A Theoretical Investigation of 2D MAXY-JRES NMR Spectroscopy of CD$_n$CD$_m$ Groups

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There exists a variety of multiple-pulse NMR experiments for spectral editing of complex molecules in solution. Maximum quantum correlation NMR (MAXY NMR) spectroscopy is one of the techniques for distinguishing CH$_n$ groups by editing $^1$H NMR spectra. Spectral assignments of 2D homonuclear $J$-resolved NMR spectroscopy become too difficult, due to complex overlapping spectra. In order to overcome this problem a new technique called 2D MAXY-JRES NMR spectroscopy, which is the combination of MAXY NMR and homonuclear $J$-resolved NMR spectroscopy, is used. In this study, product operator description of 2D MAXY-JRES NMR spectroscopy is performed for $I$S$_n$I$'$S$_m$ ($I = I' = {1\over 2}; S = S' = 1; n = 1, 2, 3; m = 1, 2$) multi-spin systems. Experimental suggestions are made and simulated spectra are presented for the 2D MAXY-JRES NMR experiment. Therefore, it is shown that 2D MAXY-JRES NMR spectroscopy can be used to distinguish CD, CD$_2$ and CD$_3$ groups from each other in CD$_n$CD$_m$ groups.

Key words: NMR; MAXY-JRES; Product Operator Formalism; Spin-1.