Symmetric Form of Coupling Coefficients for Single and Double Point Groups and the Application of Time-Reversal Symmetry

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Symmetrized coupling coefficients, the 3-Γ symbols, are investigated for an arbitrary molecular point group $G \subset SO(3)$ or ${}^dG \subset SU(2)$. The definition employs the 3-j symbols of the full covering group SO(3) [or SU(2)] and the expansion coefficients of the basis functions, $\langle j\, m \mid j\, \Gamma\, \gamma\, a \rangle$. Considerable simplification is achieved by taking into account time-reversal symmetry in conjunction with the lemma of Racah. It is found that the 3-Γ symbols have the same symmetry properties as the 3-j symbols of SO(3). The definition of 6-Γ symbols is likewise introduced. The treatment covers non-simply reducible groups and complex representations as well. For illustration, 3-Γ symbols of the point group I are calculated and presented.

1. Introduction

Recently, in conjunction with a brief account of the associated algebra, we have reviewed methods which are suitable to calculate symmetry coupling coefficients for an arbitrary molecular point group [1]. In addition, a generally applicable standardization of phase for these coefficients was suggested which is based on a lemma by Racah. However, since the behavior of symmetry coupling coefficients under an interchange of arguments is rather involved, the definition of symmetrized coefficients is desirable which would be analogous to the 3-j symbols in the three-dimensional proper rotation group SO(3). Indeed the original definition [2] of 3-j and 6-j symbols has been extended to simply reducible groups [3] and, more recently, a generalization to any finite or compact group has been proposed [4, 5]. It is evident that the definitions of Derome and Sharp [4] apply to any molecular point group as well if the group is considered on an isolated basis. This type of treatment has been provided, for crystallographic point groups, by Griffith [6]. If the group is not multiplicity free, some explicit choice of labeling for the multiplicity index has to be made. In addition, an uneasy manipulation of phase factors of the type $(-1)^{\Sigma \Gamma_j}$ is required where Γ_j denotes a specific irreducible representation of the group. If explicit calculations have to be performed, certain integers must be assigned in some way to each Γ_j.

On the other hand, the notion of group chains which has been applied to some extent in atomic spectroscopy [7, 8] greatly facilitates the calculation of Wigner coefficients of the groups involved. Now, a molecular point group is, in general, a subgroup of the rotation group in 3-space and, in some cases of low symmetry, even extended chain relations and group lattices may be set up. It is expected that symmetrized coupling coefficients for molecular point groups may be such devised as to be consistent with the general definition of Derome and Sharp [4], their properties being moreover simplified by application of at least the subgroup property $G \subset SO(3)$ for single groups and ${}^dG \subset SU(2)$ for double groups *. It will be shown below that an additional simplification may be achieved if time-reversal symmetry is taken into account.

2. Time-Reversal Symmetry and Conjugate Complex Representations

The introduction of the time-reversal operator T [2] into considerations of point symmetry groups produces various relations for irreducible representations and their basis functions which cannot be obtained by application of spatial symmetry operators alone.

If the time-reversal operator T is applied to the basis ket $\mid j\, m\rangle$ of the group SO(3), the time-reversed (Kramers conjugate) basis $\mid j\, m\rangle'$ is produced [9]

$$\mid j\, m \rangle' = T \mid j\, m \rangle = \sum_{m'} \mid j\, m' \rangle \begin{pmatrix} j \\ m\, m' \end{pmatrix}^* . \qquad (1)$$

* There is no generally accepted notation for double groups in the literature. Observe that, besides the usage followed here, symbols like G^* and G' are most common.

The 1-j symbol on the right of Eq. (1) is the metric tensor of Wigner, its basic definition being that of a unitary matrix which transforms the rotation matrix $\mathbf{D}^{(j)}(R)$ into its conjugate complex $\mathbf{D}^{(j)}(R)^*$ [3],

$$D^{(j)}_{mn}(R) = \sum_{m'n'} \begin{pmatrix} j \\ m\,m' \end{pmatrix}^* D^{(j)}_{m'n'}(R)^* \begin{pmatrix} j \\ n\,n' \end{pmatrix}. \quad (2)$$

In addition, the metric tensor within SO(3) conforms to

$$\begin{pmatrix} j \\ m\,m' \end{pmatrix} = [2j+1]^{1/2} \begin{pmatrix} j & 0 & j \\ m & 0 & m' \end{pmatrix}$$
$$= (-1)^{j-m'} \langle j\,m\,0\,0 \,|\, j - m' \rangle \quad (3)$$
$$= (-1)^{j+m}\,\delta(m, -m') = (-1)^{j-m'}\,\delta(m, -m').$$

Let us now consider an arbitrary subgroup G, i.e. $G \subset SO(3)$. In what follows, the arguments presented apply to the case ${}^{d}G \subset SU(2)$ as well. Representation $D^{(j)}$ of the basis kets $|jm\rangle$ then subduces a representation $D^{(j)}(G)$ which is, in general, reducible and thus may be decomposed according to

$$D^{(j)}(G) = \sum_i a_i^{(j)}\,\Gamma_i. \quad (4)$$

Consequently, the $|jm\rangle$ kets may be expanded into basis functions of irreducible representations Γ of G,

$$|jm\rangle = \sum_{\Gamma\gamma a} |j\,\Gamma\,\gamma\,a\rangle \langle j\,\Gamma\,\gamma\,a \,|\, j\,m\rangle. \quad (5)$$

The branching multiplicity index a is required whenever representation Γ occurs more than once in the decomposition of $D^{(j)}(G)$. Since the basis kets are orthonormal, the expansion coefficients of Eq. (5) form a unitary matrix,

$$\sum_m \langle j\,\Gamma\,\gamma\,a \,|\, j\,m\rangle \langle j\,m \,|\, j\,\Gamma'\,\gamma'\,a'\rangle = \delta(\Gamma,\Gamma')\,\delta(\gamma,\gamma')\,\delta(a,a'), \quad (6)$$
$$\sum_{\Gamma\gamma a} \langle j\,\Gamma\,\gamma\,a \,|\, j\,m\rangle \langle j\,m' \,|\, j\,\Gamma\,\gamma\,a\rangle = \delta(m,m')$$

where we employ the obvious bra-ket notation for complex conjugation, viz.

$$\langle j\,\Gamma\,\gamma\,a \,|\, j\,m\rangle^* = \langle j\,m \,|\, j\,\Gamma\,\gamma\,a\rangle.$$

