

CONFIGURATION OF EQUIVALENT f ELECTRONS.  
SOME CONSIDERATIONS ABOUT THE CLASSIFICATION OF THE TERMS.

A.B.Nascimento and G.Vicentini

Departamento de Química, Universidade Federal da  
Paraíba and Departamento de Química Fundamental,  
Instituto de Química, Universidade de São Paulo.

The term  $^2F$  given to the ions  $Ce^{3+}$  and  $Yb^{3+}$  is due to an electron or to one hole, respectively, in the  $4f$  configuration of the lanthanide elements. When the number of equivalent electrons (or holes) becomes larger than one there is an increase in the number of terms. In some cases it is possible to observe different terms, but with the same values of L and S. The  $Nd^{3+}$  configuration ( $4f^3$ ) presents the following terms:  $^4$ (IGFDS),  $^2$ (LKIP) and  $2x^2$ (HGFD). Table 1 contains the terms that occur twice and the levels with the same representations with different energies.

The examples given in Table 1 mean that a different set of quantum numbers are necessary to distinguish such levels.

Racah (1,2) showed that it is possible to classify systematically the states of a given  $f^n$  configuration using the group theory. The method consists in classifying the states of the  $f^n$  configuration through its properties, under some transformation within the group. The properties of such groups are used to simplify the calculus of the matrix elements of the tensor operators, which corresponds to

the interactions under study. The irreducible representations of the group may be used as labels to classify the transformations of a particular state under the group operations. These irreducible representations are used as additional quantum numbers.

Table 1 - Some terms and levels of the  $4f^3$  configuration

Term $2S+1_L$	Level $2S+1_{L_J}$	Term $2S+1_L$	Level $2S+1_{L_J}$
	$a_1)^2H_{11/2}$		$c_1)^2F_{7/2}$
a) $^2H$	$a_2)^2H_{11/2}$	c) $^2P$	$c_2)^2F_{7/2}$
	$a_3)^2H_{9/2}$		$c_3)^2F_{5/2}$
	$a_4)^2H_{9/2}$		$c_4)^2F_{5/2}$
	$b_1)^2G_{9/2}$		$d_1)^2D_{5/2}$
b) $^2G$	$b_2)^2G_{9/2}$	d) $^2D$	$d_2)^2D_{5/2}$
	$b_3)^2G_{7/2}$		$d_3)^2D_{3/2}$
	$b_4)^2G_{7/2}$		$d_4)^2D_{3/2}$

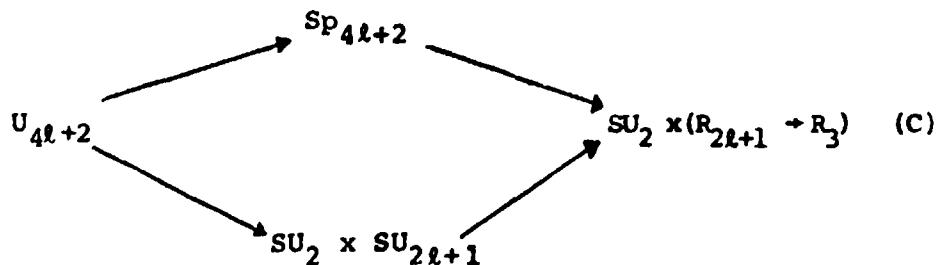
The levels  $a_1 = a_2$ ,  $a_3 = a_4$ ,  $b_1 = b_2$ ,  $b_3 = b_4$ ,  $c_1 = c_2$ ,  $c_3 = c_4$ ,  $d_1 = d_2$  and  $d_3 = d_4$  are equal, but represent different energies.

The classification of the states for equivalent electron configurations can be done using the Schur (3) functions, in terms of a simplectic group of characters.

As we know,  $\{l^n\}$  is equal to  $\sum_{\alpha=0}^{n-2\alpha} \langle l^{n-2\alpha} \rangle$  (A) with  $\alpha$  integral and  $n \geq 2\alpha$ .

The representations that corresponds to each  $\alpha$  value are given by the seniority number  $v = n - 2\alpha$  (B) (4). The number  $v$  may assume positive integral odd or even values, corresponding to configurations with an even or odd number of electrons. Each  $l^v$  term is repeated at least once in  $l^{v+2}$  and  $l^{v+4} \dots$ , and the totality of terms  $n \leq (2\ell + 1)$  presents  $v_m = n$ . The terms of a  $p^n$  configuration are determined only by  $S$  and  $L$ , that of a  $d^n$  by  $S$ ,  $L$  and  $v$  and in the case of a  $f^n$  by  $S$ ,  $L$ ,  $v$  and the quantum numbers  $W$  and  $U$  that will be explained latter.

