

# INEPT NMR Spectroscopy of $^{14}\text{ND}_n$ groups: product operator theory and simulation

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Received 19.03.2010

## Abstract

Product operator formalism is widely used for the analytical description of multi-dimensional and multiple-pulse NMR experiments for the weakly coupled spin systems having spin-1/2 and spin-1 nuclei. The INEPT NMR experiment is a polarization transfer experiment including J-coupling. In this study, the INEPT NMR experiment was analytically investigated by using product operator theory for weakly coupled  $IS_n$  ( $^{14}\text{ND}_n$ ) ( $I=1$ ,  $S=1$ ;  $n=1, 2, 3$ ) spin systems. The obtained theoretical results represent the FID values of  $^{14}\text{ND}_n$  groups. In order to make Fourier transform of the obtained FID values, a Maple program is used and then simulated spectra of the INEPT experiment are obtained for  $^{14}\text{ND}_n$  groups. Then, the experimental suggestions are made for the INEPT NMR experiment of  $^{14}\text{ND}_n$  groups. Also, it is suggested that the INEPT NMR experiment of  $IS$  ( $I=1$ ,  $S=1$ ) spin system can be used in NMR quantum computing.

**Key Words:** NMR, INEPT, product operator formalism, spin-1

## 1. Introduction

There exists a large number of one and two dimensional multi-pulse solution NMR experiments. By using polarization transfer experiments, the NMR signals of insensitive nuclear spins are enhanced [1, 2]. Distortionless Enhancement by Polarization Transfer (DEPT) and Insensitive Nuclei Enhanced by Polarization Transfer (INEPT) NMR experiments are most common polarization transfer experiments [3, 4]. In the INEPT experiment J-coupling is also performed by the multiplicity of each signal of insensitive nuclei. In NMR quantum computing, quantum logic gates are represented by the pulse sequences [5, 6]. The INEPT pulse sequence is used as CNOT logic gate in NMR quantum computing [7, 8].

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 [9–18]. 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 [19]. Experimental and theoretical investigations of  $^{13}C$  DEPT NMR spectroscopy for  $CD_n$  systems are presented elsewhere [20]. For  $CH_n$  and  $CD_n$  groups, product operator theory of 2D DEPT  $J$ -resolved NMR experiment is investigated [21, 22]. For spin systems having spin-3/2 nuclei, by using the product operator formalism, theoretical investigations of INEPT and RINEPT NMR experiments are also presented [23]. Product operator theory of high resolution solution state double quantum spectroscopy for two spin-1 AX systems are investigated [17, 24, 25]. Complete product operator for  $IS$  ( $I=1/2$ ,  $S=1$ ) and  $IS$  ( $I=1$ ,  $S=1$ ) spin systems are presented [26, 27]. Analytical descriptions of DEPT NMR spectroscopy for  $IS_n$  ( $I=1$ ;  $S=1$ ;  $n=1, 2, 3, 4$ ) spin systems are also presented [28]. By using product operator theory in NMR experiments, experimental results can be confirmed and also new experimental suggestions can be made.

The Magic Angle Spinning (MAS) NMR technique is used to perform experiments for solids [29]. Time dependent interactions in solids can be averaged by the MAS NMR technique [29, 30]. At first the INEPT was a solution NMR technique. The INEPT NMR spectroscopy for solids under the MAS is first applied by Fyfe et al. [31]. Then, the INEPT experiment of quadrupole nuclei in solids is also performed [32]. Now the INEPT experiment can be used in solids under the MAS.

In this study, by using product operator formalism, analytical description of the INEPT NMR experiment is presented for heteronuclear weakly coupled  $IS_n$  ( $^{14}ND_n$ ) ( $I=1$ ;  $S=1$ ;  $n=1, 2, 3$ ) spin systems. Then, using the obtained theoretical results and a Maple program, the simulated spectra of the experiment are obtained for  $^{14}ND_n$  groups. Simulated spectra of the INEPT NMR spectroscopy for  $^{14}ND_n$  groups are explained and experimental suggestions are made. It is pointed out that the INEPT NMR experiment of  $IS$  ( $I=1$ ,  $S=1$ ) spin system can be used as two-qutrit CNOT logic gate in NMR quantum computing.