Equation (2) may now be rewritten in terms of quantities defined within the subgroup

$$D^{(j\Gamma a)}_{\gamma\gamma'}(R) = \sum_{\Gamma_1\gamma_1 a_1\gamma'_1} \begin{pmatrix} j \\ \Gamma\,\gamma\,a\;\; \Gamma_1\,\gamma_1\,a_1 \end{pmatrix}^* D^{(j\Gamma_1 a_1)}_{\gamma_1\gamma'_1}(R)^*$$
$$\cdot \begin{pmatrix} j \\ \Gamma'\,\gamma'\,a'\;\; \Gamma_1\,\gamma'_1\,a_1 \end{pmatrix} \delta(\Gamma,\Gamma')\,\delta(a,a'). \quad (7)$$

Here, we define, in analogy to Eq. (3), a metric tensor within the subgroup G

$$\begin{pmatrix} j \\ \Gamma\,\gamma\,a\;\; \Gamma'\,\gamma'\,a' \end{pmatrix} = \sum_{mm'} \langle j\,\Gamma'\,\gamma'\,a' \,|\, j\,m'\rangle^*$$
$$\cdot \begin{pmatrix} j \\ m\,m' \end{pmatrix} \langle j\,m \,|\, j\,\Gamma\,\gamma\,a\rangle. \quad (8)$$

This relation preserves the basic definition Eq. (2) above (cf. also Eq. (3.2) of Derome and Sharp [4]). It should be observed that, consequently, the metric tensor as defined here is conjugate complex to that of Kibler [10]. Similar to SO(3), the metric tensor of Eq. (8) conforms to

$$\begin{pmatrix} j \\ \Gamma\,\gamma\,a\;\; \Gamma'\,\gamma'\,a' \end{pmatrix} = (-1)^{2j} \begin{pmatrix} j \\ \Gamma'\,\gamma'\,a'\;\; \Gamma\,\gamma\,a \end{pmatrix} \quad (9)$$

as well as to the unitarity conditions

$$\sum_{\Gamma\gamma a} \begin{pmatrix} j \\ \Gamma\,\gamma\,a\;\; \Gamma'\,\gamma'\,a' \end{pmatrix}^* \begin{pmatrix} j \\ \Gamma\,\gamma\,a\;\; \Gamma''\,\gamma''\,a'' \end{pmatrix} = \delta(\Gamma',\Gamma'')\,\delta(\gamma',\gamma'')\,\delta(a',a''), \quad (10)$$
$$\sum_{\Gamma'\gamma' a'} \begin{pmatrix} j \\ \Gamma\,\gamma\,a\;\; \Gamma'\,\gamma'\,a' \end{pmatrix}^* \begin{pmatrix} j \\ \Gamma''\,\gamma''\,a''\;\; \Gamma'\,\gamma'\,a' \end{pmatrix} = \delta(\Gamma,\Gamma'')\,\delta(\gamma,\gamma'')\,\delta(a,a'').$$

Also, Eq. (1) now assumes the form

$$|j\,\Gamma\,\gamma\,a\rangle' = T\,|j\,\Gamma\,\gamma\,a\rangle$$
$$= \sum_{\Gamma'\gamma' a'} |j\,\Gamma'\,\gamma'\,a'\rangle \begin{pmatrix} j \\ \Gamma\,\gamma\,a\;\; \Gamma'\,\gamma'\,a' \end{pmatrix}^* \quad (11)$$

as may be easily verified by introducing the expansion Equation (5). Evidently, the time-reversed function $|j\,\Gamma\,\gamma\,a\rangle'$ is basis of the conjugate complex representation $D^{(j\Gamma a)}(R)^*$. This may be demonstrated by application of the symmetry operator R to Eq. (11)

$$R\,|j\,\Gamma\,\gamma\,a\rangle' = \sum_{\Gamma'\gamma'' a'} |j\,\Gamma'\,\gamma''\,a'\rangle$$
$$\cdot \sum_{\gamma'} D^{(j\Gamma' a')}_{\gamma''\gamma'}(R) \begin{pmatrix} j \\ \Gamma\,\gamma\,a\;\; \Gamma'\,\gamma'\,a' \end{pmatrix}^*. \quad (12)$$

If Eq. (7) is now introduced, we obtain

$$R\,|j\,\Gamma\,\gamma\,a\rangle' = \sum_{\gamma'} |j\,\Gamma\,\gamma'\,a\rangle'\, D^{(j\Gamma a)}_{\gamma'\gamma}(R)^* \quad (13)$$

thus completing the proof.

On the other hand, the basis functions of the conjugate complex representation are defined according to

$$R\,|j\,\overline{\Gamma\,\gamma\,a}\rangle = \sum_{\gamma'} |j\,\overline{\Gamma\,\gamma'\,a}\rangle\, D^{(j\Gamma a)}_{\gamma'\gamma}(R)^*. \quad (14)$$

Since $|j\overline{\Gamma\gamma a}\rangle$ as well as $|j\Gamma\gamma a\rangle'$ are bases to the same representation $\overline{\Gamma}$, these functions must be related by the transformation

$$|j\Gamma\gamma a\rangle' = \sum_{\gamma a} |j\overline{\Gamma\gamma a}\rangle\langle j\overline{\Gamma\gamma a}|j\Gamma\gamma a\rangle\,. \quad (15)$$

If this is introduced into Eq. (11), the coefficient in Eq. (15) may be calculated. Then we obtain

$$T|j\Gamma\gamma a\rangle = |j\Gamma'\gamma'a'\rangle \begin{pmatrix} & j & \\ \Gamma\gamma a & & \Gamma'\gamma'a' \end{pmatrix}^* \delta(\overline{\Gamma},\Gamma')\,\delta(\bar\gamma,\gamma')\,\delta(\bar a,a')\,. \quad (16)$$

This relation is a specific form of Eq. (11), generated by application of the time-reversal operator T. Therefrom, some easy algebraic manipulations produce

$$\langle j m|j\Gamma\gamma a\rangle^* = (-1)^{j+m}\langle j-m|j\overline{\Gamma\gamma a}\rangle \begin{pmatrix} & j & \\ \Gamma\gamma a & & \overline{\Gamma\gamma a} \end{pmatrix}^* \quad (17)$$

and

$$\begin{pmatrix} & j & \\ \Gamma\gamma a & & \Gamma'\gamma'a' \end{pmatrix} = \sum_{m m'} \langle j\Gamma'\gamma'a'|j m'\rangle^* \cdot \begin{pmatrix} j \\ m\ m' \end{pmatrix} \langle j m|j\Gamma\gamma a\rangle\,\delta(\overline{\Gamma},\Gamma')\,\delta(\bar\gamma,\gamma')\,\delta(\bar a,a')\,. \quad (18)$$

For orthonormal functions, the metric tensor of Eq. (18) is of modulus one. Also, Eq. (17) will be required below in section 3, whereas Eq. (18) is the more specific form of Eq. (8) resulting from the imposition of operator T on the basis functions. The time-reversal operator affects, in addition, a few more of the equations given above, e. g. Eq. (10), in a similar fashion.

