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Additional symmetry of Clebsch-Gordan coefficients for corepresentations

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Abstract. The concept of associated representations is generalised for the case of corepresentations. Symmetry relations for the Clebsch–Gordan coefficients based on the association of corepresentations are derived. This additional symmetry not only reduces the volume of the calculations and the tables of coupling coefficients, but it also improves the correlation between the coefficients. A simple method for obtaining the Clebsch–Gordan coefficients for odd (under space inversion) basis functions is proposed.

1. Introduction

Group theory, and particularly the method of irreducible tensorial sets, is widely applied in atomic, molecular and solid state spectroscopy (Griffith 1962, Sviridov *et al* 1964, Sviridov and Smirnov 1977). The basic elements of the algebra of irreducible tensorial sets for systems with magnetic symmetry are the Clebsch–Gordan coefficients (CGC) for the irreducible corepresentations (coreps) of the anti-unitary Shubnikov magnetic groups (Wigner 1959, Bradley and Cracknell 1972, Kotzev 1972, Kotzev and Aroyo 1977). Some of their properties, such as the permutational symmetry of the CGC for coreps $[\alpha_1 a_1 \alpha_2 a_2|\alpha r_\alpha a]$ and $[\alpha_2 a_2 \alpha_1 a_1|\alpha r_\alpha a]$ which reduce the corep product $D^{\alpha_1}\times D^{\alpha_2}$ and $D^{\alpha_2}\times D^{\alpha_1}$ corespondingly is discussed in detail elsewhere (Kotzev and Aroyo 1977, 1980, 1981, 1982a, 1982b). A new type of symmetry of the CGC for coreps, which is connected with the operation of 'corep association', was briefly considered for the first time by Kotzev and Aroyo (1982c, 1983). In fact, the study of 'associated coreps' is of general interest and is independent of the development of the Racah algebra for coreps, but here it is of practical significance because it leads to the additional symmetries of the CGC.

Griffith (1962) seems to have been the first to use the concept of 'associated representations' for crystallographic point groups. The association of the single-valued, irreducible representations of the proper octahedral group O = 432 and the symmetry of the corresponding CGC was discussed by Griffith (1962), Sviridov *et al* (1964), Sviridov and Smirnov (1977) and Harnung (1973); Lulek and Lulek (1975a, 1975b) considered the association of the representations of the double-cubic and trigonal groups and the related changes of the CGC. Symmetry relations of the symmetrised CGC, based on a special case of the association of representations were discussed by Butler and Ford (1979).

The aim of this paper is to generalise the concept of associated representations for the case of corepresentations (§ 2) and to derive symmetry relations for the corresponding CGC for coreps (§ 3). We show that the symmetry of the CGC under association

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not only reduces the volume of the calculations and the tables, but also improves the correlations between the sets of coefficients and restricts the ambiguity in their definition (§ 3). A simple method for the calculation of CGC for coreps for odd (under space inversion) basis functions is considered in § 4.

A natural, but very necessary, specification of the terminology should be made, before the presentation of the results. Throughout the paper we use the term 'a standard set of corepresentations', which means a set of the matrices of all coreps D^α of a group $\mathscr{A}$, which are chosen and fixed in a definite way. If there are no special requirements, it is advisable to choose the coreps in the so-called 'Wigner cannonical form' as the standard set of coreps (Wigner 1959, Bradley and Cracknell 1972). However, our results are not restricted to such a choice and the cases, for which it is of any importance, will be especially underlined.

2. Associated corepresentations

The concept of associated coreps is defined by Kotzev and Aroyo (1982c, 1983) analogously to the concept of associatied representations. The coreps D^α and $D^{\alpha'}$ are associated with the corep D^{A} if,

$$D^{\alpha'} \sim D^{\alpha \times \mathrm{A}} \equiv D^\alpha \times D^{\mathrm{A}}. \tag{1}$$

Here '$\sim$' means equivalent and D^{A} is one-dimensional corep, the associating corep. It is obvious that dim $D^{\alpha'}$ = dim D^α and the corep $D^{\alpha'}$ is irreducible if and only if D^α is irreducible. When $D^{\alpha'}$ is equivalent to D^α, the corep D^α is called a self-associated corep with respect to D^{A}. The associating corep D^{A} can be real or complex, but is always one dimensional. The Kronecker square of a real corep D^{A} equals the identity corep D^{α_0} and the corep, associated with $D^{\alpha'}$ by D^{A} is D^α. In this case, the coreps D^α and $D^{\alpha'}$ form an associative pair (if $D^{\alpha'} \not\sim D^\alpha$). If D^{A} is one-dimensional complex corep then its Kronecker square is not D^{α_0} and the set of coreps associated with D^{A} contains more than two members, e.g. it can form a triad $(D^\alpha, D^{\alpha'}, D^{\alpha''})$ if $D^{\alpha'} \sim D^\alpha \times D^{\mathrm{A}}$, $D^{\alpha''} \sim D^{\alpha'} \times D^{\mathrm{A}}$ and $D^{\alpha''} \times D^{\mathrm{A}} \sim D^\alpha$. Therefore, the coreps of a group can be classified into sets of associated coreps with respect to the association with a given corep D^{A_i}. It is obvious that the classification into associative sets can be different for different associating coreps D^{A_i}.

