A Theoretical Application of 3D J-Resolved NMR Spectroscopy for IS_nK_m (I = 1/2, S = 1/2 and 1, K = 3/2) Spin Systems

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In 3D J-resolved NMR spectroscopy, the chemical shift along one axis and the spin-spin coupling parameters along the two other different axes are resolved. Product operator theory is used for the analytical description of multi-dimensional NMR experiments on weakly coupled spin systems. In this study, the product operator description of heteronuclear 3D J-resolved NMR spectroscopy of weakly coupled $IS_n\ K_m$ (I = 1/2, S = 1/2 and 1, K = 3/2) spin systems is presented.

Key words: Product Operator; 3D J-Resolved NMR; Spin-3/2.

1. Introduction

There exists a large number of homo and heteronuclear multiple-pulse 1D, 2D, and 3D Nuclear Magnetic Resonance (NMR) experiments. 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 [1 – 7]. In this formalism, the spin operators themselves and their direct products, called product operators, are used. In one dimensional NMR, as the multiplets from different chemically shifted nuclei overlap, spectral assignments become too difficult. In order to resolve the chemical shift and spin-spin coupling parameters along the different axes, 2D and 3D J-resolved NMR spectroscopies are widely used [e.g. 8, 9]. In 3D J-resolved NMR spectroscopy, the chemical shift is resolved along one axis and the spin-spin coupling parameters along the two different axes. The product operator description of heteronuclear 2D J-resolved and 3D J-resolved NMR spectroscopies, respectively, for weakly coupled IS_n (I = 1/2, S = 1) and IS_nK_m (I = 1/2, S = 1/2 and 1, K = 1) spin systems has been reported in [10, 11]. The product operator theory for spin 3/2 and its application for 2D J-resolved NMR spectroscopy has recently been reported [12].

In this study, by using the product operator theory, analytical descriptions of heteronuclear 3D J-resolved NMR spectroscopy for the weakly coupled IS_nK_m(I = 1/2, S = 1/2 and 1, K = 3/2) spin systems are presented. This will be the first application of the product operator theory to 3D J-resolved NMR spectroscopy for these spin systems with spin 3/2 nuclei.

2. Theory

The density operator is expressed as a linear combination of base operators (B_S) [1]:

$$\sigma(t) = \sum_S b_S(t) B_S. \tag{1}$$

For an ISK (I = 1/2, S = 1/2 and K = 3/2) spin system the complete base set consists of 256 product operators such as $E, I_y, I_yS_z, I_xS_zK_z$. In case of an ISK (I = 1/2, S = 1 and K = 3/2) spin system the complete base set consists of 576 product operators.

The time dependency of the density matrix is given by [2, 3]

$$\sigma(t) = \exp(-iHt)\sigma(0)\exp(iHt), \tag{2}$$

where H is the total Hamiltonian, which consists of the radio frequency (r. f.) pulse, the chemical shift and the spin-spin coupling Hamiltonians, and $\sigma(0)$ is the density matrix at $t = 0$. After employing the Hausdorff formula [3]

Table 1. Evolutions of some product operators under the spin-spin coupling Hamiltonian for different spin systems. $C_{nJ} = \cos(n\pi Jt)$ and $S_{nJ} = \sin(n\pi Jt)$.

