

## Rotating and Principal-Axis Frames in Multipole NMR

B. C. SANCTUARY AND MANGALA S. KRISHNAN

*Department of Chemistry, McGill University, 801 Sherbrooke Street West,  
Montreal, Quebec, Canada H3A 2K6*

Received January 9, 1986

The use of a spherical tensor operator basis to describe the nuclear magnetic state makes it ideal for considering rotations and transformations of the density operator to different frames. In this paper it is shown how all polarizations can be transformed to different frames which display the greatest reduction of coupling. These correspond to various rotating and/or principal-axis frames. © 1986 Academic Press, Inc.

### INTRODUCTION

Spherical tensors, irreducible under the rotation group have the property (1) that they can be rotated by a Wigner rotation matrix according to

$$\phi_q^k(\Omega) = \sum_{q'} \mathcal{D}_{qq'}^{(k)}(\Omega) \phi_{q'}^k(0) \quad [1]$$

where  $\Omega$  denotes the three Euler angles,  $k$  is its tensor rank, and  $q$  the spherical component. The special case of  $k = 1$  corresponds to a vector upon which the vector model of NMR rests. Higher tensor ranks, however, also display similar behaviour and cannot be neglected in NMR. It is advantageous to retain the rotational properties not only for the physical insight they provide for higher tensor ranks but also for the same mathematical simplification afforded by the rotating frame and principal axis transformations.

The usual motivation for transformations in NMR is to simplify the Hamiltonian matrix. Consequently, a particular form of Hamiltonian is cast into a frame whereby some motion is removed, or some parametrization simplified. The transformed Hamiltonian is then used to solve a particular problem.

In contrast, the multipole formulation, discussed earlier (2-5), retains the full Hamiltonian, but transforms, wherever possible, the spherical tensor basis to a convenient frame in which the Hamiltonian is simple. This approach results in a set of coupled differential equations, the rotation of which causes the spin dynamics to partially or completely uncouple.

This fact has been pointed out again in a recent publication with a more primitive operator basis set (6). In our formulation, we have used the irreducible spherical tensor operators defined as a linear combination of the set  $|IM\rangle\langle IM'|$ , which are rotationally invariant under  $SO(3)$  and satisfy the correct time-invariance symmetry. In this paper, we treat a Hamiltonian commonly used in NMR and show how the principal axis can be found by rotating the basis set for a variety of cases. For systems with a defined

principal axis like pure quadrupolar systems or quadrupolar-Zeeman systems we shall illustrate the general approach. It must be stressed that the development is valid for any spin  $I$ . Following this, we shall illustrate special cases of rotating and doubly rotating frames. Thus we attempt to unify many possible future applications.

PRINCIPAL AXIS TRANSFORMATION

A number of treatments consider various forms of the Hamiltonian used in NMR problems. We start with the expression of Spiess (7)

$$\mathcal{H}_\lambda = C^\lambda \sum_{l=0}^2 \sum_{m=-l}^l (-1)^{l-m} T^{(l)m}(V^\lambda) \times \sum_{m'=-l}^l \rho_{lm'}^\lambda \mathcal{D}_{m'-m}^{(l)}(\alpha_\lambda \beta_\lambda \gamma_\lambda) \quad [2]$$

where  $\lambda$  refers to Zeeman, chemical shift, dipole-dipole, spin-spin coupling, spin-rotation, or quadrupole interactions.  $T^{(l)m}(V)$ 's are single-spin or multispin operators as the case may be. The coefficients  $\rho_{lm'}^\lambda$  are given by Spiess. The spin operator  $T^{(l)m}(V)$ 's differ from Spiess only by a phase, which we choose as follows

$$T^{(l)m}(V)^\dagger = (-1)^{l-m} T^{(l)-m}(V) \quad [3]$$

under the operation of operator adjoint<sup>†</sup>. For example, an explicit representation of the  $T^{(l)m}(V^\lambda)$ 's can be given either in a single spin basis  $|I m\rangle \langle I m'|$  or in a multispin basis.

$$|I_1 m_1 I_2 m_2 \dots I_n m_n\rangle \langle I_1 m'_1 I_2 m'_2 \dots I_n m'_n|$$

