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Irreducible-Tensor Theory for the Group O*. I. V and W Coefficients†

Paul A. Dobosh‡
Chemistry Department, University of Virginia, Charlottesville, Virginia 22903
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The irreducible-tensor theory is extended to the double group O*. A complex basis is used because the representations E', E'', and U' are necessarily complex, and a set of phase factors are presented. The presence of repeated representations in the reduction of direct products of representations implies that more than one set of V coefficients may be associated with a given set of representations abc. For the group O*, representations are repeated a maximum of two times in any direct product and the corresponding sets of V coefficients are labeled V_1 and V_2. This requires a modification in the standard definition of W so that the subscripts on the V coefficients are included in the definition. This in turn calls for a rederivation of the useful matrix elements of double-tensor operators and several of the more important formulas are developed with particular emphasis on matrix elements in a spin-orbit basis. Complete tables of all V and W coefficients for O* are also given.

I. INTRODUCTION

A decade ago, Griffith developed his irreducible-tensor method for molecular symmetry groups in a series of papers[1] and an excellent monograph.[2] The tensor method is invaluable for evaluating matrix elements of multideterminantal wave functions and sums of matrix elements. Griffith's work did not extend to the double-group representations, those representations which are important in odd-electron systems when spin-orbit coupling is a major element in the molecular Hamiltonian. In this paper, the irreducible-tensor method will be extended to the octahedral double group O*. There are two previous papers on this subject. The work by Golding[3] covers V coefficients, while Mauza and Batarunas[4] define W coefficients, but in a manner which we believe is inadequate.

The irreducible-tensor method for finite groups is an extension of the research by Wigner[5] and Fano and Racah[6] on the full rotation group. In the notation of Fano and Racah, the Wigner-Eckart theorem may be written

$$\langle a\alpha | O_\gamma^c | b\beta\rangle = (-1)^{a-\alpha}\, \overline{V}\begin{pmatrix} a & b & c \\ -\alpha & \beta & \gamma \end{pmatrix} \langle a \| O^c \| b\rangle , \tag{1}$$

where a, b, and c are irreducible representations of a group G and α, β, and γ are components. The $\overline{V}$ coefficients are constructed in a symmetrical form so that $\overline{V}(abc;\alpha\beta\gamma) = \pm\overline{V}(bac;\beta\alpha\gamma)$, with the sign determined by well-defined rules dependent upon the particular representations abc. The symmetry of $\overline{V}$ results in a very compact set of coupling coefficients. Of more importance is the fact that one may construct invariant sums of $\overline{V}$ coefficients which are useful in reducing matrix elements between multideterminantal wave functions to matrix elements of individual atomic or molecular orbitals.

The Wigner-Eckart theorem, as written above, depends upon the group G being simply reducible,[7] that is, the reduction of the direct product of the representations a and b contains c only once for any a, b, and c. This is true for the full rotation group and for finite groups with no representations more than threefold degenerate. The group O*, however, contains the fourfold degenerate U' representation and, as Table I shows, direct products involving this representation will have repeated representations when reduced. In these cases, the more general Wigner-Eckart theorem must be used:

$$\langle a\alpha | O_\gamma^c | b\beta\rangle = (-1)^{a-\alpha}\left[\overline{V}_1\begin{pmatrix} a & b & c \\ -\alpha & \beta & \gamma \end{pmatrix} \langle a \| O^c \| b\rangle_1 + \overline{V}_2\begin{pmatrix} a & b & c \\ -\alpha & \beta & \gamma \end{pmatrix} \langle a \| O^c \| b\rangle_2\right]. \tag{2}$$

Now in any equation containing $\overline{V}$ coefficients or invariant sums of $\overline{V}$ coefficients it will be necessary to specify whether $\overline{V}_1$ or $\overline{V}_2$ is being used for a particular triplet abc.

In this discussion, it shall be assumed that the reader is familiar with the books by Griffith[2] and Fano and Racah[6] on the irreducible-tensor theory. The notation of Griffith[2] shall be adopted throughout to accentuate the close relationship with his work. In particular, V and W will be used instead of $\overline{V}$ and $\overline{W}$, and the basis functions used are those of Griffith's Table A19.[8]

TABLE I. Representations in the direct products of O^* representations.

O^*	A_1	A_2	E	T_1	T_2	E'	E''	U'
A_1	A_1	A_2	E	T_1	T_2	E'	E''	U'
A_2	A_2	A_1	E	T_2	T_1	E''	E'	U'
E	E	E	A_1+A_2+E	T_1+T_2	T_1+T_2	U'	U'	$E'+E''+U'$
T_1	T_1	T_2	T_1+T_2	$A_1+E+T_1+T_2$	$A_2+E+T_1+T_2$	$E'+U'$	$E''+U'$	$E'+E''+2U'$
T_2	T_2	T_1	T_1+T_2	$A_2+E+T_1+T_2$	$A_1+E+T_1+T_2$	$E''+U'$	$E'+U'$	$E'+E''+2U'$
E'	E'	E''	U'	$E'+U'$	$E''+U'$	A_1+T_1	A_1+T_2	$E+T_1+T_2$
E''	E''	E'	U'	$E''+U'$	$E'+U'$	A_2+T_2	A_1+T_1	$E+T_1+T_2$
U'	U'	U'	$E'+E''+U'$	$E'+E''+2U'$	$E'+E''+2U'$	$E+T_1+T_2$	$E+T_1+T_2$	$A_1+A_2+E+2T_1+2T_2$

II. PHASE FACTORS

To construct the group O^* from the group O, the representations E', E'', and U', which are necessarily complex, are added to the representations A_1, A_2, E, T_1, and T_2, which may be chosen real or complex. Since complex representations must be used, phase conventions which follow Fano and Racah as closely as possible shall be adopted.

In the theory of the full rotation group, three types of phase factors occur naturally.

(i) $(-1)^{a+b+c}$, the factor which determines the change of sign of a V coefficient when any two representations are interchanged, i.e.,

$$V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} = (-1)^{a+b+c}\, V\begin{pmatrix} b & a & c \\ \beta & \alpha & \gamma \end{pmatrix} . \tag{3}$$

(ii) $(-1)^{2b}$, which equals $+1$ for a representation which can be constructed in real form and -1 for a representation which is necessarily complex. The factor is actually an abbreviation for $(-1)^{b+b+A_1}$.

(iii) $(-1)^{c-\gamma}$, which arises from the structure of the matrix U which transforms representations to their contragredient form.[9] When complex representations are used, U can be written in the form

$$U=\begin{bmatrix} 0 & & & & & \cdot^{\cdot^{\cdot}} \\ & & & & -1 & \\ & & & +1 & & \\ & & -1 & & & \\ & +1 & & & & \\ \cdot^{\cdot^{\cdot}} & & & & & 0 \end{bmatrix} .$$

In the full rotation group all of these factors may be evaluated by replacing a, b, and c by their J values and the components α, β, and γ by their M values and evaluating the factors algebraically. For the finite groups there are no particular numbers associated with the representations or their components and other criteria must be used to determine numerical values for phase factors.

$(-1)^{c-\gamma}$ occurs for the same reason in the finite groups as in the full rotation group and alternates from $+1$ to -1 for consecutive components of a representation. The only exception is E where both components give a $+1$ factor. The E representation is real and we interpret $-\alpha$ as α for both components. Conventional choices for values of $(-1)^{c-\gamma}$ are used and they are all listed in Table II.

The factors $(-1)^{a+b+c}$ and $(-1)^{b+b+A_1} = (-1)^{2b}$ are fixed only if two of the representations in the exponent are the same. Let us say $a=b$. If c belongs to the symmetric product[10] of $a\times a$, then $(-1)^{a+a+c}$ must equal $+1$, since a symmetric function $c\gamma$ constructed from $a\times a$ must contain $a\alpha a\beta$ and $a\beta a\alpha$ with identical coefficients. These coefficients, if one neglects normalization, are simply V coefficients and so $V(aac;\alpha\beta\gamma) = V(aac;\beta\alpha\gamma)$. Similarly, if c belongs to the antisymmetric product of $a\times a$, then $(-1)^{a+b+c} = -1$. Table III lists the representations of the symmetric and antisymmetric products of $a\times a$.

For the real representations, Griffith was able to define

$$(-1)^{A_1} = (-1)^{E} = (-1)^{T_2} = +1,$$

$$(-1)^{A_2} = (-1)^{T_1} = -1$$

and obtain a consistent set of values for $(-1)^{a+b+c}$.

TABLE II. Phase factors $(-1)^{c-\gamma}$.

c^{γ}	ι	θ	ϵ	$+1$	0	-1	α	β	κ	λ	μ	ν
A_1	1											
A_2	1											
E		1	1									
T_1				1	-1	1						
T_2				1	-1	1						
E'							1	-1				
E''							1	-1				
U'									1	-1	1	-1

TABLE III. Representations of the symmetric and antisymmetric product of $a \times a$.

a	$[a^2]$	(a^2)
A_1	A_1	
A_2	A_1	
E	A_1+E	A_2
T_1	A_1+E+T_2	T_1
T_2	A_1+E+T_2	T_1
E'	T_1	A_1
E''	T_1	A_1
U	$A_2+2T_1+T_{2a}$	A_1+E+T_{2b}

By adding

$$(-1)^{E'} = i, \quad (-1)^{E''} = (-1)^{U'} = -i \ ,$$

where $i = \sqrt{-1}$, we can also find a consistent set of values for every abc except $U'U'T_2$ when T_2 is part of the symmetric product $U' \times U'$. This problem is annoying since it means that we cannot, in general, combine exponents in products of phase factors and must carry factors such as $(-1)^{a+b+c}$ around intact. Golding has used J and M values for the parent representations from which the octahedral representations arise under an octahedral field to find phase factors and this might possibly lead to a complete set of values for phase factors without the need to consider symmetric and antisymmetric products. That approach has not been tried by the author.

The values for $(-1)^{a+b+c}$ are tabulated in Table IV. With this choice of factors, all those containing A_1, E', T_1, and U' agree with those of Fano and Racah for $J=0$, $\frac{1}{2}$, 1, and $\frac{3}{2}$, respectively. This will help ensure compatibility with $\overline{V}$ coefficients when we mix space functions with spin functions of representations irreducible under the full rotation group.