Product Operators	Evolution under $H_J = 2\pi J I_z S_z$
Spin System IS $(I = 1/2, S = 1/2)$:	
I_x	$I_x C_J + 2I_y S_z S_J$
I_y	$I_y C_J - 2I_x S_z S_J$
$2I_x S_z$	$2I_x S_z C_J + I_y S_J$
$2I_y S_z$	$2I_y S_z C_J - I_x S_J$
Spin System IS $(I = 1/2, S = 1)$:	
I_x	$I_y S_z S_{2J} + I_x \left(1 + S_z^2 \left(C_{2J} - 1\right)\right)$
I_y	$-I_x S_z S_{2J} + I_y \left(1 + S_z^2 \left(C_{2J} - 1\right)\right)$
$I_x S_z$	$I_x S_z C_{2J} + I_y S_z^2 S_{2J}$
$I_y S_z$	$I_y S_z C_{2J} - I_x S_z^2 S_{2J}$
$I_x S_z^2$	$I_x S_z^2 C_{2J} + I_y S_z S_{2J}$
$I_y S_z^2$	$I_y S_z^2 C_{2J} - I_x S_z^2 S_{2J}$
Spin System IS $(I = 1/2, S = 3/2)$:	
I_x	$I_x E_S(\pm 3/2) C_{3J} + (2/3) I_y S_z E_S(\pm 3/2) S_{3J}$ $+ I_x E_S(\pm 1/2) C_J + 2I_y S_z E_S(\pm 1/2) S_J$
I_y	$I_y E_S(\pm 3/2) C_{3J} - (2/3) I_x S_z E_S(\pm 3/2) S_{3J}$ $+ I_y E_S(\pm 1/2) C_J - 2I_x S_z E_S(\pm 1/2) S_J$
$I_x S_z$	$I_x S_z E_S(\pm 3/2) C_{3J} + (3/2) I_y E_S(\pm 3/2) S_{3J}$ $+ I_x S_z E_S(\pm 1/2) C_J + (1/2) I_y E_S(\pm 1/2) S_J$
$I_y S_z$	$I_y S_z E_S(\pm 3/2) C_{3J} - (3/2) I_x E_S(\pm 3/2) S_{3J}$ $+ I_y S_z E_S(\pm 1/2) C_J - (1/2) I_x E_S(\pm 1/2) S_J$

$$\exp(-iHt) A \exp(iHt) = A - (it)[H,A] + \frac{(it)^2}{2!}[H,[H,A]] - \frac{(it)^3}{3!}[H,[H,[H,A]]] + \cdots, \tag{3}$$

the r.f pulse, chemical shift and spin-spin coupling evolution of product operators can easily be obtained [1–6]. The evolutions of product operators under the spin-spin coupling Hamiltonian are summarized in Table 1 for different spin systems [1–6, 12]. For spin S = 3/2, the unitary matrix E_S was divided into two parts:

$$E_S = E_S\left(\pm\frac{3}{2}\right) + E_S\left(\pm\frac{1}{2}\right), \tag{4}$$

where

$$E_S\left(\pm\frac{3}{2}\right) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and (5)

$$E_S\left(\pm\frac{1}{2}\right) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

By considering this decomposition, the product operator in I_y in the $IS(I = 1/2, S = 3/2)$ spin system can be written as

$$\begin{aligned} I_y = I_y \otimes E_S &= I_y \otimes E_S\left(\pm\tfrac{3}{2}\right) + I_y \otimes E_S\left(\pm\tfrac{1}{2}\right) \\ &= I_y E_S\left(\pm\tfrac{3}{2}\right) + I_y E_S\left(\pm\tfrac{1}{2}\right). \end{aligned} \tag{6}$$

By using the Hausdorff formula, evolutions of I_x, I_y, $I_x S_z$ and $I_y S_z$ product operators under the spin-spin coupling Hamiltonian $H_J = 2\pi J I_z S_z$ can be obtained for the $IS(I = 1/2, S = 3/2)$ spin system as in Table 1 [12].

At any time during the experiment, the ensemble averaged expectation value of the spin angular momentum, e.g. for I_y, is

$$\langle I_y \rangle = \mathrm{Tr}\left(I_y \sigma(t)\right), \tag{7}$$

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

3. Results and Discussion

In this section, by using the product operator theory, the analytical description of 3D J-resolved NMR spectroscopy for IS_nK_m (I = 1/2, S = 1/2 and 1, K = 3/2) spin systems is presented. The pulse sequence illustrated in Fig. 1 is used, where the density matrix operator at each stage of the experiment is labelled with numbers. In the pulse sequence it is assumed that during t_1 and t_2 relaxation and evolution under the chemical shift does not take place. Spin-spin couplings obviously exist during the first half of t_1 (between I and S spins), and also during the first half of t_2 (between I and K spins). This section is divided into two subsections for IS_nK_m (I = 1/2, S = 1/2, K = 3/2) and IS_nK_m (I = 1/2, S = 1, K = 3/2) spin systems. For both spin systems the following abbreviations are used: $C_{nJ} = \mathrm{Cos}(n\pi J t_1/2)$, $C'_{nJ} = \mathrm{Cos}(n\pi J' t_2/2)$ and $C_I = \mathrm{Cos}\,\Omega_I t_3$, where J and J' are the spin-spin coupling parameters between the I and S spins and the I and K spins, respectively.

