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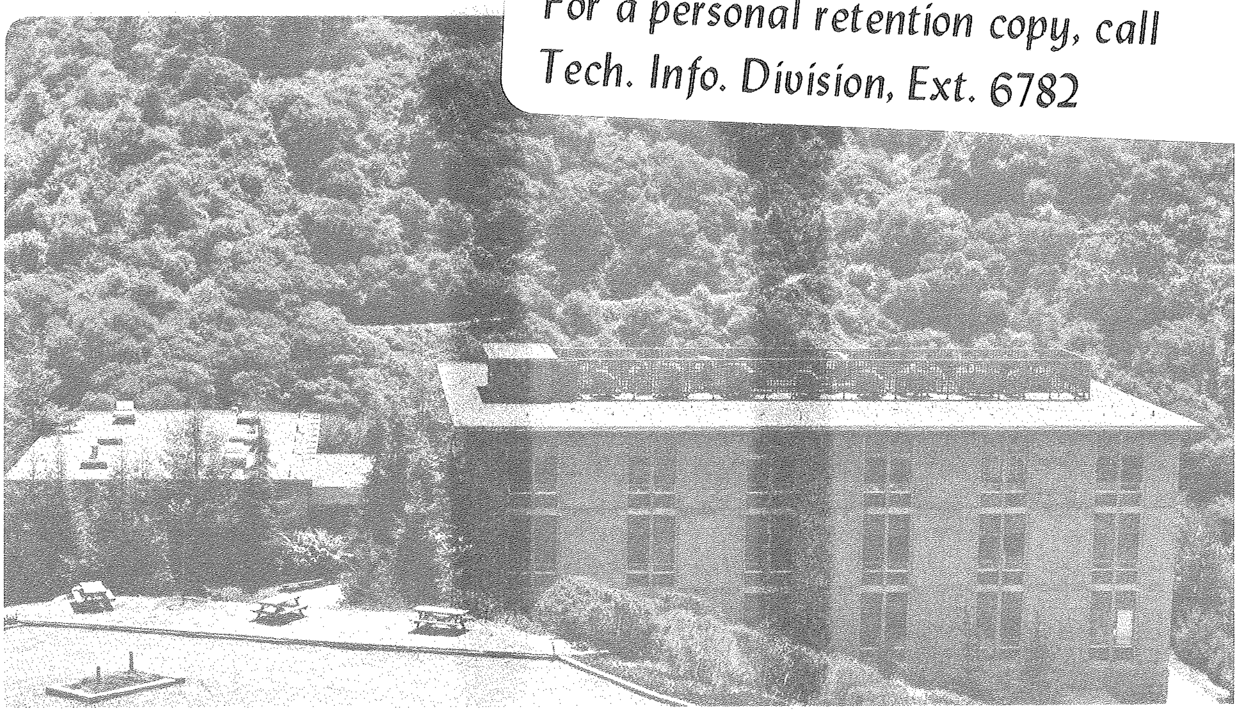

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COMPUTER GENERATION OF NUCLEAR SPIN SPECIES AND NUCLEAR SPIN STATISTICAL WEIGHTS

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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 $a_1^{b_1} a_2^{b_2}$ .... 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 $\underset{\sim}{\alpha}$ (spin up) and $\underset{\sim}{\beta}$ (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 $\underset{\sim}{\lambda}$, $\underset{\sim}{\mu}$ and $\underset{\sim}{\nu}$ is shown below.

$$f_1(1) = \underset{\sim}{\lambda}$$

$$f_1(2) = \underset{\sim}{\mu}$$

$$f_1(3) = \underset{\sim}{\nu}$$

$$f_1(4) = \underset{\sim}{\lambda}$$

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

$$gf(i) = f(g^{-1}i) \ \forall \ i \varepsilon D$$

Let us illustrate this with the map f_1 shown above and g = (1234). Since g = (1234), g^{-1} is (1432). Thus

$$gf_1(1) = f_1(g^{-1}1) = f_1(4) = \underset{\sim}{\lambda}$$

$$gf_1(2) = f_1(g^{-1}2) = f_1(1) = \underset{\sim}{\lambda}$$

$$gf_1(3) = f_1(g^{-1}3) = f_1(2) = \underset{\sim}{\mu}$$

$$gf_1(4) = f_1(g^{-1}4) = f_1(3) = \underset{\sim}{\nu}$$

Thus the nuclear spin function $\underset{\sim}{\lambda}\ \underset{\sim}{\mu}\ \underset{\sim}{\nu}\ \underset{\sim}{\lambda}$ was permuted to $\underset{\sim}{\lambda}\ \underset{\sim}{\lambda}\ \underset{\sim}{\mu}\ \underset{\sim}{\nu}$ by the action of g = (1234) on f_1. Any permutation can be characterized by its cycle structure. A permutation $g \varepsilon G$ is said to have the cycle representation

$x_1^{b_1} x_2^{b_2} \ldots\ldots x_n^{b_n}$ 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 $g \varepsilon G$ is $(b_1, b_2, \ldots, b_n)$. Consequently, a $g \varepsilon G$ which is a composite permutation-inversion operation will have the representation of the associated permutation. However, the characters corresponding to these operations could be different. Define the generalized character cycle index, hereafter, abbreviated as GCCI, corresponding to the irreducible representation Γ whose character is χ as

$$P_G^{\chi} = \frac{1}{|G|} \sum_{g \varepsilon G} \chi(g)\, x_1^{b_1} x_2^{b_2} \ldots x_n^{b_n}$$

