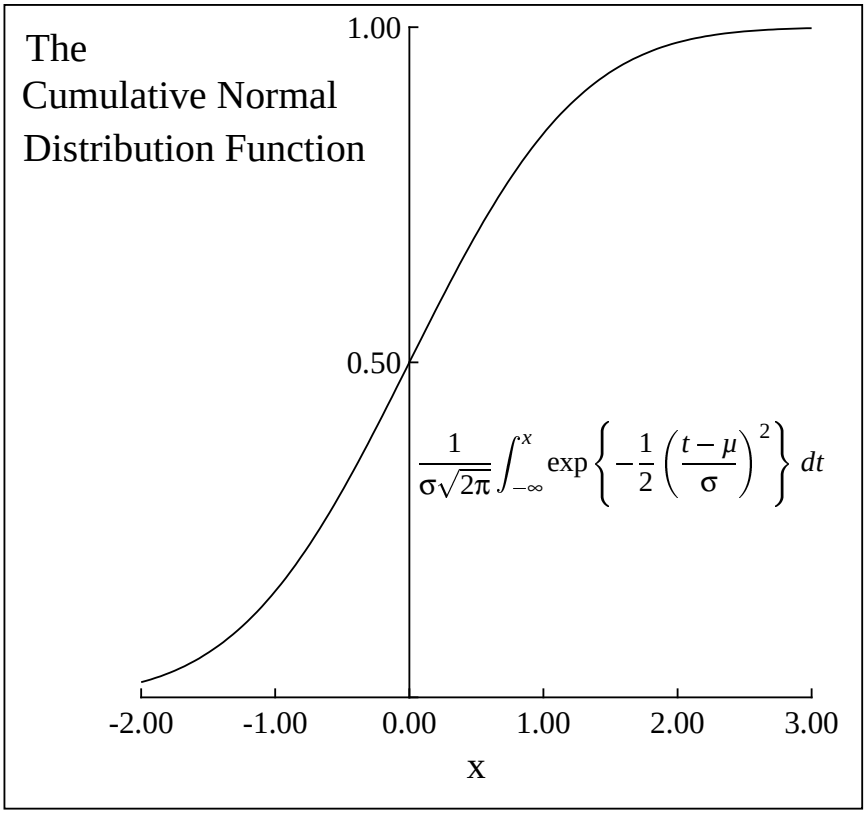
LaTeX Maths Options

You can add equations to graphs directly, but this will be a compromise, as specialized type setting techniques are required to display maths correctly. The LaTeX system is pre-eminent in the field of maths type-setting and the PSfrag system, as revised by David Carlisle and others, provides a simple way to add equations to SimFIT graphs. For the next figure **makdat** generated a Normal cdf with $\mu = 0$ and $\sigma = 1$, then **simplot** created `cdf.eps` with the key `phi(x)`, which was then used by this stand-alone code to generate the figure, where the equation substitutes for the key. LaTeX PostScript users should be aware that SimFIT PostScript file format has been specially designed to be consistent with the PSfrag package but, if you want to then use GhostScript to create graphics file, say .png from .eps, the next section should be consulted.