As an example let us consider the group $\mathrm{D}_6 \otimes \Theta = 6221'$. It has six single-valued and three double-valued coreps. With the help of the corep multiplication table of $\mathrm{D}_6 \otimes \Theta$ (see e.g. Kotzev and Aroyo 1982b) its coreps are classified into the following associative sets with respect to the one-dimensional real coreps D^2, D^3 and D^4.

$$\begin{aligned} &D^{\mathrm{A}} = D^2\colon (D^1, D^2), (D^3, D^4), (D^5), (D^6), (D^7), (D^8), (D^9) \\ &D^{\mathrm{A}} = D^3\colon (D^1, D^3), (D^2, D^4), (D^5, D^6)(D^7, D^8)(D^9) \\ &D^{\mathrm{A}} = D^4\colon (D^1, D^4), (D^2, D^3), (D^5, D^6), (D^7, D^8), (D^9). \end{aligned} \tag{2}$$

Examples of triads of associated coreps can be found in the black and white magnetic group $\mathrm{O}(T) = 4'32'$, whose coreps are classified with respect to the complex one-dimensional coreps D^2 or D^3 as follows

$$\begin{aligned} &D^2\colon (D^1, D^2, D^3), (D^4), (D^5, D^6, D^7) \\ &D^3\colon (D^1, D^3, D^2), (D^4), (D^5, D^7, D^6). \end{aligned} \tag{3}$$

By definition (1), the associated corep $D^{\alpha\times A}$ is irreducible and is equivalent to one of the irreducible coreps $D^{\alpha'}$ of the same group. In the general case, the matrices of $D^{\alpha\times A}$ will differ from the standard set of matrices of $D^{\alpha'}$. It is obvious that the corep $D^{\alpha\times A}$ can be transformed into the standard form $D^{\alpha'}$ by the matrix of CGC for coreps D^{α} and D^{A}:

$$(U^{\alpha A})^{-1}(D^{\alpha}(g)\times D^{A}_{(g)})U^{\alpha A(*)}=D^{\alpha'}(g). \tag{4}$$

Here the asterisk in parenthesis means complex conjugation, which is applied only if $g\in G$ is an anti-unitary operator. Equation (4) is a more detailed definition of the corep $D^{\alpha'}$, associated with D^{α} by D^{A}. As we always work with a 'standard set of coreps', from now on we will follow the definition given by equation (4), which is equivalent to (1).

3. Symmetry properties of CGC for associated corepresentations

CGC for coreps are defined (Kotzev 1972) as matrix elements of a unitary transformation $U^{\alpha_1\alpha_2}$ which reduce the Kronecker product $D^{\alpha_1}\times D^{\alpha_2}$ to a direct sum of irreducible coreps $D^{\alpha_3}\in D^{\alpha_1}\times D^{\alpha_2}$:

$$(U^{\alpha_1\alpha_2})^{-1}(D^{\alpha_1}(g)\times D^{\alpha_2}(g))U^{\alpha_1\alpha_2(*)}=\bigoplus_{\alpha_3}(e^{\alpha_1\alpha_2}_{\alpha_3}\times D^{\alpha_3}(g)),\qquad \forall g\in G \tag{5}$$

where $e^{\alpha_1\alpha_2}_{\alpha_3}$ is an identity matrix, whose dimension equals $(\alpha_1\alpha_2|\alpha_3)$, the multiplicity of D^{α_3} in $D^{\alpha_1}\times D^{\alpha_2}$.

From the relation between the associated coreps (4), a useful connection follows between the corresponding CGC matrices for coreps. The determination of such a relation will lead to new symmetries of the CGC (which Sviridov *et al* (1964), and Sviridov and Smirnov (1977) called 'symmetries of the second kind'). Such symmetries will not only reduce the volume of the calculation and tables of CGC for coreps, but will also improve the correlation between the 'independent' (without the relation) sets of CGC for coreps.

