

Chapter 3: Rate Laws

Excel Tutorial on Fitting logarithmic data

Example 3-1 Determination of the Activation Energy

The following table shows the raw data which you need to fit to an equation using excel

k (s⁻¹)	T (K)
0.00043	312.5
0.00103	318.47
0.0018	322.58
0.00355	327.87
0.00717	333.33


The equation is given as

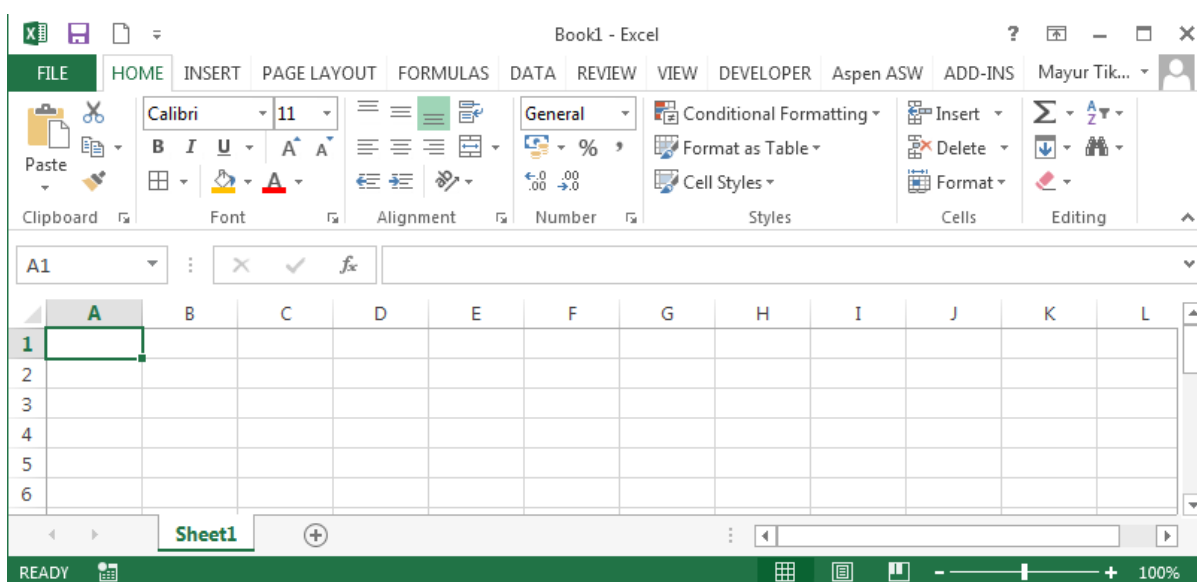
$$k = Ae^{-\frac{E}{R}\left(\frac{1}{T}\right)}$$

To find the parameter A & (E/R) , we can make the above equation linear by taking logarithm on both side,

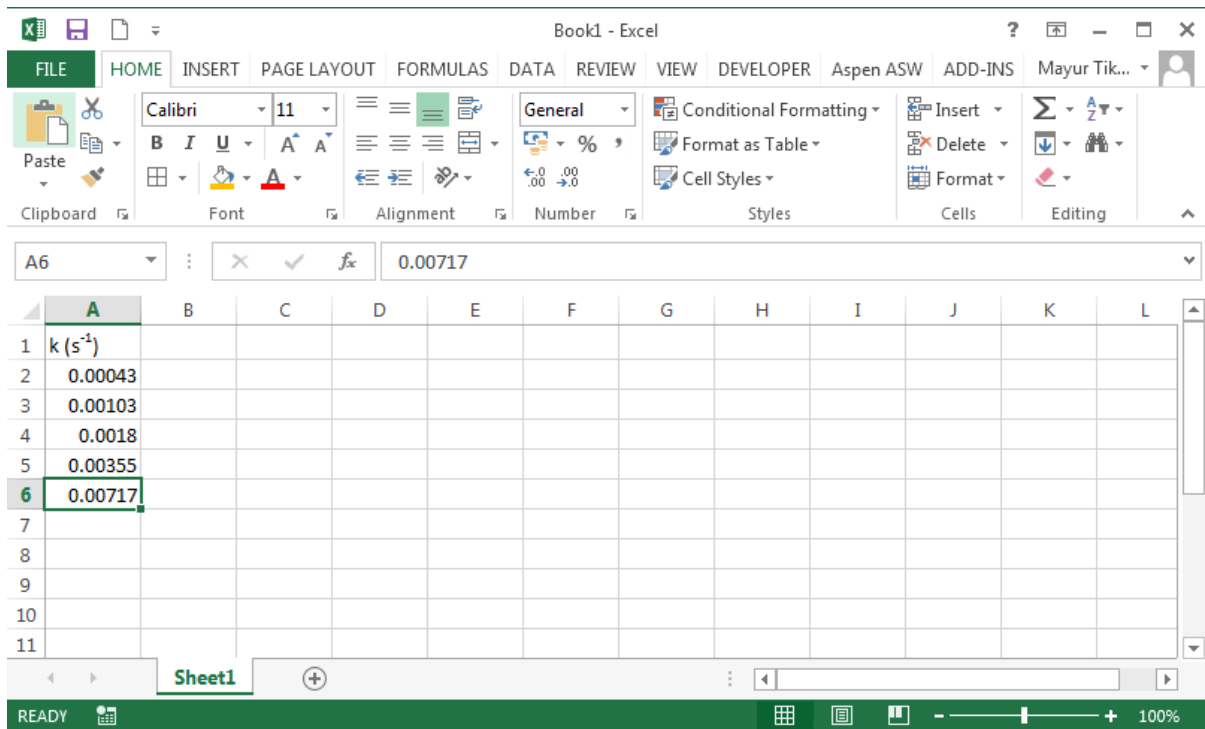
$$\ln(k) = \ln A - \frac{E}{R}\left(\frac{1}{T}\right)$$