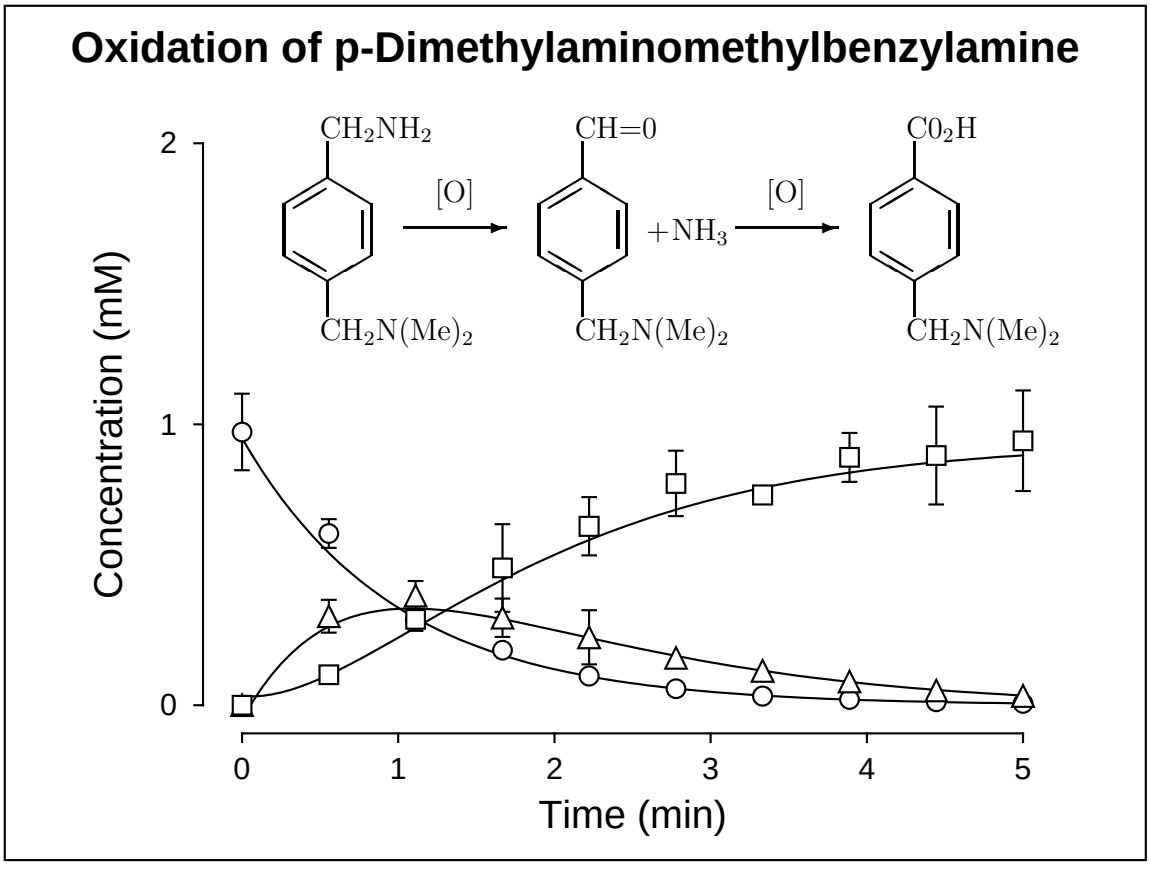
```
\documentclass[dvips,12pt]{article}
   \usepackage{graphicx}
   \usepackage{psfrag}
   \pagestyle{empty}
\begin{document}
\large
\psfrag{phi(x)}{$\displaystyle
   \frac{1}{\sigma \sqrt{2\pi}}
   \int_{-\infty}^x \exp\left\{
  -\frac{1}{2} \left( \frac{t-\mu}{\sigma} \right)^2 \right\}\,dt$}
\mbox{\includegraphics[width=6.0in]{cdf.eps}}
\end{document}
```



LaTeX Chemical FormulæOptions

LaTeX code, as below, is intended for document preparation and adds white space to the final .ps file. The easiest way round this complication is to add an outline box to the plot, as in the next figure. Then, after the .png file has been created, it can be input into, e.g., GIMP, for auto clipping to remove extraneous white space, followed by deletion of the outline box if required.

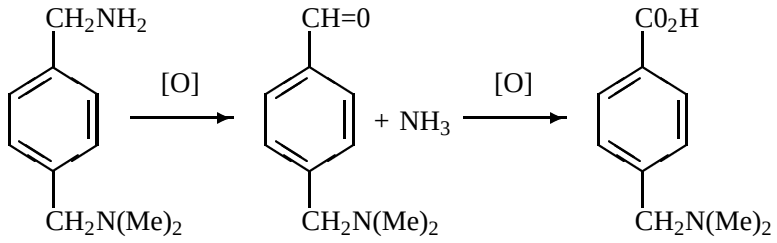
```
\documentclass[dvips,12pt]{article}
   \usepackage{graphicx}
   \usepackage{psfrag}
   \usepackage{carom}
   \pagestyle{empty}
\begin{document}
\psfrag{formula}
{\begin{picture}(3000,600)(0,0)
\thicklines
\put(0,0){\bzdrv{1==CH$_{2}$NH$_{2}$;4==CH$_{2}$N(Me)$_{2}$}}
\put(700,450){\vector(1,0){400}}
\put(820,550){[O]}
\put(1000,0){\bzdrv{1==CH=0;4==CH$_{2}$N(Me)$_{2}$}}
\put(1650,400){+}
\put(1750,400){NH$_{3}$}
\put(2000,450){\vector(1,0){400}}
\put(2120,550){[O]}
\put(2300,0){\bzdrv{1==C0$_{2}$H;4==CH$_{2}$N(Me)$_{2}$}}
\end{picture}}
\mbox{\includegraphics{chemistry.eps}}
\end{document}
```



LaTeX Composite Graphs Options

The technique used to combine sub-graphs into a composite graph is easy. First use your drawing or painting program to save the figures of interest in the form of eps files. Then the SIMFIT graphs and any component eps files are read into **editps** to move them and scale them until the desired effect is achieved. In the next figure, data were generated using **deqsol**, error was added using **adderr**, the simulated experimental data were fitted using **deqsol**, the plot was made using **simplot**, the chemical formulae and mathematical equations were generated using LaTeX and the final graph was composed using **editps**.

A kinetic study of the oxidation of *p*-Dimethylaminomethylbenzylamine



$$\frac{d}{dt}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -k_{+1} & k_{-1} & 0 \\ k_{+1} & (-k_{-1}-k_{+2}) & k_{-2} \\ 0 & k_{+2} & -k_{-2} \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix}, \begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$