We will derive this relation in a matrix form. Let us consider the most general case when association (4) is applied to all D^{α_i}, $i=1, 2, 3$ in equation (5), by different associating coreps D^{A_1}, D^{A_2} and $D^{A_3}=D^{A_1}\times D^{A_2}$. (Special cases can be found by taking the identity corep D^{α_0} as one of D^{A_i} in the final formulae.) The corresponding associated coreps will be

$$\begin{aligned}
D^{\alpha_1'}(g)&=(U^{\alpha_1A_1})^{-1}D^{\alpha_1}(g)\times D^{A_1}(g)U^{\alpha_1A_1(*)}\\
D^{\alpha_2''}(g)&=(U^{\alpha_2A_2})^{-1}D^{\alpha_2}(g)\times D^{A_2}(g)U^{\alpha_2A_2(*)}\\
D^{\alpha_3'''}(g)&=(U^{\alpha_3A_3})^{-1}D^{\alpha_3}(g)\times D^{A_3}(g)U^{\alpha_3A_3(*)}\qquad \forall g\in G.
\end{aligned} \tag{6}$$

The direct product of associated coreps $D^{\alpha_1'}\times D^{\alpha_2''}$ can be reduced into irreducible components $D^{\alpha_3''}\in D^{\alpha_1'}\times D^{\alpha_2''}$ with the CGC matrix $U^{\alpha_1'\alpha_2''}$

$$(U^{\alpha_1'\alpha_2''})^{-1}(D^{\alpha_1'}(g)\times D^{\alpha_2''}(g))U^{\alpha_1'\alpha_2''(*)}=\bigoplus_{\alpha_3''}(e^{\alpha_1'\alpha_2''}_{\alpha_3''}\times D^{\alpha_3''}(g)),\qquad \forall g\in G. \tag{7}$$

After the substitution of (6) into (7) and some elementary transformations, we get from equations (5)–(7)

$$X\left[\bigoplus_{\alpha_3'''}(e^{\alpha_1'\alpha_2''}_{\alpha_3'''}\times D^{\alpha_3'''}(g))\right]=\left[\bigoplus_{\alpha_3'''}(e^{\alpha_1\alpha_2}_{\alpha_3'''}\times D^{\alpha_3'''}(g))\right]X^{(*)} \tag{8}$$

where

$$X = X(\alpha_1, \alpha_2, A_1, A_2) = \left\{ (U^{\alpha_1 A_1} \times U^{\alpha_2 A_2})^{-1} (U^{\alpha_1\alpha_2} \times U^{A_1 A_2}) \times \left[\bigoplus_{\alpha_3} (e^{\alpha_1\alpha_2}_{\alpha_3} \times U^{\alpha_3 A_3}) \right] \right\}^{-1} U^{\alpha'_1\alpha''_2}. \tag{9}$$

It is obvious that the reducible coreps on the left- and right-hand sides of equation (8) are equivalent as they are reductions of $D^{\alpha_1} \times D^{\alpha_2} \times D^{A_1} \times D^{A_2}$ by two different schemes. For the RHS we have

$$\begin{array}{l} (D^{\alpha_1} \times D^{\alpha_2}) \times (D^{A_1} \times D^{A_2}) \\ \quad\Big\downarrow (U^{\alpha_1\alpha_2} \times U^{A_1 A_2}) \\ \left[\bigoplus_{\alpha_3} (e^{\alpha_1\alpha_2}_{\alpha_3} \times D^{\alpha_3}) \right] \times D^{A_3} \\ \quad\Big\downarrow \bigoplus_{\alpha_3} (e^{\alpha_1\alpha_2}_{\alpha_3} \times U^{\alpha_3 A_3}) \\ \bigoplus_{\alpha'''_3} (e^{\alpha_1\alpha_2}_{\alpha'''_3} \times D^{\alpha'''_3}), \end{array} \tag{10}$$

while the reduction in the LHS is according to the scheme

$$\begin{array}{l} (D^{\alpha_1} \times D^{A_1}) \times (D^{\alpha_2} \times D^{A_2}) \\ \quad\Big\downarrow U^{\alpha_1 A_1} \times U^{\alpha_2 A_2} \\ D^{\alpha'_1} \times D^{\alpha''_2} \\ \quad\Big\downarrow U^{\alpha'_1\alpha''_2} \\ \bigoplus_{\alpha'''_3} (e^{\alpha'_1\alpha''_2}_{\alpha'''_3} \times D^{\alpha'''_3}). \end{array} \tag{11}$$

