A Complete Product Operator Theory for IS ($I = 1$, $S = 1$) Spin System and Application to 3D HMQC-COSY NMR Experiment

İrfan Şaka, Sedat Gümüş, and Azmi Gençten

Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139, Samsun, Turkey

Reprint requests to A. G.; Fax: +90 362 4576081; E-mail: gencten@omu.edu.tr

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There exist a variety of multi-pulse NMR experiments for spectral assignment of complex molecules in solution. The conventional heteronuclear multiple-quantum coherence (HMQC) NMR experiment provides correlation between weakly coupled hetero-nuclei. The COSY is one of the most popular two-dimensional NMR experiment which is used to correlate J-coupled homo-nuclei of spectral assignment. The combination of the conventional HMQC and COSY NMR experiments yields a new experiment called 3D HMQC-COSY NMR experiment. The product operator theory is widely used for the analytical descriptions of multi-pulse NMR experiments for weakly coupled spin systems in liquids. In this study, complete product operator theory for weakly coupled IS ($I = 1$, $S = 1$) spin system is presented by obtaining the evolutions of the product operators under the spin-spin coupling Hamiltonian. As an application and a verification, analytical descriptions of 3D HMQC-COSY NMR experiment are obtained for weakly coupled $IS_nI'S'_m$ ($I = I' = 1/2$; $S = S' = 1$; $n = 1, 2, 3$; $m = 1, 2$) multi-spin systems. Then the estimated spectra of this experiment for various multi-spin systems are explained in detail.

Key words: Product Operator Theory; Spin-1; 3D HMQC-COSY; NMR.