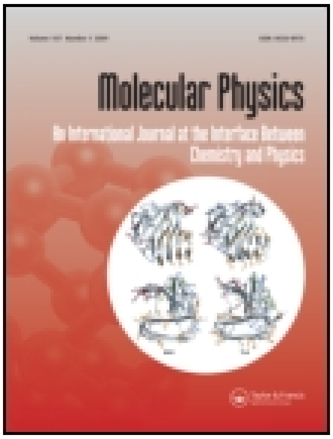

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Some investigations in the theory of open-shell ions

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Some investigations in the theory of open-shell ions
Part II. *V, W* and *X* coefficients

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V, W, and X coefficients analogous to Racah's $\bar{V}$, $\bar{W}$ and $\bar{X}$ coefficients and Wigner's $3j$, $6j$ and $9j$ symbols are defined for certain finite groups and their properties examined. Tables of values of these coefficients are given for the one-valued representations of the octahedral group.

1. Introduction

In the theory of angular momenta the Wigner coefficients $\langle j_1 j_2 j_3 m_3 | j_1 j_2 m_1 m_2 \rangle$ are known to possess symmetry with respect to the interchange of any pair of the three momenta $\mathbf{j}_1$, $\mathbf{j}_2$ and $\mathbf{j}_3$. This symmetry is made particularly obvious by the expression of the Wigner coefficients in terms of certain 'reduced' quantities, the Wigner $3j$ symbols or Racah $\bar{V}$ coefficients. Like the $\langle j_1 j_2 j_3 m_3 | j_1 j_2 m_1 m_2 \rangle$, these give the numerical details of the reduction to irreducible components of the direct product of two irreducible representations of the unitary unimodular group U_2. Alternatively, and more significantly, they show the way in which the unit representation occurs in the decomposition of the direct product of three irreducible representations.

Because of their relationship to the unit representation, the $\bar{V}$ coefficients may be regarded as three-suffix tensors. We can think of such a unit representation as an invariant which is the inner product of a $\bar{V}$ tensor with three 'vectors' $|j_1 m_1\rangle$, $|j_2 m_2\rangle$ and $|j_3 m_3\rangle$. From this point of view it is natural to consider invariants constructed solely from the $\bar{V}$. The two simplest non-trivial invariants of this kind are the $\bar{W}$ and $\bar{X}$ coefficients ($6j$ and $9j$ symbols respectively). They prove to be extremely useful for two main reasons. First, most matrix elements of interest in systems containing coupled angular momenta can be expressed very simply in terms of them and the $\bar{V}$. Secondly, although they are related to recoupling matrix elements and satisfy similar equations they have the great advantage of being highly symmetrical with respect to permutation of their constituent j symbols.

The preceding description is phrased so as to suggest that analogous quantities might be defined for finite groups and their properties usefully investigated. This is done in the present paper, chiefly for the octahedral group, although the V coefficients in § 2 are defined with somewhat greater generality. Before doing this I will expose the two essential facts upon which our analysis is founded. First, for the (one-valued) representations of the octahedral group as for those of U_2, the direct product of any three irreducible representations contains the unit representation at most once. Secondly it is possible to choose the phases of the coupling coefficients in such a way that the V coefficients have a highly symmetric and simple behaviour under permutation of their constituent representation symbols.

The theoretical scheme I develop in this paper is, then, largely a straightforward adaptation to the theory of ions with finite symmetry groups of a theory which has already proved itself for systems with spherical symmetry. The general equations satisfied by the V, W and X are consequently similar in form to those satisfied by Racah's coefficients and their proofs are similar. Consequently I do not give most of the proofs in detail here but merely sketch their methods. I recommend the reader who has any difficulty to read the first half of *Irreducible Tensorial Sets* by Fano and Racah ([1], henceforward referred to as FR), although in my proofs I depend much less heavily on the properties of recoupling transformations.

2. Definition of V coefficients

With application to the one-valued representations of the octahedral group O, of D_4 and of D_3 especially in mind we assume that we have three irreducible representations a, b and c such that each is equivalent to a real representation and ab contains c just once. Then we choose bases $|a\alpha\rangle$, $|b\beta\rangle$ and $|c\gamma\rangle$ which are real, write the product $|a\alpha\rangle\ |b\beta\rangle\ |c\gamma\rangle = |a\alpha, b\beta, c\gamma\rangle$ and suppose a, b, c to refer respectively to independent parts (or particles) of the system. We also make a definite choice for the matrices of each irreducible representation a and require that any set of kets, $|a\alpha\rangle$ say, spanning a shall span it according to our choice rather than to an equivalent one. We can then define coupling coefficients and take them all to be real. Finally if i is the unit representation we define always

$$\langle aai\iota|aa\alpha\alpha'\rangle = \delta_{\alpha\alpha'}\lambda(a)^{-1/2},$$
$$\langle iaa\alpha|ia\iota\alpha'\rangle = \langle aia\alpha|ai\alpha'\iota\rangle = \delta_{\alpha\alpha'}, \tag{1}$$

where $\lambda(a)$ is the degree of the representation a. The symmetric expression for $\langle aai\iota|aa\alpha\alpha'\rangle$ is a consequence of our assumption that a is equivalent to a real representation (see Frobenius and Schur [2]).

By hypothesis ab contains c once and therefore, apart from a numerical factor, there is just one linear combination of the products $|a\alpha, b\beta, c\gamma\rangle$ which is an invariant for the group, i.e. which forms a basis for the unit representation. In no matter what order we couple the kets $|a\alpha\rangle$, $|b\beta\rangle$ and $|c\gamma\rangle$ to form an invariant, that invariant is always the same apart perhaps from a numerical factor. Let us couple a to b first and then to c to give

$$|ab, c\rangle = \sum_{\alpha\beta\gamma}\lambda(c)^{-1/2}\langle ab\alpha\beta|abc\gamma\rangle|a\alpha, b\beta, c\gamma\rangle, \tag{2}$$

where we have used (1). It follows immediately that $|ab, c\rangle$ satisfies $\langle ab, c|ab, c\rangle = 1$. As the coupling coefficients are real we must therefore have, for a', b', c' any permutation of a, b, c, $|a'b', c'\rangle = \pm|ab, c\rangle$. Hence if we define

$$V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} = \lambda(c)^{-1/2}\langle ab\alpha\beta|abc\gamma\rangle, \tag{3}$$

then V is real and can at most have its sign changed by any permutation of its columns. For fixed a, b, c the sign change is independent of α, β and γ. The coupling coefficients $\langle ab\alpha\beta|abc\gamma\rangle$ are only partly determined by the constituent representations. For each distinct ordered trio abc there is an arbitrary phase factor common to all the coefficients and the factors for different ordered trios can be chosen entirely independently of one another. Similar remarks therefore apply to the V symbols.

