"Recitation"   CHMG 142   Group names:________________________

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R=0.082058 $\frac{L\ atm}{mol\ K}$ $\ln\left(\frac{k_2}{k_1}\right) = -\frac{E_a}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$

R=8.314 $\frac{J}{mol\ K}$ $k = Ae^{-\frac{E_a}{RT}}$

The following data was collected for the reaction of nitrogen gas and chlorine gas to form nitrogen trichloride gas.

Experiment	Initial Nitrogen (atm)	Initial Chlorine (atm)	Initial Rate (atm/min)	Temp (K)
1	0.250	0.250	0.012	300 K
2	0.500	0.500	0.047	300 K
3	0.500	0.250	0.011	300 K
4	0.250	0.500	0.072	500 K

Piece #1 (1/2 pt) Compare experiment 2 to experiment 3. What is the order of the reaction with respect to chlorine?

Doubling chlorine caused the rate to quadruple. 2nd order.

Piece #2 (1/2 pt) Compare experiment 1 to experiment 3. What is the order of the reaction with respect to nitrogen?

Doubling nitrogen caused essentially no change in the rate. 0th order.

Piece #3 (1/2 pt) Use the orders determined in Piece #1 and Piece #2 to construct a general rate law for the reaction.

$$Rate = k[Cl_2]^2$$

Piece #4 (1/2 pt) Use the rate law from Piece #3 and the data from Experiments 1, 2, and 3 to calculate the rate constant (k) for each of the experiments. Determine the average k from all of the data at 300 K.

$$Rate = k[Cl_2]^2$$
$$0.012\ atm/min = k_1[0.250\ atm]^2$$
$$k_1 = 0.192\frac{1}{atm\ min}$$
$$0.047\ atm/min = k_2[0.50\ atm]^2$$
$$k_2 = 0.188\frac{1}{atm\ min}$$
$$0.011\ atm/min = k_3[0.250\ atm]^2$$
$$k_3 = 0.176\frac{1}{atm\ min}$$

$$k_{avg} = 0.185\frac{1}{atm\ min}\ at\ 300\ K$$

Piece #5 (1/2 pt) Use the rate law from Piece #3 and the date from Experiment 4 to calculate the rate constant for the reaction at 500 K

$$.072\ atm/min = k_4[0.50\ atm]^2$$
$$k_4 = 0.288\frac{1}{atm\ min}\ at\ 500\ K$$

Piece #6 (1/2 pt) Use the two-point Arrhenius expression and the rate constants from Piece #4 and Piece #5 to calculate the activation energy (E_a) for the reaction.

$$\ln\left(\frac{k_2}{k_1}\right) = -\frac{E_a}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

$$\ln\left(\frac{0.288}{0.185}\right) = -\frac{E_a}{8.314\frac{J}{mol\ K}}\left(\frac{1}{500\ K} - \frac{1}{300\ K}\right)$$

$$0.4426 = -\frac{E_a}{8.314\frac{J}{mol\ K}}(-1.333 \times 10^{-3} K^{-1})$$

$$E_a = 2760\frac{J}{mol}$$

Piece #7 (1/2 pt) Use the average rate constant at 300 K from Piece #4 and the activation energy from Piece #6 to calculate the Arrhenius factor (collision frequency factor) in the Arrhenius equation.

$$k = Ae^{-\frac{E_a}{RT}}$$

$$0.185 = Ae^{-\frac{2760}{(8.314)(300\ K}}$$

$$0.185 = A(0.3307)$$

$$A = 0.559\ min^{-1}$$

Piece #8 (1/2 pt) Use the two-point Arrhenius equation to calculate the rate constant at 400 K.

$$\ln\left(\frac{k_2}{k_1}\right) = -\frac{E_a}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

$$\ln\left(\frac{0.288}{k_{400}}\right) = -\frac{2760\frac{J}{mol}}{8.314\frac{J}{mol\ K}}\left(\frac{1}{500\ K} - \frac{1}{400\ K}\right)$$

$$\ln\left(\frac{0.288}{k_{400}}\right) = -\frac{2760\frac{J}{mol}}{8.314\frac{J}{mol\ K}}(-5 \times 10^{-4} K^{-1}) = 0.16598$$

$$e^{\ln\left(\frac{0.288}{k_{400}}\right)} = e^{0.16598}$$

$$\left(\frac{0.288}{k_{400}}\right) = 1.18$$

$$k_{400} = 0.244\ min^{-1}$$

Puzzle #1 (1 pt) 0.666 atm of nitrogen gas and 0.333 atm of chlorine gas are put in a 2 L flask at 400 K. What is the initial rate of the reaction?

$$Rate = k[Cl_2]^2$$

$$Rate = (0.244\ min^{-1})[0.333\ atm]^2$$
$$Rate = 0.0271\frac{atm}{min}$$

Bonus Question (1 pt) What is the rate of the reaction from Puzzle #1 after 1 hour?

It's a second order rate law, so the integrated rate law is:

$$\frac{1}{[Cl_2]} = kt + \frac{1}{[Cl_2]_0}$$

1 hour is 60 minutes. The chlorine concentration after 1 hour is:

$$\frac{1}{[Cl_2]} = (0.244)(60\ \mathrm{min}\quad) + \frac{1}{0.333\ atm} = 17.643$$

$$[Cl_2] = 0.0567\ atm$$

$$Rate = (0.244\ min^{-1})[0.0567\ atm]^2$$
$$Rate = 7.84 \times 10^{-4}\frac{atm}{min}$$