3.1. IS_nK_m ($I = 1/2, S = 1/2, K = 3/2$) Spin System

For the ISK spin system $\sigma_0 = I_z$ is the density matrix operator at thermal equilibrium, and the pulse se-

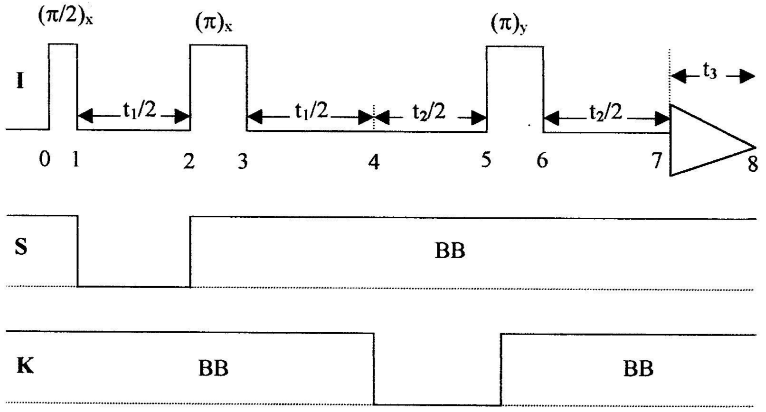

Fig. 1. The gated decoupler pulse for heteronuclear 3D J-Resolved NMR spectroscopy.

Table 2. The results of the Tr(I_yO) calculations for some of the observable product operators in (IS_nK_m) spin system (I = 1/2, S = 1/2, K = 3/2; n = 1,2, m = 1,2).

Spin System	Product Operator (O)	Tr(I_yO)
ISK	$I_yE_K\,(\pm 3/2)$	2
	$I_yE_K\,(\pm 1/2)$	2
IS_2K	$I_yE_K\,(\pm 3/2)$	4
	$I_yE_K\,(\pm 1/2)$	4
ISK_2	$I_yE_K\,(\pm 3/2,\pm 3/2)$	4
	$I_yE_K\,(\pm 3/2,\pm 1/2)$	4
	$I_yE_K\,(\pm 1/2,\pm 3/2)$	4
	$I_yE_K\,(\pm 1/2,\pm 1/2)$	4

quence in Fig. 1 obviously leads to the following density matrices for each labelled point:

$$\sigma_1 = -I_y, \sigma_2 = -I_yC_J, \tag{8}$$

$$\sigma_3 = \sigma_4 = I_yC_J \tag{9}$$

and

$$\sigma_5 = \sigma_6 = \sigma_7 = \left(I_yE_K\left(\pm\frac{3}{2}\right)C'_{3J} + I_yE_K\left(\pm\frac{1}{2}\right)C'_J\right)C_J. \tag{10}$$

Under the chemical shift evolution during t_3, the density matrix becomes

$$\sigma_8 = \sigma_7C_I. \tag{11}$$

In density matrix operators, 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 magnetization along the y-axis is proportional to $\langle I_y \rangle$ and

$$M_y(t_1,t_2,t_3)\alpha\left\langle I_y\right\rangle = \mathrm{Tr}\left(I_y\sigma_8\right). \tag{12}$$

Now it is necessary to obtain the Tr(I_yO) values of observable product operators indicated by O. For an IS_nK_m spin system (I = 1/2, S = 1/2 and K = 3/2), the Tr(I_yO) values were calculated by a computer program, the results being given in Table 2.

By using the Table 2,

$$\begin{aligned}\left\langle I_y\right\rangle (ISK) &= 2C_JC'_{3J}C_I + 2C_JC'_JC_I \qquad (13)\\ &= \frac{1}{2}\left[\mathrm{Cos}\left(\Omega_It_3 + \frac{3\pi J't_2}{2} + \frac{\pi Jt_1}{2}\right)\right.\\ &\quad + \mathrm{Cos}\left(\Omega_It_3 + \frac{3\pi J't_2}{2} - \frac{\pi Jt_1}{2}\right)\\ &\quad + \mathrm{Cos}\left(\Omega_It_3 + \frac{\pi J't_2}{2} + \frac{\pi Jt_1}{2}\right)\\ &\quad + \mathrm{Cos}\left(\Omega_It_3 + \frac{\pi J't_2}{2} - \frac{\pi Jt_1}{2}\right)\\ &\quad + \mathrm{Cos}\left(\Omega_It_3 - \frac{\pi J't_2}{2} + \frac{\pi Jt_1}{2}\right)\\ &\quad + \mathrm{Cos}\left(\Omega_It_3 - \frac{\pi J't_2}{2} - \frac{\pi Jt_1}{2}\right)\\ &\quad + \mathrm{Cos}\left(\Omega_It_3 - \frac{3\pi J't_2}{2} + \frac{\pi Jt_1}{2}\right)\\ &\quad \left. + \mathrm{Cos}\left(\Omega_It_3 - \frac{3\pi J't_2}{2} - \frac{\pi Jt_1}{2}\right)\right]\end{aligned}$$

