Chapter 3: Rate Laws
Excel Tutorial on Fitting logarithmic data

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

| 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

$$k = k_o e^{-\frac{B}{T}}$$

To find the parameter k_o B , we can make the above equation linear by taking logarithm on both side,

$$\ln(k) = \ln(k_o) - B/T$$

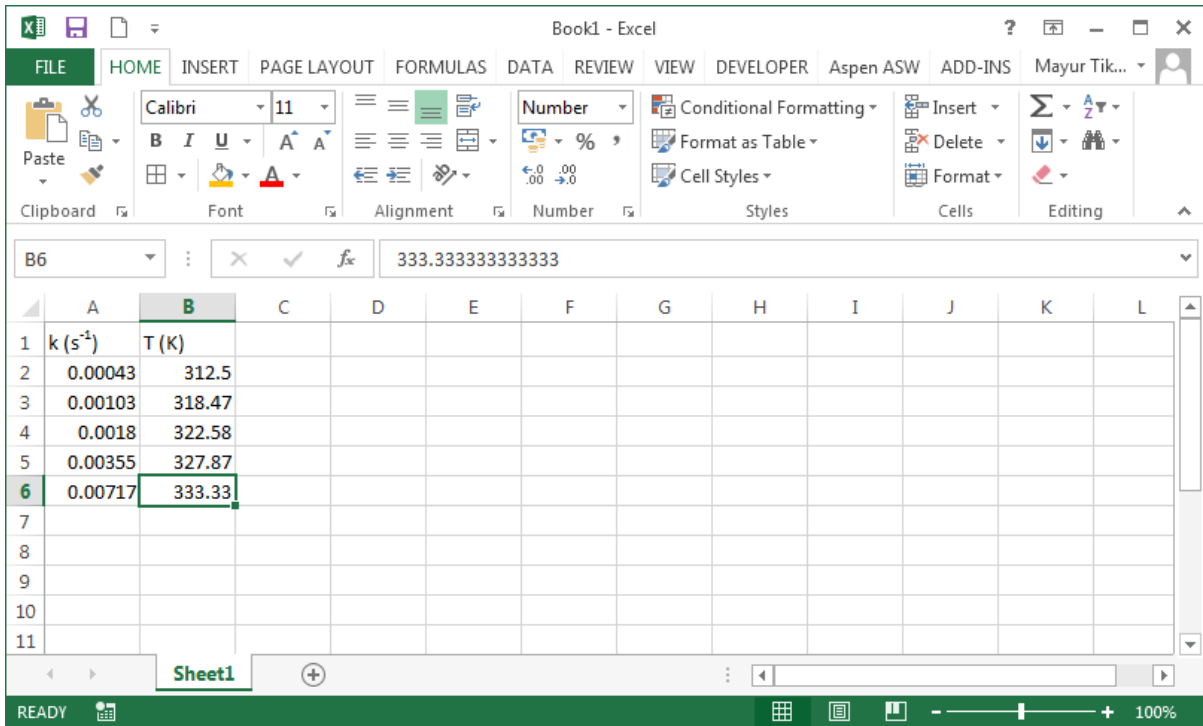So, a graph of $\ln(k)$ vs $1/T$ should yield a straight line with slope as $-B$ and intercept as $\ln k_o$