The LS terms of a  $l^n$  configuration may be classified by the chain of groups:



In the particular case of  $l = 3$ , it is necessary to use an additional sub-group  $G_2$ :

$$R_{2l+1} \rightarrow G_2 \rightarrow R_3 \quad (D)$$

In each step of the equation C it is necessary to decompose the characters  $\{l^n\}$  of  $U_{4l+2}$  in the characters of the sub-group:

$$U_{4l+2} \rightarrow SU_2 \times R_{2l+1}, \quad U_{4l+2} \rightarrow Sp_{4l+2}, \quad U_{4l+2} \rightarrow SU_{2l} \times R_3, \text{ etc.}$$

The number of totally antisymmetric functions obtained from  $n$  electrons and  $4l+2$  functions  $\Psi(s m_s m_l)$  is given by (5) :

$$C_{4l+2}^n = \frac{(4l+2)!}{n!(4l+2-n)!} \quad (E)$$

The antisymmetric representations  $\{1^n\}$  and the dimensions of the irreducible representations of  $U_{14}$  for  $l=3$  are summarized in Table 2.

Table 2 -  $\{1^n\}$  representations and dimentions  
of the irreducible representations in  $U_{14}$

$f^n$	$\{1^n\}$	$C_{14}^n = 14! / n!(14-n)!$
$f^0, f^{14}$	{0}	1
$f^1, f^{13}$	{1}	14
$f^2, f^{12}$	{1^2}	91
$f^3, f^{11}$	{1^3}	364
$f^4, f^{10}$	{1^4}	1001
$f^5, f^9$	{1^5}	2002
$f^6, f^8$	{1^6}	3003
$f^7$	{1^7}	3432

The representation of  $Sp_{4l+2}$  are defined by  $2l+1$  integral numbers  $(\sigma_1 \sigma_2 \dots \sigma_{2l+1})$  with  $\sigma_1 > \sigma_2 > \dots > \sigma_{2l+1} > 0$ .

The dimension  $D_{(v)}$  of the irreducible representation  $(11 \dots 10 \dots 0)$  of  $Sp_{4l+2}$  corresponds to a determined seniority number  $v$  given by (5):

$$D_{(v)} = 2(2l+2 - v) \frac{(4l+3)!}{v!(4l+4-v)!} \quad (F)$$

Using equation (F) and equation 80 given by Wybourne (4), it is possible to obtain the reduction  $U_{14} \rightarrow Sp_{14}$  for  $l=3$  (Table 3).

Table 3 - Reduction  $U_{14} \rightarrow Sp_{14}$  and dimensions of  $Sp_{14}$

$f^n$	Reduction $U_{14} \rightarrow Sp_{14}$	$\sum_{v=0}^7 D_{(v)} = \sum_0^7 \frac{2(8-v)15!}{v!(16-v)!} = C_{14}^n$
$f^7$	$\{1^7\} + \langle 1^7 \rangle + \langle 1^5 \rangle + \langle 1^3 \rangle + \langle 1 \rangle$	$1430 + 1638 + 350 + 14 = 3432$
$f^6$	$\{1^6\} + \langle 1^6 \rangle + \langle 1^4 \rangle + \langle 1^2 \rangle + \langle 0 \rangle$	$2002 + 910 + 90 + 1 = 3003$
$f^5$	$\{1^5\} + \langle 1^5 \rangle + \langle 1^3 \rangle + \langle 1 \rangle$	$1638 + 350 + 14 = 2002$
$f^4$	$\{1^4\} + \langle 1^4 \rangle + \langle 1^2 \rangle + \langle 0 \rangle$	$910 + 90 + 1 = 1001$
$f^3$	$\{1^3\} + \langle 1^3 \rangle + \langle 1 \rangle$	$350 + 14 = 364$
$f^2$	$\{1^2\} + \langle 1^2 \rangle + \langle 0 \rangle$	$90 + 1 = 91$
$f^1$	$\{1\} + \langle 1 \rangle$	$14 = 14$
$f^0$	$\{0\} + \langle 0 \rangle$	$1 = 1$

$\{1^n\} = \sum \langle 1^v \rangle$  and  $v$  may assume the values:

a) 1, 3, 5, 7 for a configuration with an odd number of electrons;

b) 0, 2, 4, 6 for a configuration with an even number of electrons.