In order to book-keep the number of nuclear spin states in any spin function let us introduce the concept of weight. With each $r \varepsilon R$ let us associate a formal symbol $w(r)$, which we call the weight of r. For example, we may associate the weights α and β to the spin states $\underset{\sim}{\alpha}$ and $\underset{\sim}{\beta}$ respectively. Then define the weight of any function $f \varepsilon F$ as the products of the weights of the corresponding images. In symbols,

$$W(f) = \prod_{d \varepsilon D} w(f(d)) \quad .$$

For example the weight of the spin function $\underset{\sim}{\alpha}\, \underset{\sim}{\alpha}\, \underset{\sim}{\beta}\, \underset{\sim}{\beta}$ 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:

$$G.F.^{\chi} = P_G^{\chi}(x_k \longrightarrow \sum_{r \varepsilon R} w^k(r)) \quad .$$

$G.F.^{\chi}$ is the generating function for the irreducible representation whose character is χ occurring in the set of spin functions. Equivalently, the coefficient of a typical term $w_1^{b_1} w_2^{b_2} \ldots$ in $G.F.^{\chi}$ gives the frequency of occurrence of the irreducible representation Γ whose character is χ in the set of nuclear spin functions with the weight $w_1^{b_1} w_2^{b_2} \ldots$. 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.

$$P_{O_h}^{T_{1u}} = \frac{1}{48}(3x_1^6 - 9x_2^3 + 3x_1^2x_2^2 + 6x_1^2x_4 - 6x_2x_4 + 3x_1^4x_2)$$

Then $G.F._{O_h}^{T_{1u}}$ is given by the following expression.

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

This on simplification yields,

$$\alpha^5\beta + \alpha^4\beta^2 + 2\alpha^3\beta^3 + \alpha^2\beta^4 + \alpha\beta^5 \quad .$$

Thus there is one T_{1u} representation in the set of spin functions containing 5 α's and 1 β, one T_{1u} in the set of spin functions containing 4 α's and 2 β's, 2 in the set of functions containing 3 α's and 3 β'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

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

Subroutine VEC generates all the possible vectors (powers of λ, μ and ν 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 $[1^3]$ of the symmetric group S_3.

$$\mathrm{GCCI}([1^3]) = \frac{1}{6}(x_1^3 - 3x_1^1x_2^1 + 2x_3^1)$$

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.

3	(number of terms in the GCCI)
1 -3 2	(coefficients in the GCCI)
1 3 1	(the first term)
2 1 1 1 2	(the second term)
1 1 3	(the third term)

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.

$A_1^{'+}$	A1
$B_1^{'+}$	B1
$A_2^{'+}$	A2
$B_2^{'+}$	B2
$A_1^{''+}$	A3 = $B_1^{''+}$
$A_2^{''+}$	A4 = $B_2^{''+}$
$E_1^{'+}$	E1
$E_1^{''+}$	E2

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 $x_1^{b_1} x_2^{b_2} \ldots x_n^{b_n}$, 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 $x_1^{b_1} x_2^{b_2} \ldots x_n^{b_n}$ 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), Iexp(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

$$|G|P_G^X\ (x_k \longrightarrow \sum_{r\varepsilon R} (w(r))^k)$$

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 $x_1^{b_1}\ x_2^{b_2}\ \ldots\ x_n^{b_n}$ 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 Γ^{spin}, the reducible representation spanned by all nuclear spin functions. For example, for the proton spin functions of the non-rigid triphenyl

$$\Gamma_H^{spin} = 2040\ A_1^{'+} + 1960\ B_1^{'+} + 696\ A_2^{'+} + 744\ B_2^{'+} + 1200\ A_1^{''+} + 1200\ B_1^{''+}$$
$$+ 432\ A_2^{''+} + 432\ B_2^{''+} + 2400\ E_1^{'+} + 1440\ E_1^{''+}\ .$$

When Γ_H^{spin} is known the nuclear spin statistical weights of the rovibronic levels are obtained easily by stipulating that $\Gamma^{rve} \otimes \Gamma^{spin}$ should contain

Γ^{int}, where Γ^{rve} is the species of the rovibronic level and Γ^{int} is the species of the overall internal wave function. Γ^{int} must satisfy the Pauli exclusion principle. Equivalently, Γ^{int} must be antisymmetric with respect to odd permutations for Fermions and symmetric for Bosons.

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Table 1: Input for Program POLYN

Card	Format	Input Variables	Description
1	10A8	TITLE	Alphanumeric title
2	16I5	NGCI	number of generalized cycle indices
		NSPIN	number of spin states of the same kind of nuclei in the set D
		NT	total number of nuclei in D
		MODG	order of the group
		ISPIN(I), I=1, NSPIN	spin quantum numbers. For Fermions twice the spin quantum numbers.
		IFERMI	Fermion parameter; equals 1 if the nuclei are Fermions. For Bosons set this to 0.
	for each GCCI read the following cards 3-5. For the first GCCI additional cards need to be read as per the ensuing instructions.		
3	A10	SYM	label of the irreducible representation
4	16I5	NCI	number of terms in this GCCI
5	16I5	ICOCI(I), I=1, NCI	coefficients of NCI terms in this GCCI
	if this is the first GCCI for each j = 1, NCI feed a card described as card 6.		
6	16I5	NPRO	number of distinct components in each term of the GCCI
		N(i,j), i=1, NPRO	the superfixes of each component of a term of the GCCI
		Iexp(i,j), i=1, NPRO	the suffixes of each component of a term in the GCCI

Table 2: Sample Input

Card							
1	Non-Rigid Triphenyl Proton Species						
2	8	2	14	16	-1	1	1
3	A1						
4	6						
5	1	3	3	4	4	1	
6	1	14	1				
7	2	10	2	1	2		
8	2	6	4	1	2		
9	1	7	2				
10	2	3	2	2	4		
11	2	2	6	1	2		
12	B1						
13	1	3	3	-4	-4	1	
14	A2						
15	1	-1	-1	-4	4	1	
16	B2						
17	1	-1	-1	4	-4	1	
18	A3						
19	1	1	-1	0	0	-1	
20	A4						
21	1	-3	3	0	0	-1	
22	E1						
23	2	2	-2	0	0	-2	
24	E2						
25	2	-2	-2	0	0	2	