## 2. Theory

The product operator formalism is the expansion of the density matrix operator in terms of matrix representation of angular momentum operators for individual spins. For  $IS$  ( $I=1$ ,  $S=1$ ) spin system, nine Cartesian spin angular momentum operators for  $I=1$  are  $E_I, I_x, I_y, I_z, I_z^2, [I_x, I_z]_+, [I_y, I_z]_+, [I_x, I_y]_+$  and  $(I_x^2 - I_y^2)$  [33]. Similarly, there are also nine Cartesian spin angular momentum operators for  $S=1$ . So,  $9 \times 9 = 81$  product operators are obtained with direct products of these spin angular momentum operators for  $IS$  ( $I=1$ ,  $S=1$ ) spin system. Depending on the pulse experiment,  $(I_x^2 - I_y^2)$  Cartesian spin angular momentum operator is separated into two spin angular momentum operators as  $I_x^2$  and  $I_y^2$ . In this case, there should be  $10 \times 10 = 100$  product operators for this spin system. In this study they are used in separated form.

In the liquid state and the solid state (under MAS conditions) pulse NMR experiments of weakly coupled  $IS_n$  spin systems, the total Hamiltonian consists of r.f. pulse, chemical shift and spin-spin coupling Hamiltonians can be written as

$$\mathcal{H} = \Omega_I I_z + \sum_{i=1}^n \Omega_S S_{iz} + 2\pi \sum_{i=1}^n J_i I_z S_{iz}. \quad (1)$$

Time dependence of the density matrix is governed by Liouville-von Neumann equation

$$\frac{d\sigma}{dt} = \frac{i}{\hbar} [\sigma, \mathcal{H}]. \quad (2)$$

When the Hamiltonian is time independent, the solution of equation (2) is

$$\sigma(t) = \exp(-i\mathcal{H}t)\sigma(0)\exp(i\mathcal{H}t), \quad (3)$$

where  $\sigma(0)$  is the density matrix at  $t = 0$ . After employing the Hausdorff formula [12]

$$\begin{aligned} \exp(-i\mathcal{H}t)A\exp(i\mathcal{H}t) &= A - (it)[\mathcal{H}, A] + \frac{(it)^2}{2!}[\mathcal{H}, [\mathcal{H}, A]] \\ &\quad - \frac{(it)^3}{3!}[\mathcal{H}, [\mathcal{H}, [\mathcal{H}, A]]] + \dots, \end{aligned} \quad (4)$$

evolutions of the product operators under the r.f. pulse, chemical shift and spin-spin coupling Hamiltonians can be easily obtained.

The effect of  $x$ -axis r.f. pulse on some of the Cartesian spin angular momentum operators for  $I=1$  nuclear spin are given in the following equations [18, 27]:

$$I_y \xrightarrow{\mathcal{H}_{rf}t} I_y c_\theta + I_z s_\theta, \quad (5a)$$

$$I_z \xrightarrow{\mathcal{H}_{rf}t} I_z c_\theta - I_y s_\theta, \quad (5b)$$

$$[I_x, I_y]_+ \xrightarrow{\mathcal{H}_{rf}t} [I_x, I_y]_+ c_\theta + [I_x, I_z]_+ s_\theta, \quad (5c)$$

$$[I_x, I_z]_+ \xrightarrow{\mathcal{H}_{rf}t} [I_x, I_z]_+ c_\theta - [I_x, I_y]_+ s_\theta, \quad (5d)$$

$$I_y^2 \xrightarrow{\mathcal{H}_{rf}t} \frac{1}{2}I_y^2(c_{2\theta} + 1) - \frac{1}{2}I_z^2(c_{2\theta} - 1) + \frac{1}{2}[I_y, I_z]_+ s_{2\theta}, \quad (5e)$$

where the r.f. pulse Hamiltonian for  $x$ -axes is  $\mathcal{H}_{rf} = \omega_{rf} I_x$ ,  $\theta = \omega_{rf}t$ ,  $c_{n\theta} = \cos(n\theta)$  and  $s_{n\theta} = \sin(n\theta)$ .