So, a graph of $\ln(k)$ vs $1/T$ should yield a straight line with slope as $-E/R$ and intercept as $\ln A$

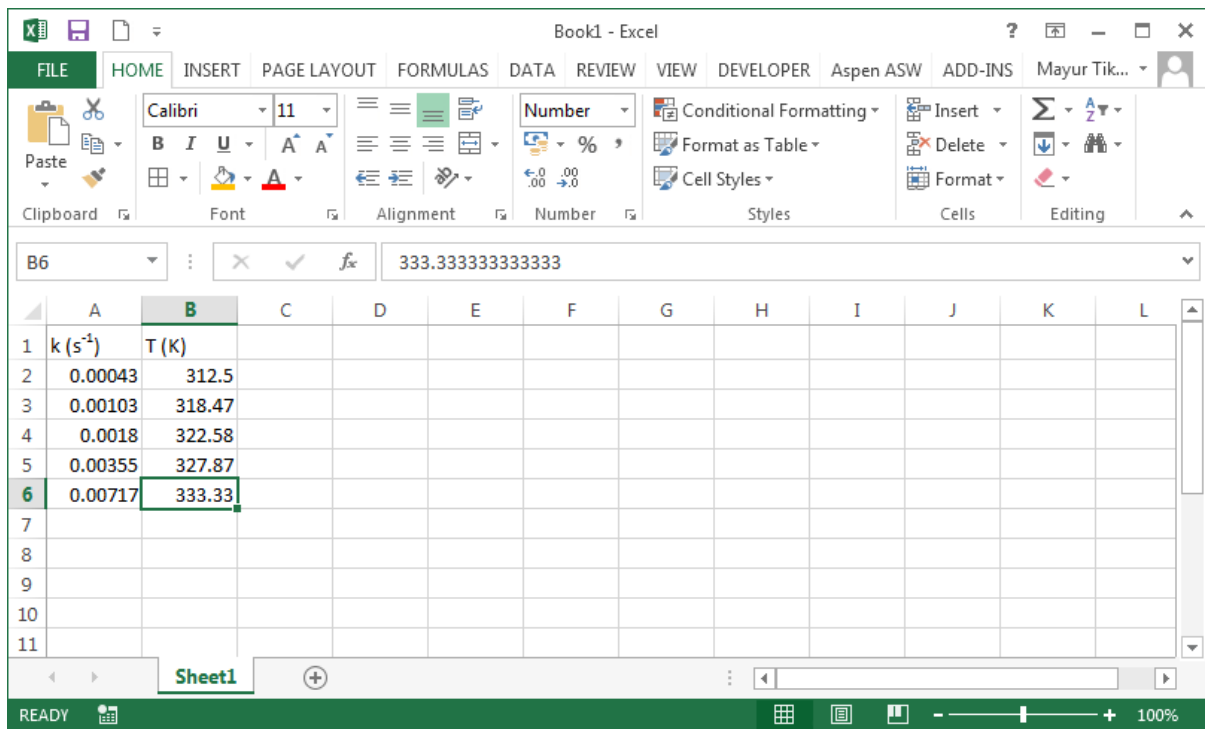
1. First, to launch Excel, choose Start, type Excel in the “Search programs and files box”. You should find Excel with icon . Click on this icon to get a blank worksheet (as shown in screenshot). If you don't have excel on your computer, then download it from Microsoft office website <https://office.microsoft.com/excel>



First enter the name of the variable in the spreadsheet. To do this, select Cell A1 and enter the variable name i.e. k (s^{-1}). Now, enter the values of k in subsequent rows starting from A2 cell to A6 cell as shown below

