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TABLES OF CLEBSCH-GORDAN COEFFICIENTS FOR INTEGER ANGULAR MOMENTUM J = 0÷6

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1. - INTRODUCTION

Clebsch-Gordan coefficients play an essential role in a variety of problems involving addition of angular momenta and in general tensor manipulation(1-12). Apart from more conventional applications in quantum mechanics Clebsch-Gordan coefficients are now often employed in material science(13,14) and in the statistical mechanics of condensed phases and in particular of anisotropic fluids such as liquid crystals(15). All of these practical applications require knowledge of the explicit values of Clebsch-Gordan coefficients of integer rank. To this effect there are already, of course, both general formulas and tables either of Clebsch-Gordan coefficients or of the closely related 3j coefficients(20-22) as well as computer programs for their evaluation(23, 24). In principle it is therefore not too difficult to obtain a certain required set of Clebsch-Gordan coefficients. In practice, however, this may still prove rather laborious. In particular the use of most tables, even if available for the ranks of interest, may still result in a somewhat time consuming and error prone exercise. For example the most commonly available tables only go up to an integral angular momentum of two(22) or four(20) and they either give the coefficients in floating point form or in terms of a string of exponents of prime numbers whose product gives the desired coefficient. Moreover they tend to make full use of the various symmetries of which the Clebsch-Gordan symbols are endowed[1]. While this can be advantageous for compactness, we think that the aim of a set of tables should be that of giving coefficients quickly while limiting the chances of trivial mistakes so that some redundancy is advisable. In the present set of tables we have chosen therefore to list Clebsch-Gordan coefficients in the most straightforward and immediately usable form, trading some extension in size against convenience of the user. In the next section the notation employed here is defined and contact is made with other widespread conventions. Some often used formulas of angular momentum and irreducible tensors technology are also listed for completeness and easy reference. Coefficients for integer angular momentum of rank up to six are listed, since there is now a number of applications in molecular physics, ranging from calculation of higher terms in intermolecular potentials[25-27] to evaluation of matrix elements arising in multiphoton spectroscopy[14], where these are required. We quote as an example the theory of hyper-Raman effect[28], where rotational averages of sixth rank tensors are involved. We shall give Clebsch-Gordan coefficients both in exact form i. e. as square roots of fractional numbers and in floating point form. We are not aware of other tables listing Clebsch-Gordan coefficiente up to this rank in this form.

2. - NOTATIONS

There is an impressive number of different conventions[29-41] for writing Clebsch-Gordan coefficients, even though many of them only differ for the symbols employed. We choose to here define a Clebsch-Gordan coefficient according to the phase convention of Rose[1] i. e. we write the coupling coefficient between two states of angular momentum J_1 and J_2 to yield a state $|J_3 m_3\rangle$ as

$$|J_3 m_3\rangle = \sum_{m_1 m_2} C(J_1, J_2, J_3; m_1, m_2, m_3)|J_1 m_1\rangle\, |J_2 m_2\rangle \qquad (1)$$

where $C(a\,b\,c; d\,e\,f)$ is a Clebsch-Gordan or vector coupling coefficient and J_1, J_2, J_3 can take non-negative integer or semi-integer values.

Clebsch-Gordan coefficients are real and can be generally written in terms of square roots of ratios of integers. In the Tables given in section 4, reproduced from computer printouts, we employ the notation

$$C(J_1, J_2, J_3; m_1, m_2, m_3) = R(N1/N2) \equiv \mathrm{sgn}(N1)\{(N1)/(N2)\}^{1/2}, \qquad (2)$$

where J_1, J_2, J_3 and N1, N2 are integers and the function sgn(M) gives the sign of its argument M. As mentioned before the results are also given for convenience in floating point form rounded to eight decimal places. The angular momentum values J_1, J_2, J_3 are said to form a triangle $\Delta(J_1 J_2 J_3)$, in the sense that the following relations hold for the allowed values

$$\Delta(J_1, J_2, J_3) : \begin{cases} J_1 + J_2 - J_3 \geqq 0 & \text{(3a)} \\ J_1 - J_2 + J_3 \geqq 0 & \text{(3b)} \\ -J_1 + J_2 + J_3 \geqq 0 & \text{(3c)} \end{cases}$$

where $(J_1 + J_2 + J_3)$ is an integer. The triangular relation is symmetric in the three angular momenta. Clebsch-Gordan coefficients formed with combinations of angular momenta not satisfying this rule are equal to zero and of course are not reported in the Tables. The angular momentum projection values m_1, m_2, m_3 can take the values

$$m_1 = -J_1, -J_1+1, .., J_1 ; \quad m_2 = -J_2, -J_2+1, .., J_2 ; \quad m_3 = -J_3, -J_3+1, .., J_3 . \qquad (4)$$

Other common notations for the same coefficients are listed below (cf. Ref. (2) and (11)).