Evidently the Kronecker multiplicities of D^{α_3} and $D^{\alpha'''_3}$ are the same, $(\alpha_1\alpha_2|\alpha_3) = (\alpha'_1\alpha''_2|\alpha'''_3)$. If the coreps $D^{\alpha'''_3}$ in the direct sums of (8) are ordered in an appropriate manner then the matrices of the reducible coreps will coincide, as all the matrices of the irreducible coreps are in a standard form. So the matrix X commutes with all the matrices of the reducible corep $[\bigoplus_{\alpha'''_3} (e^{\alpha'_1\alpha''_2}_{\alpha'''_3} \times D^{\alpha'''_3}_{(g)})]$, $\forall g \in G$ and according to the generalised Schur lemma for reducible corep (Kotzev and Aroyo 1983), it can be presented in the form of a similar direct sum by the indices α'''_3 of $D^{\alpha'''_3} \in D^{\alpha'_1} \times D^{\alpha''_2}$

$$X(\alpha_1\alpha_2 A_1 A_2) = \bigoplus_{\alpha'''_3} (X^{\alpha_1\alpha_2,\alpha'''_3} \times M^{\alpha'''_3}). \tag{12}$$

Here $X^{\alpha_1\alpha_2,\alpha'''_3}$ is an orthogonal matrix with $\dim X^{\alpha_1\alpha_2,\alpha'''_3} = (\alpha_1\alpha_2|\alpha_3) = (\alpha'_1\alpha''_2|\alpha'''_3)$. The arbitrary unitary matrices $M^{\alpha'''_3}$ commute with all the matrices of the corresponding irreducible coreps $D^{\alpha'''_3}$, i.e. they belong to its commutator algebra.

The relation demanded between the CGC matrix for coreps $U^{\alpha_1\alpha_2}$ and the matrix of the coefficients $U^{\alpha'_1\alpha''_2}$ for the associated coreps follows from equations (9) and (12):

$$U^{\alpha'_1\alpha''_2} = (U^{\alpha_1 A_1} \times U^{\alpha_2 A_2})^{-1} (U^{\alpha_1\alpha_2} \times U^{A_1 A_2}) \left[\bigoplus_{\alpha_3} (e^{\alpha_1\alpha_2}_{\alpha_3} \times U^{\alpha_3 A_3}) \right] \times \left[\bigoplus_{\alpha'''_3} (X^{\alpha_1\alpha_2,\alpha'''_3} \times M^{\alpha'''_3}) \right]. \tag{13}$$

We should note the obvious analogy of (13) with the Racah lemma generalised for coreps by (Kotzev and Aroyo (1977, 1980):

$$\left[\bigoplus_{\beta_1\beta_2}(e^{\alpha_1}_{\beta_1}\times e^{\alpha_2}_{\beta_2}\times U^{\beta_1\beta_2})\right]=(S^{\alpha_1}\times S^{\alpha_2})^{-1}U^{\alpha_1\alpha_2}\left[\bigoplus_{\alpha_3}(e^{\alpha_1\alpha_2}_{\alpha_3}\times S^{\alpha_3})\right]$$
$$\times\left[\bigoplus_{\beta_3}(\chi^{\alpha_1\alpha_2,\beta_3}\times M^{\beta_3})\right], \tag{14}$$

where $U^{\alpha_1\alpha_2}$ and $U^{\beta_1\beta_2}$ are the CGC matrices for coreps D^{α_i} of the group $\mathscr{A}$ and the corresponding CGC matrices for the coreps D^{β_i} of its subgroups $\mathscr{B}\subset\mathscr{A}$, respectively. The matrices $S^{\alpha_i}(i=1,2,3)$ are the unitary transformations of the coreps D^{α_i}, while $\chi^{\alpha_1\alpha_2,\beta_3}$ is the orthogonal matrix, whose matrix elements are known as isoscalar factors,

$$\chi^{\alpha_1\alpha_2,\beta_3}=\|(\alpha_1\beta_1S_{\beta_1},\alpha_2\beta_2S_{\beta_2};\beta_3r_{\beta_3}\|\alpha_1\alpha_2\alpha_3r_{\alpha_3}\beta_3S_{\beta_3})\|. \tag{15}$$

We can say that equation (13) is of the Racah lemma type, but drawn for a 'horizontal' transition, i.e. the transition is not from a group to one of its subgroups ('vertical' transition) but remains within the framework of the same group. We call the matrix elements of $X^{\alpha_1\alpha_2,\alpha'''_3}$ 'inner isoscalar factors' by analogy with the isoscalar factors, i.e. the matrix elements(15).

Therefore, the connection between the CGC $U^{\alpha_1\alpha_2}$ and $U^{\alpha'_1\alpha''_2}$ is determined within the following.

(i) The arbitrary unitary matrices $M^{\alpha'''_3}$, dim $M^{\alpha'''_3}=\dim D^{\alpha'''_3}$, which appear due to the generalised Schur lemma (Kotzev and Aroyo 1983). Different independent sets of CGC for coreps can be obtained for different $M^{\alpha'''_3}$. Since $M^{\alpha'''_3}$ can be arbitrary, in all our calculations we have used as a 'basic choice' $M^{\alpha'''_3}=E^{\alpha'''_3}$, the unit matrix.