3. Symmetric Coupling Coefficients for Subgroups $G \subset SO(3)$

We now consider the basis functions $|j\Gamma\gamma a\rangle$ resulting from the decomposition of the subduced representation $D^{(j)}(G)$ according to Equation (5). The collection of bases for all representations Γ of group G which are consistent with Eq. (4) will then form a possible basis for the representation $D^{(j)}$ of SO(3). The coupling of two basis kets $|j_1\Gamma_1\gamma_1 a_1\rangle$ and $|j_2\Gamma_2\gamma_2 a_2\rangle$ transforming according to irreducible representations Γ_1 and Γ_2 of $G \subset SO(3)$ follows

$$|j_1\Gamma_1\gamma_1 a_1\rangle|j_2\Gamma_2\gamma_2 a_2\rangle = \sum_{j\Gamma\gamma a} |(j_1 j_2) j\Gamma\gamma a\rangle\langle j\Gamma\gamma a|j_1\Gamma_1\gamma_1 a_1, j_2\Gamma_2\gamma_2 a_2\rangle \quad (19)$$

where $|(j_1 j_2) j\Gamma\gamma a\rangle$ will be abbreviated below by writing $|j\Gamma\gamma a\rangle$. It should be noted that the product ket is reduced here with respect to the covering group SO(3). The coupling coefficient in Eq. (19) is defined by [1]

$$\langle j\Gamma\gamma a|j_1\Gamma_1\gamma_1 a_1, j_2\Gamma_2\gamma_2 a_2\rangle = \sum_{m_1 m_2 m} \langle j m|j_1 m_1 j_2 m_2\rangle\,\langle j_1 m_1|j_1\Gamma_1\gamma_1 a_1\rangle\,\langle j_2 m_2|j_2\Gamma_2\gamma_2 a_2\rangle\,\langle j m|j\Gamma\gamma a\rangle^*\,. \quad (20)$$

We are now going to investigate the effect of an interchange of arguments on the coupling coefficient of Equation (20). From the symmetry properties of Wigner coefficients [11, 12] it follows immediately for the interchange of the indices $1 \longleftrightarrow 2$,

$$\langle j\Gamma\gamma a|j_1\Gamma_1\gamma_1 a_1, j_2\Gamma_2\gamma_2 a_2\rangle = (-1)^{j_1+j_2-j}\langle j\Gamma\gamma a|j_2\Gamma_2\gamma_2 a_2, j_1\Gamma_1\gamma_1 a_1\rangle\,. \quad (21)$$

If, in Eq. (20), the arguments $j\Gamma\gamma a \longleftrightarrow j_1\Gamma_1\gamma_1 a_1$ are interchanged, the resulting coefficient is

$$\langle j_1\Gamma_1\gamma_1 a_1|j\Gamma\gamma a, j_2\Gamma_2\gamma_2 a_2\rangle = \sum_{m_1 m_2 m} \langle j_1 m_1|j m j_2 m_2\rangle\,\langle j m|j\Gamma\gamma a\rangle\,\langle j_2 m_2|j_2\Gamma_2\gamma_2 a_2\rangle\,\langle j_1 m_1|j_1\Gamma_1\gamma_1 a_1\rangle^*\,. \quad (22)$$

We now try to bring this coefficient in relation to the original coefficient in Equation (20). The Wigner coefficient in Eq. (22) may be written

$$\langle j_1 m_1|j m j_2 m_2\rangle = (-1)^{j_2+m_2}\left[\frac{2j_1+1}{2j+1}\right]^{1/2}\langle j-m|j_1-m_1 j_2 m_2\rangle \quad (23)$$

whereas the expansion coefficients $\langle j m|j\Gamma\gamma a\rangle$ and $\langle j_1 m_1|j_1\Gamma_1\gamma_1 a_1\rangle^*$ may be expressed according to Equation (17). Putting these results together, the coefficient Eq. (22) assumes the form

$$\langle j_1 \Gamma_1 \gamma_1 a_1 | j \Gamma \gamma a, j_2 \Gamma_2 \gamma_2 a_2 \rangle \tag{24}$$
$$= (-1)^{j_1+j_2-j} \left[\frac{2j_1+1}{2j+1}\right]^{1/2} \begin{pmatrix} & j \\ \overline{\Gamma \gamma a} & \Gamma \gamma a \end{pmatrix} \begin{pmatrix} & j_1 \\ \overline{\Gamma_1 \gamma_1 a_1} & \Gamma_1 \gamma_1 a_1 \end{pmatrix}^* \langle j \overline{\Gamma \gamma a} | j_1 \overline{\Gamma_1 \gamma_1 a_1}, j_2 \Gamma_2 \gamma_2 a_2 \rangle .$$

This equation is the sought relation between the coupling coefficients of Eq. (20) and Equation (22). The expression corresponding to the third possible interchange of arguments, viz. $j \Gamma \gamma a \longleftrightarrow j_2 \Gamma_2 \gamma_2 a_2$, may be constructed from Eq. (21) and Eq. (24)

$$\langle j_2 \Gamma_2 \gamma_2 a_2 | j_1 \Gamma_1 \gamma_1 a_1, j \Gamma \gamma a \rangle \tag{25}$$
$$= (-1)^{j_1-j_2+j} \left[\frac{2j_2+1}{2j+1}\right]^{1/2} \begin{pmatrix} & j \\ \overline{\Gamma \gamma a} & \Gamma \gamma a \end{pmatrix} \begin{pmatrix} & j_2 \\ \overline{\Gamma_2 \gamma_2 a_2} & \Gamma_2 \gamma_2 a_2 \end{pmatrix}^* \langle j \overline{\Gamma \gamma a} | j_1 \Gamma_1 \gamma_1 a_1, j_2 \overline{\Gamma_2 \gamma_2 a_2} \rangle .$$