$C^{J_3 m_3}_{J_1 m_1 J_2 m_2}$	Alder[32], Jahn[33a], Jahn and Hope[33b]
$C^{J_1 J_2 J_3}_{m_1 m_2 m_3}$	Biedenharn[35], Redmond[36], Simon[39]
$C_{J_1 J_2}(J_3 m_3; m_1 m_2)$	Blatt and Weisskopf[8]
$X(J_3, m_3, J_1, J_2, m_1)$	Boys and Sahni[31]
$\langle J_1 J_2 m_1 m_2 \| J_3 m_3 \rangle$	Brink and Satchler[5], Matsen[40], Lyubarskii[41], Jerphagnon[14]
$(J_1 J_2 J_3 m_3 \| J_1 J_2 m_1 m_2)$ $(J_1 J_2 m_1 m_2 \| J_1 J_2 J_3 m_3)$	Condon and Shortley[6]
$A^{J_3 J_1 J_2}_{m_3 m_1 m_2}$	Eckart[37]

$\langle J_1 m_1, J_2 m_2 \vert (J_1 J_2) J_3 m_3 \rangle$	Fano[34]
$C^{J_1 J_2}_{J_3 m_3}(m_1 m_2)$	Fox[38]
$C^{J_3}_{m_1 m_2}$	Landau and Lifschitz[9], Van der Waerden[30]
$(J_3 m_3 \vert m_1 m_2)$ $(m_1 m_2 \vert J_3 m_3)$ $(J_1 m_1 J_2 m_2 \vert J_1 J_2 J_3 m_3)$	Racah[16], Edmonds[2]
$C(J_1 J_2 J_3 ; m_1 m_2 m_3)$ $C(J_1 J_2 J_3 ; m_1 m_2)$	Rose[1]
$\langle J_1 J_2 m_1 m_2 \vert J_1 J_2 J_3 m_3 \rangle$	Silver[11], Weissbluth[12]
$S^{J_1 J_2}_{J_3 m_1 m_2}$	Wigner[7] .

Explicit relations for the calculation of Clebsch-Gordan coefficients have been derived by Wigner[1]

$$C(J_1, J_2, J_3; m_1, m_2, m_3) = \delta_{m_3, m_1+m_2}$$

$$\times \left\{ (2J_3+1) \frac{(J_3+J_1-J_2)!\,(J_3-J_1+J_2)!\,(J_1+J_2-J_3)!\,(J_3+m_3)!\,(J_3-m_3)!}{(J_1+J_2+J_3+1)!\,(J_1-m_1)!\,(J_2-m_2)!\,(J_2+m_2)!\,(J_1+m_1)!} \right\}^{1/2}$$

$$\times \sum_v \frac{(-)^{v+J_2+m_2}\,(J_2+J_3+m_1-v)!\,(J_1-m_1+v)!}{v!\,(J_3-J_1+J_2-v)!\,(J_3+m_3-v)!\,(v+J_1-J_2-m_3)!} \qquad (5)$$

and by Racah[16]

$$C(J_1, J_2, J_3; m_1, m_2, m_3) = \delta_{m_3, m_1+m_2} \left\{ (2J_3+1) \right.$$

$$\times \left. \frac{(J_1+J_2-J_3)!\,(J_3+J_1-J_2)!\,(J_3+J_2-J_1)!\,(J_1+m_1)!\,(J_1-m_1)!\,(J_2+m_2)!\,(J_2-m_2)!\,(J_3+m_3)!\,(J_3-m_3)!}{(J_1+J_2+J_3+1)!} \right\}^{1/2}$$

$$\times \sum_v (-)^v \left\{ (J_1+J_2-J_3-v)!\,(J_1-m_1-v)!\,(J_2+m_2-v)!\,(J_3-J_2+m_1+v)!\,(J_3-J_1-m_2+v)!\,v! \right\}^{-1} \qquad (6)$$

In eqs. (5), (6) the index v takes all the integral values leaving the argument of the various factorials non negative.

