Question 2

$$N_2(g) + 3\,F_2(g) \rightarrow 2\,NF_3(g) \qquad \Delta H^\circ_{298} = -264 \text{ kJ mol}^{-1};\ \Delta S^\circ_{298} = -278 \text{ J K}^{-1} \text{ mol}^{-1}$$

The following questions relate to the synthesis reaction represented by the chemical equation in the box above.

(a) Calculate the value of the standard free energy change, ΔG°_{298}, for the reaction.

$\Delta G^\circ_{298} = \Delta H^\circ_{298} - T\Delta S^\circ_{298}$ $= -264 \text{ kJ mol}^{-1} - (298 \text{ K})(-0.278 \text{ kJ mol}^{-1} \text{ K}^{-1})$ $= -181 \text{ kJ mol}^{-1}$	One point is earned for correct substitution. One point is earned for the value of ΔG°_{298} (including kJ or J).

(b) Determine the temperature at which the equilibrium constant, K_{eq}, for the reaction is equal to 1.00. (Assume that ΔH° and ΔS° are independent of temperature.)

When $K_{eq} = 1$, then $\Delta G^\circ_T = -RT \ln(1) = 0$ If $\Delta G^\circ_T = 0$, then $0 = \Delta H^\circ - T\Delta S^\circ \Rightarrow$ $T = \dfrac{\Delta H^\circ_{298}}{\Delta S^\circ_{298}}$ $T = \dfrac{-264 \text{ kJ mol}^{-1}}{-0.278 \text{ kJ K}^{-1}\text{mol}^{-1}} = 950. \text{ K}$	One point is earned for indicating that if $K_{eq} = 1$, then $\Delta G^\circ_T = 0$. One point is earned for the answer (including the unit K).

(c) Calculate the standard enthalpy change, ΔH°, that occurs when a 0.256 mol sample of $NF_3(g)$ is formed from $N_2(g)$ and $F_2(g)$ at 1.00 atm and 298 K.

$0.256 \text{ mol } NF_3(g) \times \dfrac{-264 \text{ kJ}}{2.00 \text{ mol } NF_3(g)} = -33.8 \text{ kJ}$	One point is earned for multiplying ΔH°_{298} by the number of moles of NF_3 formed. One point is earned for recognizing that 2.00 mol of NF_3 are produced for the reaction as it is written. One point is earned for the answer (including kJ or J).

Question 2 (continued)

The enthalpy change in a chemical reaction is the difference between energy absorbed in breaking bonds in the reactants and energy released by bond formation in the products.

(d) How many bonds are formed when two molecules of NF_3 are produced according to the equation in the box above?

There are six N–F bonds formed.	One point is earned for the correct answer.

(e) Use both the information in the box above and the table of average bond enthalpies below to calculate the average enthalpy of the F – F bond.

Bond	Average Bond Enthalpy (kJ mol^{-1})
N≡N	946
N–F	272
F–F	?

$\Delta H^\circ_{298} = \Sigma E_{bonds\ broken} - \Sigma E_{bonds\ formed} = -264$ kJ mol^{-1} $= [\mathrm{BE}_{N\equiv N} + (3 \times \mathrm{BE}_{F\text{-}F})] - (6 \times \mathrm{BE}_{N\text{-}F})$ $= [946 \text{ kJ mol}^{-1} + (3 \times \mathrm{BE}_{F\text{-}F})] - 6(272 \text{ kJ mol}^{-1})$ $= -264$ kJ mol^{-1} $\Rightarrow$ 3 mol $\mathrm{BE}_{F\text{-}F} = (-264 - 946 + 1{,}632)$ kJ mol^{-1} $\Rightarrow$ $\mathrm{BE}_{F\text{-}F} = 141$ kJ mol^{-1}	One point is earned for the correct number of bonds in all three compounds multiplied by the average bond enthalpies. One point is earned for the answer (including kJ or J). <u>Note:</u> A total of one point is earned if an incorrect number of bonds is substituted in a correct equation and the answer is reasonable (i.e., positive).

$N_2(g) + 3\,F_2(g) \rightarrow 2\,NF_3(g) \qquad \Delta H^\circ_{298} = -264 \text{ kJ mol}^{-1};\ \Delta S^\circ_{298} = -278 \text{ J K}^{-1}\text{ mol}^{-1}$

2. The following questions relate to the synthesis reaction represented by the chemical equation in the box above.

   (a) Calculate the value of the standard free energy change, ΔG°_{298}, for the reaction.

