

## **Fitting Multiple Reaction Peaks**

The 1st-order, nth-order, nucleation, Gaussian distribution, and Weibull distribution models have the capability of fitting up to three parallel reactions. With up to four kinetic parameters per reaction and up to two independent fractions, there are up to 14 independent parameters. However, nonlinear regression often has trouble reliably determining more than three parameters at once. When fitting more than one reaction, we have had more success fixing all but three or four parameters, with reasonable estimates for the others. The optimized parameters can then be fixed and regression done on three or four others, and so on. Sometimes, it is useful to tie the frequency factors together by making the initial guesses the same. For well-separated reaction peaks at a constant heating rate, the data files could be split into high and low temperature components and the two peaks initially fitted independently, then the entire reaction fitted at once with the independently determined parameters as initial guesses. While these manual iteration methods sound time-consuming, the process actually goes quite fast, and reasonable rate parameters can be derived within 30 min or so.