

MENG 22100, Spring 2020

Homework Assignment 2

(Due 4/24/2020)

HW 2-1 What is activation energy? Describe two experimental methods that can be used to estimate it.

HW 2-2 Using expressions established by the collision theory, calculate the mean time between collisions experienced by an argon atom, diameter 0.29 nm, in (a) 200 kPa and (b) 200 Pa of argon gas at 298 K.

HW 2-3 Calculate the number of collisions per cubic centimeter per second between molecules A and B for a mixture containing 10 kPa of each at 300 K. The molecular diameters of A and B are 0.3 and 0.4 nm, and their atomic masses are 2 and 32 amu, respectively. Given that the experimental rate constant for the reaction is $1.07 \times 10^{-5} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K, and that the activation energy is 40 kJ mol^{-1} , (a) calculate the fraction of the collisions that result in a reaction and (b) determine the steric factor of the reaction. (Steric factor is defined as the ratio between the experimental frequency factor and that predicted by the collision theory.)

HW 2-4 For the reaction between atomic fluorine and molecular hydrogen at 300 K:



calculate the rate constant using collision theory and Polanyi equation. Additional useful information is provided as follows.

Reactants

Effective molecular diameter for H_2 : 2.5 Å

Effective atomic diameter for F: 1.7 Å

F: 19 amu

H_2 : 2 amu

Transition State for Reaction $\text{Br} + \text{H}_2 \rightarrow \text{HBr} + \text{H}$

$E_a = 552 \text{ kJ/mol}$

Linear configuration: $\text{Br} \cdots \text{H} \cdots \text{H}$

Distances: $\text{Br} \cdots \text{H}$ 1.62 Å; $\text{H} \cdots \text{H}$ 0.78 Å

Bond length for H_2 : 0.74 Å

Bond length for HBr: 1.41 Å

Heats of Formation

HF: -272.55 kJ/mol

HBr: -36.44 kJ/mol

H: 218 kJ/mol

F: 79.39 kJ/mol

Br: 111.9 kJ/mol

H_2 : 0 kJ/mol

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