Question 5 (9 points)

Answer the following questions about nitrogen, hydrogen, and ammonia.

(a) In the boxes below, draw the complete Lewis electron-dot diagrams for N₂ and NH₃.

\[
\begin{align*}
\text{N₂} & :\text{N} \equiv \text{N}: \\
\text{NH₃} & \text{H} \equiv \text{N} \equiv \text{H} \\
& \equiv \text{H}
\end{align*}
\]

The correct structures are shown in the boxes above.

Two points are earned for the correct Lewis electron-dot diagrams (1 point each).

(b) Calculate the standard free-energy change, \( \Delta G^\circ \), that occurs when 12.0 g of H₂(g) reacts with excess N₂(g) at 298 K according to the reaction represented below.

\[
\text{N}_2(g) + 3 \text{H}_2(g) \rightleftharpoons 2 \text{NH}_3(g) \quad \Delta G_{298}^\circ = -34 \text{ kJ mol}^{-1}
\]

\[
12.0 \text{ g H}_2 \times \frac{1 \text{ mol H}_2}{2.0 \text{ g H}_2} \times \frac{1 \text{ mol reaction}}{3 \text{ mol H}_2} \times \frac{-34 \text{ kJ}}{1 \text{ mol reaction}} = -68 \text{ kJ}
\]

One point is earned for the correct stoichiometry.

One point is earned for the correct answer.

(c) Given that \( \Delta H_{298}^\circ \) for the reaction is \(-92.2 \text{ kJ mol}^{-1}\), which is larger, the total bond dissociation energy of the reactants or the total bond dissociation energy of the products? Explain.

\[
\Delta H_{298}^\circ = \Sigma (\text{bond energy of the reactants}) - \Sigma (\text{bond energy of the products})
\]

Based on the equation above, for \( \Delta H_{298}^\circ \) to be negative, the total bond energy of the products must be larger than the total bond energy of the reactants.

OR

More energy is released as product bonds are formed than is absorbed as reactant bonds are broken.

One point is earned for the correct answer with the correct equation and explanation.
(d) The value of the standard entropy change, $\Delta S^\circ_{298}$, for the reaction is $-199 \text{ J mol}^{-1}\text{K}^{-1}$. Explain why the value of $\Delta S^\circ_{298}$ is negative.

All of the reactants and products in the reaction are in the gas phase, so the sign of the entropy change will depend on the number of moles of particles in the reactants and products. There are more moles of reactants (four) compared with moles of products (two), so there is a greater number of microstates in the reactants than in the products. Therefore the entropy decreases as the reaction proceeds (fewer possible microstates), and the sign of the entropy change is negative.

One point is earned for the correct explanation.

(e) Assume that $\Delta H^\circ$ and $\Delta S^\circ$ for the reaction are independent of temperature.

(i) Explain why there is a temperature above 298 K at which the algebraic sign of the value of $\Delta G^\circ$ changes.

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

As the temperature increases $|T\Delta S^\circ|$ will at some point exceed $|\Delta H^\circ|$. Because both $\Delta H^\circ$ and $\Delta S^\circ$ are negative, the sign of $\Delta G^\circ$ will then change from negative to positive.

One point is earned for the correct explanation.

(ii) Theoretically, the best yields of ammonia should be achieved at low temperatures and high pressures. Explain.

Low temperatures: The reaction is exothermic. By Le Chatelier’s principle, decreasing the temperature drives the reaction to the right to produce more heat energy, and thus more ammonia is produced.

High pressures: For this reaction, higher pressure is achieved by decreasing the volume of the container. As pressure increases, the reaction equilibrium shifts in the direction that reduces the total number of particles (by Le Chatelier’s principle). In this case, the product has fewer moles of particles than the reactants; thus product would be favored. Higher pressure therefore results in an increase in the amount of ammonia.

One point is earned for explaining increased yield at low temperatures.

One point is earned for explaining increased yield at high pressures.
Answer Question 5 and Question 6. The Section II score weighting for these questions is 15 percent each.

Your responses to these questions will be graded on the basis of the accuracy and relevance of the information cited. Explanations should be clear and well organized. Examples and equations may be included in your responses where appropriate. Specific answers are preferable to broad, diffuse responses.

5. Answer the following questions about nitrogen, hydrogen, and ammonia.

(a) In the boxes below, draw the complete Lewis electron-dot diagrams for \( N_2 \) and \( NH_3 \).

![Lewis structures](image)

(b) Calculate the standard free-energy change, \( \Delta G^\circ \), that occurs when 12.0 g of \( H_2(g) \) reacts with excess \( N_2(g) \) at 298 K according to the reaction represented below.

\[
N_2(g) + 3H_2(g) \rightarrow 2NH_3(g) \quad \Delta G_{298}^\circ = -34 \text{ kJ mol}^{-1}
\]

(c) Given that \( \Delta H_{298}^\circ \) for the reaction is \(-92.2 \text{ kJ mol}^{-1} \), which is larger, the total bond dissociation energy of the reactants or the total bond dissociation energy of the products? Explain.

