

## Product operator descriptions of INEPT and RINEPT NMR spectroscopies for $IS_n$ ( $I = 1/2$ , $S = 3/2$ ) spin systems

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### Abstract

The product operator descriptions of INEPT and reverse INEPT (RINEPT) NMR experiments are introduced for weakly coupled  $IS_n$  ( $I = 1/2$ ,  $S = 3/2$  with  $n = 1, 2, 3$ ) spin systems. Explicit expressions for polarization transfer from spin-3/2 quadrupolar nuclei to spin-1/2 nuclei (and reversed polarization transfer) are given in detail by using the evolutions of product operators under the spin–spin coupling Hamiltonian. The results calculated for the intensities and positions of the observable signals are simulated in the molecules containing the  $^{119}\text{Sn}$  ( $I = 1/2$ ) and  $^{35}\text{Cl}$  ( $S = 3/2$ ) nuclei at the coupling constant of  $J_{\text{Sn-Cl}} = 375$  Hz by using the Maple programme on computer.

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**Keywords:** NMR spectroscopy; Spin–spin coupling Hamiltonian; Polarization transfer; INEPT and RINEPT pulse sequences; Product operator formalism

### 1. Introduction

The NMR signals of insensitive nuclear spins can be enhanced by transferring polarization from a more sensitive species to which they are coupled [1]. The well-known pulse sequences as the polarization transfer techniques are insensitive nuclei enhanced by polarization transfer (INEPT), distortionless enhancement by polarization transfer (DEPT), and reverse insensitive nuclei enhanced by polarization transfer (RINEPT) [2,3]. The INEPT sequence is an alternative to the nuclear Overhauser effect. The INEPT experiment does not require any particular relaxation mechanism and therefore a better enhancement factor can be obtained [1]. Furthermore it is demonstrated that INEPT sequence can be used to determine the multiplicity of each signal in a  $^{13}\text{C}$  NMR spectrum [3]. More recently, the INEPT and DEPT experiments were used for the coherence

transfer via heteronuclear  $J$ -coupling between spin-1/2 and quadrupolar nuclei in the solids [4–6]. Fyfe et al. [4] showed that coherence transfer via the scalar coupling between spin-1/2 and quadrupolar nuclei can be obtained in the solid state by using INEPT experiment.

On the other hand to analyse and describe the multi-pulse NMR experiments an effective and useful tool is product operator theory as a simple quantum mechanical method [7,8]. The product operator formalism has been used for weakly coupled  $IS$  ( $I = 1/2$ ;  $S = 1/2, 1$ , and  $3/2$ ) spin systems [7,9–12]. The polarization transfer (PT) between spin-1/2 nuclei in an INEPT pulse sequence has been described by using product operator theory [13]. Chandrakumar [14] investigated the polarization transfer between spin-1 and spin-1/2 nuclei by using product operator formalism for INEPT and from spin-1/2 to spin-1 nuclei for refocusing INEPT experiments.

In our present work we first introduce the results of the applications of the product operators theory to the polarization transfer between spin-3/2 and spin-1/2 nuclei for INEPT and from spin-1/2 to spin-3/2 nuclei for RINEPT experiments. As one practical application of this theory we have taken the molecules that include one

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of these three organometallic compounds: trimethyltin chloride [(CH)<sub>3</sub>SnCl] (as  $IS$  spin system), dimethyltin chloride [(CH)<sub>2</sub>SnCl<sub>2</sub>] (as  $IS_2$  spin system) and methyltin trichloride [CH<sub>3</sub>SnCl<sub>3</sub>] (as  $IS_3$  spin system) containing the weakly coupled  $I = 1/2$  (<sup>119</sup>Sn with  $\gamma = -9.53 \times 10^7 \text{ T}^{-1} \text{ s}^{-1}$ ; 8.58%) and  $S = 3/2$  (<sup>35</sup>Cl with  $\gamma = 2.62 \times 10^7 \text{ T}^{-1} \text{ s}^{-1}$ ; 75.53%) nuclei [15,16]. It is well known that the scalar or indirect coupling  $J$  to the quadrupolar nuclei can be observed provided that some arrangements of ligands can cause to give low or zero electric field gradients at a point of the molecule [17,18]. In this framework by considering the values mentioned above in our selected real chemical systems the coupling constant  $J_{\text{Sn-Cl}}$  was taken as 375 Hz and simulate the intensities and positions of observable signals in INEPT and RINEPT by using Maple programme on computer [19,20].

