

Solving Integrated Rate Law Problems Using the Graphing Calculator

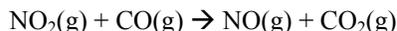
Mt. Whitney High School AP Chemistry

The old-fashioned (and tedious) method for determining the order of a reaction from experimental data was to graph the data points by hand. Since linear graphs resulting from relationships of concentration with time depend on the order of the reaction, this method usually required three separate graphs:

- Time vs. concentration for zero order reactions
- Time vs. $\ln(\text{concentration})$ for first order reactions
- Time vs. $(1/\text{concentration})$ for second order reactions

The graphing calculator greatly simplifies the process. We will use the following problem from Zumdahl, chapter 12:

The rate of the reaction



Depends only on the concentration of nitrogen dioxide below 225°C. At a temperature below 225°C the following data were collected:

Time (s)	[NO ₂] (mol/L)
0	0.500
1.20×10^3	0.444
3.00×10^3	0.381
4.50×10^3	0.340
9.00×10^3	0.250
1.80×10^4	0.174

Determine the rate law, the integrated law, and the value of the rate constant. Calculate [NO₂] at 2.70×10^4 s after the start of the reaction.

Step 1: Enter the data in a list

... → "EDIT" → 1:Edit → \leftarrow This opens the list window. If there are contents in the lists, then use the "up" cursor to move into the uppermost field – the list header (L₁, L₂, L₃...). Once there, press \leftarrow and then the "down" cursor. This clears the list field.

Now enter the values for time in L₁ and concentration in L₂. We will use L₃ and L₄ to store values corresponding to $\ln[\text{NO}_2]$.

Go to the header of L₃ and press μ y $\hat{=}$ \leftarrow . This places values of $\ln[\text{NO}_2]$ in List 3.

Go to the header of L₄ and press $\hat{=}$ \neq y $\hat{=}$ \leftarrow . This places values of $1/[\text{NO}_2]$ in List 4.

L2	L3	L4	4
.5	-.6931	2	
.444	-.8119	2.2523	
.381	-.965	2.6247	
.34	-1.079	2.9412	
.25	-1.386	4	
.174	-1.749	5.7471	
-----	-----	-----	
L4(?) =			

The contents of L₂, L₃ and L₄ should now appear as it does in the picture.

Step 2: Turn on Diagnostics

In order to analyze the linearity of our data, we need to turn on the statistical diagnostics. This will provide us with correlation coefficients when we perform a linear regression.

Open the Catalog function: y → $\hat{=}$ and then scroll down to "DiagnosticOn" and press \leftarrow , and then \leftarrow a second time. The diagnostic functions are now on.

Step 3: Perform Linear Regressions

Press ... \sim (CALC), press \downarrow . Scroll down to **4:LinReg(ax+b)** and press \downarrow .

We will now perform a linear regression on the contents of L_1 and L_2 . We would also like to store the resulting linear equation for later use. We will store it in under the σ

function. The homescreen should now say "LinReg(ax+b)". Press $y \rightarrow \text{Å} \rightarrow \text{Ç}$

$y \rightarrow \text{Å} \rightarrow \text{Ç} \rightarrow \sim$ (Y-VARS, 1:Function) \downarrow and Select "1:Y₁". Press

\downarrow . The screen should now appear as it does to the right.

Press \downarrow once again, the screen should look like it does below:

```
LinReg(ax+b) L1,
L2, Y1
```

```
LinReg
y=ax+b
a=-1.720636E-5
b=.4505445079
r2=.9011585514
r=-.9492937119
```

The values of r^2 and r give us a sense of how closely our data correlates to a linear equation. The closer these values are to 1, the better the correlation. In this case, the correlation is not very close. This indicates that there is not a linear relationship between time (t) and [NO₂], so the reaction is not zero order.

Repeat the process from the top of the page, exploring linear relationships between t (L_1) and ln[NO₂] (L_3) which would indicate a first order relationship.

Press ... \sim (CALC), press \downarrow . Scroll down to **4:LinReg(ax+b)** and press \downarrow .

We will now perform a linear regression on the contents of L_1 and L_3 .

We would also like to store the resulting linear equation for later use.

We will store it in under the σ function. The homescreen should now

say "LinReg(ax+b)". Press $y \rightarrow \text{Å} \rightarrow \text{Ç} \rightarrow y \rightarrow \text{Å} \rightarrow \text{Ç} \rightarrow \sim$ (Y-VARS,

1:Function) \downarrow and Select "1:Y₂". Press \downarrow . Press \downarrow once

again, the screen should look like it does at the right.

```
LinReg
y=ax+b
a=-5.78132E-5
b=-.7699844332
r2=.9706856708
r=-.9852338153
```

Repeat the process from the top of the page, exploring linear relationships between t (L_1) and 1/[NO₂] (L_4) which would indicate a second order relationship.

Press ... \sim (CALC), press \downarrow . Scroll down to **4:LinReg(ax+b)** and press \downarrow .

We will now perform a linear regression on the contents of L_1 and L_4 .

We would also like to store the resulting linear equation for later use.

We will store it in under the σ function. The homescreen should now

say "LinReg(ax+b)". Press $y \rightarrow \text{Å} \rightarrow \text{Ç} \rightarrow y \rightarrow \uparrow \rightarrow \text{Ç} \rightarrow \sim$ (Y-VARS,

1:Function) \downarrow and Select "1:Y₃". Press \downarrow . Press \downarrow once

again, the screen should look like it does at the right.

```
LinReg
y=ax+b
a=2.0981833E-4
b=2.012452124
r2=.9987359526
r=.9993677764
```

This last equation comes closest to a correlation of 1. The reaction is second order. You can obtain the value for k (slope = a) from the screen above, or as Y₃ under the σ function.