

A Theoretical Investigation of 2D MAXY-*J*RES NMR Spectroscopy of CD_nCD_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 1H 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-*J*RES 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-*J*RES NMR spectroscopy is performed for $IS_nI'S'_m$ ($I = I' = \frac{1}{2}$; $S = S' = 1$; $n = 1, 2, 3$; $m = 1, 2$) multi-spin systems. Experimental suggestions are made and simulated spectra are presented for the 2D MAXY-*J*RES NMR experiment. Therefore, it is shown that 2D MAXY-*J*RES NMR spectroscopy can be used to distinguish CD , CD_2 and CD_3 groups from each other in CD_nCD_m groups.

Key words: NMR; MAXY-*J*RES; Product Operator Formalism; Spin-1.