Turkish Journal of Physics

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2D MAXY--JRES NMR Spectroscopy of CH_nCH_m (CA_nCX_m) Groups: Product Operator Theory and Simulation

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Abstract: There exist a variety of multi-pulse NMR experiments for spectral editing of complex molecules in solution. Maximum quantum correlation NMR spectroscopy (MAXY NMR) 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-JRES NMR spectroscopy, which is the combination of MAXY NMR and homonuclear J-resolved NMR spectroscopy techniques, is used. In this study, product operator theory of 2D MAXY-JRES NMR spectroscopy is performed for IS_n $I'S'_m$ (I = I' = S = S' = 1\2; n = 1, 2; m = 1,2,3) multi-spin systems. By using obtained theoretical results, simulated spectra of 2D MAXY-JRES NMR spectroscopy are presented for several CH_nCH_m (CA_nCX_m) groups.

Key Words: NMR, MAXY-JRES, product operator formalism, multi-spin systems

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Turk. J. Phys., **31**, (2007), 347-354.
Full text: pdf
Other articles published in the same issue: Turk. J. Phys.,vol.31,iss.6.