### 1.1. Polarization transfer between spin-3/2 and spin-1/2 nuclei in INEPT and reverse INEPT experiments

To describe the INEPT and reverse INEPT (RINEPT) NMR experiments by using product operator formalism for weakly coupled  $IS$  ( $I = 1/2$ ,  $S = 3/2$ ) spin systems we consider that the spin multiplicity of  $I$  can be decomposed into in-phase and anti-phase coherence with the inner and outer transitions of multiplet [7,11]. For the evolutions of product operators under spin-spin coupling Hamiltonian it is convenient to use the well-known Hausdorff formula [21].

Then, the evolutions of  $I_x$ ,  $I_y$ ,  $I_x S_z$ , and  $I_y S_z$  product operators under the spin-spin coupling Hamiltonian can be written as [11]:

$$I_x \xrightarrow{2\pi J_z S_z t} I_x E_s \left( \pm \frac{3}{2} \right) \cos(3\pi J t) + \frac{2}{3} I_y S_z E_s \left( \pm \frac{3}{2} \right) \sin(3\pi J t) + I_x E_s \left( \pm \frac{1}{2} \right) \cos(\pi J t) + 2 I_y S_z E_s \left( \pm \frac{1}{2} \right) \sin(\pi J t), \quad (1a)$$

$$I_y \xrightarrow{2\pi J_z S_z t} I_y E_s \left( \pm \frac{3}{2} \right) \cos(3\pi J t) - \frac{2}{3} I_x S_z E_s \left( \pm \frac{3}{2} \right) \sin(3\pi J t) + I_y E_s \left( \pm \frac{1}{2} \right) \cos(\pi J t) - 2 I_x S_z E_s \left( \pm \frac{1}{2} \right) \sin(\pi J t), \quad (1b)$$

$$I_x S_z \xrightarrow{2\pi J_z S_z t} I_x S_z E_s \left( \pm \frac{3}{2} \right) \cos(3\pi J t) + \frac{3}{2} I_y E_s \left( \pm \frac{3}{2} \right) \sin(3\pi J t) + I_x S_z E_s \left( \pm \frac{1}{2} \right) \cos(\pi J t) + \frac{1}{2} I_y E_s \left( \pm \frac{1}{2} \right) \sin(\pi J t), \quad (1c)$$

and

$$I_y S_z \xrightarrow{2\pi J_z S_z t} I_y S_z E_s \left( \pm \frac{3}{2} \right) \cos(3\pi J t) - \frac{3}{2} I_x E_s \left( \pm \frac{3}{2} \right) \sin(3\pi J t) + I_y S_z E_s \left( \pm \frac{1}{2} \right) \cos(\pi J t) - \frac{1}{2} I_x E_s \left( \pm \frac{1}{2} \right) \sin(\pi J t). \quad (1d)$$

We used these expressions for the descriptions of INEPT and RINEPT pulse sequences. Figs. 1a and b show the mentioned pulse sequences, respectively. The labelled numbers on Fig. 1 indicate the density matrix operators at each stage of the experiments.

For the  $IS$  spin system the density matrix operators calculated at the first five stages of INEPT pulse sequence are listed in Table 1.

As seen in Table 1 and in Fig. 1b, the effects of spin-spin coupling Hamiltonian,  $H_J = 2\pi J_z S_z$ , on the product operators are considered at the intervals 1–2 and 3–4 stages for mentioned pulse sequence. Since the time interval between applied pulses  $\tau = 1/4J$ , we take  $C_{2J} = 0$  and  $S_{2J} = 1$  for  $\sigma_4$  density matrix operator. In the last stage of INEPT experiment, by considering first the chemical shift and then spin-spin coupling effects we get

$$\begin{aligned} \sigma_6 = & -2bI_y S_z E_s \left( \pm \frac{3}{2} \right) C_I C_{3J} + 3bI_x E_s \left( \pm \frac{3}{2} \right) C_I S_{3J} \\ & + 2bI_x S_z E_s \left( \pm \frac{3}{2} \right) S_I C_{3J} + 3bI_y E_s \left( \pm \frac{3}{2} \right) S_I S_{3J} \\ & - 2bI_y S_z E_s \left( \pm \frac{1}{2} \right) C_I C_J + bI_x E_s \left( \pm \frac{1}{2} \right) C_I S_J \\ & + 2bI_x S_z E_s \left( \pm \frac{1}{2} \right) S_I C_J + bI_y E_s \left( \pm \frac{1}{2} \right) S_I S_J \\ & - aI_x E_s \left( \pm \frac{3}{2} \right) S_I C_{3J} - aI_x E_s \left( \pm \frac{1}{2} \right) S_I C_J, \quad (2) \end{aligned}$$