(ii) The orthogonal transformation $X^{\alpha_1\alpha_2,\alpha'''_3}$, whose matrix elements are real,

$$X^{\alpha_1\alpha_2,\alpha'''_3}=\|(\alpha_1\alpha_2\alpha_3r_{\alpha_3},A_1A_2A_3r_{A_3},\alpha_3A_3\alpha'''_3r_{\alpha'''_3}\|\alpha_1A_1\alpha'_1,\alpha_2A_2\alpha''_2,\alpha'_1\alpha''_2\alpha'''_3r_{\alpha'''_3})\|$$
$$=\|(\alpha_1\alpha_2\alpha_3r_{\alpha_3}\|\alpha'_1\alpha''_2\alpha'''_3r_{\alpha'''_3})\| \tag{16}$$

and do not depend on the basis functions of $D^{\alpha'''_3}$. The essential difference between the isoscalar factors (15) and the inner isoscalar factors (16) is that in the case of associated coreps there is a one to one correspondence between $D^{\alpha'}$ and D^{α}, i.e. there is not a branching-type multiplicity in (16).

The inner isoscalar factors can be examined from another point of view. The matrix X, [equations (9), (12)] gives the relation between the coreps, obtained by two different coupling schemes (10) and (11). The submatrices $X^{\alpha_1\alpha_2,\alpha'''_3}$ in equation (12) are known in the quantum theory of angular momentum as X matrices of Racah. Their matrix elements, the X coefficients of Racah are equivalent to the $9j$-symbols of Wigner. In our case the X coefficients (16) can be written in the following form:

$$X\begin{pmatrix}\alpha_1 & \alpha_2 & \alpha_{12}\\ \alpha_3 & \alpha_4 & \alpha_{34}\\ \alpha_{13} & \alpha_{24} & \alpha_{1234}\end{pmatrix}\begin{matrix}r_{12}\\ r_{34}\\ r_{13,24}\end{matrix}=X\begin{pmatrix}\alpha_1 & \alpha_2 & \alpha_3\\ A_1 & A_2 & A_3\\ \alpha'_1 & \alpha''_2 & \alpha'''_3\end{pmatrix}\begin{matrix}r_{\alpha_3}\\ 1\\ r_{\alpha'''_3}\end{matrix} \tag{17}$$
$$\begin{matrix}r_{13} & r_{24} & r_{12,34}\end{matrix}\qquad\qquad\begin{matrix}1 & 1 & 1\end{matrix}$$

Consequently the matrix $X^{\alpha_1\alpha_2,\alpha'''_3}$ accomplishes the rearrangement of the vectors of the carrier spaces of the equivalent reducible coreps of both sides of equation (8). A quite natural requirement is the one-to-one correspondence between the basis vectors of these spaces for every α_3 and α_3''', which leads to a diagonal form of $X^{\alpha_1\alpha_2,\alpha_3'''}$ and $M^{\alpha_3'''}$:

$$(X^{\alpha_1\alpha_2,\alpha_3'''})_{r_{\alpha_3}r_{\alpha_3'''}}=(\alpha_1\alpha_2\alpha_3 r_{\alpha_3}\|\alpha_1'\alpha_2''\alpha_3''' r_{\alpha_3'''})=x(\alpha_1'\alpha_2''\alpha_3''' r_{\alpha'''})\delta_{r_{\alpha_3}r_{\alpha_3'''}} \tag{18}$$

where $x(\alpha_1'\alpha_2''\alpha_3''' r_{\alpha_3'''})=\pm 1$, since the matrix $X^{\alpha_1\alpha_2,\alpha_3'''}$ is orthogonal.

Hence it is reasonable to choose the CGC for coreps $U^{\alpha_1\alpha_2}$ and $U^{\alpha_1'\alpha_2''}$ in such a way so that the inner isoscalar factors are of type (18).

The CGC related by (13) with diagonal matrices $X^{\alpha_1\alpha_2,\alpha_3'''}$ (18) and the basic choice $M^{\alpha_3'''}=E^{\alpha_3'''}$ will be called 'completely associated CGC for coreps'. In this case the matrices $U^{\alpha_1\alpha_2}$ and $U^{\alpha_1'\alpha_2''}$ are related by the known $U^{\alpha_i A_i}$ and $U^{A_1A_2}$ up to a sign. We can write this symbolically as

$$U^{\alpha_1'\alpha_2''}=\pm(U^{\alpha_1A_1}\times U^{\alpha_2A_2})^{-1}(U^{\alpha_1\alpha_2}\times U^{A_1A_2})\left[\bigoplus_{\alpha_3}(e_{\alpha_3}^{\alpha_1\alpha_2}\times U^{\alpha_3A_3})\right]. \tag{19}$$

Of course, the choice of (18) is only one of the numerous possibilities, but it is the most natural one. The relations (13) and (18) are deduced for the most general case ($D^{A_1}\neq D^{A_2}\neq D^{A_3}$) and it can easily be specified for the special cases when some of the associating coreps D^{A_i} coincide or one of them is the identity corep D^{α_0}.