We prefer to use the following:

$$\mathcal{Y}^{(k)q}(I) = (i)^k \sqrt{(2I+1)(2k+1)} \sum_{M M'} (-1)^{I-M} \begin{bmatrix} I & k & I \\ -M & q & M' \end{bmatrix} |IM\rangle \langle IM'| \quad [4a]$$

where  $k$  is the tensor rank and  $q$  the spherical component of  $k$  ( $k = 0$  to  $2I$ ;  $q = -k$  to  $k$ ) for single spin operators and

$$\begin{aligned} T_{\{\bar{K}\}}^{(k)q}(k_1 k_2 \dots k_N)^{Z_{N0}} &= \frac{1}{\sqrt{(2I_1+1)(2I_2+1)\dots(2I_N+1)}} \\ &\times \sum_{\substack{q_1 q_2 \dots q_N \\ \bar{q}_1 \bar{q}_2 \dots \bar{q}_{N-2}}} \sqrt{(2\bar{K}_1+1)(2\bar{K}_2+1)\dots(2\bar{K}_{N-2}+1)(2k+1)} \\ &\times (-1)^{(\bar{K}_1+\bar{K}_2+\dots+\bar{K}_{N-2})+(k_1-k_2+\dots-k_N+k)+(\bar{q}_1-\bar{q}_2+\dots+\bar{q}_{N-2})} \\ &\times (-1)^{k-q} \begin{bmatrix} k_1 & k_2 & \bar{K}_1 \\ q_1 & q_2 & -\bar{q}_1 \end{bmatrix} \begin{bmatrix} \bar{K}_1 & k_3 & \bar{K}_2 \\ \bar{q}_1 & q_3 & -\bar{q}_2 \end{bmatrix} \dots \begin{bmatrix} \bar{K}_{N-2} & k_N & k \\ \bar{q}_{N-2} & q_N & -q \end{bmatrix} \\ &\times \mathcal{Y}^{(k_1)q_1}(I_1) \mathcal{Y}^{(k_2)q_2}(I_2) \dots \mathcal{Y}^{(k_N)q_N}(I_N) \quad [4b] \end{aligned}$$

for multispin operators.

Here  $Z_{N0}$  refers to the sequential coupling scheme  $((\dots(I_1 + I_2) + I_3) + \dots + I_N)$  with the intermediate coupling constants  $\bar{K}_1, \bar{K}_2, \dots, \bar{K}_{N-2}$ , denoted by the set  $\{\bar{K}\}$ . All of these labels are quantum numbers.

By the use of the properties of Wigner reduced rotation matrix  $d_{m' m}^{(j)}(\beta)$  ( $J$ ), for example

$$d_{m' m}^{(j)}(\beta) = (-1)^{j-m} d_{m' -m}^{(j)}(\beta + \pi) \quad [5]$$

we can rewrite the Hamiltonian matrix as

$$\mathcal{H}_\lambda = C^\lambda \sum_{lmm'} T^{(l)m}(V^\lambda) \rho_{lm'}^\lambda \mathcal{D}_{m' m}^{(l)}(\alpha^\lambda \beta^\lambda \gamma^\lambda)$$

where

$$\alpha^\lambda = -\alpha_s^\lambda, \quad \beta^\lambda = \beta_s^\lambda - \pi, \quad \text{and} \quad \gamma^\lambda = \gamma_s^\lambda \quad [6]$$

and the summation indices correspond to [2].

Expanding the density operator for spin in the multipole basis with coefficients  $\phi_m^l(v)$  gives

$$\sigma = \sum_{l,m,\{v\}} \phi_m^l(v) T^{(l)m}(v) \quad [7]$$

where  $\{v\}$  denotes the set of intermediate coupling constants, if necessary, to specify  $T^{(l)m}$  uniquely (2). This is substituted into the quantum-Liouville equation for the density operator

$$i\hbar \frac{d\sigma}{dt} = [\mathcal{H}_\lambda, \sigma] \quad [8]$$

and using the orthogonality relations of  $T^{(l)m}(v)$ 's (3) leads to

$$i\hbar \frac{d\phi_q^k}{dt}(v) = C^\lambda \sum_{\substack{lmm' \\ k'q'(v')}} \rho_{lm'}^\lambda \mathcal{D}_{m' m}^{(l)}(\alpha^\lambda \beta^\lambda \gamma^\lambda) \times \langle\langle T^{(k)q}(v^\lambda) [T^{(l)m}(v^\lambda), T^{(k')q'}(\bar{v}^\lambda)] \rangle\rangle \phi_q^{k'}(\bar{v}). \quad [9]$$