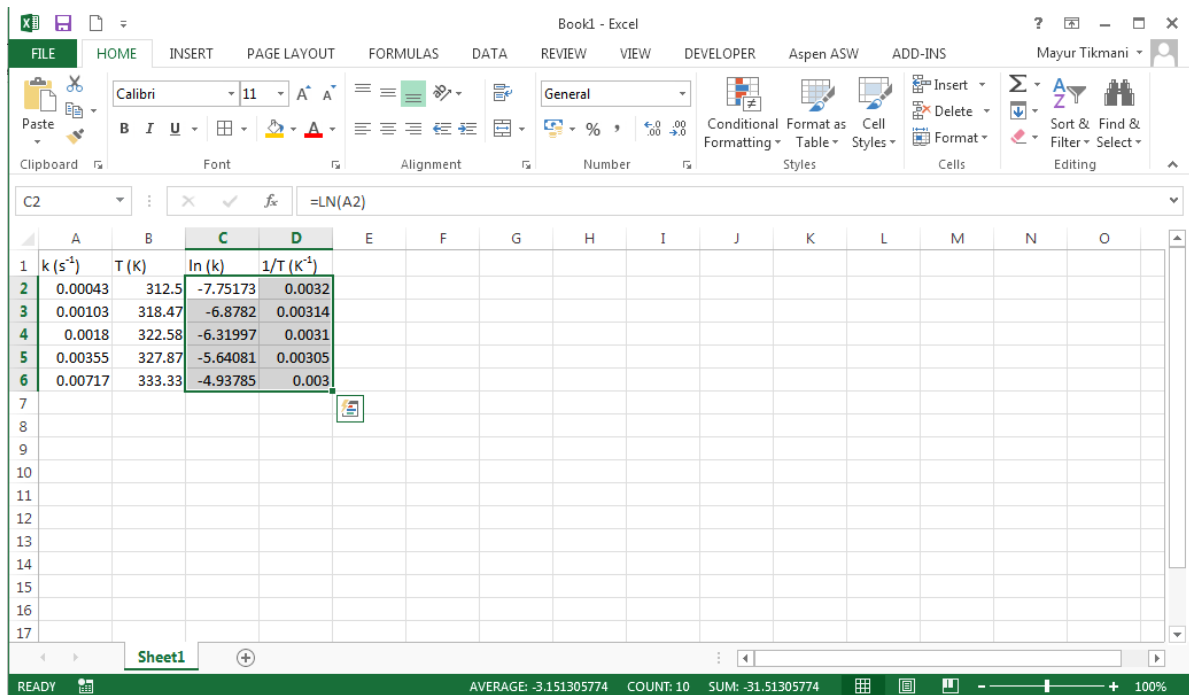




Repeat the above procedure to enter the name and values of T (K). After entering the values, your spreadsheet would look like this

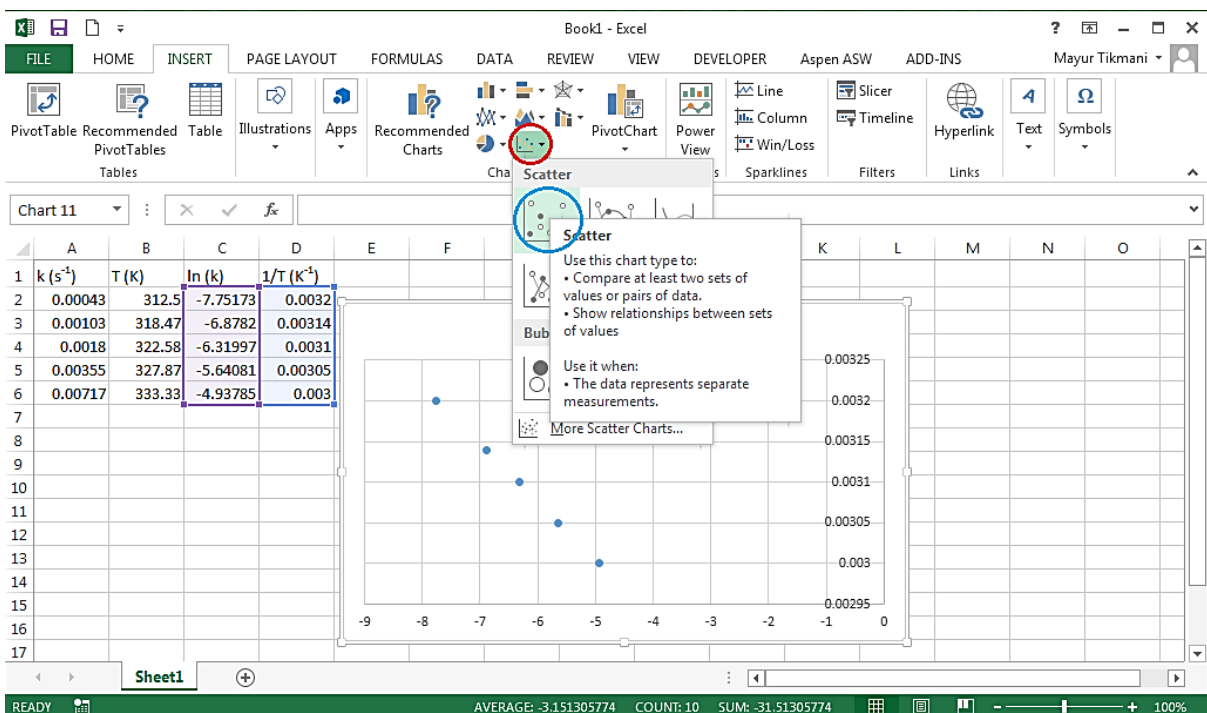


We will show how to use linear scale or logarithmic scale to find the parameters

Next, to graph the data, first select the relevant data. We want to plot $\ln(k)$ vs $1/T$. So, select the data in columns C (cell C2: C6) and D (cell D2:D6). The selected data will have an outside box covering all the data points as shown



Now, go to the Insert tab on the toolbar and under Chart menu, you will find different options for plotting your graph such as Area chart, Bar chart, column chart, pivot chart, scatter and bubble chart etc. We want to do scatter plot, so click on “scatter or bubble chart” button () shown by red circle in below screenshot. This will bring up the various chart options such as scatter, scatter with smooth lines, bubble etc which can be used to create the type of chart that you like. In this case select "scatter" which is the first () of the five options that appear (shown by blue circle in screenshot). The below spreadsheet shows the location of Scatter chart.