Table 3: The Non-Zero GCCI's of the Protons of a Non-Rigid Triphenyl

Γ	x_1^{14}	$x_1^{10}x_2^2$	$x_1^6x_2^4$	x_2^7	$x_2^3x_4$	$x_1^2x_6^2$
$A_1'^{+}$	1	3	3	4	4	1
$B_1'^{+}$	1	3	3	-4	-4	1
$A_2'^{+}$	1	-1	-1	-4	4	1
$B_2'^{+}$	1	-1	-1	4	-4	1
$A_1''^{+}$	1	1	-1	0	0	-1
$B_1''^{+}$	1	1	-1	0	0	-1
$A_2''^{+}$	1	-3	3	0	0	-1
$B_2''^{+}$	1	-3	3	0	0	-1
$E_1'^{+}$	2	2	-2	0	0	-2
$E_2''^{+}$	2	-2	-2	0	0	2

Figure Captions

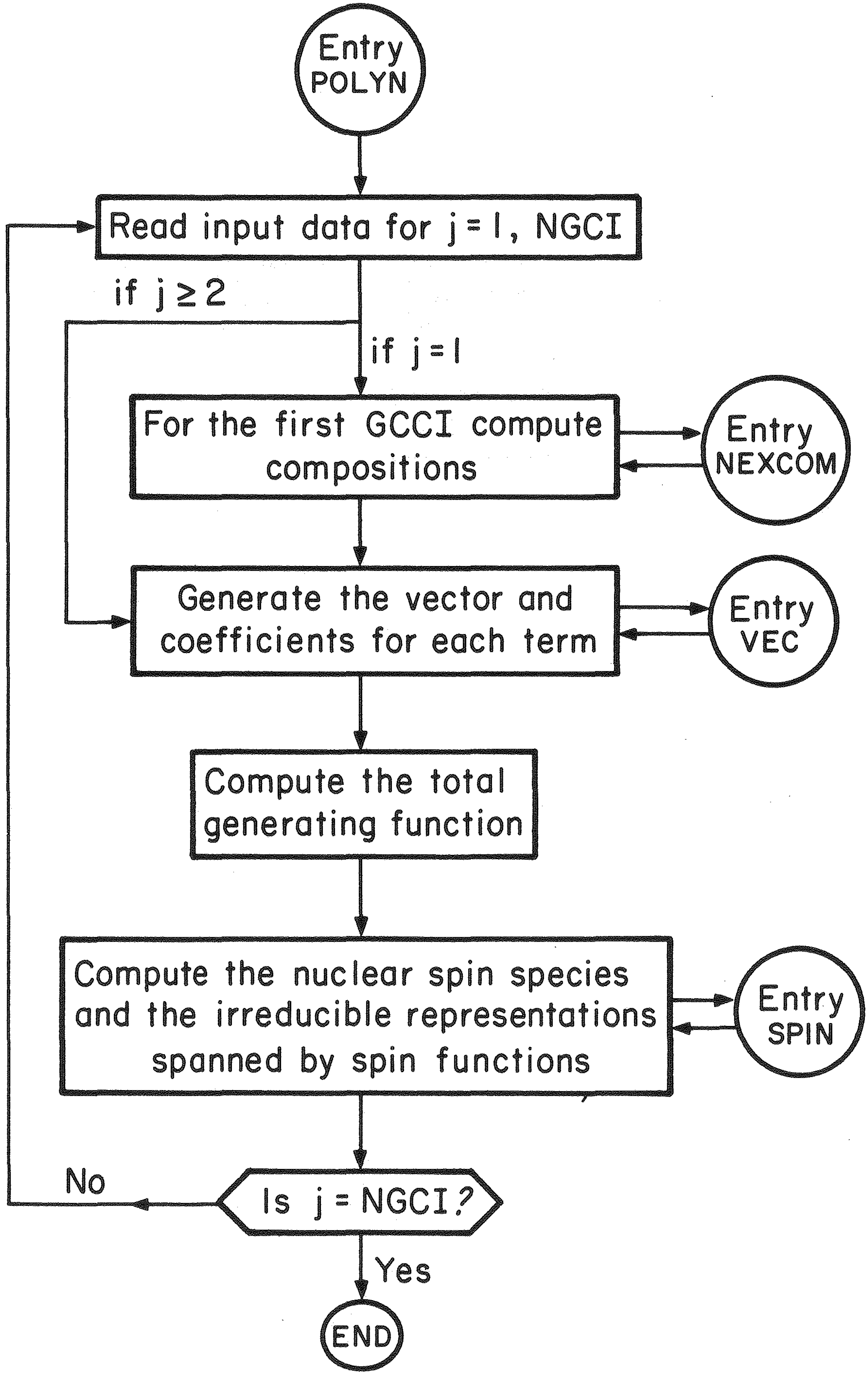
Figure 1: Flow chart of the program POLYN and subroutines.

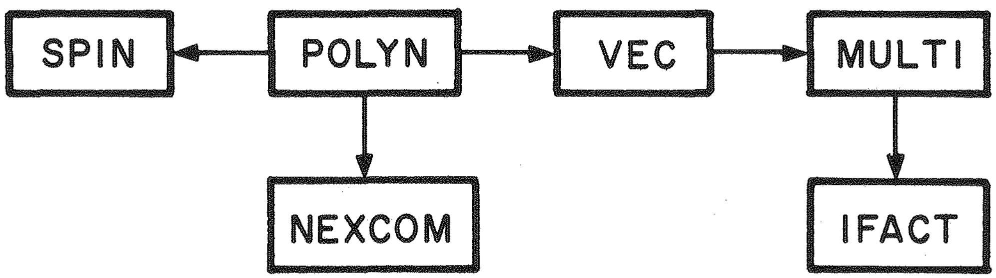
Figure 2: Organization of the main program and the various subroutines.