TABLE IV. Phase factors $(-1)^{a+b+c}$ and $(-1)^{b+b+A_1} = (-1)^{2b}$.

+1	−1
A_1^3 $A_2^2A_1$ E^2A_1	E^2A_2
$T_1^2A_1$ $T_2^2A_1$	T_1^3 $T_2^2T_1$
E^3 T_1^2E T_2^2E	
$T_1^2T_2$ T_2^3	
$A_2T_1T_2$	ET_1T_2
$E'E'T_1$ $E''E''T_1$	$E'E'A_1$ $E''E''A_1$ $U'U'A_1$
$U'U'T_{1a}$ $U'U'T_{1b}$	$U'U'E$ $U'U'T_{2b}$
$U'U'A_2$ $U'U'T_{2a}$	
$E'E''T_2$	$E'E''A_2$
$E'U'E$ $E'U'T_2$ $E''U'T_1$	$E''U'E$ $E''U'T_2$ $E'U'T_1$

III. V COEFFICIENTS

Calculating V coefficients is now a straightforward matter using the definition of Fano and Racah[11]:

$$V\begin{pmatrix} a & b & c \\ \alpha & \beta & -\gamma \end{pmatrix} = (-1)^{2b}\,(-1)^{c-\gamma}\,\lambda(c)^{-1/2} \times \langle abc\gamma | ab\alpha\beta\rangle \ , \tag{4}$$

where $\lambda(c)$ is the degeneracy of c and the $\langle abc\gamma | ab\alpha\beta\rangle$ are vector coupling coefficients. The vector coupling coefficients are the elements of the matrix which reduce the representations of $a \times b$ to the representations c. The vector coupling coefficients in Table A20 of Griffith[8] have been used as a starting point. It should be noted that if we use these vector coupling coefficients for abc to find the $V(abc)$, permute a and b in V, and then use Eq. (4) to find vector coupling coefficients for bac, the results may differ from those in Table A20 by a factor of -1. In addition, some of the vector coupling matrices of Table A20 were multiplied by -1 to obtain V coefficients compatible with $\overline{V}$ coefficients when appropriate.[12] For these reasons, the specific sections of Table A20 which were used are listed in Table V.

Griffith's coupling tables for the U' representations of $T_2 \times U'$ are unsatisfactory for our purpose. These U' representations diagonalize the spin-orbit coupling Hamiltonian $\mathcal{H}_{so}$, i.e.,

$$\langle U'_{3/2}m | \mathcal{H}_{so} | U'_{5/2}m \rangle = 0 \ ,$$

but the T_2 representations of $U' \times U'$ found with Griffith's coefficients are not symmetric and antisymmetric as they must be if we are to define V coefficients. Koster[13] points out that a linear combination of $U'_{3/2}$ and $U'_{5/2}$ may be taken (component by component) without charging the reduced form of $T_2 \times U'$. Using the linear combination

$$\begin{aligned} U'_a &= (2/\sqrt{5})\,U'_{3/2} + (1/\sqrt{5})\,U'_{5/2} \ , \\ U'_b &= (1/\sqrt{5})\,U'_{3/2} - (2/\sqrt{5})\,U'_{5/2} \ , \end{aligned} \tag{5}$$

we obtain the proper symmetric and antisymmetric

TABLE V. Sections of Table A20 of Griffith (Ref. 8) used in computing V coefficients. (−) preceding a set of representations indicates the matrix was multiplied by −1.

$A_1A_1A_1$	$T_2T_2A_1$	$A_2E'E''$	$T_1U'E'$
$A_2A_2A_1$	T_2T_2E	$A_2U'U'$	$T_1U'E''$
EEA_1	$T_2T_2T_1$	$EE'U'$	$T_2U'E'$
EEA_2	$T_2T_2T_2$	$EE''U'$	$T_2U'E''$
EEE	$T_1T_2A_2$	$EU'U'$	(−) $T_1U'U'_a$
$T_1T_1A_1$	T_1T_2E	(−) $T_1E'E'$	(−) $T_1U'U'_b$
T_1T_1E	$A_1E'E'$	(−) $T_1E''E''$	(−) $T_2U'U'_a$
$T_1T_1T_1$	$A_1E''E''$	$T_2E'E''$	(−) $T_2U'U'_b$
$T_1T_1T_2$	$A_1U'U'$		

functions for T_2.

The complete list of V coefficients for O* are presented in Table VI. In the $U' \times U'$ table, the first set of coefficients for T_1 and T_2 will be V_1 and the second set will be V_2. For T_2, the symmetric coefficients are the V_1 and the antisymmetric coefficients are the V_2.

Certain useful equations involving $\overline{V}$ coefficients carry over to V coefficients directly or with slight modification. The subscripts i, j apply when there is a choice of V_1 or V_2. We have

$$\sum_{\alpha\beta} V_i\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} V_j\begin{pmatrix} a & b & c' \\ \alpha & \beta & \gamma' \end{pmatrix} = \delta_{cc'}\,\delta_{\gamma\gamma'}\,\lambda(c)^{-1}\,\delta(a,b,c)\,\delta_{ij}\ , \quad (6)$$

where $\delta(a,b,c) = 1$ or 0 according to whether c is in $a \times b$ or not,

$$\sum_{c\gamma} \lambda(c)\, V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} V\begin{pmatrix} a & b & c \\ \alpha' & \beta' & \gamma \end{pmatrix} = \delta_{\alpha\alpha'}\,\delta_{\beta\beta'}\ , \quad (7)$$

$$\sum_{\alpha\beta\gamma} V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix}^2 = \delta(a,b,c)\ , \quad (8)$$

TABLE VI. V coefficients. $V\begin{pmatrix} A_1 & A_1 & A_1 \\ \iota & \iota & \iota \end{pmatrix} = V\begin{pmatrix} A_2 & A_2 & A_1 \\ \iota & \iota & \iota \end{pmatrix} = 1$.

(i)

$E \times E$		A_1	A_2	E	
		ι	ι	θ	ϵ
θ	θ	$1/\sqrt{2}$	$\cdots$	$-\frac{1}{2}$	$\cdots$
θ	ϵ	$\cdots$	$1/\sqrt{2}$	$\cdots$	$\frac{1}{2}$
ϵ	θ	$\cdots$	$-1/\sqrt{2}$	$\cdots$	$\frac{1}{2}$
ϵ	ϵ	$1/\sqrt{2}$	$\cdots$	$\frac{1}{2}$	$\cdots$

(ii)

$T_1 \times T_1$		A_1	E		T_1			T_2		
$(T_2 \times T_2)$		ι	θ	ϵ	1	0	-1	1	0	-1
1	1	$\cdots$	$\cdots$	$\frac{1}{2}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$-1/\sqrt{6}$	$\cdots$
1	0	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$1/\sqrt{6}$	$-1/\sqrt{6}$	$\cdots$	$\cdots$
1	-1	$1/\sqrt{3}$	$1/2\sqrt{3}$	$\cdots$	$\cdots$	$-1/\sqrt{6}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$
0	1	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$-1/\sqrt{6}$	$-1/\sqrt{6}$	$\cdots$	$\cdots$
0	0	$-1/\sqrt{3}$	$1/\sqrt{3}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$
0	-1	$\cdots$	$\cdots$	$\cdots$	$1/\sqrt{6}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$1/\sqrt{6}$
-1	1	$1/\sqrt{3}$	$1/2\sqrt{3}$	$\cdots$	$\cdots$	$1/\sqrt{6}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$
-1	0	$\cdots$	$\cdots$	$\cdots$	$-1/\sqrt{6}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$1/\sqrt{6}$
-1	-1	$\cdots$	$\cdots$	$\frac{1}{2}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$1/\sqrt{6}$	$\cdots$

(iii)

$T_1 \times T_2$		A_2	E	
		ι	θ	ϵ
1	1	$\cdots$	$\frac{1}{2}$	$\cdots$
1	0	$\cdots$	$\cdots$	$\cdots$
1	-1	$1/\sqrt{3}$	$\cdots$	$-1/2\sqrt{3}$
0	1	$\cdots$	$\cdots$	$\cdots$
0	0	$-1/\sqrt{3}$	$\cdots$	$-1/\sqrt{3}$
0	-1	$\cdots$	$\cdots$	$\cdots$
-1	1	$1/\sqrt{3}$	$\cdots$	$-1/2\sqrt{3}$
-1	0	$\cdots$	$\cdots$	$\cdots$
-1	-1	$\cdots$	$\frac{1}{2}$	$\cdots$

(iv)

$E' \times U'$		E		T_1			T_2		
		θ	ϵ	1	0	-1	1	0	-1
α'	κ	$\cdots$	$-\frac{1}{2}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$-1/\sqrt{6}$	$\cdots$
α'	λ	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$-1/2\sqrt{3}$	$-\frac{1}{2}$	$\cdots$	$\cdots$
α'	μ	$-\frac{1}{2}$	$\cdots$	$\cdots$	$1/\sqrt{6}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$
α'	ν	$\cdots$	$\cdots$	$-\frac{1}{2}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$+1/2\sqrt{3}$
β'	κ	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\frac{1}{2}$	$-1/2\sqrt{3}$	$\cdots$	$\cdots$
β'	λ	$-\frac{1}{2}$	$\cdots$	$\cdots$	$-1/\sqrt{6}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$
β'	μ	$\cdots$	$\cdots$	$1/2\sqrt{3}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\frac{1}{2}$
β'	ν	$\cdots$	$-\frac{1}{2}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$1/\sqrt{6}$	$\cdots$

(v)

$E' \times E'$		A_1	T_1		
$(E'' \times E'')$		ι	1	0	-1
α'	α'	$\cdots$	$\cdots$	$\cdots$	$1/\sqrt{3}$
α'	β'	$-1/\sqrt{2}$	$\cdots$	$-1/\sqrt{6}$	$\cdots$
β'	α'	$1/\sqrt{2}$	$\cdots$	$-1/\sqrt{6}$	$\cdots$
β'	β'	$\cdots$	$1/\sqrt{3}$	$\cdots$	$\cdots$

