

Answer on the question #63486, Chemistry / General Chemistry

Question:

In a 5.11 L container at a temperature of 24.8 C, 15.0g of C₃H₆O and 2.25atm of oxygen gas are introduced. The two combust to form carbon dioxide gas and water vapor.

Balanced equation: C₃H₆O+4O₂=3CO₂+3H₂O

I need to find the limiting reactant, calculate the enthalpy of the reaction, and determine the total amount and direction of energy flow in the reaction.

Solution:

- I. Limiting reactant.

We should write first the reaction equation and calculate the number of the moles of reagents introduced into the container:

$$\begin{aligned}C_3H_6O + 4O_2 &\rightarrow 3CO_2 + 3H_2O \\n(C_3H_6O) &= \frac{n(O_2)}{4} \\n(C_3H_6O) &= \frac{m(C_3H_6O)}{M(C_3H_6O)} = \frac{15.0 (g)}{58.08 (g \text{ mol}^{-1})} = 0.2583 \text{ mol} \\n(O_2) &= \frac{pV}{RT} = \frac{2.25(atm) \cdot 5.11(L)}{0.0822057 (L \text{ atm mol}^{-1}K^{-1}) \cdot (273.15 + 24.8)(K)} \\&= 0.4702 \text{ mol}, \frac{0.4702}{4} = 0.1176\end{aligned}$$

As

$$0.1176 < 0.2583,$$

O₂ is the limiting reactant.

- II. Enthalpy of the reaction can be calculated according to Hess' law:

$$\begin{aligned}\Delta H_{rxn} &= 3 \cdot \Delta H_f(CO_2) + 3 \cdot \Delta H_f(H_2O) - \Delta H_f(C_3H_6O), \\ \Delta H_{rxn} &= 3 \cdot (-393.52)(kJ \text{ mol}^{-1}) + 3 \cdot (-285.83)(kJ \text{ mol}^{-1}) + 249.4(kJ \text{ mol}^{-1}), \\ \Delta H_{rxn} &= -1788.65kJ \text{ mol}^{-1}.\end{aligned}$$

The data was taken from NIST chemistry webbook:

<http://webbook.nist.gov/>

The value of $\Delta H_f(C_3H_6O) = -249.4 kJ \text{ mol}^{-1}$ was taken from the webbook and corresponds to the enthalpy of formation of acetone in liquid phase.

All calculations were made in assumption that the enthalpies of formation are the same at STP conditions and the conditions given, i.e. not dependent on temperature and pressure.

- III. Energy flow in the reaction can be estimated as the Gibbs' energy change:

$$\Delta G^{mol} = \Delta H_{rxn} - T\Delta S_{rxn}$$

$$\Delta S_{rxn} = 3S_{CO_2} + 3S_{H_2O} - S_{C_3H_6O} - 4S_{O_2}$$

$$\Delta S_{rxn} = 3 \cdot 213.785(J \text{ mol}^{-1}K^{-1}) + 3 \cdot 69.95(J \text{ mol}^{-1}K^{-1}) - 200.4(J \text{ mol}^{-1}K^{-1}) - 4 \cdot 205.15(J \text{ mol}^{-1}K^{-1})$$

$$\Delta S_{rxn} = -169.795(J \text{ mol}^{-1}K^{-1})$$

$$\Delta G^{mol} = -1788.65 kJ \text{ mol}^{-1} - (273.15 + 24.8)(K) \cdot (-169.795)(J \text{ mol}^{-1}K^{-1})$$

$$\Delta G^{mol} = -1738.1 kJ/mol$$

$$\Delta G = \Delta G^{mol} \cdot \frac{n(O_2)}{4} = -1738.1 \left(\frac{kJ}{mol} \right) \cdot 0.1176(mol) = -204.34 kJ$$

As $\Delta G < 0$, the reaction is spontaneous and the energy is released from the system to surroundings.

The data on entropy was taken from NIST chemistry webbook (the link above).

Answer: The limiting reactant is oxygen, the enthalpy of the reaction is -1788.65 kJ/mol, the total amount of energy flow in the reaction is -204.34 kJ, energy flows from the system to surroundings.