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Monomial representation of point-group symmetries

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Most irreducible-matrix representations in point-group symmetries can adopt monomial form. In that case all representational matrices have only one nonzero element in each row and column. The so-obtained standard basis choice contrasts with the conventional Wigner-Racah option. Monomial representations give rise to interesting properties of the corresponding Clebsch-Gordan series: All coupling coefficients are equal in absolute value and a natural intrinsic multiplicity separation is obtained. The concept is also useful in reaching a consistent solution of the multiplicity problem in the reduction of direct products, involving the fourfold U' representation of the octahedral spinor group. Several tables of basis transformations and coupling coefficients in octahedral and icosahedral symmetries are included.

I. INTRODUCTION

Wigner and Racah have profoundly influenced the theory of matrix representations in molecular symmetry groups, by introducing a set of standard conditions, known as the $|JM\rangle$ basis of angular momentum theory.[1] From this basis set, irredicible-matrix representations along a chain of point groups are easily subduced. This approach has found general favor for several reasons.[2,3] Calculation of the so-called Clebsch-Gordan coupling coefficients (CGC's) is amenable to algorithmic standardization. Moreover, finite symmetries often arise as small distortions from parent continuous groups, suggesting an obvious parallelism between perturbation theory and subduction process. This is often the case in typical central field problems. As an example, the present interest resulted from a ligand-field-theory issue.[4–6]

The standard basis relationships of the Wigner-Racah calculus confer interesting mathematical properties on the corresponding Clebsch-Gordan series. They impose in the symmetry group a fixed inner automorphism, carrying all standard representations into their complex conjugates. As a result, all CGC's can be chosen to be real.[7,8] On the other hand, a possible drawback of uniform standardization is that alternative, equally interesting mathematical aspects of the Clebsch-Gordan series may never appear, unless a conflicting basis option is made. Monomial representations, that apply to most point groups, offer interesting perspectives in this respect. Ultimately, they might lead to additional insight in the coupling process itself.

II. MONOMIAL REPRESENTATIONS

Let $\mathfrak{C}$ be an Abelian group. A *monomial matrix* with respect to $\mathfrak{C}$ is a matrix which contains one and only one element of $\mathfrak{C}$ in each row and column, the remaining coefficients of the matrix being zeros.[9] In the present context, all matrices are unitary, and hence $\mathfrak{C}$ is the group of unimodular complex numbers; elements of $\mathfrak{C}$ will be denoted by greek lower case characters. A *monomial representation* of a symmetry group is a matrix representation, uniquely consisting of monomial matrices. The concept will also be used in conjunction with the *functional basis set* of a monomial representation. It is by no means evident that every irreducible-matrix representation is equivalent to a monomial representation.

Powerful group-theoretical techniques have been developed that deal with this problem at large. Here an algebraic outline will be preferred in order to confront the monomial concept with the conventional basis choice. The proof that a given representation is monomial reduces to verifying that the representational matrices of the group generators can be brought into monomial form, whereas a matrix product conserves the monomial property of its factors. If only one generator is present—i.e., in cyclic groups—the problem is trivial since all irreducible representations are nondegenerate and *de facto* monomial. In the less trivial case of more than one generator, the problem is to decide whether or not there exists a single unitary transformation that converts a set of generator matrices *simultaneously* into monomial equivalents. To this aim a covering set of matrix equations has to be solved. The algebra involved will be examined, starting from the conventional representation standards.

In the Fano-Racah representation,[1] one single axis of quantization, commonly identified with the z direction, enables to distinguish all partners of a given J value. In particular, adhering to an active view of rotations,[2] an n-fold axis $\mathscr{C}_n^z$ rotates the $|JM\rangle$ basis[2] according to

$$\mathscr{C}_n^z\,|JM\rangle=|JM\rangle\exp\left[-i\frac{2\pi}{n}M\right]. \quad (1)$$

As an example, a fivefold rotational axis, $\mathscr{C}_5^z$, suffices to separate the five d functions. Arranging the d basis[10] in a row vector

$$\vec{\mathrm{d}}=(\,|d2\rangle\,|d1\rangle\,|d0\rangle\,|d-1\rangle\,|d-2\rangle)$$

one obtains

$$\mathscr{C}_5^z\vec{\mathrm{d}}=\vec{\mathrm{d}}\begin{bmatrix}\bar\epsilon^2 & & & & \\ & \bar\epsilon & & & \\ & & 1 & & \\ & & & \epsilon & \\ & & & & \epsilon^2\end{bmatrix}, \quad (2)$$

where

$$\epsilon=\exp\left[\frac{2\pi i}{5}\right]$$

and the overbar symbolizes complex conjugation. The matrix in Eq. (2) will be denoted C_5 and is monomial. Limiting the group of all rotations in three dimensions to its icosahedral rotational subgroup $\mathfrak{H}$, the $J=2$ basis is subduced in a trivial way, and without loss of degeneracy, to the fivefold degenerate representation V. (The notation follows Ref. 4.)

$\mathfrak{H}$ can be generated by only two elements, including $\mathscr{C}_5^z$. However, with the exception of $\mathscr{C}_5^z$, the Fano-Racah representation does not allow other generators of $\mathfrak{H}$ to yield monomial matrices. The reason is obvious. Monomial matrices are homomorphous to permutational matrices and map basis functions precisely onto each other, changing phases when necessary. Clearly irreducibility presupposes that all components take part in this mapping. On the other hand, no symmetry element can perform a congruence operation between the $|d0\rangle$ function and any other component, because of the unique functional form of the $M=0$ partner. $|d0\rangle$ will always either be invariant, or transform into a linear combination of more than one basis function. Hence, to arrive at a monomial basis set, one is forced to take a stand that is exactly the opposite of the conventional choice. Now it is required that all basis functions coalesce under the very symmetry operation that was previously selected as a splitting field. Since the splitting field generates a cyclic subgroup, in this case of order 5, its only monomial matrix representation will either be diagonal or homomorphous to a cyclic permutation of the same order. The former alternative being discarded, let B be the unitary transformation, which carries d into a primed set $\vec{\mathrm{d}}\,'$, $\vec{\mathrm{d}}\,'=\vec{\mathrm{d}}\,B$, with

$$\vec{\mathrm{d}}\,'\equiv(\,|Va\rangle\,|Vb\rangle\,|Vc\rangle\,|Vd\rangle\,|Ve\rangle) \quad (3)$$

so that the primed analog of C_5 has the structure of a cyclic permutation. That is,

$$\bar B^{\dagger}C_5B=\begin{bmatrix}0&\kappa&0&0&0\\0&0&\lambda&0&0\\0&0&0&\mu&0\\0&0&0&0&\nu\\\pi&0&0&0&0\end{bmatrix},$$

$$\bar B^{\dagger}B=B\bar B^{\dagger}=I\,. \quad (4)$$

In Eq. (4), $\bar B^{\dagger}$ denotes the complex conjugate transposed of B, I is the 5×5 unit matrix, and the Greek lower case characters are unimodular parameters, satisfying the closure relation $\kappa\lambda\mu\nu\pi=1$. The permutational sequence in Eq. (4) is arbitrary, since $\vec{\mathrm{d}}\,'$ can only be defined within monomial equivalence. (Two monomial matrices are said to be monomially equivalent if they can be transformed into each other by a monomial matrix.) Equation (4) can be solved in a straightforward manner. Four new unimodular constants appear[11] (α, β, γ and δ):

