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Space group Clebsch–Gordan coefficients: III. Computer generated coefficients by Dirl's method

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Abstract. Using the special solutions of the multiplicity problem established in papers I and II of this series, the computer generation of space group Clebsch-Gordan (CG) coefficients by Dirl's method is described. All the elements of a CG matrix for the reduction of any Kronecker product of space group unirreps, in all 230 (single or double) space groups, are computed using a single explicit formula in terms of only the Miller and Love allowed matrix unirreps of the little groups occurring in the Kronecker product and its CG series decomposition. An example from the non-symmorphic primitive cubic space group $P2_13$ (198) is given where a complete CG matrix is displayed.

1. Introduction

In the previous papers in this series (Davies 1986a, b, hereafter referred to as DI and DII respectively) we reported that the Miller and Love (1967) (hereafter referred to as ML) space group matrix unirreps yield special solutions of the multiplicity problem for all Kronecker products in all 230 (single and double) space groups. In this paper we describe a computer program, using the method of Dirl (1979), whereby these special solutions are used to generate a complete CG matrix, where all the elements are computed using a single explicit formula in terms of only the ML allowed matrix unirreps of the little groups occurring in the Kronecker product and its CG series decomposition. An illustrative example from the non-symmorphic primitive cubic space group $P2_13$ (198) is given where a complete CG matrix is displayed. In the following, we use the same notation and definitions as in DI and DII. Equations in DI and DII are referenced by the prefix 'I' or 'II' respectively, followed by the equation number.

2. Clebsch–Gordan coefficients by Dirl's method

In DI and DII we reported that, for any Kronecker product in all 230 (single and double) space groups, there is always a special solution of the multiplicity problem, whereby for given $(\kappa_0, (\bar{\sigma}, \bar{\sigma}')\boldsymbol{q}_0)$ such that in (I.10) $m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)} > 0$, it is possible to identify the multiplicity index w with special column indices of the Kronecker product (see (I.12)). Dirl (1979) has shown that the $m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)}|\mathrm{P}:\mathrm{P}^{\boldsymbol{q}_0}|n_{\kappa_0}$ columns

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of the CG matrix indexed by $(\kappa_0(\bar{\sigma}, \bar{\sigma}')\boldsymbol{q}_0)$ may then be calculated by

$$
\begin{aligned}
C^{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}')}_{\bar{\tau}d,\bar{\tau}'d';(\kappa_0(\bar{\sigma},\bar{\sigma}')\boldsymbol{q}_0)w=(\bar{\sigma}_v,c_v;\bar{\sigma}'_v,c'_v)\bar{\sigma}_0 j} &= \| B^{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)(\bar{\sigma}_v,c_v;\bar{\sigma}'_v,c'_v)}_{\bar{e}a_0} \|^{-1} \\
&\times \delta_{\boldsymbol{q}(\bar{\tau})+\boldsymbol{q}'(\bar{\tau}'),\boldsymbol{q}_0(\bar{\sigma}_0)+\boldsymbol{Q}[\boldsymbol{q}(\bar{\tau})+\boldsymbol{q}'(\bar{\tau}')]} \frac{n_{\kappa_0}}{|\mathrm{P}^{\boldsymbol{q}_0}|} \sum_{\beta\in\mathrm{P}} \Delta^{\boldsymbol{q}_0}(\bar{\sigma}_0, \beta\bar{e})\Delta^{\boldsymbol{q}}(\bar{\tau}, \beta\bar{\sigma}_v)\Delta^{\boldsymbol{q}'}(\bar{\tau}', \beta\bar{\sigma}'_v) \\
&\times \Gamma^{(\kappa,\boldsymbol{q})}_{dc_v}[(\bar{\tau}' | \boldsymbol{\tau}(\bar{\tau}))^{-1}(\beta | \boldsymbol{\tau}(\beta))(\bar{\sigma}_v | \boldsymbol{\tau}(\bar{\sigma}_v))] \\
&\times \Gamma^{(\kappa',\boldsymbol{q}')}_{d'c'_v}[(\bar{\tau}' | \boldsymbol{\tau}(\bar{\tau}'))^{-1}(\beta | \boldsymbol{\tau}(\beta))(\bar{\sigma}'_v | \boldsymbol{\tau}(\bar{\sigma}'_v))]\Gamma^{(\kappa_0,\boldsymbol{q}_0)*}_{ja_0}[(\bar{\sigma}_0 | \boldsymbol{\tau}(\bar{\sigma}_0))^{-1}(\beta | \boldsymbol{\tau}(\beta))]
\end{aligned}
\qquad (1)
$$