The effect of the spin-spin coupling Hamiltonian on some of the product operators for a weakly coupled  $IS$  ( $I=1$ ,  $S=1$ ) spin system are given in the following equations [18, 27]:

$$I_x \xrightarrow{\mathcal{H}_J t} I_x + I_x S_z^2 (c_{2J} - 1) + I_y S_z s_{2J}, \quad (6a)$$

$$I_y \xrightarrow{\mathcal{H}_J t} I_y + I_y S_z^2 (c_{2J} - 1) - I_x S_z s_{2J}, \quad (6b)$$

$$\begin{aligned} I_x S_y \xrightarrow{\mathcal{H}_J t} &\frac{1}{2}I_x S_y (c_{2J} + 1) + \frac{1}{2}[I_y, I_z]_+ [S_x, S_z]_+ (c_{2J} - 1) \\ &+ \frac{1}{2}(I_y [S_y, S_z]_+ - [I_x, I_z]_+ S_x) s_{2J}, \end{aligned} \quad (6c)$$

$$I_x S_z \xrightarrow{\mathcal{H}_J t} I_x S_z c_{2J} + I_y S_z^2 s_{2J}, \quad (6d)$$

$$I_x S_z^2 \xrightarrow{\mathcal{H}_J t} I_x S_z^2 c_{2J} + I_y S_z s_{2J}, \quad (6e)$$

$$I_y S_z \xrightarrow{\mathcal{H}_J t} I_y S_z c_{2J} - I_x S_z^2 s_{2J}, \quad (6f)$$

$$I_y S_z^2 \xrightarrow{\mathcal{H}_J t} I_y S_z^2 c_{2J} - I_x S_z s_{2J}, \quad (6g)$$

$$I_z S_x^2 \xrightarrow{\mathcal{H}_J t} \frac{1}{2}I_z S_x^2 (c_{4J} + 1) - \frac{1}{2}I_z S_y^2 (c_{4J} - 1) + \frac{1}{2}I_z^2 [S_x, S_y]_+ s_{4J}, \quad (6h)$$

$$I_z S_y^2 \xrightarrow{\mathcal{H}_J t} \frac{1}{2} I_z S_y^2 (c_{4J} + 1) - \frac{1}{2} I_z S_x^2 (c_{4J} - 1) - \frac{1}{2} I_z^2 [S_x, S_y]_+ s_{4J}. \quad (6i)$$

In these equations  $\mathcal{H}_J = 2\pi J I_z S_z$ ,  $c_{nJ} = \cos(n\pi Jt)$  and  $s_{nJ} = \sin(n\pi Jt)$ . For  $IS$  ( $I=1, S=1$ ) spin system, evolution of all product operators under the spin-spin coupling Hamiltonian have been obtained elsewhere [27].

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

$$M_y(t) \propto \langle I_y \rangle \equiv Tr [I_y \sigma(t)]. \quad (7)$$

Where  $\sigma(t)$  is the density matrix operator calculated from Equation (3) at any time. Since  $\langle I_y \rangle$  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, product operator theory and simulated spectra of INEPT NMR spectroscopy for  $IS_n$  ( $^{14}\text{ND}_n$ ) ( $I=1, S=1; n=1, 2, 3$ ) spin systems are presented by dividing into two subsections. In the first subsection, product operator descriptions of the INEPT NMR experiment are presented for these spin systems. In the second one, simulated spectra of the INEPT NMR experiment are obtained for  $^{14}\text{ND}_n$  groups.

#### 3.1. Product operator theory

In this study, the product operator formalism is used for the analytical description of the INEPT NMR experiment for  $IS_n$  ( $^{14}\text{ND}_n$ ) ( $I=1, S=1; n=1, 2, 3$ ) spin systems. Pulse sequence of INEPT, shown in Figure 1, is used [4]. In the pulse sequence, optimum value of  $\tau$  is determined to be  $1/(8J)$  for  $IS$  ( $I=1, S=1$ ) spin system. The density matrix operator at each stage of the experiment is labeled with numbers.  $^{14}\text{N}$  is treated as spin  $I$  and D ( $^2\text{H}$ ) as spin  $S$ .

