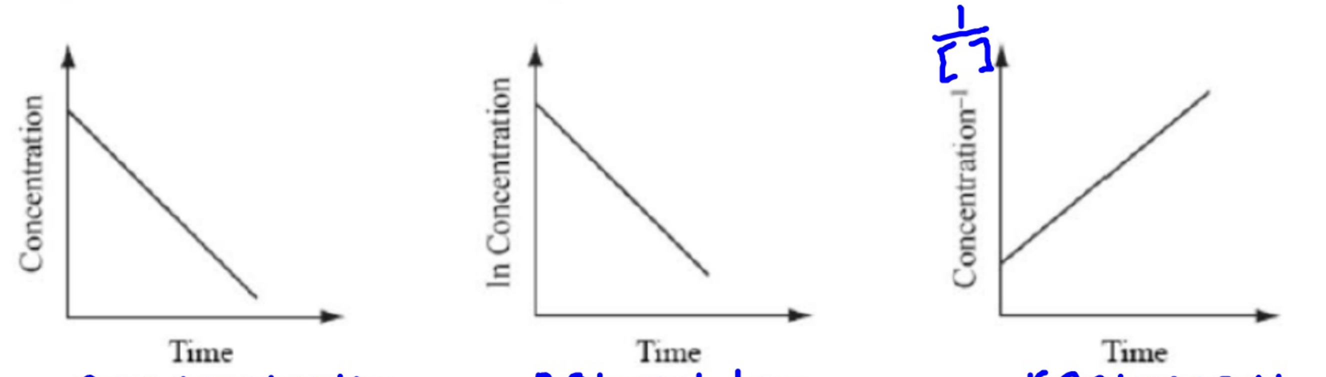
Integrated Rate Laws – use when given concentration and time data



concentration	natural log	reciprocal
Zero order k = negative slope	**First order** k = negative slope	**Second order** k = the slope

	y	=	mx	+	b
zero order	$[A]$	=	$-kt$	+	$[A_o]$
first order	$\ln[A]$	=	$-kt$	+	$\ln[A_o]$
second order	$1/[A]$	=	kt	+	$1/[A_o]$

<u>Graphing Calculator Tutorial</u> Set up your calculator so that *time* is always in L1.
Use L2, L3 and L4 to display the *y*-variables. Remember the list for what is placed on the *y*-axis is alphabetical (concentration, natural log of concentration and reciprocal concentration).

L1 = time (*x*-variable throughout!)		
L2 = concentration	[A]	straight line infers zero order
L3 = ln concentration	ln [A]	straight line infers first order
L4 = reciprocal concentration	1/[A]	straight line infers second order

Use this system to set up the data given in the following exercise:

We are going to perform 3 linear regressions to determine the order of the reactant. They will be L1,L2; L1,L3; L1,L4. Next, we will determine which regression has the best *r*-value [linear regression correlation coefficient in big people language!] We will also paste the best regression equation Y=
so that we can easily do other calculations commonly required on AP Chemistry Exam problems.

1. The decomposition of N_2O_5 in the gas phase was studied at constant temperature.

$$2\ N_2O_5(g) \rightarrow 4\ NO_2(g) + O_2(g)$$

The following results were collected:

zero r=-.94
1st r=-.99
2nd r=.94

$[N_2O_5]$	Time (s)
0.1000	0
0.0707	50
0.0500	100
0.0250	200
0.0125	300
0.00625	400

a) Determine the rate law and calculate the value of *k*.

$$rate = k[N_2O_5]^1$$

$$k = |slope| = |-6.9 \times 10^{-3}| = 6.9 \times 10^{-3}\ \frac{1}{s}$$

b) Calculate the concentration of $N_2O_5(g)$ at 250 s.

integrated rate law: $\ln[N_2O_5] = -6.9 \times 10^{-3}\ t - 2.3$

at $t = 250s$: $\ln[N_2O_5] = -6.9 \times 10^{-3}(250) - 2.3$

$\ln[N_2O_5] = -4.025$

$[N_2O_5] = e^{-4.025} = 0.018\ M$

c) Calculate the concentration of $N_2O_5(g)$ at 600 s.

$\ln[N_2O_5] = -6.9 \times 10^{-3}\ t - 2.3$

$\ln[N_2O_5] = -6.9 \times 10^{-3}(600) - 2.3$

$\ln[N_2O_5] = -6.44$

$[N_2O_5] = e^{-6.44} = 2 \times 10^{-3}\ M$

d) At what time is the concentration of $N_2O_5(g)$ equal to 0.00150 M?

$\ln(0.00150) = -6.9 \times 10^{-3}\ t - 2.3$

$t = 610\ s$

2. For the reaction of $(CH_3)_3CBr$ with OH^-,

$$(CH_3)_3CBr + OH^- \rightarrow (CH_3)_3COH + Br^-$$

The following data were obtained in the laboratory.

zero: r = -.991

1st: r = -.999

2nd: r = .992

Time (s)	$[(CH_3)_3CBr]$
0	0.100
30.0	0.074
60.0	0.055
90.0	0.041

a) Determine the order of this reaction. Sketch an appropriate graph.

1st order w/ respect to $(CH_3)_3CBr$

b) Calculate the value of the rate constant and include proper units.

$k = 9.9 \times 10^{-3} \frac{1}{s}$

c) At what time is the concentration of $(CH_3)_3CBr$ equal to [0.086]?

$\ln[(CH_3)_3CBr] = -9.9 \times 10^{-3} t - 2.3$

$\ln(0.086) = -9.9 \times 10^{-3} t - 2.3$

$t = 15 \text{ s}$

d) What is the concentration of $(CH_3)_3CBr$ after 2 minutes?

$\ln[(CH_3)_3CBr] = -9.9 \times 10^{-3}(120) - 2.3$

$\ln[(CH_3)_3CBr] = -3.488$

$[(CH_3)_3CBr] = e^{-3.488}$

$= 0.031 \text{ M}$