Work Session 16a: Massaging data graphically

Massaging" data means to manipulate data. Massaging data graphically often means to manipulate data so as to obtain a straight line.
Example: Here is some x, y data:

Data Table 1A.

y	x
4.0	1
5.0	2
6.3	3
7.9	4

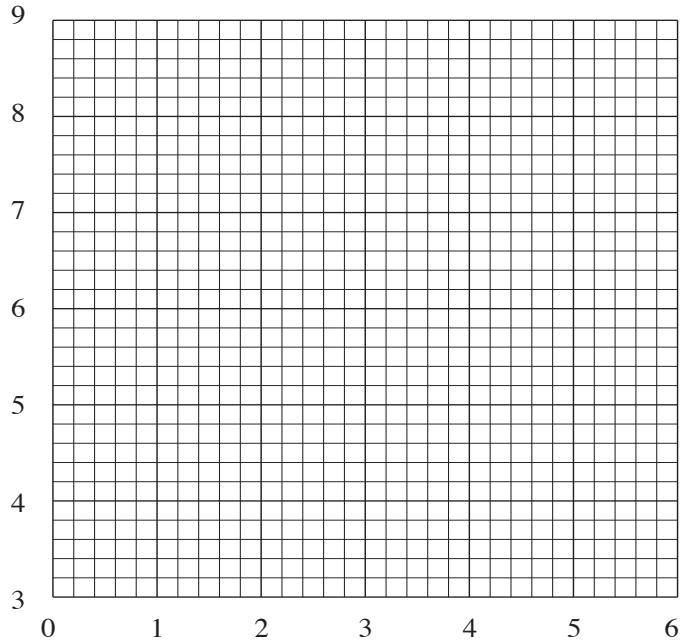
Plot y vs x on the Graph Grid 1A.
Notice that a curve, not a straight line is the result.

Now make a third column in the Data Table.
Use your calculator to obtain the log y values.

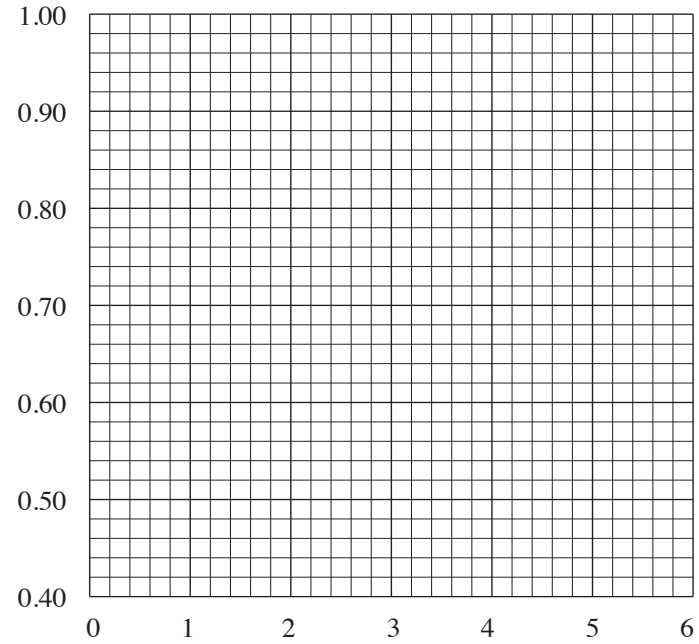
Data Table 1B.

y	log y	x
4.0	____	1
5.0	____	2
6.3	____	3
7.9	____	4

Plot log y vs x on the Graph Grid 1B. Use a ruler to get a crisp straight line. Recall that a straight line follows the mathematical relationship: y = mx + b, where m is the slope, and b is the intercept. The intercept is the value on the y axis where the x axis is at zero.



Graph Grid 1A.



Graph Grid 1B.

Whatever the form of the data that is used on the y and x axis to get a straight line goes into the straight line formula. The plot on grid 1B for this data has "log y" on the y axis, and "x" on the x axis. The straight line equation for the data would be:

$$\log y = mx + b$$

Look at the graph and estimate the value where the line crosses the y axis at x = 0. This is the value for b. The value of m can be obtained by putting log y, x, and b values into the above equation and solving for m. Use the log y and x values from one line of the data table. If you found that m = 0.1 and b = 0.5, you calculated correctly.