To find the parameters with the help of excel, open excel. You will see a blank worksheet on the screen that looks like this
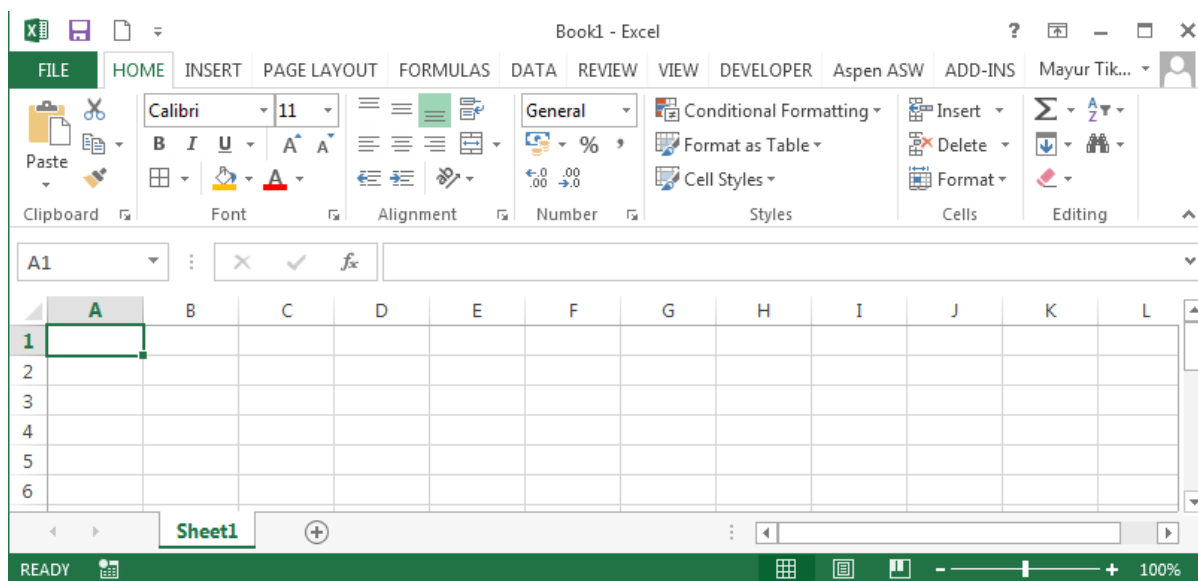
First enter the name of the variable in the spreadsheet. To do this, select Cell A1 and enter the variable name i.e. k (s⁻¹). Now, enter the values of k in subsequent rows starting from A2 cell to A6 cell as shown below
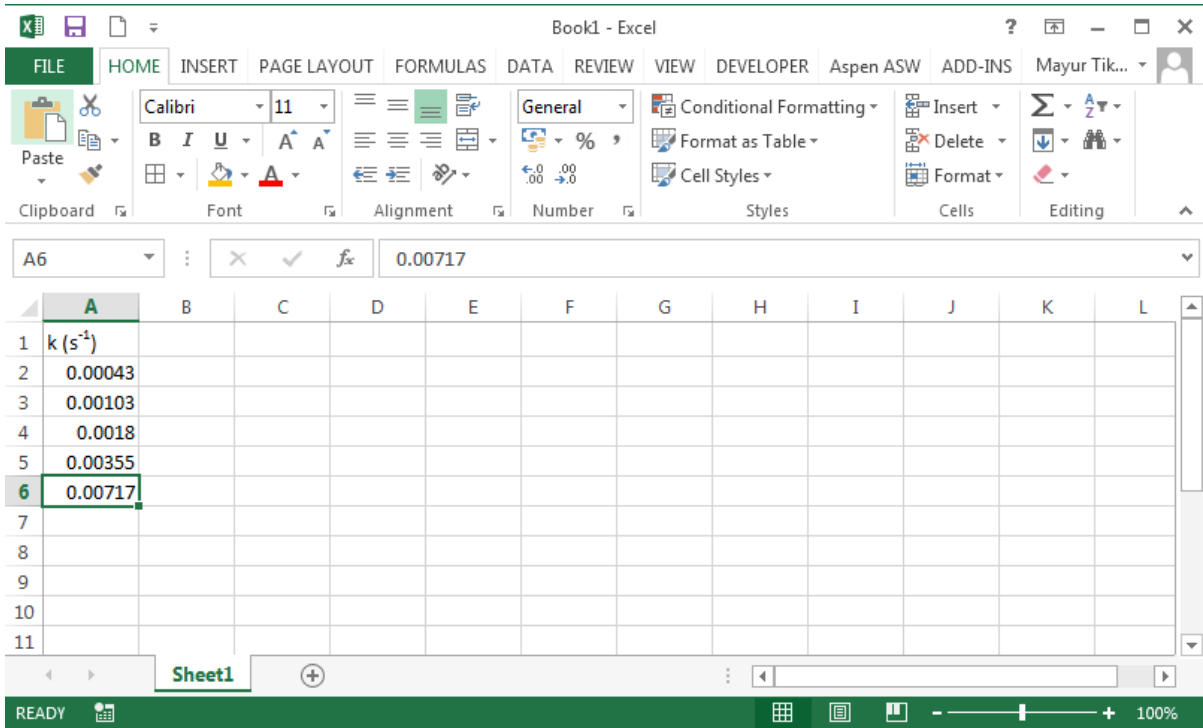

Repeat the above procedure to enter the name and values of T (K). After entering the values, your spreadsheet would look like this

To plot $\ln(k)$ vs $1/T$, we need to determine the values of $\ln(k)$ and $1/T$. To find the logarithmic value of k, use "ln ( )" function embedded in excel. Put variable name in C1 as ln (k) and then type the formula "=ln (A2)" in cell C2.

You will find that cell C2 contains logarithmic value of cell A2. Similarly, determine the value of ln (k) corresponding to remaining k values i.e. cell A3 to cell A6 using the above formula. You can also extend this formula down the line by dragging the bottom right corner of the cell (drag "+" sign) and dragging it down for as many cells as you need. In this case, drag it down to cell C6.

Now, put 1/T (K^{-1}) in cell D1 as variable name and repeat the above procedure to find the values of 1/T in column D. The formula to be used for cell D2 is "=1/B2" as shown below

Next, drag Cell D2 till D6 to find the values of 1/T at different T values

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 and D.
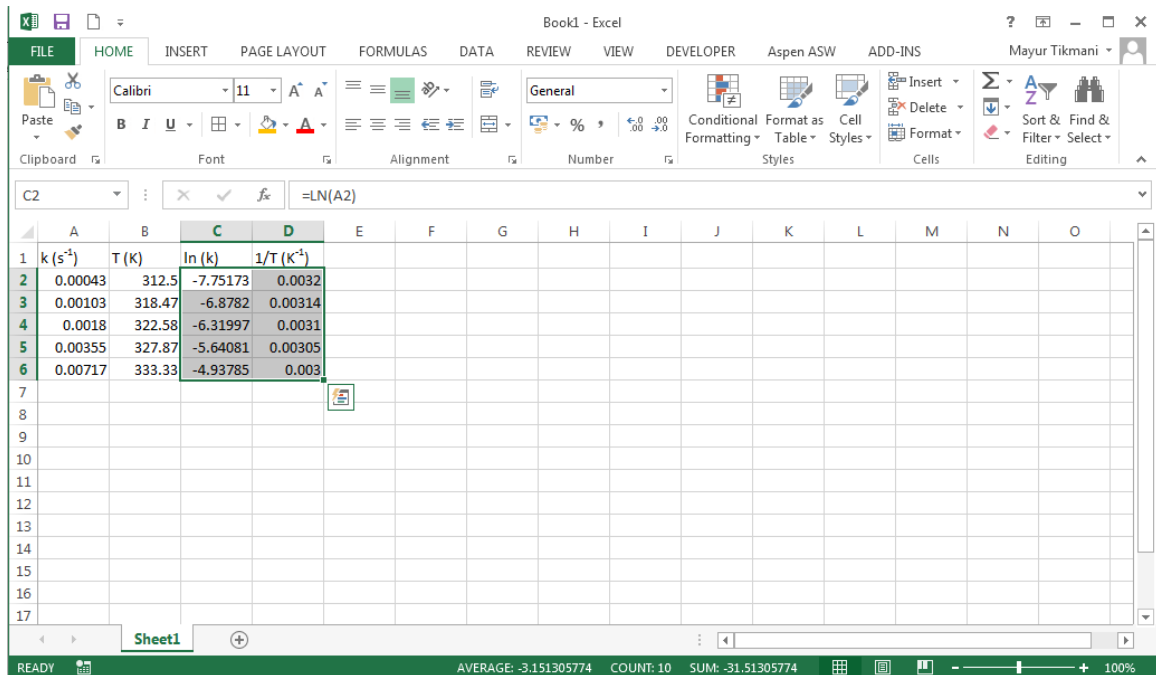