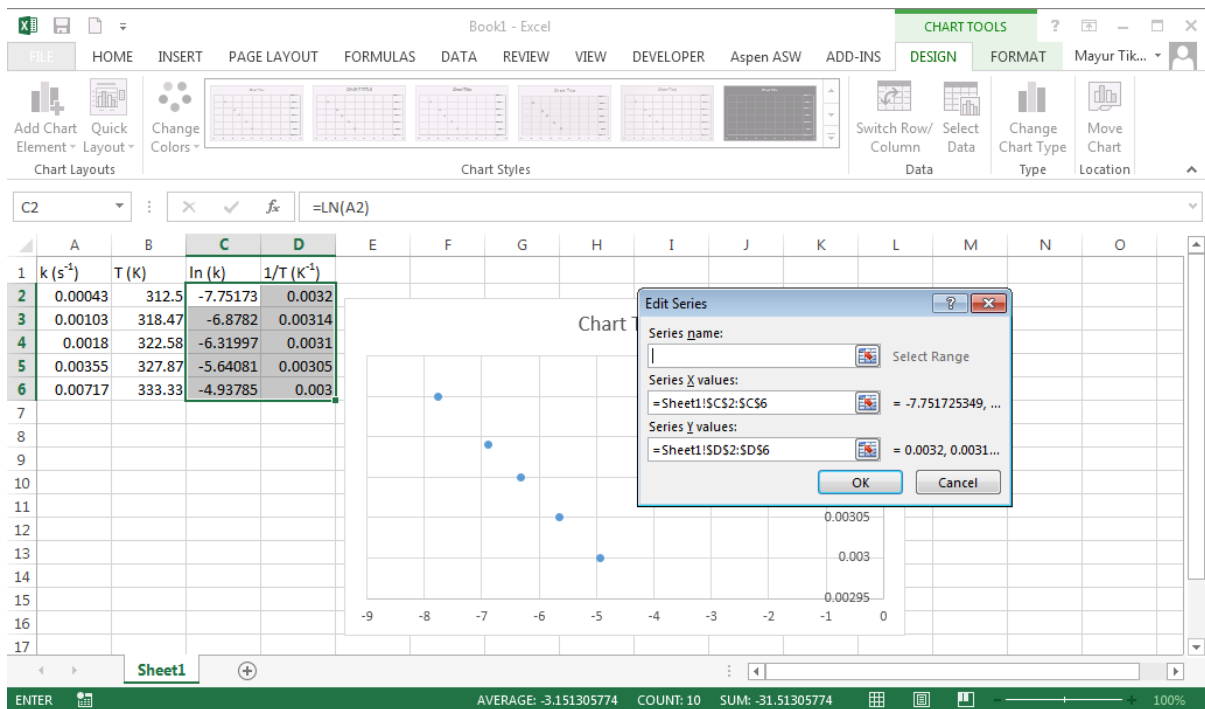
This plots $\ln(k)$ on X axis and $1/T$ on Y axis. However, we want $1/T$ on X axis and $\ln(k)$ on Y axis.

To switch X and Y axis, right click on the graph anywhere and among the list of options, select “Select Data...”. A dialog box will appear on the screen. The “Chart data range” shows the location of your selected data. In this case, you have selected Cell C2: C6 and Cell D2:D6 from sheet 1. So complete data set is represented as Sheet1! \$C\$2:\$D\$6. Using the dollar sign (\$) before the row and column coordinates makes an absolute cell reference that won’t change. Without the \$ sign, the reference is relative and will change. So, in our case, with \$ sign, Chart data range will always refer to cell C2: D6

The screenshot shows the 'Select Data Source' dialog box in Microsoft Excel. The dialog box is open over a chart area, and the 'Chart data range' is set to '=Sheet1!\$C\$2:\$D\$6'. The 'Switch Row/Column' button is highlighted. The 'Horizontal (Category) Axis Labels' list contains values: -7.751725349, -6.878196477, -6.319968614, -5.640807675, and -4.937849624. The background spreadsheet shows columns for k (s^{-1}), T (K), $\ln(k)$, and $1/T$ (K^{-1}) with data points for rows 2 through 6.

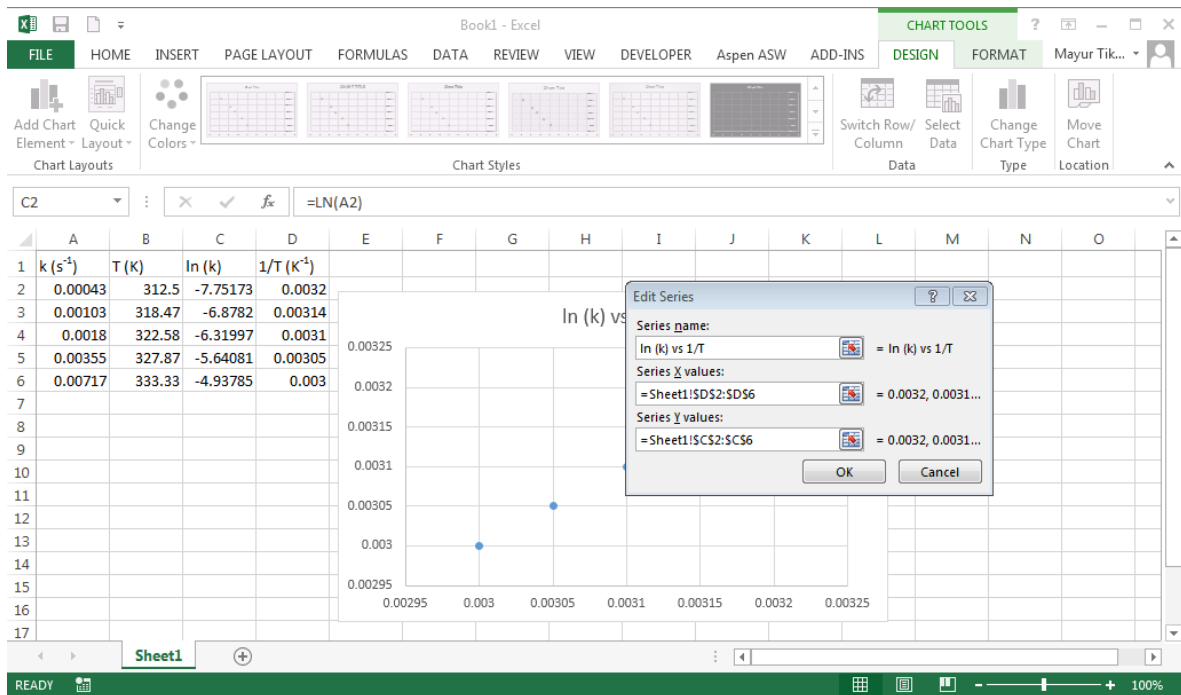
	A	B	C	D	E	F
1	k (s^{-1})	T (K)	$\ln(k)$	$1/T$ (K^{-1})		
2	0.00043	312.5	-7.75173	0.0032		
3	0.00103	318.47	-6.8782	0.00314		
4	0.0018	322.58	-6.31997	0.0031		
5	0.00355	327.87	-5.64081	0.00305		
6	0.00717	333.33	-4.93785	0.003		

