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Publication Date
2012-09-17
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May 1981

Prepared for the U.S. Department of Energy under Contract W-7405-ENG-48
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COMPUTER GENERATION OF NUCLEAR SPIN SPECIES
AND NUCLEAR SPIN STATISTICAL WEIGHS

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Abstract

This paper develops computer programs for computer generation of nuclear spin species and nuclear spin statistical weights of rovibronic levels. The programs developed here generate nuclear spin species and statistical weights from the group structures known as Generalized Character Cycle Indices (GCCI's) which are easily computed from the character table of the PI group of the molecule under consideration. Procedures are illustrated with examples.
1. Introduction

The nuclear spin statistics of rovibronic levels are of fundamental importance in molecular spectroscopy. The nuclear spin statistical weights of the rovibronic levels yield information on the intensities of spectral lines and the hyperfine splitting of rovibronic levels. The conventional technique for finding the statistical weights involves finding the character of the reducible representation spanned by the nuclear spin functions and then taking the inner product of the rovibronic species and nuclear spin species which should contain the species of overall internal wave function. The symmetry species of overall internal wave function must be antisymmetric with respect to exchange of particles for Fermions and should be symmetric for Bosons. For a molecule containing \( b_1 \) nuclei of the type 1, \( b_2 \) nuclei of the type 2, etc., with their possible number of spin states being \( a_1 \), \( a_2 \), etc., there are \( a_1^{b_1} a_2^{b_2} \ldots \) spin functions. Even for a simple molecule like \(^{13}\)C Triphenylene there are 1073741824 nuclear spin functions. Thus it is quite difficult to enumerate all these spin functions, find their character and then find the statistical weights. We undertake the present investigation to develop computer programs which will yield the irreducible representations spanned by the set of nuclear spin functions and the nuclear spin species with minimal input.

The nuclear spin statistical weights of the rotational levels in the rotational subgroup have been discussed by Placzek and Teller (1), Wilson (2,3), Schäfer (4) and Mizushima (5). Hougen (6) pointed out the necessity of obtaining these nuclear spin statistical weights in the complete symmetry group (point group or permutation-inversion group) and correlated the nuclear spin statistical weights to the point groups. The topic has been reviewed by Herzberg (7) and more recently by Bunker (8).
Galbraith (9) obtained the nuclear spin statistical weights using the unitary group approach and Schur's theorem. Recently, Weber (10,11) discussed the nuclear spin statistical weights of symmetry top molecules belonging to point groups $D_{nh}$ or $D_{nd}$ ($n \leq 6$). The present author (12) recently developed a general method for the nuclear spin statistics of molecules belonging to any point group. In this paper we computerize this method with the intent of making it useful and readily available for spectroscopists. In Sec. 2 we shall briefly review this method.

The present author (13-22) has been employing combinatorial and group theoretical techniques for problems in chemical physics. This paper uses a theorem of Williamson (23) recently generalized by Merris (24). Even though this paper is self-contained, a better account of preliminaries and definitions can be found in the text books (25-28).

In recent years chemical applications of non-numerical computational methods are becoming important in several areas (29-32). This paper considers another such application to molecular spectroscopy.

In Sec. 2 we outline the theory and methods; Sec. 3 describes the computer programs and subroutines for nuclear spin statistics.

2. Theory and Methods

Let $D$ be the set of nuclei of the same kind in the molecule and let $R$ be the set of possible spin states of the nuclei in the set $D$. We will treat each kind of nuclei separately and obtain their nuclear spin species individually. The overall spin species is the direct product of different kinds of nuclear spin species. To illustrate, $D$ can be considered as the set of all hydrogen nuclei in a molecule and $R$ as the set consisting of 2 elements, namely $\uparrow$ (spin up) and $\downarrow$ (spin down). Let $G$ be the PI
(permutation-inversion) group of the molecule as defined by Longuet-Higgins (33). Each element $g$ in $G$ (permutation followed by inversion has the same effect as permutation on the nuclei) permutes the nuclei in $D$.

If one considers the set of functions $F$, from $D$ to $R$ then $g$ also permutes the functions in $F$. For example, a map $f_1$ from a set containing 4 deuterium nuclei with their possible spin states being $\check{\lambda}$, $\check{\nu}$ and $\check{\gamma}$ is shown below.

\[
\begin{align*}
  f_1(1) &= \check{\lambda} \\
  f_1(2) &= \check{\nu} \\
  f_1(3) &= \check{\gamma} \\
  f_1(4) &= \check{\lambda}
\end{align*}
\]

A typical $g \in G$ acts on a $f \in F$ by the procedure shown below.

\[
gf(1) = f(g^{-1}i) \quad i \in D
\]

Let us illustrate this with the map $f_1$ shown above and $g = (1234)$. Since $g = (1234)$, $g^{-1}$ is $(4321)$. Thus

\[
\begin{align*}
  gf_1(1) &= f_1(g^{-1}1) = f_1(4) = \check{\lambda} \\
  gf_1(2) &= f_1(g^{-1}2) = f_1(1) = \check{\lambda} \\
  gf_1(3) &= f_1(g^{-1}3) = f_1(2) = \check{\nu} \\
  gf_1(4) &= f_1(g^{-1}4) = f_1(3) = \check{\gamma}
\end{align*}
\]

