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NAME: ______________

General Chemistry
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Thermodynamics Calculations, Part II

Solve the following problems. Show formulas, units, and work for problems requiring calculations.

Suppose that 1.00 mol of C_3H_8 (g) reacts completely with O_2 (g) to produce CO_2 (g) and H_2O (g) (g).

Reactants

Products

1. **Write the balanced chemical equation for this reaction.**

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$$

2. **Calculate the enthalpy change of this reaction. Don't forget the correct units.**

$$\Delta H^o_{rxn} = [PRODUCTS] - [REACTANTS]$$

$$= [(4)(H_2O) + (3)(CO_2)] - [(1)(C_3H_8) + (5)(O_2)]$$

$$= [(4)(-241.82) + (3)(-393.5)] - [(1)(-103.85) + (5)(0)]$$

$$= [-967.28 + (-1180.5)] - [-103.85]$$

$$= [-2147.78] - [-103.85]$$

$$= -2043.93 \text{ kJ/mol}$$

3. **Is this reaction exothermic or endothermic? How do you know?**

EXOTHERMIC, because the sign of ΔH is $-$.

4. **Is this enthalpy change favorable or unfavorable?**

FAVORABLE.

5. **Calculate the ΔS° for the reaction in #1. Use the correct units.**

$$\Delta S^o_{rxn} = [PRODUCTS] - [REACTANTS]$$

$$\Delta S^o_{rxn} = [(4)(H_2O) + (3)(CO_2)] - [(1)(C_3H_8) + (5)(O_2)]$$

$$= [(4)(188.83) + (3)(213.6)] - [(1)(269.9) + (5)(205.0)]$$

$$= [755.32 + 640.8] - [269.9 + 1025]$$

$$= 1396.12 - 1294.9$$

$$= 101.22 \frac{J}{mol \cdot Kelvin}$$

6. **Is this entropy change favorable or unfavorable? How do you know?**

Favorable. When ΔS_{rxn} is a positive number, the entropy change is favorable.

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7. **Calculate the ΔG° for this reaction at 298 K. You may use either of the two formulas to calculate ΔG°. Make sure that you keep track of the units -- ΔS° usually has "J" as part of its units, but ΔH° usually has "kJ"!**

Option #1: use $\Delta G = \Delta H - T\Delta S$

$$\Delta G^o_{rxn} = \left[-2043.93 \frac{kJ}{mol}\right] - \left[(298 \cancel{Kelvins})\left(0.10122 \frac{kJ}{mol \cdot \cancel{Kelvin}}\right)\right]$$

answer from question #2

given above in this problem

answer from #5, but it had to be converted to kJ to match the units of ΔH.

$$101.22 \frac{\cancel{J}}{mol \cdot K} \times \frac{1 \, kJ}{1000 \, \cancel{J}} = 0.10122 \frac{kJ}{mol \cdot K}$$

$$\Delta G^o_{rxn} = \left[-2043.93 \frac{kJ}{mol}\right] - \left[30.16 \frac{kJ}{mol}\right]$$

$$= -2074.09 \frac{kJ}{mol}$$

or

Option #2: use the "products - reactants" method again.

$$\Delta G^o_{rxn} = [\text{PRODUCTS}] - [\text{REACTANTS}]$$

$$= [(4)(H_2O) + (3)(CO_2)] - [(1)(C_3H_8) + (5)(O_2)]$$

$$= [(4)(-228.57) + (3)(-394.4)] - [(1)(-23.47) + (5)(0)]$$

$$= [-914.28 + -1183.2] - [-23.47]$$

$$= [-2097.48] - [-23.47]$$

$$= -2074.01 \frac{kJ}{mol}$$

As you can see, you get the same answer using this method (to 4 sig figs, at least).

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8. **Is the reaction spontaneous or not? How do you know?**

It is spontaneous. It released more energy than it requires. The sign of ΔG is $-$.

9. **Consider the following reaction:**

$$X + 2W \rightarrow Y \qquad \Delta G^\circ = 40.9 \text{ kJ/mol}$$

Here is what this expression really means: In this reaction, if 1 mol of X is reacted with 2 mol of W, then 1 mol of Y is produced and this requires 40.9 kJ of energy. Therefore, in order to produce 2.96 mol of Y, how many kJ of energy must be used? Show work. Include units.

$$2.96 \text{ mol of } Y \times \frac{40.9 \text{ kJ}}{1 \text{ mol of } Y} = 121.1 \text{ kJ}$$

10. **In all of the calculations above (excluding #9), you assumed that 1.00 mol of C_3H_8 reacted. Now, re-calculate the ΔG° from #7 assuming that**

   a. **Only 0.393 mol of C_3H_8 reacts.**

$$0.393 \text{ mol } C_3H_8 \times \frac{-2074 \text{ kJ}}{1 \text{ mol } C_3H_8} = -815.1 \text{ kJ}$$

answer from #7

   b. **Only 0.393 g of C_3H_8 reacts.**

$$0.393 g \times \frac{1 \text{ mol}}{44.1 g} = 0.008916 \text{ mol} \times \frac{-2074 \text{ kJ}}{1 \text{ mol}} = -18.5 \text{ kJ}$$

use periodic table

$C_3 = 3 \times 12.0$

$H_8 = 8 \times 1.01$