One direct and useful application of the associative symmetry of the CGC for coreps (19) is in the problem of the ambiguity of the CGC. (From definition (5) it follows that the CGC are determined within an orthogonal transformation, whose dimension equals the sum of the Kronecker multiplicities of the resultant coreps $D^{\alpha_3}\in D^{\alpha_1}\times D^{\alpha_2}$). It follows from (19) that this type of ambiguity for all completely associated CGC for coreps, i.e. CGC, which couple associated coreps and satisfy (19), is reduced to only one orthogonal transformation for the whole set of associated CGC for coreps.

For example, in equation (3) the seven coreps of the group $O(T)=4'32'$ are classified into three associative sets. The total number of CGC matrices $U^{\alpha_1\alpha_2}$ is 49. We can arrange them in table 1, where we have used '$\alpha_1\alpha_2$' instead of $U^{\alpha_1\alpha_2}$.

Table 1. Matrices of CGC.

11	12	13	14	15	16	17
21	22	23	24	25	26	27
31	32	33	34	35	36	37
41	42	43	44	45	46	47
51	52	53	54	55	56	57
61	62	63	64	65	66	67
71	72	73	74	75	76	77

Due to the permutation symmetry between the matrices $U^{\alpha_1\alpha_2}$ and $U^{\alpha_2\alpha_1}$ the number of independent matrices is reduced to 28 (the upper part of the table 1). After the use of relation (18) between the completely associated CGC for coreps, the number of independent $U^{\alpha_1\alpha_2}$ (in the sense of an independent choice of the orthogonal transformation by the Kronecker multiplicity) is reduced to 9 matrices only—the encircled $\alpha_1\alpha_2$ in the table 1. For example, using (19) and the associating corep D^2, we can determine up to a sign all the CGC of the matrices U^{56}, U^{57}, U^{66}, U^{67}, and U^{77} from those of U^{55} only.

4. CGC for corepresentations for even and odd sets of basis functions

It is well known that a number of physical quantities and wavefunctions are transformed as basis functions which are characterised by a definite parity in respect to space inversion, even in the cases when the inversion itself is not an element of the group (e.g. the electric and magnetic dipole moments, dipole active normal vibrations in molecules and crystals, etc). Using the generalised Racah lemma we have shown that the CGC for coreps, which are necessary for the coupling of odd and odd or odd and even basis function can be chosen to coincide up to a sign with the corresponding CGC for even basis (Kotzev and Aroyo 1981, 1982a, 1982b). The same statement can be proved quite independently with the help of associated coreps and associated CGC.

We will consider the following two cases

(i) Centrosymmetrical group $G \times C_i$; the space inversion is an element of the group, and the even and the odd quantities are transforming by unequivalent coreps $D^{\alpha+}$ and $D^{\alpha-}$ respectively.

(ii) Anti-unitary groups containing improper rotations in the unitary subgroup $H\Delta G$; the even the odd quantities are transformed by equivalent coreps but the corresponding CGC are different.

In the remaining two cases, namely, the pure rotation groups, or the groups containing improper rotations as anti-unitary elements only, the even and odd quantities are transformed by equivalent coreps with identical choice of the corep matrices, and the corresponding CGC of coreps coincide.

4.1. Case (i). Centrosymmetrical groups.

All coreps of these groups can be classified into associative sets of the type ($D^{\alpha+}$, $D^{\alpha-}$) with respect to the one-dimensional real corep $D^{\alpha_{\bar 0}}$, the pseudoscalar corep, where $D^{\alpha-} = D^{\alpha+} \times D^{\alpha_{\bar 0}}$. The connection between the CGC matrices $U^{\alpha_1^- \alpha_2^-}$ and $U^{\alpha_1^+ \alpha_2^+}$ can be obtained directly from (13):

$$U^{\alpha_1^-\alpha_2^-} = (U^{\alpha_1^+\alpha_0^-} \times U^{\alpha_2^+\alpha_0^-})(U^{\alpha_1^+\alpha_2^+} \times U^{\alpha_0^-\alpha_0^-})\left[\bigoplus_{\alpha_3^+} (e^{\alpha_1^+\alpha_2^+}_{\alpha_3^+} \times U^{\alpha_3^+\alpha_0^-})\right]$$

$$\times\left[\bigoplus_{\alpha_3^+} (X^{\alpha_1^+\alpha_2^+,\alpha_3^+} \times M^{\alpha_3^+})\right]. \tag{20}$$