Now, press the Insert tab on the toolbar and click on "scatter chart" present ( ) on the chart menu. This will bring up the various chart options which can be used to create the type of chart that you like. In this case select "XY (Scatter)" which is the first option ( ) of the five options that appear. The below spreadsheet shows the location of Scatter chart.
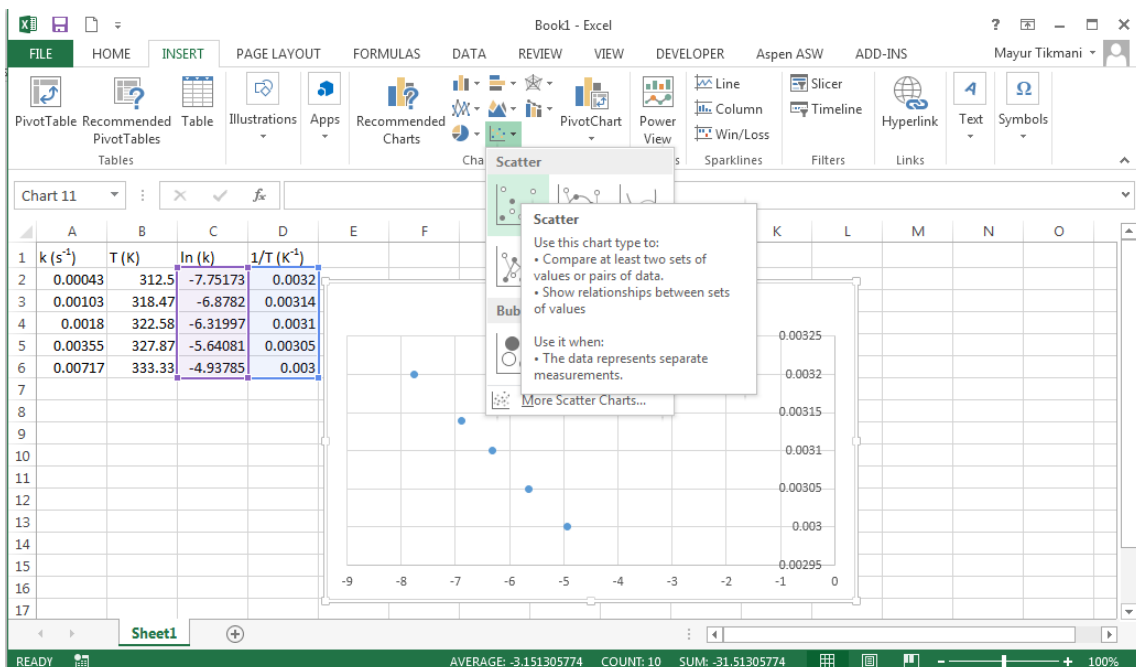

This plots ln (k) on X axis and 1/T on Y axis. However, we want 1/T on X axis and ln (k) on Y axis.