$$B=\frac{1}{\sqrt5}\begin{bmatrix}\epsilon\alpha\bar\kappa\bar\lambda & \bar\epsilon^2\alpha\bar\lambda & \alpha & \epsilon^2\alpha\mu & \bar\epsilon\alpha\mu\nu\\ \bar\epsilon^2\beta\bar\kappa\bar\lambda & \bar\epsilon\beta\bar\lambda & \beta & \epsilon\beta\mu & \epsilon^2\beta\mu\nu\\ \bar\kappa\bar\lambda & \bar\lambda & 1 & \mu & \mu\nu\\ \epsilon^2\gamma\bar\kappa\bar\lambda & \epsilon\gamma\bar\lambda & \gamma & \bar\epsilon\gamma\mu & \bar\epsilon^2\gamma\mu\nu\\ \bar\epsilon\delta\bar\kappa\bar\lambda & \epsilon^2\delta\bar\lambda & \delta & \bar\epsilon^2\delta\mu & \epsilon\delta\mu\nu\end{bmatrix}. \quad (5)$$

This result is quite general: Any $\{\,|JM\rangle\}$ basis, with integral J value, can similarly be transformed into an equivalent orthonormal basis of indistinguishable partners. The loss of individuality in the partners reveals a true characteristic of a monomial basis, e.g., all V components have the same self-repulsion integral.

Still B has a considerable internal degree of freedom, since all phase factors in Eq. (4), ϵ excepted, are as yet undefined. The next step is to obtain the B transform of the other group generator representations, yielding matrices containing the unknown phase factors as variables. The problem whether or not these phases can be fixed so that the resulting matrices are monomial, can now, in principle, be solved by linear algebra, although the resulting

TABLE I. Behavior of basis kets belonging to irreducible monomial representations of the octahedral ($\mathfrak{O}$) and icosahedral ($\mathfrak{H}$) group under useful symmetry elements. (See also Fig. 1.) The monomial E components can be obtained from the real quadrupole functions: $|E_b^a\rangle = 1/\sqrt{2}(|d_{z^2}\rangle \pm i\,|d_{x^2-y^2}\rangle)$. For the relation between the monomial V components and the d functions, see text. All rotations are counterclockwise and rotate functions, not coordinate systems, e.g., $\mathscr{C}_4^x\,|Ea\rangle = \bar{\omega}\,|Eb\rangle$; $\omega = \exp(2\pi i/3)$.

$\mathfrak{O}$	$\mathscr{C}_4^z$	$\mathscr{C}_4^x$	$\mathscr{C}_3^{xyz}$	$\mathscr{C}_2^y$
$\lvert Ea\rangle$	$\lvert Eb\rangle$	$\bar{\omega}\lvert Eb\rangle$	$\bar{\omega}\lvert Ea\rangle$	$\lvert Ea\rangle$
$\lvert Eb\rangle$	$\lvert Ea\rangle$	$\omega\lvert Ea\rangle$	$\omega\lvert Eb\rangle$	$\lvert Eb\rangle$
$\lvert T_1x\rangle$	$\lvert T_1y\rangle$	$\lvert T_1x\rangle$	$\lvert T_1y\rangle$	$-\lvert T_1x\rangle$
$\lvert T_1y\rangle$	$-\lvert T_1x\rangle$	$\lvert T_1z\rangle$	$\lvert T_1z\rangle$	$\lvert T_1y\rangle$
$\lvert T_1z\rangle$	$\lvert T_1z\rangle$	$-\lvert T_1y\rangle$	$\lvert T_1x\rangle$	$-\lvert T_1z\rangle$
$\lvert T_2yz\rangle$	$-\lvert T_2xz\rangle$	$-\lvert T_2yz\rangle$	$\lvert T_2xz\rangle$	$-\lvert T_2yz\rangle$
$\lvert T_2xz\rangle$	$\lvert T_2yz\rangle$	$-\lvert T_2xy\rangle$	$\lvert T_2xy\rangle$	$\lvert T_2xz\rangle$
$\lvert T_2xy\rangle$	$-\lvert T_2xy\rangle$	$\lvert T_2xz\rangle$	$\lvert T_2yz\rangle$	$-\lvert T_2xy\rangle$
$\mathfrak{H}$	$\mathscr{C}_5^z$	$\mathscr{C}_3^{111}$	$\mathscr{C}_3^{\bar{1}11}$	$\mathscr{C}_2^y$
$\lvert Va\rangle$	$\omega\lvert Ve\rangle$	$\omega\lvert Va\rangle$	$\bar{\omega}\lvert Va\rangle$	$\lvert Vc\rangle$
$\lvert Vb\rangle$	$\omega\lvert Va\rangle$	$\lvert Vd\rangle$	$\omega\lvert Vc\rangle$	$\lvert Vb\rangle$
$\lvert Vc\rangle$	$\bar{\omega}\lvert Vb\rangle$	$\bar{\omega}\lvert Vc\rangle$	$\lvert Ve\rangle$	$\lvert Va\rangle$
$\lvert Vd\rangle$	$\bar{\omega}\lvert Vc\rangle$	$\lvert Ve\rangle$	$\omega\lvert Vd\rangle$	$\lvert Ve\rangle$
$\lvert Ve\rangle$	$\lvert Vd\rangle$	$\lvert Vb\rangle$	$\bar{\omega}\lvert Vb\rangle$	$\lvert Vd\rangle$

equations are rather intricate because of the large number of unknowns.

At this point it is preferable to recur to the group-theoretical results, that allow to predict when and how a given irreducible representation can be made monomial. First we note that an induced[12] representation always will be monomial if it is induced from a one-dimensional or monomial subgroup representation; however, will it be irreducible? While this is not necessarily so, the reverse implication is an important lemma of induction[13]: *any irreducible monomial representation is an induced monomial representation.* This lemma provides a sufficient criterion to determine the monomial representations in the point group of interest.

