[물리화학2] Homework 4

1. A bimolecular elementary reaction in gas phase is

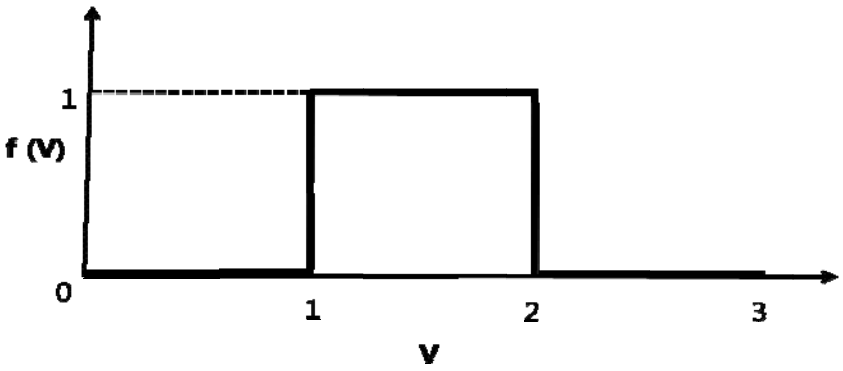
$$A + B \xrightarrow{k_2} P$$

The rate of reaction is described as:

$$k_2 = N_A \int_0^\infty \sigma(\varepsilon) v_{rel} f(\varepsilon) d\varepsilon$$

(1) Express σ(ε) in terms of σ (collision cross-section) and ε_a (threshold kinetic energy)

(2) Derive k_2 when the distribution of molecular speeds is given as:



2. For the gas-phase reaction A+A → A_2 , the experimental rate constant, k_2 , has been fitted to the Arrehenius equation with the pre-exponential factor A = 4.07 × 10^5 $dm^3mol^{-1}s^{-1}$ at 300 K and an activation energy of 65.43 $kJmol^{-1}$. Calculate Δ^{+}S, Δ^{+}H, and Δ^{+}U for the reaction.

3. Derive the Eyring equation $\left(k_2 K \frac{kT}{h} \overline{K_c^{\ddagger}} \right)$ in activated complex theory.

$$\boxed{A + B \leftrightarrow C^{\ddagger} \rightarrow P}$$

$V = k^{\ddagger}[C^{\ddagger}]$, $v = k_2[A][B]$

4. Derive material balance equation $\frac{\partial[J]}{\partial t} = D\frac{\partial^2[J]}{\partial x^2} - v\frac{\partial[J]}{\partial x} - k[J]$ under pseudo 1st order reaction and forced convection velocity v.

5. The rate constant for the dissociation of ethane is given by k = 5 × 10^{16} $e^{-368kJ/RT}$ between 823 and 893 K, where Ea = -368 kJ. Calculate the enthalphy and the entropy of activation for this reaction at 850 K.

$$\boxed{C_2H_6 \leftrightarrow (CH_3 - CH_3)^{\ddagger} \rightarrow 2CH_3}$$