The irreducible representations for the unitary group  $U_{2l+1}$  are labeled by the division of  $n$  in  $2l+1$  integral numbers, where  $|\lambda| = |\lambda_1, \lambda_2 \dots \lambda_{2l+1}|$ , with  $\lambda_1 > \lambda_2 > \dots > 0$  and  $\lambda_1 + \lambda_2 + \dots = n$ . The dimension  $D_{|\lambda|}$  is calculated according to Weyl (6) (page 201):

$$D_{\lambda} = \frac{2l+1}{\prod_{j>i=1}^{2l+1}} \frac{\lambda_1 - \lambda_j - i + j}{j - i} \quad (G)$$

or, according to Judd (5), by:

$$\frac{(2s+1)(l+2)!(2l+1)!}{(2l+2-b)!(2l+1-a)!(a+1)!b!} \quad (G-1)$$

$$\text{with } a = \frac{1}{2}n + s \quad \text{and} \quad b = \frac{1}{2} - s .$$

The irreducible representations of  $U_{2l+1}$  may be decomposed in the irreducible representation of  $R_{2l+1}$  (continuous group of rotations in  $2l+1$  dimensions) using the tables presented by Young (7). The irreducible representations  $W$  of  $R_{2l+1}$  are labeled by  $l$  integral numbers  $(w_1 w_2 \dots w_l)$  with  $2 \geq w_1 \geq w_2 \geq \dots \geq w_l \geq 0$ . The irreducible representations of  $U_{2l+1}$  are designated to the corresponding Young partitions and that of  $R_{2l+1}$  for  $W(w_1 w_2 \dots w_l)$ . For the  $R_3$  group, the spectroscopic symbol  $(S, P, D, \dots)$  in which the  $2L+1$  multiplicity gives the dimension of this irreducible representation.

In the case of  $l = 3$ , the irreducible representations of  $R_7$  are characterized by the division of  $n$  in three integral numbers:  $W = (w_1, w_2, w_3)$  in which  $2 \geq w_1 \geq w_2 \geq w_3 \geq 0$ .  $W(w_1 w_2 w_3)$  constitutes an additional quantum number for the  $4f^n$  configuration. Table 4 shows the decomposition for the reduction  $U_7 \rightarrow R_7$  together with its representations. This makes easy the reduction  $U_{14} \rightarrow SU_2 \times U_7$  (see equation C).

Table 4 - Reduction  $U_7 \rightarrow R_7$ 

$U_7 \rightarrow R_7$					
$f^n$	$2S+1_w\{w_1w_2w_3\}$	v	Dimension	$2S+1_w\{w_1w_2w_3\}$	Dimension
$f^0$	$^1\{000\}$	0	1	$^1 000 $	1
$f^1$	$^2\{100\}$	1	7	$^2 100 $	7
$f^2$	$^3\{110\}$	2	21	$^3 110 $	21
	$^1\{200\}$	2	28	$[ ^1 200 $	27
		0		$[  000 $	1
$f^3$	$^4\{111\}$	3	35	$^4 111 $	35
	$^2\{210\}$	3	112	$[ ^2 210 $	105
		1		$[ ^2 100 $	7
$f^4$	$^5\{111\}$	4	35	$^5 111 $	35
	$^3\{211\}$	4	210	$[ ^3 211 $	189
		2		$[ ^3 110 $	21
	$^1\{220\}$	4	196	$[ ^1 220 $	168
		2		$[ ^1 200 $	27
		0		$[ ^1 000 $	1
$f^5$	$^6\{110\}$	5	21	$^6 110 $	21
	$^4\{221\}$	5	224	$[ ^4 211 $	189
		3		$[ ^4 111 $	35
	$^2\{221\}$	5	490	$[ ^2 221 $	378
		3		$[ ^2 210 $	105
		1		$[ ^2 100 $	7

(continue)