Clebsch-Gordan coefficients are related to the often used and more symmetric 3j symbols introduced by Wigner[7]

$$C(J_1, J_2, J_3; m_1, m_2, m_3) = (-)^{-J_1+J_2-m_3} (2J_3+1)^{1/2} \begin{pmatrix} J_1 & J_2 & J_3 \\ m_1 & m_2 & -m_3 \end{pmatrix} \tag{7}$$

3. - SOME USEFUL RELATIONS

We report here (Sections 3.1-3.4) for easy reference some useful properties of Clebsch-Gordan coefficients and (Section 3.5) a small collection of frequently employed formulas involving vector coupling coefficients. Applications to Wigner matrices and irreducible tensors are given in Sections 3.7 and 3.8.

3. 1. - Symmetries

There are various symmetry relations that can be derived e. g. from the general explicit expression for the Clebsch-Gordan coefficients given by Racah[1,16]. We have in particular :

$$C(J_1, J_2, J_3; m_1, m_2, m_3) =$$

$$= (-)^{J_1+J_2-J_3} C(J_1, J_2, J_3; -m_1, -m_2, -m_3) \tag{8a}$$

$$= (-)^{J_1+J_2-J_3} C(J_2, J_1, J_3; m_2, m_1, m_3) \tag{8b}$$

$$= (-)^{J_1-m_1} \left\{(2J_3+1)/(2J_2+1)\right\}^{1/2} C(J_1, J_3, J_2; m_1, -m_3, -m_2) \tag{8c}$$

From these relations some other useful equations can in turn be derived

$$C(J_1, J_2, J_3; m_1, m_2, m_3) =$$

$$= (-)^{J_2+m_2} \left\{(2J_3+1)/(2J_1+1)\right\}^{1/2} C(J_3, J_2, J_1; -m_3, m_2, -m_1) \tag{9a}$$

$$= (-)^{J_1-m_1} \left\{(2J_3+1)/(2J_2+1)\right\}^{1/2} C(J_3, J_1, J_2; m_3, -m_1, m_2) \tag{9b}$$

$$= (-)^{J_2+m_2} \left\{(2J_3+1)/(2J_1+1)\right\}^{1/2} C(J_2, J_3, J_1; -m_2, m_3, m_1) \tag{9c}$$

3. 2. - Orthogonality

The Clebsch-Gordan coefficients are elements of a unitary transformation and they satisfy orthogonality relations. These can be written as

$$\sum_{m_1, m_2} C(J_1, J_2, J; m_1, m_2, m)\, C(J_1, J_2, J'; m_1, m_2, m') = \delta_{JJ'}\, \delta_{mm'} \qquad (10a)$$

or

$$\sum_{m_1} C(J_1, J_2, J; m_1, m-m_1, m)\, C(J_1, J_2, J'; m_1, m-m_1, m) = \delta_{JJ'} \; . \qquad (10b)$$

We also have

$$\sum_{J, m} C(J_1, J_2, J; m_1, m_2, m)\, C(J_1, J_2, J; m_1', m_2', m) = \delta_{m_1 m_1'}\, \delta_{m_2 m_2'} \qquad (11a)$$

or

$$\sum_{J} C(J_1, J_2, J; m_1, m-m_1, m)\, C(J_1, J_2, J; m_1', m'-m_1', m') = \delta_{m_1 m_1'}\, \delta_{mm'} \; . \qquad (11b)$$

3. 3. - Sum rules

Some useful formulas are:

$$\sum_m C(J_1, J_2, J_1; -m, 0, -m)\, C(J_1', J_2, J_1'; m-M, 0, m-M) =$$

$$= \frac{(-)^{2M+J_2-2J_1-2J_1'}}{(2J_2+1)} \left[\frac{(2J_1+1)(2J_1'+1)(2J_1-J_2)!\,(2J_1'+J_2+1)!}{(2J_1'-J_2)!\,(2J_1+J_2+1)!} \right]^{1/2} \qquad (12) \quad \text{(cf. Ref. 42)}$$

$$\sum_{m_1, m_2, m} C(J_1, J_2, J; m_1, m_2, m)^2 = (2J+1) \qquad (13)$$

$$\sum_m (-)^m C(J, J, L; m, -m, 0) = (-)^J (2J+1)^{1/2}\, \delta_{0L} \; . \qquad (14)$$