According to the conventions used in our calculations (similar to the conventions adopted in the quantum theory of angular momentum) $U^{\alpha_i\alpha_0} = E^{\alpha_i}$, $M^{\alpha_i} = E^{\alpha_i} (i = 1, 2, 3)$ and as $D^{\alpha-} = D^{\alpha+} \times D^{\alpha_{\bar 0}}$ are in a standard form, then $U^{\alpha_i^+\alpha_0^-} = E^{\alpha_i}$. All of the CGC tabulated by us are completely associated, i.e. they are fulfiling (19). From these considerations and (19), we get

$$U^{\alpha_1^-\alpha_2^-} = \pm U^{\alpha_1^+\alpha_2^+}. \tag{21}$$

The exact sign (the inner isoscalar factors) is determined for each $\alpha_3 r_{\alpha_3}$-block of $U^{\alpha_1^+\alpha_2^-}$ by a comparison between the coefficients obtained and the corresponding Wigner coefficients for which we have $U^{j_1^- j_2^-} = U^{j_1^+ j_2^+}$.

The same result can be obtained for the CGC $U^{\alpha_1^+\alpha_2^-}$ and $U^{\alpha_1^-\alpha_2^+}$, i.e.

$$U^{\alpha_1^+\alpha_2^+} = U^{\alpha_1^-\alpha_2^+} = U^{\alpha_1^+\alpha_2^-} = U^{\alpha_1^-\alpha_2^+}. \tag{22}$$

4.2. *Case (ii). Non-centrosymmetrical groups*

To make things clearer, the discussion of the Shubnikov groups, whose unitary subgroups contain improper rotations, will be carried out for a definite group—the 'grey' group $T_d \otimes \Theta$ (or its isomorphic 'black and white' group $O_h(T_d)$). They are subgroups of the centrosymmetrical group $O_h \otimes \Theta$. The subduction of every irreducible coreps of $O_h \otimes \Theta$ on the group $T_d \otimes \Theta$ is an irreducible corep of $T_d \otimes \Theta$ and it is given in table 2.

Table 2. Compatibility table.

$O_h \otimes \Theta$	$D^{\alpha\pm}$	D^{1+}	D^{2+}	D^{3+}	D^{4+}	D^{5+}	D^{6+}	D^{7+}	D^{8+}	D^{1-}	D^{2-}	D^{3-}	D^{4-}	D^{5-}	D^{6-}	D^{7-}	D^{8-}
	$\psi^{\alpha\pm}$	ψ^{1+}	ψ^{2+}	ψ^{3+}	ψ^{4+}	ψ^{5+}	ψ^{6+}	ψ^{7+}	ψ^{8+}	ψ^{1-}	ψ^{2-}	ψ^{3-}	ψ^{4-}	ψ^{5-}	ψ^{6-}	ψ^{7-}	ψ^{8-}
$T_d \otimes \Theta$	D^{β}	D^1	D^2	D^3	D^4	D^5	D^6	D^7	D^8	D^2	D^1	D^3	D^5	D^4	D^7	D^6	D^8
	ψ^{β}	ψ^{1e}	ψ^{2e}	ψ^{3e}	ψ^{4e}	ψ^{5e}	ψ^{6e}	ψ^{7e}	ψ^{8e}	ψ^{2o}	ψ^{1o}	ψ^{3o}	ψ^{5o}	ψ^{4o}	ψ^{7o}	ψ^{6o}	ψ^{8o}

As we have already noted the even $\psi^{\alpha+}$ and odd $\psi^{\alpha-}$ basis functions are transformed by inequivalent coreps $D^{\alpha+}$ and $D^{\alpha-}$ respectively, but the corresponding CGC for coreps (22) coincide. It is seen from table 2 that two types of basis functions are transforming by every corep D^{β} of $T_d \otimes \Theta$: even, ψ^{β^e}, obtained from the corresponding functions $\psi^{\alpha+}$ of $D^{\alpha+}$, and odd, ψ^{β^o}, obtained from $\psi^{\alpha-}$ of $D^{\alpha-}$. In the general case, a given D^{β} can be deduced from non-equivalent coreps $D^{\alpha+}$ and $D^{\alpha'-}$, $(D^{\alpha+} \downarrow \mathscr{B}) = (D^{\alpha'-} \downarrow \mathscr{B}) = D^{\beta}$. We shall underline the fact that ψ^{β^o} and ψ^{β^e} are transformed by one and the same D^{β}. The CGC $U^{\beta_1^o\beta_2^o}$, $U^{\beta_1^e\beta_2^o}$, $U^{\beta_1^o\beta_2^e}$ which couple odd and odd, even and odd and odd and even basis functions respectively, can be chosen to be completely associated (19) with the $U^{\beta_1\beta_2}$, using $D^1 = (D^{2-} \downarrow \mathscr{B})$ as an associating corep with an odd basis function ψ^{1^o}.