$U_7 \rightarrow R_7$					
$\omega^n$	$2S+1 \omega\{w_1 w_2 w_3\}$	v	Dimension	$2S+1 \omega\{w_1 w_2 w_3\}$	Dimension
$f^6$	$^7\{100\}$	6	7	$^7 110 $	7
	$^5\{210\}$	6		$^5 210 $	105
		4		$^5 111 $	35
	$^3\{221\}$	6	588	$^3 221 $	378
		4		$^3 221 $	189
		2		$^3 110 $	21
		6		$^2 222 $	294
		4		$^2 220 $	168
		2		$^1 200 $	27
				$^1 000 $	1
$f^7$	$^8\{000\}$	7	1	$ 000 $	1
	$^6\{200\}$	1		$^6 200 $	27
		5	48	$^6 110 $	21
	$^4\{220\}$	7		$^4 220 $	168
		5		$^4 211 $	189
		3	392	$^4 111 $	35
	$^2\{222\}$	7		$ 222 $	294
		5		$^2 221 $	378
		3		$^2 210 $	105
		1		$^2 100 $	7

The use of equations numbers 128 and 132 given by Wybourne (4) gives immediately the reduction  $Sp_{14} \rightarrow SU_2 \times U_7$ . For example, in the reduction  $U_{14} \rightarrow SU_2 \times U_7$  the representation  $\{1^4\} \rightarrow \{5\}_{111} + \{3\}_{211} + \{2\}_{220}$  and under  $U_7 \rightarrow R_7$  (see table 4) we have:

$$\{5\}_{111} \rightarrow \{5\}_{111}$$

$$\{3\}_{111} \rightarrow \{3\}_{211} + \{3\}_{110}$$

$$\{1\}_{220} \rightarrow \{1\}_{220} + \{1\}_{200} + \{1\}_{000}$$

The irreducible representation  $\{1^4\}$ ,  $\{1^2\}$  and  $\{0\}$  of  $Sp_{14}$  may be decomposed in that of  $SU_2 \times R_7$ , given:

$$\{1^4\} \rightarrow \{5\}_{111} + \{3\}_{211} + \{1\}_{220}$$

$$\{1^2\} \rightarrow \{3\}_{110} + \{1\}_{200}$$

$$\{0\} \rightarrow \{1\}_{000}$$

When  $R_7$  is restrict to the subgroup  $G_2$ , the irreducible representations may be characterized by the division of  $n$  into two integrals  $U(u_1 u_2)$  with  $2 > U_1 > U_2 > 0$  (exception for  $U(u_1 u_2) = U(30)$ ,  $U(31)$  and  $U(40)$ ). The decomposition  $R_7 \rightarrow G_2$  is indicated in Table 5 (1). The dimension of the  $G_2$  representations were calculated by:

$$D(u_1 u_2) = (u_1 + u_2 + 3)(u_1 + 2)(2u_1 + u_2 + 5) \times (u_1 + 2u_2 + 4)(u_1 - u_2 + 1)(u_2 + 1)/120 \quad (5)$$

those of the  $R_7$  by the formula:

$$\begin{aligned} D(w_1 w_2 w_3) &= (w_1 + w_2 + 4)(w_1 + w_3 + 3)(w_2 + w_3 + 2) \\ &\times (w_1 - w_2 + 1)(w_1 - w_3 + 2)(w_2 - w_3 + 1) \\ &\times (2w_1 + 5)(2w_2 + 3)(2w_3 + 1)/720. \end{aligned}$$

Table 5 - Decomposition  $R_7 \rightarrow G_2$

$z = 3$	$R_7 \rightarrow G_2$		
$f^n$	$2S+1 [w_1 w_2 w_3]$	$G(u_1 u_2)$	Dimension of $G_2$
$f^0$	$1 000 $	$1(00)$	1
$f^1$	$2 100 $	$1(10)$	7
$f^2$	$3 110 $	$\begin{bmatrix} 3(10) \\ 3(11) \end{bmatrix}$	$\begin{matrix} 7 \\ 14 \end{matrix}$
	$1 200 $	$1(20)$	27
	$1 000 $	$1(00)$	1
$f^3$	$4 111 $	$\begin{bmatrix} 4(00) \\ 4(10) \\ 4(20) \end{bmatrix}$	$\begin{matrix} 1 \\ 7 \\ 27 \end{matrix}$
	$2 210 $	$\begin{bmatrix} 2(11) \\ 2(20) \\ 2(21) \end{bmatrix}$	$\begin{matrix} 14 \\ 27 \\ 64 \end{matrix}$
	$2 100 $	$2(10)$	7
$f^4$	$5 111 $	$\begin{bmatrix} 5(00) \\ 5(10) \\ 5(20) \end{bmatrix}$	$\begin{matrix} 1 \\ 7 \\ 27 \end{matrix}$
	$3 211 $	$\begin{bmatrix} 3(10) \\ 3(11) \\ 3(20) \\ 3(21) \\ 3(30) \end{bmatrix}$	$\begin{matrix} 7 \\ 14 \\ 27 \\ 54 \\ 77 \end{matrix}$
	$3 110 $	$\begin{bmatrix} 3(10) \\ 3(11) \end{bmatrix}$	$\begin{matrix} 7 \\ 14 \end{matrix}$
	$1 220 $	$\begin{bmatrix} 1(20) \\ 1(21) \\ 1(22) \end{bmatrix}$	$\begin{matrix} 27 \\ 64 \\ 77 \end{matrix}$
	$1 200 $	$1(20)$	27
	$1 000 $	$1(00)$	1