Thus the nuclear spin function $\check{\lambda} \check{\nu} \check{\gamma} \check{\lambda}$ was permuted to $\check{\lambda} \check{\lambda} \check{\nu} \check{\gamma}$ by the action of $g = (1234)$ on $f_1$. Any permutation can be characterized by its cycle structure. A permutation $g \in G$ is said to have the cycle representation.
if it has \( b_1 \) cycles of length 1, \( b_2 \) cycles of length 2, 
..., \( b_n \) cycles of length \( n \). Equivalently, the cycle type of \( g \in G \) is 
\( (b_1, b_2, ..., b_n) \). Consequently, a \( g \in G \) which is a composite permutation-
 inversion operation will have the representation of the associated per-
mutation. However, the characters corresponding to these operations 
could be different. Define the generalized character cycle index, here-
after, abbreviated as GCCI, corresponding to the irreducible representa-
tion \( \Gamma \) whose character is \( \chi \) as
\[
p^G \chi = \frac{1}{|G|} \sum_{g \in G} \chi(g) x_1^{b_1} x_2^{b_2} ... x_n^{b_n}
\]

In order to book-keep the number of nuclear spin states in any spin 
function let us introduce the concept of weight. With each \( r \in R \) let us 
associate a formal symbol \( w(r) \), which we call the weight of \( r \). For ex-
ample, we may associate the weights \( \alpha \) and \( \beta \) to the spin states \( \alpha \) and \( \beta \) 
respectively. Then define the weight of any function \( f \in F \) as the products 
of the weights of the corresponding images. In symbols,
\[
W(f) = \prod_{d \in D} w(f(d)).
\]

For example the weight of the spin function \( \alpha \alpha \beta \beta \) corresponding to 4 
protons is \( \alpha^2 \beta^2 \).

In this set up Williamson (23) proved the following theorem for 
one-dimensional representations which was recently generalized by Merris 
(24) to irreducible representations of any dimension.

**Theorem 1:**
\[
G.F. \chi = P^G \chi(x_k) \rightarrow \sum_{r \in R} w^k(r).
\]
G.F.\(^{X}\) is the generating function for the irreducible representation whose character is \(\chi\) occurring in the set of spin functions. Equivalently, the coefficient of a typical term \(w_1 \ b_1^1 \ w_2 \ b_2^2 \ ...\) in G.F.\(^{X}\) gives the frequency of occurrence of the irreducible representation \(\Gamma\) whose character is \(\chi\) in the set of nuclear spin functions with the weight \(w_1 \ w_2 \ ...\). However, to obtain this all that we needed is the set of cycle indices which can be easily read-off by looking at the character table.

Before we proceed further let us illustrate the above theorem with an example. Consider an aggregate of Fermions with spin 1/2 arranged in \(O_h\) symmetry. Let \(T_{1u}\) be the irreducible representation under consideration.

\[
G.F. \left( \frac{T_{1u}}{O_h} \right) = \frac{1}{48} \left( 3x_1^6 - 9x_2^3 + 3x_1^2x_2^2 + 6x_1^2x_4 - 6x_2^2x_4 + 3x_1^4x_2 \right)
\]

Then G.F.\(^{T_{1u}}\)\(^{O_h}\) is given by the following expression.

\[
G.F. \left( \frac{T_{1u}}{O_h} \right) = \frac{1}{48} \left[ 3(\alpha + \beta)^6 - 9(\alpha^2 + \beta^2)^3 + 3(\alpha + \beta)^2(\alpha^2 + \beta^2)^2 
+ 6(\alpha + \beta)^2(\alpha^4 + \beta^4) - 6(\alpha^2 + \beta^2)(\alpha^4 + \beta^4) + 3(\alpha + \beta)^4(\alpha^2 + \beta^2) \right]
\]

This on simplification yields,

\[
\alpha^5\beta + \alpha^4\beta^2 + 2\alpha^3\beta^3 + \alpha^2\beta^4 + \alpha\beta^5
\]

Thus there is one \(T_{1u}\) representation in the set of spin functions containing 5 \(\alpha\)'s and 1 \(\beta\), one \(T_{1u}\) in the set of spin functions containing 4 \(\alpha\)'s and 2 \(\beta\)'s, 2 in the set of functions containing 3 \(\alpha\)'s and 3 \(\beta\)'s and so on. The elegance of this method lies in the fact that it did not require the character of the set of spin functions to decompose it into its irreducible components.
3. Program Description

The program POLYN which is the main program reads the input data, checks the input data for obvious errors, calls several subroutines which compute the generating functions, generate and printout the nuclear spin species. All the integer inputs are read in 16I5 format. The organization of this program is shown in the flow chart in Fig. 1.

3.1. Summary of Subroutines and Function Subprograms

Subroutine VEC generates the vector and coefficient by a multinomial expansion of each multinomial in the generating function. For example, if one considers a term $x_2^2 x_4^2$ in the GCCI for a Boson problem involving 12 nuclei then the two multinomials involved in this term are in the product

$$\left(\lambda^2 + \mu^2 + \nu^2\right)^2 \left(\lambda^4 + \mu^4 + \nu^4\right)^2.$$

Subroutine VEC generates all the possible vectors (powers of $\lambda$, $\mu$ and $\nu$ in the above expansion) and the corresponding coefficients which are products of several multinomial numbers. To compute the coefficients in the multinomial expansion the subroutine VEC calls a function subprogram MULTI. MULTI gives the multinomial of the argument of the function with the integers in the array K. For this purpose it calls a function subprogram IFACT which computes the factorial of the argument in the function.

Subroutine NEXCOM generates the next composition from a given composition. It is initialized by setting the logical variable MTC to false and calling the routine in a loop. The subroutine sets MTC to false if the generated composition is the last composition. Then one comes out of the loop and proceeds to the next set of instructions. Otherwise the subroutine is called again. This subroutine returns the composition in the
integer array R every time it is called. The vector thus returned in the array R is stored in the array KN. For details of this subroutine see Nijenhuis and Wilf (34).