On the basis of the three relations thus derived, viz. Eq. (21), Eq. (24), and Eq. (25), a symmetric coupling coefficient for the subgroup $G \subset SO(3)$ may be defined by

$$\begin{pmatrix} j_1 & j_2 & j \\ \Gamma_1 \gamma_1 a_1 & \Gamma_2 \gamma_2 a_2 & \Gamma \gamma a \end{pmatrix} = (-1)^{j_1-j_2+j} [2j+1]^{-1/2} \begin{pmatrix} & j \\ \Gamma \gamma a & \overline{\Gamma \gamma a} \end{pmatrix} \langle j \overline{\Gamma \gamma a} | j_1 \Gamma_1 \gamma_1 a_1, j_2 \Gamma_2 \gamma_2 a_2 \rangle . \tag{26}$$

It is easy to verify that the symmetric coupling coefficient of Eq. (26) shows the same behavior with respect to an interchange of columns as the 3-j symbol. Also the unitarity conditions for these coefficients follow easily from those of the coupling coefficients involved (cf. Eq. (43) of Reference [1]). On the other hand, it should be observed that the $\bar{f}$ coefficient introduced by Kibler [10] is conjugate complex to the coefficient of Eq. (26) and that a sum over $\overline{\Gamma \gamma a}$ is implied. In addition, it has been pointed out above [cf. Section 2 and Eq. (8)] that the metric tensor employed here is the conjugate complex of that involved in the $\bar{f}$ coefficient. Both quantities share the direct dependence on j_1, j_2, and j which is the major reason that they are not particularly useful in actual calculations. In fact, it has been shown [10] that the $\bar{W}_f$ coefficient which is essentially the sum of products of four coefficients $\bar{f}$ is identical to the quantity $\bar{W}$ of Racah [13] and thus is equal to the 6-j symbol. Similarly the X_f coefficient of Kibler (sum of products of six $\bar{f}$) is identical to the X coefficient [13] or the 9-j symbol. It follows that the coefficient of Eq. (26) is nothing more than the 3-j symbol for a subgroup basis in $G \subset SO(3)$ and, indeed, we may write

$$\begin{pmatrix} j_1 & j_2 & j \\ \Gamma_1 \gamma_1 a_1 & \Gamma_2 \gamma_2 a_2 & \Gamma \gamma a \end{pmatrix} = \sum_{m_1 m_2 m} \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix} \langle j_1 m_1 | j_1 \Gamma_1 \gamma_1 a_1 \rangle \langle j_2 m_2 | j_2 \Gamma_2 \gamma_2 a_2 \rangle \langle j m | j \Gamma \gamma a \rangle . \tag{27}$$

4. 3-Γ'Symbols for Arbitrary Point Groups

In considering an arbitrary point group G, we are free to choose any basis $|\Gamma \gamma\rangle$ for a given representation Γ which shows the required transformation properties. We may decide to use, in particular, the basis functions $|j \Gamma \gamma a\rangle$ of the previous section. The coupling of two basis kets transforming according to irreducible representation Γ_1 and Γ_2, respectively, may then be described by

$$|j_1 \Gamma_1 \gamma_1 a_1\rangle |j_2 \Gamma_2 \gamma_2 a_2\rangle = \sum_{\Gamma \gamma b} |(j_1 \Gamma_1 a_1, j_2 \Gamma_2 a_2) \Gamma \gamma b\rangle \langle \Gamma \gamma b | \Gamma_1 \gamma_1 \Gamma_2 \gamma_2 \rangle . \tag{28}$$

Here the ket $|(j_1 \Gamma_1 a_1, j_2 \Gamma_2 a_2) \Gamma \gamma b\rangle$ may be written more concisely as $|\Gamma \gamma b\rangle$ and a similar statement applies for the kets on the right of Equation (28). Also it should be observed that, in contrast to Eq. (19), the product ket has been reduced here with respect to group G only. Finally, the label b in Eq. (28) is a Kronecker multiplicity index which is required whenever representation Γ occurs more than once in the decomposition of the Kronecker product

$$\Gamma_1 \otimes \Gamma_2 = \sum_{\Gamma} b_\Gamma \Gamma . \tag{29}$$

Obviously, the ket vectors $|(j_1 \Gamma_1 a_1, j_2 \Gamma_2 a_2) \Gamma \gamma b\rangle$ form a basis for representation Γ of G. Provided that $G \subset SO(3)$, linear combinations of these vectors have to be taken in order to construct bases which are irreducible under SO(3),

$$|(j_1 \Gamma_1 a_1, j_2 \Gamma_2 a_2) \Gamma \gamma b\rangle = \sum_{ja} |(j_1 j_2) j \Gamma \gamma a\rangle \, (j \Gamma a b \,|\, j_1 \Gamma_1 a_1, j_2 \Gamma_2 a_2). \tag{30}$$

Here the coefficients are independent of the γ_i. If now Eq. (30) is used in Eq. (19) and the outcoming expression is compared with Eq. (28), the result may be written as

$$\langle j \Gamma \gamma a \,|\, j_1 \Gamma_1 \gamma_1 a_1, j_2 \Gamma_2 \gamma_2 a_2\rangle = \sum_b (j \Gamma a b \,|\, j_1 \Gamma_1 a_1, j_2 \Gamma_2 a_2) \langle \Gamma \gamma b \,|\, \Gamma_1 \gamma_1 \Gamma_2 \gamma_2\rangle . \tag{31}$$

This is the lemma of Racah [14] thus connecting the coupling coefficients of two groups which are related as, e. g., in the present case where $G \subset \mathrm{SO}(3)$.

We may now return to the original intention to define a symmetrized coupling coefficient for an arbitrary point group G and write, in complete analogy to Eq. (26),

$$\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma \\ \gamma_1 & \gamma_2 & \gamma \end{pmatrix}_b = (-1)^{j_1 - j_2 + j} [d_\Gamma]^{-1/2} \begin{pmatrix} & j \\ \Gamma \gamma a & \overline{\Gamma \gamma a} \end{pmatrix} \langle \Gamma \gamma b \,|\, \Gamma_1 \gamma_1 \Gamma_2 \gamma_2\rangle \tag{32}$$

where the metric tensor is defined by the basis of the irreducible representation Γ. This quantity will be called, for obvious reasons, a 3-Γ symbol. In Eq. (32), b is the Kronecker multiplicity index introduced above and d_Γ the dimension of representation Γ. The relation between labels Γ_i and j_i which is needed in the application of Eq. (32) is provided by Equation (31). The 3-Γ symbol is different from zero subject to the following conditions:

(i) j_1, j_2, and j conform to the triangular condition;
(ii) the irreducible representations Γ_i of G are contained within $D^{(j_i)}(G)$;
(iii) the inner direct product $\Gamma_1 \otimes \Gamma_2 \otimes \Gamma$ contains the totally symmetric representation.