We now define the phases of the coupling coefficients so as to exhibit the natural symmetry of V as clearly as possible. Three cases arise according to the extent to which the representations in V are the same. First if a, b and c are all different then each V is a multiple of a different coupling coefficient so we can choose the phases so that V is invariant to all permutations of its columns. However, we can also choose the phases so that V is multiplied by the parity of a permutation and it is sometimes advantageous to adopt this apparently perverse choice.

Next let $a=b\neq c$. Then c must belong either to the symmetrized square $[a^2]$ or the antisymmetrized square (a^2) of a. So

$$V\begin{pmatrix} a & a & c \\ \beta & \alpha & \gamma \end{pmatrix} = \epsilon V\begin{pmatrix} a & a & c \\ \alpha & \beta & \gamma \end{pmatrix}$$

where $\epsilon=+1$ if c belongs to $[a^2]$ and -1 otherwise. We now define the phases of the coupling of ac to a and ca to a so that

$$V\begin{pmatrix} c & a & a \\ \gamma & \beta & \alpha \end{pmatrix} = \epsilon V\begin{pmatrix} a & a & c \\ \alpha & \beta & \gamma \end{pmatrix} = \epsilon V\begin{pmatrix} a & c & a \\ \beta & \gamma & \alpha \end{pmatrix}.$$

It then easily follows that V is invariant to all permutations P of its columns when $\epsilon=+1$ and is multiplied by the parity of P when $\epsilon=-1$.

Lastly suppose $a=b=c$ and that the sets of kets $|a\alpha\rangle$, $|a\beta\rangle$, $|a\gamma\rangle$ are identical. Then a permutation P of α, β and γ must multiply $|aa,a\rangle$ by ± 1. Hence $|aa,a\rangle$ is a basis for a representation of degree one of the symmetric group S_3. So it is either the unit or the alternating representation. Therefore V is either invariant to permutations P of its columns or multiplied by the parity of P, this behaviour depending on a but being independent of α, β and γ.

We have given V the required high degree of symmetry. The associative property of Racah's $\bar{V}$ (FR, equation (10.4)) reads $|ab,c\rangle=|bc,a\rangle$ in our notation and is true because V is always invariant to even permutation of its columns. The fact that the definition (3) of V does not contain any minus signs while the definition of $\bar{V}$ does so even for j integral is simply a consequence of our assumption that our representations are actually real and not merely equivalent to real ones.

For the groups D_3, D_4 and O the change of sign of V under odd permutations necessarily occurs for each group for A_2E^2 and for O also for $T_1{}^3$ and $T_1T_2{}^2$. For O we also define it to happen for ET_1T_2. This enables us to give a simple explicit formula for the effect of an odd permutation on V for each of these groups.

$$V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix}$$

is multiplied by $(-1)^{a+b+c}$, where we interpret a representation symbol, a say, as 0 in this context unless $a=A_2$ or T_1 when we interpret it as 1. For example $(-1)^{A_2}=-1$, but $(-1)^{T_2}=+1$. Clearly $(-1)^{2a}=1$ always. One should note that the high symmetry we have assumed for V is inconsistent with the universal rule

$$\langle abc\gamma|ab\alpha\beta\rangle=\langle bac\gamma|ba\beta\alpha\rangle$$

for $a\neq b$, just as for Wigner coefficients in U_2.

For example we must have

$$\langle A_2EE\theta|A_2Ea\epsilon\rangle = -\langle EA_2E\theta|EA_2\epsilon a\rangle$$

for O (see table 1).

The V satisfy the relations

$$\left.\begin{aligned}\sum_{\alpha\beta} V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} V\begin{pmatrix} a & b & c' \\ \alpha & \beta & \gamma' \end{pmatrix} &= \lambda(c)^{-1}\delta_{cc'}\delta_{\gamma\gamma'}\delta(a,b,c), \\ \sum_{c\gamma} \lambda(c) V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} V\begin{pmatrix} a & b & c \\ \alpha' & \beta' & \gamma \end{pmatrix} &= \delta_{\alpha\alpha'}\delta_{\beta\beta'},\end{aligned}\right\} \tag{4}$$

where $\delta(a,b,c)=1$ when abc contains the unit representation and $\delta(a,b,c)=0$ otherwise. $\lambda(c)$ is the degree of the representation c and corresponds to the quantity $2j+1$ in the theory of angular momenta. Equations (4) follow immediately from the orthonormality properties of the coupling coefficients (compare FR, equations (10.17) and (10.18)). $V=0$ when c is not contained in ab. Summation of the first equation of (4) over γ yields the equation

$$\sum_{\alpha\beta\gamma} V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix}^2 = \delta(a,b,c). \tag{5}$$

When c is the unit representation i we deduce from (1) that

$$V\begin{pmatrix} a & b & i \\ \alpha & \beta & \iota \end{pmatrix} = \delta_{ab}\delta_{\alpha\beta}\lambda(a)^{-1/2}. \tag{6}$$

Another equation which is sometimes useful is obtained by putting $c'=i$ in the first of equations (4) and is

$$\sum_{\alpha} V\begin{pmatrix} a & a & c \\ \alpha & \alpha & \gamma \end{pmatrix} = \lambda(a)^{1/2}\delta_{ci}. \tag{7}$$

Thus far we have described properties of the V which exactly parallel those of Racah's $\bar{V}$. As well as these the V possess further symmetry and of a kind quite different from that discussed earlier. Suppose a group possesses a representation of degree one (assumed real) distinct from the unit representation and let a function η be a basis for it. For example A_2 is such a representation for the octahedral group. Then η^2 is a basis for the unit representation and

$$|a'\alpha'\rangle = \eta|a\alpha\rangle = |\eta a\alpha\rangle,$$

say, is a basis for an irreducible representation a' which may or may not be the same as a. The components, classified by α', are not necessarily in accord with the standard choice for components of a'. If $a=a'$ it may not be possible to choose them so. We now show that V symbols for abc are simply related to those for $a'b'c$, $ab'c'$ and $a'bc'$.