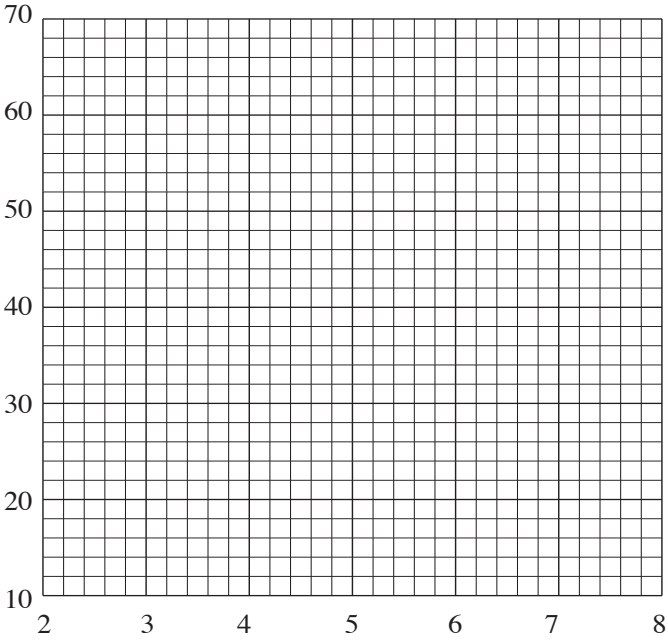
You will more often get the slope by triangulation, which does not require knowing the "b" value. If the points are spread out, then the slope is best obtained by triangulation, as you will see on graph grid 3.

Here is another set of data.

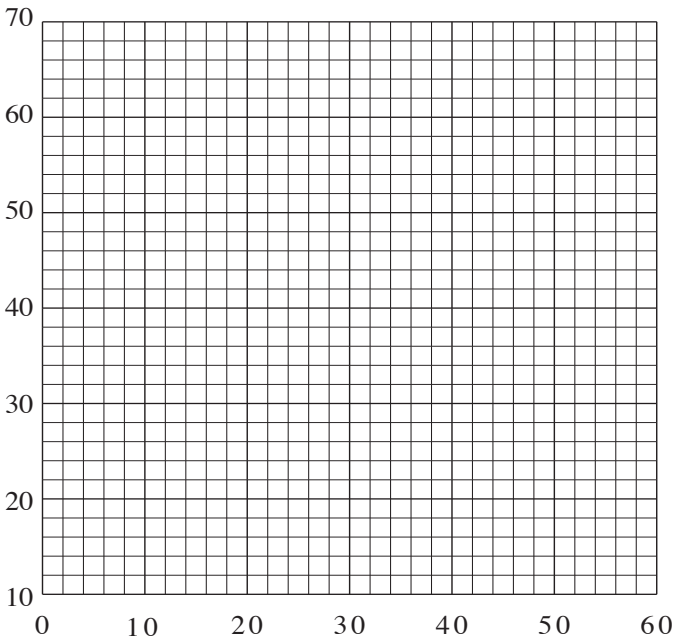
Data Table 2.

y	x	x^2
21.8	3	____
41.0	5	____
54.2	6	____
69.8	7	____

Disregard the third column for now. Plot the points on Graph Grid 2A. If you have access to a French curve, use it to get a smooth curve.



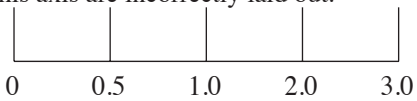
Graph Grid 2A



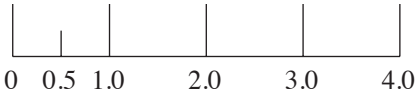
Graph Grid 2B.

Table 2 data follows the relationship: $y = mx^2 + b$. To get a straight line out of the data, first fill in the third column on Data Table 2 labeled x^2. Plot y vs x^2 on Graph Grid 2B. Calculate b and m as before. Did you get m = 1.2 and b = 11? Good. Notice how for the grids in 1A & B and 2A & B, the numbers are put on the heavier grid marks so things work out evenly and most of the grid is used. For the rest of this work sheet, number the grids as seems proper. The left-hand corner does not have to be zero, zero. Each axis can start at whatever value is appropriate to the spread of the data. Each axis can have its own increments, but make sure that each increment along an axis has the same value.