(vi)

$E' \times E''$		A_2	T_2		
		ι	1	0	-1
α'	α''	$\cdots$	$\cdots$	$\cdots$	$1/\sqrt{3}$
α'	β''	$-1/\sqrt{2}$	$\cdots$	$-1/\sqrt{6}$	$\cdots$
β'	α''	$1/\sqrt{2}$	$\cdots$	$-1/\sqrt{6}$	$\cdots$
β'	β''	$\cdots$	$1/\sqrt{3}$	$\cdots$	$\cdots$

(vii)

$E'' \times U'$		E		T_1			T_2		
		θ	ϵ	1	0	-1	1	0	-1
α''	κ	$-\frac{1}{2}$	$\cdots$	$\cdots$	$-1/\sqrt{6}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$
α''	λ	$\cdots$	$\cdots$	$-\frac{1}{2}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$1/2\sqrt{3}$
α''	μ	$\cdots$	$\frac{1}{2}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$-1/\sqrt{6}$	$\cdots$
α''	ν	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$1/2\sqrt{3}$	$\frac{1}{2}$	$\cdots$	$\cdots$
β''	κ	$\cdots$	$\cdots$	$-1/2\sqrt{3}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$-\frac{1}{2}$
β''	λ	$\cdots$	$\frac{1}{2}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$1/\sqrt{6}$	$\cdots$
β''	μ	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\frac{1}{2}$	$-1/2\sqrt{3}$	$\cdots$	$\cdots$
β''	ν	$-\frac{1}{2}$	$\cdots$	$\cdots$	$1/\sqrt{6}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$

TABLE VI. (*Continued*)

(viii)

$U' \times U'$		A_1 ι	A_2 ι	E θ	E ϵ	T_{1a} 1	T_{1a} 0	T_{1a} -1	T_{1b} 1	T_{1b} 0	T_{1b} -1	T_{2a} 1	T_{2a} 0	T_{2a} -1	T_{2b} 1	T_{2b} 0	T_{2b} -1
κ	κ	⋯	⋯	⋯	⋯	⋯	⋯	⋯	$-\sqrt{5}/2\sqrt{6}$	⋯	⋯	⋯	⋯	$1/2\sqrt{2}$	⋯	⋯	⋯
κ	λ	⋯	$-\frac{1}{2}$	⋯	$-1/2\sqrt{2}$	⋯	⋯	⋯	⋯	⋯	⋯	⋯	$1/2\sqrt{3}$	⋯	⋯	$1/2\sqrt{3}$	⋯
κ	μ	⋯	⋯	⋯	⋯	⋯	⋯	$-1/\sqrt{10}$	⋯	⋯	$-1/2\sqrt{10}$	$-1/2\sqrt{6}$	⋯	⋯	$1/\sqrt{6}$	⋯	⋯
κ	ν	$-\frac{1}{2}$	⋯	$-1/2\sqrt{2}$	⋯	⋯	$\sqrt{3}/2\sqrt{5}$	⋯	⋯	$-1/2\sqrt{15}$	⋯	⋯	⋯	⋯	⋯	⋯	⋯
λ	κ	⋯	$-\frac{1}{2}$	⋯	$1/2\sqrt{2}$	⋯	⋯	⋯	⋯	⋯	⋯	⋯	$1/2\sqrt{3}$	⋯	⋯	$-1/2\sqrt{3}$	⋯
λ	λ	⋯	⋯	⋯	⋯	⋯	⋯	$\sqrt{2}/\sqrt{15}$	⋯	⋯	$-\sqrt{3}/2\sqrt{10}$	$-1/2\sqrt{2}$	⋯	⋯	⋯	⋯	⋯
λ	μ	$\frac{1}{2}$	⋯	$-1/2\sqrt{2}$	⋯	⋯	$-1/2\sqrt{15}$	⋯	⋯	$-\sqrt{3}/2\sqrt{5}$	⋯	⋯	⋯	⋯	⋯	⋯	⋯
λ	ν	⋯	⋯	⋯	⋯	$-1/\sqrt{10}$	⋯	⋯	$-1/2\sqrt{10}$	⋯	⋯	⋯	⋯	$-1/2\sqrt{6}$	⋯	⋯	$-1\sqrt{6}$
μ	κ	⋯	⋯	⋯	⋯	⋯		$-1/\sqrt{10}$	⋯	⋯	$-1/2\sqrt{10}$	$-1/2\sqrt{6}$	⋯	⋯	$-1/\sqrt{6}$	⋯	⋯
μ	λ	$-\frac{1}{2}$	⋯	$1/2\sqrt{2}$	⋯	⋯	$-1/2\sqrt{15}$	⋯	⋯	$-\sqrt{3}/2\sqrt{5}$	⋯	⋯	⋯	⋯	⋯	⋯	⋯
μ	μ	⋯	⋯	⋯	⋯	$\sqrt{2}/\sqrt{15}$	⋯	⋯	$-\sqrt{3}/2\sqrt{10}$	⋯	⋯	⋯	⋯	$-1/2\sqrt{2}$	⋯	⋯	⋯
μ	ν	⋯	$\frac{1}{2}$	⋯	$-1/2\sqrt{2}$	⋯	⋯	⋯	⋯	⋯	⋯	⋯	$1/2\sqrt{3}$	⋯	⋯	$-1/2\sqrt{3}$	⋯
ν	κ	$\frac{1}{2}$	⋯	$1/2\sqrt{2}$	⋯	⋯	$\sqrt{3}/2\sqrt{5}$	⋯	⋯	$-1/2\sqrt{15}$	⋯	⋯	⋯	⋯	⋯	⋯	⋯
ν	λ	⋯	⋯	⋯	⋯	$-1/\sqrt{10}$	⋯	⋯	$-1/2\sqrt{10}$	⋯	⋯	⋯	⋯	$-1/2\sqrt{6}$	⋯	⋯	$1/\sqrt{6}$
ν	μ	⋯	$\frac{1}{2}$	⋯	$1/2\sqrt{2}$	⋯	⋯	⋯	⋯	⋯	⋯	⋯	$1/2\sqrt{3}$	⋯	⋯	$1/2\sqrt{3}$	⋯
ν	ν	⋯	⋯	⋯	⋯	⋯	⋯	⋯	⋯	⋯	$-\sqrt{5}/2\sqrt{6}$	$1/2\sqrt{2}$	⋯	⋯	⋯	⋯	⋯

$$V\begin{pmatrix} a & b & c \\ -\alpha & -\beta & -\gamma \end{pmatrix} = (-1)^{a-\alpha+b-\beta+c-\gamma}\, V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} . \quad (9)$$

Notice in Eq. (9) that the factor is $(-1)^{a-\alpha+b-\beta+c-\gamma}$ and not $(-1)^{a+b+c}$, as in Eq. (14) of Golding.[3] In the full rotation group $\alpha+\beta+\gamma=0$ for nonzero $\overline{V}$, but this is not necessarily true for O*.

IV. *W* COEFFICIENTS

The most important of the invariant sums of V coefficients is the W coefficient. The Fano and Racah definition is[14]

$$W\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix} = \sum_{\alpha\beta\gamma\delta\epsilon\phi} (-1)^{a-\alpha+b-\beta+c-\gamma+d-\delta+e-\epsilon+f-\phi} \times V\begin{pmatrix} a & b & c \\ -\alpha & -\beta & -\gamma \end{pmatrix} V\begin{pmatrix} a & e & f \\ \alpha & \epsilon & -\phi \end{pmatrix} \times V\begin{pmatrix} b & f & d \\ \beta & \phi & -\delta \end{pmatrix} V\begin{pmatrix} c & d & e \\ \gamma & \delta & -\epsilon \end{pmatrix} . \quad (10)$$

We shall use the same formula but now we must not only specify W via the six representations, but we must specify whether the constituent V coefficients are V_1 or V_2 when there is a choice. In the worst possible case four labels are required, a point which was apparently overlooked by Mauza and Batarunas.[4] We shall define W as

$$W\begin{pmatrix} a_i & b & c_l \\ d_k & e & f_j \end{pmatrix} = \sum_{\alpha\beta\gamma\delta\epsilon\phi} (-1)^{a-\alpha+b-\beta+c-\gamma+d-\delta+e-\epsilon+f-\phi} . \times V_i\begin{pmatrix} a & b & c \\ -\alpha & -\beta & -\gamma \end{pmatrix} V_j\begin{pmatrix} a & e & f \\ \alpha & \epsilon & -\phi \end{pmatrix} \times V_k\begin{pmatrix} b & f & d \\ \beta & \phi & -\delta \end{pmatrix} V_l\begin{pmatrix} c & d & e \\ \gamma & \delta & -\epsilon \end{pmatrix} . \quad (11)$$

It should be clearly understood that the subscript i, as an example, does not label a but instead refers to the three representations abc together. Let us suppose we form $U'_{3/2}$ from $T_1 \times U'$ and then take the direct product of $U'_{3/2} \times T_1$ to form $U'_{5/2}$. In the second direct product, it does not matter whether we start with $U'_{3/2}$, as we have, or with $U'_{5/2}$. The subscript has meaning only in the context of the first direct product. For the first product V_1 would be used and for the second product V_2 would be used. This point will be made clearer in the example in Sec. VI.