If required, Eq. (32) may be explicitly derived by studying the interchange of arguments in the coupling coefficients of group G, i. e. $\langle \Gamma \gamma b \,|\, \Gamma_1 \gamma_1 \Gamma_2 \gamma_2\rangle$. The method consists of using the detailed results of the previous section in conjunction with the lemma, Equation (31). Observe that without taking account of the time-reversal symmetry, a sum over $\Gamma' \gamma'$ would occur on the right of Eq. (32), $\overline{\Gamma \gamma}$ being replaced simultaneously by $\Gamma' \gamma'$.

The 3-Γ symbols form the elements of a unitary matrix. The corresponding conditions which are stated below follow easily from the unitarity relations of the coupling coefficients involved [viz. Eq. (7) and Eq. (8) of [1]]. It is

$$\sum_{\gamma_1 \gamma_2} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma \\ \gamma_1 & \gamma_2 & \gamma \end{pmatrix}_b^* \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma' \\ \gamma_1 & \gamma_2 & \gamma' \end{pmatrix}_b = [d_\Gamma]^{-1} \delta(\Gamma, \Gamma') \, \delta(\gamma, \gamma') \delta(b, b'), \tag{33}$$

$$\sum_{\Gamma \gamma b} [d_\Gamma] \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma \\ \gamma_1 & \gamma_2 & \gamma \end{pmatrix}_b^* \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma \\ \gamma_1' & \gamma_2' & \gamma \end{pmatrix}_b = \delta(\gamma_1, \gamma_1') \delta(\gamma_2, \gamma_2'). \tag{34}$$

Similar to the lemma of Racah, the 3-Γ symbols and the 3-j symbols over a subgroup basis, Eq. (26), are related. The expression which is equivalent to Eq. (31) may be written

$$\begin{pmatrix} j_1 & j_2 & j \\ \Gamma_1 \gamma_1 a_1 & \Gamma_2 \gamma_2 a_2 & \Gamma \gamma a \end{pmatrix} = \sum_b \begin{pmatrix} j_1 & j_2 & j \\ \Gamma_1 a_1 & \Gamma_2 a_2 & \Gamma a \end{pmatrix}_b \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma \\ \gamma_1 & \gamma_2 & \gamma \end{pmatrix}_b . \tag{35}$$

The coefficient in Eq. (35) again has unitary properties as may be verified by application of the known relations for the 3-Γ and 3-j symbols. It should be observed that the coefficients involved in Eq. (31) and Eq. (35) are sometimes called isoscalar factors [7].

The position of the multiplicity index b in the 3-Γ symbol of Eq. (32) is of no importance. This may be demonstrated easily by looking at the frequency of the resulting representation. Thus, on the basis of a relation equivalent to Eq. (25), the coefficient $\langle \Gamma_2 \gamma_2 b \,|\, \Gamma_1 \gamma_1 \Gamma \gamma\rangle$, e. g., is related to $\langle \overline{\Gamma \gamma b} \,|\, \Gamma_1 \gamma_1 \overline{\Gamma_2 \gamma_2}\rangle$ which coefficient corresponds to the reduction $\Gamma_1 \otimes \overline{\Gamma}_2 = \Sigma \, n_{\overline{\Gamma}} \overline{\Gamma}$. The frequency of $\overline{\Gamma}$ is now given by

$$n_{\overline{\Gamma}} = 1/g \sum_R \chi_{\Gamma_1}(R) \chi_{\overline{\Gamma}_2}(R) \chi_{\overline{\Gamma}}(R)^* . \tag{36}$$

Since $\chi_{\overline{\Gamma}}(R)^* = \chi_\Gamma(R)$ and similarly $\chi_{\overline{\Gamma}_2}(R) = \chi_{\Gamma_2}(R)^*$, Eq. (36) is identical to the relation for n_{Γ_2} in the reduction $\Gamma_1 \otimes \Gamma = \Sigma\, n_{\Gamma_2} \Gamma_2$. It follows that the index b may be placed outside the 3-Γ symbol, in agreement with the usage for non-simply reducible finite groups [4].

As a consequence of the structure of the 3-Γ symbol and its relation to the 3-j symbol, as expressed by Eq. (35) and Eq. (27), the properties of the 3-Γ symbol with respect to an interchange of columns are equivalent to those of the 3-j symbol provided a positive and real isoscalar factor is assumed. Thus an even permutation of the columns leaves the numerical value unaltered,

$$\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma \\ \gamma_1 & \gamma_2 & \gamma \end{pmatrix}_b = \begin{pmatrix} \Gamma_2 & \Gamma & \Gamma_1 \\ \gamma_2 & \gamma & \gamma_1 \end{pmatrix}_b = \begin{pmatrix} \Gamma & \Gamma_1 & \Gamma_2 \\ \gamma & \gamma_1 & \gamma_2 \end{pmatrix}_b \tag{37}$$

whereas an odd permutation introduces the factor $(-1)^{j_1+j_2+j}$,

$$\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma \\ \gamma_1 & \gamma_2 & \gamma \end{pmatrix}_b = (-1)^{j_1+j_2+j} \begin{pmatrix} \Gamma_2 & \Gamma_1 & \Gamma \\ \gamma_2 & \gamma_1 & \gamma \end{pmatrix}_b. \tag{38}$$

The result of Eq. (38) should be compared with that obtained if group G is considered on an isolated basis. Thus the treatment of Derome and Sharp [4] would give the phase factor $(-1)^{\Gamma_1+\Gamma_2+\Gamma}$ which is useful only if additional definitions are introduced [6].

Except for certain modifications deriving from the group-subgroup relation $G \subset SO(3)$, the 3-Γ symbols conform to the general definitions introduced for any finite and compact group [4]. Since the corresponding expressions are easily converted to the present case, these will not be given in detail. As an example we list below the relation between the 3-Γ symbols for conjugate complex representations,

$$\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma \\ \gamma_1 & \gamma_2 & \gamma \end{pmatrix}_b^* = \begin{pmatrix} & j_1 & \\ \Gamma_1\gamma_1 a_1 & & \overline{\Gamma_1\gamma_1 a_1} \end{pmatrix}^* \begin{pmatrix} & j_2 & \\ \Gamma_2\gamma_2 a_2 & & \overline{\Gamma_2\gamma_2 a_2} \end{pmatrix}^* \begin{pmatrix} & j & \\ \Gamma\gamma a & & \overline{\Gamma\gamma a} \end{pmatrix}^* \begin{pmatrix} \overline{\Gamma}_1 & \overline{\Gamma}_2 & \overline{\Gamma} \\ \overline{\gamma}_1 & \overline{\gamma}_2 & \overline{\gamma} \end{pmatrix}_b. \tag{39}$$

This expression is the lemma of Sharp [4] applied to the 3-Γ symbols of Equation (32).