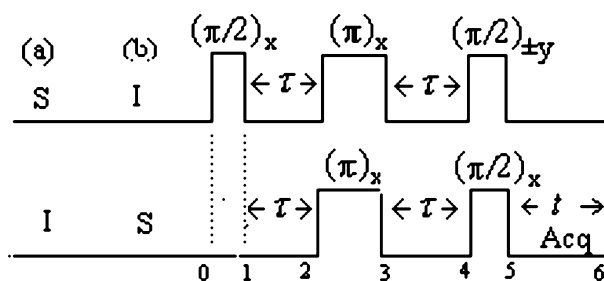


Fig. 1. (a) Conventional INEPT pulse sequence for the polarization from  $S = 3/2$  nuclei to  $I = 1/2$  nuclei and (b) reversed INEPT (RINEPT) pulse sequence for the polarization from  $I = 1/2$  nuclei to  $S = 3/2$  nuclei ( $\tau = 1/4J$ ).

Table 1

For  $IS$  ( $I = 1/2$ ,  $S = 3/2$ ) spin systems, the calculated first five density matrix operators in INEPT pulse sequence

INEPT
$\sigma_0 = bS_z + aI_z$
$\sigma_1 = -bS_y + aI_z$
$\sigma_2 = -b(S_y C'_J - 2I_z S_x S'_J) + aI_z$
$\sigma_3 = -\sigma_2$
Using $\cos(2\pi J \tau) = 0$ , $\sin(2\pi J \tau) = 1$ since $\tau = 1/4J$ ,
$\sigma_4 = -2bI_z S_x - aI_z$
$\sigma_5 = -2bI_y S_z E_s \left( \pm \frac{3}{2} \right) - 2bI_x S_z E_s \left( \pm \frac{1}{2} \right) + a[I_y E_s \left( \pm \frac{3}{2} \right) + I_x E_s \left( \pm \frac{1}{2} \right)]$

Where  $C'_{nJ} = \cos(n\pi J \tau)$  and  $S'_{nJ} = \sin(n\pi J \tau)$ .

where  $C_{nJ} = \cos(n\pi Jt)$ ,  $S_{nJ} = \sin(n\pi Jt)$ ,  $C_I = \cos(\Omega_I t)$ , and  $S_I = \sin(\Omega_I t)$ . On the other hand since we take only single quantum terms and detect along  $y$ -axis, we have

$$\begin{aligned} \sigma_6 = & 3bI_y E_s \left( \pm \frac{3}{2} \right) S_I S_{3J} + bI_y E_s \left( \pm \frac{1}{2} \right) S_I S_J \\ & + aI_y E_s \left( \pm \frac{3}{2} \right) C_I C_{3J} + aI_y E_s \left( \pm \frac{1}{2} \right) C_I C_J. \end{aligned} \quad (3)$$

If a second experiment is performed with a  $90_{-y}^0$  pulse instead  $90_y^0$  pulse on  $S$  spin, then we can write

$$\begin{aligned} \sigma_6 = & -b \left[ 3I_y E_s \left( \pm \frac{3}{2} \right) S_{3J} S_I + I_y E_s \left( \pm \frac{1}{2} \right) S_J S_I \right] \\ & + a \left[ I_y E_s \left( \pm \frac{3}{2} \right) C_{3J} C_I + I_y E_s \left( \pm \frac{1}{2} \right) C_J C_I \right]. \end{aligned} \quad (4)$$

When the second  $\sigma_6$  is subtracted from the first the final result becomes

$$\sigma_f = 6bI_y E_s \left( \pm \frac{3}{2} \right) S_{3J} S_I + 2bI_y E_s \left( \pm \frac{1}{2} \right) S_J S_I. \quad (5)$$

