

# 2D MAXY–JRES NMR Spectroscopy of $\text{CH}_n\text{CH}_m$ ( $\text{CA}_n\text{CX}_m$ ) 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  $\text{CH}_n$  groups by editing  $^1\text{H}$  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 techniques, is used. In this study, product operator theory of 2D MAXY-JRES NMR spectroscopy is performed for  $IS_nI'S'_m$  ( $I = I' = S = S' = \frac{1}{2}$ ;  $n = 1, 2$ ;  $m = 1, 2, 3$ ) multi-spin systems. By using obtained theoretical results, simulated spectra of 2D MAXY-JRES NMR spectroscopy are presented for several  $\text{CH}_n\text{CH}_m$  ( $\text{CA}_n\text{CX}_m$ ) groups.

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

## 1. Introduction

There exists a large number of homo and heteronuclear multiple-pulse 1D, 2D and 3D Nuclear Magnetic Resonance (NMR) experiments. Maximum quantum correlation NMR spectroscopy (MAXY NMR) is one of the techniques for distinguishing  $\text{CH}_n$  groups by editing  $^1\text{H}$  NMR spectra [1-7].  $^{13}\text{C}$  NMR spectroscopy is also widely used in editing methods such as DEPT [8] and SEMUT [9]. Editing and selective detection methods for  $^1\text{H}$  NMR spectroscopy are reviewed elsewhere [10]. In homonuclear J-resolved NMR spectroscopy, the chemical shift and spin-spin coupling parameters are resolved along the two different axes for the same kind of coupled nuclei such as  $^1\text{H}$ . Sometimes, 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 and homonuclear J-resolved NMR spectroscopy techniques, is used [3]. This technique is used for the identifications of  $\text{CH}_n\text{CH}_m$  groups in complex samples such as biological fluids [3].

As NMR is a quantum mechanical phenomenon, nuclear spin systems can be treated by quantum mechanical methods. The product operator formalism, as a simple quantum mechanical method, has been developed for the analytical description of multiple-pulse NMR experiments on weakly coupled spin systems

in liquids having spin  $1/2$  and spin 1 nuclei [11–19]. In this formalism, the spin operators themselves and their direct products, called product operators, are used. By using product operator theory, SEMUT NMR spectroscopy is applied to  $CD_n$  groups [20]. Experimental and theoretical investigations of  $^{13}C$  DEPT NMR spectroscopy for  $CD_n$  systems are presented elsewhere [21]. For  $CH_n$  and  $CD_n$  groups, product operator theory of 2D DEPT J-resolved NMR experiment is investigated [22–23]. Product operator theory for spin  $3/2$  and its application for 2D J-resolved NMR spectroscopy is reported [24]. For spin systems having spin  $3/2$  nuclei, by using the product operator formalism, theoretical investigations of 3D J-resolved, DEPT, SEMUT, INEPT and RINEPT NMR experiments are also presented [25–27].

In this study, by using product operator formalism, theoretical results are obtained for 2D MAXY-JRES NMR experiment for  $IS_nI'S'_m$  ( $I = I' = S = S' = \frac{1}{2}$ ;  $n = 1, 2$ ;  $m = 1, 2, 3$ ) multi-spin systems. Then, by using these theoretical results, simulated spectra of 2D MAXY–JRES NMR experiment for various groups are obtained. Therefore, by using this technique, the identifications of  $CH_nCH_m$  ( $CA_nCX_m$ ) groups are clearly explained.

## 2. Theory

The density matrix operator is expressed as a linear combination of base operators  $B_S$  [11],

$$\sigma(t) = \sum_S b_S(t)B_S. \quad (1)$$

For  $IS$  ( $I = 1/2$ ,  $S = 1/2$ ) spin system, the complete base set consists of 16 product operators such as  $E, I_y, I_yS_z, I_xS_z$ .