The matrix element of the above, denoted by  $\langle\langle [ \quad , \quad ] \rangle\rangle$  can be treated using the Wigner-Eckart theorem to give a product of a reduced matrix element and a Wigner coefficient as ( $J$ )

$$\begin{aligned} & \langle\langle T^{(k)q}(v^\lambda) [T^{(l)m}(v^\lambda), T^{(k')q'}(\bar{v}^\lambda)] \rangle\rangle \\ &= (-1)^{k-q} \begin{bmatrix} k & l & k' \\ -q & m & q' \end{bmatrix} \langle\langle T^{(k)}(v^\lambda) [T^{(l)}(v^\lambda), T^{(k')}(\bar{v}^\lambda)] \rangle\rangle \\ &= (-1)^{k-q} \begin{bmatrix} k & l & k' \\ -q & m & q' \end{bmatrix} f(klk'v^\lambda v^\lambda \bar{v}^\lambda) \end{aligned} \quad [10]$$

where  $f(klk'v^\lambda v^\lambda \bar{v}^\lambda)$  is shorthand for the reduced matrix element.

In view of this, Eq. [9] can now be cast into the form

$$\begin{aligned} i\hbar \frac{d\phi_q^k}{dt}(v) = C^\lambda \sum_{\substack{lmm' \\ k'q'(v')}} \{ & (-1)^{k-q} \begin{bmatrix} k & l & k' \\ -q & m & q' \end{bmatrix} \rho_{lm'}^\lambda \\ & \times \mathcal{D}_{m' m}^{(l)}(\alpha^\lambda \beta^\lambda \gamma^\lambda) f(klk'v^\lambda v^\lambda \bar{v}^\lambda) \} \phi_q^{k'}(\bar{v}). \end{aligned} \quad [11]$$

At this point, a great deal of coupling exists as seen by the sum and [11] is not easy to solve. The utility of any basis is to remove such couplings as much as possible. One approach is to start initially with a Hamiltonian in a principal axis, or rotating frame. Situations exist, however, when the angle dependence of [6] is needed. The procedure here is to simplify the set of equations [11] as much as possible, solve the coupled equation using well-known techniques of differential equations, and transform the results back to the original basis. Rotation of the  $\phi_q^k(v)$ 's to a different orientation can be shown to eliminate the  $mm'$  summation in special cases. We define a rotated basis quite generally by

$$\Psi_{\bar{q}}^k(v) = \sum_q \mathcal{D}_{\bar{q}q}^{(k)}(\alpha''\beta''\gamma'')\phi_q^k(v) \quad [12]$$

and its inverse

$$\phi_q^k(v) = \sum_{\bar{q}'} \mathcal{D}_{\bar{q}'q}^{(k)*}(\alpha''\beta''\gamma'')\Psi_{\bar{q}'}^k(v). \quad [13]$$

By virtue of the property (I)

$$\begin{aligned} \sum_{qq'} \mathcal{D}_{\bar{q}q}^{(k)}(\alpha\beta\gamma)(-1)^{k-q} \begin{bmatrix} k & l & k' \\ -q & m & q' \end{bmatrix} \mathcal{D}_{\bar{q}'q'}^{(k')*}(\alpha\beta\gamma) \\ = (-1)^{k'-q'}(-1)^{l-m} \begin{bmatrix} k & k' & l \\ -\bar{q} & \bar{q}' & m'' \end{bmatrix} \mathcal{D}_{m''m}^{(l)}(\gamma\beta\alpha) \end{aligned} \quad [14]$$

Eq. [11] can be simplified to

$$i\hbar \frac{\partial \Psi_{\bar{q}}^k(v)}{\partial t} = C^\lambda \sum_{\substack{l\bar{v}^\lambda \\ kq'}} (-1)^{l-m''} (-1)^{k'-\bar{q}'} \begin{bmatrix} k & k' & l \\ -\bar{q} & \bar{q}' & m'' \end{bmatrix} \times \rho_{l\bar{m}''}^\lambda \Psi_{\bar{q}}^{k'}(v) f(klk'v^\lambda v^\lambda \bar{v}^\lambda) \quad [15]$$

only for the choice of angles

$$\alpha'' = -\alpha^\lambda, \quad \beta'' = \beta^\lambda, \quad \text{and} \quad \gamma'' = -\gamma^\lambda$$

which determine the frame in which the problem displays maximum simplicity. For the Hamiltonian [6], apart from the imposition of additional, say point-group, symmetry, no further decoupling can occur without imposing approximations. The choice of angles  $\alpha''$ ,  $\beta''$ , and  $\gamma''$  in the transformation [12] clearly depends upon the angle of the particular mechanism in the Hamiltonian ( $\alpha^\lambda$ ,  $\beta^\lambda$ ,  $\gamma^\lambda$ ) (6). This is the principal-axis coordinate frame. Equation [15] is further simplified when the tensor rank of the Hamiltonian interaction is restricted by the mechanism to be  $l = 1$  or  $2$ .