Subroutine SPIN generates the nuclear spin species and the frequency of occurrence of each nuclear spin species. First the coefficients in the overall generating function are sorted according to their total spin quantum number. Then it branches to subsections depending on whether the nuclei are Bosons or Fermions. In each section the possible multiplicities and the occupations are obtained using the sorted coefficients. For Fermions there are 2 cases depending on if the total number of nuclei is odd or even. It also prints out all the nuclear spin species and the frequency of occurrence of each nuclear spin species in parentheses in an appropriate format.

The overall organization of all the subroutines and main program are shown in Fig. 2.

3.2. Input Description

The main program POLYN reads the input cards. The input should be in Tape 5 and the output is in Tape 6. Table 1 gives the description of the input for this program with formats and descriptions of the various variables. Here we would like to expound further on some of the variables. Consider a GCCI of the representation $[3^1]$ of the symmetric group $S_3$.

$$\text{GCCI}([3^1]) = \frac{1}{6} (x_1^3 - 3x_1x_2^1 + 2x_3^1)$$

For this GCCI, $NCI =$ number of terms in the GCCI and that is 3. The coefficients ICOCI for all the terms in the GCCI are 1, -3 and 2. For each term in the GCCI NPRO, N(i,j), Iexp(i,j) are to be fed in the same order as the coefficients. For example, NPRO, the number of distinct components
in the second term, is 2 because these are \(x_1^1\) and \(x_2^1\). For each of the NPRO terms \(N(i,j)\), the superfixes and \(Iexp(i,j)\), the suffixes are to be read in. To illustrate, cards 4-8 are shown below for this GCCI.

\[
\begin{array}{cccc}
3 & \text{(number of terms in the GCCI)} \\
1 & -3 & 2 & \text{(coefficients in the GCCI)} \\
1 & 3 & 1 & \text{(the first term)} \\
2 & 1 & 1 & 1 & 2 & \text{(the second term)} \\
1 & 1 & 3 & \text{(the third term)}
\end{array}
\]

A complete sample input is given in Table 2 for the proton spin species of a non-rigid triphenyl. The GCCI's of this molecule are shown in Table 3. For the coefficients and the various terms in the GCCI, Table 3 should be consulted. Even though there are 10 GCCI's for this molecule, Table 2 contains only 8 of them. This is because the pairs \((A_1^{++}, B_1^{++})\) and \((A_2^{++}, B_2^{++})\) have the same GCCI. For computational convenience the symmetry species are labelled as follows.

\[
\begin{array}{ll}
A_1^{++} & A_1 \\
B_1^{++} & B_1 \\
A_2^{++} & A_2 \\
B_2^{++} & B_2 \\
A_1^{++} & A_3 = B_1^{++} \\
A_2^{++} & A_4 = B_2^{++} \\
E_1^{++} & E_1 \\
E_1^{++} & E_2
\end{array}
\]
Since the PI group of this molecule is a direct product of permutation and inversion groups, the statistical weights and nuclear spin species of this molecule are unaffected by the ± labels. Also, there are only nuclear spin species which correspond to the + species. The output which corresponds to this input is shown in Table 4.

3.3. Limitations and Required Modifications to Circumvent the Limitations

Arrays in the common blocks B1-B5 are dimensioned to sufficiently large numbers to handle most of the chemically interesting cases. In case the problem requires arrays of greater lengths, these common blocks should be suitably altered. The present program can handle nuclei with up to 10 spin states. For nuclei with more than 10 spin states the arrays KN, IVEC, ITVEC and R have to be appropriately modified. The present program can handle GCCI's with any typical term $x_1^{b_1} x_2^{b_2} \cdots x_n^{b_n}$, for $n \leq 5$. For $n \geq 6$ a message is printed out by the subroutine VEC specifying this limitation. The subroutine contains comment statements giving instructions as to where the modifications are necessary.

3.4. Error Messages

This program is capable of detecting a number of inconsistent input errors. For example, it checks each typical term $x_1^{b_1} x_2^{b_2} \cdots x_n^{b_n}$ for correctness. Any such typical term in the GCCI should satisfy the condition

$$\sum_{i=1}^{n} i b_i = NT$$

where NT is the total number of nuclei. If this condition is not satisfied by the input then it prints out an error message "Input error for this term."
Check \( N(I), I_{\exp}(I) \). Then the user should check this term just printed out for consistency and correct it. The program will not proceed until this error is corrected. The second error message is based on the condition that the sum of all the coefficients of any term in the polynomial

\[
|G| \prod_{\sigma \in \mathbb{R}} (x_k \rightarrow \sum (w(r))^k)
\]

should be divisible by \( |G| \). If it is not divisible by \( |G| \), the program prints out an error message "ICO(JJ) is not divisible by MODG. Input error." Most probably, the error is in the set of coefficients in the array ICOCI. The user should carefully check these coefficients and correct them. If no error is detected in the coefficients then the error is in the terms

\[
b_1 x_1 \quad b_2 x_2 \quad \ldots \quad b_n x_n
\]

that is otherwise not detectable by the earlier criterion. When this error message is printed out the program branches to a stop.

A complete listing of the program can be found in Table 5.