   (b) Determine the temperature at which the equilibrium constant, K_{eq}, for the reaction is equal to 1.00. (Assume that ΔH° and ΔS° are independent of temperature.)

   (c) Calculate the standard enthalpy change, ΔH°, that occurs when a 0.256 mol sample of $NF_3(g)$ is formed from $N_2(g)$ and $F_2(g)$ at 1.00 atm and 298 K.

   The enthalpy change in a chemical reaction is the difference between energy absorbed in breaking bonds in the reactants and energy released by bond formation in the products.

   (d) How many bonds are formed when two molecules of NF_3 are produced according to the equation in the box above?

   (e) Use both the information in the box above and the table of average bond enthalpies below to calculate the average enthalpy of the F – F bond.

Bond	Average Bond Enthalpy (kJ mol^{-1})
N≡N	946
N–F	272
F–F	?

(a) $\Delta G = \Delta H - T\Delta S$

$\Delta G = -264 - 298(-0.278)$

$\Delta G = -181$ kJ

(b) $\Delta G = -RT\ln K$

K = 1 at equilibrium $\Delta G = 0$

$\Delta G = \Delta H - T\Delta S$

$\Delta H = T\Delta S$

$\frac{\Delta H}{\Delta S} = T$

$T = \frac{-264}{-0.278}$

T = 950. K

(c) $N_2 + 3F_2 \rightarrow 2NF_3$

$0.256 \text{ mol } NF_3 \left| \frac{-264 \text{ kJ}}{2 \text{ mol } NF_3} \right| = -33.8$ kJ

$\Delta H = -33.8$ kJ

(d) $N_2 + 3F_2 \rightarrow 2NF_3$

N≡N F–F F–N(–F)–F

N≡N F–F

F–F F–N(–F)–F

6 bonds formed

GO ON TO THE NEXT PAGE.

2A2

(e) $\Delta H = \Delta H_{\text{bonds broken}} - \Delta H_{\text{bonds formed}}$

$-264 = 946 + 3\Delta H_{F_2} - 6(272)$

$3\Delta H_{F_2} = 422$

$\Delta H_{F_2} = 141 \frac{kJ}{mol}$

$F-F: \quad 141 \frac{kJ}{mol}$

2B1

$N_2(g) + 3\,F_2(g) \rightarrow 2\,NF_3(g)$ $\quad \Delta H^\circ_{298} = -264$ kJ mol^{-1}; $\Delta S^\circ_{298} = -278$ J K^{-1} mol^{-1}

2. The following questions relate to the synthesis reaction represented by the chemical equation in the box above.

(a) Calculate the value of the standard free energy change, ΔG°_{298}, for the reaction.

(b) Determine the temperature at which the equilibrium constant, K_{eq}, for the reaction is equal to 1.00. (Assume that ΔH° and ΔS° are independent of temperature.)

(c) Calculate the standard enthalpy change, ΔH°, that occurs when a 0.256 mol sample of $NF_3(g)$ is formed from $N_2(g)$ and $F_2(g)$ at 1.00 atm and 298 K. 25°

The enthalpy change in a chemical reaction is the difference between energy absorbed in breaking bonds in the reactants and energy released by bond formation in the products.

(d) How many bonds are formed when two molecules of NF_3 are produced according to the equation in the box above?

(e) Use both the information in the box above and the table of average bond enthalpies below to calculate the average enthalpy of the F – F bond.

Bond	Average Bond Enthalpy (kJ mol^{-1})
N≡N	946
N–F	272
F–F	?

a) $\Delta G = \Delta H - T\Delta S$

$= (-264) - (298)(-278)$

$\Delta G^\circ_{298} = 82,580$

b) reaction in equilibrium when $\Delta G = 0$

$0 = (-264) - T(-278)$

$264 = -T(-278)$

$\frac{264}{278} = T$

when $T = .95$ K $\rightarrow \Delta G = 0$

GO ON TO THE NEXT PAGE.