(continue)

$\ell = 3$	$R_7 \rightarrow G_2$		
$f^n$	$2S+1(w_1w_2w_3)$	$G(u_1u_2)$	Dimension of $G_2$
	$6 110 $	$\begin{bmatrix} 6 \\ 6 \end{bmatrix} (10) \\ (11)$	7 14
	$4 211 $	$\begin{bmatrix} 4 \\ 4 \\ 4 \\ 4 \\ 4 \end{bmatrix} (10) \\ (11) \\ (20) \\ (21) \\ (30)$	7 14 27 64 77
	$4 111 $	$\begin{bmatrix} 2 \\ 2 \\ 2 \end{bmatrix} (00) \\ (10) \\ (20)$	1 7 27
$f^5$	$2 221 $	$\begin{bmatrix} 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \end{bmatrix} (10) \\ (11) \\ (20) \\ (21) \\ (30) \\ (31)$	7 14 27 64 77 189
	$2 210 $	$\begin{bmatrix} 2 \\ 2 \\ 2 \end{bmatrix} (11) \\ (20) \\ (21)$	14 27 54
	$2 100 $	$2 (10)$	7

(continue)

$\ell = 3$	$R_7 \rightarrow G_2$		
$f^n$	$2S+1[w_1w_2w_3]$	$G(u_1u_2)$	Dimension of $G_2$
$f^6$	$^7 100 $	$^7(10)$	7
	$^5 210 $	$\begin{cases} ^5(11) \\ ^5(20) \\ ^5(21) \end{cases}$	$14 \\ 27 \\ 64$
	$^5 111 $	$\begin{cases} ^5(00) \\ ^5(10) \\ ^5(20) \end{cases}$	$1 \\ 7 \\ 27$
	$^3 221 $	$\begin{cases} ^3(10) \\ ^3(11) \\ ^3(20) \\ ^3(21) \\ ^3(30) \\ ^3(31) \end{cases}$	$7 \\ 14 \\ 27 \\ 64 \\ 77 \\ 189$
		$\begin{cases} ^3(10) \\ ^3(11) \\ ^3(20) \\ ^3(21) \\ ^3(30) \end{cases}$	$7 \\ 14 \\ 27 \\ 64 \\ 77$
		$\begin{cases} ^3(10) \\ ^3(11) \end{cases}$	$7 \\ 14$
	$^3 110 $	$\begin{cases} ^1(00) \\ ^1(10) \\ ^1(20) \\ ^1(30) \\ ^1(40) \end{cases}$	$1 \\ 7 \\ 27 \\ 77 \\ 182$
		$\begin{cases} ^1(20) \\ ^1(21) \\ ^1(22) \end{cases}$	$27 \\ 64 \\ 77$
		$^1(20)$	27
		$^1(00)$	1

(continue)

$\ell = 3$	$R_7 \rightarrow G_2$		
$f^n$	$2S+1[w_1w_2w_3]$	$G(u_1u_2)$	Dimension of $G_2$
$f^7$	$^8 000 $	$^8(00)$	1
		$^6(20)$	27
	$^6 110 $	$[^6(10)$	7
		$[^6(11)$	14
	$^4 220 $	$[^4(20)$	27
		$[^4(21)$	64
		$[^4(22)$	77
		$[^4(10)$	7
		$[^4(11)$	14
$f^7$	$^4 211 $	$[^4(20)$	27
		$[^4(21)$	64
		$[^4(30)$	77
		$[^4(00)$	1
		$[^4(10)$	7
	$^2 222 $	$[^4(20)$	27
		$[^2(00)$	1
		$[^2(10)$	7
		$[^2(20)$	27
		$[^2(30)$	77
$f^7$	$^2 221 $	$[^2(40)$	182
		$[^2(10)$	7
		$[^2(11)$	14
		$[^2(20)$	27
		$[^2(21)$	64
	$^2 210 $	$[^2(30)$	77
		$[^2(31)$	189
		$[^2(11)$	14
		$[^2(20)$	27
		$[^2(21)$	64
$f^7$	$^2 100 $	$[^2(10)$	7