While one might hope that a W would be zero unless the $ijkl$ were all 1 or 2; this is not the case. Mauza and Batarunas[4] did not realize that for some choices of six representations, as many as 16 W coefficients may occur and in some applications all of them can prove useful. All of the nonzero W coefficients for O* are listed in Table VII except for two special cases. Any W containing an A_1 representation may be computed with a modified version of Griffith's Eq. (4.2) (Ref. 2) which we write as

$$W\begin{pmatrix} A_1 & b & c_l \\ d_k & e & f \end{pmatrix} = \frac{(-1)^{b+f+d}}{\lambda(b)^{1/2}\lambda(e)^{1/2}}\,\delta_{bc}\,\delta_{ef}\,\delta(b,f,d)\,\delta_{k,l}\ . \tag{12}$$

Also, any W containing only T_1 and T_2 representations is equal to $\frac{1}{6}$.[2]

The $\overline{W}$ coefficients of Fano and Racah and the W coefficients of Griffith are invariant under several permutations of the six constituent representations. Allowed permutations include the permutation of columns and the simultaneous turning upside down of any two columns. This invariance holds in most cases for O* also. When permuting representations, however, one must consider how the subscripts are permuted since they are not attached to the representations. The rules are

$$W\begin{pmatrix} a_i & b & c_l \\ d_k & e & f_j \end{pmatrix} = W\begin{pmatrix} d_k & b & f_j \\ a_i & e & c_l \end{pmatrix}\ , \tag{13a}$$

TABLE VII. W coefficients. All nonzero W coefficients are listed except those containing A_1, which are evaluated using Eq. (12), and those containing only T_1 and T_2, which are equal to $\frac{1}{6}$. The coefficients are divided into sections according to the number and distribution of U' representations. Within each section, coefficients are ordered by first assigning the numbers 1–8 to the representations A_1 through U', then permuting representations so that $a<b<c$ in $W(abc/def)$, and finally ordering the W's according to the numbers abc or ad. When a trio of representations possesses a V_1 and a V_2 coefficient, the coefficient used is represented by an asterisk for V_2 and no asterisk for V_1. All coefficients which change sign under permutation are preceded by −. A number in parentheses is to be raised to the $\frac{1}{2}$ power.

$W(abc/def)$: coefficients are ordered by the number ad									
$\begin{matrix} A_2 & E & E \\ A_2 & E & E \end{matrix}$	$\frac{1}{2}$	$\begin{matrix} A_2 & T_1 & T_2 \\ A_2 & T_1 & T_2 \end{matrix}$	$\frac{1}{3}$	$\begin{matrix} A_2 & E' & E'' \\ A_2 & E' & E'' \end{matrix}$	$-\frac{1}{2}$	$\begin{matrix} A_2 & E & E \\ E & E & E \end{matrix}$	$\frac{1}{2}$	$\begin{matrix} A_2 & T_1 & T_2 \\ E & T_1 & T_2 \end{matrix}$	$\frac{1}{3}$
$\begin{matrix} A_2 & T_1 & T_2 \\ E & T_2 & T_1 \end{matrix}$	$\frac{1}{3}$	$\begin{matrix} A_2 & E & E \\ T_1 & T_1 & T_2 \end{matrix}$	$\frac{-1}{(6)}$	$\begin{matrix} A_2 & T_1 & T_2 \\ T_1 & T_1 & T_2 \end{matrix}$	$\frac{1}{3}$	$\begin{matrix} A_2 & T_1 & T_2 \\ T_1 & T_2 & T_1 \end{matrix}$	$-\frac{1}{3}$	$\begin{matrix} A_2 & E' & E' \\ T_1 & E'' & E'' \end{matrix}$	$\frac{1}{2}$
$\begin{matrix} A_2 & E & E \\ T_2 & T_1 & T_2 \end{matrix}$	$\frac{1}{(6)}$	$\begin{matrix} A_2 & T_1 & T_2 \\ T_2 & T_1 & T_2 \end{matrix}$	$\frac{-1}{3}$	$\begin{matrix} A_2 & T_1 & T_2 \\ T_2 & T_2 & T_1 \end{matrix}$	$\frac{1}{3}$	$\begin{matrix} A_2 & E' & E'' \\ T_2 & E' & E'' \end{matrix}$	$\frac{1}{2}$	$\begin{matrix} A_2 & T_1 & T_2 \\ E' & E'' & E' \end{matrix}$	$\frac{-1}{(6)}$
$\begin{matrix} A_2 & T_1 & T_2 \\ E'' & E' & E'' \end{matrix}$	$\frac{-1}{(6)}$	$\begin{matrix} E & T_1 & T_1 \\ E & T_1 & T_1 \end{matrix}$	$\frac{1}{3}$	$\begin{matrix} E & T_1 & T_2 \\ E & T_1 & T_2 \end{matrix}$	$\frac{1}{3}$	$\begin{matrix} E & T_1 & T_1 \\ E & T_2 & T_2 \end{matrix}$	$\frac{-1}{3}$	$\begin{matrix} E & T_2 & T_2 \\ E & T_2 & T_2 \end{matrix}$	$\frac{1}{3}$
$\begin{matrix} E & E & E \\ T_1 & T_1 & T_1 \end{matrix}$	$\frac{1}{2(3)}$	$\begin{matrix} E & E & E \\ T_1 & T_1 & T_2 \end{matrix}$	$\frac{1}{2(3)}$	$\begin{matrix} E & E & E \\ T_1 & T_2 & T_2 \end{matrix}$	$\frac{1}{2(3)}$	$\begin{matrix} E & T_1 & T_1 \\ T_1 & T_1 & T_1 \end{matrix}$	$\frac{1}{6}$	$\begin{matrix} E & T_1 & T_1 \\ T_1 & T_1 & T_2 \end{matrix}$	$\frac{-1}{2(3)}$
$\begin{matrix} E & T_1 & T_2 \\ T_1 & T_1 & T_2 \end{matrix}$	$-\frac{1}{6}$	$\begin{matrix} E & T_1 & T_1 \\ T_1 & T_2 & T_2 \end{matrix}$	$\frac{-1}{6}$	$\begin{matrix} E & T_1 & T_2 \\ T_1 & T_2 & T_1 \end{matrix}$	$\frac{-1}{6}$	$\begin{matrix} E & T_1 & T_2 \\ T_1 & T_2 & T_2 \end{matrix}$	$\frac{1}{2(3)}$	$\begin{matrix} E & T_2 & T_2 \\ T_1 & T_2 & T_2 \end{matrix}$	$\frac{1}{6}$
$\begin{matrix} E & E & E \\ T_2 & T_2 & T_2 \end{matrix}$	$\frac{1}{2(3)}$	$\begin{matrix} E & T_1 & T_1 \\ T_2 & T_1 & T_1 \end{matrix}$	$\frac{-1}{6}$	$\begin{matrix} E & T_1 & T_1 \\ T_2 & T_1 & T_2 \end{matrix}$	$\frac{1}{2(3)}$	$\begin{matrix} E & T_1 & T_2 \\ T_2 & T_1 & T_2 \end{matrix}$	$\frac{1}{6}$	$\begin{matrix} E & T_1 & T_1 \\ T_2 & T_2 & T_2 \end{matrix}$	$\frac{1}{6}$
$\begin{matrix} E & T_1 & T_2 \\ T_2 & T_2 & T_1 \end{matrix}$	$\frac{1}{6}$	$\begin{matrix} E & T_1 & T_2 \\ T_2 & T_2 & T_2 \end{matrix}$	$\frac{-1}{2(3)}$	$\begin{matrix} E & T_2 & T_2 \\ T_2 & T_2 & T_2 \end{matrix}$	$-\frac{1}{6}$	$\begin{matrix} T_1 & E' & E' \\ T_1 & E' & E' \end{matrix}$	$\frac{1}{6}$	$\begin{matrix} T_1 & E'' & E'' \\ T_1 & E'' & E'' \end{matrix}$	$\frac{1}{6}$
$\begin{matrix} T_1 & E' & E' \\ T_2 & E'' & E'' \end{matrix}$	$\frac{1}{6}$	$\begin{matrix} T_1 & T_1 & T_1 \\ E' & E' & E' \end{matrix}$	$-\frac{1}{3}$	$\begin{matrix} T_1 & T_2 & T_2 \\ E' & E'' & E'' \end{matrix}$	$-\frac{1}{3}$	$\begin{matrix} T_1 & T_1 & T_1 \\ E'' & E'' & E'' \end{matrix}$	$-\frac{1}{3}$	$\begin{matrix} T_1 & T_2 & T_2 \\ E'' & E' & E' \end{matrix}$	$-\frac{1}{3}$
$\begin{matrix} T_2 & E' & E'' \\ T_2 & E' & E'' \end{matrix}$	$\frac{1}{6}$								
$W(abc/deU)$, $W(abc/dUf)$, $W(abc/Uef)$: coefficients are ordered by the number abc									
$\begin{matrix} A_2 & E & E \\ U & E' & E'' \end{matrix}$	$\frac{1}{2}$	$\begin{matrix} A_2 & T_1 & T_2 \\ U & E' & E'' \end{matrix}$	$\frac{1}{(6)}$	$\begin{matrix} A_2 & T_1 & T_2 \\ U & E'' & E' \end{matrix}$	$\frac{-1}{(6)}$	$\begin{matrix} E & T_1 & T_1 \\ E' & E' & U \end{matrix}$	$\frac{1}{2(3)}$	$\begin{matrix} E & T_1 & T_1 \\ E'' & E'' & U \end{matrix}$	$\frac{1}{2(3)}$
$\begin{matrix} E & T_1 & T_2 \\ E' & E'' & U \end{matrix}$	$\frac{-1}{2(3)}$	$\begin{matrix} E & T_1 & T_2 \\ E'' & E' & U \end{matrix}$	$\frac{1}{2(3)}$	$\begin{matrix} E & T_1 & T_2 \\ E' & U & E' \end{matrix}$	$\frac{1}{2(3)}$	$\begin{matrix} E & T_1 & T_2 \\ E'' & U & E'' \end{matrix}$	$\frac{-1}{2(3)}$	$\begin{matrix} E & T_2 & T_2 \\ E' & E'' & U \end{matrix}$	$\frac{-1}{2(3)}$
$\begin{matrix} E & T_2 & T_2 \\ E'' & E' & U \end{matrix}$	$\frac{-1}{2(3)}$	$\begin{matrix} T_1 & T_1 & T_1 \\ E' & E' & U \end{matrix}$	$-\frac{1}{6}$	$\begin{matrix} T_1 & T_1 & T_1 \\ E'' & E'' & U \end{matrix}$	$\frac{1}{6}$	$\begin{matrix} T_1 & T_1 & T_2 \\ E' & E'' & U \end{matrix}$	$\frac{1}{2(3)}$	$\begin{matrix} T_1 & T_1 & T_2 \\ E'' & U & E'' \end{matrix}$	$\frac{-1}{2(3)}$
$\begin{matrix} T_1 & T_2 & T_2 \\ E' & E'' & U \end{matrix}$	$-\frac{1}{6}$	$\begin{matrix} T_1 & T_2 & T_2 \\ U & E' & E' \end{matrix}$	$\frac{1}{6}$	$\begin{matrix} T_1 & T_2 & T_2 \\ U & E'' & E'' \end{matrix}$	$-\frac{1}{6}$	$\begin{matrix} T_1 & T_2 & T_2 \\ E'' & E' & U \end{matrix}$	$\frac{1}{6}$	$\begin{matrix} T_1 & E' & E' \\ T_1 & E' & U \end{matrix}$	$-\frac{1}{3}$
$\begin{matrix} T_1 & E' & E' \\ T_2 & E'' & U \end{matrix}$	$\frac{1}{3}$	$\begin{matrix} T_1 & E'' & E'' \\ T_1 & E'' & U \end{matrix}$	$-\frac{1}{3}$	$\begin{matrix} T_1 & E'' & E'' \\ T_2 & E' & U \end{matrix}$	$\frac{1}{3}$	$\begin{matrix} T_2 & T_2 & T_2 \\ E' & E'' & U \end{matrix}$	$\frac{1}{2(3)}$	$\begin{matrix} T_2 & E' & E'' \\ T_2 & E' & U \end{matrix}$	$-\frac{1}{3}$
$W(abU/deU)$: coefficients are ordered by the number ad									
$\begin{matrix} E & E' & U \\ E & E' & U \end{matrix}$	$-\frac{1}{4}$	$\begin{matrix} E & E' & U \\ E & E'' & U \end{matrix}$	$\frac{1}{4}$	$\begin{matrix} E & E'' & U \\ E & E'' & U \end{matrix}$	$-\frac{1}{4}$	$\begin{matrix} E & E' & U \\ T_1 & E' & U \end{matrix}$	$\frac{1}{4}$	$\begin{matrix} E & E' & U \\ T_1 & E'' & U \end{matrix}$	$\frac{1}{4}$
$\begin{matrix} E & E'' & U \\ T_1 & E'' & U \end{matrix}$	$\frac{1}{4}$	$\begin{matrix} E & E' & U \\ T_2 & E' & U \end{matrix}$	$\frac{1}{4}$	$\begin{matrix} E & E' & U \\ T_2 & E'' & U \end{matrix}$	$-\frac{1}{4}$	$\begin{matrix} E & E'' & U \\ T_2 & E'' & U \end{matrix}$	$\frac{1}{4}$	$\begin{matrix} T_1 & E' & U \\ T_1 & E' & U \end{matrix}$	$\frac{-1}{12}$
$\begin{matrix} T_1 & E' & U \\ T_1 & E'' & U \end{matrix}$	$-\frac{1}{4}$	$\begin{matrix} T_1 & E'' & U \\ T_1 & E'' & U \end{matrix}$	$\frac{-1}{12}$	$\begin{matrix} T_1 & E' & U \\ T_2 & E' & U \end{matrix}$	$\frac{1}{4}$	$\begin{matrix} T_1 & E' & U \\ T_2 & E'' & U \end{matrix}$	$\frac{-1}{12}$	$\begin{matrix} T_1 & E'' & U \\ T_2 & E'' & U \end{matrix}$	$\frac{1}{4}$
$\begin{matrix} T_2 & E' & U \\ T_2 & E' & U \end{matrix}$	$\frac{-1}{12}$	$\begin{matrix} T_2 & E' & U \\ T_2 & E'' & U \end{matrix}$	$-\frac{1}{4}$	$\begin{matrix} T_2 & E'' & U \\ T_2 & E'' & U \end{matrix}$	$\frac{-1}{12}$				