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, NGCI
if j ≥ 2
if j = 1
For the first GCCI compute compositions
Entry
NEXCOM
Generate the vector and coefficients for each term
Entry
VEC
Compute the total generating function
Compute the nuclear spin species and the irreducible representations spanned by spin functions
Entry
SPIN
No
Is j = NGCI?
Yes
END


SPIN
POLYN
VEC
MULTI
NEXCOM
IFACT

```
 NON-RIGID TRIPHENYL PROTON SPECIES
   2   -1    1
A1
NPRO,N(I),I=1,NPRO     1   14
 IEXPS     1
NPRO,N(I),I=1,NPRO     2   10     2
 IEXPS     1    2
NPRO,N(I),I=1,NPRO     2    6     4
 IEXPS     1    2
NPRO,N(I),I=1,NPRO     1    7
 IEXPS     2
NPRO,N(I),I=1,NPRO     2    3     2
 IEXPS     2    4
NPRO,N(I),I=1,NPRO     2    2     6
 IEXPS     1    2
 SPIN IRREP COMPONENT       2040
    THE GENERATING FUNCTION FOR NUCLEAR SPIN SPECIES
 COEFFICIENT           VECTOR
             1         14     0
             4         13     1
            21         12     2
            58         11     3
           142         10     4
           244          9     5
           356          8     6
           388          7     7
           356          6     8
           244          5     9
           142          4    10
            58          3    11
            21          2    12
             4          1    13
             1          0    14
   1               3               5               7               9               11              13              15
    A1(        32)  A1(       112)  A1(       102)  A1(        84)  A1(        37)  A1(        17)  A1(         3)  A1(         1)
B1
 SPIN IRREP COMPONENT       1960
    THE GENERATING FUNCTION FOR NUCLEAR SPIN SPECIES
 COEFFICIENT           VECTOR
             0         14     0
             4         13     1
            16         12     2
            58         11     3
           129         10     4
           244          9     5
           335          8     6
           388          7     7
           335          6     8
           244          5     9
           129          4    10
            58          3    11
            16          2    12
             4          1    13
             0          0    14
   1               3               5               7               9               11              13              15
    B1(        53)  B1(        91)  B1(       115)  B1(        71)  B1(        42)  B1(        12)  B1(         4)  B1(         0)
A2
 SPIN IRREP COMPONENT        696
    THE GENERATING FUNCTION FOR NUCLEAR SPIN SPECIES
 COEFFICIENT           VECTOR
             0         14     0
             0         13     1
```

```
              1        12     2
             12        11     3
             36        10     4
             88         9     5
            131         8     6
            160         7     7
            131         6     8
             88         5     9
             36         4    10
             12         3    11
              1         2    12
              0         1    13
              0         0    14
  1           3          5          7          9          11          13          15
   A2(      29)  A2(       43)  A2(       52)  A2(       24)  A2(       11)  A2(       1)  A2(       0)  A2(       0)
B2
 SPIN IRREP COMPONENT      744
   THE GENERATING FUNCTION FOR NUCLEAR SPIN SPECIES
 COEFFICIENT           VECTOR
              0        14     0
              0        13     1
              3        12     2
             12        11     3
             44        10     4
             88         9     5
            145         8     6
            160         7     7
            145         6     8
             88         5     9
             44         4    10
             12         3    11
              3         2    12
              0         1    13
              0         0    14
  1           3          5          7          9          11          13          15
   B2(      15)  B2(       57)  B2(       44)  B2(       32)  B2(       9)  B2(       3)  B2(       0)  B2(       0)
A3
 SPIN IRREP COMPONENT     1200
   THE GENERATING FUNCTION FOR NUCLEAR SPIN SPECIES
 COEFFICIENT           VECTOR
              0        14     0
              1        13     1
              7        12     2
             28        11     3
             75        10     4
            147         9     5
            218         8     6
            248         7     7
            218         6     8
            147         5     9
             75         4    10
             28         3    11
              7         2    12
              1         1    13
              0         0    14
  1           3          5          7          9          11          13          15
   A3(      30)  A3(       71)  A3(       72)  A3(       47)  A3(       21)  A3(       6)  A3(       1)  A3(       0)
A4
 SPIN IRREP COMPONENT      432
   THE GENERATING FUNCTION FOR NJCLEAR SPIN SPECIES
 COEFFICIENT           VECTOR
              0        14     0
```

```
                0       13     1
                0       12     2
                4      -11     3
               20       10     4