Time dependency of the density matrix is given by [15,17]

$$\sigma(t) = \exp(-i\mathcal{H}t)\sigma(0)\exp(i\mathcal{H}t), \quad (2)$$

where  $\mathcal{H}$  is the total Hamiltonian which consists of radio frequency (r.f.) pulse, chemical shift and spin-spin coupling Hamiltonians and  $\sigma(0)$  is the density matrix at  $t=0$ . After employing the Hausdorff formula [15],

$$\begin{aligned} \exp(-i\mathcal{H}t)A\exp(i\mathcal{H}t) = & A - (it)[\mathcal{H}, A] + \frac{(it)^2}{2!}[\mathcal{H}, [\mathcal{H}, A]] \\ & - \frac{(it)^3}{3!}[\mathcal{H}, [\mathcal{H}, [\mathcal{H}, A]]] + \dots \end{aligned} \quad (3)$$

evolutions of product operators under the r.f. pulse, chemical shift and spin-spin coupling Hamiltonians can easily be obtained [11–16]. At any time during the experiment, the ensemble averaged expectation value of the spin angular momentum, e.g. for  $I_y$ , is

$$\langle I_y \rangle = \text{Tr}[I_y\sigma(t)], \quad (4)$$

where  $\sigma(t)$  is the density matrix operator calculated from equation (2) at any time. As  $\langle I_y \rangle$  is proportional to the magnitude of the  $y$ -magnetization, it represents the signal detected on  $y$ -axis. So, in order to estimate the free induction decay (FID) signal of a multi-pulse NMR experiment, density matrix operator should be obtained at the end of the experiment.

## 3. Results and Discussion

In this section, the analytical descriptions of 2D MAXY-JRES NMR experiment for  $CH_nCH_m$  groups are presented by using product operator formalism. This section is divided into two subsections. In the first subsection, theoretical results of analytical description for 2D MAXY-JRES NMR experiment are presented. In the second one, simulated spectra of 2D MAXY-JRES NMR experiment are obtained for several  $CH_nCH_m$  ( $CA_nCX_m$ ) groups having weak coupling between H nuclei.

### 3.1. Product operator theory

Pulse sequence illustrated in Figure 1 is used for the product operator description of 2D MAXY-JRES NMR experiment [3]. The density matrix operator at each stage of experiment is labelled with numbers.  $^{13}\text{C}$  is treated as spin  $I$  and  $I'$ ; and  $^1\text{H}$  as spin  $S$  and  $S'$  in Figure 1. In the pulse sequence, optimum value of  $\Delta$  is  $1/(2J_{IS})$ ,  $\Delta'$  is a short compensation delay,  $t_1$  is the incremented evolution delay during which homonuclear weak spin-spin coupling Hamiltonian ( $\mathcal{H}_J(S'S') = 2\pi J_{S'S'}S_zS'_z$ ) takes place between  $S$  and  $S'$  spins. This Hamiltonian can be applied for  $\text{CH}_n\text{CH}_m$  ( $\text{CA}_n\text{CX}_m$ ) groups having weak coupling between H nuclei.  $t_2$  is the acquisition time for  $S$  and  $S'$  spins. Starting from the density matrix operator at thermal equilibrium, one should apply the required Hamiltonians during the pulse sequence and obtain the density matrix operators for each stage of the experiment. To follow these processes by hand becomes too difficult for multi-spin systems. In order to overcome this problem a computer program in Mathematica is written in this study [28-29]. This program is used to obtain the density matrix operator at the end of the experiment for different spin systems.

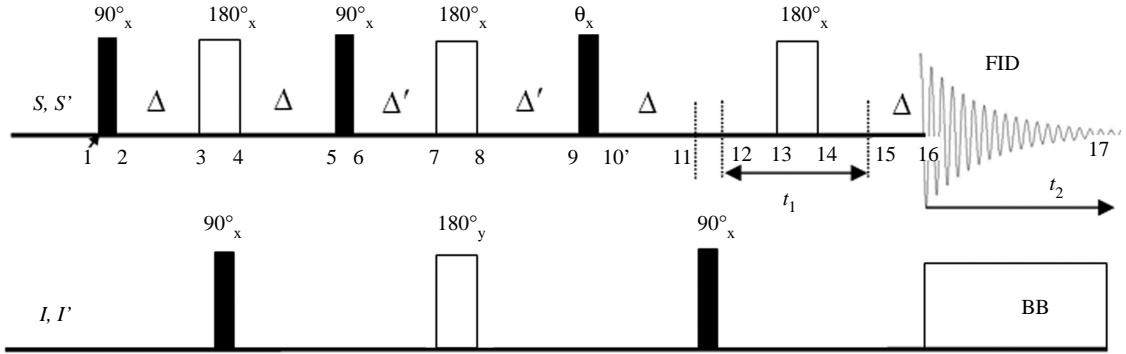


Figure 1. 2D MAXY-JRES NMR pulse sequence.