Thus the observable magnetization for INEPT experiment is

$$M_x(t) \propto \langle I_y \rangle = \text{Tr} [I_y \sigma_f], \quad (6)$$

and for the  $IS$  ( $I = 1/2$  and  $S = 3/2$ ) spin system by substituting Eq. (5) into Eq. (6) we have the coefficients

$$\text{Tr} \left[ I_y I_y E_s \left( \pm \frac{3}{2} \right) \right] = \text{Tr} \left[ I_y I_y E_s \left( \pm \frac{1}{2} \right) \right] = 1 \quad (7)$$

and we obtain

$$\begin{aligned} \langle I_y \rangle (IS) = & 3b [\cos(\Omega_I - 3\pi J)t - \cos(\Omega_I + 3\pi J)t] \\ & + b [\cos(\Omega_I - \pi J)t - \cos(\Omega_I + \pi J)t]. \end{aligned} \quad (8)$$

This equation represents four signals at the coordinates of  $(\frac{3J}{2}, \Omega_I)$ ,  $(\frac{J}{2}, \Omega_I)$ ,  $(-\frac{J}{2}, \Omega_I)$ , and  $(-\frac{3J}{2}, \Omega_I)$  with an intensity distribution of  $(-3:-1:1:3)$ .

For the  $IS_2$  ( $I = 1/2$ ,  $S = 3/2$ ) spin systems in INEPT pulse sequences we can divide  $I_y$  into four parts as

$$\begin{aligned} I_y = & I_y E_s \left( \pm \frac{3}{2}, \pm \frac{3}{2} \right) + I_y E_s \left( \pm \frac{3}{2}, \pm \frac{1}{2} \right) \\ & + I_y E_s \left( \pm \frac{1}{2}, \pm \frac{1}{2} \right) + I_y E_s \left( \pm \frac{1}{2}, \pm \frac{3}{2} \right), \end{aligned} \quad (9)$$

where, for example,

$$I_y E_s \left( \pm \frac{3}{2}, \pm \frac{1}{2} \right) = I_y \otimes E_{s1} \left( \pm \frac{3}{2} \right) \otimes E_{s2} \left( \pm \frac{1}{2} \right). \quad (10)$$

By using the same considerations at every single stage of INEPT experiment seen in Fig. 1A we obtain the observable signal as

$$\begin{aligned} \langle I_y \rangle (IS_2) = & b \{ 6 [\cos(\Omega_I - 6\pi J)t - \cos(\Omega_I + 6\pi J)t] \\ & + 8 [\cos(\Omega_I - 4\pi J)t - \cos(\Omega_I + 4\pi J)t] \\ & + 6 [\cos(\Omega_I - 2\pi J)t - \cos(\Omega_I + 2\pi J)t] \}. \end{aligned} \quad (11)$$

Thus we have seven signals at the coordinates of  $(3J, \Omega_I)$ ,  $(2J, \Omega_I)$ ,  $(J, \Omega_I)$ ,  $(0, \Omega_I)$ ,  $(-J, \Omega_I)$ ,  $(-2J, \Omega_I)$ , and  $(-3J, \Omega_I)$  with an intensity of  $(-3:-4:-3:0:3:4:3)$ .

For the  $IS_3$  spin system in INEPT experiment we can divide  $I_y$  into eight parts as

$$\begin{aligned} I_y = & I_y E_s \left( \pm \frac{3}{2}, \pm \frac{3}{2}, \pm \frac{3}{2} \right) + I_y E_s \left( \pm \frac{3}{2}, \pm \frac{3}{2}, \pm \frac{1}{2} \right) \\ & + I_y E_s \left( \pm \frac{3}{2}, \pm \frac{1}{2}, \pm \frac{3}{2} \right) + I_y E_s \left( \pm \frac{3}{2}, \pm \frac{1}{2}, \pm \frac{1}{2} \right) \\ & + I_y E_s \left( \pm \frac{1}{2}, \pm \frac{3}{2}, \pm \frac{3}{2} \right) + I_y E_s \left( \pm \frac{1}{2}, \pm \frac{3}{2}, \pm \frac{1}{2} \right) \\ & + I_y E_s \left( \pm \frac{1}{2}, \pm \frac{1}{2}, \pm \frac{3}{2} \right) + I_y E_s \left( \pm \frac{1}{2}, \pm \frac{1}{2}, \pm \frac{1}{2} \right), \end{aligned} \quad (12)$$

where, for instance,

$$\begin{aligned} I_y E_s \left( \pm \frac{3}{2}, \pm \frac{3}{2}, \pm \frac{1}{2} \right) \\ = I_y \otimes E_{s1} \left( \pm \frac{3}{2} \right) \otimes E_{s2} \left( \pm \frac{3}{2} \right) \otimes E_{s3} \left( \pm \frac{1}{2} \right). \end{aligned} \quad (13)$$