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 as shown
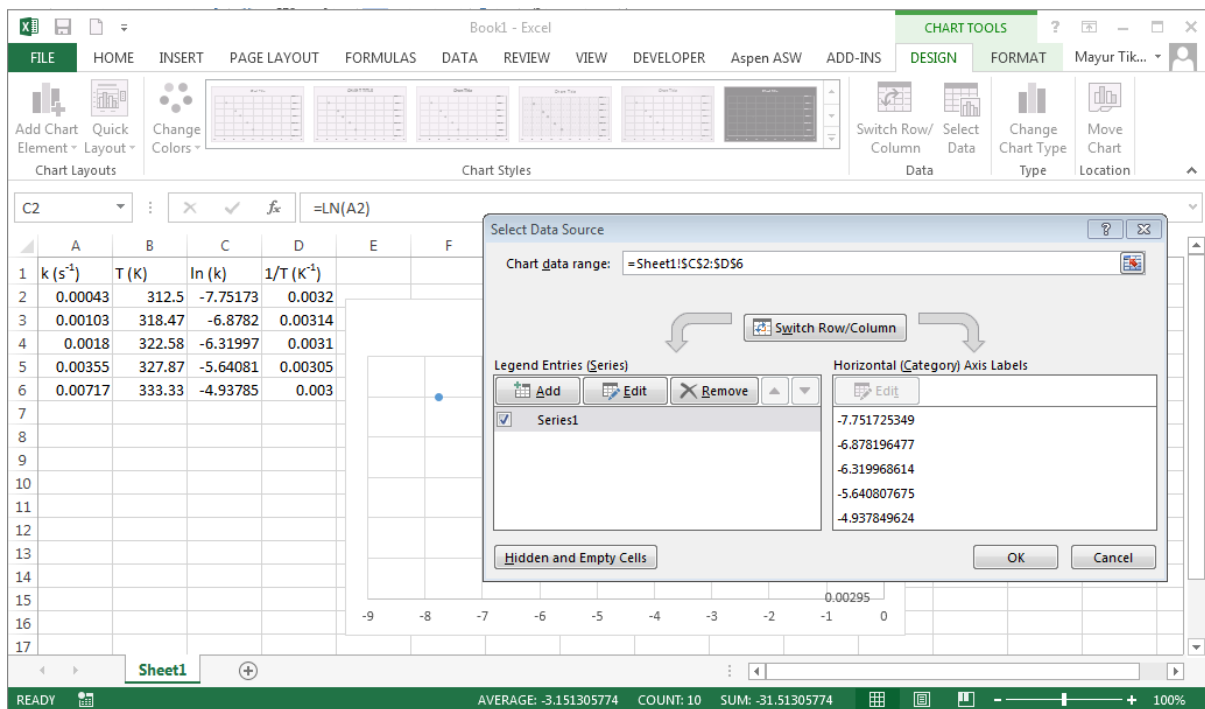

Now click on the Edit tab which again opens up another dialog box with name "Edit series". Here, we can edit Series Name, and Series X and Y values
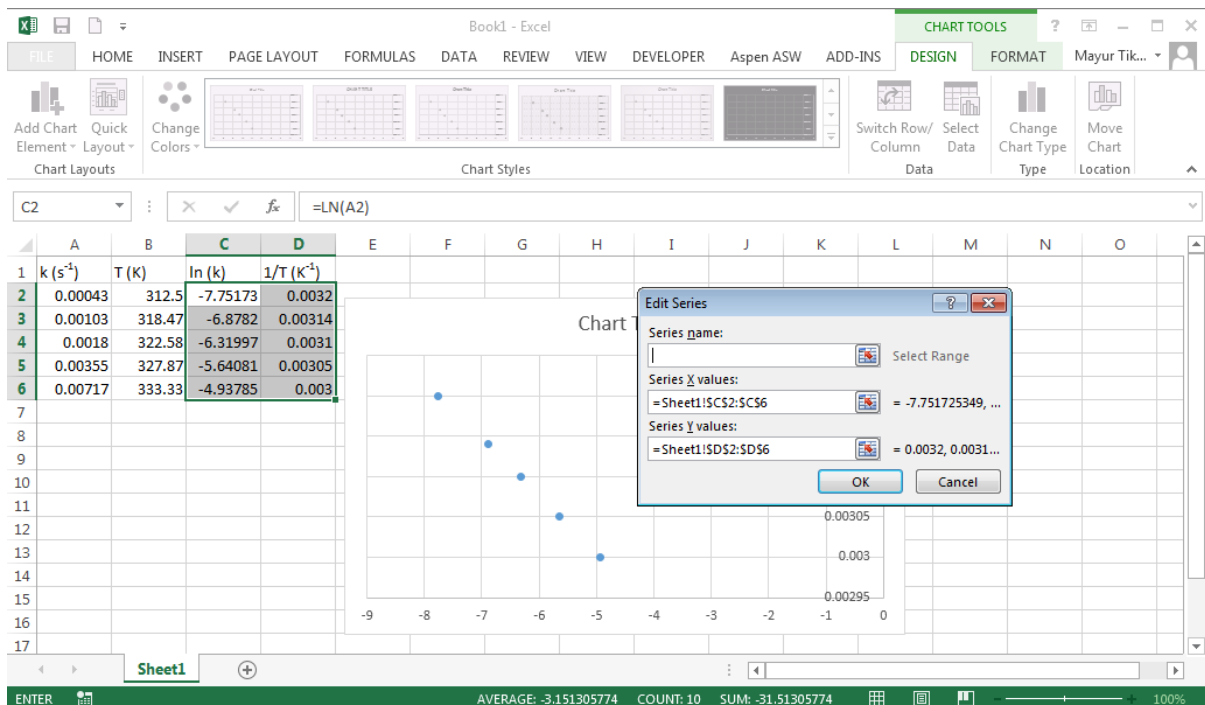

Currently, the X values window reads "=Sheet1!$C$2:$C$6" while it should read "=Sheet1!$D$2:$D$6". The same is the case for Y values.

To switch the values, simply, change C to D and the D to C in both the X values box and 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