The decomposition of  $G_2$  in  $R_3$  is made using equations 131 and 132 of reference (4) (Table 6). The representation  $U(u_1 u_2)$  of  $G_2$  gives the additional third quantum number of the  $f^n$  configuration.

In the  $Nd^{3+}(4f^3)$  where the terms  $^2D$ ,  $^2F$ ,  $^2G$ ,  $^2H$  occur twice,  $v = 0$  and 3. The decomposition  $U_{14} \rightarrow Sp_{14}$  gives:

$$(1^3) \rightarrow <1> + <1^3> \quad (\text{see equation C and Table 3})$$

In the reduction  $Sp_{14} \rightarrow SU_2 \times R_7$  (Table 4) we have

$$<1^3> \rightarrow ^4|111| + ^2|210|$$

$$<1> \rightarrow ^2|100|.$$

Using Table 5 it is possible to obtain the reduction  $R_7 \rightarrow G_2$ :

$$|111| \rightarrow (00) + (10) + (20)$$

$$|210| \rightarrow (11) + (20) + (21)$$

$$|100| \rightarrow (10)$$

The decomposition  $G_2 \rightarrow R_3$  is made by using Table 6. In our example we have:

$$(00) \rightarrow S$$

$$(10) \rightarrow F$$

$$(11) \rightarrow PH$$

$$(20) \rightarrow DGI$$

$$(21) \rightarrow DFGHKL$$

Table 6 - Reduction  $G_2 \rightarrow R_3$

$G_2$	DIMENSION	$\rightarrow R_3$	DIMENSION	L	$G_2$	DIMENSION	$\rightarrow R_3$	DIMENSION	L
(00)	1	S	1	0			S	1	0
(10)	7	F	7	3			D	5	2
(11)	14	P H	$\begin{bmatrix} 3 \\ 11 \end{bmatrix}$	1 5			F	7	3
(20)	27	D G I	$\begin{bmatrix} 5 \\ 9 \\ 13 \end{bmatrix}$	2 4 6	(40)	182	G G H I I K L	9 9 11 13 13 15 17	4 4 5 6 6 7 8
(21)	64	D F G H K L	$\begin{bmatrix} 5 \\ 7 \\ 9 \\ 11 \\ 15 \\ 17 \end{bmatrix}$	2 3 4 5 7 8			L M N Q	17 19 21 25	8 9 10 12
(30)	77	P F G H I K M	$\begin{bmatrix} 3 \\ 7 \\ 9 \\ 11 \\ 13 \\ 15 \\ 19 \end{bmatrix}$	1 3 4 5 6 7 9	(31)	189	P D F G H H I I K	3 5 7 7 9 11 11 13 13 15	1 2 3 3 4 5 5 6 6 7
(22)	77	S D G H I L N	$\begin{bmatrix} 1 \\ 5 \\ 9 \\ 11 \\ 13 \\ 17 \\ 21 \end{bmatrix}$	0 2 4 5 6 8 10			K L M N O	15 17 19 21 23	7 8 9 10 11

It is possible to note that the  $v$  quantum number separates the  $^2F$  states into two, with  $v = 1$  and  $v = 3$ . The states  $^2D$ ,  $^2G$  and  $^2H$ , with the same seniority ( $v$ ), are distinguished by the quantum numbers  $W$  and  $U$ :

$$\begin{aligned} ^2F &= |100|(10) ^2F, |210|(21) ^2F; v_1 = 1 \text{ and } v = 3 \\ ^2D &= |210|(20) ^2D, |210|(21) ^2D \\ ^2G &= |210|(20) ^2G, |210|(21) ^2G \\ ^2H &= |210|(11) ^2H, |210|(21) ^2H \end{aligned} \quad \left. \begin{array}{l} \\ \\ \end{array} \right\} \quad v = 3$$

Equation C may be alternatively used as  $U_{14} \rightarrow SU_2 \times U_7$ . In this case,

$$\{1^3\} \rightarrow ^4\{111\} + ^2\{210\}$$

and, under  $U_7 \rightarrow R_7$ , we have:

$$\{111\} \rightarrow |111|$$

$$\{210\} \rightarrow |210| + |100|.$$

Table 7 illustrates alternative procedures. The quantum number  $v$  is used as label for the  $Sp_{14}$  representations.