where $\bar{\tau}\in\mathrm{P}:\mathrm{P}^{\boldsymbol{q}}$, $d=1, 2, \ldots, n_\kappa$, $\bar{\tau}'\in\mathrm{P}:\mathrm{P}^{\boldsymbol{q}'}$, $d'=1, 2, \ldots, n_{\kappa'}$; $v=1, 2, \ldots, m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)}$, $\bar{\sigma}_0\in\mathrm{P}:\mathrm{P}^{\boldsymbol{q}_0}$, $j=1, 2, \ldots, n_{\kappa_0}$, and where

$$
\begin{aligned}
\| B^{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)(\bar{\sigma}_v,c_v;\bar{\sigma}'_v,c'_v)}_{\bar{e}a_0} \|^2 &= \frac{n_{\kappa_0}}{|\mathrm{P}^{\boldsymbol{q}_0}|} \sum_{\substack{\beta\in\mathrm{P}^{\boldsymbol{q},\boldsymbol{q}',\boldsymbol{q}_0} \\ \bar{\sigma},\bar{\sigma}'}} \\
&\times \Gamma^{(\kappa,\boldsymbol{q})}_{c_v c_v}[(\bar{\sigma}_v | \boldsymbol{\tau}(\bar{\sigma}_v))^{-1}(\beta | \boldsymbol{\tau}(\beta))(\bar{\sigma}_v | \tau(\bar{\sigma}_v))]\Gamma^{(\kappa',\boldsymbol{q}')}_{c'_v c'_v} \\
&\times [(\bar{\sigma}'_v | \boldsymbol{\tau}(\bar{\sigma}'_v))^{-1}(\beta | \boldsymbol{\tau}(\beta))(\bar{\sigma}'_v | \boldsymbol{\tau}(\bar{\sigma}'_v))]\Gamma^{(\kappa_0,\boldsymbol{q}_0)*}_{a_0 a_0}[(\beta | \boldsymbol{\tau}(\beta))].
\end{aligned}
\qquad (2)
$$

In (1) and (2) we have preferred to use the allowed matrix unirreps $\Gamma^{(\kappa'',\boldsymbol{q}'')}$ of the little groups $\mathrm{G}^{\boldsymbol{q}''}$, $\kappa''=\kappa, \kappa', \kappa_0$, $\boldsymbol{q}''=\boldsymbol{q}, \boldsymbol{q}', \boldsymbol{q}_0$, instead of the projective matrix unirreps $R^{\kappa''}$ of the little co-groups $\mathrm{P}^{\boldsymbol{q}''}$ $(\simeq\mathrm{G}^{\boldsymbol{q}''}/\mathrm{T})$ (see § 2 of DII). By using (1) and (2) for all $(\kappa_0, (\bar{\sigma}, \bar{\sigma}')\boldsymbol{q}_0)$, such that in (I.10) $m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)}>0$, all columns of the CG matrix may be calculated.

As in DI, the generalisation of (1) and (2) to 'double' space groups is trivial (Dirl 1981).

3. Program

We have written a program in ALGOL 60 for a DEC System 10 computer to calculate CG coefficients for Kronecker products of (single or double) space group unirreps and the algorithm for the first stage of this program, the search for special solutions of the multiplicity problem, is described in DII. The algorithm for the second stage, the actual calculation of the CG coefficients themselves, may be very briefly described as follows.

Step (c)(iii) of DII is followed immediately by:

(c)(iv) for each value of the multiplicity index

$$w=(\bar{\sigma}_v, c_v; \bar{\sigma}'_v, c'_v) \qquad v=1, 2, \ldots, m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)}$$

in (I.12), compute the norm of the corresponding vector $B^{(k,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)(\bar{\sigma}_v,c_v;\bar{\sigma}'_v,c'_v)}_{\bar{e}a_0}$ using (2).