*Axially symmetric interactions.* In the case that an interaction is characterized by one constant  $C^\lambda$ , the Hamiltonian [6] simplifies to

$$\mathcal{H}_\lambda = \sum_m C_{lm}^\lambda T^{(l)m}(v^\lambda) \quad [16]$$

where

$$C_{lm}^\lambda = C^\lambda \mathcal{D}_{m0}^{(l)}(O\beta^\lambda\gamma^\lambda)$$

The Hamiltonian, for example, can be written as

$$\mathcal{H}_Q = -\gamma \hbar I_z H_z + \frac{\hbar e^2 Qq}{2I(2I-1)} \{3I_z^2 - I(I+1)\} \quad [17]$$

In the rotating frame  $\mathcal{H}_Q$  satisfies [16]. Equation [15] then takes the form

$$i\hbar \frac{\partial \Psi_{\bar{q}}^k}{\partial t} = C^{\lambda} \sum_{k' \bar{q}'} f(klk'v^{\lambda}v^{\lambda}\bar{v}^{\lambda}) \times (-1)^{k'-\bar{q}} \begin{bmatrix} k & k' & I \\ -\bar{q} & \bar{q} & 0 \end{bmatrix} \Psi_{\bar{q}}^k \quad [18]$$

which is diagonal in  $\bar{q}$ . For an axially symmetric quadrupole interaction of a single spin, this equation has been solved for  $I \leq \frac{5}{2}$  and coefficients  $f(klk'v^{\lambda}v^{\lambda}\bar{v}^{\lambda})$  have been given elsewhere (4).

*Quadrupole-Zeeman systems with arbitrary asymmetry.* In this section, we give a more explicit representation for the  $f(klk'v^{\lambda}v^{\lambda}\bar{v}^{\lambda})$ . The full Hamiltonian consists of the pure quadrupolar terms and the Zeeman field in a direction  $\theta\phi$  to the axis of symmetry and can be written as

$$\mathcal{H} = -\gamma \hbar H_0 (I_z \cos \theta + I_x \sin \theta \cos \phi + I_y \sin \theta \sin \phi) + \hbar \frac{e^2 Qq}{4I(2I-1)} \left[ (3I_z^2 - I^2) + \frac{\eta}{2} (I_+^2 + I_-^2) \right]. \quad [19]$$

In the basis set of  $\mathcal{Y}^{(k)q}(I)$ 's as defined earlier by [4], we can rewrite the Hamiltonian as

$$\begin{aligned} \mathcal{H} = i\hbar\omega_0 \left[ \cos \theta \sqrt{\frac{I(I+1)}{3}} \mathcal{Y}^{(1)0}(I) + \frac{\sin \theta}{2} e^{i\phi} \times \sqrt{\frac{2I(I+1)}{3}} \mathcal{Y}^{(1)-1}(I) \right. \\ \left. - \frac{\sin \theta}{2} e^{-i\phi} \sqrt{\frac{2I(I+1)}{3}} \mathcal{Y}^{(1)1}(I) \right] - \frac{\hbar e^2 Qq}{4} \sqrt{\frac{(2I+3)(I+1)}{5I(2I-1)}} \\ \times \left\{ \mathcal{Y}^{(2)0}(I) + \frac{\eta}{\sqrt{6}} (\mathcal{Y}^{(2)2}(I) + \mathcal{Y}^{(2)-2}(I)) \right\}. \quad [20] \end{aligned}$$

The spin-density operator in our basis set, expressed as

$$\sigma = \frac{1}{(2I+1)} \sum_{k=0}^{2I} \sum_{q=-k}^k \mathcal{Y}^{(k)q}(I) \phi_q^{(k)}$$

where

$$\phi_q^{(k)} = \langle \langle \mathcal{Y}^{(k)q}(I) | \sigma \rangle \rangle = T\gamma \{ [\mathcal{Y}^{(k)q}]^{\dagger} \sigma \} \quad [21]$$

leads to the following differential equation for  $\phi_q^{(k)}$ 's. Details of this method for the pure quadrupolar system ( $\omega_0 = 0$ ) has been described elsewhere (5) and the equation below follows from straightforward application of Clebsch-Gordan algebra.