For  $ISI'S'$  multi-spin system, the density matrix at thermal equilibrium is  $\sigma_1 = S_z + S'_z$ . By using the computer program following density matrices for each labelled point are obtained:

$$\sigma_1 \xrightarrow{90_x^0(S,S')} -S_y - S'_y \equiv \sigma_2, \quad (5)$$

$$\sigma_2 \xrightarrow{\mathcal{H}_J(IS)\Delta + \mathcal{H}'_J(I'S')\Delta} 2I_zS_x + 2I'_zS'_x = \sigma_3, \quad (6)$$

$$\sigma_3 \xrightarrow{180_x^0(S,S') + 90_x^0(I,I')} 2I_yS_x + 2I'_yS'_x = \sigma_4, \quad (7)$$

$$\sigma_{10} = -2I_yS_x - 2I'_yS'_x, \quad (8)$$

$$\sigma_{12} = 2I_zS_x + 2I'_zS'_x, \quad (9)$$

$$\sigma_{12} \xrightarrow{\mathcal{H}_J(S-S')t_1/2 + 180_x^0(S,S') + \mathcal{H}_J(S-S')t_1/2} 2I_zS_xc_J + 2I'_zS'_xc_J + 4I_zS_yS'_zS_J + 4I'_zS'_yS'_zS'_J, \quad (10)$$

$$\sigma_{17} = S_yc_Jc_S + S'_yc_Jc'_S - S_xc_Js_S - S'_xc_Js'_S - 2S_yS'_zs_Js_S - 2S_zS'_ys_Js'_S - 2S_xS'_zc_Js_S - 2S_zS'_xc_Js'_S, \quad (11)$$

where  $\mathcal{H}_J(IS) = 2\pi J_{IS}I_zS_z$ ,  $\mathcal{H}'_J(I'S') = 2\pi J_{I'S'}I'_zS'_z$ ,  $\mathcal{H}_J(SS') = 2\pi J_{SS'}S_zS'_z$ ,  $c_J = \cos(\pi J_{SS'}t_1)$ ,  $s_J = \sin(\pi J_{SS'}t_1)$ ,  $c_S = \cos(\Omega_S t_2)$ ,  $s_S = \sin(\Omega_S t_2)$ ,  $c'_S = \cos(\Omega'_S t_2)$  and  $s'_S = \sin(\Omega'_S t_2)$ . In density matrix operator, only the terms with observable product operators are kept, as they are the only ones that contribute to the signal on  $y$ -axis detection. Then, the density matrix operator for  $ISI'S'$  is equals to  $\sigma_{17} = S_y c_J c_S + S'_y c_J c'_S$ . The density matrix operators obtained at the end of the experiment for  $ISI'S'$ ,  $ISI'S'_2$ ,  $ISI'S'_3$ ,  $IS_2I'S'_2$  and  $IS_2I'S'_3$  multi-spin systems are given in Table 1.

**Table 1.** Density matrix operators at end of the 2D MAXY-JRES NMR experiment for various spin systems.

Spin system	$\sigma_{17}$
$ISI'S'$	$S_y c_J c_S + S'_y c_J c'_S$
$ISI'S'_2$	$S_y c_J^2 c_S - (S'_{1y} + S'_{2y}) c_J c'_S \sin(\theta)$
$ISI'S'_3$	$S_y c_J^3 c_S + (S'_{1y} + S'_{2y} + S'_{3y}) c_J c'_S \sin^2(\theta)$
$IS_2I'S'_2$	$-(S_{1y} + S_{2y}) c_J^2 c_S \sin(\theta) - (S'_{1y} + S'_{2y}) c_J^2 c'_S \sin(\theta)$
$IS_2I'S'_3$	$-(S_{1y} + S_{2y}) c_J^3 c_S \sin(\theta) + (S'_{1y} + S'_{2y} + S'_{3y}) c_J^2 c'_S \sin^2(\theta)$