For example: The increments shown on this axis are incorrectly laid out:

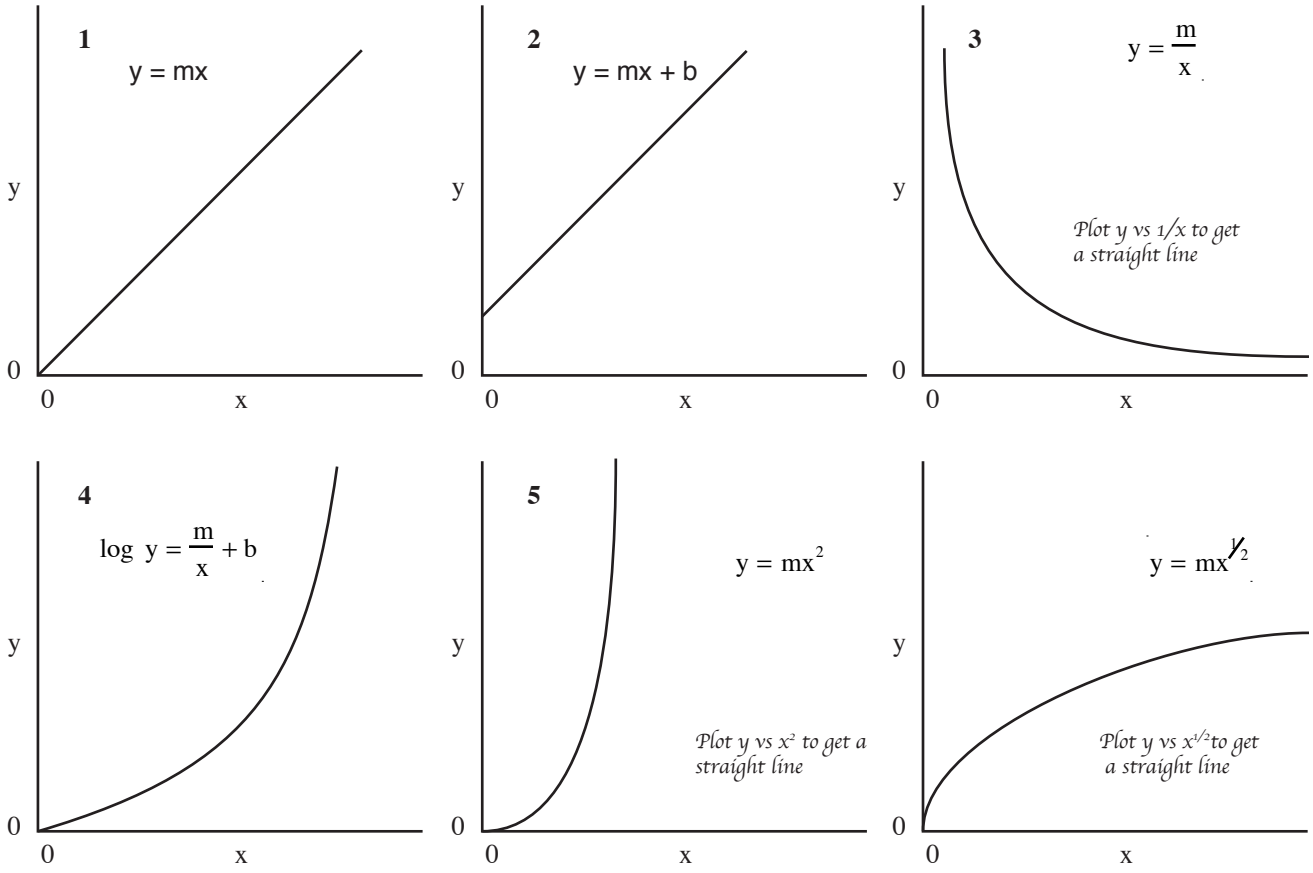


Do you spot the error? The distance between 0 and 0.5 is the same as the distance between 1.0 and 2.0. Each increment along an axis must have the same distance. The next axis has the increments laid out correctly:



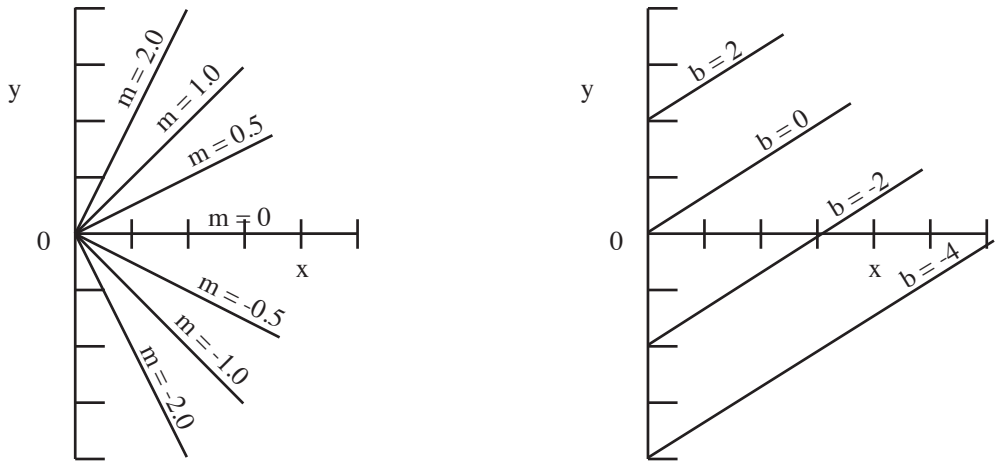
The 0.5 would not be shown as it appears here, for consistency with the rest of the axis. It is shown to emphasize the need for uniformity on an axis. The y-axis and the x-axis can each have their own set of increments. Each must be consistent within.