$$\begin{aligned} \frac{\partial \phi_q^k}{\partial t} = i\omega_0 \cos \theta q \phi_q^k + i\omega_0 e^{i\phi} \frac{\sin \theta}{2} \sqrt{(k-q)(k+q+1)} \phi_{q+1}^k \\ + i\omega_0 e^{-i\phi} \frac{\sin \theta}{2} \sqrt{(k+q)(k-q+1)} \phi_{q-1}^k \end{aligned}$$

$$\begin{aligned}
 & + \frac{3}{2} \hat{Q} \sqrt{\frac{(2I+k+2)(2I-k)[(k+1)^2 - q^2]}{I^2(2I-1)^2(2k+1)(2k+3)}} \phi_q^{k+1} \\
 & + \frac{\hat{Q}\eta}{4} \sqrt{\frac{(k-q+1)(k-q+2)(k-q+3)(k+q)(2I+k+2)(2I-k)}{I^2(2I-1)^2(2k+1)(2k+3)}} \phi_{q-2}^{k-1} \\
 & - \frac{\hat{Q}\eta}{4} \sqrt{\frac{(k+q+1)(k+q+2)(k+q+3)(k-q)(2I+k+2)(2I-k)}{I^2(2I-1)^2(2k+1)(2k+3)}} \phi_{q+2}^{k-1} \\
 & - \frac{3}{2} \hat{Q}q \sqrt{\frac{(k^2 - q^2)(2I+k+1)(2I-k+1)}{I^2(2I-1)^2(2k+1)(2k-1)}} \phi_q^{k-1} \\
 & + \frac{\hat{Q}\eta}{4} \sqrt{\frac{(k+q-2)(k+q-1)(k+q)(k-q+1)(2I+k+1)(2I-k+1)}{I^2(2I-1)^2(2k+1)(2k-1)}} \phi_{q-2}^{k-1} \\
 & - \frac{\hat{Q}\eta}{4} \sqrt{\frac{(k-q-2)(k-q-1)(k-q)(k+q+1)(2I+k+1)(2I-k+1)}{I^2(2I-1)^2(2k+1)(2k-1)}} \phi_{q-2}^{k-1}
 \end{aligned} \quad [22]$$

where  $\hat{Q} = e^2 Q q / 2$ . A complete analysis of the differential equation will not be considered here. We point out the simple feature of this equation as follows:

$$\frac{\partial \phi_q^k}{\partial t} = \sum_{q'} A_{q'} \phi_{q'}^k + \sum_{q'} B_{q'} \phi_{q'}^{k+1} + \sum_{q'} C_{q'} \phi_{q'}^{k-1} \quad [23]$$

with  $q'$  summed over approximate  $q$  values and  $A, B, C$  the corresponding coefficients. This set of equations is quite general to all single-spin-1 problems and contains all the information we need to know about a fairly complicated Hamiltonian. If we recall that  $\phi_1^1$  and  $\phi_{-1}^1$  are related directly to the observable magnetization  $M_x + iM_y$ , this provides us a tool for analyzing the effect of a pulse or a series of pulses on almost any system with any initial state of preparation where single-spin approximation is valid and relaxation effects can be neglected. Thus a system of coupled differential equations with constant coefficients is all that is necessary to work with. A phenomenological approach including relaxation effects and an exact method for the dipolar effects in a multispin basis operators are in progress. The method also illustrates the generality of spherical tensors to a Hamiltonian which has been transformed into a principal axis frame. The next two sections consider the case where such a simplification is not available and where rotating and doubly rotating frames defined from the basis set come in handy for solutions.