               52        9     5
               88        8     6
              104        7     7
               88        6     8
               52        5     9
               20        4    10
                4        3    11
                0        2    12
                0        1    13
                0        0    14
   1              3              5               7               9              11              13              15
    A4(        16)  A4(        36)  A4(        32)  A4(        16)  A4(         4)  A4(         0)  A4(         0)  A4(         0)
E1
 SPIN IRREP COMPONENT     2400
    THE GENERATING FUNCTION FOR NJCLEAR SPIN SPECIES
 COEFFICIENT          VECTOR
                0       14     0
                2       13     1
               14       12     2
               56       11     3
              150       10     4
              294        9     5
              436        8     6
              496        7     7
              436        6     8
              294        5     9
              150        4    10
               56        3    11
               14        2    12
                2        1    13
                0        0    14
   1              3              5               7               9              11              13              15
    E1(        60)  E1(       142)  E1(       144)  E1(        94)  E1(        42)  E1(        12)  E1(         2)  E1(         0)
E2
 SPIN IRREP COMPONENT     1440
    THE GENERATING FUNCTION FOR NUCLEAR SPIN SPECIES
 COEFFICIENT          VECTOR
                0       14     0
                0       13     1
                4       12     2
               24       11     3
               80       10     4
              176        9     5
              276        8     6
              320        7     7
              276        6     8
              176        5     9
               80        4    10
               24        3    11
                4        2    12
                0        1    13
                0        0    14
   1              3              5               7               9              11              13              15
    E2(        44)  E2(       100)  E2(        96)  E2(        56)  E2(        20)  E2(         4)  E2(         0)  E2(         0)
```

```
POLY                   ** PROGRAM POLY(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE8)**

     0000008B           PROGRAM POLY(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE8)
     0015448           COMMON /B1/N(10,20),NP(10,20),NPP,NFIR,NPPO,INDEX
     001544B           COMMON /B3/IC,KN(5,3,200),IEXP(5,20),ICO(1000),IVEC(5,1000)
     001544B           COMMON /B4/ITVEC(10,1000),ICOT(1000)
     001544B           COMMON /B5/SYM,NSPIN,ISPIN(20),NT,IFERMI
     001544B            INTEGER R(3),ICOCI(30) ,SYM,TITLE(10)
     001544B            LOGICAL MTC
     001544B           READ(5,772)(TITLE(I),I=1,10)
     001627B           WRITE(6,772)(TITLE(I),I=1,10)
     001636B   772      FORMAT(10A8)
     001636B           READ(5,90)NGCI,NSPIN,NT,MODG,(ISPIN(IL),IL=1,NSPIN),IFERMI
     001654B           NFIR=NSPIN
     001654B            WRITE(6,90)NSPIN,(ISPIN(I),I=1,NSPIN)
     001667B           DO 1000 IJK=1,NGCI
     001671B            READ(5,81)SYM
     001676B   81      FORMAT(A10)
     001676B           WRITE(6,82)SYM
     001702B   82      FORMAT(* *,A10)
     001702B            IF(IJK-1)15,15,16
     001704B   15      READ(5,90)NCI
     001710B   16      READ(5,90)(ICOCI(L),L=1,NCI)
     001720B            ISTAT=0
     001720B            DO 100 IC=1,NCI
     001723B           IF(IJK-1)17,17,18
     001726B   18       READ(8)NPRO,(((KN(I,ISUB,L),ISUB=1,NSPIN),L=1,NP(I,IC)),I=1,NPRO)
     001767B           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 8.FOR ALL SUBSEQUENT
               C       GCCI'S THEY ARE READ FROM TAPE 8.
     001767B   17      DO 14 I=1,10
     001771B           N(I,IC)=0
     001772B   14       NP(I,IC)=0
     001775B           READ(5,90)NPRO,(N(I,IC),I=1,NPRO),(IEXP(I,IC),I=1,NPRO)
     002020B           WRITE(6,191)NPRO,(N(I,IC),I=1,NPRO)
     002033B           WRITE(6,98)(IEXP(I,IC),I=1,NPRO)
     002045B    191      FORMAT(X,*NPRO,N(I),I=1,NPRO*,16I5)
     002045B   98      FORMAT(2X,*IEXPS*,16I5)
     002045B           ISUM=0
     002045B           DO 13 I=1,NPRO
     002050B   13       ISUM=ISUM+N(I,IC)*IEXP(I,IC)
               C       CHECK FOR INPUT ERROR.
     002057B           IF(ISUM-NT)192,193,192
     002061B   192      WRITE(6,194)
     002065B           STOP
     002066B   194     FORMAT(2X,*INPUT ERROR FOR THIS TERM.CHECK N(I),IEXP(I)*)
     002066B   90      FORMAT(16I5)
     002066B   193     DO 11 I=1,NPRO
     002070B           MTC=.FALSE.
     002070B            J=0
               C       SUBROUTINE NEXCOM GENERATES THE NEXT COMPOSITION OF N(I,IC) IN TO
               C       NSPIN PARTS IN THE ARRAY R.
     002071B   8       CALL NEXCOM(N(I,IC),NSPIN,R,MTC)
     002101B            J=J+1
     002102B            DO 9 ISUB=1,3
     002104B   9       KN(I,ISUB,J)=R(ISUB)
     002113B           IF(MTC) GO TO 8
     002114B             NP(I,IC)=J
```

```