As an example, all more-dimensional irreducible representations in the group $\mathfrak{O}$, describing the rotations of the octahedron, can easily be induced from one-dimensional subgroup representations, and are consequently monomial. Corresponding standard basis choices are listed in Table I (see also Ref. 4). T_1 and T_2 are induced from, respectively, the A_2 and B_2 representation in the dihedral subgroup $\mathfrak{D}_4$. E can be obtained by induction from the one-dimensional complex representation Γ_2 in the tetrahedral subgroup $\mathfrak{T}$. The same Γ_2 representation also directly induces V in $\mathfrak{H}$. Hence the fivefold degenerate representation in the icosahedron is monomial.[9] Table I contains the transformational properties of V for several generators of $\mathfrak{H}$. Their orientation in a dodecahedron is displayed in Fig. 1. From Table I both representations (E and V) induced from Γ_2 are seen to be monomial with respect to the cyclic Abelian group $\mathfrak{C}_3 = \{\omega, \bar{\omega}, 1\}$. Having

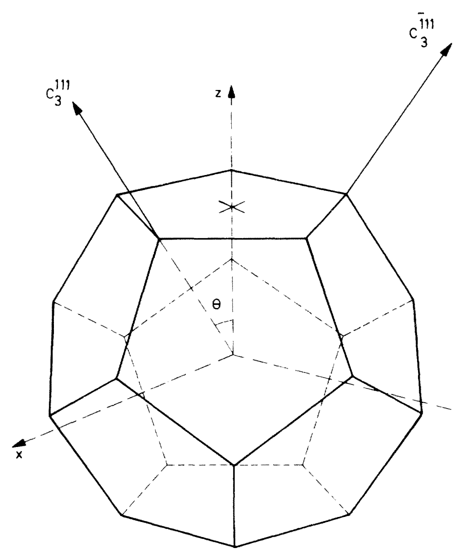

FIG. 1. Coordinate system in a dodecahedron. The z direction coincides with a fivefold rotation axis, the y direction with a twofold axis of rotation (cf. Table I). $\mathscr{C}_3^{111}$ and $\mathscr{C}_3^{\bar{1}11}$ are generators of a tetrahedral subgroup. The Miller indices in superscript refer to the standard coordinate frame for this subgroup; $\tan\theta = 2(\sqrt{5}-1)/(\sqrt{5}+1)$.

established the representational matrices, we can identify κ,λ,μ,ν from the table and use common projection techniques to solve B completely. A new unimodular constant ξ thereby appears:

$$\xi \equiv \frac{1}{2^{3/2}}(\sqrt{3},\sqrt{5}) = \frac{1}{\sqrt{6}}(1+\epsilon\omega+\bar{\epsilon}\omega+\epsilon^2\bar{\omega}+\bar{\epsilon}^2\bar{\omega}) ,$$

$$B = \frac{1}{\sqrt{5}} \begin{bmatrix} \bar{\epsilon}^2\xi & \xi\omega & \epsilon^2\xi & \bar{\epsilon}\xi\bar{\omega} & \epsilon\xi\bar{\omega} \\ \bar{\epsilon}\bar{\xi} & \bar{\xi}\omega & \epsilon\bar{\xi} & \epsilon^2\bar{\xi}\bar{\omega} & \bar{\epsilon}^2\bar{\xi}\bar{\omega} \\ 1 & \omega & 1 & \bar{\omega} & \bar{\omega} \\ -\epsilon\bar{\xi} & -\bar{\xi}\omega & -\bar{\epsilon}\bar{\xi} & -\bar{\epsilon}^2\bar{\xi}\bar{\omega} & -\epsilon^2\bar{\xi}\bar{\omega} \\ \epsilon^2\xi & \xi\omega & \bar{\epsilon}^2\xi & \epsilon\xi\bar{\omega} & \bar{\epsilon}\xi\bar{\omega} \end{bmatrix} . \tag{6}$$

Most point groups are completely covered by monomial irreducible representations. Quite remarkably $\mathfrak{H}$ is an exception. Indeed, since $\mathfrak{T}$ is its largest nontrivial subgroup, the dimension of the left-coset space of $\mathfrak{T}$, i.e., $|\mathfrak{H}|/|\mathfrak{T}|=5$, puts a lower limit to the dimension of induced representations.[14] Consequently, induction cannot generate the icosahedral three- or fourfold degenerate representations directly in reduced form. Therefore according to the lemma, these representations cannot actualize monomial form.

III. COUPLING OF MONOMIAL REPRESENTATIONS

A. Preliminary definitions

Let $|\Gamma_1\gamma_1\rangle$ be a ket function transforming as the γ_1 component of Γ_1. $\Gamma_1(\mathscr{R})_{\gamma_1\gamma_1'}$ is an element of the corresponding representation matrix for symmetry operation $\mathscr{R}$ in $\mathfrak{G}$. That is,

$$\mathscr{R}\,|\Gamma_1\gamma_1\rangle = \sum_{\gamma_1'} \Gamma_1(\mathscr{R})_{\gamma_1'\gamma_1}\,|\Gamma_1\gamma_1'\rangle . \tag{7}$$

The inner Kronecker product of two irreducible representations Γ_1 and Γ_2 can be decomposed according to the well-known formula,

$$\Gamma_1\times\Gamma_2 = \sum_{\Gamma} c_\Gamma \Gamma , \tag{8}$$

c_Γ being a multiplicity index, denoting the frequency of Γ in the decomposition. The CGC's, denoted

$$\langle \Gamma_1\gamma_1\Gamma_2\gamma_2\,|\,\Gamma\gamma\rangle ,$$

are elements of a transformation matrix, that reduces the direct product[6,15] as expressed in Eq. (9):

$$|\Gamma\gamma\rangle = \sum_{\gamma_1\gamma_2} \langle \Gamma_1\gamma_1\Gamma_2\gamma_2\,|\,\Gamma\gamma\rangle\,|\Gamma_1\gamma_1\rangle\,|\Gamma_2\gamma_2\rangle . \tag{9}$$

Define a supermatrix A, with elements

$$A_{gg'} = \frac{1}{|\mathfrak{G}|} \sum_{\mathscr{R}} \Gamma_1(\mathscr{R})_{\gamma_1\gamma_1'}\,\Gamma_2(\mathscr{R})_{\gamma_2\gamma_2'}\,\bar{\Gamma}(\mathscr{R})_{\gamma\gamma'} , \tag{10}$$

where the labels g and g' are shorthand notations for the triads $\gamma_1\gamma_2\gamma$ and $\gamma_1'\gamma_2'\gamma'$, respectively. Henceforth, A will be limited to a submatrix of A, formed by those g values, for which the diagonal elements A_{gg} differ from zero. Indeed the remaining part of A only contains zeros. The selected labels will be called "allowed" g values.

The CGC's that appear in Eq. (9) can be calculated fairly easily:

$$\langle \Gamma_1\gamma_1\Gamma_2\gamma_2\,|\,\Gamma\gamma\rangle = \frac{|\Gamma|^{1/2}}{(A_{g'g'})^{1/2}} A_{gg'} , \tag{11}$$

where $|\Gamma|$ is the dimension of Γ. In Eq. (11), the primed label can be any allowed triangle $\gamma_1'\gamma_2'\gamma'$; its choice corresponds to a phase choice for the entire Clebsch-Gordan series.[16] According to the equation, coupling coefficients that describe the coupling of Γ_1 and Γ_2 to a resulting Γ are proportional to elements of A. The entire Clebsch-Gordan series is contained in every column of A.