By following the same calculations steps we get:

$$\begin{aligned} \langle I_y \rangle (IS_3) = & 9b [\cos(\Omega_I - 9\pi J)t - \cos(\Omega_I + 9\pi J)t] \\ & + 21b [\cos(\Omega_I - 7\pi J)t - \cos(\Omega_I + 7\pi J)t] \\ & + 30b [\cos(\Omega_I - 5\pi J)t - \cos(\Omega_I + 5\pi J)t] \\ & + 30b [\cos(\Omega_I - 3\pi J)t - \cos(\Omega_I + 3\pi J)t] \\ & + 12b [\cos(\Omega_I - \pi J)t - \cos(\Omega_I + \pi J)t]. \end{aligned} \quad (14)$$

This equation denotes 10 signals at the coordinates of  $(\frac{9J}{2}, \Omega_I)$ ,  $(\frac{7J}{2}, \Omega_I)$ ,  $(\frac{5J}{2}, \Omega_I)$ ,  $(\frac{3J}{2}, \Omega_I)$ ,  $(\frac{1J}{2}, \Omega_I)$ ,  $(-\frac{1J}{2}, \Omega_I)$ ,  $(-\frac{3J}{2}, \Omega_I)$ ,  $(-\frac{5J}{2}, \Omega_I)$ ,  $(-\frac{7J}{2}, \Omega_I)$ , and  $(-\frac{9J}{2}, \Omega_I)$  with an intensity distribution  $(-3:-7:-10:-10:-4:4:10:10:7:3)$ . Figs. 2A–C show the plots of signals obtained for  $IS$ ,  $IS_2$ , and  $IS_3$  spin systems, respectively in which were performed in Maple by considering the typical coupling constant value of  $J_{\text{Sn-Cl}} = 375$  Hz and the transverse relaxation time value of 0.01 s and the chemical shift value  $\delta_{\text{Sn}} = 0$  ppm for the selected molecules containing  $^{119}\text{Sn}$   $\{^{35}\text{Cl}\}$  nuclei [19,20].

As for reverse INEPT (or RINEPT) experiment in which polarization transfer (PT) is from spin-1/2 nuclei to spin-3/2 nuclei, we follow the similar ways and considerations in order to get the signals for  $IS$  ( $I = 1/2$ ,  $S = 3/2$ ) spin system. In this framework, both the chemical shift Hamiltonian  $H_{CS} = \Omega_S S_z$  and spin-spin coupling Hamiltonian  $H_J = 2\pi J_z S_z$  are applied on the spin density operator  $\sigma_5$  in Table 2 during acquisition time  $t$  and by considering single quantum terms and the phase cycling for reverse INEPT pulse sequences we obtain