Analogously to the case of centrosymmetrical groups, we can show that these relations are of the type:

$$U^{\beta_1^o\beta_2^o} = \pm U^{\beta_1^e\beta_2^e}. \tag{23}$$

As in case (i), the necessary sign is obtained by a comparison with the phases of the corresponding coefficients $U^{\alpha_1\pm\alpha_2\pm}$, or with the Wigner coefficients. (In the general case $U^{\beta_1^o\beta_2^o}$ and $U^{\beta_1^e\beta_2^o}$ are related to different matrices of Wigner coefficients.) Consequently, the CGC coupling odd and even basis functions for Shubnikov groups with improper rotations in the unitary subgroup can be chosen to coincide up to a sign for each triad $(\beta_1\beta_2\beta_3 r_3)$. This choice is made in all our calculations of CGC for coreps of all 90 anti-unitary Shubnikov point groups (Kotzev and Aroyo, 1981, 1982a, 1982b). The only exception is the group $T_d \otimes \Theta$, where we have not observed the choice (19) for some parts of the matrices U^{48} and U^{88}. This leads to non-fulfilment of (23) for the triads $(\beta_1\beta_2\beta_3) = (4, 8, 8)$, $(8, 8, 4)$, $(8, 8, 5)$. The completely associated CGC for these triads, satisfying (19) are given in table 3. The relations of type (23) for U^{48}, U^{88} are given in table 4. If the CGC of table 5a of Kotzev and Aroyo (1981) are substituted by the ones given in table 3, then the corresponding rows in table 6 (Kotzev and Aroyo 1981) should be replaced by the factors given in table 4 and table 7 in Kotzev and Aroyo (1981) is not necessary.

The complete tables of the inner isoscalar factors ± 1, giving the connection between the even and odd basis for coreps of all anti-unitary point groups of the type discussed are published in Kotzev and Aroyo (1981, 1982a, 1982b).

Table 3. Completely associated CGC for the corep triads $(D^8 \times D^8 : D^4)$, $(D^8 \times D^8 : D^5)$, $(D^4 \times D^4 : D^8)$ of $\mathrm{T_d} \otimes \Theta$ and $\mathrm{O_h}(\mathrm{T_d})$.

81 81 413 −1/2	84 84 411 −1/2	42 82 822 1/3
81 81 423 −1/8	84 84 421 −1/8	42 83 813 −1/3*
81 83 421 −3/8	41 81 814 2/3*	42 83 823 −1/3
81 84 412 −1/4	41 81 824 1/6	42 84 814 1/3*
81 84 422 −1/4	41 82 821 −1/2	42 84 824 −1/3
82 82 411 −1/2	41 83 812 2/3*	43 81 822 1/2
82 82 421 1/8	41 83 822 −1/6	43 82 813 −2/3*
82 83 412 −1/4	41 84 823 −1/6	43 82 823 1/6
82 83 422 1/4	42 81 811 −1/3*	43 83 824 1/2
82 84 424 −3/8	42 81 821 1/3	43 84 811 −2/3*
83 83 413 −1/2	42 82 812 1/3*	43 84 821 −1/6
83 83 423 1/8		

Table 4. Inner isoscalar factors for U^{48}, U^{58} and U^{88} for odd bases of $\mathrm{T_d} \otimes \Theta$ and $\mathrm{O_h}(\mathrm{T_d})$.

$\alpha_1 \times \alpha_2$	$\alpha_1^{\mathrm{o}} \times \alpha_2^{\mathrm{o}}$	$\alpha_1^{\mathrm{o}} \times \alpha_2^{\mathrm{e}}$	$\alpha_1^{\mathrm{e}} \times \alpha_2^{\mathrm{o}}$
48	$\bar{6}^* - \bar{7}^* + 8_1 + 8_2^*$	$6 + 7 + 8_1^* + \bar{8}_2$	$6^* + \bar{7}^* + 8_1 + \bar{8}_2^*$
58	$6 + 7 + 8_1^* + \bar{8}_2$	$\bar{6}^* + \bar{7}^* + \bar{8}_1 + 8_2^*$	$\bar{6} + \bar{7} + \bar{8}_1^* + 8_2$
88	$1^* + 2 + \bar{3}^* + \bar{4}_1 + 4_2 + 5_1^* + \bar{5}_2$	$\bar{1} + \bar{2}^* + \bar{3}^* + \bar{4}_1^* + \bar{4}_2 + 5_1 + 5_2$	$\bar{1} + 2^* + 3^* + 4_1^* + \bar{4}_2 + 5_1 + 5_2$

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