The magnetisation along the  $y$ -axis is proportional to  $\langle S_y \rangle + \langle S'_y \rangle$  and

$$M_y(t_1, t_2) \propto \langle S_y \rangle + \langle S'_y \rangle = \text{Tr}[S_y \sigma_{17}] + \text{Tr}[S'_y \sigma_{17}]. \quad (12)$$

Now it is necessary to obtain  $\text{Tr}[S_y O]$  and  $\text{Tr}[S'_y O']$  values of observable product operators indicated by  $O$  and  $O'$ .  $\text{Tr}[S_y O]$  and  $\text{Tr}[S'_y O']$  values are calculated by a computer program and the results for several spin systems are given in Table 2.

**Table 2.**  $\sum_{i=1}^n \text{Tr}[S_{iy} O]$  and  $\sum_{j=1}^m \text{Tr}[S'_{jy} O']$  values for observable product operators of  $IS_n I' S'_m$  ( $I = I' = S = S' = \frac{1}{2}$ ;  $n = 1, 2$ ;  $m = 1, 2, 3$ ) multi-spin systems.

Spin system	Product operator ( $O$ )	Product operator ( $O'$ )	$\sum_{i=1}^n \text{Tr}[S_{iy} O]$	$\sum_{j=1}^m \text{Tr}[S'_{jy} O']$
$ISI'S'$	$S_y$	$S'_y$	4	4
$ISI'S'_2$	$S_y$	$S'_{1y} + S'_{2y}$	8	16
$IS_2I'S'_2$	$S_{1y} + S_{2y}$	$S'_{1y} + S'_{2y}$	32	32
$ISI'S'_3$	$S_y$	$S'_{1y} + S'_{2y} + S'_{3y}$	16	48
$IS_2I'S'_3$	$S_{1y} + S_{2y}$	$S'_{1y} + S'_{2y} + S'_{3y}$	64	96

By using Table 2, the relationship

$$\langle S_y \rangle + \langle S'_y \rangle = 4c_J s_S + 4c_J c'_S. \quad (13)$$

is obtained for  $ISI'S'$  spin system. This equation shows that the spin-spin coupling information appears on F1 axis and represents two coherences for both  $S$  and  $S'$  spins with phases of  $\pi J t_1 \pm \Omega_S t_2$  and  $\pi J t_1 \pm \Omega'_S t_2$ ; and half of the amplitude in each component. Therefore, they both give doublets signals at the coordinates of  $(J/2, \Omega_S)$  and  $(-J/2, \Omega_S)$  for  $S$  spin and at the coordinates of  $(J/2, \Omega'_S)$  and  $(-J/2, \Omega'_S)$  for  $S'$  spin with the same intensity distribution of 1 : 1.

The  $\sum_{i=1}^n \text{Tr}[S_{iy} \sigma_{17}]$  and  $\sum_{j=1}^m \text{Tr}[S'_{jy} \sigma_{17}]$  values represent the FID signals of 2D MAXY-JRES NMR experiment for  $S$  and  $S'$  spins, respectively.  $\sum_{i=1}^n \text{Tr}[S_{iy} \sigma_{17}]$  values and their signal coordinates with the intensity distribution are presented in Table 3 for  $S$  spins. For  $S'$  spins,  $\sum_{j=1}^m \text{Tr}[S'_{jy} \sigma_{17}]$  values and their signal coordinates with the intensity distribution are presented in Table 4.

**Table 3.**  $\sum_{i=1}^n \text{Tr} [S_{iy}\sigma_{17}]$  values and their signal coordinates with the intensity distribution for  $S$  spins of  $IS_nI'S'_m$  ( $I = I' = S = S' = \frac{1}{2}$ ;  $n = 1, 2$ ;  $m = 1, 2, 3$ ) multi-spin systems.