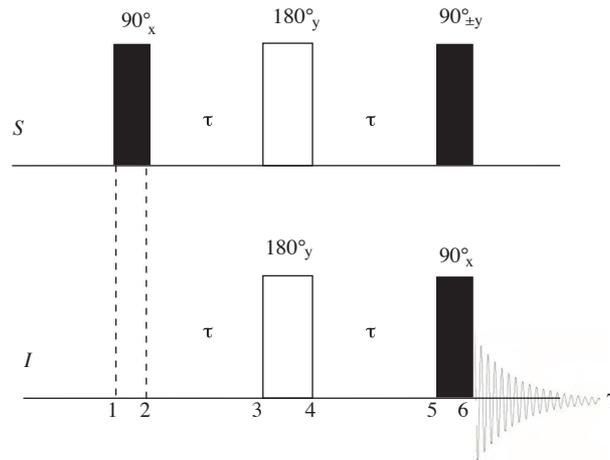


Figure 1. Pulse sequence of INEPT NMR experiment.

### 3.1.1. IS spin system

$\sigma_1$  is the density matrix operator at thermal equilibrium for  $IS$  spin system. Evolutions of density matrix operator for each labeled point are obtained:

$$\sigma_1 = aI_z + bS_z, \quad (8)$$

$$\sigma_1 \xrightarrow{(90^\circ)_x^S} aI_z - bS_y = \sigma_2, \quad (9)$$

$$\sigma_2 \xrightarrow{2\pi J\tau I_z S_z} aI_z + \frac{1}{\sqrt{2}}bI_z S_x - bS_y + \left(1 - \frac{1}{\sqrt{2}}\right)bI_z^2 S_y = \sigma_3, \quad (10)$$

$$\sigma_3 \xrightarrow{(180^\circ)_y^I + (180^\circ)_y^S} -aI_z + \frac{1}{\sqrt{2}}bI_z S_x - bS_y + \left(1 - \frac{1}{\sqrt{2}}\right)bI_z^2 S_y = \sigma_4, \quad (11)$$

$$\sigma_4 \xrightarrow{2\pi J\tau I_z S_z} -aI_z + bI_z S_x + bI_z^2 S_y - bS_y = \sigma_5, \quad (12)$$

$$\sigma_5 \xrightarrow{(90^\circ)_x^I + (90^\circ)_y^S} \sigma_6 \left[ (90^\circ)_y^S \right], \quad (13)$$

$$\sigma_6 \left[ (90^\circ)_y^S \right] = aI_y + bI_y S_z + bI_y^2 S_y - bS_y. \quad (14)$$

In order to remove the asymmetry in the spectrum, phase cycling should be applied. In the second experiment,  $(90^\circ)_y^S$  pulse is replaced with the  $(90^\circ)_{-y}^S$  pulse. Then,

$$\sigma_6 \left[ (90^\circ)_{-y}^S \right] = aI_y - bI_y S_z + bI_y^2 S_y - bS_y \quad (15)$$

is found. After the subtraction of two results we obtain

$$\sigma_6 [Sub] = \sigma_6 \left[ (90^\circ)_{+y}^S \right] - \sigma_6 \left[ (90^\circ)_{-y}^S \right] = 2bI_y S_z. \quad (16)$$

At the end of the experiment

$$\sigma_6(Sub) \xrightarrow{2\pi JI_z S_z t + \Omega_s I_s t} 2bI_y S_z c_I c_{2J} - 2bI_x S_z s_I c_{2J} - 2bI_x S_z^2 c_I s_{2J} - 2bI_y S_z^2 s_I s_{2J} = \sigma_7. \quad (17)$$

is obtained.  $\sigma_7$  is the density matrix operator at the end of the experiment. In the density matrix operator theory, only the last term of  $\sigma_7$  contributes to the signal as the acquisition is taken along y-axes. Now it is necessary to obtain the  $Tr [I_y O]$  values of the observables product operators indicated by  $O$ . For  $IS_n$  ( $I=1$ ,  $S=1$ ,  $n=1,2,3$ ) spin systems,  $Tr [I_y O]$  values of all the observables product operators are calculated and the results are given in Table 1. By using Table 1 and equation (7)

$$\langle M_y \rangle \propto Tr [I_y \sigma_7] = -2bs_I s_{2J} = 2b [\cos(\Omega_I t + 2\pi Jt) - \cos(\Omega_I t - 2\pi Jt)] \quad (18)$$

is found. In this and in the following equations,  $s_I = \sin(\Omega_I t)$  and  $s_{nJ} = \sin(n\pi Jt)$ . Therefore the INEPT experiment for  $IS$  ( $I=1$ ,  $S=1$ ) spin system give doublet signals with opposite direction and no signal for central peak. The signal coordinates are  $(\Omega_I + J)$ ,  $(\Omega_I)$  and  $(\Omega_I - J)$  with the intensity distribution of 1:0:-1, respectively.

