Exercise 4.63 – Gibbs free energy calculations

Q463-01 For the reaction:

$3HC{\equiv}CH(g) \longrightarrow C_6H_6(g)$ H = - 597.3 kJ and S = - 0.33 kJ K^{-1}.

This reaction:

A. is spontaneous at 300 K and becomes non-spontaneous at higher temperatures.
B. is spontaneous at 300 K and becomes non-spontaneous at lower temperatures.
C. is non-spontaneous at 300 K and becomes spontaneous at higher temperatures.
D. is non-spontaneous at 300 K and becomes spontaneous at lower temperatures.

Q463-02 For the process:

$C_6H_6(l) \longrightarrow C_6H_6(s)$

$\Delta H^{\ominus}$ = -9.83 $kJmol^{-1}$ and $\Delta S^{\ominus}$ = -35.2 J K^{-1} mol^{-1}.

a) Predict and explain the effect of an increase in temperature of the spontaneity of the process.
b) Calculate the temperature (in ºC) at which $\Delta G = 0$ for the above process and explain the significance of this temperature.

Q463-03 Decomposition of solid barium carbonate is given by the following equation:

$BaCO_3(s) \longrightarrow BaO(s) + CO_2(g)$

compound	$BaCO_3(s)$	$CO_2(g)$	$BaO(s)$
$\Delta Hf^{\ominus}$/$kJmol^{-1}$	-1219	-394	-558
$S^{\ominus}$ /JK^{-1} mol^{-1}	+112	+214	+70

a) Calculate the value of $\Delta G^{\ominus}$ in kJ mol^{-1} at 25ºC
b) State with a reason whether the reaction is spontaneous at 25ºC
c) Determine the minimum temperature above which the reaction is spontaneous.

Q463-04 Methanol can be made from synthesis gas, produced by the reaction:

$CH_4(g) + H_2O(g) \longrightarrow 3H_2(g) + CO(g)$

For this reaction $\Delta H^{\ominus}$ = +210kJ and $\Delta S^{\ominus}$ = 216 JK^{-1}

a) Use these values to explain why this reaction is not spontaneous at 298K.
b) Calculate the temperature at which it becomes spontaneous.

Q463-05 When solid blue copper (II) sulphate pentahydrate $CuSO_4.5H_2O$ loses water, the white solid copper (II) sulphate monohydrate $CuSO_4.H_2O$ is produced as represented by the equation:

$CuSO_4.5H_2O(s) \longrightarrow CuSO_4.H_2O(s) + 4H_2O(g)$

The thermodynamic data for the substances involved in the reversible process are:

	$\Delta H^{\ominus}f$ / $kJmol^{-1}$	$S^{\ominus}$ / J K^{-1} mol^{-1}
$CuSO_4.5H_2O$ (s)	-2278	305
$CuSO_4.H_2O$ (s)	-1084	150
H_2O (g)	-242	189

a) Calculate the value of $\Delta H^{\ominus}$ for the reaction above and state what information the sign of $\Delta H^{\ominus}$ provides about this reaction.
b) Calculate $\Delta S^{\ominus}$ for the reaction and state the meaning of the sign of $\Delta S^{\ominus}$ obtained.
c) Identify a thermodynamic function that can be used to predict the reaction spontaneity and state its units.
d) Use the values obtained in the above to determine whether the reaction is spontaneous or non-spontaneous at 25ºC.

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Q463-06 Using the answers in question 7 above:
a) identify which compound $CuSO_4.5H_2O(s)$, or $CuSO_4.H_2O$ (s) is more stable at 25ºC
b) Use the values obtained in question 7 to determine the centigrade temperature above which the other compound is more stable.

Q463-07 Consider the following reaction:

$$N_2(g) + 3H_2(g) \longrightarrow 2NH_3(g)$$

a) Using average bond enthalpies values below, calculate the standard enthalpy change for this reaction.
Bond enthalpies (kJ mol^{-1}) : N≡N, 942; H-H, 432; N-H, 386.
The absolute entropy values, S, at 300K for $N_2(g)$, $H_2(g)$ and $NH_3(g)$ are 193, 131 and 192 JK^{-1} mol^{-1} respectively.
b) Calculate $\Delta S^{\ominus}$ for the reaction and explain the sign of $\Delta S^{\ominus}$
c) Calculate $\Delta G^{\ominus}$ for the reaction at 300K.

Q463-08 The enthalpy change for the combustion of butanoic acid at 25ºC is - 2183.5 kJ mol^{-1}. The combustion reaction is:

$$C_3H_7COOH(l) + 5O_2(g) \longrightarrow 4CO_2(g) + 4H_2O(l)$$

a) Write the balanced equation for the formation of butanoic acid from its elements.
b) Using the data below, calculate the standard enthalpy of formation, $H^{\ominus}f$, for butanoic acid.

Substance	Standard Enthalpy of Formation, $H^{\ominus}f$ / kJ mol^{-1}	Absolute Entropy, S, / J mol^{-1} K^{-1}
C(s)	0	5.7
$CO_2(g)$	-393.5	213.6
H2(g)	0	130.6
$H_2O(l)$	-285.9	60.9
$O_2(g)$	0	205.0
$C_3H_7COOH(l)$		226.3

c) Calculate the standard entropy change, $S^{\ominus}f$, for the formation of butanoic acid at 25ºC
d) Calculate the standard free energy of formation, $G^{\ominus}f$, for butanoic acid at 25ºC
e) Is this reaction spontaneous at 25ºC? Explain your answer

Q463-09 Consider the following reaction:

$$N_2(g) + 3H_2(g) \longrightarrow 2NH_3(g)$$

The enthalpy change, $\Delta H^{\ominus}$ for this reaction = -92 kJ. The magnitude of the entropy change ΔS, at 27ºC for the reaction is -202 J K^{-1} mol^{-1}. Calculate ΔG for this reaction at 27ºC and determine whether this reaction is spontaneous at this temperature.

Q463-10 The equation for the decomposition of calcium carbonate is given below:

$$CaCO_3(s) \longrightarrow CaO(s) + CO_2(g)$$

At 500K, ΔH for this reaction is +177 kJ mol^{-1} and ΔS is 161 JK^{-1} mol^{-1}. Calculate the value of ΔG at 500K and determine, giving a reason, whether or not the reaction is spontaneous.