As one can see from the output for each irreducible representation (Cf. Table 4), the frequency of occurrence of that irreducible representation in the set of spin functions is also computed by this program and printed out with the leading message "SPIN IRREP COMPONENT." One can immediately infer the irreducible representations contained in \( \Gamma_{\text{spin}} \), the reducible representation spanned by all nuclear spin functions. For example, for the proton spin functions of the non-rigid triphenyl

\[
\Gamma_{\text{spin}}^H = 2040 \ A_1^+ + 1960 \ B_1^+ + 696 \ A_2^+ + 744 \ B_2^+ + 1200 \ A_1''^+ + 1200 \ B_1''^+ + 432 \ A_2''^+ + 432 \ B_2''^+ + 2400 \ E_1^+ + 1440 \ E_1''^+.
\]

When \( \Gamma_{\text{spin}}^H \) is known the nuclear spin statistical weights of the rovibronic levels are obtained easily by stipulating that \( \Gamma_{\text{rov}} \otimes \Gamma_{\text{spin}} \) should contain
Γ^\text{int}_r$, where $Γ^\text{rve}$ is the species of the rovibronic level and $Γ^\text{int}$ is the species of the overall internal wave function. $Γ^\text{int}$ must satisfy the Pauli exclusion principle. Equivalently, $Γ^\text{int}$ must be antisymmetric with respect to odd permutations for Fermions and symmetric for Bosons.

References

20. K. Balasubramanian, Submitted for publication.
Acknowledgments

The author thanks Professor Kenneth S. Pitzer for his encouragement. This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the U. S. Department of Energy under Contract Number W-7405-ENG-48.
Table 1: Input for Program POLYN

<table>
<thead>
<tr>
<th>Card</th>
<th>Format</th>
<th>Input Variables</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10A8</td>
<td>TITLE</td>
<td>Alphanumeric title</td>
</tr>
<tr>
<td>2</td>
<td>16I5</td>
<td>NGCI</td>
<td>number of generalized cycle indices</td>
</tr>
<tr>
<td></td>
<td></td>
<td>NSPIN</td>
<td>number of spin states of the same kind of nuclei in the set D</td>
</tr>
<tr>
<td></td>
<td></td>
<td>NT</td>
<td>total number of nuclei in D</td>
</tr>
<tr>
<td></td>
<td></td>
<td>MODG</td>
<td>order of the group</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ISPIN(I), I=1,</td>
<td>spin quantum numbers. For Fermions twice the spin quantum numbers.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>NSPIN</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>IFERMI</td>
<td>Fermion parameter; equals 1 if the nuclei are Fermions. For Bosons set this to 0.</td>
</tr>
</tbody>
</table>

For each GCCI read the following cards 3-5. For the first GCCI additional cards need to be read as per the ensuing instructions.

<table>
<thead>
<tr>
<th>Card</th>
<th>Format</th>
<th>Input Variables</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>A10</td>
<td>SYM</td>
<td>label of the irreducible representation</td>
</tr>
<tr>
<td>4</td>
<td>16I5</td>
<td>NCI</td>
<td>number of terms in this GCCI</td>
</tr>
<tr>
<td>5</td>
<td>16I5</td>
<td>ICOCI(I), I=1,</td>
<td>coefficients of NCI terms in this GCCI</td>
</tr>
<tr>
<td></td>
<td></td>
<td>NCI</td>
<td></td>
</tr>
</tbody>
</table>

if this is the first GCCI for each $j = 1$, NCI feed a card described as card 6.

<table>
<thead>
<tr>
<th>Card</th>
<th>Format</th>
<th>Input Variables</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>16I5</td>
<td>NPRO</td>
<td>number of distinct components in each term of the GCCI</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$N(i, j), i=1, NPRO$ the superfixes of each component of a term of the GCCI</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$I\exp(i, j), i=1, NPRO$ the suffixes of each component of a term in the GCCI</td>
</tr>
</tbody>
</table>
Table 2: Sample Input

<table>
<thead>
<tr>
<th>Card</th>
<th>Non-Rigid Triphenyl Proton Species</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>8 2 14 16 -1 1 1</td>
</tr>
<tr>
<td>3</td>
<td>A1</td>
</tr>
<tr>
<td>4</td>
<td>6</td>
</tr>
<tr>
<td>5</td>
<td>1 3 3 4 4 1</td>
</tr>
<tr>
<td>6</td>
<td>1 14 1</td>
</tr>
<tr>
<td>7</td>
<td>2 10 2 1 2</td>
</tr>
<tr>
<td>8</td>
<td>2 6 4 1 2</td>
</tr>
<tr>
<td>9</td>
<td>1 7 2</td>
</tr>
<tr>
<td>10</td>
<td>2 3 2 2 4</td>
</tr>
<tr>
<td>11</td>
<td>2 2 6 1 2</td>
</tr>
<tr>
<td>12</td>
<td>B1</td>
</tr>
<tr>
<td>13</td>
<td>1 3 3 -4 -4 1</td>
</tr>
<tr>
<td>14</td>
<td>A2</td>
</tr>
<tr>
<td>15</td>
<td>1 -1 -1 -4 4 1</td>
</tr>
<tr>
<td>16</td>
<td>B2</td>
</tr>
<tr>
<td>17</td>
<td>1 -1 -1 4 -4 1</td>
</tr>
<tr>
<td>18</td>
<td>A3</td>
</tr>
<tr>
<td>19</td>
<td>1 1 -1 0 0 -1</td>
</tr>
<tr>
<td>20</td>
<td>A4</td>
</tr>
<tr>
<td>21</td>
<td>1 -3 3 0 0 -1</td>
</tr>
<tr>
<td>22</td>
<td>E1</td>
</tr>
<tr>
<td>23</td>
<td>2 2 -2 0 0 -2</td>
</tr>
<tr>
<td>24</td>
<td>E2</td>
</tr>
<tr>
<td>25</td>
<td>2 -2 -2 0 0 2</td>
</tr>
</tbody>
</table>
Table 3: The Non-Zero GCCI's of the Protons of a Non-Rigid Triphenyl