Spin system	$\sum_{i=1}^n \text{Tr} [S_{iy}\sigma_{17}]$ values	Signal coordinates	Intensity distribution
$ISI'S'$	$4c_Jc_S$	$(J/2, \Omega_S), (-J/2, \Omega_S)$	1 : 1
$ISI'S'_2$	$8c_J^2c_S$	$(J, \Omega_S), (\Omega_S), (-J, \Omega_S)$	1 : 2 : 1
$ISI'S'_3$	$16c_J^3c_S$	$(3J/2, \Omega_S), (J/2, \Omega_S), (-J/2, \Omega_S), (-3J/2, \Omega_S)$	1 : 3 : 3 : 1
$IS_2I'S'_2$	$-32c_J^2c_S \sin(\theta)$	$(J, \Omega_S), (\Omega_S), (-J, \Omega_S)$	1 : 2 : 1
$IS_2I'S'_3$	$-64c_J^3c_S \sin(\theta)$	$(3J/2, \Omega_S), (J/2, \Omega_S), (-J/2, \Omega_S), (-3J/2, \Omega_S)$	1 : 3 : 3 : 1

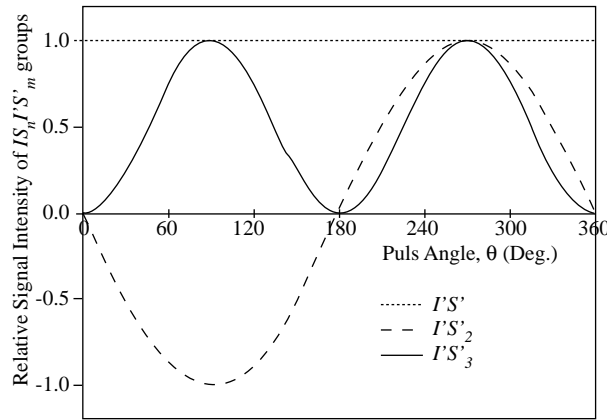
**Table 4.**  $\sum_{j=1}^m \text{Tr} [S'_{jy}\sigma_{17}]$  values and their signal coordinates with the intensity distribution for  $S'$  spins of  $IS_nI'S'_m$  ( $I = I' = S = S' = \frac{1}{2}$ ;  $n = 1, 2$ ;  $m = 1, 2, 3$ ) multi-spin systems.

Spin system	$\sum_{j=1}^m \text{Tr} [S'_{jy}\sigma_{17}]$ values	Signal coordinates	Intensity distribution
$ISI'S'$	$4c_Jc'_S$	$(J/2, \Omega'_S), (-J/2, \Omega'_S)$	1 : 1
$ISI'S'_2$	$16c_Jc'_S \sin(\theta)$	$(J/2, \Omega'_S), (-J/2, \Omega'_S)$	1 : 1
$ISI'S'_3$	$48c_Jc'_S \sin^2(\theta)$	$(J/2, \Omega'_S), (-J/2, \Omega'_S)$	1 : 1
$IS_2I'S'_2$	$32c_J^2c'_S \sin(\theta)$	$(J, \Omega'_S), (\Omega'_S), (-J, \Omega'_S)$	1 : 2 : 1
$IS_2I'S'_3$	$96c_J^2c'_S \sin^2(\theta)$	$(J, \Omega'_S), (\Omega'_S), (-J, \Omega'_S)$	1 : 2 : 1

The total FID values can be generalized as following:

$$\begin{aligned} \sum_{i=1}^n \text{Tr} [S_{iy}\sigma_{17}] + \sum_{j=1}^m \text{Tr} [S'_{jy}\sigma_{17}] = & (-1)^{n+1} n 2^{n+m} c_J^n \sin^{n-1}(\theta) c_S \\ & + (-1)^{m+1} m 2^{n+m} c_J^m \sin^{m-1}(\theta) c'_S. \end{aligned} \quad (14)$$