is obtained. This equation represents the FID signals of 3D J-resolved NMR spectroscopy for an ISK spin system. These are the eight signals at ($J/4$, $3J'/4$, Ω_I), ($-J/4$, $3J'/4$, Ω_I), ($J/4$, $J'/4$, Ω_I), ($-J/4$, $J'/4$, Ω_I), ($J/4$, $-J'/4$, Ω_I), ($-J/4$, $-J'/4$, Ω_I), ($J/4$, $-3J'/4$, Ω_I), and ($-J/4$, $-3J'/4$, Ω_I) with the same relative intensities. In these signal representations, the first, second and third terms are the values at the F_1, F_2, and

F_3 axes, respectively. Since the gated decoupler pulse sequence is used, the spin-spin couplings in F_1 and F_2 dimensions are scaled by a factor of 0.5.

For the IS_2K spin system, by using the same pulse sequence we obtain

$$\sigma_7 = \left[I_y E_K \left(\pm\frac{3}{2} \right) C'_{3J} + I_y E_K \left(\pm\frac{1}{2} \right) C'_J \right] C_J^2 \tag{14}$$

and

$$\sigma_8 = \sigma_7 C_I. \tag{15}$$

By using the results in Table 2, the signal representation becomes

$$\left\langle I_y \right\rangle (IS_2K) = 4C_J^2 C'_{3J} C_I + 4C_J^2 C'_J C_I. \tag{16}$$

This equation represents the signals at ($J/2$, $3J'/4$, Ω_I), ($J/2$, $J'/4$, Ω_I), ($J/2$, $-J'/4$, Ω_I), ($J/2$, $-3J'/4$, Ω_I), (0, $3J'/4$, Ω_I), (0, $J'/4$, Ω_I), (0, $-J'/4$, Ω_I), (0, $-3J'/4$, Ω_I), ($-J'/2$, $3J'/4$, Ω_I), ($-J/2$, $J'/4$, Ω_I), ($-J/2$, $-J'/4$, Ω_I), and ($-J/2$, $-3J'/4$, Ω_I) with the relative intensities 1 : 1 : 1 : 1 : 2 : 2 : 2 : 2 : 1 : 1 : 1 : 1.

For the ISK_2 spin system, by applying the same procedure,

$$\begin{aligned} \sigma_8 = {} & I_y E_K (\pm 3/2, \pm 3/2) {C'_{3J}}^2 C_J C_I \\ & + I_y E_K (\pm 1/2, \pm 1/2) {C'_J}^2 C_J C_I \\ & + \Big[I_y E_K (\pm 3/2, \pm 1/2) \\ & \quad + I_y E_K (\pm 1/2, \pm 3/2) \Big] C'_{3J} C'_J C_J C_I \end{aligned} \tag{17}$$

is obtained. Then, by using the Table 2,

$$\left\langle I_y \right\rangle (ISK_2) = 4C_J {C'_{3J}}^2 C_I + 8C_J C'_{3J} C'_J C_I + 4C_J {C'_J}^2 C_I \tag{18}$$

is found. This equation represents fourteen signals at ($J/4$, $3J'/2$, Ω_I), ($-J/4$, $3J'/2$, Ω_I), ($J/4$, J', Ω_I), ($-J/4$, J', Ω_I), ($J/4$, $J'/2$, Ω_I), ($-J/4$, $J'/2$, Ω_I), ($J/4$, 0, Ω_I), ($-J/4$, 0, Ω_I), ($J/4$, $-J'/2$, Ω_I), ($-J/4$, $-J'/2$, Ω_I), ($J/4$, $-J'$, Ω_I), ($-J/4$, $-J'$, Ω_I), ($J/4$, $-3J'/2$, Ω_I), and ($-J/4$, $-3J'/2$, Ω_I) with the relative intensities 1 : 1 : 2 : 2 : 3 : 3 : 4 : 4 : 3 : 3 : 2 : 2 : 1 : 1.

