

Using the TI89 to perform a linear regression and graph the results

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In this document, I will walk you through the use of your TI89 calculator to solve a problem in which you need to carry out a linear regression and plot the results. Specifically, we will work through example 8.12 from my textbook, *A Life Scientist's Guide to Physical Chemistry*

1. First, you need to be clear as to what you are hoping to accomplish. In this case, we will get the slope of a graph of $\ln K$ vs T^{-1} in order to obtain the enthalpy of reaction, using equation (8.12).
2. To enter the statistics list editor, press the `APPS` key, then select `Stats/List E...` and press `ENTER`.
3. I suggest you start by clearing all lists, so that you're starting with your calculator in a reasonably clean state. The simplest way I have found to do this is to select each list name at the top of the table one at a time, press `ENTER` to edit the entire list, then press `CLEAR` and `ENTER`.
4. My first step is usually to enter the data directly as provided in the problem. Go to `list1` and enter the temperatures (in $^{\circ}\text{C}$, as given) in this column, then enter the K values in `list2`.
5. We need T^{-1} , with T in Kelvin. You can do this in one or two steps. I'm going to do it in one step, but you should be able to adapt this

method to do it in two steps if you like. Move the cursor to highlight `list3` in the table heading, then press `ENTER`. At the bottom of the screen, it should say

`list3={}`

You can type a formula to calculate `list3`. Here is the formula you want, as it will appear at the bottom of the screen:

`list3=(list1+273.15)-1`

To get `list1`, press `2ND VAR-LINK`, scroll down to find and select `list1`, then hit `enter`.

6. Using the same technique, calculate $\ln K$ for all your data, storing the result in `list4`.
7. While you're here, note the minimum and maximum values of T^{-1} and of $\ln K$. You will need these for graphing later. In this case, T^{-1} goes from 0.00341 to 0.0036, and $\ln K$ goes from -1.347 to -0.357 .
8. It's now time to do the linear regression. The values you want to plot on your x axis are the T^{-1} values in `list3`. The y values are the $\ln K$ values in `list4`. Press `F4:Calc`, use the cursor to highlight `3:Regressions`, then choose `2:LinReg(ax+b)` and hit `ENTER`. This will bring up a dialog box. For the X List, enter `list3`, and for the Y List, enter `list4`. You also need to set `Store RegEqn` to: `y1(x)`. To do this, highlight this option and hit the right arrow. Select `y1(x)` and press `ENTER`. You can now press `ENTER` to complete the calculation. After a second or two, a box will pop up containing the slope and intercept, as well as some regression statistics. The value of `a` is the slope, while `b` is the intercept. Press `ENTER`.
9. It's time to set up the plot. Press `F2:Plots`, select `1:Plot Setup` and press `ENTER`. There should be a checkmark next to `Plot1`. If there isn't, select `Plot1` and press `F4:✓`. With `Plot1` selected, press `F1:Define`. Set `x` to `list3` and `y` to `list4` using `2ND VAR-LINK`... Make sure the `Mark` is set to something visible (not `Dot`). Press `ENTER` twice to return to the list editor.

10. Now we need to set up the visible window. Press the yellow diamond key followed by `WINDOW`. We previously determined that the x (T^{-1}) values run from 0.00341 to 0.0036. A reasonable plotting range would therefore be 0.0033 to 0.0037, with tic marks every 0.0001. This is of course not the only sensible choice, but you do need to make sure your points are visible inside the plotting area, so don't set the window too tight. Set `xmin=0.0033`, `xmax=0.0037` and `xsc1=0.0001`. Similarly, set `ymin=-1.5`, `ymax=0` and `yscl=0.5`.
11. If you now press the yellow diamond key followed by `GRAPH`, you should get your graph. The tic marks set above will help you figure out the scale.
12. Once you have used the graph (e.g. copying it reasonably carefully into an exam paper), you may want to get the slope or intercept and to do some arithmetic with them. In this case, we want to calculate

$$\Delta_r H_m^\circ = -R(\text{slope}).$$

Return to the regular calculator mode by pressing `HOME`. The slope can be retrieved by pressing `2ND VAR-LINK`, then scrolling down (quite a long way) to the `STATVARS` section, and selecting `a`. This will print `statvars\ a` on your screen which you can then multiply by $-R$ in the usual way to get the enthalpy of (in this case) the transfer process.