2B2

c) per mole at 298 K −264 kJ is the ΔH°

0.256 * −264 = ΔH° for 0.256 moles at 298 K

$\frac{-67.6 \text{ kJ}}{2}$

−33.8 kJ

d)

$1 N \equiv N 1 + 3(F - F) \rightarrow 2(N - F_3)$

6 bonds are formed

e)

−264 = ΣH_f° products − ΣH_f° reactants (bond these)

−264 = 2(272) − [3(x) + 946]

−808 = −3x − 946

138 = −3x

x = −46 kJ/mol = ΔH bond ave. F–F

2C₁

$N_2(g) + 3\,F_2(g) \rightarrow 2\,NF_3(g)$ $\Delta H^\circ_{298} = -264$ kJ mol^{-1}; $\Delta S^\circ_{298} = -278$ J K^{-1} mol^{-1}

2. The following questions relate to the synthesis reaction represented by the chemical equation in the box above.

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(c) Calculate the standard enthalpy change, ΔH°, that occurs when a 0.256 mol sample of $NF_3(g)$ is formed from $N_2(g)$ and $F_2(g)$ at 1.00 atm and 298 K.

The enthalpy change in a chemical reaction is the difference between energy absorbed in breaking bonds in the reactants and energy released by bond formation in the products.

(d) How many bonds are formed when two molecules of NF_3 are produced according to the equation in the box above?

(e) Use both the information in the box above and the table of average bond enthalpies below to calculate the average enthalpy of the F – F bond.

Bond	Average Bond Enthalpy (kJ mol^{-1})
N≡N	946
N–F	272
F–F	?

a) $\Delta G = \Delta H - T\Delta S$

$\Delta G = -264$ kJ/mol $- 298$K $\cdot (-278$ J/mol K$)$

$\Delta G = -264000$ J/mol $+ 82844$ J/mol

$\Delta G = 346844$ J/mol $= 346.844$ kJ/mol ≈ 347 kJ/mol

b) $\Delta G = -RT \ln K$

$\Delta G = -8.314 \cdot x \cdot \ln(1)$

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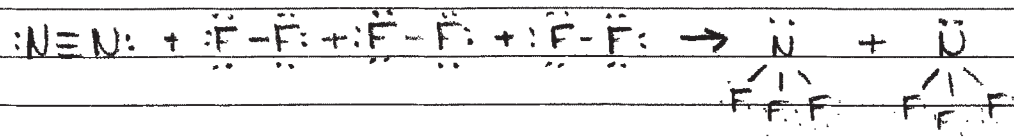
2C2

c) $\Delta H^\circ_{298} = \frac{-264\ kJ}{mol}$

$.256\ mol \,\Big|\, \frac{-264\ kJ}{mol} \,\Big\|\, -67.584\ kJ \approx -67.6\ kJ$

d) 

6 bonds are formed (3 in each molecule)

e) $2(3(N-F)) - 3(F-F) - (N\equiv N) = -264\ kJ/mol$

$2(3(272\ kJ/mol)) - 3(x) - 946\ kJ/mol = -264\ kJ/mol$

$-3x = 950\ kJ/mol$

$x = 316.6\ kJ/mol \approx 317\ kJ/mol$

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Question 2

Overview

The intent of this question was to assess students' understanding of thermodynamics for a particular reaction. Students were asked to calculate ΔG°_{298} using thermodynamic data provided, to predict the temperature at which the reaction is at equilibrium, to calculate the enthalpy for a specific number of moles of product, and to relate the number of bonds broken and formed to bond energies and reaction enthalpy in order to calculate the average enthalpy of the F–F bond.

Sample: 2A
Score: 10

This response earned all 10 points: 2 for part (a), 2 for part (b), 3 for part (c), 1 for part (d), and 2 for part (e).

Sample: 2B
Score: 7

In part (a) only 1 out of 2 points was earned because there is no conversion between kJ and J, leading to an incorrect answer. In part (b) both points were earned because the error is the same conversion error made in part (a), thus no penalty was associated with a second occurrence of the same error. All points were earned in parts (c) and (d). In part (e) no points were earned because the number of N–F bonds used in the calculation is incorrect, and the bond energy is calculated by using products minus reactants. The latter mistake was a common error in responses to this question.

Sample: 2C
Score: 5

In part (a) 1 out of 2 points was earned because the student neglects to include the negative sign on the ΔH when adding. In part (b) no points were earned because the student does not recognize that $\Delta G = 0$ when $K_{eq} = 1$ and therefore does not use $\Delta H = T\Delta S$ to calculate temperature; this was one of the most common errors students made on this question. Only 2 out of 3 points were earned in part (c) because the response does not consider the stoichiometry of the chemical equation in determining the enthalpy. (Note that using −264 kJ for each mole of NF_3 in part (c) is inconsistent with using −264 kJ for 2 moles of NF_3 in the responses to parts (a) and (e).) The point was earned in part (d). In part (e) only 1 out of 2 points was earned because the relationship of bonds broken to bonds formed is reversed.