To add axis titles, legends or other labels to your chart, you can click on (+) appearing on top right corner of the graph. Let's tick mark Axis titles to add title to axis.
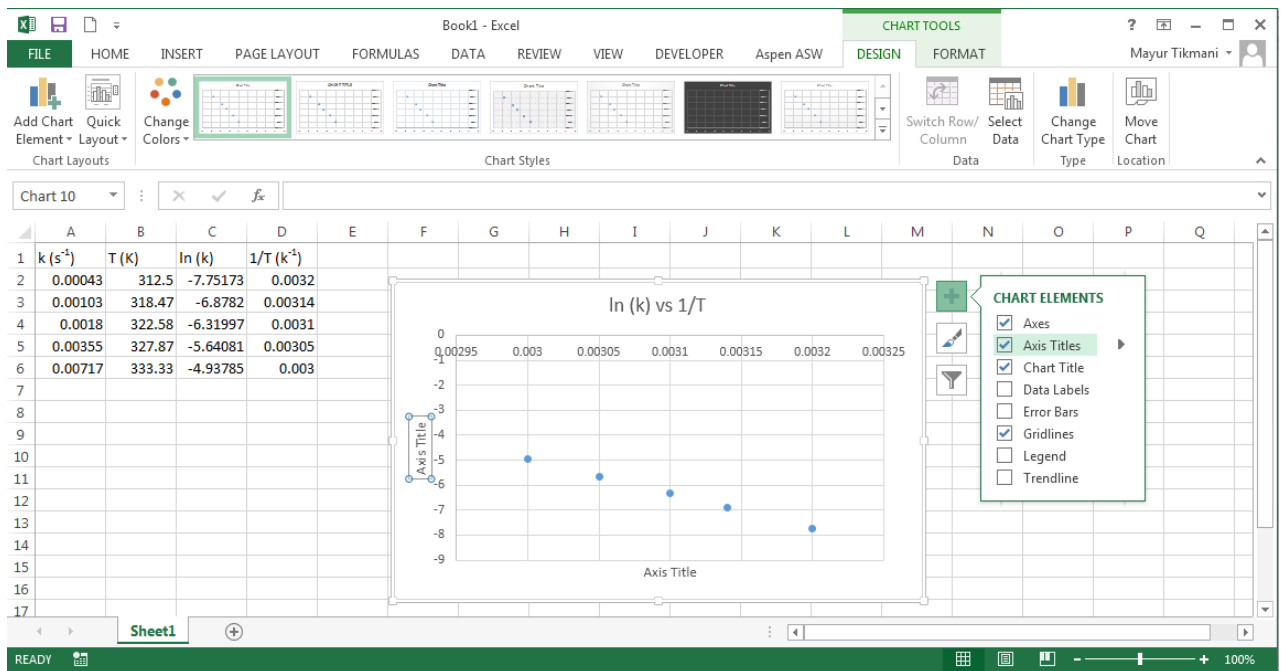

