

The fitting of NMR relaxation decays of sugar/water mixtures

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Serious errors can be introduced in the estimation of the concentration and decay time of immobile and mobile components in samples, if appropriate functions are not used for the fitting of simple free induction decays (FID). The proton FID's of maltose water mixtures at low temperatures exhibit a pronounced oscillation and the usual combination of Gaussian and exponential functions is inappropriate. A sinc function multiplied by a Gaussian has frequently been used to fit these data, however more appropriate functions can be found by examining the origin of the oscillation in the FID. The origin of the FID lies in the distribution of magnetic fields experienced by resonant nuclei. The local field distribution is dominated by near neighbour interactions and broadened by interaction with more distant nuclei. The decay is the Fourier transform of this combination. Whereas the sinc function assigns a rectangular function to the interaction between near neighbours, a Pake function represents the interaction of the magnetic fields between neighbouring nuclei. Furthermore, a distribution of pake functions corresponding to different near neighbour distances is more realistic for a carbohydrate water mixture having many different inter-proton distances. A series of fits to maltose water mixtures over a temperature range of 190 – 270K is presented showing the improved fits which are possible using the above functions.

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