Steinborn and Filter[43] have derived:

$$\sum_{J_1} \left\{ C(J_1 J_2 J_3;\, 0\,0\,0) \right\}^2 = (2J_3+1) \left\{ (J_1+J_2-J_3-1)!!\,(J_1+J_2+J_3)!! \right\} / \left\{ (J_1+J_2-J_3)!!\,(J_1+J_2+J_3+1)!! \right\} \qquad (15)$$

where $(-1)!! = 1$ is implied. A few recent results are: Din's formula[44, 45]

$$\sum_{\substack{J_1 = |J_3-J_2| \\ J_1 \neq k}}^{J_2+J_3} (2J_1+1) \left\{ C(J_1 J_2 J_3;\, 0\,0\,0) \right\}^2 / \left\{ J_1(J_1+1) - k(k+1) \right\} = 0; \qquad (16)$$

where $J_3 - J_2 \leq k \leq J_2 + J_3$ and $k + J_2 + J_3$ odd, and the following two obtained by Morgan III[46]

$$\sum_{J_2=0}^{J_1} \left\{(-)^{J_1-J_2} C(J_1 J_2 (J_1-J_2); 0\,0\,0)\right\}^2 / (2J_1 - 2J_2 + 1) = \left\{(2J_1)!!/(2J_1+1)!!\right\} \qquad (17)$$

$$\sum_{J_2=0}^{J_1} \left\{(-)^{J_1-J_2} C(J_1 J_2 (J_1-J_2); 0\,0\,0)\right\}^2 / \left\{(2J_1 - 2J_2 + 1)(2J_2-1)^2\right\} \qquad (18)$$

$$= \begin{cases} 1; \text{ if } J_1 = 0 \\ \left\{(2J_1)!!(2J_1-2)!!\right\} / \left\{(2J_1+1)!!(2J_1-1)!!\right\}; \text{ if } J_1 \text{ is a positive integer number.} \end{cases}$$

3. 4. - Recurrence relations

We give here two recurrent equations[1] that may prove useful in further extending the present Tables if necessary. The first allows changing the angular momentum J

$$\left\{m_1 - m\,\frac{J_1(J_1+1) - J_2(J_2+1) + J(J+1)}{2J(J+1)}\right\} C(J_1, J_2, J; m_1, m-m_1, m) =$$

$$= \left\{\frac{(J^2-m^2)(J-J_1+J_2)(J+J_1-J_2)(J_1+J_2+J+1)(J_1+J_2-J+1)}{4J^2(2J-1)(2J+1)}\right\}^{1/2} C(J_1, J_2, J-1; m_1, m-m_1, m)$$

$$+ \left\{\frac{\left[(J+1)^2-m^2\right](J+1-J_1+J_2)(J+1+J_1-J_2)(J_1+J_2+J+2)(J_1+J_2-J)}{4(J+1)^2(2J+1)(2J+3)}\right\}^{1/2} C(J_1, J_2, J+1; m_1, m-m_1, m) \qquad (19)$$

The second relates Clebsch-Gordan coefficients with the same angular momentum J_1, J_2, J but different components:

$$\left\{J(J+1) - J_1(J_1+1) - J_2(J_2+1) - 2m(M-m)\right\} \quad C(J_1, J_2, J; m, M-m, M) =$$

$$= \left\{(J_1-m+1)(J_1+m)(J_2+M-m+1)(J_2-M+m)\right\}^{1/2} C(J_1, J_2, J; m-1, M-m+1, M)$$

$$+ \left\{(J_1+m+1)(J_1-m)(J_2-M+m+1)(J_2+M-m)\right\}^{1/2} C(J_1, J_2, J; m+1, M-m-1, M) \qquad (20)$$

Recurrent relations especially useful for large ($J \sim 30$-40) angular momentum have been obtained by Schulten and Gordon[19] both for 3j and 6j symbols.

3.5. - Some special formulas

Formulas giving certain classes of vector coupling coefficients in algebraic form can be obtained specializing the general eqs. (5) and (6). Explicit formulas for coefficients with one of the angular momentum rank $J = 1, 2$ can be found in the celebrated book by Condon and Shortley[6]. As for semi-integer ranks, formulas for $J = 1/2$ are reported, e.g. by Rose[1] while formulas for $J = 3/2,\ 5/2$ are given by Saito and Morita[47]. Here we present a small collection of relations mainly chosen according to what we have found most useful.