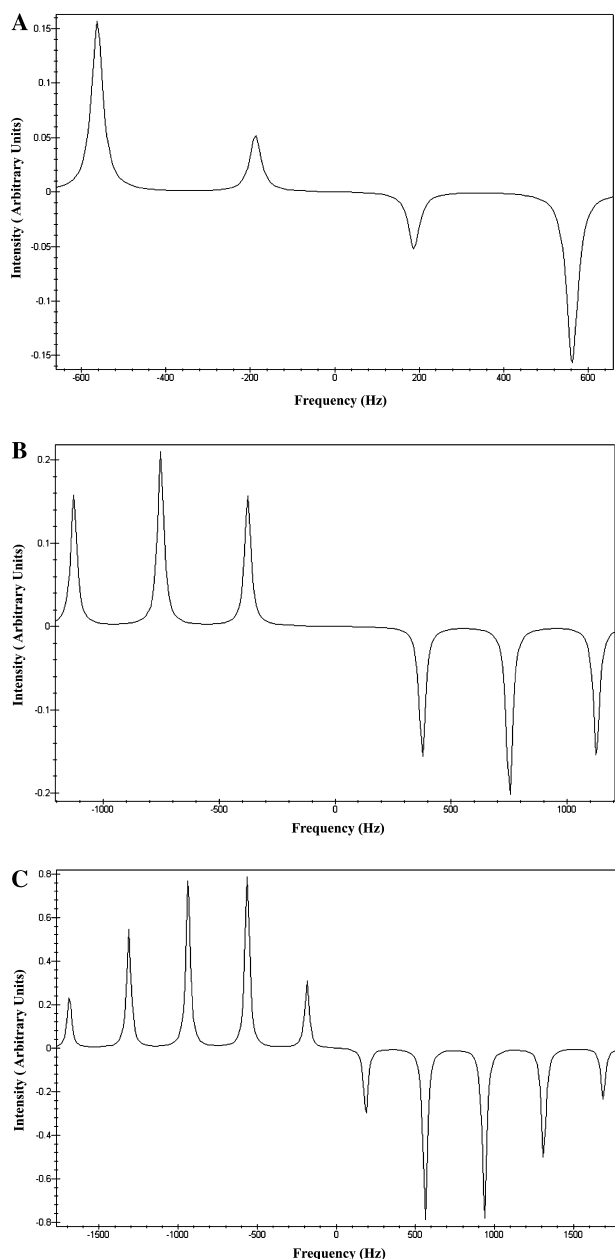


Fig. 2. Simulated spectra of weakly coupled  $^{119}\text{Sn}\{^{81}\text{Cl}\}$  INEPT NMR of the selected molecules (A) for the  $IS$  ( $I = 1/2$ ,  $S = 3/2$ ) spin system, (B) for the  $IS_2$  spin system, and (C) for the  $IS_3$  spin system.

Table 2

For  $IS$  ( $I = 1/2$ ,  $S = 3/2$ ) spin systems, the calculated first five density matrix operators in reverse INEPT (RINEPT) pulse sequence

REVERSE INEPT
$\sigma_0 = aI_z + bS_z$
$\sigma_1 = -aI_y + bS_x$
$\sigma_2 = -aI_y E_s \left(\pm \frac{3}{2}\right) C'_{3J} + \frac{2}{3} aI_x S_z E_s \left(\pm \frac{3}{2}\right) S'_{3J}$ $- aI_z E_s \left(\pm \frac{1}{2}\right) C'_J + 2aI_x S_z E_s \left(\pm \frac{1}{2}\right) S'_J + bS_x$
$\sigma_3 = -\sigma_2$
Using $\cos(2\pi J\tau) = 0$ , $\sin(2\pi J\tau) = 1$ since $\tau = 1/4J$ ,
$\sigma_4 = +\frac{2}{3} aI_x S_z E_s \left(\pm \frac{3}{2}\right) - 2aI_x S_z E_s \left(\pm \frac{1}{2}\right) - bS_x$
$\sigma_5 = \frac{2}{3} aI_z S_y E_s \left(\pm \frac{3}{2}\right) - 2aI_z S_y E_s \left(\pm \frac{1}{2}\right) + bS_y$

Where  $C'_{nJ} = \cos(n\pi J\tau)$  and  $S'_{nJ} = \sin(n\pi J\tau)$ .

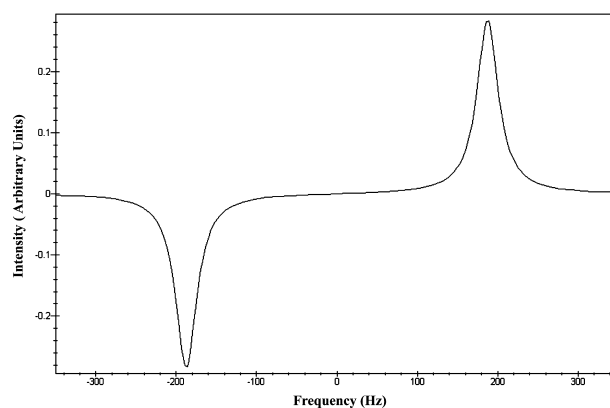


Fig. 3. Simulated spectrum of weakly coupled  $^{119}\text{Sn}\{^{35}\text{Cl}\}$  RINEPT NMR of the selected molecule (as the  $IS$  ( $I = 1/2$ ,  $S = 3/2$ ) spin system).

$$\sigma_f = -\frac{2}{3} aS_y E_s \left(\pm \frac{3}{2}\right) S_S S_J + 2aS_y E_s \left(\pm \frac{1}{2}\right) S_S S_J. \quad (15)$$