In a previous communication,[6] several general properties of A have been reported: A is Hermitian, idempotent, and its trace equals its rank, c_Γ. Similarly, Damhus[8] investigated the reality of A, in connection to the Wigner and Racah basis choice. The formalism will now be further specified to deal with monomial representations. If $\Gamma(\mathscr{R})$ is monomial, one has

$$\Gamma(\mathscr{R})_{\gamma\gamma'} = \mathscr{g}(\mathscr{R})_{\gamma'}\,\delta(\gamma,\sigma_{\gamma'}^{\Gamma(\mathscr{R})}) , \tag{12}$$

$$\Gamma(\mathscr{R}^{-1})_{\gamma\gamma'} = \bar{\mathscr{g}}(\mathscr{R})_{\gamma}\,\delta(\gamma,\sigma_{\gamma'}^{\Gamma(\mathscr{R}^{-1})}) = \bar{\mathscr{g}}(\mathscr{R})_{\gamma}\,\delta(\gamma',\sigma_{\gamma}^{\Gamma(\mathscr{R})}) . \tag{13}$$

$\mathscr{g}(\mathscr{R})$ is a vector, carrying the nonzero elements of $\Gamma(\mathscr{R})$, ordered as they occur from left to right in the matrix; e.g., for the V representation matrix in Eq. (4) one could write

$$\mathscr{g}(\mathscr{C}_5^{\xi}) = (\pi,\kappa,\lambda,\mu,\nu) .$$

$\sigma_{\gamma'}^{\Gamma(\mathscr{R})}$ symbolizes the permutation, associated with $\Gamma(\mathscr{R})$, operating on the γ' component. Of course the inverse rotation $\mathscr{R}^{-1}$ induces the inverse permutation.

The coupling of monomial representations is characterized by two interesting properties.

B. Property 1: If $c_\Gamma = 1$ and A is the projection matrix of three monomial representations, all elements of A are equal except for phase

Proof: In the definition of A [Eq. (10)] $\mathscr{R}$ can safely be replaced by $\mathscr{S}^{-1}\mathscr{R}$, $\mathscr{S}$ being a fixed element of $\mathfrak{G}$. Factorization yields

$$A_{gg'} = \frac{1}{|\mathfrak{G}|}\sum_{\mathscr{R}} \Gamma_1(\mathscr{S}^{-1}\mathscr{R})_{\gamma_1\gamma_1'} \times \Gamma_2(\mathscr{S}^{-1}\mathscr{R})_{\gamma_2\gamma_2'}\bar{\Gamma}(\mathscr{S}^{-1}\mathscr{R})_{\gamma\gamma'}$$
$$= \bar{\varphi}_1(\mathscr{S})_{\gamma_1}\bar{\varphi}_2(\mathscr{S})_{\gamma_2}\varphi(\mathscr{S})_{\gamma}A_{\sigma_g g'} \quad (14)$$

Again σ_g symbolizes a contraction of a triad,

$$\sigma_{\gamma_1}^{\Gamma_1(\mathscr{S})}\sigma_{\gamma_2}^{\Gamma_2(\mathscr{S})}\sigma_{\gamma}^{\Gamma(\mathscr{S})} .$$

The product of φ elements in Eq. (14) is a product of unimodular constants. Hence $A_{gg'}$ and $A_{\sigma_g g'}$ are equal in absolute value, but may have different phases. Similarly column indices can be changed, substituting $\mathscr{R}$ by $\mathscr{R}\mathscr{S}$:

$$A_{gg'} = \frac{1}{|\mathfrak{G}|}\sum_{\mathscr{R}} \Gamma_1(\mathscr{R}\mathscr{S})_{\gamma_1\gamma_1'}\Gamma_2(\mathscr{R}\mathscr{S})_{\gamma_2\gamma_2'}\bar{\Gamma}(\mathscr{R}\mathscr{S})_{\gamma\gamma'}$$
$$= \varphi_1(\mathscr{S})_{\gamma_1'}\varphi_2(\mathscr{S})_{\gamma_2'}\bar{\varphi}(\mathscr{S})_{\gamma'}A_{g\sigma_{g'}} . \quad (15)$$

Next consider completeness. Given two elements in the same column, $A_{gg'}$ and $A_{g''g'}$, assume that there is no $\mathscr{S}$ in $\mathfrak{G}$ that can turn g into g''. More precisely, for all $\mathscr{S}$ in $\mathfrak{G}$,

$$\delta(\gamma_1,\sigma_{\gamma_1''}^{\Gamma_1(\mathscr{S})})\delta(\gamma_2,\sigma_{\gamma_2''}^{\Gamma_2(\mathscr{S})})\delta(\gamma,\sigma_{\gamma''}^{\Gamma(\mathscr{S})}) = 0 . \quad (16)$$

From the definition of monomial matrices [Eq. (12)] the off-diagonal element $A_{gg''}$ can be written more explicitly:

$$A_{gg''} = \frac{1}{|\mathfrak{G}|}\sum_{\mathscr{R}}[\varphi_1(\mathscr{R})_{\gamma_1''}\varphi_2(\mathscr{R})_{\gamma_2''}\bar{\varphi}(\mathscr{R})_{\gamma''}\delta(\gamma_1,\sigma_{\gamma_1''}^{\Gamma_1(\mathscr{R})})\delta(\gamma_2,\sigma_{\gamma_2''}^{\Gamma_2(\mathscr{R})})\delta(\gamma,\sigma_{\gamma''}^{\Gamma(\mathscr{R})})] . \quad (17)$$

Clearly, in view of the assumption in Eq. (16), all Kronecker deltas in Eq. (17) will be zero, and hence $A_{gg''}=0$. Consequently, the 2×2 minor in Eq. (18) does not vanish, since both g and g'' are allowed labels:

$$\begin{vmatrix} A_{gg} & A_{gg''} \\ A_{g''g} & A_{g''g''} \end{vmatrix} = A_{gg}A_{g''g''} \neq 0 . \quad (18)$$

If $c_\Gamma = 1$, this result is contradictory.[17] Hence our premise was false, and this completes the proof for $c_\Gamma = 1$. Table II provides an example of the A matrix, for $T_1 \times E = T_2$.

C. Property 2: If $c_\Gamma > 1$, and A is the projection of three monomial representations, A will be in reduced form. Each block in A will have rank one, and hence property 1

Proof: The preceding equations [(14) and (15)] have shown how to change, respectively, row and column labels and effectuate vertical and lateral shifts in A. We now add one more type of operator, corresponding to diagonal shifts. Indeed, if one substitutes $\mathscr{R}$ by its $\mathscr{S}^{-1}$ transform in the definition of A, one obtains

$$A_{gg'} = \frac{1}{|\mathfrak{G}|}\sum_{\mathscr{R}} \Gamma_1(\mathscr{S}^{-1}\mathscr{R}\mathscr{S})_{\gamma_1\gamma_1'}\Gamma_2(\mathscr{S}^{-1}\mathscr{R}\mathscr{S})_{\gamma_2\gamma_2'} \times \bar{\Gamma}(\mathscr{S}^{-1}\mathscr{R}\mathscr{S})_{\gamma\gamma'}$$
$$= \bar{\varphi}_1(\mathscr{S})_{\gamma_1}\varphi_1(\mathscr{S})_{\gamma_1'}\bar{\varphi}_2(\mathscr{S})_{\gamma_2}\varphi_2(\mathscr{S})_{\gamma_2'} \times \varphi(\mathscr{S})_{\gamma}\bar{\varphi}(\mathscr{S})_{\gamma'}A_{\sigma_g\sigma_{g'}} . \quad (19)$$

Combining Eqs. (14), (15), and (19) into one minor, yields zero:

TABLE II. A matrix for the coupling $T_1 \times E = T_2$ in the octahedral group $\mathfrak{O}$. All representations are in monomial form, as defined in Table I. All matrix elements are to be divided by 6; [$\omega = \exp(2\pi i/3)$].