$$C(J, J', 0; m, -m, 0) = (-)^{J-m}\, \delta_{JJ'}/(2J+1)^{1/2} \tag{21}$$

$$C(J_1, 0, J_2; m_1, m_2, m_1+m_2) = \delta_{J_1, J_2}\, \delta_{m_2, 0} \tag{22}$$

$$C(1, 1, 0; m, -m, 0) = (-)^{1-m}/3^{1/2} \tag{23}$$

$$C(1, 1, 1; m, -m, 0) = m/2^{1/2} \tag{24}$$

$$C(1, 1, 2; m, -m, 0) = (1/2)^{|m|}\,(2/3)^{1/2} \tag{25}$$

$$C(J, 1, J; 0, m, m) = -C(1, J, J; m, 0, m) = -m/2^{1/2}\ ; \qquad J > 0 \tag{26}$$

$$C(J, 1, J+1; 0, m, m) = C(1, J, J+1; m, 0, m) = \{(J+2)/(2(2J+1))\}^{1/2}; \quad m \neq 0 \tag{27}$$

$$C(J, 1, J-1; 0, m, m) = C(1, J, J-1; m, 0, m) = \{(J-1)/(2(2J+1))\}^{1/2}; \ J > 0,\ m \neq 0 \tag{28}$$

$$C(2, 2, 0; m, -m, 0) = (-)^m/5^{1/2} \tag{29}$$

$$C(2, 2, 2; m, -m, 0) = (-)^m C(2, 2, 2; 0, m, m) = (-)^m (m^2-2)/14^{1/2} \tag{30}$$

$$C(2, 2, 4; m, -m, 0) = 24/\{70^{1/2}(2+m)!\,(2-m)!\} \tag{31}$$

$$C(2, 2, J; 0, 0, 0) = (-12)^{J/2}\{(2J+1)(4-J)!\,/(5+J)!\}^{1/2}\ , \tag{32}$$

if $J = 0, 2, 4$ and zero otherwise

$$C(4,4,2; m,-m, 0) = (-)^m (5/9)^{1/2} C(4,2,4; m,0,m) = (-)^m (3m^2-20)/(693^{1/2}2) \tag{33}$$

$$C(J_1, 3, J; m, 0, m) = \left\{ \frac{5(J_1+m+3)(J_1+m+2)(J_1-m+3)(J_1-m+2)(J_1-m+1)(J_1+m+1)}{(J_1+2)(J_1+3)(2J_1+2)(2J_1+3)(2J_1+5)(2J_1+1)} \right\}^{1/2}; \tag{34}$$

if $J = J_1+3$

$$C(J_1,3,J;m_1,3,m) = \left\{ \frac{(J_1+m_1+6)(J_1+m_1+5)(J_1+m_1+4)(J_1+m_1+3)(J_1+m_1+2)(J_1+m_1+1)}{(2J_1+1)(2J_1+2)(2J_1+3)(2J_1+4)(2J_1+5)(2J_1+6)} \right\}^{1/2} ; \quad \text{if } J = J_1+3 \qquad (35)$$

Eqs. (34), (35) have been given, albeit incorrectly, in Ref. (48).

$$C(J_1,J_2,(J_1+J_2);m_1,m_2,m_1+m_2) = \left\{ \frac{(2J_1)!(2J_2)!(J_1+J_2+m_1+m_2)!(J_1+J_2-m_1-m_2)!}{(2J_1+2J_2)!(J_1+m_1)!(J_1-m_1)!(J_2+m_2)!(J_2-m_2)!} \right\}^{1/2} \qquad (36)$$

$$C(J_1,J_2,J_3;0\,0\,0) = \begin{cases} 0, & \text{if } J_1+J_2+J_3 \text{ is odd} \\ (-)^{(J_1+J_2+J_3)/2} \left\{ \dfrac{2J_3+1}{J_1+J_2+J_3+1} \right\}^{1/2} \dfrac{\Gamma(J_1+J_2+J_3)}{\Gamma(J_1+J_2-J_3)\Gamma(J_1-J_2+J_3)\Gamma(-J_1+J_2+J_3)} & \end{cases} \qquad (37)$$

where $\Gamma(x) = (x/2)!/(x!)^{1/2}$, if $J_1+J_2+J_3$ is an even integer.

3. 6. - Asymptotic results

A classical result due to Brussaard and Toloehk[49]:

$$C(J_1,J_2,J;m_1,m_2,m) \cong (-)^{J_1+J_2-J}\, d^{J_1}_{m_1,\,J-J_2}(\vartheta) ; \qquad (38)$$

where the small Wigner matrix d^J_{mn} is defined in (1) and $\cos\vartheta = m/J$; $J \gg 1$, $J_1 \ll J$ and of course $m = m_1+m_2$.