**Table 1.**  $Tr [I_y O]$  values of some of the observable product operators for  $IS_n$  ( $I=1, S=1; n = 1, 2, 3$ ) spin systems.

Spin System	Product Operators ( $O$ )	$Tr [I_y O]$
$IS$	$I_y S_z^2$	1
$IS_2$	$I_y (S_{1z}^2 + S_{2z}^2)$	6
	$I_y S_{1z}^2 S_{2z}^2$	2
$IS_3$	$I_y (S_{1z}^2 + S_{2z}^2 + S_{3z}^2)$	27
	$I_y (S_{1z}^2 S_{2z}^2 + S_{1z}^2 S_{3z}^2 + S_{2z}^2 S_{3z}^2)$	18
	$I_y S_{1z}^2 S_{2z}^2 S_{3z}^2$	4

### 3.1.2. $IS_2$ spin system

For  $IS_2$  spin system  $\sigma_1 = aI_z + bS_{1z} + bS_{2z}$  is the density matrix operator at thermal equilibrium. Evolution of the density matrix operators during the experiment progressed as follows:

$$\sigma_1 \xrightarrow{(90^\circ)_x^S} aI_z - b(S_{1y} - S_{2y}) = \sigma_2, \quad (19)$$

$$\sigma_2 \xrightarrow{2\pi J\tau(I_z S_{1z} + I_z S_{2z}) + (180^\circ)_y^I + (180^\circ)_y^S} \sigma_4, \quad (20)$$

$$\begin{aligned} \sigma_4 &\xrightarrow{2\pi J\tau(I_z S_{1z} + I_z S_{2z}) + (90^\circ)_x^I + (90^\circ)_{+y}^S} aI_y \\ &+ b(I_y S_{1z} + I_y S_{2z} + I_y^2 S_{1y} + I_y^2 S_{2y} - S_{1y} - S_{2y}) = \sigma_6 \left[ (90^\circ)_{+y}^S \right]. \end{aligned} \quad (21)$$

And similarly,

$$\sigma_6 \left[ (90^\circ)_{-y}^S \right] = aI_y + b(-I_y S_{1z} - I_y S_{2z} + I_y^2 S_{1y} + I_y^2 S_{2y} - S_{1y} - S_{2y}) \quad (22)$$

is found. Then,

$$\sigma_6 [Sub] = \sigma_6 \left[ (90^\circ)_{+y}^S \right] - \sigma_6 \left[ (90^\circ)_{-y}^S \right] = 2bI_y S_{1z} + 2bI_y S_{2z} \quad (23)$$

is obtained. For the last step we can obtain

$$\sigma_7 = [-2I_y(S_{1z}^2 + S_{2z}^2) + 4I_y(S_{1z}^2 S_{2z}^2)] s_{2J} s_I - 2I_y S_{1z}^2 S_{2z}^2 s_{4J} s_I. \quad (24)$$

Using Table 1,

$$\langle M_y \rangle \propto Tr [I_y \sigma_7] (IS_2) = -16s_I (s_{2J} + s_{4J}) \quad (25)$$

is found. This result represent five signals at the coordinates of  $(\Omega_I + 2J)$ ,  $(\Omega_I + J)$ ,  $(\Omega_I)$ ,  $(\Omega_I - J)$  and  $(\Omega_I - 2J)$  with intensity distribution of 1:1:0:-1:-1.