$\mathfrak{O}$	*xayz*	*yaxz*	*zaxy*	*xbyz*	*ybxz*	*zbxy*
xayz	1	ω	$\bar{\omega}$	$-\omega$	-1	$-\bar{\omega}$
yaxz	$\bar{\omega}$	1	ω	-1	$-\bar{\omega}$	$-\omega$
zaxy	ω	$\bar{\omega}$	1	$-\bar{\omega}$	$-\omega$	-1
xbyz	$-\bar{\omega}$	-1	$-\omega$	1	$\bar{\omega}$	ω
ybxy	-1	$-\omega$	$-\bar{\omega}$	ω	1	$\bar{\omega}$
zbxy	$-\omega$	$-\bar{\omega}$	-1	$\bar{\omega}$	ω	1

$$\begin{vmatrix} A_{gg'} & A_{g\sigma_{g'}} \\ A_{\sigma_g g'} & A_{\sigma_g \sigma_{g'}} \end{vmatrix} = 0 \; . \qquad (20)$$

Since a minor of 2×2 vanishes, this can only mean that the labels involved circumscribe a block of rank 1. Completeness is easily established as well. If two allowed labels g and g'' cannot be connected by symmetry elements, they will belong to separate blocks, since in that case, according to Eqs. (16) and (17), their off-diagonal element $A_{gg''}$ will equal zero. Consequently A is fully reduced into submatrices of rank 1.

D. Discussion

The monomial concept imparts a peculiar transparency to the coupling phenomenon. According to the first property, the coupling problem is limited to a problem in phase space. The phases of interest belong to the direct sum of the Abelian groups that constitute the field of the monomial matrices involved. According to the second property, non-simply-reducible groups will, in fact, be reduced. The irreducible form of A represents the natural intrinsic multiplicity separation, and no recurrence to extrinsic labeling criteria, e.g., those involving higher-order groups, is required.

Two examples will be commented upon. First consider the triple product $T\times T=2T$ in the tetrahedral group $\mathfrak{T}$. The A matrix is resumed[6] in Table III. All even permutations of component labels go together into one block, and all odd ones into the other. This multiplicity separation differs from the classical differentiation into a symmetrized and an antisymmetrized direct product,[4] $[T^2]$ and (T^2). Instead in the present classification a triple symmetrization is achieved based upon the permutational structure of the T matrices. These are homorphous to permutational matrices of the alternating group of three elements. Hence they do not provide odd permutations that could turn a label of the first block into one of the second. Such labels thus must belong to disjunct blocks.

A somewhat similar cause differentiates the $V\times V=2V$ direct product in the $\mathfrak{H}$ group. Again A is reduced into two blocks.

(i) There is one block of dimensions 20×20, based upon all g values of the type $\langle iij \rangle$, where i and j stand for any component label of V. ($i,j=a$, b, c, d, or e, and $i\neq j$.) Each element in this block has absolute value $\frac{1}{20}$.

(ii) There is one block of dimension 60×60, based upon all possible g values of the type $\langle ijk \rangle$. ($i,j,k=a$, b, c, d, or e, and $i\neq j\neq k$.) Each element has abolsute value $\frac{1}{60}$.

TABLE III. A matrix for $T\times T=2T$ in the tetrahedral group. The behavior of the T components under relevant group generators ($\mathcal{C}_3^{xyz},\mathcal{C}_2^{y}$) is consistent with the x, y, and z functions in Table I. All matrix elements are to be divided by 3.

$\mathfrak{T}$	xyz	yzx	zxy	xzy	zyx	yxz
xyz	1	1	1	0	0	0
yzx	1	1	1	0	0	0
zxy	1	1	1	0	0	0
xzy	0	0	0	1	1	1
zyx	0	0	0	1	1	1
yxz	0	0	0	1	1	1

Moreover, the only phase factors that occur in A, belong to the cyclic group of order 3: $(\omega,\bar{\omega},1)$. The V matrices (see Table I) are isomorphous to the permutational matrices of the alternating group in five dimensions.[9] Hence they can perform all even permutations of a given quintuple $\langle ijklm \rangle$, and thus certainly generate all even and all odd permutations of a triad $\langle ijk \rangle$. However, they cannot turn a label $\langle iij \rangle$ into $\langle ijk \rangle$, and therefore such labels will cause a natural multiplicity separation.

IV. MULTIPLICITY SEPARATION IN THE OCTAHEDRAL SPINOR GROUP

Turning attention to spin irreducible representations, based on half-integer J values, at first sight, the monomial concept does not appear to be very promising. A fundamental representation, such as E' in $\mathfrak{O}^*$, describing the electron spin in an octahedral field, defies all attempts to monomial reduction.[6] Indeed one can find pairs of octahedral group generators (e.g., two fourfold axes, $\mathcal{C}_4^{z}$ and $\mathcal{C}_4^{x}$), for which the E' representational matrices have nonzero character. Matrix homomorphism to the permutational group of order 2 is therefore impossible. On the other hand spinor subgroups, such as $\mathfrak{D}_3^*$ and $\mathfrak{D}_4^*$, have monomial spin representations. Nevertheless, even in the octahedral spinor group $\mathfrak{O}^*$ the monomial concept is not devoid of interest, as we intend to show in this section.

In the $\mathfrak{O}^*$ group, the fourfold degenerate representation U' poses a rather unique problem of direct product multiplicity. Four cases of repeated representations occur:

$$U'\times U'=2T_1 \; , \quad U'\times U'=2T_2 \; , \qquad (21a)$$

$$U'\times T_1=2U' \; , \quad U'\times T_2=2U' \; . \qquad (21b)$$

These cases are of considerable importance in the description of spin-orbit coupling interactions for odd-electron systems in octahedral fields.[4,18] Several criteria for multiplicity separation have been proposed. For the resolution of the product $U' \times T_1 = 2U'$, one can make profitable use of the continuous parent group labels.[4] T_1 corresponds to $J=1$, and U' (the quartet spin state) has a value of $J=\frac{3}{2}$. According to the well-known Wigner rules, these J values couple to $J=\frac{5}{2}(U'+E'')$, $J=\frac{3}{2}(U')$, and $J=\frac{1}{2}(E')$. Hence the two resulting U' representations can unambiguously be distinguished by their J parentage.

