

(FORMATIVE) WRITTEN TEST n°1 – CHEMISTRY 2 (1h30)

The 2 exercises can be treated independently. No documents allowed. Any type of calculator allowed.

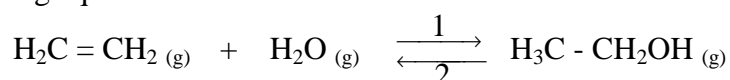
All answers must be justified.

All gases may be considered as ideal.

For numerical applications, take : $R = 8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$; $1 \text{ atm} = 1.013 \text{ bar} = 101325 \text{ Pa}$; $T_0 = 0^\circ\text{C} = 273\text{K}$

Exercise I – Chemical equilibria – Industrial synthesis of ethanol (12 points)

Ethanol may be prepared by hydration of ethylene (C_2H_4) in the gaseous phase, at a temperature of 300°C (573K) under a pressure of 70 bars, in presence of a catalyst (to speed up the reaction) according to the following equilibrium:


A. Study of the equilibrium state

- 1- Calculate the molar standard enthalpy change, entropy change and free enthalpy change at 298K for the reaction taken in the forward direction (1).
- 2- Calculate the equilibrium constant of the reaction at 300°C (573K) neglecting the impact of the heat capacities.
- 3- Actually, if we take into account the heat capacities of the reagent, one would find $K_{573}^0 = 3.4 \cdot 10^{-3}$ (*use this value to solve the rest of the exercise*). Is it reasonable, in this case, to neglect the impact of the heat capacities?
- 4- Predict for this reaction, the impact of changing
 - Temperature while keeping P constant,
 - Pressure while keeping T constant.

Comment on the experimental conditions applied in industry.

B. Equilibrium state. Change of the equilibrium.

The reaction is performed at 300°C (573K) under 70 bars, from a mixture made of 2 moles of water and 2 moles of ethylene.

- 1- Determine the variance of the system in these conditions. Show that its value is in agreement with a set of equations that link together all the intensive parameters needed to define the system.

- 2- The molar advancement, noted ξ , is defined by the following equation: $\xi = \left| \frac{n_i - n_{i0}}{\nu_i} \right|$

n_i is the number of mole of a reactant or a product i for the molar advancement ξ ,

n_{i0} is the initial number of mole of a reactant or a product i for the molar advancement ξ ,

ν_i is the stoichiometric coefficient of a reactant or a product i according to the equation.

Calculate the value of the molar advancement of the reaction at equilibrium (ξ_e).

- 3- Express literally the yield in ethanol for the given reaction, as a function of ξ_e . Calculate its value in the given conditions (300°C , 70 bars).

- 4- **To the mixture at equilibrium obtained in the previous questions**, we add 1 mole of water, at constant T and pressure (300°C , 70 bars).

Give the table of advancement (or ICE table) and calculate the quotient of the reaction *after addition of water but before further evolution*. In which direction will evolve the chemical system? (no further computation is requested at this stage)

Data:

C : $12 \text{ g}\cdot\text{mol}^{-1}$

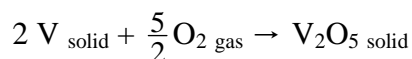
H : $1.0 \text{ g}\cdot\text{mol}^{-1}$

O : $16 \text{ g}\cdot\text{mol}^{-1}$

	$\Delta_f \bar{H}_{298}^0$ ($\text{kJ}\cdot\text{mol}^{-1}$)	\bar{S}_{298}^0 ($\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$)
Ethanol : $\text{CH}_3\text{CH}_2\text{OH}$ (g)	- 235.1	282.7
H_2O (g)	- 241.4	188.8
Ethylene : C_2H_4 (g)	52.3	219.5

Exercise II – Thermochemistry – Dry oxidation of Vanadium (8 points)

Vanadium (V) is extremely explosive and when it is as a powder, it burns easily in air according to the reaction:



- 1) Calculate the standard molar enthalpy change of the reaction at 298 K.
- 2) Calculate the standard molar internal energy change of the reaction at 298 K.

In an experiment, an operator uses a calorimeter which **volume is constant**. The initial temperature is 298 K and the initial pressure is set at 2 bars. The reaction is ignited and it is supposed that the reaction is fast and total.

- 3) Calculate **the final temperature** if initially the operator uses 0.2 mole of vanadium and 0.4 mole of O₂ supplied by air (reminder: air is supposed to be made of 80 % of N₂ and 20 % of O₂ in volume). The calorimeter is supposed to be perfectly adiabatic in this question (thermally isolated). Set a table of advancement (or ICE table).
- 4) Calculate the final temperature and the final pressure if initially the operator uses 0.2 mole of vanadium and 0.4 mole of O₂ supplied by air, taking into account that the heat capacity of the calorimeter is 836 J.K⁻¹.

Data:

	V solid	V ₂ O ₅ solid	O ₂	N ₂
$\Delta_f H^\circ_{298} \text{ (kJ.mol}^{-1}\text{)}$	0	-1255	0	0
$C_v^\circ \text{ (J.K}^{-1}\text{.mol}^{-1}\text{)}$	26.3	122.0	20.8	20.1