POLY                        ** PROGRAM POLY(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE8)**

0021158  11     CONTINUE
0021218        WRITE(8)NPRO,(((KN(I,ISUB,L),ISUB=1,NSPIN),L=1,NP(I,IC)),I=1,NPRO)
0021638  177     IF(IC-1)5,5,6
0021658  5     NPP=NP(1,IC)
0021678         DO 200 II=1,NFIR
0021728         DO 200 JJ=1,NPP
0021758  200    ITVEC(II,JJ)=KN(1,II,JJ)
0022108        DO 300 II=1,NP(1,IC)
         C     ICOT IS THE ARRAY OF TOTAL COEFFICIENTS INITIALISED TO ZERO.
0022168  300     ICOT(II)=0
         C     SUBROUTINE VEC RETURNS THE ARRAY OF VECTORS AND THE ARRAY OF
         C     COEFFICIENTS FOR EACH TERM IN THE GCCI.THESE ARRAYS ARE IVEC AND
         C     ICO ,RESPECTIVELY.
0022208  6      CALL VEC
0022238        DO 450 JVEC=1,INDEX
         C     MATCHES THE VECTOR GENERATED BY THE SUBROUTINE VEC WITH THE
         C     PRINCIPAL VECTOR ITVEC.
         C     WHEN THERE IS A MATCH THE CORRESPONDING COEFFICIENT GENERATED BY
         C     VEC IS MULTIPLIED BY THE COEFFICIENT OF THIS TERM IN THE GCCI AND
         C     ADDED TO ICOT,THE ARRAY OF TOTAL COEFFICIENTS.
0022258         DO 400 J1=1,NPP
0022308         DO 350 I1=1,NFIR
0022338         IF(ITVEC(I1,J1)-IVEC(I1,JVEC))400,350,400
0022338  350    CONTINUE
0022458          ICOT(J1)=ICOT(J1)+ICO(JVEC)*ICOCI(IC)
0022518  400      CONTINUE
0022548  450    CONTINUE
         C     COMPUTATION OF THE FREQUENCY OF OCCURANCE OF THE IRREDUCIBLE
         C     REPRESENTATION SYM IN THE REPRESENTATION SPANNED BY ALL SPIN
         C     FUNCTIONS.
0022578        INPRO=1
0022608         DO 373 II=1,NPRO
0022628  373    INPRO=INPRO*(NSPIN**N(II,IC))
0022778        ISTAT=ISTAT+INPRO*ICOCI(IC)
0023018  100     CONTINJE
0023048        REWIND 8
0023068         ISTAT=ISTAT/MODG
0023108           WRITE(6,374)ISTAT
0023158  374     FORMAT(2X,*SPIN IRREP COMPONENT*,I9)
0023158        WRITE(6,178)
0023208  178   FORMAT(2X,*   THE GENERATING FUNCTION FOR NUCLEAR SPIN SPECIES*)
0023208        WRITE(6,179)
0023238  179    FORKAT(2X,*COEFFICIENT*,10X,*VECTOR*)
0023238         DO 900 J=1,NPP
         C     CHECKS FOR INPUT ERROR.
0023258        IF((ICOT(J)/MODG)*MODG-ICOT(J))197,198,197
0023318  197     WRITE(6,199)
0023358  199   FORMAT(2X,*ICO(JJ) IS NOT DIVISIBLE BY MCDG.INPUT ERROR*)
0023358        STOP
0023368  198     ICOT(J)=ICOT(J)/MODG
0023418  900    WRITE(6,97)ICOT(J),(ITVEC(I,J),I=1,NFIR)
0023608  97    FORMAT(10X,I5,3X,16I5)
         C     SUBROUTINE SPIN COMPUTES AND PRINTS OUT THE NUCLEAR SPIN SPECIES
         C     FROM THE GENERATING FUNCTION.
0023608        CALL SPIN
0023628  1000    CONTINUE
0023648        STOP
0023658         END

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VEC                      **  SUBROUTINE VEC**

0000008             SUBROUTINE VEC
0000008            COMMON /B1/N(10,20),NP(10,20),NPP,NFIR,NPRO,INDEX
0000008            COMMON /33/IC,KN(5,3,200),IEXP(5,20),ICO(1000),IVEC(5,1000)
0000008             COMMON /B2/K(1000)
0000008            DO 498 J1=1,200
000001B             ICO(J1)=0
000001B            DO 498 I1=1,NFIR
000004B             IVEC(I1,J1)=0
000004B     498     CONTINUE
            C      THIS SUBROUTINE CAN HANDLE ATMOST 5 TERMS IN EACH MONOMIAL OF THE
            C      GCCI.HOWEVER,IT CAN BE EASILY MODIFIED.
000013B            IF(NPRO-5)1,1,2
000016B     2       WRITE(6,99)
000021B            STOP
000022B     99     FORMAT(2X,*THIS PROGRAM CAN HANDLE ATMOST NPRO=5.IF NPRO≥6 MODIFY
                  CSUBROUTIVE VEC AT THIS LINE WHERE THIS WRITE STATEMENT IS EXECUTED
                  C*)
000022B     1       IND=0
            C      CONSTRUCTION OF THE VECTOR FOR EACH MONOMIAL.
000022B            DO 500 J5=1,NP(5,IC)
000030B            DO 490 J4=1,NP(4,IC)
000036B            DO 480 J3=1,NP(3,IC)
000044B            DO 470 J2=1,NP(2,IC)
000052B            DO 460 J1=1,NP(1,IC)
000060B             IND=IND+1
000061B            DO 450 II=1,NFIR
000064B             ISUM=0
000064B            DO 400 I=1,NPRO
000067B            GO TO (8,9,10,11,12) I
000076B     8      ISUM=ISUM+IEXP(I,IC)*KN(I,II,J1)
000105B             GO TO 400
000106B     9      ISUM=ISUM+IEXP(I,IC)*KN(I,II,J2)
000116B             GO TO 400
000117B     10     ISUM=ISUM+IEXP(I,IC)*KN(I,II,J3)
000127B            GO TO 400
000130B     11     ISUM=ISUM+IEXP(I,IC)*KN(I,II,J4)
000140B            GO TO 400
000141B     12     ISUM=ISUM+IEXP(I,IC)*KN(I,II,J5)
000151B     400    CONTINUE
000154B     450     IVEC(II,IND)=ISUM
000162B             IPRO=1
000163B             DO 457 I=1,NPRO
000165B            DO 455 II=1,NFIR
000170B            GO TO (13,14,15,16,17) I
000177B     13     K(II)=KN(I,II,J1)
000203B             GO TO 455
000205B     14     K(II)=KN(I,II,J2)
000211B             GO TO 455
000213B     15      K(II)=KN(I,II,J3)
000217B             GO TO 455
000221B     16      K(II)=KN(I,II,J4)
000225B             GO TO 455
000227B     17      K(II)=KN(I,II,J5)
000233B     455     CONTINUE
            C      CONSTRUCTION OF THE COEFFICIENT FOR EACH MONOMIAL BY MULTINOMIAL
            C      EXPANSION.MULTI IS THE FUNCTION SUBPROGRAM THAT GENERATES THE
            C      MULTINOMIAL OF IARG WITH THE INTEGERS IN THE ARRAY K.