Another type of differentiation is possible for the case $U' \times U' = 2T_2$. Indeed the resulting kets can be resolved in a symmetrized $[U'^2]$ and an antisymmetrized (U'^2) direct product.[7,19] Either of these multiplicity separations fails, when applied to the other cases, and *ad hoc* procedures have to be invoked. A satisfactory solution of this problem can only be achieved if the A matrix can be reduced. To that end T_1 and T_2 will be represented in monomial form (cf. Table I). The U' matrix cannot be reduced in the same way, but an alternative to the standard basis choice can be considered. Note that $E \times E' = U'$ (U' contains the spin-orbit components of a ^2E state). So in the construction of U', we can—at least partially—introduce monomial properties by using the monomial E components $|Ea\rangle$ and $|Eb\rangle$. Consequently we define

$$
\begin{aligned}
|U'1\rangle &= |Ea\rangle\,|E'\alpha\rangle\ ,\\
|U'2\rangle &= |Eb\rangle\,|E'\alpha\rangle\ ,\\
|U'3\rangle &= i\,|Ea\rangle\,|E'\beta\rangle\ ,\\
|U'4\rangle &= -i\,|Eb\rangle\,|E'\beta\rangle\ .
\end{aligned}
\tag{22}
$$

In Eq. (22) the U' component labels are mere sequential numbers. This choice explicitly intends to preclude any reference to extrinsic labeling criteria. The $U'(\mathscr{R})$ matrices can now be obtained from $E(\mathscr{R})$ and $E'(\mathscr{R})$, as expressed in Eq. (23) (the $\mathscr{R}$ argument is not repeated in the right-hand side of the equation):

$$
U'(\mathscr{R}) = \begin{bmatrix}
E_{aa}E'_{\alpha\alpha} & E_{ab}E'_{\alpha\alpha} & iE_{aa}E'_{\alpha\beta} & -iE_{ab}E'_{\alpha\beta}\\
E_{ba}E'_{\alpha\alpha} & E_{bb}E'_{\alpha\alpha} & iE_{ba}E'_{\alpha\beta} & -iE_{bb}E'_{\alpha\beta}\\
-iE_{aa}E'_{\beta\alpha} & -iE_{ab}E'_{\beta\alpha} & E_{aa}E'_{\beta\beta} & -E_{ab}E'_{\beta\beta}\\
iE_{ba}E'_{\beta\alpha} & iE_{bb}E'_{\beta\alpha} & -E_{ba}E'_{\beta\beta} & E_{bb}E'_{\beta\beta}
\end{bmatrix} . \tag{23}
$$

New standard basis relations for the modified U' basis are represented in Table IV. In the Frobenius-Schur classification U' is an irreducible representation of the second kind,[20,21] and has an antisymmetric conjugating matrix, for example, Q. That is,

$$QU'(\mathscr{R})Q^{-1} = \bar{U}'(\mathscr{R})\ . \tag{24}$$

Since the present choice is incompatible with the Fano-Racah convention, Q does not coincide with $U'(\mathscr{C}_2^y)$, but, nevertheless, it meets the standard format[7]:

$$
Q = \begin{bmatrix}
0 & 0 & 0 & -1\\
0 & 0 & 1 & 0\\
0 & -1 & 0 & 0\\
1 & 0 & 0 & 0
\end{bmatrix} . \tag{25}
$$

Introducing the tilde to symbolize reflection of row or column indices, $\tilde{k} = 5-k$, Eq. (24) can be rewritten as follows:

$$\bar{U}'(\mathscr{R})_{ij} = (-1)^{i+j}U'(\mathscr{R})_{\tilde{i}\tilde{j}}\ . \tag{26}$$

TABLE IV. Behavior of modified basis kets belonging to the fourfold spin-irreducible representation U' of the octahedral group under useful symmetry elements; $\eta = \exp(2\pi i/24)$.

$\mathfrak{O}^*$	$\mathscr{C}_4^z$	C_3^{xyz}	$\mathscr{C}_2^y$
$\lvert U'1\rangle$	$\frac{1}{\sqrt{2}}(1-i)\lvert U'2\rangle$	$\frac{1}{\sqrt{2}}(\bar{\eta}^{11}\lvert U'1\rangle+\eta^{7}\lvert U'3\rangle)$	$-i\lvert U'3\rangle$
$\lvert U'2\rangle$	$\frac{1}{\sqrt{2}}(1-i)\lvert U'1\rangle$	$\frac{1}{\sqrt{2}}(\eta^{5}\lvert U'2\rangle+\eta^{11}\lvert U'4\rangle)$	$i\lvert U'4\rangle$
$\lvert U'3\rangle$	$-\frac{1}{\sqrt{2}}(1+i)\lvert U'4\rangle$	$\frac{1}{\sqrt{2}}(\bar{\eta}^{11}\lvert U'1\rangle+\bar{\eta}^{5}\lvert U'3\rangle)$	$-i\lvert U'1\rangle$
$\lvert U'4\rangle$	$-\frac{1}{\sqrt{2}}(1+i)\lvert U'3\rangle$	$\frac{1}{\sqrt{2}}(\bar{\eta}^{7}\lvert U'2\rangle+\eta^{11}\lvert U'4\rangle)$	$i\lvert U'2\rangle$

TABLE V. Nonzero blocks in the A matrix for the coupling $U' \times U' = 2T_1$. All matrix elements are to be divided by 12; $\omega = \exp(2\pi i/3)$.

	$11x$	$11y$	$13z$	$22x$	$22y$	$24z$	$33x$	$33y$	$31z$	$44x$	$44y$	$42z$
$11x$	1	$i\bar{\omega}$	$-i\omega$	$\bar{\omega}$	i	$i\omega$	1	$-i\bar{\omega}$	$-i\omega$	$\bar{\omega}$	$-i$	$i\omega$
$11y$	$-i\omega$	1	$-\bar{\omega}$	$-i$	ω	$\bar{\omega}$	$-i\omega$	-1	$-\bar{\omega}$	$-i$	$-\omega$	$\bar{\omega}$
$13z$	$i\bar{\omega}$	$-\omega$	1	$i\omega$	$-\bar{\omega}$	-1	$i\bar{\omega}$	ω	1	$i\omega$	$\bar{\omega}$	-1
$22x$	ω	i	$-i\bar{\omega}$	1	$i\omega$	$i\bar{\omega}$	ω	$-i$	$-i\bar{\omega}$	1	$-i\omega$	$i\bar{\omega}$
$22y$	$-i$	$\bar{\omega}$	$-\omega$	$-i\bar{\omega}$	1	ω	$-i$	$-\bar{\omega}$	$-\omega$	$-i\bar{\omega}$	-1	ω
$24z$	$-i\bar{\omega}$	ω	-1	$-i\omega$	$\bar{\omega}$	1	$-i\bar{\omega}$	$-\omega$	-1	$-i\omega$	$-\bar{\omega}$	1
$33x$	1	$i\bar{\omega}$	$-i\omega$	$\bar{\omega}$	i	$i\omega$	1	$-i\bar{\omega}$	$-i\omega$	$\bar{\omega}$	$-i$	$i\omega$
$33y$	$i\omega$	-1	$\bar{\omega}$	i	$-\omega$	$-\bar{\omega}$	$i\omega$	1	$\bar{\omega}$	i	ω	$-\bar{\omega}$
$31z$	$i\bar{\omega}$	$-\omega$	1	$i\omega$	$-\bar{\omega}$	-1	$i\bar{\omega}$	ω	1	$i\omega$	$\bar{\omega}$	-1
$44x$	ω	i	$-i\bar{\omega}$	1	$i\omega$	$i\bar{\omega}$	ω	$-i$	$-i\bar{\omega}$	1	$-i\omega$	$i\bar{\omega}$
$44y$	i	$-\bar{\omega}$	ω	$i\bar{\omega}$	-1	$-\omega$	i	$\bar{\omega}$	ω	$i\bar{\omega}$	1	$-\omega$
$42z$	$-i\bar{\omega}$	ω	-1	$-i\omega$	$\bar{\omega}$	1	$-i\bar{\omega}$	$-\omega$	-1	$-i\omega$	$-\bar{\omega}$	1