### 3.1.3. $IS_3$ spin system

For  $IS_3$  spin system, density matrix at thermal equilibrium is

$$\sigma_1 = aI_z + bS_{1z} + bS_{2z} + bS_{3z}. \quad (26)$$

Applying the same procedure, we obtain

$$\langle M_y \rangle \propto Tr [I_y \sigma_7] (IS_3) = -(48s_{2J} + 48s_{4J} + 24s_{6J}) s_I. \quad (27)$$

As seen in this equation there exists seven signals at the coordinates of  $(\Omega_I + 3J)$ ,  $(\Omega_I + 2J)$ ,  $(\Omega_I + J)$ ,  $(\Omega_I)$ ,  $(\Omega_I - J)$ ,  $(\Omega_I - 2J)$  and  $(\Omega_I - 3J)$  with the relative intensities of 1:2:2:0:-2:-2:-1.

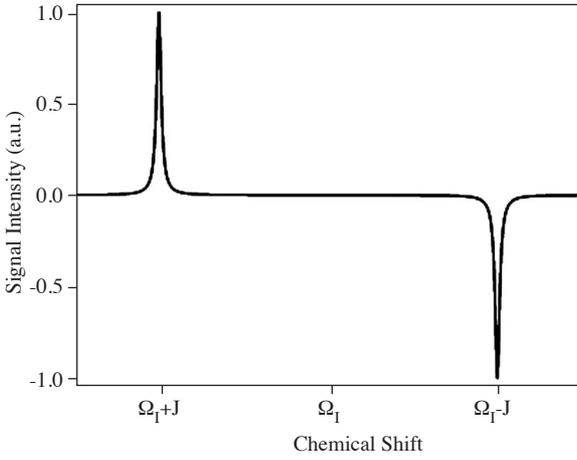
### 3.2. Simulated spectra

The INEPT experiment of  $IS_n(^{14}\text{ND}_n)$  ( $I=1$ ;  $S=1$ ;  $n=1, 2, 3$ ) spin systems can be used in partially deuterated ammonium containing molecules such as  $(\text{NH}_{4-4x}\text{D}_{4x})_2\text{ACl}_6$  ( $x=0.5, 0.75$  and  $1$ ;  $A=\text{Te, Sn}$ ) [34,35]. A computer program was written by Kanters et al. for product operator description of NMR experiments and for the simulations of FID signals [36, 37]. This is called Product Operator Formalism (POF.M) using Maple. In this study, in order to obtain the simulated spectra of the FID results, POF.M program is implemented for this experiment.  $Tr [I_y \sigma_7] (IS_n)$  values, signal coordinates and signal intensities obtained for  $IS$ ,  $IS_2$  and  $IS_3$  spin systems are given in Table 2. They represent the FID signals of INEPT NMR spectroscopy for  $^{14}\text{ND}_n$  groups (under MAS conditions for solids). By using  $Tr [I_y \sigma_7] (IS_n)$  values, simulated spectra of this experiment are obtained and they are given in Figures 2, 3 and 4 for  $^{14}\text{ND}$ ,  $^{14}\text{ND}_2$  and  $^{14}\text{ND}_3$  groups, respectively.

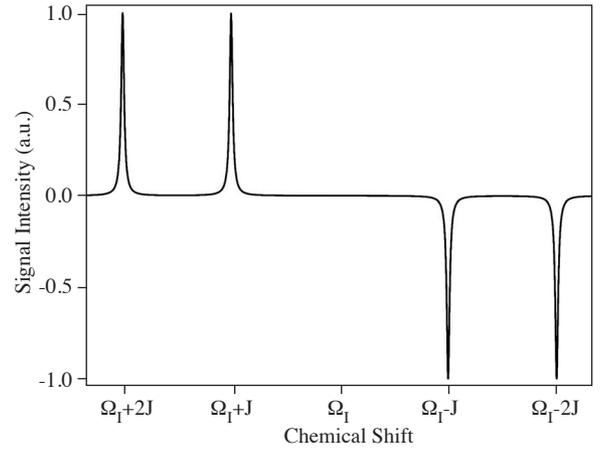
It can be seen from the theoretical results and the simulated spectra that the INEPT NMR experiment can be used to identify  $^{14}\text{ND}$ ,  $^{14}\text{ND}_2$  and  $^{14}\text{ND}_3$  groups from each other and also to determine the spin-spin coupling constant between  $^{14}\text{N}$  and  $\text{D}$  nuclei in molecules containing  $^{14}\text{ND}_n$  groups such as  $(\text{NH}_{4-4x}\text{D}_{4x})_2\text{ACl}_6$  ( $x = 0.5, 0.75$  and  $1$ ;  $A = \text{Te, Sn}$ ).