(d) The value of the standard entropy change, \( \Delta S_{298}^\circ \), for the reaction is \(-199 \text{ J mol}^{-1}K^{-1} \). Explain why the value of \( \Delta S_{298}^\circ \) is negative.

(e) Assume that \( \Delta H^\circ \) and \( \Delta S^\circ \) for the reaction are independent of temperature.

(i) Explain why there is a temperature above 298 K at which the algebraic sign of the value of \( \Delta G^\circ \) changes.

(ii) Theoretically, the best yields of ammonia should be achieved at low temperatures and high pressures. Explain.
(b) 12.0 g of H₂ is approximately equal to 6 mol.
Therefore, \( \frac{6}{3} = 2 \) mol of nitrogen will react, since the hydrogen is the limiting reactant.
Therefore, \( \Delta G = -34 \times 2 = -68 \text{kJ} \).

(c) AH of any reaction is equal to AH of the reaction where you dissociate all the reactants' bonds, and put them all back together to make the product. This is true by the Hess's Law, which suggests that AH is same as long as the reactants and the products are same between the 2 reactions.

**Path does not matter**

Therefore, \( \Delta H = \sum \text{(reactants' bond dissociation energy)} \)

\[ + \Delta H \text{ (putting together)} \]

\[ - \Sigma \text{(products' total bond formation energy)} \]

Since \( \Delta H \text{(bond formation)} = -\Delta H \text{(bond dissociation)} \)

So since \( \Delta H < 0 \), \( \Sigma \text{(reactants)} < \Sigma \text{(products)} \)

(d) The entropy is the scale of randomness, and therefore will be in proportional to the amount of gas, because more the gases, more random it can get, mathematically.
(ii) Le Chatelier's Principle suggests that when an environmental change is done on a system with an equilibrium, the equilibrium will shift to reduce the change. Therefore, if we lower the temperature, the system would try to raise it by exothermic reaction, which in this case is making ammonia.

Also when we increase the pressure, the system would try to decrease it by reducing the molecules of the gas, since in an ideal gas, $P\cdot V = n\cdot R\cdot T$. This is also done by making ammonia.
Answer Question 5 and Question 6. The Section II score weighting for these questions is 15 percent each.

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5. Answer the following questions about nitrogen, hydrogen, and ammonia.

(a) In the boxes below, draw the complete Lewis electron-dot diagrams for \( \text{N}_2 \) and \( \text{NH}_3 \).

![Lewis electron-dot diagrams for \( \text{N}_2 \) and \( \text{NH}_3 \)]

(b) Calculate the standard free-energy change, \( \Delta G^\circ \), that occurs when 12.0 g of \( \text{H}_2(g) \) reacts with excess \( \text{N}_2(g) \) at 298 K according to the reaction represented below.

\[
\text{N}_2(g) + 3 \text{H}_2(g) \rightleftharpoons 2 \text{NH}_3(g) \quad \Delta G^\circ_{298} = -34 \text{ kJ mol}^{-1}
\]

(c) Given that \( \Delta H^\circ_{298} \) for the reaction is \(-92.2 \text{ kJ mol}^{-1} \), which is larger, the total bond dissociation energy of the reactants or the total bond dissociation energy of the products? Explain.

(d) The value of the standard entropy change, \( \Delta S^\circ_{298} \), for the reaction is \(-199 \text{ J mol}^{-1}\text{K}^{-1} \). Explain why the value of \( \Delta S^\circ_{298} \) is negative.

(e) Assume that \( \Delta H^\circ \) and \( \Delta S^\circ \) for the reaction are independent of temperature.

(i) Explain why there is a temperature above 298 K at which the algebraic sign of the value of \( \Delta G^\circ \) changes.

(ii) Theoretically, the best yields of ammonia should be achieved at low temperatures and high pressures. Explain.

\[
\Delta G^\circ = 
\begin{array}{c}
12.0 \text{ g} \cdot \frac{1\text{ mol H}_2}{2.029\text{ g}} \cdot \frac{2\text{ mol NH}_3}{3\text{ mol H}_2} \cdot -39 \text{ kJ} \\
\Delta G^\circ = -136 \text{ kJ}
\end{array}
\]

(c) The total bond dissociation energy of the products is larger when \( \Delta H^\circ < 0 \), the reaction is exothermic, so bonds...

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GO ON TO THE NEXT PAGE.
are formed. \[ \Delta H^0 = \sum \text{bond energy of reactants} - \sum \text{bond energy of products} \]

Thus, since \( \Delta H^0 < 0 \), the total bond dissociation energy of the products is greater.

d) \( \Delta S^{\circ} \) is negative. There are 4 moles of gas reactants and 2 moles of gas products. Therefore, the products are more orderly, causing a decrease in entropy, which explains why \( \Delta S^{\circ} < 0 \)

e) (i) \( \Delta G^0 = \Delta H^0 - T \Delta S^0 \). Since \( \Delta H^0 \) and \( \Delta S^0 \) are both negative,

\[ \Delta G^0 = - T (-) \]

Therefore, at high temperatures, the value of \( \Delta G^0 \) will be more positive, which causes \( \Delta G^0 \) to be positive.