<table>
<thead>
<tr>
<th>Γ</th>
<th>$x_1^{14}$</th>
<th>$x_1 x_2^{10}$</th>
<th>$x_1 x_2^{6}$</th>
<th>$x_2^{4}$</th>
<th>$x_2 x_4^{7}$</th>
<th>$x_1 x_6^{3}$</th>
<th>$x_1 x_6^{2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{1}^{1+}$</td>
<td>1</td>
<td>3</td>
<td>3</td>
<td>4</td>
<td>4</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$B_{1}^{1+}$</td>
<td>1</td>
<td>3</td>
<td>3</td>
<td>-4</td>
<td>-4</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$A_{2}^{1+}$</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-4</td>
<td>4</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$B_{2}^{1+}$</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>4</td>
<td>-4</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$A_{1}^{1'}$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>0</td>
<td>0</td>
<td>-1</td>
<td></td>
</tr>
<tr>
<td>$B_{1}^{1'}$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>0</td>
<td>0</td>
<td>-1</td>
<td></td>
</tr>
<tr>
<td>$A_{2}^{1'}$</td>
<td>1</td>
<td>-3</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>-1</td>
<td></td>
</tr>
<tr>
<td>$B_{2}^{1'}$</td>
<td>1</td>
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Figure Captions

Figure 1: Flow chart of the program POLYN and subroutines.

Figure 2: Organization of the main program and the various subroutines.

Table Captions

Table 4: The computer output for the sample input is Table 2.

Table 5: Complete listing of the computer programs for nuclear spin statistics.
Entry POLYN

Read input data for $j = 1, \text{NGCI}$

if $j \geq 2$

if $j = 1$

For the first GCCI compute compositions

Generate the vector and coefficients for each term

Compute the total generating function

Compute the nuclear spin species and the irreducible representations spanned by spin functions

Is $j = \text{NGCI}$?

END
NCN-RIGID TRIPHENYL PROTON SPECIES

\begin{align*}
\text{SPIN IRREP COMPONENT } & 2040 \\
\text{THE GENERATING FUNCTION FOR NUCLEAR SPIN SPECIES} \\
\text{COEFFICIENT VECTOR} \\
& 1 \ 0 \\
& 4 \ 1 \\
& 21 \ 2 \\
& 58 \ 3 \\
& 142 \ 4 \\
& 244 \ 5 \\
& 396 \ 6 \\
& 396 \ 7 \\
& 244 \ 8 \\
& 142 \ 9 \\
& 58 \ 10 \\
& 21 \ 11 \\
& 4 \ 12 \\
& 1 \ 13 \\
& 0 \ 14 \\
\end{align*}

\begin{align*}
\text{SPIN IRREP COMPONENT } & 1960 \\
\text{THE GENERATING FUNCTION FOR NUCLEAR SPIN SPECIES} \\
\text{COEFFICIENT VECTOR} \\
& 0 \ 0 \\
& 4 \ 1 \\
& 16 \ 2 \\
& 58 \ 3 \\
& 129 \ 4 \\
& 244 \ 5 \\
& 335 \ 6 \\
& 335 \ 7 \\
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& 16 \ 11 \\
& 4 \ 12 \\
& 0 \ 13 \\
\end{align*}

\begin{align*}
\text{SPIN IRREP COMPONENT } & 696 \\
\text{THE GENERATING FUNCTION FOR NUCLEAR SPIN SPECIES} \\
\text{COEFFICIENT VECTOR} \\
& 0 \ 0 \\
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\end{align*}
### Spin Irrep Component 744
**The Generating Function for Nuclear Spin Species Coefficient Vector**

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**Spin IRREP Component 2400**

**The Generating Function for Nuclear Spin Species**

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**Spin IRREP Component 1440**

**The Generating Function for Nuclear Spin Species**

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**Spin IRREP Component 441**

**The Generating Function for Nuclear Spin Species**

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**PROGRAM POLY(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE7=INPUT)**