Now click on the Edit tab which again opens up another dialog box with name “Edit series”. Here, we can edit Series Name, and Series X and Y values

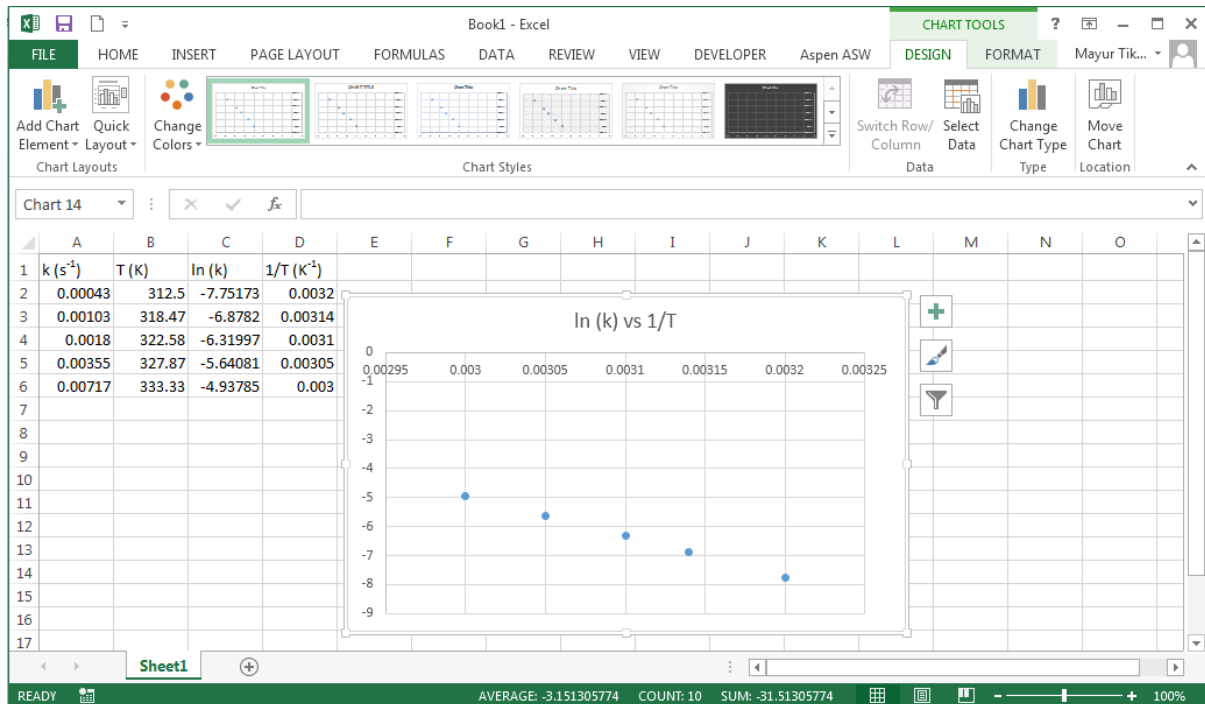


Currently, the X values window reads "`=Sheet1!C2:C6`" which means that X axis takes data from cell C2:C6 of sheet 1, which is the value of $\ln k$. However, we want X values to be from column D (cell D2:D6) which is the value of $1/T$. Thus, Series X values should read "`=Sheet1!D2:D6`" instead of "`=Sheet1!C2:C6`". The same is the case for Y values.