5. 6-Γ Symbols for Point Groups

The definition of the higher 3 n-Γ symbols may be accomplished in the usual way. Thus a 6-Γ symbol will now depend on four multiplicity indices, one for each of the inherent 3-Γ symbols *,

$$\begin{aligned} \begin{Bmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \Gamma_4 & \Gamma_5 & \Gamma_6 \end{Bmatrix}_{b_1b_2b_3b_4} = \sum_{\substack{\gamma_1\gamma_2\gamma_3\\ \gamma_4\gamma_5\gamma_6}} & \begin{pmatrix} & j_1 & \\ \overline{\Gamma_1\gamma_1} & & \Gamma_1\gamma_1 \end{pmatrix}^* \begin{pmatrix} & j_2 & \\ \overline{\Gamma_2\gamma_2} & & \Gamma_2\gamma_2 \end{pmatrix}^* \begin{pmatrix} & j_3 & \\ \overline{\Gamma_3\gamma_3} & & \Gamma_3\gamma_3 \end{pmatrix}^* \\ & \cdot \begin{pmatrix} & j_4 & \\ \overline{\Gamma_4\gamma_4} & & \Gamma_4\gamma_4 \end{pmatrix}^* \begin{pmatrix} & j_5 & \\ \overline{\Gamma_5\gamma_5} & & \Gamma_5\gamma_5 \end{pmatrix}^* \begin{pmatrix} & j_6 & \\ \overline{\Gamma_6\gamma_6} & & \Gamma_6\gamma_6 \end{pmatrix}^* \begin{pmatrix} \overline{\Gamma}_4 & \Gamma_5 & \Gamma_3 \\ \overline{\gamma}_4 & \gamma_5 & \gamma_3 \end{pmatrix}_{b_1} \\ & \cdot \begin{pmatrix} \Gamma_4 & \Gamma_2 & \overline{\Gamma}_6 \\ \gamma_4 & \gamma_2 & \overline{\gamma}_6 \end{pmatrix}_{b_2} \begin{pmatrix} \Gamma_1 & \overline{\Gamma}_5 & \Gamma_6 \\ \gamma_1 & \overline{\gamma}_5 & \gamma_6 \end{pmatrix}_{b_3} \begin{pmatrix} \overline{\Gamma}_1 & \overline{\Gamma}_2 & \overline{\Gamma}_3 \\ \overline{\gamma}_1 & \overline{\gamma}_2 & \overline{\gamma}_3 \end{pmatrix}_{b_4} \end{aligned} \tag{40}$$

or expressed in a more simple form,

$$\begin{aligned} \begin{Bmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \Gamma_4 & \Gamma_5 & \Gamma_6 \end{Bmatrix}_{b_1b_2b_3b_4} = \sum_{\substack{\gamma_1\gamma_2\gamma_3\\ \gamma_4\gamma_5\gamma_6}} & \begin{pmatrix} & j_4 & \\ \overline{\Gamma_4\gamma_4} & & \Gamma_4\gamma_4 \end{pmatrix}^* \begin{pmatrix} & j_5 & \\ \overline{\Gamma_5\gamma_5} & & \Gamma_5\gamma_5 \end{pmatrix}^* \begin{pmatrix} & j_6 & \\ \overline{\Gamma_6\gamma_6} & & \Gamma_6\gamma_6 \end{pmatrix}^* \\ & \cdot \begin{pmatrix} \overline{\Gamma}_4 & \Gamma_5 & \Gamma_3 \\ \overline{\gamma}_4 & \gamma_5 & \gamma_3 \end{pmatrix}_{b_1} \begin{pmatrix} \Gamma_4 & \Gamma_2 & \overline{\Gamma}_6 \\ \gamma_4 & \gamma_2 & \overline{\gamma}_6 \end{pmatrix}_{b_2} \begin{pmatrix} \Gamma_1 & \overline{\Gamma}_5 & \Gamma_6 \\ \gamma_1 & \overline{\gamma}_5 & \gamma_6 \end{pmatrix}_{b_3} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_{b_4}^*. \end{aligned} \tag{41}$$

These two equations are connected by the lemma of Sharp, Eq. (39), the former expression conforming also to the definition of Derome and Sharp [4]. Obviously, these definitions may be related to the unitary

* For convenience of presentation, the indices a_i in the metric tensors are not explicitly written. In addition, it has been always assumed that $D^{j\Gamma a}(R) \equiv D^{j'\Gamma a'}(R)$ for all j, a, j', a', cf. Eq. (18) of [3].

matrix between two different coupling schemes of three basis kets of a given point group G,

$$\langle (\Gamma_1 \Gamma_2) \Gamma_{12} b_{12} \Gamma_3; \Gamma b \mid \Gamma_1 (\Gamma_2 \Gamma_3) \Gamma_{23} b_{23}; \Gamma b' \rangle$$

$$= [d_{\Gamma_{12}} d_{\Gamma_{23}}]^{1/2} (-1)^{(j_3 + j - j_{12})_b + (2 j_3)_{b23} + (2 j_{23})_{b'} + (j_1 - j_2 + j_{12})_{b12}} \begin{Bmatrix} \bar{\Gamma}_1 & \bar{\Gamma}_2 & \Gamma_{12} \\ \bar{\Gamma}_3 & \bar{\Gamma} & \bar{\Gamma}_{23} \end{Bmatrix}_{b b_{23} b' b_{12}} . \quad (42)$$

Here, the phase factor $(-1)^{(j)_b}$ is defined by that particular value j within the basis function $|j \Gamma \gamma a\rangle$ which has been employed to calculate the 3-Γ symbol with index b. The 6-Γ symbols are the elements of a unitary matrix and satisfy thus the condition

$$\sum_{\Gamma_6} [d_{\Gamma_3}][d_{\Gamma_6}] \begin{Bmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \Gamma_4 & \Gamma_5 & \Gamma_6 \end{Bmatrix}^*_{b_1 b_2 b_3 b_4} \begin{Bmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3' \\ \Gamma_4 & \Gamma_5 & \Gamma_6 \end{Bmatrix}_{b_1' b_2 b_3 b_4'} = \delta(\Gamma_3, \Gamma_3') \, \delta(b_1, b_1') \, \delta(b_4, b_4') \, . \quad (43)$$