Since the observable magnetization is defined as

$$M_y(t) \propto \langle S_y \rangle = \text{Tr}[S_y \sigma_f] \quad (16)$$

and using the coefficients

$$\text{Tr} \left[ S_y S_y E_s \left(\pm \frac{3}{2}\right) \right] = \frac{3}{2}$$

and

$$\text{Tr} \left[ S_y S_y E_s \left(\pm \frac{1}{2}\right) \right] = \frac{7}{2},$$

finally we get

$$\langle S_y \rangle (IS) = 6aS_S S_J \\ = 3a[\cos(\Omega_s - \pi J)t - \cos(\Omega_s + \pi J)t]. \quad (17)$$

Therefore, for RINEPT pulse sequences we have only two signals at the coordinates of  $(\frac{J}{2}, \Omega_s)$  and  $(-\frac{J}{2}, \Omega_s)$  with an intensity distribution of  $(-1:1)$ . The simulations of these two signals for the selected molecule, trimethyltinchloride  $[(\text{CH})_3\text{SnCl}]$  (as  $IS$  spin system), are shown in Fig. 3.

For RINEPT experiment we have only two signals for  $IS_2$  and  $IS_3$  ( $I = 1/2$ ,  $S = 3/2$ ) spin systems as we detect always on the spin-3/2 nuclei along  $y$ -axis. The simulations of these two signals are shown in Fig. 3.

## 2. Results and discussion

It is well known that the INEPT NMR experiment is one of the most popular heteronuclear multi-pulse experiments and was initially designed to enhance the sensitivity of observing low- $\gamma$  nuclei by means of polarization transfer. In this study first we have presented the descriptions of INEPT NMR experiment for  $IS_n$  ( $I = 1/2$ ,  $S = 3/2$  with  $n = 1, 2, 3$ ) and reverse INEPT

(or RINEPT) NMR experiment for  $IS$  ( $I = 1/2$ ,  $S = 3/2$ ) weakly coupled spin systems by using the product operator formalism. Approximately two-thirds of the NMR active nuclei in the periodic table are quadrupolar and therefore the NMR studies of quadrupolar nuclei are crucial. However,  $J$  coupling to these fast relaxing nuclei can not be often observable. But when the quadrupolar nuclei have zero electric field gradient in some symmetries of molecules, multiplet structure can be arisen from spin–spin coupling and observed [17]. In INEPT NMR experiment the final spectrum should contain responses from those spin-3/2 nuclei which are coupled to spin-1/2 nuclei. This case can be satisfy by using phase cycling schemes of the mentioned pulse sequences. In this framework Rinaldi and Baldwin [22] showed that the polarization transfer from low gamma quadrupolar nuclei ( $^1\text{H}\{^{11}\text{B}\}$ ) to  $I = 1/2$  nucleus in the ( $^1\text{H}\{^{11}\text{B}\}$ ) INEPT experiment can produce the maximum enhancement in theoretical base.

Since the INEPT experiment is usually recommended for nuclei having negative  $\gamma$  values,  $^{29}\text{Si}$ ,  $^{119}\text{Sn}$ , and  $^{15}\text{N}$  being three examples and should be used only if one  $J$  value is involved and its magnitude is know, in three organotin complexes we have taken as the real chemical systems, namely, trimethyltinchloride [ $(\text{CH}_3)_3\text{SnCl}$ ] (as  $IS$  spin system), dimethyltinchloride [ $(\text{CH}_3)_2\text{SnCl}_2$ ] (as  $IS_2$  spin system) and methyltintrichloride [ $\text{CH}_3\text{SnCl}_3$ ] (as  $IS_3$  spin system) these conditions could be satisfied.

In our work for weakly coupled  $IS$  ( $I = 1/2$ ,  $S = 3/2$ ) spin system in INEPT experiment in which PT is from spin-3/2 to spin-1/2 nuclei by using phase cycling we obtained four signals with an intensity distribution of (–3:–1: 1:3). This result is in very good agreement with some experimental results [22]. Furthermore the simulations of the signal intensities calculated of a selected molecules containing  $^{119}\text{Sn}$   $\{^{35}\text{Cl}\}$  nuclei by using INEPT and RINEPT pulse sequences were performed in the Maple programme on computer and the spectra obtained justify the above discussions.

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