TABLE VII. (*Continued*)

$W(abc/dUU)$, $W(abc/UeU)$, $W(abc/UUf)$: coefficients are ordered by the number abc

A_2 E E	E' U U	$\frac{1}{2(2)}$
A_2 E E	E'' U U	$\frac{-1}{2(2)}$
A_2 T_1 T_2	E' U U	$\frac{1}{2(3)}$
A_2 T_1 T_2	E'' U U	$\frac{1}{2(3)}$
A_2 E' E''	E U U	$\frac{-1}{2(2)}$
A_2 E' E''	T_1 U U	$\frac{-1}{2(2)}$
A_2 E' E''	T_2 U U	$\frac{-1}{2(2)}$
E E E	E' U U	$\frac{1}{2(2)}$
E E E	E'' U U	$\frac{1}{2(2)}$
E T_1 T_1	E' U U	$\frac{-1}{2(6)}$
E T_1 T_1	U E' U	$\frac{1}{2(30)}$
E T_1 T_1	U^* E' U	$\frac{3}{2(30)}$
$-E$ T_1 T_2	U U E'	$\frac{1}{2(6)}$
E T_1 T_2^*	U U E'	$\frac{-1}{2(6)}$
E T_1 T_1	E'' U U	$\frac{-1}{2(6)}$
E T_1 T_1	U E'' U	$\frac{-3}{2(30)}$
E T_1 T_1	U^* E'' U	$\frac{1}{2(30)}$
E T_1 T_2	E' U U	$\frac{1}{2(6)}$
E T_1 T_2	U E' U	$\frac{3}{2(30)}$
E T_1 T_2	U^* E' U	$\frac{-1}{2(30)}$
E T_1 T_2	E'' U U	$\frac{-1}{2(6)}$
E T_1 T_2	U E'' U	$\frac{1}{2(30)}$
E T_1 T_2	U^* E'' U	$\frac{3}{2(30)}$
$-E$ T_1 T_2	U U E''	$\frac{-1}{2(6)}$
E T_1 T_2	U U E''	$\frac{-1}{2(6)}$
E T_2 T_2	E' U U	$\frac{-1}{2(6)}$
$-E$ T_2 T_2	U E' U	$\frac{-1}{2(6)}$
E T_2 T_2	U^* E' U	$\frac{1}{2(6)}$
E T_2 T_2	E'' U U	$\frac{-1}{2(6)}$
$-E$ T_2 T_2	U E'' U	$\frac{-1}{2(6)}$
E T_2 T_2	U^* E'' U	$\frac{-1}{2(6)}$
T_1 T_1 T_1	E' U U	$\frac{5}{6(10)}$
T_1 T_1 T_1	E'' U U	$\frac{1}{2(10)}$
T_1 T_1 T_1	E'' U U^*	$\frac{2}{3(10)}$
T_1 T_1 T_2	E' U U	$\frac{-1}{2(30)}$
T_1 T_1 T_2	E' U U^*	$\frac{1}{(30)}$
T_1 T_2 T_2^*	U U E'	$\frac{-1}{2(6)}$
T_1 T_1 T_2	E'' U U	$\frac{-1}{2(30)}$
T_1 T_1 T_2	E'' U U^*	$\frac{1}{(30)}$
T_1 T_1 T_2^*	U U E''	$\frac{1}{2(6)}$
T_1 T_2 T_2	E' U U	$\frac{1}{2(10)}$
T_1 T_2 T_2	E' U U^*	$\frac{2}{3(10)}$
$-T_1$ T_2 T_2	U E' U	$\frac{-1}{3(2)}$
T_1 T_2 T_2	U^* E' U	$\frac{-1}{6(2)}$
T_1 T_2 T_2	E'' U U	$\frac{5}{6(10)}$
$-T_1$ T_2 T_2	U E'' U	$\frac{1}{3(2)}$
T_1 T_2 T_2	U^* E'' U	$\frac{-1}{6(2)}$
T_2 T_2 T_2	E' U U^*	$\frac{1}{2(6)}$
T_2 T_2 T_2	E'' U U^*	$\frac{-1}{2(6)}$
T_1 E' E'	E U U	$\frac{1}{2(10)}$
T_1 E' E'	E U U^*	$\frac{-1}{(10)}$
T_1 E' E'	T_1 U U	$\frac{5}{6(10)}$
T_1 E' E'	T_2 U U	$\frac{1}{2(10)}$
T_1 E' E'	T_2 U U^*	$\frac{2}{3(10)}$
T_2 E' E''	E U U^*	$\frac{1}{2(2)}$
T_1 E'' E''	E U U	$\frac{-1}{2(10)}$
$-T_2$ E' E''	T_1 U U	$\frac{1}{3(2)}$
T_2 E' E''	T_1 U U^*	$\frac{-1}{6(2)}$
$-T_2$ E' E''	T_2 U U	$\frac{-1}{3(2)}$
T_2 E' E''	T_2 U U^*	$\frac{-1}{6(2)}$
T_1 E'' E''	E U U^*	$\frac{1}{(10)}$
T_1 E'' E''	T_1 U U	$\frac{1}{2(10)}$
T_1 E'' E''	T_1 U U^*	$\frac{2}{3(10)}$
T_1 E'' E''	T_2 U U	$\frac{5}{6(10)}$

