Spontaneity and Gibbs free energy

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At 298K:

$$\Delta G^{\ominus}_{reaction} = \Sigma \Delta G^{\ominus}_{f \, (products)} - \Sigma \Delta G^{\ominus}_{f \, (reactants)}$$

At any temperature:

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

1. What is the standard free energy change, $\Delta G^{\ominus}$, in kJ, for the following reaction at 298K?

$$C_2H_5OH_{(l)} + 3O_{2(g)} \rightarrow 2CO_{2(g)} + 3H_2O_{(g)} \quad \text{kJ/mol}$$
$$\text{-175} \qquad 0 \qquad \text{-394} \quad \text{-229}$$
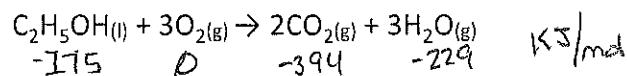
Compound	$\Delta G_f^{\ominus}$ (kJ mol^{-1})
$C_2H_5OH_{(l)}$	−175
$CO_{2(g)}$	−394
$H_2O_{(g)}$	−229
$O_{2(g)}$	0

$\Delta G^{\circ}_{rxn} =$

$$\left[3\tfrac{mol}{mol\,rxn}\left(-229\tfrac{kJ}{mol}\right) + 2\tfrac{mol}{mol\,rxn}\left(-394\tfrac{kJ}{mol}\right)\right] - \left[1\tfrac{mol}{mol\,rxn}\left(-175\tfrac{kJ}{mol}\right)\right]$$

$$\Delta G^{\circ}_{rxn} = -1475\tfrac{kJ}{mol\,rxn} + 175\,^{kJ}/_{mol\,rxn}$$

$$\boxed{\Delta G^{\ominus}_{rxn} = -1300\,^{kJ}/_{mol\,rxn}}$$

2. A reaction has a standard enthalpy change, ΔH, of +10.00 kJ mol^{-1} at 298 K. The standard entropy change, ΔS, for the same reaction is +10.00 J K^{-1} mol^{-1}. What is the value of ΔG for the reaction in kJ mol^{-1}?

Given:

$\Delta H = +10.00\,kJ/mol$

@ T = 298K

$\Delta S = 10.00\,J/mol\,K$

$\Delta G = ?\,kJ/mol$

Soln: $\Delta G^{\circ} = \Delta H - \Delta TS$

$$= 10.00\tfrac{kJ}{mol} - \left[(298K)\left(\tfrac{10.00\,J}{mol\,K}\right)\left(\tfrac{1\,kJ}{1000\,J}\right)\right]$$

$$= 10.00\tfrac{kJ}{mol} - 2.98\tfrac{kJ}{mol}$$

$$\boxed{\Delta G^{\circ} = 7.02\tfrac{kJ}{mol}}$$

3. The equation for the decomposition of calcium carbonate is given below.

$$CaCO_{3(s)} \rightarrow CaO_{(s)} + CO_{2(g)}$$
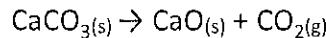
At 500 K, ΔH for this reaction is +177 kJmol^{-1} and ΔS is 161 J K^{-1} mol^{-1}

Given $\Delta H = 177$ KJ/mol $\Delta S = 161 \frac{J}{K \cdot mol}$
@ T = 500K

(a) Explain why ΔH for the reaction above cannot be described as $\Delta H_f^\ominus$

Cannot be ΔH_f° as conditions are not standard and not formation from Elements

(b) State the meaning of the term ΔS.

ΔS means $\rightarrow$ Change in Entropy (degree disorder)

(c) Calculate the value of ΔG at 500 K and determine, giving a reason, whether or not the reaction will be spontaneous.

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

$= 177 \frac{KJ}{mol} - 500K \left(161 \frac{J}{K \cdot mol}\right)\left(\frac{1KJ}{1000J}\right)$

$\Delta G = 177 \frac{KJ}{mol} - 80.5 \frac{KJ}{mol}$

$\Delta G = 97 \frac{KJ}{mol}$

NoN Thermodynamically Favorable due to $\Delta G = +$

4. Consider the following reaction:

$$N_{2(g)} + 3H_{2(g)} \rightleftharpoons 2NH_{3(g)} \quad \Delta H = -92.4 \text{ kJmol}^{-1}$$
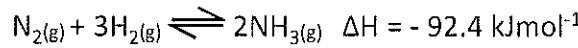
$\Delta S = $ 192 131   193 J/K·mol

4 moles gas $\rightarrow$ 2 moles GAS

(i) The absolute entropy values, S, at 238 K for $N_{2(g)}$, $H_{2(g)}$ and $NH_{3(g)}$ are 192, 131 and 193 J K^{-1} mol^{-1} respectively. Calculate $\Delta S^\ominus$ for the reaction and explain the sign of $\Delta S^\ominus$.