3. 7. - The coupling of Wigner rotation matrices

Wigner rotation matrices or generalized spherical harmonics $D^J_{mn}(\alpha\,\beta\,\gamma)$ represent matrix elements of the operator performing a coordinate system rotation of Euler angles $(\alpha\,\beta\,\gamma)$ in an angular momentum basis. Thus following Rose[1] convention

$$D^J_{mn}(\alpha\,\beta\,\gamma) = \langle Jm|\exp(-i\alpha J_z)\exp(-i\beta J_y)\exp(-i\gamma J_z)|Jn\rangle , \qquad (39)$$

where $0 \leqq \alpha \leqq 2\pi$, $0 \leqq \beta \leqq \pi$, $0 \leqq \gamma \leqq 2\pi$. The Wigner rotation matrices form an orthogonal basis set in the Euler angles space. As such they are often used for writing down expansions of anisotropic quantities in the molecular theories of crystals[14], liquid crystals[15] and polymers[13].

Clebsch-Gordan coefficients arise naturally when we want to rewrite a product of Wigner rotation matrices [1] of the same argument and of rank J_1, J_2 in terms of a single rotation matrix. The coupling rule for these matrices can be written as

$$D^{J_1}_{m_1 n_1}(\alpha\,\beta\,\gamma)\,D^{J_2}_{m_2 n_2}(\alpha\,\beta\,\gamma)$$

$$= \sum_J C(J_1, J_2, J; m_1, m_2, m)C(J_1, J_2, J; n_1, n_2, n)\,D^J_{m_1+m_2,\, n_1+n_2}(\alpha\,\beta\,\gamma) \qquad (40)$$

In particular, since spherical harmonics Y_{Jm} are just special cases of Wigner rotation matrices

$$D^J_{m0}(\alpha\,\beta\,0) = \left\{4\pi/(2J+1)\right\}^{1/2} Y_{Jm}(\alpha\,\beta)^*, \qquad (41)$$

we have the useful coupling relation for spherical harmonics,

$$Y_{J_1 m_1}(\alpha\,\beta)Y_{J_2 m_2}(\alpha\,\beta) = \sum_J \left\{(2J_1+1)(2J_2+1)/(4\pi(2J+1))\right\}^{1/2}$$

$$\times\ C(J_1, J_2, J; m_1, m_2, m)C(J_1, J_2, J; 0, 0, 0)Y_{Jm}(\alpha\,\beta) \qquad (42)$$

Remembering that $D^J_{00}(0\beta 0) = P_J(\cos\beta)$ we also find at once the coupling relation for the Legendre polynomials P_J i. e.

$$P_{J_1}(\cos\beta)\,P_{J_2}(\cos\beta) = \sum_J C(J_1, J_2, J; 0, 0, 0)^2\, P_J(\cos\beta) \qquad (43)$$

Notice that the coupling of even rank polynomials only gives even rank P_J since (cf. eq. (37)) the Clebsch-Gordan coefficient $C(J_1, J_2, J_3; 0, 0, 0)$ is zero unless $(J_1+J_2+J_3)$ is even.

Conversely we can decompose a Wigner rotation matrix as a linear combination of products of Wigner functions of lower rank,

$$D^J_{mn} = \sum C(J_1, J_2, J; m_1, m_2, m)\,C(J_1, J_2, J; n_1, n_2, n)D^{J_1}_{m_1 n_1}D^{J_2}_{m_2 n_2}\,\delta_{m_1+m_2,\,m}\,\delta_{n_1+n_2,\,n} \qquad (44)$$

$$= \sum C(J_1, J_2, J; m_1, m-m_1, m)C(J_1, J_2, J; n_1, n-n_1, n)D^{J_1}_{m_1 n_1}D^{J_2}_{m-m_1,\, n-n_1} \qquad (45)$$

where the sum is extended to all indices not appearing on the left hand side.