(ii) At low temperatures, \( \Delta G^0 < 0 \), so the reaction is spontaneous. At high pressures, the \( \text{N}_2 \) and \( \text{NH}_3 \) molecules have a greater tendency to collide and form \( \text{NH}_3 \).
Answer Question 5 and Question 6. The Section II score weighting for these questions is 15 percent each.

Your responses to these questions will be graded on the basis of the accuracy and relevance of the information cited. Explanations should be clear and well organized. Examples and equations may be included in your responses where appropriate. Specific answers are preferable to broad, diffuse responses.

5. Answer the following questions about nitrogen, hydrogen, and ammonia.

(a) In the boxes below, draw the complete Lewis electron-dot diagrams for \( \text{N}_2 \) and \( \text{NH}_3 \).

\[ \begin{align*}
\text{N}_2 & :N \equiv N : \\
\text{NH}_3 & \end{align*} \]

(b) Calculate the standard free-energy change, \( \Delta G^\circ \), that occurs when 12.0 g of \( \text{H}_2(g) \) reacts with excess \( \text{N}_2(g) \) at 298 K according to the reaction represented below.

\[ \text{N}_2(g) + 3 \text{H}_2(g) \rightarrow 2 \text{NH}_3(g) \quad \Delta G_{298}^\circ = -34 \text{ kJ mol}^{-1} \]

(c) Given that \( \Delta H_{298}^\circ \) for the reaction is -92.2 kJ mol\(^{-1}\), which is larger, the total bond dissociation energy of the reactants or the total bond dissociation energy of the products? Explain.

(d) The value of the standard entropy change, \( \Delta S_{298}^\circ \), for the reaction is -199 J mol\(^{-1}\)K\(^{-1}\). Explain why the value of \( \Delta S_{298}^\circ \) is negative.

(e) Assume that \( \Delta H^\circ \) and \( \Delta S^\circ \) for the reaction are independent of temperature.

(i) Explain why there is a temperature above 298 K at which the algebraic sign of the value of \( \Delta G^\circ \) changes.

(ii) Theoretically, the best yields of ammonia should be achieved at low temperatures and high pressures. Explain.

\[ \text{(b)} \quad \text{NH}_3 \rightarrow 17 \text{g} / \text{mol} \hspace{1cm} 12.9 \text{ g} \hspace{0.2cm} \frac{17}{11} \text{mol} \]

\[ \Delta G_{298}^\circ \times \frac{17}{11} = -24 \text{kJ} \]

\[ \text{(c)} \quad \Delta H_{298}^\circ = \Sigma E_{\text{bond \ before}} - \Sigma E_{\text{bond \ after}} = -892.2 \text{kJ/mol} \]

\[ \therefore \text{Bond dissociation energy of reactants is larger than products' energy.} \]
(d) Because the coefficient of equation is decrease when this react, value of $\Delta S^{\text{zag}}$ is negative.

(e) (ii) Because $\Delta G = \Delta H - T \Delta S$, $\Delta G$ changes because of change of temperature.

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

To make $\Delta G$ negative, $T$ should be low because $\Delta S$ is negative.

And high pressures make react low $\Delta S$.

Because $\Delta S$ is negative, high pressures makes react make more $NH_3$. 
Question 5

Sample: 5A
Score: 9

This response earned all 9 points: 2 for part (a), 2 for part (b), 1 for part (c), 1 for part (d), 1 for part (e)(i), and 2 for part (e)(ii). In part (d) the point was earned for relating the negative change in entropy, associated with randomness, to the change in the number of moles of gas in the reaction.

Sample: 5B
Score: 6

This response earned 6 of the possible 9 points. In part (a) both points were earned for acceptable Lewis electron-dot diagrams of nitrogen gas and ammonia. In part (b) 1 point was earned for the application of an appropriate mass-to-mole conversion followed by the application of a ratio of moles to energy. Because the calculation includes an inappropriate conversion of moles of hydrogen to ammonia for the mole-to-energy conversion that follows, the response did not earn the second point. In part (c) 1 point was earned for a correct answer and explanation. In part (d) 1 point was earned for a correct answer with explanation. In part (e)(i) 1 point was earned for a correct explanation. In part (e)(ii) an incorrect explanation did not earn either of the possible points.

Sample: 5C
Score: 2

This response earned 2 of the possible 9 points. In part (a) both points were earned for acceptable Lewis electron-dot diagrams of nitrogen gas and ammonia. In part (b) the incorrect use of a mass-to-mass ratio with no mole-to-energy ratio did not earn either point. In part (c) the response presents a correct equation but interprets it incorrectly and thus did not earn the point. In part (d) there is reference to a decrease in the number of moles, but no mention of gas, randomness, or entropy; consequently no point was earned. In part (e)(i) presentation of the Gibb–Helmholtz equation, with an inadequate explanation, did not earn a point. In part (e)(ii) the response refers incorrectly to free energy, and while it mentions increased pressures favoring low entropy, it does not relate this to decreased gas pressure; hence, neither point was earned.