Multiply the invariant $|ab,c\rangle$ of equation (2) through by η^2 to give

$$\begin{aligned}|ab,c\rangle' &= \sum_{\alpha\beta\gamma} V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix}|\eta a\alpha, \eta b\beta, c\gamma\rangle \\ &= \sum_{\alpha'\beta'\gamma} V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix}|a'\alpha', b'\beta', c\gamma\rangle.\end{aligned}$$

So $|ab,c\rangle'$ is, apart perhaps from sign, the invariant corresponding to $a'b'$ coupled with c. Therefore

$$V\begin{pmatrix} a' & b' & c \\ \alpha' & \beta' & \gamma \end{pmatrix} = \omega V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix},$$

where $\omega = \pm 1$ is independent of α, β and γ but may depend on the ordered set (a, b, c). An equation of analogous form holds if we incorporate η not with ab but with either ac or bc. It is convenient to write

$$V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix}'_{\mu\nu}$$

to indicate that the μth and νth columns have been 'dashed'. Generalizing the last equation we have

$$V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix}'_{\mu\nu} = \omega(abc)_{\mu\nu} V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix}. \tag{8}$$

Because the V coefficients are invariant to even permutations of their columns it follows that $\omega(abc)_{\mu\nu}$ is invariant to even permutations applied simultaneously to a, b, c and to $\mu\nu$, i.e. for example

$$\omega(abc)_{12} = \omega(bca)_{13}.$$

The order of μ and ν is irrelevant.

We now pass from this somewhat formal and abstract discussion to consider the octahedral group O. Here A_2 is the unique non-trivial representation of degree one and $A_1' = A_2$, $E' = E$, $T_1' = T_2$. Of course $a'' = a$ always. For the group O the relation $a \to a'$ is the same, via the isomorphism with the permutation group S_4, as the well-known passage between associated representations obtained by reflecting the Young tableau corresponding to the representation in its main diagonal.

We can define our components so that $|T_1'M'\rangle = |T_2M\rangle$, $|T_2'M'\rangle = |T_1M\rangle$ and of course $|A_1'a'\rangle = |A_2a\rangle$ and $|A_2'a'\rangle = |A_1a\rangle$. However, for the self-associated representation E we must make a choice such as $\theta' = \epsilon$, $\epsilon' = -\theta$ (θ, ϵ transform as d_{z^2}, $d_{x^2-y^2}$ respectively.) We make the obvious definition here that

$$V\begin{pmatrix} E & b & c \\ -\theta & \beta & \gamma \end{pmatrix} = -V\begin{pmatrix} E & b & c \\ \theta & \beta & \gamma \end{pmatrix}; \text{ etc.}$$

Consider for example $a = b = c = E$. There are four non-zero V which we take as

$$V\begin{pmatrix} E & E & E \\ \theta & \epsilon & \epsilon \end{pmatrix} = V\begin{pmatrix} E & E & E \\ \epsilon & \theta & \epsilon \end{pmatrix} = V\begin{pmatrix} E & E & E \\ \epsilon & \epsilon & \theta \end{pmatrix} = -V\begin{pmatrix} E & E & E \\ \theta & \theta & \theta \end{pmatrix} = \tfrac{1}{2}. \tag{9}$$

Then replacing the first two columns of V we find

$$\tfrac{1}{2} = V\begin{pmatrix} E & E & E \\ \theta & \epsilon & \epsilon \end{pmatrix} = \omega V\begin{pmatrix} E & E & E \\ \theta' & \epsilon' & \epsilon \end{pmatrix} = -\omega V\begin{pmatrix} E & E & E \\ \epsilon & \theta & \epsilon \end{pmatrix} = -\tfrac{1}{2}\omega$$

and so $\omega = -1$. Therefore we have also

$$V\begin{pmatrix} E & E & E \\ \theta & \theta & \theta \end{pmatrix} = -V\begin{pmatrix} E & E & E \\ \theta' & \theta' & \theta \end{pmatrix} = -V\begin{pmatrix} E & E & E \\ \epsilon & \epsilon & \theta \end{pmatrix}$$

agreeing with equation (9). In this case $\omega = -1$ for replacement of either of the other pairs of columns also. On the other hand for V symbols involving only the representations A_1, A_2, T_1 and T_2 we can insist that $|ab, c\rangle'$ is identical in form with $|ab, c\rangle$ and then have the simpler relations

$$V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix}'_{\mu\nu} = V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix}. \tag{10}$$

We conclude this section by tabulating a set of values of V and ω. For the rest of the paper only the octahedral group O without inversion is explicitly treated. The inclusion of inversion is, of course, trivial. First, then, the V.