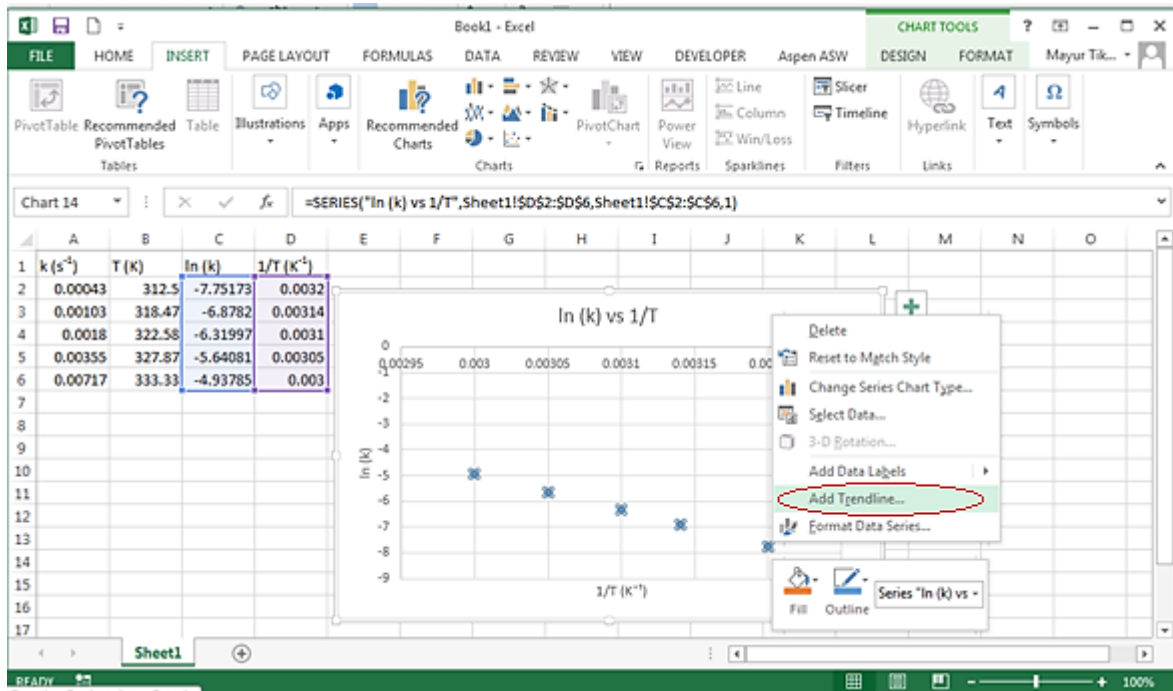
To switch the values, simply change C to D in X values box. Now the X axis will take value from cell D2 to D6 and similarly change D to C in the Y values box. You can also put the chart title by writing in the rectangular box provided under “Series Name”. In this, we have chosen title as “ln (k) vs 1/T”.



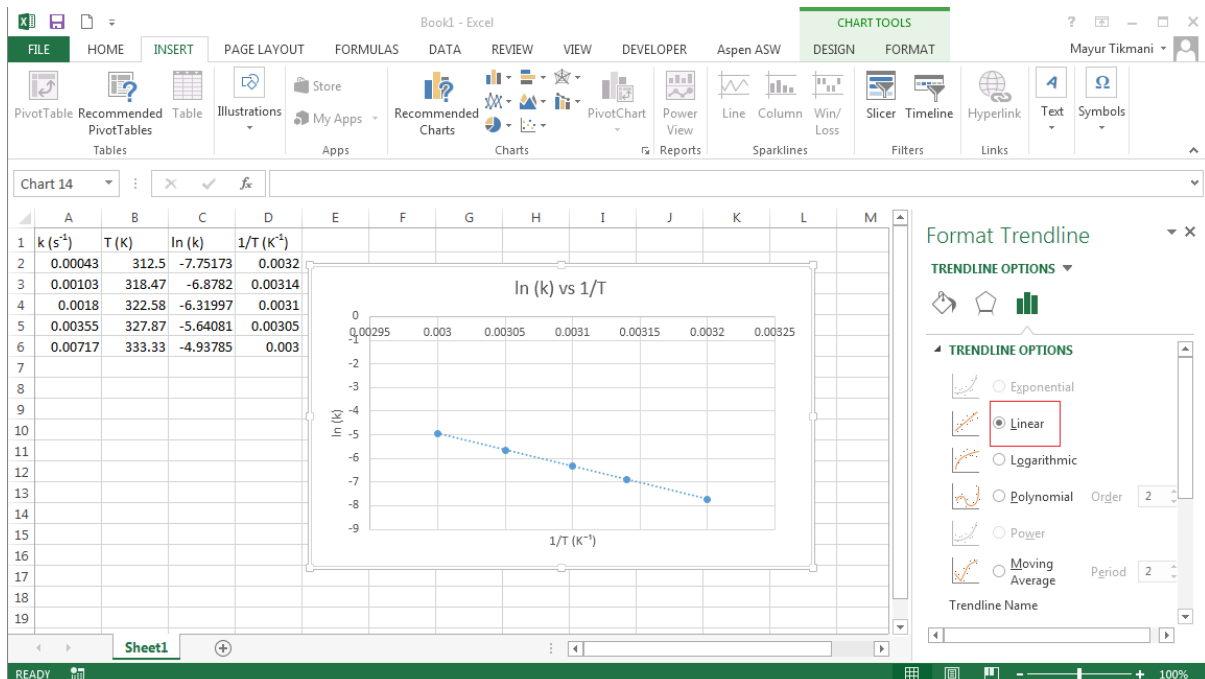
Next, click on the "Ok" button. You should see a graph between $\ln(k)$ and $1/T$ that look like this