$\Delta S_{rxn} = \Sigma \Delta S_P - \Sigma \Delta S_R$

$= \left[\frac{2mol}{mol_{rxn}}\left(193 J/K \cdot mol\right)\right] - \left[3\frac{mol}{mol_{rxn}}\left(131\frac{J}{K \cdot mol}\right) + \frac{1mol}{mol_{rxn}}\left(192\frac{J}{K \cdot mol}\right)\right] = 386 - 585$

$\boxed{\Delta S_{rxn} = -199 \text{ J/K} \cdot mol}$ 4 moles gas $\rightarrow$ 2 mole gas a decrease in disorder

(ii) Calculate $\Delta G^\ominus$ for the reaction at 238 K. State and explain whether the reaction is spontaneous.

$\therefore -\Delta S$

@ T = 238K

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

$= -92.4 \frac{KJ}{mol} - \left[(238K)\left(\frac{-199J}{K \cdot mol}\right)\left(\frac{1KJ}{1000J}\right)\right]$

fewer molecules of GAS

$= -92.4 - (-47.4)$

$\Delta G = -45 \frac{KJ}{mol}$ Reaction is Thermodynamically Favorable due to $-\Delta G$

WKST – Spontaneity and Gibbs free energy

5. Hex-1-ene gas, C_6H_{12}, burns in oxygen to produce carbon dioxide and water vapour. Assume 25°C

(a) Write an equation to represent this reaction.

$$C_6H_{12\,(g)} + 9O_{2\,(g)} \xrightarrow{\Delta} 6\,CO_{2\,(g)} + 6\,H_2O_{(g)}$$
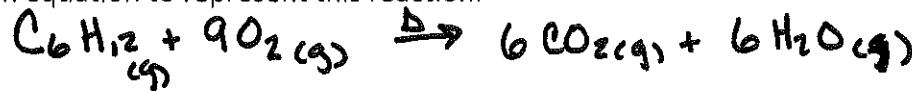
(b) Use the data below to calculate the values of $\Delta H_c^{\ominus}$ and $\Delta S^{\ominus}$ for the combustion of hex-1-ene.

Substance	$O_{2(g)}$	$C_6H_{12(g)}$	$CO_{2(g)}$	$H_2O_{(g)}$
Standard enthalpy of formation, $\Delta H_f^{\ominus}$ (kJmol^{-1})	0.0	−43	−394	−242
Entropy, $S^{\ominus}$ (J K^{-1} mol^{-1})	205	385	214	189

(i) Value of $\Delta H_c^{\ominus}$

$$\Delta H_c = \Sigma H_p - \Sigma H_R$$
$$= \left[6\,\tfrac{mol}{molrxn}\left(-394\,\tfrac{KJ}{mol}\right) + 6\,\tfrac{mol}{mol}\left(-242\,\tfrac{KJ}{mol}\right)\right] - \left[1\,\tfrac{mol}{molrxn}\left(-43\,\tfrac{KJ}{mol}\right) + 0\right]$$
$$= [(-3816)] - [-43]$$
$$\boxed{\Delta H_c = -3773\ \tfrac{KJ}{mol}}$$

(ii) Value of $\Delta S^{\ominus}$

$$\Delta S^{\circ} = \Sigma S_p - \Sigma S_R$$
$$= \left[6\,\tfrac{mol}{molrxn}\left(214\,\tfrac{J}{Kmol}\right) + 6\,\tfrac{mol}{molrxn}\left(189\,\tfrac{J}{Kmol}\right)\right] - \left[1\,\tfrac{mol}{molrxn}\left(385\,\tfrac{J}{Kmol}\right) + 9\,\tfrac{mol}{molrxn}\left(205\,\tfrac{J}{Kmol}\right)\right]$$
$$= +2418 - (2230)$$
$$\boxed{\Delta S^{\circ} = 188\ \tfrac{J}{Kmol}}$$

(c) Calculate the standard free energy change for the combustion of hex-1-ene.

$$\Delta G = \Delta H - T\Delta S$$
$$= -3773\,\tfrac{KJ}{mol} - \left[(298K)\left(\tfrac{188J}{Kmol}\right)\left(\tfrac{1\,KJ}{1000J}\right)\right]$$
$$= -3773 - 56.0$$

$$\boxed{\Delta G = -3829\ \tfrac{KJ}{mol}}$$

(d) State and explain whether or not the combustion of hex-1-ene is spontaneous at 25°C.

The reaction is Thermodynamical Favorable due to $-\Delta G$