Taking the components of T_1 to transform as x, y and z we obtain the useful formulae

$$\left.\begin{aligned} V\begin{pmatrix} T_1 & T_1 & T_1 \\ \alpha & \beta & \gamma \end{pmatrix} = V\begin{pmatrix} T_2 & T_2 & T_1 \\ \alpha & \beta & \gamma \end{pmatrix} = -\frac{1}{\sqrt{6}}\epsilon_{\alpha\beta\gamma}, \\ V\begin{pmatrix} T_1 & T_1 & T_2 \\ \alpha & \beta & \gamma \end{pmatrix} = V\begin{pmatrix} T_2 & T_2 & T_2 \\ \alpha & \beta & \gamma \end{pmatrix} = -\frac{1}{\sqrt{6}}|\epsilon_{\alpha\beta\gamma}|, \end{aligned}\right\} \tag{11}$$

where $\epsilon_{\alpha\beta\gamma} = \pm 1$ or 0 is the usual alternating tensor in three variables. Note that the components of T_2 are also labelled x, y and z not, as previously, ξ, η and ζ. The V which are not included in equations (6) and (11) are given in table 1. $\omega(abc)_{\mu\nu} = 1$ unless at least one of a, b, c is E. Remembering the invariance to even permutations, table 2 gives a sufficient collection of values of ω.

A_2EE

$\alpha\beta \backslash \gamma$	θ	ϵ
$a\theta$	0	$1/\sqrt{2}$
$a\epsilon$	$-1/\sqrt{2}$	0

EEE

$\alpha\beta \backslash \gamma$	θ	ϵ
$\theta\theta$	$-\frac{1}{2}$	0
$\theta\epsilon$	0	$\frac{1}{2}$
$\epsilon\theta$	0	$\frac{1}{2}$
$\epsilon\epsilon$	$\frac{1}{2}$	0

$A_2T_1T_2$

	x	y	z
ax	$1/\sqrt{3}$	.	.
ay	.	$1/\sqrt{3}$	.
az	.	.	$1/\sqrt{3}$

T_2ET_1

	x	y	z
$x\theta$	$-\frac{1}{2}$	.	.
$y\theta$	.	$\frac{1}{2}$	.
$z\theta$	.	.	.
$x\epsilon$	$-1/2\sqrt{3}$	.	.
$y\epsilon$	.	$-1/2\sqrt{3}$	.
$z\epsilon$	.	.	$1/\sqrt{3}$

T_1ET_1

	x	y	z
$x\theta$	$1/2\sqrt{3}$	.	.
$y\theta$	.	$1/2\sqrt{3}$	.
$z\theta$	.	.	$-1/\sqrt{3}$
$x\epsilon$	$-\frac{1}{2}$	.	.
$y\epsilon$	.	$\frac{1}{2}$	.
$z\epsilon$	.	.	.

Table 1. Values of $V\begin{pmatrix} abc \\ \alpha\beta\gamma \end{pmatrix}$. For those containing three T representations see equation (11).

a b c	ij 12	13	23
E E A_2	1	1	-1
E A_2 E	-1	1	1
A_2 E E	1	-1	1
E E E	-1	-1	-1
E T_1 T_1	1	-1	1
E T_1 T_2	1	1	-1
E T_2 T_1	-1	-1	-1
E T_2 T_2	-1	1	1

Table 2. Values of $\omega(abc)_{ij}$.

3. W COEFFICIENTS

The W coefficients are defined by the formula

$$W\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix} = \sum_{\alpha\beta\gamma\delta\epsilon\phi} V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} V\begin{pmatrix} a & e & f \\ \alpha & \epsilon & \phi \end{pmatrix} V\begin{pmatrix} b & f & d \\ \beta & \phi & \delta \end{pmatrix} V\begin{pmatrix} c & d & e \\ \gamma & \delta & \epsilon \end{pmatrix}. \tag{12}$$

Strictly W should be defined so as to be invariant in form with respect to orthonormal transformations of the basic kets $|a\alpha\rangle$, etc., in analogy with equation (11.6) of FR for $\bar{W}$. This can easily be done but W is then a more complicated expression and, as we shall not consider such orthonormal transformations, we use the simpler formula (12).

It follows immediately from (12) that W is invariant both to even permutations of its columns and to turning any pair of columns upside down. For example

$$W\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix} = W\begin{pmatrix} b & c & a \\ e & f & d \end{pmatrix} = W\begin{pmatrix} d & b & f \\ a & e & c \end{pmatrix},$$

etc. Next, W is multiplied by $(-1)^{2(a+b+c+d+e+f)} = 1$, i.e. is also invariant, on odd permutation of its columns. These symmetry operations are all well-known for $\bar{W}$.

The other symmetry operations for W are the 'dashing' of any of the four trios (def), (dbc), (eca), (fab) or the three quartets $(abde)$, $(bcef)$, $(acdf)$. Each such operation multiplies W by ± 1 and those W which do not involve an E representation are left invariant. Thus

$$W\begin{pmatrix} T_1 & T_1 & T_1 \\ T_1 & T_1 & T_1 \end{pmatrix} = W\begin{pmatrix} T_1 & T_2 & T_2 \\ T_1 & T_2 & T_2 \end{pmatrix} = W\begin{pmatrix} T_1 & T_1 & T_1 \\ T_2 & T_2 & T_2 \end{pmatrix}.$$

When an E is present we use the values of ω in table 2 to deduce the relation between W and W'. For example

$$W\begin{pmatrix} E & T_2 & T_1 \\ T_2 & T_1 & T_1 \end{pmatrix} = \omega(ET_2T_1)_{12}\,\omega(ET_1T_1)_{12}\,W\begin{pmatrix} E & T_1 & T_1 \\ T_1 & T_2 & T_1 \end{pmatrix}$$
$$= -W\begin{pmatrix} E & T_1 & T_1 \\ T_1 & T_2 & T_1 \end{pmatrix},$$

where we simply multiply together those ω which involve an E. The minus sign in the relation $\epsilon' = -\theta$ causes no difficulty because when it occurs in (12) it always appears twice and hence cancels out.