	$12x$	$12y$	$14z$	$21x$	$21y$	$23z$	$34x$	$34y$	$32z$	$43x$	$43y$	$41z$
$12x$	1	i	i	1	i	$-i$	-1	i	$-i$	-1	i	i
$12y$	$-i$	1	1	$-i$	1	-1	i	1	-1	i	1	1
$14z$	$-i$	1	1	$-i$	1	-1	i	1	-1	i	1	1
$21x$	1	i	i	1	i	$-i$	-1	i	$-i$	-1	i	i
$21y$	$-i$	1	1	$-i$	1	-1	i	1	-1	i	1	1
$23z$	i	-1	-1	i	-1	1	$-i$	-1	1	$-i$	-1	-1
$34x$	-1	$-i$	$-i$	-1	$-i$	i	1	$-i$	i	1	$-i$	$-i$
$34y$	$-i$	1	1	$-i$	1	-1	i	1	-1	i	1	1
$32z$	i	-1	-1	i	-1	1	$-i$	-1	1	$-i$	-1	-1
$43x$	-1	$-i$	$-i$	-1	$-i$	i	1	$-i$	i	1	$-i$	$-i$
$43y$	$-i$	1	1	$-i$	1	-1	i	1	-1	i	1	1
$41z$	$-i$	1	1	$-i$	1	-1	i	1	-1	i	1	1

Surprisingly, this is not the only type of conjugacy relationship that can be defined for U'. At this point, the partial monomial character of the newly defined $U'(\mathscr{R})$ matrices [Eq. (23)] appears on the scene. This character can take on two different forms, according to whether $\mathscr{R}$ does or does not permute the partners $|Ea\rangle$ and $|Eb\rangle$. The former symmetry elements will be called odd, $\mathscr{R}_o$, the latter even, $\mathscr{R}_e$:

$$U'(\mathscr{R}_e)_{ij} = U'(\mathscr{R}_e)_{ij}\delta(1,(-1)^{i+j}) ,$$
$$U'(\mathscr{R}_o)_{ij} = U'(\mathscr{R}_o)_{ij}\delta(-1,(-1)^{i+j}) . \tag{27}$$

Combining Eqs. (26) and (27) a new type of conjugacy relationship results:

$$SU'(\mathscr{R}_e)S^{-1} = \bar{U}'(\mathscr{R}_e) ,$$
$$SU'(\mathscr{R}_o)S^{-1} = -\bar{U}'(\mathscr{R}_o) , \tag{28}$$

where S is the standard counterdiagonal symmetric matrix

$$S = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} . \tag{29}$$

The parity property is a true group characteristic. The even elements form a subgroup, and all odd elements are contained in one single coset of this subgroup. This result can directly be obtained from Eq. (28). The proof is very similar to the resolution of the permutation group into its alternating subgroup and a coset of odd permutations.

These results will now be introduced in the relevant A matrices. The summation over $\mathscr{R}$ in A can thereby be partitioned in partial sums, A^e and A^o, over $\mathscr{R}_e$ and $\mathscr{R}_o$, respectively. First consider the coupling $U' \times U'$ [Eq. (21a)]. i,j and i',j' are, respectively, row and column labels of U'; t,t' refer to T_1 or T_2:

$$
\begin{aligned}
A_{ijt,i'j't'} &= \delta(1,(-1)^{i+i'})\delta(1,(-1)^{j+j'})A^{e}_{ijt,i'j't'} + \delta(-1,(-1)^{i+i'})\delta(-1,(-1)^{j+j'})A^{\mathscr{O}}_{ijt,i'j't'} \\
&= \delta((-1)^{i+i'},(-1)^{j+j'})A_{ijt,i'j't'} \\
&= \delta((-1)^{i+j},(-1)^{i'+j'})A_{ijt,i'j't'} \; . \qquad (30)
\end{aligned}
$$

Equation (30) requires that the sum of row indices $i+j$ has the same parity as the sum of column indices $i'+j'$. No intertwining elements will occur. Accordingly, A will be reduced. This is confirmed in Tables V and VI. Surprisingly, A also incorporates property 1 of the projection matrix of monomial representations (see Sec. III). Only part of this result can be explained from monomial features.

Several further observations can be made.

(a) The A matrices, pertaining to the coupling $U'\times T$ [Eq. (21b)] can easily be derived from the present set. Indeed, using Eq. (26), one will verify

$$A^{U'TU'}_{itj,i't'j'} = (-1)^{j+j'} A^{U'U'T}_{i\bar{j}t,i'\bar{j}'t'} \; . \qquad (31)$$

(b) We recall that the A matrices give rise to the construction of Clebsch-Gordan series [Eq. (11)]. Therefrom the resulting ket vectors can be obtained [Eq. (9)]. That is,

$$|\, Tt;g' \rangle = \frac{|\, T\,|^{1/2}}{(A_{g'g'})^{1/2}} \sum_{i,j} A_{ijt,g'} \,|\, U'_i \rangle \,|\, U'_j \rangle \; . \qquad (32)$$

In this case the additional label g' symbolizes the triad $i'j't'$. Notice that g' not only reflects a phase choice but also a multiplicity choice. The latter choice basically consists in the parity $(-1)^{i'+j'}$. The summation is restricted to those i,j combinations that conserve this parity. Evidently $(i \Longleftrightarrow j)$ ex-

TABLE VI. Nonzero blocks in the A matrix for the coupling $U'\times U' = 2T_2$. All matrix elements are to be divided by 12; $\omega = \exp(2\pi i/3)$.