1. 0000000
   PROGRAM POLY(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE7=INPUT)
2. 0015448
   COMMON /B1/N10,20,100,APP,IFER,NPPI,INDEX
3. 0015448
   COMMON /B3/NCH,NCH,200,EXP5,20,EXP5,1000,IVEC(5,1000)
4. 0015448
   COMMON /B49/IVEC10,1000,10,CT(1000)
5. 0015448
   COMMON /B5/SYM,NSPIN,ISPIN(20),T1,IFERMI
6. 0015448
   INTEGER N111,ICC111,SYM,TITLE111
7. 0015448
   LOGICAL MTC
8. 0015448
   READ5(772)(TITLE111,I=1,10)
9. 0016279
   WRITE6(772)(TITLE111,I=1,10)
10. 0016308
    FORMAT(10A)
11. 0016308
    READ5(90,NCH,NPNI,IFER,NPPI,ISPIN),I=1,NPPI,IFERMI
12. 0016548
    WRITE6(90,NPPI,ISPIN),I=1,NPPI
13. 0016548
    DO 100 I=10,100
14. 0016678
    READ5(81)SYM
15. 0016718
    FORMAT(A10)
16. 0016718
    WRITE6(A10)
17. 0016718
    FORMAT(A10)
18. 0017028
    FORMAT(A10)
19. 0017028
    IF(IJK-L115.15.16)
20. 0017046
    READ5(90,NCI)
21. 0017108
    READ5(90,NC1,LYC1L),L=1,NCI
22. 0017208
    ISTAT=0
23. 0017208
    DO 100 IC=1,NCI
24. 0017233
    IF(IJK-L117.17.18)
25. 0017268
    READ6(16PRO),I(KNI1,ISUB),J=1,NPNI,IXP11,IC1),I=1,NPNI
26. 0017678
    GO TO 177
C FOR THE FIRST GCCI THE COMPOSITIONS FOR VARIOUS TERMS IN THIS GCCI
C ARE GENERATED THEN THEY ARE WRITTEN ON TAPE A. FOR ALL SUBSEQUENT
C GCCI'S THEY ARE READ FROM TAPE B.
27. 0017678
    DO 14 I=1,10
28. 0017718
    NEX1,IC1)=0
29. 0017728
    NPRO1,IC1)=0
30. 0017759
    READ5(90,NPRO,111,111,IC1,I=1,NPNI,IXP11,IC1),I=1,NPNI
31. 0020208
    WRITE6(16PRO,111,IC1,I=1,NPNI,IXP11,IC1),I=1,NPNI
32. 0021088
    WRITE6(16PRO,111,IC1,I=1,NPNI,IXP11,IC1),I=1,NPNI
33. 0020458
    FORMAT16PRO,111,1615)
34. 0020458
    DO 15 I=1,NPNI
35. 0020458
    ISUM=ISUM+NPRO1,IC1)
36. 0020458
    IF(ISUM-L1192.193.192)
37. 0020458
    WRITE6(16PRO,194)
38. 0020458
    STOP
39. 0020458
    FORMAT16PRO,#INPUT ERROR FOR THIS TERM.CHECK N11,IXP11+)
40. 0020468
    DO 15 I=1,NPNI
41. 0020468
    ISUM=ISUM+NPRO1,IC1)
42. 0020468
    IF(ISUM-L1192.193.192)
43. 0020468
    WRITE6(16PRO)
44. 0020468
    MTC=FALSE.
45. 0020468
    J=0
C SUBROUTINE NEXTCOM GENERATES THE NEXT COMPOSITION OF N11,IC1 IN TO
C NPNI PARTS IN THE ARRAY A.
46. 0021088
    CALL NEXTCOM111,IC1,NPNI,A,MTC)
47. 0021088
    J=1
48. 0021088
    DO 9 ISUB=1,3
49. 0021088
    KNI1(ISUB)=K(ISUB)
50. 0021138
    IF(MTC) GO TO 0
51. 0021148
    NPNI,IC1)=J
** PROGRAM POLY

** INPUT, OUTPUT, TAPE5 (INPUT), TAPE6 (OUTPUT), TAPE7 **

52. 0021150 11 CONTINUE
53. 0021210 WRITE(NPRO, ( \( I(j=1), Isum=1, Ispn=1, Ivec(i=1), I(i=1), I=1, I=npro \) )
54. 0021330 177 IF (I=15,5,6)
55. 0021580 9 NPP+NPL(I,IC)
56. 0021678 DO 200 I=1,NFIR
57. 0021728 DO 200 J=1,NPP
58. 0021758 200 IVEC(I,J,J)=KN1(I,1,1,1)
59. 0021210 CONTINUE DO 300 I=1,NPL(I,IC)
60. 0021160 300 ICO(TI)=0
61. 0021200 6 CALL VEC
62. 0021308 DO 350 III=1,NPP
63. 0021378 ICO(TI)=ICO(TI)+VEC(III,1,1,1,1,1)
64. 0021398 CONTINUE
65. 0021458 CONTINUE
66. 0021338 350 CONTINUE
67. 0021548 ICO(TI)=ICO(TI)+ICOC(I,IC)
68. 0021518 CONTINUE
69. 0021348 450 CONTINUE

** COMPUTATION OF THE FREQUENCY OF OCCURRENCE OF THE IRREDUCIBLE
** REPRESENTATION SPIN IN THE REPRESENTATION SPANNED BY ALL SPIN
** FUNCTIONS.

70. 0021578 I=1
71. 0021608 DO 373 III=1,NPP
72. 0021628 INPRO=INPRO+INSPIN*INPRO
73. 0021778 ISTAT=ISTAT+INPRO*ICOC(I,IC)
74. 0021210 CONTINUE
75. 0021308 DO 373 III=1,NPP
76. 0021378 ICO(TI)=ICO(TI)+VEC(III,1,1,1,1,1)
77. 0021398 CONTINUE
78. 0021458 CONTINUE
79. 0021338 373 CONTINUE
80. 0021548 ICO(TI)=ICO(TI)+ICOC(I,IC)
81. 0021518 CONTINUE
82. 0021348 473 CONTINUE

** IFICO(TI,J,J) MODG NOT DIVISIBLE BY NPP, INPUT ERROR.
** CHECKS FOR INPUT ERROR.

83. 0021258 IF (ICO(TI,J,J) MODG=1,199)
84. 0021318 197 WRITE(199)
85. 0021378 IF (ICO(TI,J,J) MODG=1,199)
86. 0021398 STOP
87. 0021338 158 ICO(TI,J,J) MODG
88. 0021358 WRITE(199)
89. 0021398 STOP
90. 0021368 97 FORMAT(I10,E5.5)
91. 0021388 C subroutine SPIN computes and prints out the nuclear spin species
92. 0021398 C from the generating function.
93. 0021308 CALL SPIN
94. 0021348 CONTINUE
95. 0021368 STOP
96. 0021388 END
SUBROUTINE VEC

COMMON /81/N10,201,NP110,201,NPR1,INDEX
COMMON /33/I5,NI5,3,2001,1f.XI'I'>
COMMON /E4/I4,E4,10001
COMMON /K8/K8,10001
COMMON /H30/H30,2001
DO 498 J4=1,NPR
CONTINUE

THIS SUBROUTINE CAN HANDLE AT MOST 5 TERMS IN EACH MONOMIAL OF THE
GCCIT. HOWEVER, IT CAN BE EASILY MODIFIED.