When one of the symbols in W is the unit representation it is easy to show that

$$W\begin{pmatrix} a & b & A_1 \\ d & e & f \end{pmatrix} = (-1)^{a+d+f}\lambda(a)^{-1/2}\lambda(d)^{-1/2}\delta_{ab}\delta_{de}\delta(a,d,f). \tag{13}$$

Next, using the relation

$$\sum_{\alpha} \epsilon_{\alpha\beta\gamma}\epsilon_{\alpha\epsilon\phi} = \delta_{\beta\epsilon}\delta_{\gamma\phi} - \delta_{\beta\phi}\delta_{\gamma\epsilon}, \tag{14}$$

for the alternating tensor (do not confuse the two kinds of ϵ), we deduce from (11) that

$$W\begin{pmatrix} T_1 & T_1 & T_1 \\ h & T_1 & T_1 \end{pmatrix} = \tfrac{1}{6}\sum_{\beta\gamma\epsilon\phi\theta}(\delta_{\beta\epsilon}\delta_{\gamma\phi} - \delta_{\beta\phi}\delta_{\gamma\epsilon}) V\begin{pmatrix} T_1 & T_1 & h \\ \beta & \phi & \theta \end{pmatrix} V\begin{pmatrix} T_1 & h & T_1 \\ \gamma & \theta & \epsilon \end{pmatrix}$$
$$= \tfrac{1}{6}\sum_{\beta\gamma\theta} V\begin{pmatrix} T_1 & T_1 & h \\ \beta & \gamma & \theta \end{pmatrix}^2 - \tfrac{1}{6}\sum_{\beta\gamma\theta} V\begin{pmatrix} T_1 & T_1 & h \\ \beta & \beta & \theta \end{pmatrix} V\begin{pmatrix} T_1 & T_1 & h \\ \gamma & \gamma & \theta \end{pmatrix}$$
$$= \tfrac{1}{6} - \tfrac{1}{2}\delta_{hA_1}, \tag{15}$$

where we used (5) and (7), except for $h=A_2$ when $W=0$. Apart from the W given by formulae (13) and (15) there are only eight other genuinely distinct ones except those which are zero because of $\delta(a,b,c)\delta(a,e,f)d(b,f,d)\delta(c,d,e)=0$. All others can be turned into one of these by the symmetry operations described earlier for the W. These eight and a few other useful values are given in table 3.

$$W\begin{pmatrix} E & E & E \\ E & E & A_2 \end{pmatrix}=W\begin{pmatrix} E & E & A_2 \\ E & E & A_2 \end{pmatrix}=\frac{1}{2}, \quad W\begin{pmatrix} E & E & E \\ E & E & E \end{pmatrix}=0, \quad W\begin{pmatrix} E & E & A_2 \\ T_1 & T_2 & T_1 \end{pmatrix}=-\frac{1}{\sqrt{6}},$$
$$W\begin{pmatrix} E & E & E \\ T_1 & T_1 & T_1 \end{pmatrix}=W\begin{pmatrix} E & E & E \\ T_1 & T_1 & T_2 \end{pmatrix}=-W\begin{pmatrix} E & T_2 & T_1 \\ T_1 & T_1 & T_1 \end{pmatrix}=\frac{1}{2\sqrt{3}}, \quad W\begin{pmatrix} E & T_2 & T_1 \\ E & T_1 & T_1 \end{pmatrix}=0,$$
$$W\begin{pmatrix} E & T_1 & T_1 \\ E & T_1 & T_1 \end{pmatrix}=\frac{1}{3}, \quad W\begin{pmatrix} E & T_1 & T_1 \\ T_1 & T_1 & T_1 \end{pmatrix}=W\begin{pmatrix} E & T_2 & T_1 \\ T_2 & T_2 & T_1 \end{pmatrix}=-W\begin{pmatrix} E & T_1 & T_1 \\ T_2 & T_1 & T_1 \end{pmatrix}$$
$$=-W\begin{pmatrix} E & T_2 & T_1 \\ T_1 & T_2 & T_1 \end{pmatrix}=\frac{1}{6}.$$

Table 3. Values of $W\begin{pmatrix} a\,b\,c \\ d\,e\,f \end{pmatrix}$. All W with six T representations equal $\frac{1}{6}$.

There are a number of important equations satisfied by V and W. We lead into these by considering the relationship between the matrix element

$$\langle e,fb(d)c\gamma|ef(a),bc'\gamma'\rangle$$

representing the recoupling of the three representations e, f and b. For group-theoretic reasons it has a factor $\delta_{cc'}\delta_{\gamma\gamma'}$ and is independent of γ. Expansion in terms of the V coefficients then gives the two relations

$$\langle e,fb(d)c\gamma|ef(a),bc\gamma\rangle=\lambda(a)^{1/2}\lambda(d)^{1/2}(-1)^{b+c+e+f}W\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix}, \tag{16}$$

$$\sum_{\alpha\beta\delta\epsilon\phi} V\begin{pmatrix} a & b & c' \\ \alpha & \beta & \gamma' \end{pmatrix}V\begin{pmatrix} a & e & f \\ \alpha & \epsilon & \phi \end{pmatrix}V\begin{pmatrix} b & f & d \\ \beta & \phi & \delta \end{pmatrix}V\begin{pmatrix} c & d & e \\ \gamma & \delta & \epsilon \end{pmatrix}=\lambda(c)^{-1}\delta_{cc'}\delta_{\gamma\gamma'}W\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix}. \tag{17}$$

From (17), using equations (4), we can deduce a series of other equations. Multiply through by

$$\lambda(c')V\begin{pmatrix} a & b & c' \\ \alpha' & \beta' & \gamma' \end{pmatrix}$$

and sum over c' and γ'. Dropping the dashes on α and β this yields

$$\sum_{\delta\epsilon\phi} V\begin{pmatrix} a & e & f \\ \alpha & \epsilon & \phi \end{pmatrix} V\begin{pmatrix} b & f & d \\ \beta & \phi & \delta \end{pmatrix} V\begin{pmatrix} c & d & e \\ \gamma & \delta & \epsilon \end{pmatrix}=W\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix} V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix}.$$