Table 7 - Classification of the  $4f^3$  Configuration

$U_{14}$	$Sp_{14}$	$SU_2 \times U_7$	$v$	$SU_2 \times R_7$	$SU_2 \times G_2$	$SU_2 \times R_3$
$\{1^3\}$	$\left\{ \begin{array}{l} \langle 1^3 \rangle \\ \langle 1 \rangle \end{array} \right\}$	$\left\{ \begin{array}{ll} ^4\{111\} & 3 \\ ^2\{210\} & 3 \\ \langle 1 \rangle & 1 \end{array} \right\}$		$\begin{array}{l} ^4 111  \\ ^2 210  \\ ^2 100  \end{array}$	$\begin{array}{l} ^4(00) \\ ^4(10) \\ ^4(20) \\ ^2(11) \\ ^2(20) \\ ^2(21) \\ ^2(10) \end{array}$	$\begin{array}{l} ^4S \\ ^4F \\ ^4DGI \\ ^2PH \\ ^2DGI \\ ^2DFGHKL \\ ^2F \end{array}$

For the terms that occurs twice, with the same symbols of the  $4f^n$  configuration for example (30 and (40) it is necessary to introduce an additional label  $\tau$ . If the irreducible representation of  $R_7$ , the symbols used are  $W$  and  $U$  for  $G_2$ , the terms for  $f^n$  are  $f^n \tau vWUSL$ . According to Pauli, the classifications for  $f^{14-n}$  will be identical to that of  $f^n$ , so, it is only necessary to use  $n \leq 7$ . Table 8 shows the relation of the  $R_7$  and  $G_2$  representation.

Considering the fact that configurations with an odd number of electrons have an even multiplicity or vice-versa, we draw the Figure 1 to correlate the  $W$ ,  $U$  and  $v$  quantum numbers. It is easy to observe in this figure that for the reduction  $Sp_{14} \rightarrow SU_2 \times R_7$  is given by:

$$\begin{aligned}
 <0> & |000| \\
 <1> & ^2|100| \\
 <1^2> & ^3|110| + ^1|200| \\
 <1^3> & ^4|111| + ^2|210| \\
 <1^4> & ^5|111| + ^3|211| + ^1|220| \\
 <1^5> & ^6|110| + ^4|211| + ^2|221| \\
 <1^6> & ^7|100| + ^5|210| + ^3|221| + ^1|222| \\
 <1^7> & ^8|000| + ^6|200| + ^4|220| + ^2|222|.
 \end{aligned}$$

In the case of  $Nd^{3+}(4f^3)$ ,  $^4|111|$  gives 5 quartets:  $^4S$ ,  $^4F$ ,  $^4DGI$ ;  $^2|210|$  gives 11 terms:  $^2(PH)$ ,  $^2(DGI)$ ,  $^2(DFGHKL)$  and  $^2|100|$  gives only one term  $^2F$ . The results of Table 7 are clearly observed in Figure 1. For the coupling designated by  $(v_1 s_1)$  and  $(v_2 s_2)$  we obtain (1):

$$v_1 + 2s_2 = v_2 + 2s_1 = 2\ell + 1 \quad (H).$$

For the representation  $|110|$ ,  $|211|$  and  $|111|$  the  $(v,s)$  couplings are  $(5, 5/2)$ ,  $(5, 3/2)$ ,  $(3, 3/2)$  for the configuration  $f^5$  and  $(2,1)$ ,  $(4,1)$ ,  $(4,2)$  for  $f^4$ .