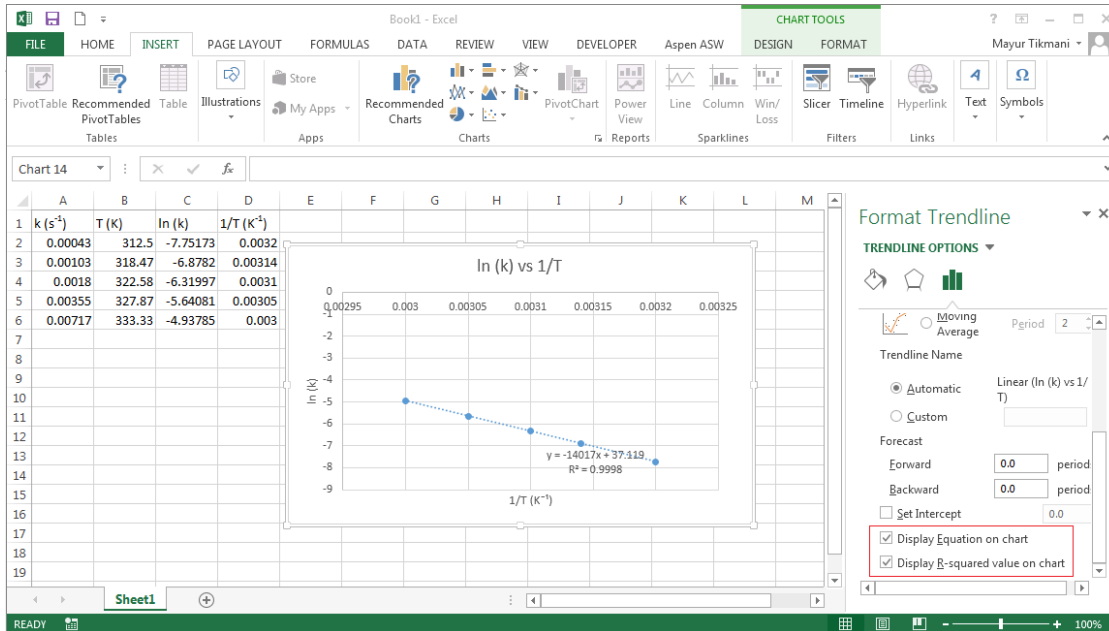
Now, to fit this graph, you need to add trendline. To add trendline, right click on any of the data point and select “Add Trendline”.



You should find that a menu bar opens on the right side where you can format your trendline. You can choose the type of curve you want to fit such as exponential, Linear, Logarithmic, Polynomial etc. In this case, we want to do a linear fit. So select “Linear button” (shown below by red rectangular box).



Now, to add equation and R^2 value to your graph, tick mark on the check-boxes corresponding to “Display Equation on chart” and “Display R-squared value on chart” as shown below. After selecting these boxes, graph equation and R^2 value is displayed on the chart.



The graph equation displayed is

$$y = -14017x + 37.2$$

As mentioned before that the slope and intercept of the graph is $-E/R$ and $\ln A$ respectively, so, from the graph equation