WRITE(6,99)
STOP

FORMAT*, THIS PROGRAM CAN HANDLE AT MOST 5 PRO-6, IF NPR06 MODIFY
C SUBROUTINE VEC AT THIS LINE WHERE THIS WRITE STATEMENT IS EXECUTED C#

IND=0
CONSTRUCTION OF THE VECTOR FOR EACH MONOMIAL.
DO 500 J5=1,NPI5,1CI
DO 490 J4=1,NPI4t1CI
DO 480 JJ=1,NPI3,1CI
DO 470 J2=1,NPI21CI
DO 460 J1=1,NPI11CI
INO•INO>l
ISUM=0
OD 4CJO ala,NPRO
GO TO 18,9,10,11,121 I
SUM=SUM+1EXPI,ICI*KNII,II,J21
GO TO 400
ISUM=ISUM+IEXPI!,ICI*KNII,II,Jll
GO TO 400
ISUM=ISUM+IEXPI!,ICI*KNII,II,J41
GO TO 400
ISUM=ISUM+IEXPI!,ICI*KNII,II,J51
CONTINUE
IVEC(II,IND)=ISUM

CONSTRUCTION OF THE COEFFICIENT FOR EACH MONOMIAL BY MULTINOMIAL
EXPANSION. MULTI IS THE FUNCTION SUBPROGRAM THAT GENERATES THE
MULTINOMIAL OF IARG WITH THE INTEGERS IN THE ARRAY K.
** SUBROUTINE VEC **

50. 0002378 IF(IN(I,IC))457,457,18
51. 0002448 IARG=IN(+1,IC)
52. 0002478 IPRO=IARG*MULTI(IARG)
53. 0002518 CONTINUE
54. 0002548 ICOI(INO)=IPRO
55. 0002578 CONTINUE
56. 0002618 CONTINUE
57. 0002648 CONTINUE
58. 0002678 CONTINUE
59. 0002728 CONTINUE
60. 0002758 INDEX=IND

C SORTING OF THE VECTOR. IF A NEWLY GENERATED VECTOR IS EQUAL TO AN
C ALREADY GENERATED VECTOR THE COEFFICIENT GENERATED FOR THE NEW
C VECTOR IS ADDED TO THE COEFFICIENT CORRESPONDING TO THE OLD VECTOR
C AND THE NEW VECTOR IS PUSHED OUT.

61. 0002768 INDEX=INDEX+1
62. 0002778 DO 538 JL=1,IND-1
63. 0003018 DO 537 JJ=JL+1,IND
64. 0003048 DO 536 JS=JS+1,IND
65. 0003078 CONTINUE
66. 0003088 CONTINUE
67. 0003128 ICD(JL)=ICD(JL)+ICD(JL)
68. 0003158 ICD(JL)=ICD(JL)+ICD(JL)
69. 0003188 DO 539 JS=JS+1,IND
70. 0003218 DD 539 JS=JS+1,IND
71. 0003248 DO 538 JL=1,IND
72. 0003278 DD 538 JL=1,IND
73. 0003318 DD 538 JL=1,IND
74. 0003348 DO 537 JS=JS+1,IND
75. 0003378 DO 536 JS=JS+1,IND
76. 0003418 CONTINUE
77. 0003448 CONTINUE
78. 0003478 CONTINUE
79. 0003518 INDEX=INDEX-1
80. 0003548 CONTINUE

C UNIQUE VECTORS ARE RETURNED IN THE ARRAY IVEC.

90. 0003628 RETURN
91. 0003648 END

760C Compilation -- MNF4 Level 5.24 25 Mar 81 10:48:10
FUNCTION MULTIFIARG**

1. FUNCTION MULTIFIARG
   C THIS FUNCTION SUBPROGRAM GENERATES MULTINOMIAL
   C IARG IARG
   C K(1),K(2),.....K(NFIR)
   C NFIR+NSPIN IS THE NUMBER OF SPIN STATES.
   2. COMMON /1//K(10),NPRO,NFIR,NPRO,INDEX
   3. COMMON /N2/K(1000)
   4. IF(ARG)1,1,2
   5. MULTI=1
   6. RETURN
   7. RETURN
   8. DO 100 I=1,NFIR
   9. IF(ARG)1,1,2
   10. RETURN
   11. RETURN
   12. END

FUNCTION IFACT(IN)**

1. FUNCTION IFACT(IN)
   C THIS FUNCTION SUBPROGRAM GENERATES THE FACTORIAL OF N.
   2. IF(IN)1,1,2
   3. IFAC=1
   4. RETURN
   5. IPRO=1
   6. DO 100 I=1,N
   7. IPRO=IPRO*IN
   8. IFAC=IPRO
   9. RETURN
   10. END

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** SUBROUTINE NEXCMIN,K,R,NTC**

1. 0000008

**NEXCM**

SUBROUTINE NEXCM(N,K,P .MT(J)

C THIS SUBROUTINE GENERATES THE NEXT COMPOSITION OF J INTO K PARTS.