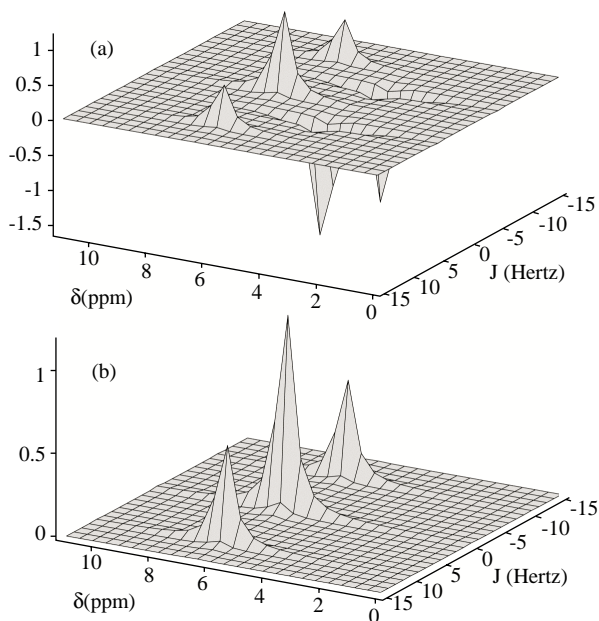
The relative signal intensity plots of 2D  $^1\text{H}$  MAXY-JRES NMR experiment for  $IS_nI'S'_m$  ( $I = I' = S = S' = \frac{1}{2}$ ;  $n = 1, 2$ ;  $m = 1, 2, 3$ ) multi-spin systems as functions of the edited-pulse angle  $\theta$  are presented in Figure 2. In order to identify  $\text{CH}_n\text{CH}_m$  groups, by using 2D  $^1\text{H}$  MAXY-JRES NMR experiment, the FID signals can be taken for three different angles of  $90^\circ$ ,  $180^\circ$  and  $270^\circ$ . As one can see from Figure 2, only signals coming from CH groups are observed for the angle of  $180^\circ$ . When the experiment is performed for an angle of  $90^\circ$ , the signals for CH and  $\text{CH}_3$  groups are positive and for  $\text{CH}_2$  groups are negative. For the angle of  $270^\circ$ , all groups give positive signals.


**Figure 2.** Relative signal intensity plots of 2D  $^1\text{H}$  MAXY-JRES NMR spectroscopy for  $IS_nI'S'_m$  spin systems as functions of the selective pulse angle  $\theta$ .

### 3.2. Simulated spectra

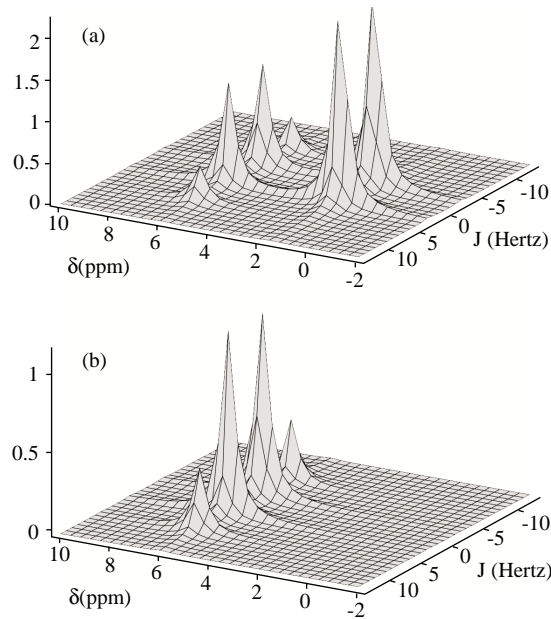
One should be aware of the fact that this experiment can be applied only for  $\text{CH}_n\text{CH}_m$  ( $\text{CA}_n\text{CX}_m$ ) groups having weak coupling between H nuclei. In simulated spectra, chemical shift values of  $^1\text{H}$  nuclei are set to 6.5, 4 and 1.5 ppm for CH,  $\text{CH}_2$  and  $\text{CH}_3$  groups, respectively. Spin-spin coupling constants between two H nuclei are assumed to be 10, 5 and 8 Hz in  $\text{CHCH}_2$ ,  $\text{CHCH}_3$  and  $\text{CH}_2\text{CH}_3$  groups, respectively.

For product operator description of NMR experiment, a computer program is written by Kanters et al. [30–31]. This is called Product Operator Formalism using Maple (POF.M). In order to obtain the simulated spectra, POF.M is implemented for Fourier transformation of theoretical representations of FID signals obtained in this study. Simulated spectra of 2D  $^1\text{H}$  MAXY-JRES NMR experiment for various groups are given in Figures 3, 4 and 5.