Table 8 - Relation between Groups  $R_7$  and  $G_2$

L	v	w	u
S	0;7	000	00
F	1;6	100	10
F PH	2;5	110	10 11
DGI	2;7	200	20
S F DGI	3;4	111	00 10 20
PH DGI DFGHKL	3;6	210	11 20 21
F PH DGI DFGHKL PFGHIKM	4;5	211	10 11 20 21 30
DGI DFGHKL SDGHILN	4;7	220	20 21 22
F PH DGI DFGHKL PFGHIKM PDFFGHHIIKKLMNO	5;6	221	10 11 20 21 30 31
S F DGI PFGHIKM SDFGGHHIIKKLMNO	6;7	222	00 10 20 30 40

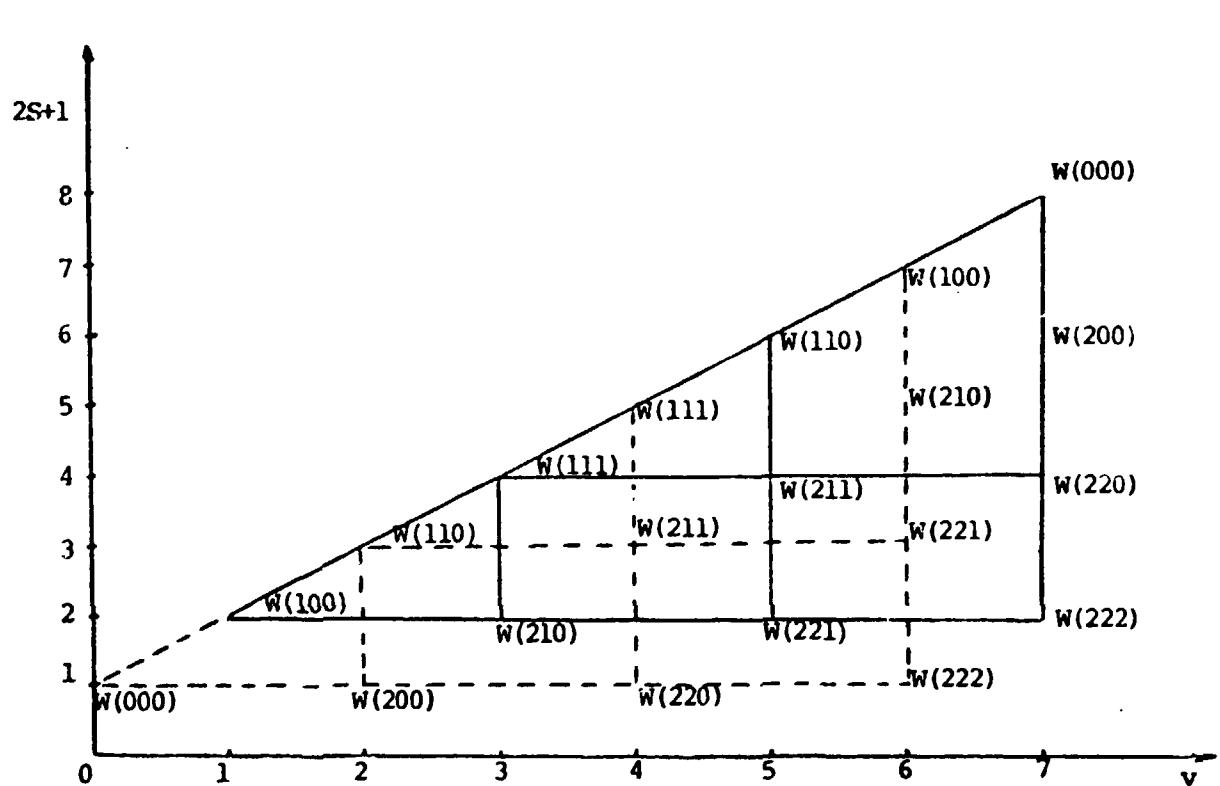


Figure 1 - Illustrative correlation between the configuration  $4f^n$ ,  $W$ ,  $U$ ,  $v$  and the multiplicity of the terms.

REFERENCES

1. RACAH, G., (1949), Theory of Complex Spectra IV, Phys. Rev., 76, 1352-1365.
2. RACAH, G., (1951), Group Theory and Spectroscopy, mimeographed notes, Princeton. These notes are available as a CERN (Geneva) reprint.
3. WYBOURNE, G., (1974), Classical Groups for Physicists, Wiley, New York.
4. WYBOURNE, G., (1970), Symmetry Principles and Atomic Spectroscopy, Wiley, New York.
5. JUDD, R., (1973), Operator Techniques in Atomic Spectroscopy, McGraw-Hill, New York.
6. WEYL, H., (1946), The Classical Groups (Princeton University Press, Princeton, N.J.).
7. LITTLEWOOD, D.E., (1950), The Theory of Group Characters, Oxford University Press, New York, 2nd ed..