The symmetry properties of the 6-Γ symbols under interchanges of rows and columns may be expressed as follows:

$$\text{(i)} \quad \begin{Bmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \Gamma_4 & \Gamma_5 & \Gamma_6 \end{Bmatrix}_{b_1 b_2 b_3 b_4} = (-1)^{(2j_4)_{b_1} + (2j_6)_{b_2} + (2j_2)_{b_4}} \begin{Bmatrix} \bar{\Gamma}_1 & \Gamma_5 & \bar{\Gamma}_6 \\ \bar{\Gamma}_4 & \Gamma_2 & \bar{\Gamma}_3 \end{Bmatrix}_{b_2 b_1 b_4 b_3} ; \quad (44)$$

$$\text{(ii)} \quad \begin{Bmatrix} \Gamma_a & \Gamma_b & \Gamma_c \\ \bar{\Gamma}_d & \bar{\Gamma}_e & \bar{\Gamma}_f \end{Bmatrix}_{\beta_1 \beta_2 \beta_3 \beta_4} = M_i(\bar{\Gamma}_4 \Gamma_5 \Gamma_3)_{\beta_1 b_1} \, M_i(\Gamma_4 \Gamma_2 \bar{\Gamma}_6)_{\beta_2 b_2} \cdot M_i(\Gamma_1 \bar{\Gamma}_5 \Gamma_6)_{\beta_3 b_3} \, M_i(\Gamma_1 \Gamma_2 \Gamma_3)_{\beta_4 b_4} \begin{Bmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \Gamma_4 & \Gamma_5 & \Gamma_6 \end{Bmatrix}_{b_1 b_2 b_3 b_4} \quad (45)$$

with a third condition for the cyclic permutation of arguments which is similar to (ii) except for the complex conjugations on the left. The M_i in Eq. (45) are interchange matrices defining any interchange of the arguments specified. On the basis of the above, most definitions for 6-j symbols for an arbitrary group [4] may be conveniently carried over to 6-Γ symbols. Similar statements apply to the higher 3 n-G symbols.

6. 3-Γ Symbols for the Point Group I. — An Example

The point group I of the icosahedron is non-simply reducible thus providing a convenient example to demonstrate the calculation of 3-Γ symbols with the added complication of a multiplicity index. It should be noted that the latter index b is required whenever the irreducible representation $H(\Gamma_5)$ occurs at least twice in the Kronecker product.

The actual procedure is based on Eq. (27) and Equation (35). First of all, the basis functions employed here are specified in Table 1. The expansion coefficients involved and the appropriate 3-j symbols are then inserted into Eq. (27) and the 3-j symbols for the subgroup $I \subset SO(3)$ are obtained. Subsequently, Eq. (35) is used to generate the 3-Γ symbols, the required isoscalar factors being determined by a renormalization as described elsewhere [1]. The resulting non-zero 3-Γ symbols are presented in Table 2. In this example, all metric tensors are of value unity.

It should be observed that if several 3-Γ symbols are connected on the basis of general symmetry properties or by similar relations, only one 3-Γ

Table 1. Basis functions for point group I.

$\lvert j \Gamma \gamma a \rangle$	Basis functions [a] $\sum_m \langle j m \mid j \Gamma \gamma a \rangle \mid j m \rangle$	Time-inverted basis [b] $\lvert j \overline{\Gamma \gamma a} \rangle$
$\lvert 0A_1 11\rangle$	$\lvert 00\rangle$	$\lvert 0A_1 11\rangle$
$\lvert 1T_1 01\rangle$	$i \lvert 10\rangle$	$\lvert 1T_1 01\rangle$
$\lvert 1T_1 11\rangle$	$- \lvert 11\rangle$	$\lvert 1T_1 -11\rangle$
$\lvert 2H01\rangle$	$\lvert 20\rangle$	$\lvert 2H01\rangle$
$\lvert 2H11\rangle$	$i \lvert 21\rangle$	$\lvert 2H-11\rangle$
$\lvert 2H21\rangle$	$- \lvert 22\rangle$	$\lvert 2H-21\rangle$
$\lvert 3T_2 01\rangle$	$i \lvert 30\rangle$	$\lvert 3T_2 01\rangle$
$\lvert 3T_2 11\rangle$	$-i\sqrt{3/5} \lvert 32\rangle - \sqrt{2/5} \lvert 3-3\rangle$	$\lvert 3T_2 -11\rangle$
$\lvert 3G11\rangle$	$\lvert 31\rangle$	$\lvert 3G-11\rangle$
$\lvert 3G21\rangle$	$-i\sqrt{2/5} \lvert 32\rangle + \sqrt{3/5} \lvert 3-3\rangle$	$\lvert 3G-21\rangle$
$\lvert 4G12\rangle$	$-\sqrt{7/15} \lvert 41\rangle - i\sqrt{8/15} \lvert 4-4\rangle$	$\lvert 4G-12\rangle$
$\lvert 4G22\rangle$	$-i\sqrt{14/15} \lvert 42\rangle + 1/\sqrt{15} \lvert 4-3\rangle$	$\lvert 4G-22\rangle$
$\lvert 4H02\rangle$	$\lvert 40\rangle$	$\lvert 4H02\rangle$
$\lvert 4H12\rangle$	$-i\sqrt{8/15} \lvert 41\rangle - \sqrt{7/15} \lvert 4-4\rangle$	$\lvert 4H-12\rangle$
$\lvert 4H22\rangle$	$-1/\sqrt{15} \lvert 42\rangle + i\sqrt{14/15} \lvert 4-3\rangle$	$\lvert 4H-22\rangle$

[a] Basis functions are such chosen that all metric tensors are of value unity. Positive rotation of the coordinates assumed. The basis functions are according to A. G. McLellan, J. Chem. Phys. **34**, 1350 [1961].

[b] The time-inverted basis may be constructed by application of Equation (16).