Using equations (4) we then obtain successively

$$\sum_{\phi} V\begin{pmatrix} a & e & f \\ \alpha & \epsilon & \phi \end{pmatrix} V\begin{pmatrix} b & f & d \\ \beta & \phi & \delta \end{pmatrix}=\sum_{c\gamma}\lambda(c)W\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix} V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} V\begin{pmatrix} c & d & e \\ \gamma & \delta & \epsilon \end{pmatrix}, \tag{19}$$

$$\delta_{fg}\lambda(f)^{-1}\delta(a,e,f)V\begin{pmatrix} b & g & d \\ \beta & \eta & \delta \end{pmatrix}=\sum_{c\gamma\alpha\epsilon}\lambda(c)W\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix} V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} V\begin{pmatrix} c & d & e \\ \gamma & \delta & \epsilon \end{pmatrix} V\begin{pmatrix} a & e & g \\ \alpha & \epsilon & \eta \end{pmatrix}, \tag{20}$$

$$\sum_{c}\lambda(c)W\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix}W\begin{pmatrix} a & b & c \\ d & e & g \end{pmatrix}=\lambda(f)^{-1}\delta_{fg}\delta(a,e,f)\delta(b,d,f). \tag{21}$$

As well as (21) there are other equations satisfied by the W alone which may sometimes be useful. From its connection with recoupling transformations

(FR, p. 57) the first may be called the associative law. We prove it as follows:

$$\sum_c(-1)^c\lambda(c)W\begin{pmatrix}a&b&c\\d&e&f\end{pmatrix}W\begin{pmatrix}a&b&c\\e&d&g\end{pmatrix}$$

$$=\sum_{c\alpha\beta\gamma}(-1)^c\lambda(c)W\begin{pmatrix}a&b&c\\d&e&f\end{pmatrix}V\begin{pmatrix}a&b&c\\\alpha&\beta&\gamma\end{pmatrix}W\begin{pmatrix}a&b&c\\e&d&g\end{pmatrix}V\begin{pmatrix}a&b&c\\\alpha&\beta&\gamma\end{pmatrix}$$

$$=(-1)^{f+g}W\begin{pmatrix}a&d&g\\b&e&f\end{pmatrix}, \tag{22}$$

using equation (18). On putting $g=A_1$ we obtain the useful result

$$\sum_c\lambda(c)W\begin{pmatrix}a&b&c\\a&b&f\end{pmatrix}=\delta(a,b,f). \tag{23}$$

Our final equation is the analogy in our theory of an equation for the $\bar{W}$ obtained by Biedenharn and Elliott (FR, p. 159). It can be proved in very similar way to the associative law, using first (4) then successively (18) twice, (19) once, (18) twice and finally (4) again giving

$$(-1)^{a+b+c+d+e+f+\bar{d}+\bar{e}+\bar{f}}W\begin{pmatrix}a&b&c\\d&e&f\end{pmatrix}W\begin{pmatrix}a&b&c\\\bar{d}&\bar{e}&\bar{f}\end{pmatrix}$$

$$=\sum_g(-1)^g\lambda(g)W\begin{pmatrix}g&\bar{e}&e\\a&f&\bar{f}\end{pmatrix}W\begin{pmatrix}g&\bar{f}&f\\b&d&\bar{d}\end{pmatrix}W\begin{pmatrix}g&\bar{d}&d\\c&e&\bar{e}\end{pmatrix}. \tag{24}$$

4. X COEFFICIENTS

The X coefficients are defined by the formula

$$X\begin{bmatrix}a&b&c\\d&e&f\\g&h&k\end{bmatrix}=\sum_{\alpha\beta\gamma\delta\epsilon\phi\eta\theta\kappa}V\begin{pmatrix}a&b&c\\\alpha&\beta&\gamma\end{pmatrix}V\begin{pmatrix}d&e&f\\\delta&\epsilon&\phi\end{pmatrix}V\begin{pmatrix}g&h&k\\\eta&\theta&\kappa\end{pmatrix}$$

$$V\begin{pmatrix}a&d&g\\\alpha&\delta&\eta\end{pmatrix}V\begin{pmatrix}b&e&h\\\beta&\epsilon&\theta\end{pmatrix}V\begin{pmatrix}c&f&k\\\gamma&\phi&\kappa\end{pmatrix}. \tag{25}$$

It follows from (25) that X is invariant to transposition, i.e. reflection in its main diagonal, and to even permutation of rows or columns. Odd permutations of the rows or columns multiply it by $(-1)^{a+b+c+d+e+f+g+h+k}$. Evidently X has some similarity with a 3×3 determinant and we see, for example, that

$$X\begin{bmatrix}T_1T_1T_1\\T_1T_1T_1\\T_1T_1T_1\end{bmatrix}=0$$

because of this. Quite a number of X can be shown to be zero by the same sort of elementary argument which shows certain determinants to be zero. All the X in table 4 (a) may be evaluated by such procedures supplemented, on occasion, by the dashing operation. This latter symmetry operation on X involves dashing the four symbols which represent the intersections of any pair of rows with any pair of columns or any six symbols which are such that the remaining three lie one in each row and one in each column. As with W, we have $X'=X$ when X contains no E and $X'=\pm X$ otherwise with $\pm$ the product of the relevant ω values. For example

$$X\begin{bmatrix}A_2E\ E\\E\ A_2E\\E\ E\ A_2\end{bmatrix}=X\begin{bmatrix}A_2E\ E\\E\ A_1E\\E\ E\ A_1\end{bmatrix}$$

because

$$\{\omega(EA_2E)_{23}\omega(EEA_2)_{23}\}^2=1.$$

When one of the symbols in X, say k, is A_1, equation (25) simplifies to give

$$X\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & A_1 \end{bmatrix} = \lambda(c)^{-1/2}\lambda(g)^{-1/2}\delta_{cf}\delta_{gh}(-1)^{b+d+f+h}W\begin{pmatrix} a & b & c \\ e & d & g \end{pmatrix}. \qquad (26)$$