3. 8. - Irreducible tensors coupling

An irreducible tensor operator of rank J can be defined as a set of (2J+1) quantities $T^{J,m}$, $(m = -J, -J+1, \ldots, J)$ which transform under the (2J+1) dimensional representation of the full rotation group $O^+(3)$ as

$$(T^{J,m})_{MOL} = \sum_n D^{J*}_{mn}(M-L)(T^{J,n})_{LAB} \qquad (46)$$

where the LAB and MOL subscript refer to laboratory and rotated or "molecular" frame. The components $T^{J,m}$ of a rank J irreducible tensor verify the Racah[16] relations

$$J_z^x T^{J,m} = m T^{J,m} , \qquad (47)$$

$$J_\pm^x T^{J,m} = \left\{ (J\mp m)(J\pm m+1) \right\}^{1/2} T^{J,m\pm 1} , \qquad (48)$$

where the x superscript indicates the commutation superoperator: $A^x B = [A,B]$, while J_z, $J_\pm$ are the usual angular momentum projection operators. Eqs. (47), (48) can be written more concisely as

$$J_n^x T^{J,m} = (-)^n C(J,1,J;m+n,-n,m) \left\{ J(J+1) \right\}^{1/2} T^{J,m+n}; \quad n = 0, \pm 1 \qquad (49)$$

A tensor of rank J can be constructed from two tensors of rank J_1 and J_2 when they are coupled as follows:

$$T^{J,m}(A_1,A_2) = \sum_{m_1} C(J_1,J_2,J;m_1,m-m_1,m) T^{J_1,m_1}(A_1) T^{J_2,m-m_1}(A_2) \qquad (50)$$

where the symbols A_1 and A_2 represent all the variables upon which the tensors depend.

3.9. - Wigner-Eckart theorem

The calculation of matrix elements $<J_1 m_1 | T^{J,m} | J_2 m_2>$ of an irreducible tensor operator $T^{J,m}$ over an angular momentum basis set is simplified by the Wigner-Eckart theorem[1] according to which

$$<J_1 m_1 | T^{J,m} | J_2 m_2> = K_{J_1 J_2} C(J_2,J,J_1;m_2,m,m_1) \qquad (51)$$

where the quantity $K_{J_1 J_2}$, often written as $(J_1 || T^J || J_2)$, is called a reduced matrix element of the set of operator T^J and is independent on the angular momentum projection numbers. Notice that the Clebsch-Gordan coefficient implicity contains a δ_{m_2+m,m_1} which in turn guarantees conservation of angular momentum.

3.10. - Gaunt formula

This gives the integral of three Wigner rotation matrices as

$$\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin\beta \int_0^{2\pi} d\gamma\, D^{J_1}_{m_1 n_1}(\alpha\,\beta\,\gamma)\, D^{J_2}_{m_2 n_2}(\alpha\,\beta\,\gamma)\, D^{J_3}_{m_3 n_3}(\alpha\,\beta\,\gamma)^{*} =$$

$$= 8\pi^2\, \delta_{m_1+m_2,m_3}\, \delta_{n_1+n_2,n_3}\, C(J_1,J_2,J_3;m_1,m_2,m_3)C(J_1,J_2,J_3;n_1,n_2,n_3)/(2J_3+1). \quad (52)$$

4. - TABLES OF CLEBSCH-GORDAN COEFFICIENTS FOR INTEGER ANGULAR MOMENTUM J = 0÷6

Here we employ the notation

$$C(J_1, J_2, J_3; m_1, m_2, m_3) = R(N1/N2) \equiv \mathrm{sgn}(N1)\{(N1)/(N2)\}^{1/2}$$

where J_1, J_2, J_3 and N1, N2 are integers and the function sgn(M) gives the sign of its argument M. As mentioned before the results are also given for convenience in floating point form rounded to eight decimal places.

REFERENCES

(1) - M. E. Rose, Elementary Theory of Angular Momentum (Wiley, 1957).

(2) - A. R. Edmonds, Angular Momentum in Quantum Mechanics (Princeton University Press, 1957).

(3) - C. G. Gray, Can. J. Phys. 54, 505 (1976).

(4) - U. Fano and G. Racah, Irreducible Tensorial Sets (Academic Press, 1959).

(5) - D. M. Brink and G. R. Satchler, Angular Momentum (Oxford University Press, 1968).

(6) - E. U. Condon and G. H. Shortley, The Theory of Atomic Spectra (Cambridge University Press, 1935).

(7) - E. P. Wigner, Group Theory (Academic Press, 1959).

(8) - J. M. Blatt and V. F. Weisskopf, Theoretical Nuclear Physics (Wiley, 1952).

(9) - L. D. Landau and E. M. Lifschitz, Quantum Mechanics (Pergamon Press, 1959).