$$\ln A = 37.2$$

$$\text{and } (-E/R) = 14017$$

Therefore, the equation becomes

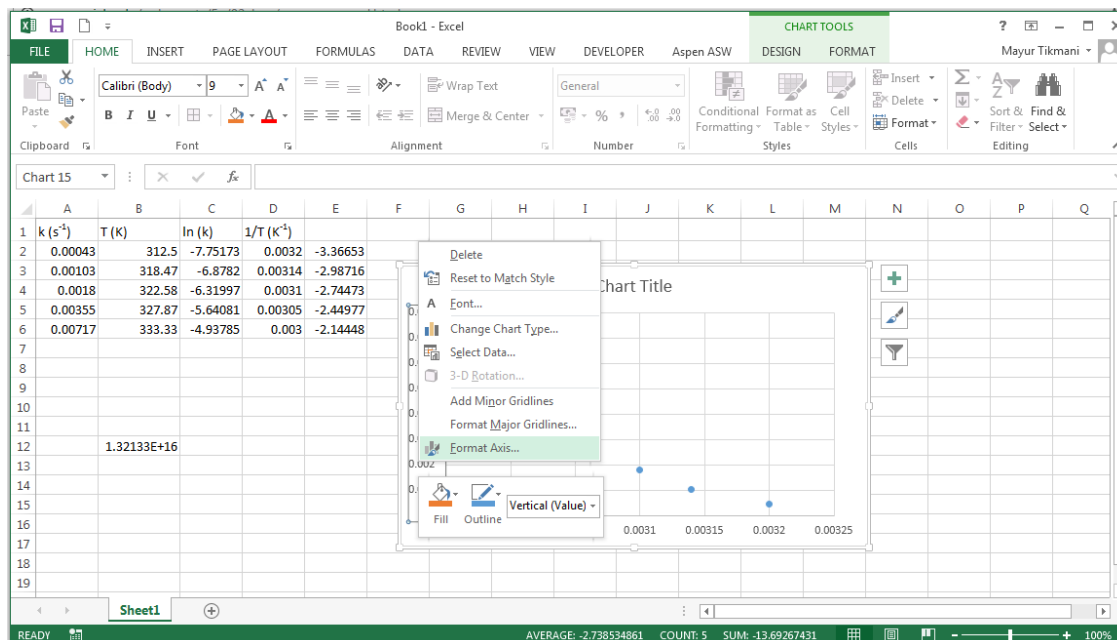
$$\ln(k) = 37.2 - 14017/T$$

Or,

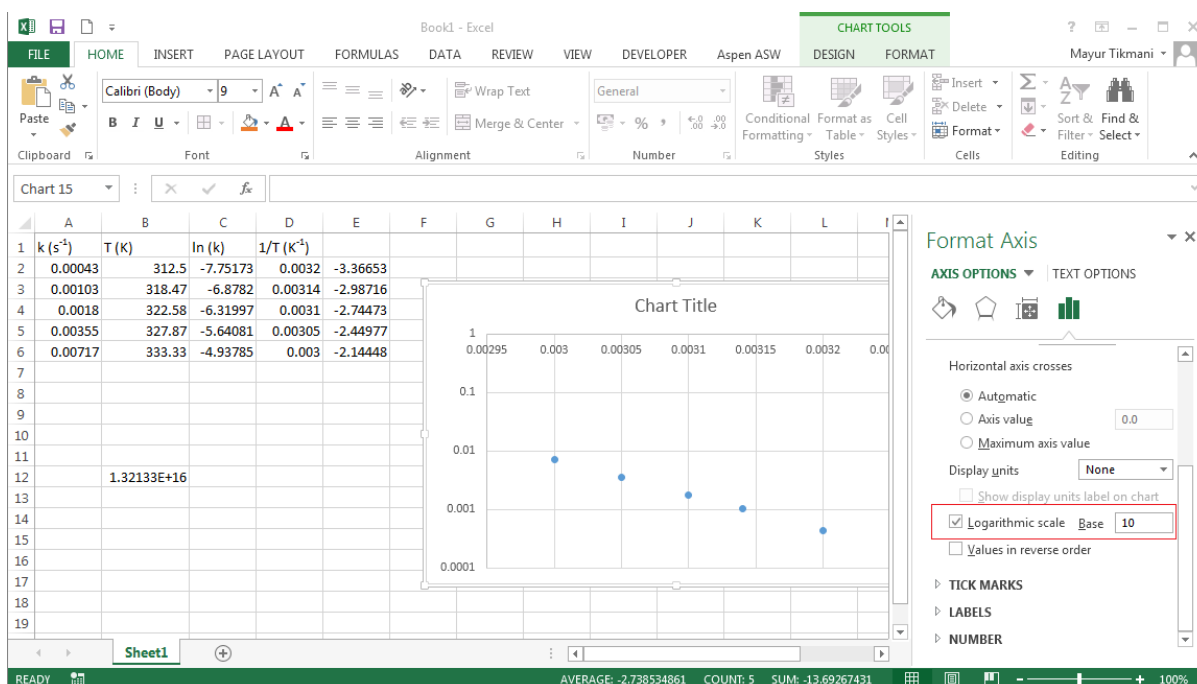
$$k = 1.32 \times 10^{16} e^{-\frac{14017}{T}}$$

Logarithmic Scale

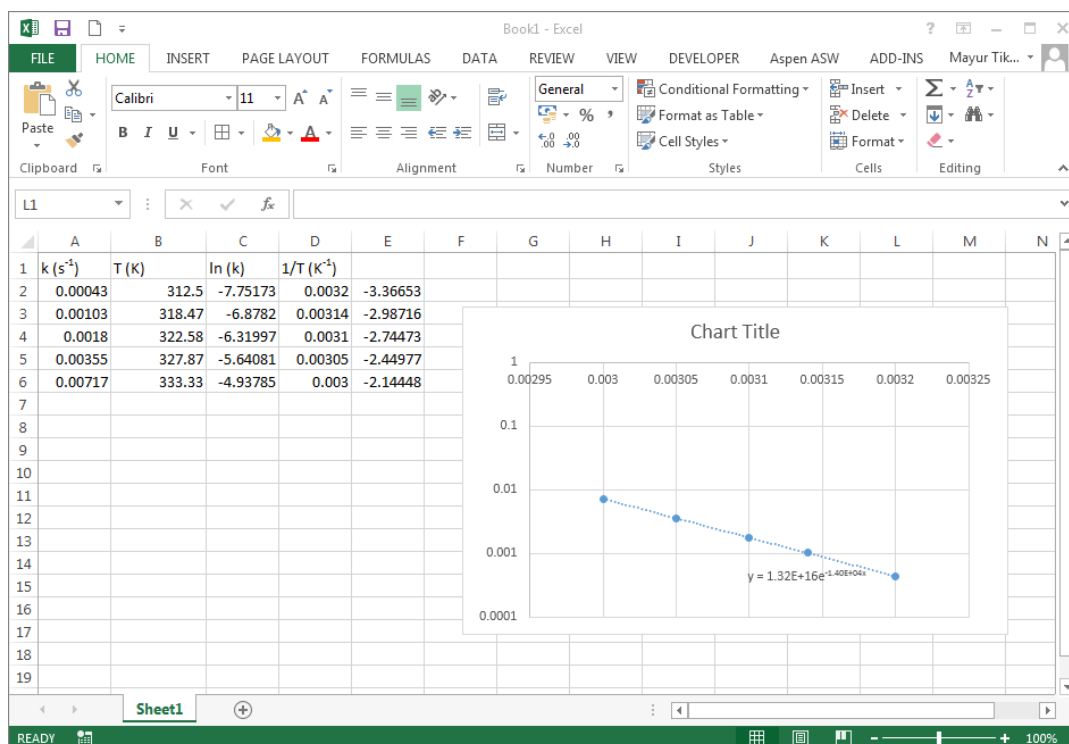
Now we should try graphing in Excel using logarithmic axes. Create a new chart exactly the same as the last one except using columns A and D instead of C and D. Make sure that the X and Y axes are referencing the correct columns; the X column should be referencing the D column. To put this chart on a semi log axis, right-click on the Y axis, and select "Format Axis" from the menu.



This will bring up the "Format Axis" menu. Now, check the "Logarithmic Scale" box at the bottom of the window. You can choose the base of the logarithmic scale by entering the value in the box provided next to Base. In this case, we have chosen 10. Your chart should now have Y axis converted to logarithmic scale and should look something like this.



Now we just need to add the trendline. You can do this by again right-clicking a point in the series, and selecting "Add Trendline" from the menu. This time instead of a linear trendline though, we need an exponential trendline, so select "Exponential" from the choices. Then, check the box for "Display Equation on chart" as was done earlier. You should see an equation on the graph



The equation in the above graph is

$$k = 1.32 \times 10^{16} e^{\frac{-14017}{T}}$$

Which is same as was obtained on a linear scale.