	$11yz$	$11xz$	$13xy$	$22yz$	$22xz$	$24xy$	$33yz$	$33xz$	$31xy$	$44yz$	$44xz$	$42xy$
$11yz$	1	$i\bar{\omega}$	$-i\omega$	$-\bar{\omega}$	$-i$	$-i\omega$	1	$-i\bar{\omega}$	$-i\omega$	$-\bar{\omega}$	i	$-i\omega$
$11xz$	$-i\omega$	1	$-\bar{\omega}$	i	$-\omega$	$-\bar{\omega}$	$-i\omega$	-1	$-\bar{\omega}$	i	ω	$-\bar{\omega}$
$13xy$	$i\bar{\omega}$	$-\omega$	1	$-i\omega$	$\bar{\omega}$	1	$i\bar{\omega}$	ω	1	$-i\omega$	$-\bar{\omega}$	1
$22yz$	$-\omega$	$-i$	$i\bar{\omega}$	1	$i\omega$	$i\bar{\omega}$	$-\omega$	i	$i\bar{\omega}$	1	$-i\omega$	$i\bar{\omega}$
$22xz$	i	$-\bar{\omega}$	ω	$-i\bar{\omega}$	1	ω	i	$\bar{\omega}$	ω	$-i\bar{\omega}$	-1	ω
$24xy$	$i\bar{\omega}$	$-\omega$	1	$-i\omega$	$\bar{\omega}$	1	$i\bar{\omega}$	ω	1	$-i\omega$	$-\bar{\omega}$	1
$33yz$	1	$i\bar{\omega}$	$-i\omega$	$-\bar{\omega}$	$-i$	$-i\omega$	1	$-i\bar{\omega}$	$-i\omega$	$-\bar{\omega}$	i	$-i\omega$
$33xz$	$i\omega$	-1	$\bar{\omega}$	$-i$	ω	$\bar{\omega}$	$i\omega$	1	$\bar{\omega}$	$-i$	$-\omega$	$\bar{\omega}$
$31xy$	$i\bar{\omega}$	$-\omega$	1	$-i\omega$	$\bar{\omega}$	1	$i\bar{\omega}$	ω	1	$-i\omega$	$-\bar{\omega}$	1
$44yz$	$-\omega$	$-i$	$i\bar{\omega}$	1	$i\omega$	$i\bar{\omega}$	$-\omega$	i	$i\bar{\omega}$	1	$-i\omega$	$i\bar{\omega}$
$44xz$	$-i$	$\bar{\omega}$	$-\omega$	$i\bar{\omega}$	-1	$-\omega$	$-i$	$-\bar{\omega}$	$-\omega$	$i\bar{\omega}$	1	$-\omega$
$42xy$	$i\bar{\omega}$	$-\omega$	1	$-i\omega$	$\bar{\omega}$	1	$i\bar{\omega}$	ω	1	$-i\omega$	$-\bar{\omega}$	1

	$12yz$	$12xz$	$14xy$	$21yz$	$21xz$	$23xy$	$34yz$	$34xz$	$32xy$	$43yz$	$43xz$	$41xy$
$12yz$	1	i	i	-1	$-i$	i	-1	i	$-i$	1	$-i$	$-i$
$12xz$	$-i$	1	1	i	-1	1	i	1	-1	$-i$	-1	-1
$14xy$	$-i$	1	1	i	-1	1	i	1	-1	$-i$	-1	-1
$21yz$	-1	$-i$	$-i$	1	i	$-i$	1	$-i$	i	-1	i	i
$21xz$	i	-1	-1	$-i$	1	-1	$-i$	-1	1	i	1	1
$23xy$	$-i$	1	1	i	-1	1	i	1	-1	$-i$	-1	-1
$34yz$	-1	$-i$	$-i$	1	i	$-i$	1	$-i$	i	-1	i	i
$34xz$	$-i$	1	1	i	-1	1	i	1	-1	$-i$	-1	-1
$32xy$	i	-1	-1	$-i$	1	-1	$-i$	-1	1	i	1	1
$43yz$	1	i	i	-1	$-i$	i	-1	i	$-i$	1	$-i$	$-i$
$43xz$	i	-1	-1	$-i$	1	-1	$-i$	-1	1	i	1	1
$41xy$	i	-1	-1	$-i$	1	-1	$-i$	-1	1	i	1	1

change in Eq. (32) does not alter this multiplicity choice. The resulting T ket vectors are therefore necessarily symmetric or antisymmetric with respect to product symmetrization.

(c) More importantly, the resulting T ket vectors also diagonalize the Kramers star operator.[4] First consider the effect of the Kramers star operator on the basic components. The spin functions $|E'\alpha\rangle$ and $|E'\beta\rangle$ still are in the Wigner convention and therefore[22]

$$|E'\alpha\rangle^* = i\,|E'\beta\rangle \,,$$
$$|E'\beta\rangle^* = -i\,|E'\alpha\rangle \,. \quad (33)$$

The $|Ea\rangle$ and $|Eb\rangle$ representations were defined from real functions (Table I) and hence

$$|Ea\rangle^* = |Eb\rangle \,,$$
$$|Eb\rangle^* = |Ea\rangle \,. \quad (34)$$

Combining these results with Eq. (22) yields the effect on the U' components:

$$|U'k\rangle^* = (-1)^k\,|U'\tilde{k}\rangle \,. \quad (35)$$

The ket products in Eq. (32) are thus transformed as follows:

$$|Tt;g'\rangle^* = \frac{|T|^{1/2}}{(A_{g'g'})^{1/2}} \sum_{ij} \bar{A}_{ijt,g'}(-1)^{i+j} \times |U'\tilde{i}\rangle\,|U'\tilde{j}\rangle \,. \quad (36)$$

Again this transformation is not able to change the parity condition, implied in the multiplicity choice. Indeed

$$(-1)^{\tilde{i}+\tilde{j}} = (-1)^{10-i-j} = (-1)^{i+j} \,. \quad (37)$$

The resulting ket vectors thus are invariant under the star operation, except for a phase factor, dependent on the choice of g'.

V. PHYSICAL APPLICATIONS

In practical calculations the use of a Wigner-Racah basis usually is preferable whenever the physical operator can be characterized by a definite symmetry. In that case the operator acts as a splitting field and a symmetry-adapted basis will diagonalize its interactions.

However, if several operators with different symmetries are considered simultaneously, there is no distinct advantage in using a basis that is adapted to only one operator. One rather tends to construct an interaction matrix that is "highly symmetrical" in appearance. Here symmetrical refers to the requirement that if the interaction matrix is solved for one component, expressions for the other components can simply be obtained by permuting terms in the solution. Evidently a monomial basis choice is extremely well oriented to meet this criterion. Typical examples are offered by Jahn-Teller problems, where two vibrational modes of different symmetries are both active. In their original paper on the $T\times(e+t)$ Jahn-Teller coupling in cubic symmetries, Öpik and Pryce[23] suggested to replace the usual nonmonomial e coordinates, transforming as z^2 and x^2-y^2, by a new set of three more symmetrical coordinates, transforming as x^2, y^2, and z^2. However, these new functions are not normal coordinates in the Lagrangian sense. Hence the most satisfactory solution of the problem can be arrived at by using the true monomial e components, that are given in Table I.

Finally it should be noted that the multiplicity separation proposed here also has clearcut advantages when dealing with chains of groups. Indeed in this case Racah's lemma, that relates coupling coefficients in continuous groups to their finite group counterparts,[7] takes a particularly simple form. Usually the lemma implies a summation over all repeated representations of a product multiplicity. However, in the present formalism, where a complete multiplicity separation has been achieved, only one term of this sum will survive, as determined by the particular triad $\langle \gamma_1\gamma_2\gamma \rangle$, one is looking at.

VI. CONCLUSION

In an algebraic sense monomiality is a joint property of a limited set of matrices. In an enlarged group-theoretical sense the concept refers to a peculiar set of totally equivalent partners, somewhat similar to the geometric points that give rise to point groups.

Clebsch-Gordan coefficients, based on monomial representations, adopt an especially simple form, somehow reminding the simplicity of Wigner's grand orthogonality theorem. The A matrices, displayed in Tables V and VI, suggest that these properties might even be extended to triple products of other representations as well.

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