平成 28 年度　反応の化学b　期末試験問題

以下の問に答えよ。問題文は英語でも、解答の文章は日本語で良い。
数値は 3 桁まで求めよ。

問 1.　Calculating ΔG_{rxn} under Nonstandard Conditions

Consider the following reaction at 298 K:

$$2\,NO\,(g) + O_2(g) \longrightarrow 2\,NO_2(g) \quad \Delta G^\circ_{rxn} = -71.2\,kJ$$

Compute ΔG_{rxn} under the following conditions:

$$P_{NO} = 0.200\ atm;\ P_{O_2} = 0.400\ atm;\ P_{NO_2} = 8.00\ atm$$

Is the reaction more or less spontaneous under these conditions than under standard conditions?

気体定数 $R = 8.31\ J\ mol^{-1}\ K^{-1}$.

問 2.　Finding Equilibrium Concentrations from Initial Concentrations in Cases with a Small Equilibrium Constant

Consider the following reaction for the decomposition of hydrogen disulfide:

$$2\,H_2S(g) \rightleftharpoons 2\,H_2(g) + S_2(g)$$

$$K_c = 1.67 \times 10^{-7} \text{ at } 800\,^\circ C$$

A 0.500-L reaction vessel initially contains 0.0125 mol of H_2S at 800 °C. Find the equilibrium concentrations of H_2 and S_2.

注） decomposition ; 分解, sulfide ; 硫化物, vessel 容器

問 3.

Using the Two-Point Form of the Arrhenius Equation

The reaction between nitrogen dioxide and carbon monoxide is given by the following equation:

$$NO_2(g) + CO(g) \longrightarrow NO(g) + CO_2(g)$$

The rate constant at 701 K was measured as 2.57 $M^{-1} \cdot s^{-1}$ and that at 895 K was measured as 567 $M^{-1} \cdot s^{-1}$. Find the activation energy for the reaction in kJ/mol.

気体定数　$R = 8.31\ J\ K^{-1}\ mol^{-1}$

問 4.

Consider the following gas-phase reaction:

$$H_2(g) + I_2(g) \longrightarrow 2\,HI(g)$$

The reaction was experimentally determined to be first order in H_2 and first order in I_2. Consider the following proposed mechanisms.

Proposed mechanism I:

$H_2(g) + I_2(g) \longrightarrow 2\,HI(g)$　　Single step

Proposed mechanism II:

$I_2(g) \underset{k_2}{\overset{k_1}{\rightleftharpoons}} 2\,I(g)$　　Fast

$H_2(g) + 2\,I(g) \xrightarrow[k_3]{} 2\,HI(g)$　　Slow

Proposed mechanism III:

$I_2(g) \underset{k_2}{\overset{k_1}{\rightleftharpoons}} 2\,I(g)$　　Fast

$H_2(g) + I(g) \underset{k_4}{\overset{k_3}{\rightleftharpoons}} H_2I(g)$　　Fast

$H_2I(g) + I(g) \xrightarrow[k_5]{} 2\,HI(g)$　　Slow

問. Proposed mechanism II, III のいずれにおいても、rate law が

$$\text{Rate} = k[I_2][H_2]$$

と、Proposed mechanism I と同じになることを示しなさい。