In each of the previous cases, you have been told how to graph the data to get a straight line. Usually there are a few things to try depending on the way the plot of the raw data looks. Here are a few examples of typical curves obtained from plotting the raw data. For graphs 3, 5, and 6, directions are given to show you how to rework the data to get a straight line. There is no note on graph 4. You will be told to rework the data contained in Data Table 4 to get a straight line. Use the examples above as well as the example on page 1 to do this.

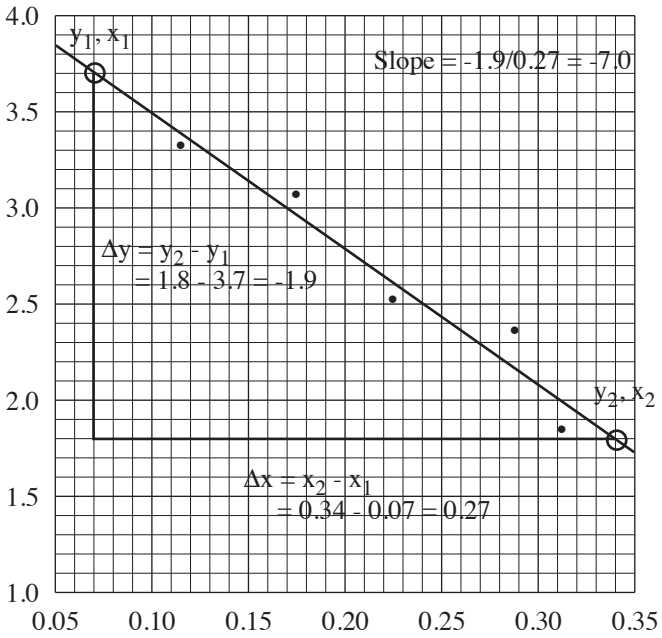


General Graphs

The effect on Graphs 1 and 2 caused by varying values of m and b are shown below.



Experimental data will often give a graph that looks like the example on the right. The points are somewhat scattered, but in the general direction of a straight line. The 5 data points are shown, and a straight line is drawn as evenly as possible through them. If you look at the graph by holding the sheet up to your eye so that you are looking down the line, the points should appear evenly scattered to the right and the left of the line. Drawing the line is best done with a transparent ruler. After the line is drawn, the slope is found by triangulation. Choose two positions on the line, one near each end of the line, and circle these positions. It helps if you can find a position near the end of the line right on a grid mark, as has been done in the example. Call the left position y_1, x_1 and the right position y_2, x_2. Now draw a triangle, and calculate the y length (Δy) and x length (Δx) of the triangle. The slope is $\Delta y/\Delta x$. If the line slopes down, it will have a negative slope. The numbers cause this to happen. If the line slopes up, it will have a positive slope.



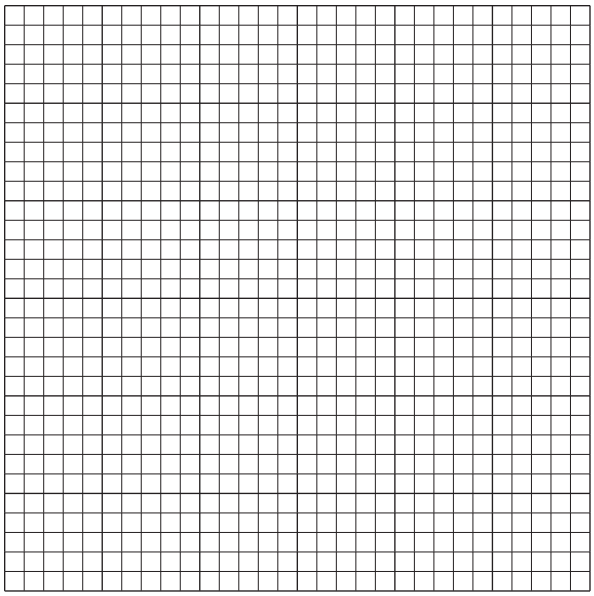
Many calculators will do this automatically. Use the linear regression function. Excel will do this if you tell it to add a trendline.

