

$$IE_1(Al) = V_\infty - V_{1\text{Å}} = 0 - \frac{Z_{eff}(e)(-e)}{4\pi\varepsilon_0(1\text{Å})} = \frac{2(1.602\times10^{-12}\,C)^2}{4\pi(8.85\times10^{-12}\frac{C^2}{Jm})(10^{-10}m)}$$

$$= \boxed{28.8\ eV}$$

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4. (30 pts) The diatomic molecule XY has an equilibrium bond length of 2 Å. The ionization energies of X and Y are 400 kJ/mol and 1000 kJ/mol, respectively, while their electron affinities are 40 kJ/mol and 100 kJ/mol. The % ionic character of the XY molecule is 75%.
   a. Which atom ends up positively charged in the diatomic molecule? Why?
   b. Calculate the bond energy of XY, in kJ/mol, using the information provided and the classical description of ionic bonding.

a)

$$IE_1(X) + EA(X) = 400 \frac{kJ}{mol} + 40 \frac{kJ}{mol} = 440 \frac{kJ}{mol}$$

$$IE_1(Y) + EA(Y) = 1000 \, kJ/mol + 100 \frac{kJ}{mol} = 1100 \frac{kJ}{mol}$$

since $IE_1(Y) + EA(Y) > IE_1(X) + EA(X)$, Y will end up negatively charged,

so $\boxed{\text{X atom ends up positively charged in the diatomic molecule}}$

b) using the equation $BE_{ionic} = -V_{AB}(r) - (IE(A) - EA(Y))$

$$BE_{ionic} = -\frac{e(-e)\delta^2}{4\pi\varepsilon_0 (2Å)} - \delta(IE(X) - EA(Y))$$

$$= \frac{(1.602\times10^{-19}C)^2(0.75)^2}{4\pi(8.85\times10^{-12}\frac{C^2}{Jm})(2\times10^{-10}m)} - \left(400\frac{kJ}{mol} - 100\frac{kJ}{mol}\right)(0.75)$$

$$= 390.7 \frac{kJ}{mol} - 0.75(400-100)\frac{kJ}{mol} = \boxed{165.7 \frac{kJ}{mol}}$$

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