*Zeeman Interaction.* For a single spin of arbitrary magnitude, an operator basis has been defined by  $\mathcal{Y}^{(k)q}(I)$  (3-5) and the Zeeman Hamiltonian in the rotating frame of the rf-field of frequency  $\omega$ , is

$$= ih \sqrt{\frac{I(I+1)}{3}} \left[ \Delta \omega \mathcal{Y}^{(1)0}(I) + \frac{1}{\sqrt{2}} \omega_1 e^{-i\omega t} \mathcal{Y}^{(1)1}(I) - \frac{1}{\sqrt{2}} \omega_1 e^{i\omega t} \mathcal{Y}^{(1)-1}(I) \right] \quad [24]$$

or

$$= i\hbar\Omega \sqrt{\frac{I(I+1)}{3}} \sum_m \mathcal{D}_{mb}^{(I)}(0\theta - \phi) \mathcal{Y}^{(I)m}(I) \quad [25]$$

where  $\Omega = \sqrt{\Delta\omega^2 + \omega_1^2}$ ,  $\Delta\omega = \omega - \omega_0$  and  $\cos\theta = \Delta\omega/\Omega$ ,  $\sin\theta = \omega_1/\Omega$ . After transforming to the frame defined by the effective field angles  $\theta$  and  $\phi$ , the multipole polarizations obey

$$\frac{d\Psi_q^k}{dt} = i\Omega\bar{q}\Psi_q^k \quad [26]$$

thereby generalizing, to tensors of arbitrary rank rotating with multi-quantum frequencies  $\bar{q}\Omega$  about the effective field, the vector model of rotation about the effective field in the rotating frame. The effective field defines the principal-axis frame of the rf Hamiltonian. Although the transformation to an effective field is common, it has been only done for vector quantities; Eq. [26], however, is valid for all spin magnitudes of all tensor ranks, and also for off-resonant cases, for the choice of angles shown above.

*Doubly rotating frame.* When more than one mechanism exists it is possible to transform to a frame in which one part, say that which gives the dominant contribution, is simplest. Such a transformation causes the other part of the Hamiltonian to become more off-diagonal, but these can usually be treated as perturbations.

Consider an rf field and a nuclear quadrupole acting simultaneously, but with the former dominant. The first rotating frame transforms all tensor polarizations to the rf frame

$$\phi_q^k(v) = e^{-i\omega_1 t} \phi_q^k(v). \quad [27]$$

Next the transformation [12] leads to [26] for the rf part, but introduces additional terms arising from the rotation of the quadrupole part to the effective field. The doubly rotating frame removes the precession about the effective field,

$$\Psi_q^k = \exp[-i\bar{q}\Omega t] \Psi_q^k \quad [28]$$

eliminating the rf field completely and leaving only the quadrupole part with considerable off-diagonality. For example, an initial axially symmetric quadrupole becomes effectively asymmetric in the doubly rotating frame. This, however, can be solved using perturbation theory and the results then transformed back to the original frame (7).

#### CONCLUSION

In treating NMR spin-dynamics problems in multipole formulation, rotating frames and principal-axis transformations lead to simplifications in analogy to conventional approaches such as average Hamiltonian theory. The techniques used here are to be contrasted, however, with treatments in which the Hamiltonian is written in terms of tensor operators, and it alone is transformed and rotated. Although this is an alternative approach, such subsequent analyses usually treat the transformed Hamiltonian in a basis which does not display rotational symmetry, thereby losing some of the advantages gained from transforming the Hamiltonian.

The advantages gained, in addition, by using a spherical operator basis are clear when it is seen that the vector model is generalized to all tensor polarizations which are being increasingly the object of study in NMR. Hence the advantages of the vector model are carried over to higher tensor polarizations as seen from [12], [21], and [22]. Within a spherical basis, these transformations optimize the rotational properties. Further simplifications are possible, especially for multispin systems, by the application of point-group symmetry.

## REFERENCES

1. A. R. EDMONDS, "Angular Momentum in Quantum Mechanics," Princeton Univ. Press, Princeton, N.J., 1974.
2. A. P. YUTSIS, I. B. LEVINSON, AND V. V. VANAGAS, "Mathematical Apparatus of the Theory of Angular Momentum" (translated from Russian by the Israel Program for Scientific Translations), 1962.
3. B. C. SANCTUARY, *Mol. Phys.* **48**, 1155 (1983).
4. B. C. SANCTUARY, T. K. HALSTEAD, AND P. A. OSMENT, *Mol. Phys.* **49**, 753 (1983).
5. M. S. KRISHNAN AND B. C. SANCTUARY, *Z. Naturforsch. A* **41**, 353 (1986).
6. J. PH. GRIVET, *J. Magn. Reson.* **62**, 269 (1985).
7. H. N. SPIESS, "NMR Basis Principles and Progress," Vol. 15, p. 55 Springer-Verlag, Berlin, 1978.
8. B. C. SANCTUARY, *Mol. Phys.* **49**, 785 (1983).