Let's write X axis title as 1/T (K^{-1}) and Y axis as ln (k). Your graph will now have axes title and should look like this
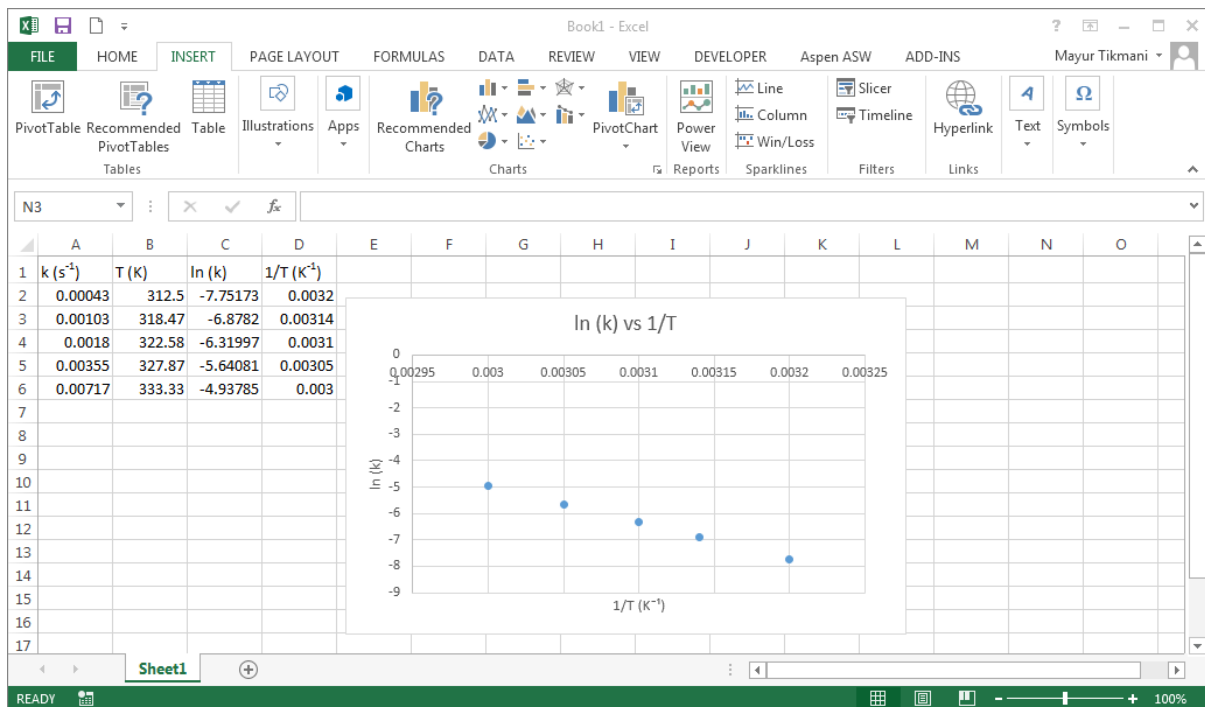
Now, to fit this graph, you need to add trendline. To add trendline, right click on any of the data point and select "Add Trendline".
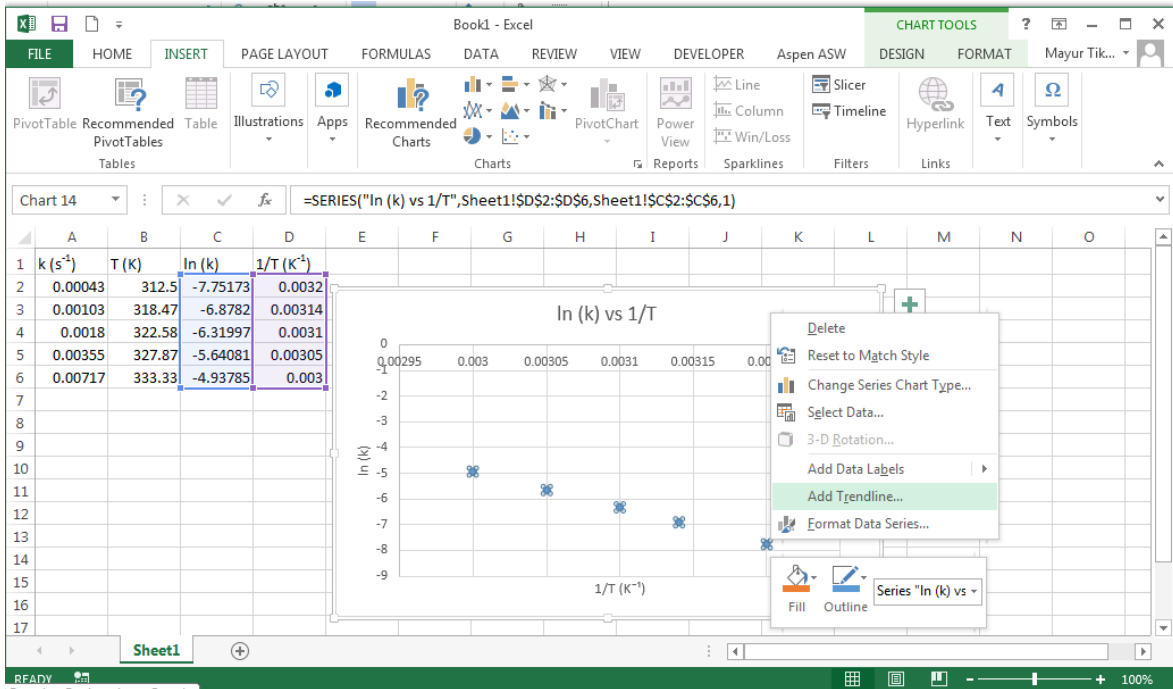
You should find that a menu bar opens on the right side where you can format your trendline. You can choose the type of curve you want to fit such as exponential, Linear, Logarithmic, Polynomial etc. In this case, we want to do a linear fit. So select "Linear button" (shown below by red rectangular box).
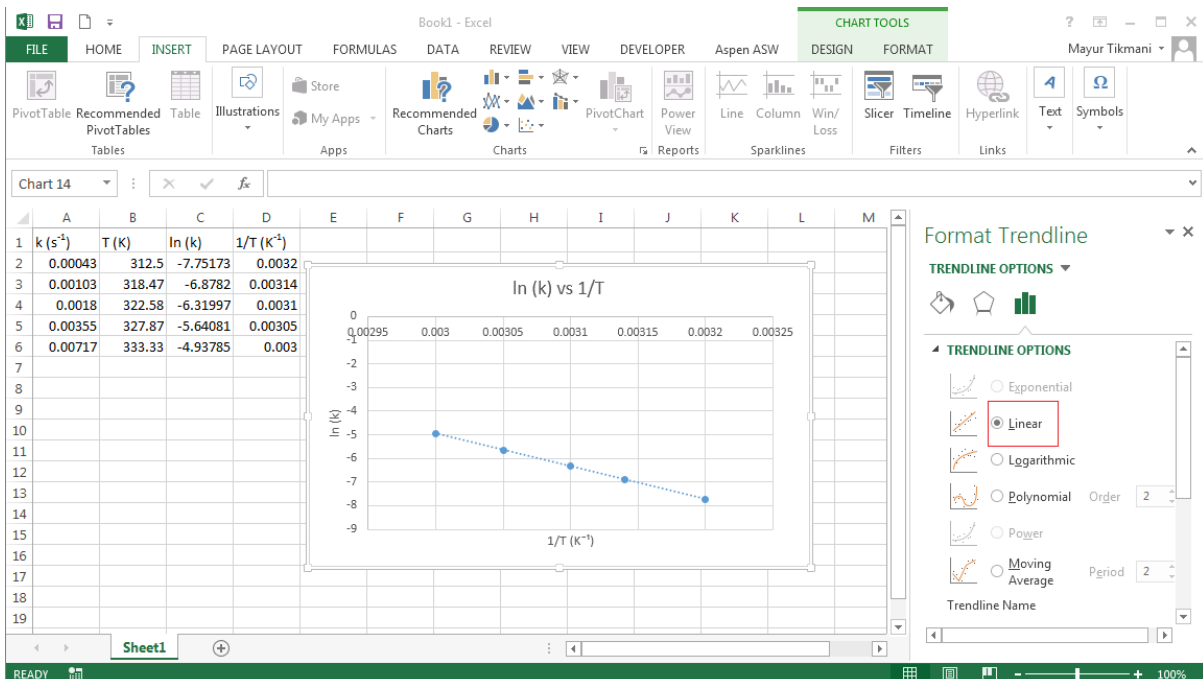
Now, to add equation and R^2 value to your graph, tick mark on the check-boxes corresponding to "Display Equation on chart" and "Display R-squared value on chart" as shown below. After selecting these boxes, graph equation and R^2 value is displayed on the chart.
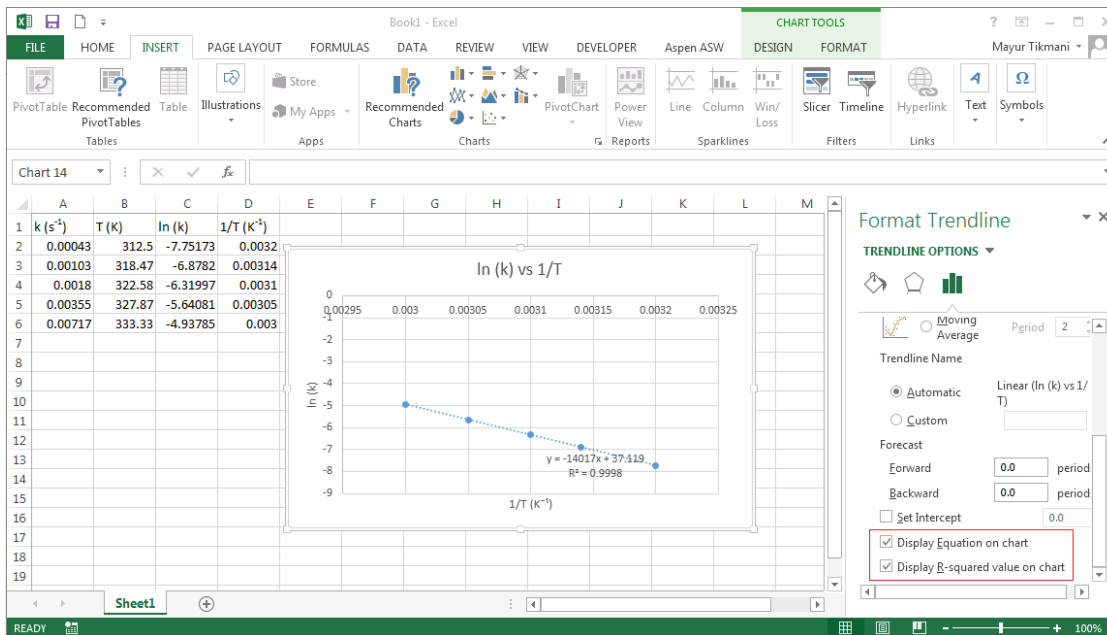
The graph equation displayed is