Equation (26) together with the dashing operation means that we can easily obtain the value of any X which contains at least one A_1 or A_2 representation. Another special case, analogous to equation (15), is

$$X\begin{bmatrix} a & b & T_1 \\ d & e & T_1 \\ T_1 & T_1 & T_1 \end{bmatrix} = \tfrac{1}{6}\lambda(b)^{-1}\delta_{bd} - \tfrac{1}{6}\lambda(a)^{-1}\delta_{ae}(-1)^{b+d}, \qquad (27)$$

providing that $\delta(a, b, T_1)\delta(d, e, T_1)\delta(a, d, T_1)\delta(b, e, T_1) = 1$. A general X can be evaluated in terms of the W using the relation

$$X\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & k \end{bmatrix} = \sum_p \lambda(p)W\begin{pmatrix} a & b & c \\ h & p & e \end{pmatrix}W\begin{pmatrix} d & e & f \\ p & g & a \end{pmatrix}W\begin{pmatrix} g & h & k \\ c & f & p \end{pmatrix}, \qquad (28)$$

which follows from (25) together with (19), (18) and (4). The sum in (28) is over at most four values of p and hence any X is calculated without difficulty. Another useful formula for calculating X is given by putting $a = f$ and $b = k$ in (25), multiplying by $\lambda(c)$ and summing over c, whence

$$\sum_c \lambda(c)X\begin{bmatrix} a & b & c \\ d & e & a \\ g & h & b \end{bmatrix} = \lambda(e)^{-1}\delta_{eg}\delta(b, e, h). \qquad (29)$$

I have tabulated a sufficient collection of X in table 4 so that any X which does not contain A_1 can be turned into one of this collection, or into one containing A_1, by permutation of rows and columns, transposition and dashing. Those containing A_1 are readily calculated using equation (26).

There is a series of equations involving V and X paralleling (17)–(20). A typical one is

$$\sum_{\alpha\beta\delta\epsilon} V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix}V\begin{pmatrix} d & e & f \\ \delta & \epsilon & \phi \end{pmatrix}V\begin{pmatrix} a & d & g \\ \alpha & \delta & \eta \end{pmatrix}V\begin{pmatrix} b & e & h \\ \beta & \epsilon & \theta \end{pmatrix}$$
$$= \sum_{k\kappa} \lambda(k)X\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & k \end{bmatrix}V\begin{pmatrix} c & f & k \\ \gamma & \phi & \kappa \end{pmatrix}V\begin{pmatrix} g & h & k \\ \eta & \theta & \kappa \end{pmatrix}. \qquad (30)$$

It can be proved by a straightforward but lengthy series of operations. First express the right-hand side in terms of W by (28) and then eliminate the W using equations (18) and (19). Having obtained (30) we can deduce the rest of the series from it using (4). The most useful ones are

$$\sum_{\alpha\beta\delta\epsilon\eta\theta} V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix}V\begin{pmatrix} d & e & f \\ \delta & \epsilon & \phi \end{pmatrix}V\begin{pmatrix} g & h & k \\ \eta & \theta & \kappa \end{pmatrix}V\begin{pmatrix} a & d & g \\ \alpha & \delta & \eta \end{pmatrix}V\begin{pmatrix} b & e & h \\ \beta & \epsilon & \theta \end{pmatrix}$$
$$= X\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & k \end{bmatrix}V\begin{pmatrix} c & f & k \\ \gamma & \phi & \kappa \end{pmatrix}, \qquad (31)$$

(*a*) X which are zero for symmetry reasons

$$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} \quad \begin{bmatrix} T_2 & T_2 & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} \quad \begin{bmatrix} T_2 & \cdot & \cdot \\ \cdot & T_2 & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} \quad \begin{bmatrix} E & T_2 & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} \quad \begin{bmatrix} E & T_2 & \cdot \\ \cdot & \cdot & T_2 \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$\begin{bmatrix} E & E & E \\ T_2 & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} \quad \begin{bmatrix} A_2 & E & E \\ E & E & E \\ E & E & E \end{bmatrix} \quad \begin{bmatrix} A_2 & E & E \\ E & \cdot & \cdot \\ E & \cdot & \cdot \end{bmatrix} \quad \begin{bmatrix} A_2 & E & E \\ E & T_2 & \cdot \\ E & \cdot & T_2 \end{bmatrix} \quad \begin{bmatrix} A_2 & E & E \\ E & T_2 & T_2 \\ E & \cdot & \cdot \end{bmatrix}$$

(*b*) X with an A_2.

$$\begin{bmatrix} A_2 & E & E \\ E & A_2 & E \\ E & E & E \end{bmatrix} = \frac{1}{4}, \begin{bmatrix} A_2 & E & E \\ E & A_2 & E \\ E & E & A_2 \end{bmatrix} = -\frac{1}{4}, \begin{bmatrix} A_2 & E & E \\ \cdot & A_2 & T_2 \\ T_2 & E & \cdot \end{bmatrix} = \frac{1}{6}, \begin{bmatrix} A_2 & E & E \\ T_2 & A_2 & \cdot \\ \cdot & E & \cdot \end{bmatrix} = -\frac{1}{6},$$

$$\begin{bmatrix} A_2 & E & E \\ \cdot & E & \cdot \\ T_2 & E & \cdot \end{bmatrix} = \begin{bmatrix} A_2 & E & E \\ \cdot & E & \cdot \\ T_2 & E & T_2 \end{bmatrix} = -\frac{1}{6\sqrt{2}}, \begin{bmatrix} A_2 & E & E \\ \cdot & E & T_2 \\ T_2 & E & \cdot \end{bmatrix} = \begin{bmatrix} A_2 & E & E \\ \cdot & \cdot & \cdot \\ T_2 & \cdot & \cdot \end{bmatrix} = \begin{bmatrix} A_2 & E & E \\ \cdot & T_2 & T_2 \\ T_2 & \cdot & \cdot \end{bmatrix} = \frac{1}{6\sqrt{2}},$$

$$\begin{bmatrix} A_2 & E & E \\ \cdot & T_2 & \cdot \\ T_2 & \cdot & \cdot \end{bmatrix} = \frac{1}{6\sqrt{6}}, \begin{bmatrix} A_2 & E & E \\ E & T_2 & \cdot \\ E & \cdot & \cdot \end{bmatrix} = \frac{1}{6},$$

(*c*) X without A_1 or A_2.