**Table 2.**  $Tr [I_y \sigma_7] (IS_n)$  values, the signal coordinates and the signal intensities for  $IS$ ,  $IS_2$  and  $IS_3$  spin systems.

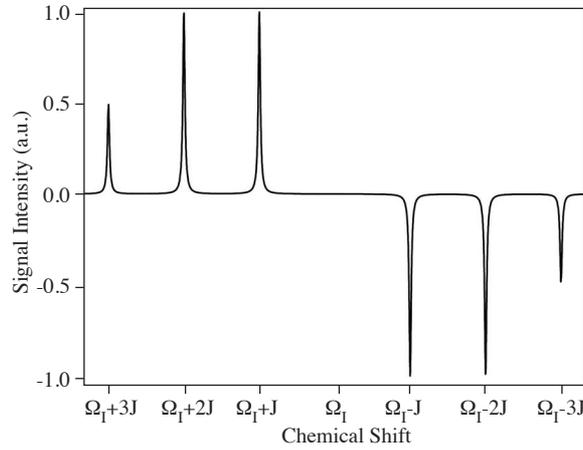
Spin system	$Tr [I_y \sigma_7] (IS_n)$ values	Signal coordinates	Signal intensities
$IS$	$\cos(\Omega_I t + 2\pi J t) - \cos(\Omega_I t - 2\pi J t)$	$(\Omega_I + J)$ , $(\Omega_I)$ , $(\Omega_I - J)$	1:0:-1
$IS_2$	$\cos(\Omega_I t + 4\pi J t) - \cos(\Omega_I t - 4\pi J t)$ $+ \cos(\Omega_I t + 2\pi J t) - \cos(\Omega_I t - 2\pi J t)$	$(\Omega_I + 2J)$ , $(\Omega_I + J)$ , $(\Omega_I)$ , $(\Omega_I - J)$ , $(\Omega_I - 2J)$	1:1:0:-1:-1
$IS_3$	$24[(\cos \Omega_I t + 2\pi J t) - (\cos \Omega_I t - 2\pi J t)]$ $+ 24[\cos(\Omega_I t + 4\pi J t) - \cos(\Omega_I t - 4\pi J t)]$ $+ 12[(\cos \Omega_I t + 6\pi J t) - (\cos \Omega_I t - 6\pi J t)]$	$(\Omega_I + 3J)$ , $(\Omega_I + 2J)$ , $(\Omega_I + J)$ , $(\Omega_I)$ , $(\Omega_I - J)$ , $(\Omega_I - 2J)$ , $(\Omega_I - 3J)$	1:2:2:0:-2:-2:-1



**Figure 2.** Simulated spectrum of the INEPT NMR experiment for  $^{14}\text{ND}$  group.



**Figure 3.** Simulated spectrum of the INEPT NMR experiment for  $^{14}\text{ND}_2$  group.



**Figure 4.** Simulated spectrum of the INEPT NMR experiment for  $^{14}\text{ND}_3$  group.

## 4. Conclusions

In this study, by using product operator theory, analytical description of INEPT NMR experiment is presented for  $^{14}\text{ND}_n$  groups. The obtained theoretical results represent the FID values of  $^{14}\text{ND}_n$  groups. Simulated spectra of the INEPT NMR spectroscopy are obtained for  $^{14}\text{ND}_n$  groups by using the Fourier transformations of the FID values. It is shown that, by using the INEPT NMR experiment,  $^{14}\text{ND}_n$  groups can be identified from each other and  $^1J(^{14}\text{N},\text{D})$  coupling constants can be determined in some molecules such as partially deuterated ammonium containing molecules.  $IS$  ( $I=1$ ,  $S=1$ ) spin system is represented as two-qutrit states in quantum computing [38]. So, the INEPT NMR experiment of  $IS$  ( $I=1$ ,  $S=1$ ) spin system can be also used as two-qutrit CNOT logic gate in NMR quantum computing.

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