Follow the example above to correctly plot the following data. This data fits General Graph #2. You do not have to write on the grid when you are calculating the slope. Write it in the white space on this sheet if you wish.

Date Table 3.

y	x
1.4	1.0
2.2	2.0
2.4	3.0
3.2	4.0
3.4	5.0

Plot the data on Graph Grid 3 by drawing the best straight line possible through the midst of the points. Find the values of m and b. Show it in the equation form: y = _____ x + _____



Also, use a computer to graph the data. Open the Massaging Data Excel template on a computer that has Excel installed, and enter the data points into the data table. Put your name and the date on the graph.
If you are doing this on your own computer wothout the template, check out the Excel and Graphs handout, if necessary. If you use a different graphing program, no problem. Check to see how Excel placed the line compared to how you did. Comment on the placement of the line and the slope calculated, comparing your hands-on graph to the Excel graph:

Graph Grid 3.

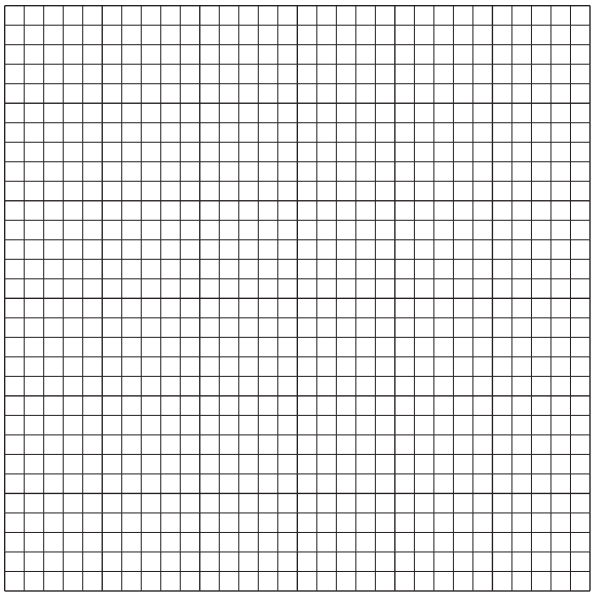
(m = 0.50? Good!)

Here is some more data.

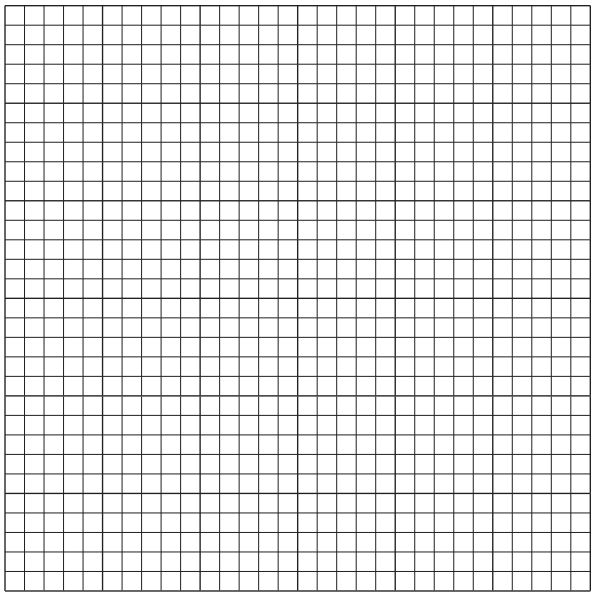
Data Table 4.

y	x	1/x	x^2	
0.10	1.0	___	___	___
31.6	2.0	___	___	___
215	3.0	___	___	___
562	4.0	___	___	___