$W(abc/UUU)$: coefficients are ordered by the number abc

A_2 E E	U U U	$\frac{1}{2(2)}$
$-A_2$ T_1 T_2	U U U	$\frac{-1}{(15)}$
A_2 T_1 T_2^*	U^* U U	$\frac{1}{(15)}$
$-A_2$ T_1 T_2	U^* U U	$\frac{-1}{2(15)}$
A_2 T_1 T_2^*	U U U	$\frac{-1}{2(15)}$
E T_1 T_1	U U U	$\frac{-2}{5(6)}$
E T_1 T_1^*	U^* U U	$\frac{2}{5(6)}$
E T_1 T_1	U^* U U	$\frac{3}{10(6)}$
E T_2 T_1^*	U U U	$\frac{3}{10(6)}$
$-E$ T_1 T_2	U U U	$\frac{1}{2(30)}$
E T_1 T_2^*	U^* U U	$\frac{1}{2(30)}$
$-E$ T_1 T_2	U^* U U	$\frac{-1}{(30)}$
E T_1 T_2^*	U U U	$\frac{1}{(30)}$
$-E$ T_2 T_2	U^* U U	$\frac{-1}{2(6)}$
$-E$ T_2 T_2^*	U U U	$\frac{1}{2(6)}$
T_1 T_1 T_1	U U U	$\frac{-1}{3(10)}$
T_1 T_1 T_1^*	U^* U U	$\frac{1}{2(10)}$
T_1 T_1 T_1^*	U U U^*	$\frac{1}{2(10)}$
T_1 T_1 T_1	U^* U U^*	$\frac{1}{2(10)}$
T_1 T_1 T_1^*	U^* U U^*	$\frac{-1}{3(10)}$
$-T_1$ T_1 T_2	U U U^*	$\frac{1}{2(6)}$
$-T_1$ T_1 T_2	U^* U U	$\frac{-1}{2(6)}$
T_1 T_1 T_2^*	U U U	$\frac{-2}{5(6)}$
T_1 T_1 T_2^*	U^* U U	$\frac{-1}{5(6)}$
T_1 T_1 T_2^*	U U U^*	$\frac{-1}{5(6)}$
T_1 T_1 T_2^*	U^* U U^*	$\frac{-1}{10(6)}$
T_1 T_2 T_2	U U U	$\frac{-1}{6(10)}$
T_1 T_2 T_2	U U U^*	$\frac{1}{3(10)}$
$-T_1$ T_2 T_2	U^* U U	$\frac{-1}{3(10)}$
$-T_1$ T_2 T_2^*	U U U	$\frac{1}{3(10)}$
T_1 T_2 T_2^*	U^* U U	$\frac{-1}{3(10)}$
$-T_1$ T_2 T_2^*	U U U^*	$\frac{1}{6(10)}$
$-T_1$ T_2 T_2	U^* U U^*	$\frac{-1}{6(10)}$
T_1 T_2 T_2^*	U^* U U^*	$\frac{2}{3(10)}$
T_2 T_2 T_2	U U U^*	$\frac{-1}{2(6)}$
T_2 T_2 T_2	U^* U U	$\frac{-1}{2(6)}$
T_2 T_2 T_2^*	U U U	$\frac{-1}{2(6)}$

$W(abU/dUU)$: coefficients are ordered by the number ad

E E' U	E U U	$-\frac{1}{4}$
E E'' U	E U U	$-\frac{1}{4}$
E E' U	T_1 U U	$\frac{-1}{(20)}$
E E' U^*	T_1 U U	$\frac{-1}{2(20)}$
E E'' U	T_1 U U	$\frac{1}{(20)}$
E E'' U^*	T_1 U U	$\frac{1}{2(20)}$
$-E$ E' U	T_2 U U	$\frac{1}{4}$
$-E$ E'' U	T_2 U U	$\frac{1}{4}$
T_1 E' U	T_1 U U	$\frac{1}{6}$
T_1 E' U^*	T_1 U U^*	$-\frac{1}{4}$
T_1 E'' U	T_1 U U	$\frac{-1}{10}$
T_1 E'' U^*	T_1 U U^*	$\frac{1}{60}$
T_1 E'' U	T_1 U U^*	$\frac{1}{5}$
T_1 E'' U^*	T_1 U U	$\frac{1}{5}$
T_1 E' U^*	T_2 U U^*	$\frac{-1}{3(20)}$
$-T_1$ E' U	T_2 U U^*	$\frac{-5}{6(20)}$
T_1 E' U^*	T_2 U U	$\frac{1}{(20)}$
$-T_1$ E'' U	T_2 U U	$\frac{2}{3(20)}$
T_1 E'' U^*	T_2 U U^*	$\frac{1}{(20)}$
$-T_1$ E'' U	T_2 U U^*	$\frac{-1}{2(20)}$
T_1 E'' U^*	T_2 U U	$\frac{1}{3(20)}$
T_2 E' U	T_2 U U	$\frac{1}{12}$
T_2 E' U^*	T_2 U U^*	$-\frac{1}{6}$
$-T_2$ E' U	T_2 U U^*	$\frac{1}{6}$
$-T_2$ E' U^*	T_2 U U	$\frac{1}{6}$
T_2 E'' U	T_2 U U	$\frac{1}{12}$
T_2 E'' U^*	T_2 U U^*	$-\frac{1}{6}$
$-T_2$ E'' U	T_2 U U^*	$-\frac{1}{6}$
$-T_2$ E'' U^*	T_2 U U	$-\frac{1}{6}$

TABLE VII. (*Continued*)

$W(aUU/dUU)$: coefficients are ordered by the number ad

$\begin{matrix} A_2 & U & U \\ A_2 & U & U \end{matrix}$	$-\frac{1}{4}$	$\begin{matrix} A_2 & U & U \\ E & U & U \end{matrix}$	$-\frac{1}{4}$	$\begin{matrix} A_2 & U & U \\ T_1 & U & U \end{matrix}$	$\frac{3}{20}$	$\begin{matrix} A_2 & U & U^* \\ T_1^* & U & U \end{matrix}$	$-\frac{3}{20}$	$\begin{matrix} A_2 & U & U \\ T_1^* & U & U \end{matrix}$	$\frac{1}{5}$
$\begin{matrix} A_2 & U & U^* \\ T_1 & U & U \end{matrix}$	$\frac{1}{5}$	$\begin{matrix} A_2 & U & U \\ T_2 & U & U \end{matrix}$	$\frac{1}{4}$	$\begin{matrix} A_2 & U & U^* \\ T_2^* & U & U \end{matrix}$	$\frac{1}{4}$	$\begin{matrix} E & U & U \\ T_1 & U & U \end{matrix}$	$\frac{1}{20}$	$\begin{matrix} E & U & U^* \\ T_1^* & U & U \end{matrix}$	$\frac{1}{5}$
$\begin{matrix} E & U & U \\ T_1^* & U & U \end{matrix}$	$-\frac{1}{10}$	$\begin{matrix} E & U & U^* \\ T_1 & U & U \end{matrix}$	$-\frac{1}{10}$	$\begin{matrix} E & U & U^* \\ T_2^* & U & U \end{matrix}$	$\frac{1}{4}$	$\begin{matrix} T_1 & U & U \\ T_1 & U & U \end{matrix}$	$-\frac{11}{60}$	$\begin{matrix} T_1^* & U & U^* \\ T_1^* & U & U^* \end{matrix}$	$-\frac{1}{30}$
$\begin{matrix} T_1 & U & U^* \\ T_1^* & U & U \end{matrix}$	$\frac{3}{20}$	$\begin{matrix} T_1 & U & U^* \\ T_2 & U & U^* \end{matrix}$	$-\frac{1}{10}$	$\begin{matrix} T_1^* & U & U^* \\ T_1 & U & U \end{matrix}$	$-\frac{1}{10}$	$\begin{matrix} T_1^* & U & U \\ T_1^* & U & U \end{matrix}$	$-\frac{1}{10}$	$\begin{matrix} T_1^* & U & U \\ T_1 & U & U^* \end{matrix}$	$\frac{3}{20}$
$\begin{matrix} T_1 & U & U \\ T_1^* & U & U^* \end{matrix}$	$-\frac{1}{10}$	$\begin{matrix} T_1 & U & U^* \\ T_1^* & U & U^* \end{matrix}$	$-\frac{1}{10}$	$\begin{matrix} T_1^* & U & U^* \\ T_1^* & U & U \end{matrix}$	$-\frac{1}{10}$	$\begin{matrix} T_1^* & U & U^* \\ T_1 & U & U^* \end{matrix}$	$-\frac{1}{10}$	$\begin{matrix} T_1^* & U & U \\ T_1^* & U & U^* \end{matrix}$	$-\frac{1}{10}$
$\begin{matrix} T_1 & U & U \\ T_2 & U & U \end{matrix}$	$\frac{3}{20}$	$\begin{matrix} T_1^* & U & U^* \\ T_2^* & U & U^* \end{matrix}$	$-\frac{1}{20}$	$\begin{matrix} T_1^* & U & U \\ T_2 & U & U \end{matrix}$	$\frac{1}{30}$	$\begin{matrix} T_1 & U & U \\ T_2 & U & U^* \end{matrix}$	$\frac{1}{30}$	$\begin{matrix} T_1 & U & U^* \\ T_2^* & U & U \end{matrix}$	$\frac{1}{20}$
$\begin{matrix} -T_1 & U & U^* \\ T_2 & U & U^* \end{matrix}$	$-\frac{1}{6}$	$\begin{matrix} -T_1^* & U & U^* \\ T_2 & U & U \end{matrix}$	$\frac{1}{6}$	$\begin{matrix} -T_1^* & U & U \\ T_2^* & U & U \end{matrix}$	$-\frac{1}{6}$	$\begin{matrix} T_1^* & U & U \\ T_2 & U & U^* \end{matrix}$	$\frac{1}{10}$	$\begin{matrix} -T_1 & U & U \\ T_2^* & U & U^* \end{matrix}$	$\frac{1}{6}$
$\begin{matrix} T_1 & U & U^* \\ T_2^* & U & U^* \end{matrix}$	$\frac{1}{15}$	$\begin{matrix} T_1^* & U & U^* \\ T_2^* & U & U \end{matrix}$	$\frac{1}{15}$	$\begin{matrix} T_2 & U & U \\ T_2 & U & U \end{matrix}$	$-\frac{1}{6}$	$\begin{matrix} T_2^* & U & U^* \\ T_2^* & U & U^* \end{matrix}$	$\frac{1}{12}$	$\begin{matrix} T_2 & U & U^* \\ T_2^* & U & U \end{matrix}$	$\frac{1}{12}$
$\begin{matrix} T_2 & U & U^* \\ T_2 & U & U^* \end{matrix}$	$-\frac{1}{6}$	$\begin{matrix} T_2^* & U & U^* \\ T_2 & U & U \end{matrix}$	$-\frac{1}{6}$	$\begin{matrix} T_2^* & U & U \\ T_2^* & U & U \end{matrix}$	$-\frac{1}{6}$	$\begin{matrix} T_2^* & U & U \\ T_2 & U & U^* \end{matrix}$	$\frac{1}{12}$	$\begin{matrix} T_2 & U & U \\ T_2^* & U & U^* \end{matrix}$	$-\frac{1}{6}$

$$W\begin{pmatrix} a_i & b & c_l \\ d_k & e & f_j \end{pmatrix} = W\begin{pmatrix} c_i & b & a_j \\ f_k & e & d_l \end{pmatrix} , \tag{13b}$$

$$W\begin{pmatrix} a_i & b & c_l \\ d_k & e & f_j \end{pmatrix} = W\begin{pmatrix} b_i & c & a_j \\ e_l & f & d_k \end{pmatrix} . \tag{13c}$$

