

Bain AD, Rex DM, Smith RN. Fitting dynamic NMR lineshapes. *Magn Reson Chem* 2001; 39: 122-126.

#### ABSTRACT

The lineshapes in an NMR spectrum, due to dynamic processes within the sample, provide an excellent way of measuring the rates of these processes. As the process speeds up, lines broaden, coalesce and finally sharpen into an average peak. Mathematical techniques for simulating these lineshapes have long been available, and rates can be extracted by fitting the calculated lineshape to the experiment. This is often done by manual iteration and visual comparison. The principal iterative program, DNMR5, is somewhat clumsy by modern standards. A recent reformulation of the theory of the lineshapes, which describes the spectrum as a sum of transitions, simplifies setting up the iterative process. This approach is described in general, and illustrated with the two-site equally-populated case.