$$y = -14017x + 37.2$$

As mentioned before that the slope and intercept of the graph is $-B$ and $\ln(k_o)$ respectively, so, from the graph equation

$\ln(k_o) = 37.2$

$and\ B = 14017$

Therefore, the equation becomes

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

Or,

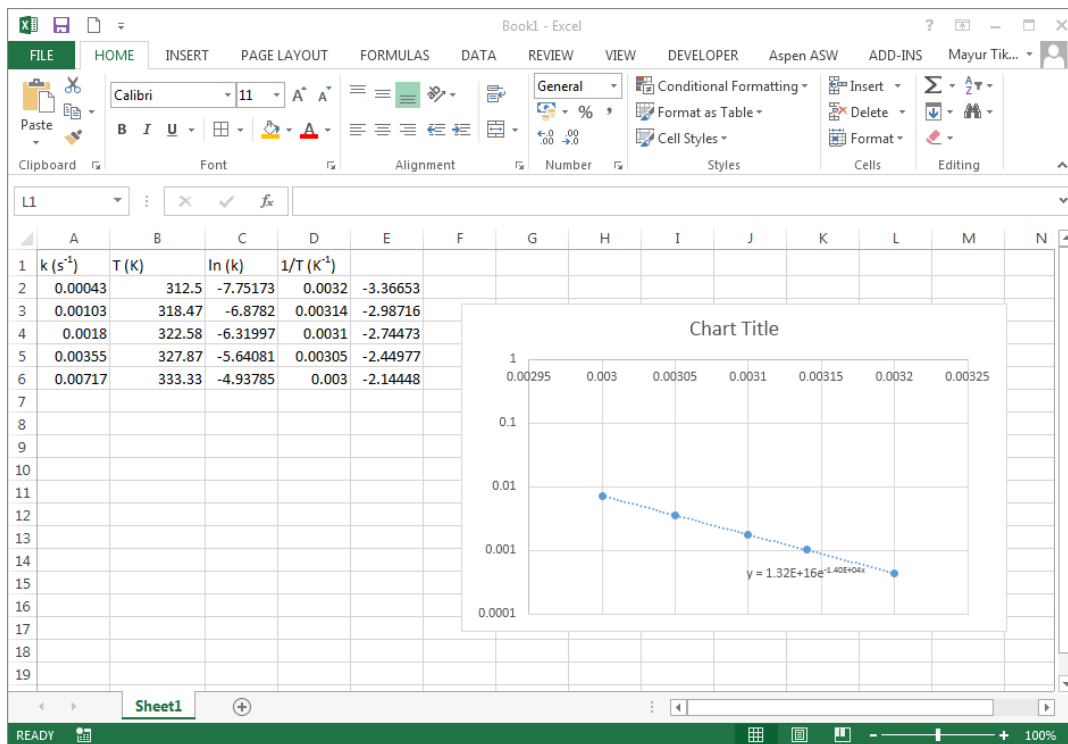$$k = 1.32\ x\ 10^{16} e^{\frac{-14017}{T}}$$