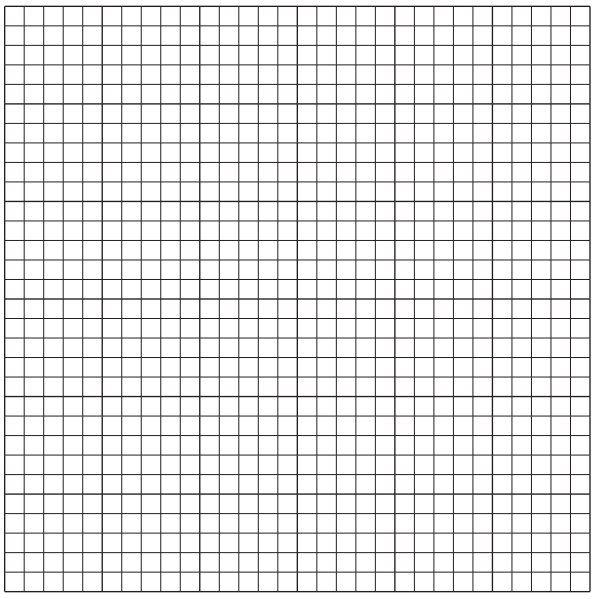
If you want to "massage the data" to see which relationship holds, you would add columns to the raw data in Data Table 4, and calculate values to fill in the column in a way that will give a straight line. For example, to see if the data fits General Graph #3 on page 3, calculate the value of 1/x, then graph y versus 1/x on Graph Grid 4A. An appropriate set of numbers on the x axis would be 0, 0.25, 0.50, 0.75, and 1.0 on the heavier lines. To see if the data fits General Graph #5 on page 3, calculate the values of x^2, then plot y vs x^2 on Graph Grid 4B. Actually, the data fits General Graph #4 on page 3. You will need to add another column of values to your Data Table. What will the title of the column be? Look at General Graph 4, and use the terms for y and x in the equation shown there. Graph the properly altered y and the altered x on Graph Grid 4C to get a straight line.



Graph Grid 4A



Graph Grid 4B.



Graph Grid 4C.

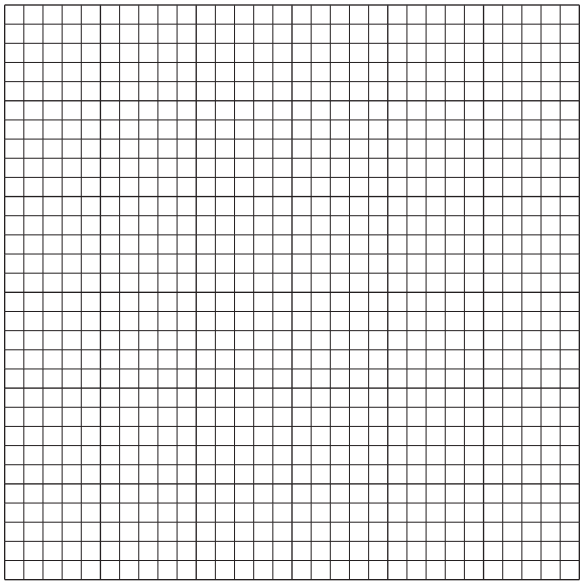
Find the slope and intercept and show the equation for this data. (If done correctly, m should be -5 and b should be 4.) Write the equation using the y–axis and x-axis terms (that is, the form used for the data on the y and the x axis):

Equation: _____

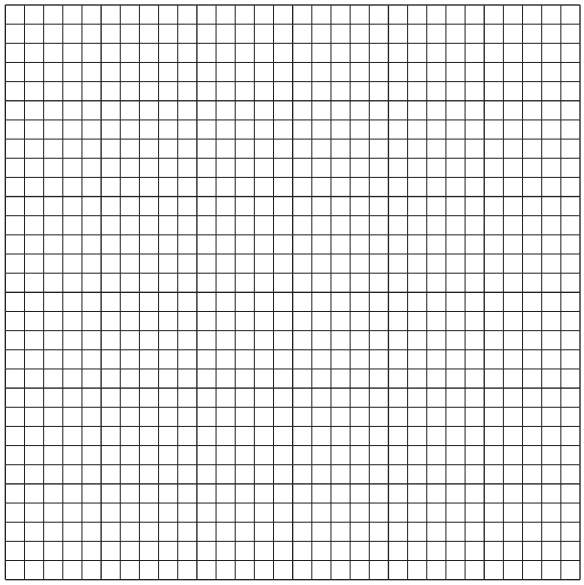
The following data was obtained by measuring the concentrations of Ag^+ and CrO_4^{2-} in some saturated solutions of Ag_2CrO_4 :

Data Table 5. *Note: $[CrO_4^{2-}]$/M means that the numbers listed give the concentration in Molarity.*	$[CrO_4^{2-}]$/M	$[Ag^+]$/M	$\frac{1}{[Ag^+]^2}$ / M^{-2}
	1.0×10^{-4}	1.0×10^{-4}	
	0.25×10^{-4}	2.0×10^{-4}	
	0.11×10^{-4}	3.0×10^{-4}	
	0.067×10^{-4}	4.0×10^{-4}	

Plot the $[CrO_4^{2-}]$ vs the $[Ag^+]$ on Graph Grid 5A (0.2×10^{-4} divisions on y, 1×10^{-4} divisions on x).



Graph Grid 5A



Graph Grid 5B.