The cases for which the representations are not invariant involve V_1 and V_2 for $U'\,U'\,T_2$ as might be expected. Specifically, an odd permutation of columns introduces a factor

$$W\begin{pmatrix} a_i & b & c_l \\ d_k & e & f_j \end{pmatrix} = (-1)^{2d+2e+2f}\,(-1)^{a+b+c_i}\,(-1)^{a+e+f_j} \times (-1)^{b+f+d_k}\,(-1)^{c+d+e_l}\, W\begin{pmatrix} c_i & b & a_j \\ f_k & e & d_l \end{pmatrix} .$$

The factor is always equal to $+1$ for the full rotation group and the single groups. With our choice of phase factors, it is always $+1$ for O* unless an odd number of the triplets abc, aef, bfd, and cde which form W are $U'\,U'\,T_{2a}$. In this case the factor is -1. Equation (13b) should be rewritten as

$$W\begin{pmatrix} a_i & b & c_l \\ d_k & e & f_j \end{pmatrix} = (-1)^{n(U'U'T_{2a})}\, W\begin{pmatrix} c_i & b & a_j \\ f_k & e & d_l \end{pmatrix} , \tag{13b'}$$

where $n(U'\,U'\,T_{2a})$ is the number of $U'\,U'\,T_{2a}$ triplets. In Table VII any W coefficient which changes sign under an odd permutation of columns is preceded by a minus sign.

There are several relationships between V and W coefficients which are useful in applications of tensor theory. They are generally derived from a variation of the definition of W:

$$\delta_{\gamma\gamma'}\,\delta_{cc'}\,\lambda(c)^{-1}\, W\begin{pmatrix} a_i & b & c_l \\ d_k & e & f_j \end{pmatrix} = \sum_{\alpha\beta\delta\epsilon\phi} (-1)^{a-\alpha+b-\beta+c-\gamma+d-\delta+e-\epsilon+f-\phi} \times V_i\begin{pmatrix} a & b & c \\ -\alpha & -\beta & -\gamma \end{pmatrix} V_j\begin{pmatrix} a & e & f \\ \alpha & \epsilon & -\phi \end{pmatrix} \times V_k\begin{pmatrix} b & f & d \\ \beta & \phi & -\delta \end{pmatrix} V_l\begin{pmatrix} c' & d & e \\ \gamma' & \delta & -\epsilon \end{pmatrix} . \tag{14}$$

Multiplying both sides by $\lambda(c)V(abc;\alpha'\beta'\gamma)$ and summing over c and γ, we find that

$$\sum_c \delta_{cc'}\, V\begin{pmatrix} a & b & c \\ \alpha' & \beta' & \gamma \end{pmatrix} W\begin{pmatrix} a & b & c_l \\ d_k & e & f_j \end{pmatrix} = \sum_{\alpha\beta\gamma\delta\epsilon\phi,c} (-1)^{d-\delta+e-\epsilon+f-\phi}\,\lambda(c)\, V\begin{pmatrix} a & b & c \\ \alpha' & \beta' & \gamma \end{pmatrix} \times V\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} V_j\begin{pmatrix} a & e & f \\ \alpha & \epsilon & -\phi \end{pmatrix} \times V_k\begin{pmatrix} b & f & d \\ \beta & \phi & -\delta \end{pmatrix} V_l\begin{pmatrix} c' & d & e \\ \gamma' & \delta & -\epsilon \end{pmatrix} . \tag{15}$$

We drop the subscript i since the sum over c is over all the representations contained in $a\times b$ and both V_1 and V_2 would appear in the sum if c were a repeated representation. Using Eq. (7) and then dropping the primes we obtain the most important of the V, W equations:

$$V_1\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} W\begin{pmatrix} a_1 & b & c_l \\ d_k & e & f_j \end{pmatrix} + V_2\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} W\begin{pmatrix} a_2 & b & c_l \\ d_k & e & f_j \end{pmatrix} = \sum_{\delta\epsilon\phi} (-1)^{d-\delta+e-\epsilon+f-\phi}\, V_j\begin{pmatrix} a & e & f \\ \alpha & \epsilon & -\phi \end{pmatrix} \times V_k\begin{pmatrix} b & f & d \\ \beta & \phi & -\delta \end{pmatrix} V_l\begin{pmatrix} c & d & e \\ \gamma & \delta & -\epsilon \end{pmatrix} . \tag{16}$$

The form of the equation above is the most general and occurs if c is a repeated representation in $a\times b$. If this were not the case, the left-hand side of Eq. (16) would contain only one term.

V. DOUBLE-TENSOR OPERATORS

The real power of the irreducible-tensor method lies in the formulas for the evaluation of double-tensor operators. If we have two spaces A and B, we may combine functions in the two spaces to form irreducible representations in their direct-product space C using vector coupling coefficients

$$|abc\gamma\rangle = \sum_{\alpha\beta} \langle abc\gamma | ab\alpha\beta\rangle \, |ab\alpha\beta\rangle \; . \tag{17}$$

In an identical manner, operators D and E which operate only in the spaces A and B, respectively, may be combined to form irreducible-tensor operators in the direct-product space

$$(D^d \times E^e)^f_\phi = \sum_{\delta\epsilon} \langle def\phi | de\delta\epsilon\rangle D^d_\delta E^e_\epsilon \; . \tag{18}$$

We would like to be able to express matrix elements of operators in the combined space as functions of matrix elements in the separate spaces. An often encountered case is that of A being xyz coordinate space and B being spin space. If the functions in these spaces form bases for irreducible representations of the groups O and SU(2), respectively, the product group is O*. If, as is the case with O and SU(2), the groups are simply reducible, a matrix element in which the functions and operators are simple products may be written

$$\langle ab\alpha\beta | D^d_\delta E^e_\epsilon | a'b'\alpha'\beta'\rangle = (-1)^{a-\alpha+b-\beta} \, V\begin{pmatrix} a & a' & d \\ -\alpha & \alpha' & \delta \end{pmatrix} V\begin{pmatrix} b & b' & e \\ -\beta & \beta' & \epsilon \end{pmatrix} \langle a \| D^d \| a'\rangle \langle b \| E^e \| b'\rangle \; . \tag{19}$$

The V in each case would be those appropriate to the groups G_A and G_B in the spaces A and B. As discussed in an earlier section, the V coefficients for O* have been chosen so that they are identical to those of Fano and Racah for SU(2) for spins of 0 to $\frac{3}{2}$.

A matrix element written in terms of irreducible-tensorial sets of the product space would be

$$\begin{aligned} \langle abc_i\gamma | (D^d \times E^e)^f_\phi \, | a'b'c'_j\gamma'\rangle = {} & (-1)^{c-\gamma} V_1\begin{pmatrix} c & c' & f \\ -\gamma & \gamma' & \phi \end{pmatrix} \langle abc_i \| (D^d \times E^e)^f \| a'b'c'_j\rangle_1 \\ & + (-1)^{c-\gamma} V_2\begin{pmatrix} c & c' & f \\ -\gamma & \gamma' & \phi \end{pmatrix} \langle abc_i \| (D^d \times E^e)^f \| a'b'c'_j\rangle_2 \; . \end{aligned} \tag{20}$$

Multiplying both sides by $(-1)^{c-\gamma} V_k(ccf; -\gamma\gamma'\phi)$ and summing over γ, γ', ϕ, we find

$$\langle abc_i \| (D^d \times E^e)^f \| a'b'c'_j\rangle_k = \sum_{\gamma\gamma'\phi} \langle abc_i\gamma | (D^d \times E^e)^f_\phi \, | a'b'c'_j\gamma'\rangle (-1)^{c-\gamma} V_k\begin{pmatrix} c & c' & f \\ -\gamma & \gamma' & \phi \end{pmatrix} \; , \tag{21}$$

where k is equal to 1 or 2 as in Eq. (2). Using Eqs. (17)–(19), this becomes

$$\begin{aligned} \langle abc_i \| (D^d \times E^e)^f \| a'b'c'_j\rangle_k = {} & \sum_{\alpha\beta\delta\epsilon\alpha'\beta'\gamma\gamma'\phi} (-1)^{c-\gamma} V_k\begin{pmatrix} c & c' & f \\ -\gamma & \gamma' & \phi \end{pmatrix} (-1)^{a-\alpha} V\begin{pmatrix} a & a' & d \\ -\alpha & \alpha' & \delta \end{pmatrix} \langle a \| D^d \| a'\rangle \\ & \times (-1)^{b-\beta} V\begin{pmatrix} b & b' & e \\ -\beta & \beta' & \epsilon \end{pmatrix} \langle b \| E^e \| b'\rangle \langle abc_i\gamma | ab\alpha\beta\rangle \langle a'b'c'_j\gamma' | a'b'\alpha'\beta'\rangle \langle def\phi | de\delta\epsilon\rangle \; . \end{aligned} \tag{22}$$

Finally, replacing the vector coupling coefficients with V coefficients according to Eq. (4), we may write the matrix element as

$$\begin{aligned} \langle abc_i \| (D^d \times E^e)^f \| a'b'c'_j\rangle_k = {} & \lambda(c)^{1/2} \lambda(c')^{1/2} \lambda(f)^{1/2} \langle a \| D^d \| a'\rangle \langle b \| E^e \| b'\rangle (-1)^{2b+2b'+2e} \\ & \times \sum_{\alpha\beta\delta\epsilon\alpha'\beta'\gamma\gamma'\phi} (-1)^{c'-\gamma'+f-\phi+a-\alpha+b-\beta} \left[V_i\begin{pmatrix} a & b & c \\ \alpha & \beta & -\gamma \end{pmatrix} V\begin{pmatrix} d & e & f \\ \delta & \epsilon & -\phi \end{pmatrix} V_j\begin{pmatrix} a' & b' & c' \\ \alpha' & \beta' & -\gamma' \end{pmatrix} \right. \\ & \left. V_k\begin{pmatrix} c & c' & f \\ -\gamma & \gamma' & \phi \end{pmatrix} V\begin{pmatrix} a & a' & d \\ -\alpha & \alpha' & \delta \end{pmatrix} V\begin{pmatrix} b & b' & e \\ -\beta & \beta' & \epsilon \end{pmatrix} \right] \; . \end{aligned} \tag{23}$$