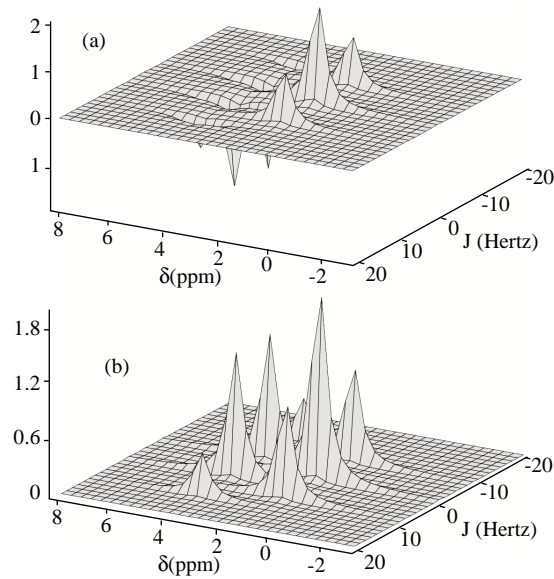


**Figure 3.** Simulated 2D  $^1\text{H}$  MAXY-JRES NMR spectra for  $IS1'S2'$  ( $\text{CHCH}_2$ ) spin systems for the angles of (a)  $\theta=90^\circ$  and (b)  $\theta=180^\circ$ .

Simulated spectra of  $IS1'S2'$  ( $\text{CHCH}_2$  groups) performed for  $90^\circ$  and  $180^\circ$  are presented in Figure 3(a) and Figure 3(b), respectively. For an angle of  $90^\circ$ , positive triplet for CH groups and negative doublet for  $\text{CH}_2$  groups are obtained. For the angle of  $180^\circ$ , while positive triplets are observed for CH groups, there is no signal coming from  $\text{CH}_2$  groups. In Figure 4(a) and Figure 4(b), simulated spectra of  $IS1'S3'$  ( $\text{CHCH}_3$  groups) performed for the angle of  $90^\circ$  and  $180^\circ$  are given, respectively. For the angle of  $90^\circ$  positive quartet for CH and positive doublet for  $\text{CH}_3$  groups are found. For the angle of  $180^\circ$  only positive quartet for CH groups are obtained. As shown in simulated spectra (Figures 3, 4 and 5) that one can easily identify CH,  $\text{CH}_2$  and  $\text{CH}_3$  groups from each other in  $\text{CH}_n\text{CH}_m$  groups by performing 2D MAXY-JRES NMR experiment for the angles of  $90^\circ$ ,  $180^\circ$  and  $270^\circ$ .



**Figure 4.** Simulated 2D <sup>1</sup>H MAXY-JRES NMR spectra for  $ISI'S'_3$  ( $\text{CHCH}_3$ ) spin systems for the angles of (a)  $\theta=90^\circ$  and (b)  $\theta=180^\circ$ .



**Figure 5.** Simulated 2D <sup>1</sup>H MAXY-JRES NMR spectra for  $IS_2I'S'_3$  ( $\text{CH}_2\text{CH}_3$ ) spin systems for the angles of (a)  $\theta=90^\circ$  and (b)  $\theta=270^\circ$ .

## 4. Conclusion

By using a computer program written in Mathematica, the product operator theory is applied for the analytical description of 2D MAXY-JRES NMR experiment for  $IS_nI'S'_m$  ( $I = I' = S = S' = \frac{1}{2}$ ;  $n = 1, 2$ ;  $m = 1, 2, 3$ ) multi-spin systems. Then, simulated spectra of this experiment are obtained for various groups by implementing POF.M program. It is shown that 2D MAXY-JRES NMR experiment can be easily used for identification of CH, CH<sub>2</sub> and CH<sub>3</sub> groups from each other in CH<sub>n</sub>CH<sub>m</sub> groups. As the

product operator theory can be used for weakly coupled spin systems, this experiment can be applied only for  $\text{CH}_n\text{CH}_m$  ( $\text{CA}_n\text{CX}_m$ ) groups having weak coupling between H nuclei.

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