In Data Table 5, calculate the values for the column $1/[Ag^+]^2/M^{-2}$. (Note that when you square the first $[Ag^+]$ and take the inverse, the value comes out to 1×10^8 M^{-2}. Write each of the other values with the exponent set to 10^8. The second inverse square would be written as 0.25×10^8 M^{-2}. The first column of data for $[CrO_4^{2-}]$ lists data in this manner. Keeping the exponent the same on a string of data often eases the process of graphing.) Now graph $[CrO4^{-2}]$ versus $1/[Ag+]^2$ on Graph Grid 5B. (Put 0.2×10^8 divisions on the x axis.) What is the slope of the line obtained?

Slope = _____ (should be around $10^{-12}M^3$)

What is the equation showing how $[CrO_4^{2-}]$ and $[Ag^+]$ are related? Use the concentration symbols as used on the y and x axis, not y and x, in the equation.

Equation : _____

Graphical methods are commonly used to find the *order* of a reaction in kinetics. The order of a reaction states the way in which the concentration of a material influences the rate of the reaction. For the generic reaction: A B + C, here are three equations showing how [A], the concentration of A, varies with time, depending on the order of the reaction (slope terms are shaded):

Zero order: $[A] = -k \cdot t + [A]_0$

First order: $\ln[A] = -k \cdot t + \ln[A]_0$

Second order: $\frac{1}{[A]} = k \cdot t + \frac{1}{[A]_0}$

Note that [A] and t are the variables, since $[A]_0$, the initial concentration, remains the same. Also note that on the right side of the equation, t is the x and the $[A]_0$ term is the b. (b stands for a different expression of $[A]_0$ in each case: $[A]_0$ or ln $[A]_0$ or $1/[A]_0$ for 0°, 1° or 2°). The m stands for -k for zero and first order, k for second order.

Here is some data for a typical reaction:

Data Table 6.

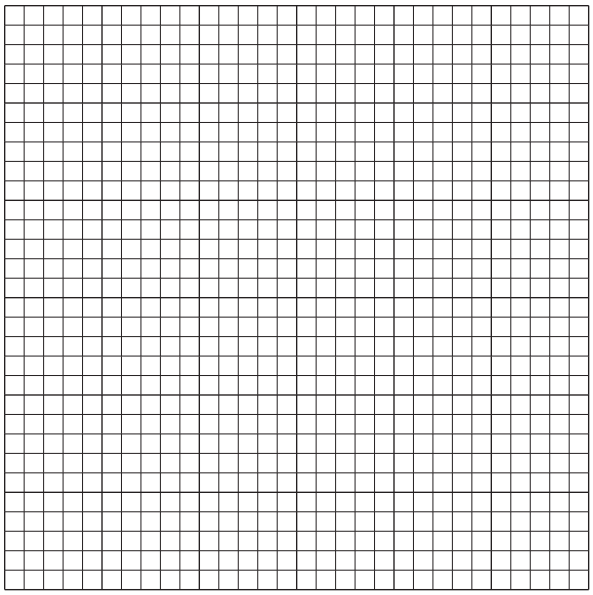
[A]/M	t/min	ln [A]	$1/[A]/M^{-1}$
1.00	0	_____	_____
0.80	1	_____	_____
0.63	2	_____	_____
0.50	3	_____	_____
0.40	4	_____	_____
0.32	5	_____	_____

Calculate the values for each column: ln [A] and $1/[A]/M^{-1}$.

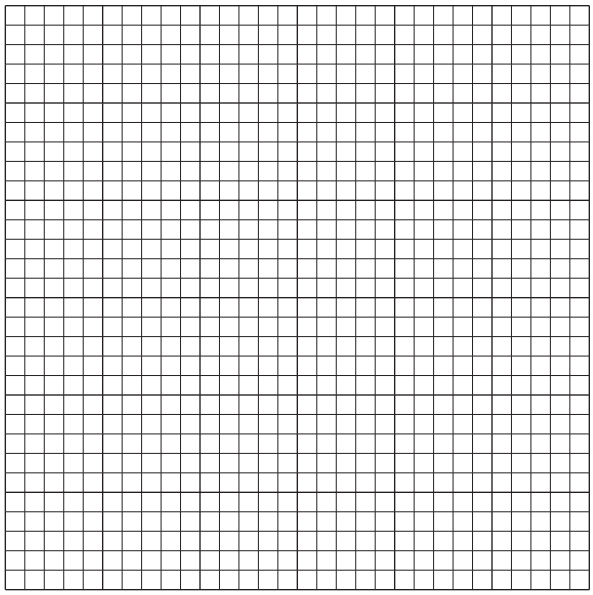
Plot [A] vs t on Graph Grid 6A.