Two important special cases occur whenever either E or D is the scalar operator 1. Using the fact that $V(bbA_1; -\beta\beta\iota) = (-1)^{b-\beta}/\lambda(b)^{1/2}$, Eq. (23) reduces in the first case to

$$\langle abc_i \| D^d \| a'b'c'_j\rangle_k = \lambda(c)^{1/2} \lambda(c')^{1/2} \delta_{bb'} (-1)^{a+b+c_i} (-1)^{c+c'+d_k} (-1)^{2a+2c+2a'} \, W\begin{pmatrix} c_k & d & c'_j \\ a' & b & a_i \end{pmatrix} \langle a \| D^d \| a'\rangle \tag{24}$$

and in the second case to

$$\langle abc_i \| E^e \| a'b'c'_j\rangle_k = \lambda(c)^{1/2}\lambda(c')^{1/2}\delta_{aa'}(-1)^{a'+b'+c'_j}(-1)^{c+c'+e_k}(-1)^{2c'+2e}\, W\begin{pmatrix} c_k & e & c'_j \\ b' & a & b_i \end{pmatrix}\langle b \| E^e \| b'\rangle . \quad (25)$$

An interesting variation of the special cases occurs if either of the groups to which a, a' and b, b' belong are not simply reducible. For example, if the group in space A is O^*, Eq. (19) would have to be rewritten in the more general form

$$\langle ab\alpha\beta | D^d_\delta E^e_\epsilon | a'b'\alpha'\beta'\rangle = (-1)^{b-\beta} V\begin{pmatrix} b & b' & e \\ -\beta & \beta' & \epsilon \end{pmatrix}\langle b \| E^e \| b'\rangle$$
$$\times(-1)^{a-\alpha}\left[V_1\begin{pmatrix} a & a' & d \\ -\alpha & \alpha' & \delta \end{pmatrix}\langle a \| D^d \| a'\rangle_1 + V_2\begin{pmatrix} a & a' & d \\ -\alpha & \alpha' & \delta \end{pmatrix}\langle a \| D^d \| a'\rangle_2\right] . \quad (26)$$

Carrying this through, we find Eq. (24) would become

$$\langle abc_i \| D^d \| a'b'c'_j\rangle_k = \lambda(c)^{1/2}\lambda(c')^{1/2}\delta_{bb'}(-1)^{a+b+c_i}(-1)^{c+c'+d_k}(-1)^{2a+2c+2a'}$$
$$\times\left[W\begin{pmatrix} c_k & d & c'_j \\ a'_1 & b & a_i \end{pmatrix}\langle a \| D^d \| a'\rangle_1 + W\begin{pmatrix} c_k & d & c'_j \\ a'_2 & b & a_i \end{pmatrix}\langle a \| D^d \| a'\rangle_2\right] . \quad (27)$$

This particular equation plays an important part in the development of the theory of j-j coupling in an octahedral molecule in the strong-field limit. This theory will be presented in a subsequent paper.

VI. SPIN-ORBIT COUPLING

Matrix elements for functions in a spin-orbit basis, designated $Sht\tau$, are easily expressed in terms of matrix elements in the L-S coupling basis, designated by $ShM\theta$, with the use of W coefficients when the operator is a one-electron operator. For the spin-orbit Hamiltonian operator $\mathcal{H}_{so}$ the relation is expressed using $\Omega_{JJ'}$ coefficients:

$$\langle Sht_J\tau | \mathcal{H}_{so} | S'h't_{J'}\tau\rangle = \Omega_{JJ'}\begin{pmatrix} S & S' & T_1 \\ h' & h & t \end{pmatrix}\langle Sh \| \mathcal{H}_{so} \| S'h'\rangle . \quad (28)$$

Griffith[2] showed that for $S = 0$ or 1, the Ω coefficient is proportional to a W coefficient. In fact, the relationship holds for spins of $\frac{1}{2}$ and $\frac{3}{2}$ as well:

$$\Omega_{JJ'}\begin{pmatrix} S & S' & T_1 \\ h' & h & t \end{pmatrix} = (-1)^{2S}(-1)^{S+S'+T_{1a}}(-1)^{S+h+t_J} \times W\begin{pmatrix} S_1 & T_1 & S' \\ h'_{J'} & t & h_J \end{pmatrix} . \quad (29)$$

In the above expression, one replaces the spins S and S' by the appropriate representation A_1, E', T_1, or U'. When S and S' equal $\frac{3}{2}$, the correct $U'U'T_1$ to use is $U'U'T_{1a}$. In using this formula and others involving spin-orbit coupling, one must remember that our U' functions arising from ${}^4T_2$ are not the states which diagonalize $\mathcal{H}_{so}$ and we must transform back to the U' functions of Griffith[8] in most physical problems.

The double-tensor formulas derived in Sec. V may be applied directly to the calculation of one-electron operators which operate only on the space or only on the spin portion of a spin-orbit wave function. This is an extension of Griffith's Sec. 9.7.[2] To illustrate the application of the formulas and to clarify the W coefficient notation, all of the reduced matrix elements of the U' states of ${}^4T_1$ for the magnetic moment operator $\mu = -\beta L - 2\beta S$ shall be evaluated in some detail in terms of matrix elements in the L-S basis. From Eq. (2) there are two reduced matrix elements for any pair of U' states. Abbreviating $\langle T_1 \| -\beta L \| T_1\rangle$ as $\langle L\rangle$ and $\langle\frac{3}{2} \| -2\beta S \| \frac{3}{2}\rangle$ as $\langle S\rangle$, we may write

$$\langle U'_i \| \mu \| U'_j\rangle_k = \lambda(U')(-1)^{2U'}(-1)^{U'+U'+T_{1k}}$$
$$\times\left[(-1)^{U'+U'+T_{1i}}\, W\begin{pmatrix} U'_k & T_1 & U'_j \\ T_1 & U' & T_{1i} \end{pmatrix}\langle L\rangle + (-1)^{U'+U'+T_{1j}}\, W\begin{pmatrix} U'_k & T_2 & U'_j \\ U'_1 & T_1 & U'_i \end{pmatrix}\langle S\rangle\right] . \quad (30)$$

In writing the subscripts for the U' representations of $T_1 \times U'$, Griffith[8] uses the $\frac{3}{2}, \frac{5}{2}$ notation while we use 1 and 2, respectively, in the W coefficient to indicate which V coefficients are being used to form the representations. Using Eqs. (13), we may rearrange the W coefficients

$$W\begin{pmatrix} U'_k & T_1 & U'_j \\ T_1 & U' & T_{1i} \end{pmatrix} = W\begin{pmatrix} T_1 & T_1 & T_{1i} \\ U'_k & U' & U'_j \end{pmatrix}$$

and

$$W\begin{pmatrix} U'_k & T_1 & U'_j \\ U'_1 & T_1 & U'_i \end{pmatrix} = W\begin{pmatrix} T_{1k} & U' & U'_i \\ T_{1j} & U' & U'_1 \end{pmatrix}$$

to facilitate use of Table VII. The subscript 1 in the above W coefficient arises from the spin matrix element $\langle\frac{3}{2} \| -2\beta S \| \frac{3}{2}\rangle$. Using the tables we find

$$\langle U'_{3/2} \| \mu \| U'_{3/2}\rangle_1 = -4\left((-1/3\sqrt{10})\langle L\rangle + \tfrac{-11}{60}\langle S\rangle\right) ,$$

$$\langle U'_{3/2} \| \mu \| U'_{3/2} \rangle_2 = -4\,(0\langle L\rangle + 0\langle S\rangle)\,,$$

$$\langle U'_{3/2} \| \mu \| U'_{5/2} \rangle_1 = -4\,(0\langle L\rangle + 0\langle S\rangle)\,,$$

$$\langle U'_{3/2} \| \mu \| U'_{5/2} \rangle_2 = -4\left((1/2\sqrt{10})\langle L\rangle + \tfrac{-1}{10}\langle S\rangle\right),$$

$$\langle U'_{5/2} \| \mu \| U'_{5/2} \rangle_1 = -4\left((1/2\sqrt{10})\langle L\rangle + \tfrac{3}{20}\langle S\rangle\right),$$

$$\langle U'_{5/2} \| \mu \| U'_{5/2} \rangle_2 = -4\left((-1/3\sqrt{10})\langle L\rangle + \tfrac{-1}{10}\langle S\rangle\right).$$

VII. CONCLUSIONS

Elements of the irreducible-tensor theory for the octahedral double group O* have been presented. The choice of phase factors is such that the theory is compatible with the work of Fano and Racah for spin functions. In addition, W coefficients and phase factors involving the representations A_1, A_2, E, T_1, and T_2 agree with those of Griffith[2] and his formulas may be used for evaluating reduced matrix elements for these representations. All of these formulas must be altered to some extent for the E', E'', and U' representations, as will be done in future papers in conjunction with two particularly interesting applications. The first is the development of a theory of j-j coupling in octahedral molecules in the strong-field limit. Here, octahedral symmetry orbitals are first combined with spin functions to form e', e'', and u' molecular spin-orbitals which are then used to form configurations. The second application, and the one which initially prompted this investigation, is the calculation of the Faraday-effect parameters A/D, B/D, and C/D for electronic and vibronic transitions.

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‡Present address: Department of Chemistry, Mt. Holyoke College, South Hadley, Mass. 01075.

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$$\overline{V}(j_1 j_2 j_3; m_1 m_2 m_3) = (-1)^{j_1+j_2+j_3}(j_1 j_2 j_3; m_1 m_2 m_3).$$

[13]G. F. Koster, Phys. Rev. 109, 227 (1958).

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