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.
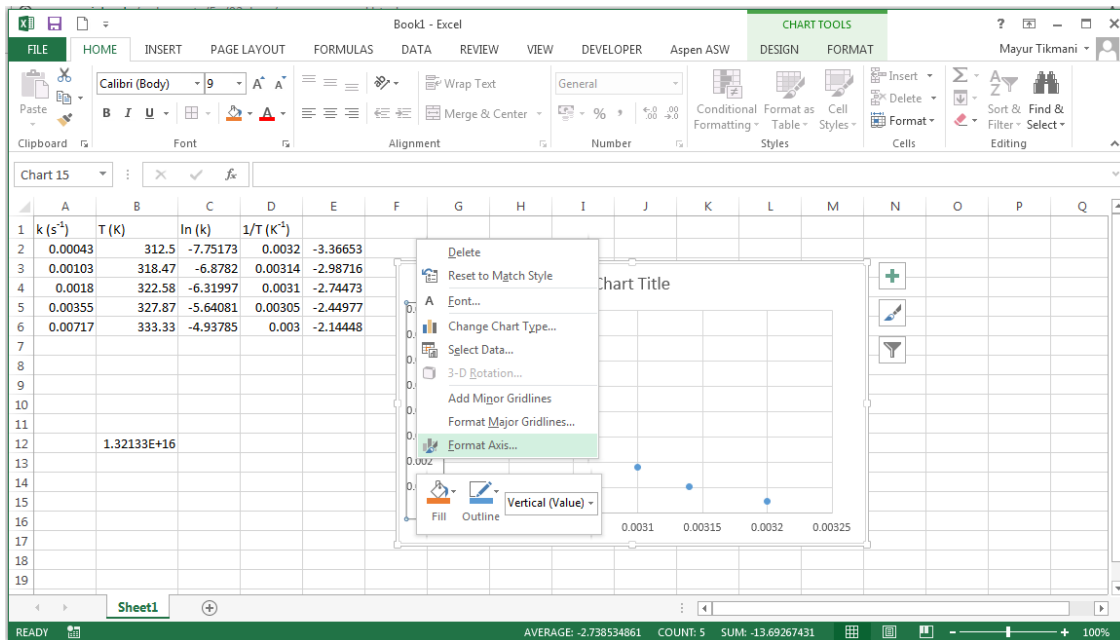
This will bring up the "Format Axis" menu. Now, check the "Logarithmic Scale" box at the bottom of the window. You can choose the base of the logarithmic scale by entering the value in the box provided next to Base. In this case, we have chosen 10. Your chart should now have Y axis converted to logarithmic scale and should look something like this.
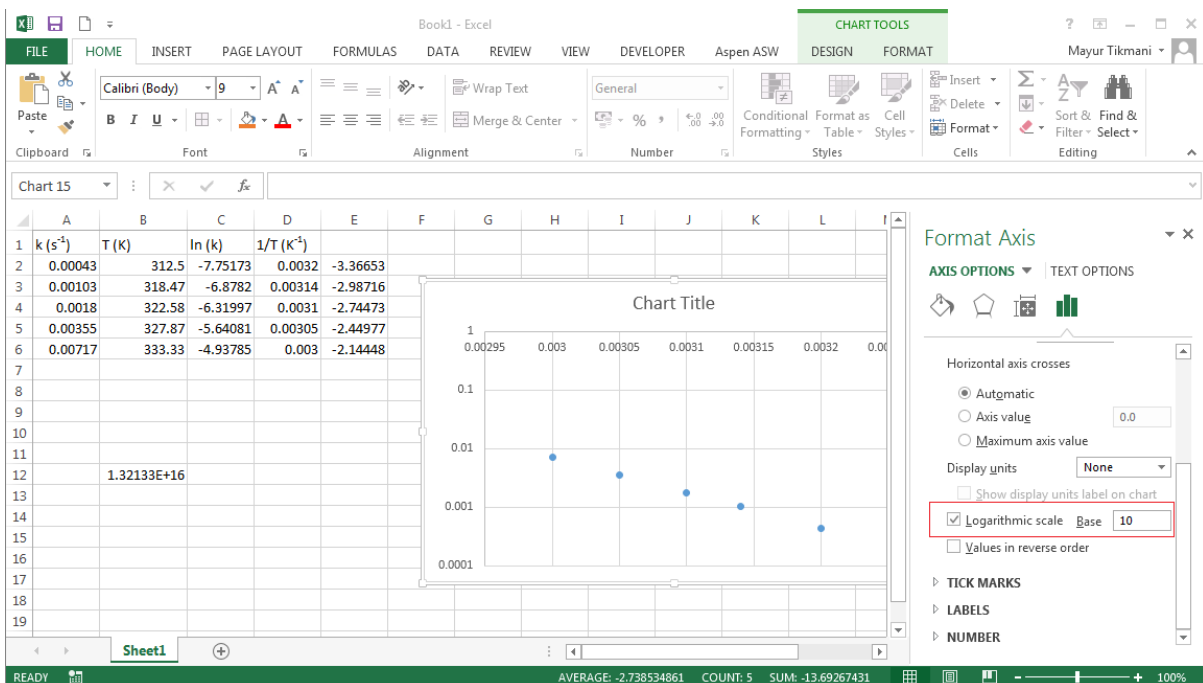
Now we just need to add the trendline. You can do this by again right-clicking a point in the series, and selecting "Add Trendline" from the menu. This time instead of a linear trendline though, we need an exponential trendline, so select "Exponential" from the choices. Then, check the box for "Display Equation on chart" as was done earlier. You should see an equation on the graph

The equation in the above graph is

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

Which is same as was obtained on a linear scale.