

Decomposition of Butadiene

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This is a Mathematica notebook to illustrate the analysis of data concerning the decomposition of butadiene.

The times at which concentration data was taken (seconds):

```
In[18]:= times = {0, 1000, 1800, 2800, 3600, 4400, 5200, 6200}
```

The measured concentration (moles per liter) at each time:

```
In[19]:= data = {0.01, 0.00625, 0.00476, 0.0037, 0.00313, 0.0027, 0.00241, 0.00208}
```

Make a logarithmic transformation of the concentrations

```
In[20]:= logdata = Log[data]
```

And plot (first install into 2 x 6 matrix "pdata"):

```
In[23]:= pdata = Transpose[{times, logdata}];  
plt1 = ListPlot[pdata,  
  AxesLabel → {"time (seconds)", "log(concentration)"}, AxesOrigin → {0, -4.5}]
```

This is not a straight line, so this is not first order. Still, fit a line and see how it looks

```
In[25]:= line = Fit[pdata, {1, x}, x]
```

Evaluate line at each time, superimpose a graph of the line on a plot with the log data

```
In[26]:= plt2 = Plot[line, {x, 0, 6200}, PlotStyle → {Red}];  
Show[plt1, plt2,  
  AxesLabel → {"time (seconds)", "log(concentration)"}, AxesOrigin → {0, -4.5}]
```

Perhaps it's second order...