$$\begin{bmatrix} T_2 & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} = \begin{bmatrix} T_2 & T_2 & T_2 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} = \begin{bmatrix} T_2 & \cdot & \cdot \\ \cdot & T_2 & \cdot \\ \cdot & \cdot & T_2 \end{bmatrix} = \begin{bmatrix} E & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} = \begin{bmatrix} E & \cdot & \cdot \\ \cdot & T_2 & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} = \begin{bmatrix} E & \cdot & \cdot \\ \cdot & T_2 & \cdot \\ \cdot & \cdot & T_2 \end{bmatrix} = -\begin{bmatrix} E & T_2 & T_2 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} = \frac{1}{18}$$

$$-\begin{bmatrix} E & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & E \end{bmatrix} = \begin{bmatrix} E & \cdot & \cdot \\ \cdot & T_2 & \cdot \\ \cdot & \cdot & E \end{bmatrix} = \frac{1}{36}, \quad -\begin{bmatrix} E & \cdot & T_2 \\ \cdot & T_2 & \cdot \\ \cdot & \cdot & E \end{bmatrix} = \begin{bmatrix} E & \cdot & T_2 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & E \end{bmatrix} = \begin{bmatrix} E & E & E \\ E & \cdot & \cdot \\ E & \cdot & \cdot \end{bmatrix} = \frac{1}{12}, \begin{bmatrix} E & T_2 & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & E \end{bmatrix} = -\frac{1}{12\sqrt{3}}$$

$$\begin{bmatrix} E & \cdot & \cdot \\ \cdot & E & \cdot \\ \cdot & \cdot & E \end{bmatrix} = \frac{1}{9}, \quad \begin{bmatrix} E & T_2 & \cdot \\ \cdot & E & \cdot \\ \cdot & \cdot & E \end{bmatrix} = 0, \quad \begin{bmatrix} E & E & E \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix} = \begin{bmatrix} E & E & E \\ T_2 & \cdot & \cdot \\ T_2 & \cdot & \cdot \end{bmatrix} = \frac{1}{6\sqrt{3}}, \quad \begin{bmatrix} E & E & E \\ E & E & E \\ E & E & E \end{bmatrix} = \frac{1}{4}.$$

Table 4. Values of X. A dot always signifies T_1 and the symbol X is omitted.

$$\sum_{\alpha\delta} V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} V\begin{pmatrix} d & e & f \\ \delta & \epsilon & \phi \end{pmatrix} V\begin{pmatrix} a & d & g \\ \alpha & \delta & \eta \end{pmatrix}$$
$$= \sum_{hk\theta\kappa} \lambda(h)\lambda(k) X\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & k \end{bmatrix} V\begin{pmatrix} c & f & k \\ \gamma & \phi & \kappa \end{pmatrix} V\begin{pmatrix} g & h & k \\ \eta & \theta & \kappa \end{pmatrix} V\begin{pmatrix} b & e & h \\ \beta & \epsilon & \theta \end{pmatrix} \quad (32)$$

and the orthonormality rule for the X:

$$\sum_{gh} \lambda(g)\lambda(h) X\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & k \end{bmatrix} X\begin{bmatrix} a & b & c' \\ d & e & f' \\ g & h & k \end{bmatrix}$$
$$= \lambda(c)^{-1}\lambda(f)^{-1}\delta_{cc'}\delta_{ff'}\delta(a,b,c)\delta(d,e,f)\delta(c,f,k). \quad (33)$$

If we multiply (31) by

$$V\begin{pmatrix} c & f & k' \\ \gamma & \phi & \kappa' \end{pmatrix}$$

and sum over γ and ϕ we obtain equation (25) with X on the left-hand side replaced by $X\delta_{kk'}\delta_{\kappa\kappa'}$ and the second k, and κ on the right-hand side replaced by k' and κ'. Just as with equation (17) this result can be given a group-theoretic significance in terms of recoupling transformations (see FR, p. 60).

Finally, there is also an associative law for X which reads

$$\sum_{gh} (-1)^h \lambda(g)\lambda(h) X\begin{bmatrix} a & d & g \\ b & e & h \\ c & f & k \end{bmatrix} X\begin{bmatrix} a & d & g \\ e & b & h \\ l & m & k \end{bmatrix} = (-1)^{f+m} X\begin{bmatrix} a & b & c \\ e & d & f \\ l & m & k \end{bmatrix} \quad (34)$$

and can be deduced from equation (31).

5. Discussion

We have now forged a mathematical tool and its use will be demonstrated in subsequent papers. The reader who is familiar with the corresponding one for the unitary unimodular group U_2 will have no difficulty in using it for himself already. Here I mention that our present theory is welded into the usual ligand field theory chiefly through equation (3), which expresses the coupling coefficients in terms of V, and equation (16) giving the three-representation recoupling coefficients in terms of W. Incidentally equations (16), (13) and (15) together with table 3 give implicitly the values of all these recoupling coefficients. We shall see in a later paper that the X are proportional to more complicated recoupling coefficients (as in FR, Chapter 12) and also to certain sums which occur in the theory of the vibration-induced electric dipole intensities of Laporte-forbidden electronic transitions in centrosymmetric ions. It will appear that the V, W and X are most useful in problems, such as the latter, where the states of interest are defined by coupling two or more sets of states of sub-systems each forming bases for irreducible representations, and which are complicated mainly because of the presence of these couplings and of summations over the components of irreducible representations. The relationship to methods directly involving coupling and recoupling coefficients will also be shown.

From our present viewpoint the most important difference between the representations of the octahedral group O and those of its associated spinor group O* is that the direct product of two of the latter, but not of the former, may contain a repeated representation. Therefore if it proves possible at all usefully to define V symbols for O^* they will be essentially more complicated and not at all a trivial generalization of those of the present paper. Hence our present method is not immediately applicable to general calculations with spin-orbit coupling. However it can be used in some cases and we shall see that general two-electron systems provide a straightforward example, spin functions with given S transforming as the irreducible representations A_1 or T_1 according to whether they represent singlets or triplets.

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