Table 3. The results of the $\mathrm{Tr}\left(I_y O\right)$ calculations for some of the observable product operators in (IS_nK_m) spin system ($I = 1/2, S = 3/2, K = 3/2; n = 1, 2, m = 1, 2$).

Spin System	Product Operator (O)	$\mathrm{Tr}(I_y O)$
ISK	$I_y E_K (\pm 3/2)$	3
	$I_y E_K (\pm 1/2)$	3
	$I_y S_z^2 E_K (\pm 3/2)$	2
	$I_y S_z^2 E_K (\pm 1/2)$	2
IS_2K	$I_y E_K (\pm 3/2)$	9
	$I_y E_K (\pm 1/2)$	9
	$I_y \left(S_{lz}^2 + S_{2z}^2 \right) E_K (\pm 3/2)$	12
	$I_y \left(S_{lz}^2 + S_{2z}^2 \right) E_K (\pm 1/2)$	12
	$I_y \left(S_{lz}^2 + S_{2z}^2 \right) E_K (\pm 3/2)$	4
	$I_y \left(S_{lz}^2 + S_{2z}^2 \right) E_K (\pm 1/2)$	4
ISK_2	$I_y E_K (\pm 3/2, \pm 3/2)$	6
	$I_y E_K (\pm 3/2, \pm 1/2)$	6
	$I_y E_K (\pm 1/2, \pm 3/2)$	6
	$I_y E_K (\pm 1/2, \pm 1/2)$	6
	$I_y S_z^2 E_K (\pm 3/2, \pm 3/2)$	4
	$I_y S_z^2 E_K (\pm 3/2, \pm 1/2)$	4
	$I_y S_z^2 E_K (\pm 1/2, \pm 3/2)$	4
	$I_y S_z^2 E_K (\pm 1/2, \pm 1/2)$	4

3.2. IS_nK_m ($I = 1/2, S = 1, K = 3/2$) *Spin System*

For the ISK spin system, $\sigma_0 = I_z$ is the density matrix operator at thermal equilibrium, and the density matrices for each labelled point are

$$\sigma_4 = I_y, \left(I + {S_z}^2 (C_{2J} - I) \right) \tag{19}$$

and

$$\begin{aligned} \sigma_5 = \sigma_6 = \sigma_7 = {} & \left[I_y E_K (\pm 3/2) C'_{3J} + I_y E_K (\pm 1/2) C'_J \right] \\ & \cdot \left[I + S_z^2 (C_{2J} - I) \right]. \end{aligned} \tag{20}$$

Under the chemical shift evolution during t_3, the density matrix becomes

$$\begin{aligned} \sigma_8 = \sigma_7 C_I = {} & \left[I_y E_K (\pm 3/2) C'_{3J} + I_y E_K (\pm 1/2) C'_J \right] \\ & \cdot \left[I + S_z^2 (C_{2J} - I) \right] C_I. \end{aligned} \tag{21}$$

For the IS_nK_m spin system (I = 1/2, S = 1, K = 3/2, n = 1,2, m = 1/2), the calculated $\mathrm{Tr}(I_y O)$ values are given in Table 3. By using Table 3,

$$\left\langle I_y \right\rangle (ISK) = C'_{3J} C_I + C'_J C_I \; + 2C'_{2J} C'_{3J} C_I + 2C'_{2J} C'_I C_I \tag{22}$$

is obtained. This equation represents the FID signals of 3D J-resolved NMR spectroscopy for the ISK spin system. These are the twelve signals at ($J/2$, $3J'/4$,

Ω_I), $(J/2, J'/4, \Omega_I)$, $(J/2, -J'/4, \Omega_I)$, $(J/2, -3J'/4, \Omega_I)$, $(0, 3J'/4, \Omega_I)$, $(0, J'/4, \Omega_I)$, $(0, -J'/4, \Omega_I)$, $(0, -3J'/4, \Omega_I)$, $(-J/2, 3J'/4, \Omega_I)$, $(-J/2, J'/4, \Omega_I)$, $(-J/2, -J'/4, \Omega_I)$, and $(-J/2, -3J'/4, \Omega_I)$ with the same relative intensities.