C THE COMPOSITION IS RETURNED AS A VECTOR IN THE ARRAY K,NTC IS A

C LOGICAL VARIABLE WHICH IS INITIALIZED TO FALSE.This gives the

C FIRST COMPOSITION. X0,0,0,...

C ALL THE SUBSEQUENT COMPOSITIONS ARE GENERATED IN A LExicographic

C ORDER WHEN CALLED SUCCESSIVELY. NTc IS SET TO FALSE BY THE

C SUBROUTINE WHEN IT GENERATES THE LAST COMPOSITION.

C FOR REFERENCE SEE A.NIJEHUIS AND H.S.KULP,*COMBINATORIAL

C ALGORITHMS*, ACADEMIC PRESS, 1975.

2. 0000008

INTEGER AK1,T,N

3. 0000008

LOGICAL NTc

4. 0000008

IF (NTC) GO TO 20

5. 0000038

K=1

6. 0000038

WHET

7. 0000040

H=0

8. 0000058

IF (K.EQ.1) GO TO 15

9. 0000108

DO 15 IT=2,K

10. 0000128

11 K(K)=H

11. 0000148

15 NTc=K(J).NE.N

12. 0000178

RETURN

13. 0000228

20 IF (IT.GT.1) H=0

14. 0000298

H=H+1

15. 0000268

T=K(IT)

16. 0000228

R(1)=H

17. 0000278

R(IT)=1

18. 0000308

R(IT)=R(1)+1

19. 0000318

GO TO 20

20. 0000328

END

7600 Compilation -- NMF4 Level 5.24. 25 Mar 81 10:48:10
**SUBROUTINE SPIN**

SUBROUTINE SPIN

THIS SUBROUTINE GENERATES ALL THE NUCLEAR SPIN SPECIES AND THE
CORRESPONDING FREQUENCIES OF OCCURRENCE FROM THE GENERATING
FUNCTION.

COMMON /81/ NI(10,20), NP(10,20), NPP, NPPR, NPPR, INK
COMMON /84/ ITVEC(10,100), IGO(1000)
INTEGER NMUL(50), MULT(50), MULT(50)
INTEGER SYM

DO 7 J = 1, NT + 1
MULT(J) = 0
DO 100 I = 1, NSPIN
ITSPIN = ITSPIN + ISPIN(I) * ITVEC(I, J)
IF (ITSPIN .LT. 0) GO TO 7
MULT (ITSPIN) = MULT (ITSPIN) + 1
CONTINUE

IF (IFERMI .EQ. 1) THE NUCLEI ARE FERMIONS; OTHERWISE THEY ARE BOSONS.
IF (IFERMI .NE. 1) GO TO 7.

CONSTRUCTION OF BOSON SPECIES, MULT IS THE ARRAY THAT GIVES THE
MULTIPLET STRUCTURE OF THE SPIN SPECIES. MULT IS THE ARRAY OF
FREQUENCIES OF OCCURRENCE OF THE CORRESPONDING MULTIPLETS.

DO 200 I = 1, NT + 1
MULT(I) = 2 * NT + 1 - I
IF (MULT(I) .LT. 0) GO TO 200
MULT(I) = MULT(I) + 1
CONTINUE

IF (NT .EQ. 2 * IT / 2) CONSTRUCTION OF FERMION SPECIES WITH
EVEN NUMBER OF NUCLEI AND HENCE EVEN MULTIPLETS.

WRITE (*, 910) MULT, SYM, NT
RETURN

30. 003649 33 CONTINUE
31. 003649 RETURN
32. 003649 C CONSTRUCTION OF THE FERMION SPECIES. THERE ARE 2 CASES DEPENDING
33. 003649 ON THE TOTAL NUMBER OF NUCLEI NT IS ODD OR EVEN. IF NT IS ODD GO
34. 003649 TO 3. ELSE GO TO 9.
35. 003708 7 IF (NT .LT. 2) NT = NT + 4
36. 003758 9 IF (NT .EQ. 1)
37. 003758 CONSTRUCTION OF FERMION SPECIES WITH EVEN NUMBER OF NUCLEI
38. 003758 AND HENCE ODD MULTIPLETS.
39. 003758 40 DO 99 I = 1, NT + 2
40. 003758 41 DO 99 I = 1, NT + 2
SUBROUTINE SPIN

** **

IF (I1/E1) E1, I2, E1
GO TO 400

CONTINUE
IF (I1/E1) E1, I2
DO 36 INITI = I1, INITI
INI = INITI + 1
INI = INITI + I6
IFI INI = I40, I40, I41
WRITE 16, 9011 MULT, INITI, I, 1, I
WRITE 16, 9111 SVM, MULT, I, I, 2
GO TO 39
WRITE 16, 9011 MULT, INITI, I, 1, I
WRITE 16, 9111 SVM, MULT, INITI, I, 2
CONTINUE
FORM4TI2X, 8113VIXI21
RETURN
END

CONSTRUCTION OF FERMION SPECIES WITH DDD NUMBER OF NUCLEI AND
HENCE EVEN MULTIPlicITIES.

DO 300 I = 1, I2, I2
INI = INITI + 1
INI = INITI + I6
IFI INI = I40, I40, I41
WRITE 16, 9011 MULT, INITI, I, 1, I
WRITE 16, 9111 SVM, MULT, INITI, I, 2
GO TO 39
WRITE 16, 9011 MULT, INITI, I, 1, I
WRITE 16, 9111 SVM, MULT, INITI, I, 2
CONTINUE
FORM4TI2X, 8113VIXI21
RETURN
END