(10) - B. R. Judd, Operator Techniques in Atomic Spectroscopy (McGraw-Hill, 1963).

(11) - C. L. Biedenharn and H. Van Dam (Eds.), Quantum Theory of Angular Momentum (Academic Press, 1963); B. Silver, Irreducible Tensor Methods (Academic Press, 1976).

(12) - M. Weissbluth, Atoms and Molecules (Academic Press, 1978).

(13) - V. J. McBrierty, J. Chem. Phys. 57, 3287 (1972).

(14) - J. Jerphagnon, D. Chemla and R. Bonneville, Adv. in Phys. 27, 609 (1978).

(15) - G. R. Luckhurst and G. W. Gray (Eds.), The Molecular Physics of Liquid Crystals (Academic Press, 1979).

(16) - G. Racah, Phys. Rev. 62, 438 (1942).

(17) - Ya. A. Smorodinskii and L. A. Shelepin, Sov. Phys.-Uspekhi 15, 1 (1972).

(18) - A. P. Yutsis, I. B. Levinson and V. V. Vanagas, Mathematical Apparatus of the Theory of Angular Momentum (Israel Program for Scientific Translation, 1962).

(19) - K. Schulten and R. G. Gordon, J. Math. Phys. 16, 1961 (1975) (a); 16, 1971 (1975) (b).

(20) - M. Rotenberg, R. Bivins, N. Metropolis and J. K. Wooten Jr., The 3-j and 6-j Symbols (Technology Press MIT, 1959).

(21) - M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions (Dover, 1965).

(22) - C. Bricman et al., Rewiev of Particle Properties, Particle Data Group (CERN).

(23) - cf. for example CERN Library of computer programs and routines.

(24) - G. Rudnicki-Bujnowski, Comp. Phys. Comm. 10, 245 (1975).

(25) - A. D. Buckingham, Adv. Chem. Phys. 12, 107 (1967).

(26) - G. Gray and B. W. N. Lo, Chem. Phys. 14, 73 (1976).

(27) - R. P. Leavitt, J. Chem. Phys. 72, 3472 (1980).

(28) - D. L. Andrews and T. Thirunamachandran, J. Chem. Phys. 67, 5026 (1977).

(29) - B. L. Van der Waerden, Die Gruppentheoretische Methode in der Quantenmechanik (Springer, 1931).

(30) - B. L. Van der Waerden, Moderne Algebra (Springer, 1950).

(31) - S. F. Boys and R. S. Sahni, Phil. Trans. Roy. Soc. A246, 463 (1954).

(32) - K. Alder, Helv. Phys. Acta 25, 235 (1952).

(33) - H. A. Jahn, Proc. Roy. Soc. A205, 192 (1951) (a); H. A. Jahn and J. Hope, Phys. Rev. 93, 318 (1954) (b).

(34) - U. Fano, Report 1214, U. S. Nat. Bur. Standard (unpublished, 1951).

(35) - L. C. Biedenharn, Tables of the Racah Coefficients, Oak Ridge National Laboratory, Physics Division, ORNL-1098 (1952).

(36) - P. J. Redmond, Proc. Roy. Soc. A222, 84 (1954).

(37) - C. Eckart, Revs. Mod. Phys. 2, 305 (1930).

(38) - V. A. Fox, ZhETF (JETP) 10, 383 (1940) (in Russian).

(39) - A. Simon, Oak Ridge National Laboratory, ORNL-1718 (1954).

(40) - F. A. Matsen, Vector Spaces and Linear Algebra for Chemistry and Physics (Holt, Rinehart and Winston, 1970).

(41) - G. Ya. Lyubarskii, The Application of Group Theory in Physics (Pergamon Press, 1960).

(42) - B. I. Dunlap and B. R. Judd, J. Math. Phys. 16, 318 (1975).

(43) - E. O. Steinborn and E. Filter, Theor. Ch. Acta 38, 247 (1975).

(44) - A. M. Din, Lett. Math. Phys. 5, 207 (1981).

(45) - R. Askey, Lett. Math. Phys. 6, 299 (1982).

(46) - J. D. Morgan III, J. Phys. A: Math. Gen. 10, 1059 (1977).

(47) - R. Saito and M. Morita, Prog. Theor. Phys. 13, 540 (1955).

(48) - G. J. Davies and M. Evans, J. Chem. Soc. Farad. II, 71, 1291 (1975).

(49) - P. J. Brussaard and H. A. Tolhoek, Physica 23, 955 (1957).