For the ISK_2 spin system,

$$\sigma_4 = I_y \left(I + S_z^2 \left(C_{2J} - I \right) \right) \tag{23}$$

and

$$\left\langle I_y \right\rangle (ISK_2) = \mathrm{Tr}\,(I_y \sigma_8) \tag{24}$$

$$= 2{C'_{3J}}^2 C_I + 2{C'_J}^2 C_I + 4C'_{3J} C'_J C_I + 8C_{2J} C'_{3J} C'_J C_I + C_{2J} {C'_{3J}}^2 C_I + 4C_{2J} {C'_J}^2 C_I$$

is found. This equation represents twenty one signals at $(J/2, 3J'/2, \Omega_I)$, $(0, 3J'/2, \Omega_I)$, $(-J/2, 3J'/2, \Omega_I)$, $(J/2, J', \Omega_I)$, $(0, J', \Omega_I)$, $(-J/2, J', \Omega_I)$, $(J/2, J'/2, \Omega_I)$, $(0, J'/2, \Omega_I)$, $(-J/2, J'/2, \Omega_I)$, $(J/2, 0, \Omega_I)$, $(0, 0, \Omega_I)$, $(-J/2, 0, \Omega_I)$, $(J/2, -J'/2, \Omega_I)$, $(0, -J'/2, \Omega_I)$, $(-J/2, -J'/2, \Omega_I)$, $(J/2, -J', \Omega_I)$, $(0, -J', \Omega_I)$, $(-J/2, -J', \Omega_I)$, $(J/2, -3J'/2, \Omega_I)$, $(0, -3J'/2, \Omega_I)$, and $(-J/2, -3J'/2, \Omega_I)$ with the relative intensities of 1 : 1 : 1 : 2 : 2 : 2 : 3 : 3 : 3 : 4 : 4 : 4 : 3 : 3 : 3 : 2 : 2 : 2 : 1 : 1 : 1.

For the IS_2K spin system

$$\left\langle I_y \right\rangle (IS_2K) = C'_{3J} C_I + 4C'_{3J} C_{2J} C_I + 4C'_{3J} C_{2J}^2 C_I + C'_J C_I + 4C'_J C_{2J} C_I + 4C'_J C_{2J}^2 C_I \tag{25}$$

is found. As seen in this equation, there exist twenty signals at $(J, 3J'/4, \Omega_I)$, $(J, J'/4, \Omega_I)$, $(J, -J'/4, \Omega_I)$, $(J, -3J'/4, \Omega_I)$, $(J/2, 3J'/4, \Omega_I)$, $(J/2, J'/4, \Omega_I)$, $(J/2, -J'/4, \Omega_I)$, $(J/2, -3J'/4, \Omega_I)$, $(0, 3J'/4, \Omega_I)$, $(0, J'/4, \Omega_I)$, $(0, -J'/4, \Omega_I)$, $(0, -3J'/4, \Omega_I)$, $(-J/2, 3J'/4, \Omega_I)$, $(-J/2, J'/4, \Omega_I)$, $(-J/2, -J'/4, \Omega_I)$, $(-J/2, -3J'/4, \Omega_I)$, $(-J, 3J'/4, \Omega_I)$, $(-J, J'/4, \Omega_I)$, $(-J, -J'/4, \Omega_I)$, and $(-J, -3J'/4, \Omega_I)$ with the relative intensities of 1 : 1 : 1 : 1 : 2: 2 : 2 : 2 : 3 : 3 : 3 : 3 : 2 : 2 : 2 : 2 : 1 : 1 : 1 : 1.

4. Conclusion

3D J-resolved NMR spectroscopy is widely used for resolving the chemical shift along one axis and the spin-spin coupling parameters along the two other axes. The product operator formalism became a technique used in the analytical description of multi-dimensional and multiple-pulse NMR experiments of weakly coupled spin systems having spin $1/2$ and spin 1. Therefore, by using the product operator theory an analytical description of heteronuclear 3D J-resolved NMR spectroscopy for both IS_nK_m (I = 1/2, S = 1/2, K = 3/2; n = 1,2, m = 1,2) and IS_nK_m (I = 1/2, S = 1, K = 3/2; n = 1,2, m = 1,2) spin systems is presented in this study. One can easily show that the results obtained in this study are consistent with those of the classical formalism.

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