Kinetics Worksheet

Although kinetics problems may seem complicated, all of the information to solve them comes from concentration-time plots: start a reaction, start the stopwatch, and then monitor how the products and reactant concentrations (molarity) change over time. You collect a set of x-y data pairs at increasing time.

Listed below are three sets of concentration-time data collected at two different temperatures for each reaction

$$C \rightarrow D$$

Note here that the coefficient for C is 1 in all calculations. (In cC, the c=1).

This is all the kinetic data you need to be able to calculate:
   The instantaneous rate at any time: $\Delta C/\Delta t$
   The reaction order (use both method of initial rates and curve fitting): x
   rate constant at each temperature: k_1, k_2
   half life at each temperature: $t_{1/2}$
   initial concentration at each temperature: $[C_0]$
   activation energy: E_a
   pre-exponential factor: A

On other words, you can assign all the bolded constants to the following rate law:

$$-\Delta C/\Delta t = rate = k[C]^x = A \exp(-E_a/RT) [C]^x$$

To give you plenty of practice, the data have been obtained for three reactions each of which has a different order. The concentration-time data for each set of reactions is shown below:

Problem set 1.
Find rates, C_0, k, $t_{1/2}$, A, E_a and reaction order at each temperature.

Data at 300K			Data at 310K		
time (s)	[C]		time (s)	[C]	
0	Unknown C_0		0	Unknown C_0	
1	.12		1	.074	
2	.074		2	.027	
3	.044		3	.009	
4	.027		4	.0036	
5	.016		5	.0013	
6	.009		6	5.0×10^{-4}	
8	.0036		8	6.7×10^{-5}	
10	.0013		10	9.1×10^{-6}	

Problem set 2.
Find rates, C_0, k, $t_{1/2}$, A, E_a and reaction order at each temperature.

Data at 300K			Data at 313K		
time (s)	[C]		time (s)	[C]	
0	**Unknown C_0**		0	**Unknown C_0**	
1	.182		1	.166	
2	.166		2	.142	
3	.153		3	.125	
4	.142		4	.111	
5	.133		5	.1	
6	.125		6	.09	
8	.111		8	.076	
10	.1		10	.066	

Problem set 3.
Find rates, C_0, k, $t_{1/2}$, A, E_a and reaction order at each temperature.

Data at 300K			Data at 305K		
time (s)	[C]		time (s)	[C]	
0	**Unknown C_0**		0	**Unknown C_0**	
.05	.1875		.05	.175	
.1	.175		.1	.15	
.15	.1625		.15	.125	
.2	.15		.2	.1	
.25	.1375		.25	.075	
.3	.125		.3	.05	
.35	.1125		.35	.025	
.4	1		.4	0	

Problem set 2 solutions.
Find rates, C_0, k, $t_{1/2}$, A, E_a and reaction order at each temperature.

Data at 300K			Data at 313K		
time (s)	[C]	1/[C]	time (s)	[C]	1/[C]
0	**Unknown C_0**		0	**Unknown C_0**	
1	.182	5.5	1	.166	6
2	.166	6	2	.142	7
3	.153	6.5	3	.125	8
4	.142	7	4	.111	9
5	.133	7.5	5	.1	10
6	.125	8	6	.09	11
8	.111	9	8	.076	13
10	.1	10	10	.066	15

Calculate **order** from method of initial rates (see handout on order of reaction) or from functional relationships of integrated rate law. Notice in this case that the 1/[C] result in the data table above is a straight line, indicating that this reaction is order $x = 2$ in [C]. So rate = k $[C]^2$.

Solve for rate constant, **k**, and initial concentration, C_0, directly knowing the order, using integrated rate law:
$1/[C] = kt + 1/[C_0]$ so slope = k and y intercept = $1/[C_0]$

At **300K** curve fit yields y = 0.5 x + 5   At **313 K** curve fit yields y = 1.0 x + 5
k = 0.5 $M^{-1}sec^{-1}$ and $1/[C_0] = 5$, **$[C_0] = 0.2$ M**   **k = 1.0 $M^{-1}sec^{-1}$** and $1/[C_0] = 5$, **$[C_0] = 0.2$ M**

Solve for half life, $t_{1/2}$, for second order reaction: $t_{1/2} = 1/k[A_0]$ and for 0.2 M
At **300 K, $t_{1/2}$** = 1/((.2)(.5)) = **10 sec**   at **313K, $t_{1/2}$** = 1/((.2)(1)) = **5 sec**

Solve for activation energy, **Ea** using the combined Arrhenius equation :
          ln $(k_2/k_1) = (Ea/R)(1/T_1 - 1/T_2)$ so   ln(1.0/0.5) = **(Ea**/8.3)(1/300 - 1/313)
          and substituting, **Ea** = 41,600 J or **41.6 kJ**

Solve for pre-exponential term, **A**: k = Aexp(-Ea/RT) so   0.5 = Aexp(-41,600/8.3*300)
          Rearrange and solve for **A = 8.7 x 10^6**

Problem set 3 solutions.
Find rates, C_0, k, $t_{1/2}$, A, E_a and reaction order at each temperature.

Data at 300K			Data at 305K		
time (s)	[C]		time (s)	[C]	
0	**Unknown C_0**		0	**Unknown C_0**	
.05	.1875		.05	.175	
.1	.175		.1	.15	
.15	.1625		.15	.125	
.2	.15		.2	.1	
.25	.1375		.25	.075	
.3	.125		.3	.05	
.35	.1125		.35	.025	
.4	.1		.4	0	

Calculate **order** from method of initial rates (see handout on order of reaction) or from functional relationships of integrated rate law. Notice in this case that the[C] result in the data table above is already a straight line, indicating that this reaction is order x = 0 in [C]. So rate = k.

Solve for rate constant, **k**, and initial concentration, C_0, directly knowing the order, using integrated rate law: $C = -kt + C_0$
so slope = -k and y intercept = C_0

At **300K** curve fit yields y = - 0.25 x -.2   At **305 K** curve fit yields y = - .5 x - .2
k = 0.25 Msec^{-1} and [C$_0$] = 0.2 M   k = 0.5 Msec^{-1} and [C$_0$] = 0.2 M

Solve for half life, $t_{1/2}$, for first order reaction: $t_{1/2} = C_0/2k$
At **300 K**, **$t_{1/2}$ = 0.2/((2)(0.25)) = 0.4 sec   at 310K, $t_{1/2}$ = 0.2/((2)(.5))= 0.2 sec**

Solve for activation energy, **Ea** using the combined Arrhenius equation :
          ln (k_2/k_1) = (**Ea**/R)(1/T$_1$ - 1/T$_2$)   so   ln(.5/.25) = (**Ea**/8.3)(1/300 - 1/305)
          and substituting, **Ea** = 105,400 J or **105.4 kJ**
Solve for pre-exponential term, **A**: k = Aexp(-Ea/RT) so   0.5 = Aexp(-105,400/8.3*300)
          Rearrange and solve for **A = 1.1 x 10^9**