Table 2. 3-Γ Symbols for Point Group I.[a]

T_1	T_1	T_1	3-Γ[b]
0	1	−1	$i/\sqrt{6}$

T_1	T_1	H	3-Γ
0	0	0	$-\sqrt{2/15}$
0	1	−1	$-1/\sqrt{10}$
1	1	−2	$-1/\sqrt{5}$
1	−1	0	$1/\sqrt{30}$

T_1	T_2	G	3-Γ[b]
0	1	−2	$i/\sqrt{6}$
1	0	−1	$i/\sqrt{6}$
1	1	2	$-i/\sqrt{12}$
1	−1	1	$-i/\sqrt{12}$

T_1	T_2	H	3-Γ
0	0	0	$1/\sqrt{5}$
0	1	−2	$1/\sqrt{15}$
1	0	−1	$-1/\sqrt{15}$
1	1	2	$-\sqrt{2/15}$
1	−1	1	$\sqrt{2/15}$

T_1	G	G	3-Γ[b]
0	1	−1	$i/\sqrt{12}$
0	2	−2	$-i/\sqrt{12}$
1	1	−2	$i/\sqrt{6}$

T_1	G	H	3-Γ
0	1	−1	$-\sqrt{2/15}$
0	2	−2	$1/\sqrt{30}$
1	1	−2	$1/\sqrt{60}$
1	−1	0	$-1/\sqrt{10}$
1	2	2	$\sqrt{3/20}$
1	−2	1	$1/\sqrt{15}$

T_1	H	H	3-Γ[b]
0	1	−1	$i/\sqrt{30}$
0	2	−2	$i\sqrt{2/15}$
1	0	−1	$-i/\sqrt{10}$
1	1	−2	$-i/\sqrt{15}$

T_2	T_2	T_2	3-Γ[b]
0	1	−1	$-i/\sqrt{6}$

T_2	T_2	H	3-Γ
0	0	0	$-\sqrt{2/15}$
0	1	−2	$1/\sqrt{10}$
1	1	1	$1/\sqrt{5}$
1	−1	0	$1/\sqrt{30}$

T_2	G	G	3-Γ[b]
0	1	−1	$-i/\sqrt{12}$
0	2	−2	$-i/\sqrt{12}$
1	1	2	$-i/\sqrt{6}$

T_2	G	H	3-Γ
0	1	−1	$1/\sqrt{30}$
0	2	−2	$\sqrt{2/15}$
1	1	2	$1/\sqrt{15}$
1	−1	−1	$\sqrt{3/20}$
1	2	1	$-1/\sqrt{60}$
1	−2	0	$-1/\sqrt{10}$

T_2	H	H	3-Γ[b]
0	1	−1	$-i\sqrt{2/15}$
0	2	−2	$i/\sqrt{30}$
1	0	−2	$i/\sqrt{10}$
1	1	2	$i/\sqrt{15}$

G	G	G	b	3-Γ
1	1	−2	4	$-i/\sqrt{12}$
1	2	2	4	$-i/\sqrt{12}$

G	G	H	3-Γ
1	1	−2	$-\sqrt{2/15}$
1	−1	0	$-1/\sqrt{20}$
1	2	2	$-1/\sqrt{30}$
1	−2	1	$1/\sqrt{30}$
2	2	1	$-\sqrt{2/15}$
2	−2	0	$1/\sqrt{20}$

H	H	G	3-Γ[b]
0	1	−1	$i/\sqrt{20}$
0	2	−2	$-i/\sqrt{20}$
1	2	2	$-i\sqrt{3/40}$
1	−2	1	$i\sqrt{3/40}$

H	H	G	b	3-Γ
0	1	−1	4	$-i/\sqrt{20}$
0	2	−2	4	$-i/\sqrt{20}$
1	1	−2	4	$-2i/\sqrt{30}$
1	2	2	4	$i/2\sqrt{30}$
1	−2	1	4	$-i/2\sqrt{30}$
2	2	1	4	$-2i/\sqrt{30}$

H	H	H	3-Γ
0	0	0	$-\sqrt{2/35}$
0	1	−1	$-1/\sqrt{70}$
0	2	−2	$\sqrt{2/35}$
1	1	−2	$-\sqrt{3/35}$

H	H	H	b	3-Γ
0	0	0	4	$6/5\sqrt{14}$
0	1	−1	4	$-4/5\sqrt{14}$
0	2	−2	4	$1/5\sqrt{14}$
1	1	−2	4	$2/5\sqrt{21}$
1	2	2	4	$-7/5\sqrt{21}$

[a] The 3-Γ symbols have been calculated, in general, employing basis functions of the minimum value of j. Where this is not the case, the index $b=j$ has been added for the basis representation Γ within $\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma \\ \gamma_1 & \gamma_2 & \gamma \end{pmatrix}_b$.

[b] The 3-Γ symbol changes sign under odd permutation of columns.

symbol is listed. Thus, according to Eq. (37) and Eq. (38), the 3-Γ symbols are invariant against even permutations of columns, odd permutations introducing the phase factor $(-1)^{j_1+j_2+j}$. Also, conjugate complex 3-Γ symbols are related by Equation (39). Finally, 3-Γ symbols containing the totally symmetric representation A_1 may be written as

$$\begin{pmatrix} A_1 & \Gamma_2 & \Gamma \\ a_1 & \gamma_2 & \gamma \end{pmatrix} = [d_\Gamma]^{-1/2} \, \delta(\Gamma_2, \Gamma) \, \delta(\gamma_2, \bar{\gamma}) \qquad (46)$$

and are therefore not separately listed.

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[1] E. König and S. Kremer, Theor. Chim. Acta **32**, 27 [1973].
[2] E. P. Wigner, Group Theory and its Application to the Quantum Mechanics of Atomic Spectra, Academic Press, New York 1959.
[3] E. P. Wigner, On the Matrices which Reduce the Kronecker Product of Representations of S. R. Groups (unpublished manuscript, 1940), reprinted in L. C. Biedenharn and H. Van Dam, Quantum Theory of Angular Momentum, Academic Press, New York 1965.
[4] J. R. Derome and W. T. Sharp, J. Math. Phys. **6**, 1584 [1965].
[5] J. R. Derome, J. Math. Phys. **7**, 612 [1966].
[6] J. S. Griffith, The Irreducible Tensor Method for Molecular Symmetry Groups, Englewood Cliffs, N. J., Prentice-Hall 1962.
[7] B. G. Wybourne, Symmetry Principles and Atomic Spectroscopy, Wiley-Intersci., New York 1970.
[8] B. R. Judd, in E. M. Loebl, Group Theory and Its Applications, Vol. 1, Academic Press, New York 1968.
[9] R. J. Elliott and K. W. H. Stevens, Proc. Roy. Soc. **A 218**, 553 [1953].
[10] M. Kibler, J. Mol. Spectrosc. **26**, 111 [1968].
[11] A. R. Edmonds, Angular Momentum in Quantum Mechanics, Princeton University Press, Princeton 1960.
[12] M. E. Rose, Elementary Theory of Angular Momentum, John Wiley, New York 1957.
[13] U. Fano and G. Racah, Irreducible Tensorial Sets, Academic Press, New York 1959.
[14] G. Racah, Phys. Rev. **76**, 1352 [1949].