Plot ln [A] vs t on Graph Grid 6B.
(For 6B: Mark the y axis from -1.2 on the bottom using 0.2 increments.)

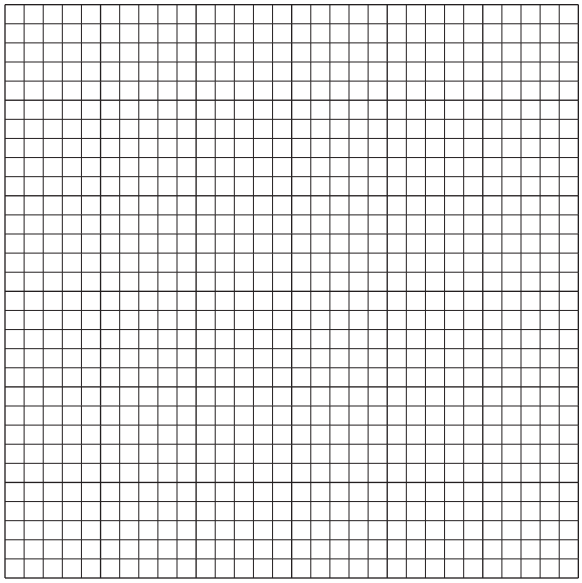
Plot $\frac{1}{[A]}$ vs t on Graph Grid 6C.



Graph Grid 6A



Graph Grid 6B.



Graph Grid 6C.

If one of these is a straight line, you will conclude what order the reaction is from what you had to plot to get a straight line.

So if the straight line comes from:

[A] vs t, it is 0°;

ln [A] vs t, it is 1°;

$\frac{1}{[A]}$ vs t, it is 2°

For the straight line, find the slope and use that to calculate the value of k.

Look at the order equations on the previous page and figure out the proper way to obtain k from the slope.

Slope = _____

k = _____

Name_____ Grade_____ Date_____

Finally, activation energies, E_a, are frequently found graphically.
The Arrhenius equation:

$$\ln k = \frac{-E_a}{R} \cdot \frac{1}{T} + C$$

(slope term shaded)

is used. Values of k, the rate constant, are measured at various temperatures, then ln k and 1/T are calculated and plotted. Here is some typical data:

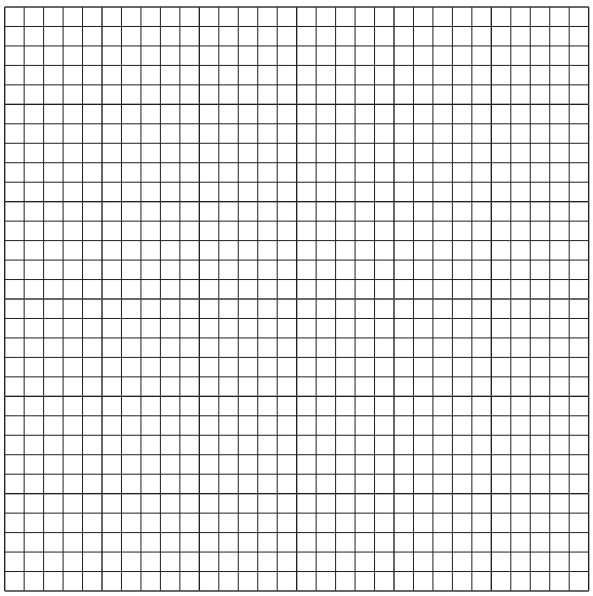
Note: t/°C means temperature with units in Celsius. T/K means temperature with units in Kelvin. 1/T/K^{-1} means inverse Kelvin with units K^{-1}.

Data Table 7.

k/s^{-1}	ln k	t/°C	T/K	1/T/K^{-1}
_____	_____	_____	_____	_____
2.00 x 10^{-5}	_____	20.0	_____	_____
7.30 x 10^{-5}	_____	30.0	_____	_____
2.70 x 10^{-4}	_____	40.0	_____	_____
9.10 x 10^{-4}	_____	50.0	_____	_____
2.90 x 10^{-3}	_____	60.0	_____	_____

Fill in the values for the columns left blank, then plot ln k vs 1/T on Graph Grid 7.

(Note:
Start the y axis at -11 on the bottom up to -5 on the top. Mark the x axis as 0.00300 on the left, then 0.00310, 0.00320, etc. on to the right)



Graph Grid 7.

Calculate the slope and E_a (R = 8.3 J·mol^{-1}K^{-1})

(the slope will be around -12000K).

Slope = _____

E_a = _____