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```
VEC                          **  SUBROUTINE VEC**

0002378            IF(N(I,IC))457,457,18
0002448     18     IARG=N(I,IC)
0002478              IPRO=IPRO*MULTI(IARG)
000251B    457      CONTINUE
0002548              ICO(IND)=IPRO
000255B    460      CONTINUE
000261B    470      CONTINUE
000264B    480      CONTINUE
000267B    490      CONTINUE
000272B    500      CONTINUE
000275B              INDEX=IND
              C     SORTING OF THE VECTOR.IF A NEWLY GENERATED VECTOR IS EQAL 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.
000276B            IND1=INDEX
000276B             DO 538 JL=1,IND1-1
000301B            DO 537 JJ=JL+1,IND1
000304B            DO 536 II=1,NFIR
000307B             IF(IVEC(II,JL)-IVEC(II,JJ))537,536,537
000307B    536      CONTINUE
000321B                ICO(JL)=ICO(JL)+ICO(JJ)
000323B            IF(JJ-INDEX)24,23,23
000326B     24     DO 539 JM=JJ,INDEX-1
000331B             DO 539 IM=1,NFIR
000334B            ICO(JM)=ICO(JM+1)
000335B    539        IVEC(IM,JM)=IVEC(IM,JM+1)
000344B            DO 542 IM=1,NFIR
000346B            ICO(INDEX)=0
000346B    542         IVEC(IM,INDEX)=-INDEX
000352B     23     INDEX=INDEX-1
000354B    537     CONTINUE
000357B    538      CONTINUE
              C     UNIQUE VECTORS ARE RETURNED IN THE ARRAY IVEC.
000362B              RETURN
000364B              END

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MULTI                       ** FUNCTION MULTI(IARG)**

   1.    000000B             FUNCTION MULTI(IARG)
                       C    THIS FUNCTION SUBPROGRAM GGENERATES MULTINOMIAL
                       C                 IARG
                       C   (                           )
                       C    K(1),K(2),.....,K(NFIR)
                       C    NFIR=NSPIN IS THE NUMBER OF SPIN STATES.
   2.    000000B            COMMON /B1/N(10,20),NP(10,20),NPP,NFIR,NPRO,INDEX
   3.    000000B             COMMON /B2/K(1000)
   4.    000000B             IF(IARG)1,1,2
   5.    000002B       1     MULTI=1
   6.    000003B             RETURN
   7.    000006B       2     IPRO=1
   8.    000006B            DO 100 I=1,NFIR
                       C    IFACT IS THE FUNCTION SUBPROGRAM WHICH GEWNERATES THE FACTORIAL OF
                       C    THE ARGUEMENT
   9.    000011B       100    IPRO=IPRO*IFACT(K(I))
  10.    000021B             MULTI=IFACT(IARG)/IPRO
  11.    000026B            RETURN
  12.    000030B             END

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IFACT                       **FUNCTION IFACT(N)**

   1.    000000B            FUNCTION IFACT(N)
                       C    THIS FUNCTION SUBPROGRAM GENERATES THE FACTORIAL OF N.
   2.    000000B             IF(N)1,1,2
   3.    000002B       1      IFACT=1
   4.    000003B              RETURN
   5.    000006B       2     IPRO=1
   6.    000006B             DO 100 I=1,N
   7.    000011B       100   IPRO=IPRO*I
   8.    000015B             IFACT=IPRO
   9.    000015B            RETURN
  10.    000020B              END

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NEXCOM                      ** SUBROUTINE NEXCOM(N,K,R,MTC)**

    0000008              SUBROUTINE NEXCOM(N,K,R,MTC)
                 C      THIS SUBROUTINE GENERATES THE NEXT COMPOSITION OF N INTO K PARTS.
                 C      THE COMPOSITION IS RETURNED AS A VECTOR IN THE ARRAY R.MTC IS A
                 C      LOGICAL VARIABLE WHICH IS INITIALISED TO FALSE.THIS GIVES THE
                 C      FIRST COMPOSITION N,0,0,0,...... .
                 C      ALL THE SUBSEQUENT COMPOSITIONS ARE GENERATED IN A LEXICOGRAPHIC
                 C      ORDER WHEN CALLED SUCCESSIVELY.MTC IS SET TO FALSE BY THE
                 C      SUBROUTINE WHEN IT GENERATES THE LAST COMPOSITION.
                 C      FOR REFERENCE SEE A.NIJENHUIS AND H.S.WILF,'COMBINATURIAL
                 C      ALGOIRTHMS',ACADEMIC 1975.
    000000B              INTEGER R(K),T,H
    000000B             LOGICAL MTC
    000000B             IF(MTC)GO TO 20
    000003B               R(1)=N
    000003B             T=N
    000004B              H=0
    000005B             IF(K.EQ.1)GO TO 15
    000010B              DO 11 I=2,K
    000012B      11     R(I)=0
    000014B      15      MTC=R(K).NE.N
    000017B             RETURN
    000022B      20     IF(T.GT.1) H=0
    000025B              H=H+1
    000026B             T=R(H)
    000027B              R(H)=0
    000027B              R(1)=T-1
    000030B              R(H+1)=R(H+1)+1
    000031B              GO TO 15
    000032B               END

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SPIN                        ** SUBROUTINE SPIN**

  1.    000000B              SUBROUTINE SPIN
                       C    THIS SUBROUTINE GENERATES ALL THE NUCLEAR SPIN SPECIES AND THE
                       C    CORRESPONDING FREQUENCIES OF OCCURANCE FROM THE GENERATING
                       C    FUNCTION.
  2.    000000B             COMMON /B1/N(10,20),NP(10,20),NPP,NFIR,NPRO,INDEX
  3.    000000B             COMMON /B4/ITVEC(10,1000),ICOT(1000)
