Butadiene Decomposition

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Worksheet for examining second order chemical reaction data for decomposition of butadiene.

```
> restart;
  with(plots) : #Load in plots package
  with(CurveFitting) : #Maple's curve fitting package
```

Times at which data was taken (seconds)

```
> times := [0, 1000, 1800, 2800, 3600, 4400, 5200, 6200]; #Times, in seconds
```

Butadiene concentration, moles per liter at each time above

```
> data := [0.01, 0.00625, 0.00476, 0.0037, 0.00313, 0.0027, 0.00241, 0.00208];
      #Butadiene concentrations, moles per liter
```

Number of data points

```
> N := nops(data)
```

Plot the data versus time. Call the plot "plot1".

```
> plot1 := pointplot([seq([times[j], data[j]], j = 1 ..N)], symbol = solidcircle, symbolsize = 20)
```

Does not look 0th order. Is it first order? Try a logarithmic transformation of the data (as was done for H2O2).

```
> log_of_data := [seq(ln(data[j]), j = 1 ..N)]
```

Fit a line y = -k*t+b to this data. We'll use Maple's built-in curve fitting (and examine how it works in Chapter 3).

```
> bestline := LeastSquares(times, log_of_data, t, curve = -k·t + b)
```

Plot this line and display with plot of log data

```
> plot1log := pointplot([seq([times[j], log_of_data[j]], j = 1 ..N)], symbol = solidcircle,
      symbolsize = 20) :
  plot2 := plot(bestline, t = 0 ..6000, color = blue) :
  display(plot1log, plot2)
```

Hmm, not too good. Doesn't appear to be first order...

```
>
```