Reconstruction of Two-Dimensional Spectra from One-Dimensional Projections—Examples from Solid State NMR.

Bibhuti B. Das1, K. V. Ramanthan2, Daniel H. Arcos1, John P. Staab1, J.B. Spitzmesser1, Laura L. Holte1, and F. David Doty1

1. Doty Scientific Inc. 700 Clemson Rd, Columbia, SC, USA
2. Indian Institute of Science, Bangalore, India

The use of Projection Reconstruction (PR) to obtain two dimensional (2D) spectra from one-dimensional (1D) data in the solid state is illustrated. The method exploits multiple 1D spectra obtained using magic angle spinning and off-magic angle spinning. The spectra recorded under the influence of scaled heteronuclear scalar and dipolar couplings in the presence of homonuclear dipolar decoupling sequences have been used to reconstruct J/D Resolved 2D-NMR spectra. The use of just two 1D spectra is observed sufficient to reconstruct a J-resolved 2D-spectrum while a Separated Local Field (SLF) 2D-NMR spectrum could be obtained from three 1D spectra. The experimental techniques for recording the 1D spectra and procedure of reconstruction are discussed and the reconstructed results are compared with 2D experiments recorded in traditional methods. The application of the technique has been made to small molecules in solid polycrystalline samples and partially oriented in magnetic field. Implementation of PR-NMR in solid state provides high-resolution spectra as well as leads to significant reduction in experimental time. The experiments are relatively simple and are devoid of several technical complications involved in performing the 2D experiments.