  4.    000000B             COMMON /B5/SYM,NSPIN,ISPIN(20),NT,IFERMI
  5.    000000B             INTEGER NMULTI(50),MULTIP(50),NULTI(50)
  6.    000000B              INTEGER SYM
  7.    000000B              DO 75 I=1,NT+1
  8.    000231B        75    NULTI(I)=0
  9.    000233B             DO 100 J=1,VPP
                       C    SORTING OF THE ARRAY OF COEFFICIENTS ACCORDING TO THEIR TOTAL SPIN
                       C    QUANTUM NUMBER.
 10.    000236B              ITSPIN=0
 11.    000236B             DO 50 I=1,NSPIN
 12.    000241B        50    ITSPIN=ITSPIN+ISPIN(I)*ITVEC(I,J)
 13.    000247B             IF(ITSPIN)100,1,1
 14.    000250B        1     NULTI(ITSPIN+1)=NULTI(ITSPIN+1)+ICOT(J)
 15.    000253B        100   CONTINUE
                       C    IF IFERMI=1,THE NUCLEI ARE FERMIONS.OTHERWISE THEY ARE BOSONS.
 16.    000256B             IF(IFERMI.EQ.1) GO TO 7
                       C    CONSTRUCTION OF BOSON SPECIES.MULTIP IS THE ARRAY THAT GIVES THE
                       C    MULTIPLICITIES OF THE SPIN SPECIES.NMULTI IS THE ARRAY OF
                       C    FREQUENCIES OF OCCURANCE OF THE CORRESPONDING MULTIPLETS.
 17.    000260B             DO 200 I=1,NT+1
 18.    000263B             MULTIP(I)=2*(I-1)+1
 19.    000264B              II=NT+2-I
 20.    000266B             IF(II-NT-1)3,2,2
 21.    000272B        2     NMULTI(II)=NULTI(II)
 22.    000273B              GO TO 200
 23.    000274B        3     NMULTI(II)=NULTI(II)-NULTI(II+1)
 24.    000276B        200    CONTINUE
 25.    000302B             IF=NT+1
 26.    000303B             IFI=(IF/8)+1
 27.    000304B              INITI=0
 28.    000305B             DO 33 INDA=1,IFI
 29.    000310B              INI=INITI+1
 30.    000311B             INITI=INITI+8
 31.    000312B             IF(INITI-IF)34,34,35
 32.    000315B        34   WRITE(6,90)(MULTIP(I),I=INI,INITI)
 33.    000325B             WRITE(6,91)(SYM,NMULTI(I),I=INI,INITI)
 34.    000340B             GO TO 33
 35.    000340B        35   WRITE(6,90)(MULTIP(I),I=INI,IF)
 36.    000351B             WRITE(6,91)(SYM,NMULTI(I),I=INI,IF)
 37.    000364B        33   CONTINUE
 38.    000366B               RETURN
                       C    CONSTRUCTION OF THE FERMION SPECIES.THERE ARE 2 CASES DEPENDING
                       C    ON  THE TOTAL NUMBER OF NUCLEI NT IS ODD OR EVEN.IF NT IS ODD GO
                       C    TO 8.ELSE GO TO 9.
 39.    000370B        7    IF((NT/2)*2-NT)8,9,8
                       C    CONSTRUCTION OF FERMION SPECIES WITH EVEN NUMBER OF NUCLEI AND
                       C    HENCE ODD MULTIPLICITIES.
 40.    000372B        9     IF=NT+1
 41.    000373B             DO 400 I=1,IF,2
 42.    000375B             MULTIP(I)=I
 43.    000375B               II=NT+2-I
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```
SPIN                          ** SUBROUTINE SPIN**

      000377B                 IF(II-IF)11,12,12
      000403B   12            NMULTI(II)=NULTI(II)
      000404B                 GO TO 400
      000405B   11            NMULTI(II)=NULTI(II)-NULTI(II+2)
      000407B   400            CONTINUE
      000413B                  IFI=(IF/16)+1
      000414B                 INITI=-1
      000415B                 DO 36 INDA=1,IFI
      000420B                 INI=INITI+2
      000421B                 INITI=INITI+16
      000422B                 IF(INITI-IF)37,37,38
      000425B   37            WRITE(6,90)(MULTIP(I),I=INI,INITI,2)
      000437B                 WRITE(6,91)(SYM,NMULTI(I),I=INI,INITI,2)
      000452B                 GO TO 36
      000452B   38            WRITE(6,90)(MULTIP(I),I=INI,IF,2)
      000464B                 WRITE(6,91)(SYM,NMULTI(I),I=INI,IF,2)
      000477B   36             CONTINUE
      000501B                  RETURN
                C             CONSTRUCTION OF FERMION SPECIES WITH ODD NUMBER OF NUCLEI AND
                C             HENCE EVEN MULTIPLICITIES.
      000503B   8              IF=NT+1
      000504B   10             DO 300 I=2,IF,2
      000507B                  MULTIP(I)=I
      000507B                  II=NT+3-I
      000511B                 IF(II-IF)4,5,5
      000514B   5             NMULTI(II)=NULTI(II)
      000516B                 GO TO 300
      000517B   4             NMULTI(II)=NULTI(II)-NULTI(II+2)
      000521B   300            CONTINUE
      000525B                 IFI=(IF/16)+1
      000526B                 INITI=0
      000527B                 DO 39 INDA=1,IFI
      000532B                 INI=INITI+2
      000533B                  INITI=INITI+16
      000534B                 IF(INITI-IF)40,40,41
      000537B   40            WRITE(6,90)(MULTIP(I),I=INI,INITI,2)
      000551B                 WRITE(6,91)(SYM,NMULTI(I),I=INI,INITI,2)
      000564B                  GO TO 39
      0005E4B   41            WRITE(6,90)(MULTIP(I),I=INI,IF,2)
      000576B                 WRITE(6,91)(SYM,NMULTI(I),I=INI,IF,2)
      000611B   39             CONTINUE
      000613B   90             FORMAT(2X,8(I3,12X))
      000613B   91            FORMAT(5X,8(A2,*(*,I9,*)*,2X))
      000613B                 RETURN
      000615B                 END

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