(c)(v) Using (1) compute the columns of the CG matrix for $v=1, 2, \ldots, m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)}$, $\bar{\sigma}_0\in\mathrm{P}:\mathrm{P}^{\boldsymbol{q}_0}$, $j=1, 2, \ldots, n_{\kappa_0}$.

The whole CG matrix is completed by repeating steps (c)(iv) and c(v) above for every $m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)}>0$ in (I.10).

(d) Finally, check that the computed CG matrix correctly reduces the Kronecker product matrix as given by (I.10). It is sufficient to carry out this check for all the generating elements of G.

The program, which has been designed to run for any space group, has been tested on a representative selection of space groups. The run time varies considerably according to the size of the group. For high-dimensional Kronecker products, the most time consuming part is the block diagonalisation check given by step (d) above.

For the non-symmorphic primitive cubic space group P2$_1$3 (198), the total run time for actually calculating the CG matrices for all Kronecker products for all $\boldsymbol{q}$ vectors (having non-trivial little co-groups) in the fundamental domain of the first Brillouin zone (see Cracknell *et al* 1979, Davies and Cracknell 1979) is approximately 25 min.

4. Example

We take as our example a Kronecker product from the non-symmorphic primitive cubic space group G = P2$_1$3 (198) (see also Davies and Dirl 1984). The symmetry operators, multiplication table, special $\boldsymbol{q}$ vectors (i.e. $\boldsymbol{q}$ vectors with non-trivial little co-groups), allowed matrix unirreps, etc, are given in Cracknell *et al* (1979) (hereafter referred to as CDML) and we adopt the notation of this reference for our example. In the following, the special $\boldsymbol{q}$ vectors $\boldsymbol{GM} = (0,0,0)$, $\boldsymbol{X} = (0,\frac{1}{2},0)$, $\boldsymbol{M} = (\frac{1}{2},\frac{1}{2},0)$ appear (where the coordinates are relative to primitive reciprocal lattice vectors). The symmetry operators and allowed matrix unirreps of the little groups $G^{\boldsymbol{q}}$ ($\boldsymbol{q} = \boldsymbol{GM}, \boldsymbol{X}, \boldsymbol{M}$) are given in CDML, pp 592-4. The symmetry elements of G are labelled using the notation of ML and the set consists of:

$$G = \{(1),(2,2),(3,3),(4,1),(5),(6,2),(7,3),(8,1),(9),(10,2),(11,3),(12,1)\} \tag{3}$$

together with all possible products with elements of the translation group T, of the primitive cubic lattice. The correspondence between the ML notation and that used by Bradley and Cracknell (1972) may be found in table (3.1) of CDML. In (3), a symmetry element denoted by a single integer denotes a point group symmetry element. Where a symmetry element in (3) consists of a pair of integers separated by a comma, the first integer denotes a point group symmetry element and the second integer denotes the associated non-primitive lattice translation according to the code: $1 = (\frac{1}{2},0,\frac{1}{2})$, $2 = (\frac{1}{2},\frac{1}{2},0)$, $3 = (0,\frac{1}{2},\frac{1}{2})$ (where the coordinates are relative to conventional lattice vectors). For example, (1), (5), (9) in the Bradley and Cracknell (1972) notation are respectively: $\{E|\boldsymbol{0}\}$, $\{C_{31}^-|\boldsymbol{0}\}$, $\{C_{31}^+|\boldsymbol{0}\}$. Similarly (2, 2), (3, 3), (4, 1) are respectively: $\{C_{2x}|(\frac{1}{2},\frac{1}{2},0)\}$, $\{C_{2y}|(0,\frac{1}{2},\frac{1}{2})\}$, $\{C_{2z}|(\frac{1}{2},0,\frac{1}{2})\}$.

We consider the Kronecker product $\Lambda^{(1,\boldsymbol{X})}\otimes\Lambda^{(1,\boldsymbol{X})}$. The WVSR (see (I.7)) and the corresponding multiplicities for this Kronecker product are tabulated on p 104 and 801, respectively, of Davies and Cracknell (1979). There are three WVSR and the corresponding terms $(\bar{\sigma},\bar{\sigma}')\boldsymbol{q}_0$ (in (I.7)) are

$$((\bar{1}),(\bar{1}))\boldsymbol{GM} \qquad ((\bar{1}),(\bar{5}))\boldsymbol{M} \qquad ((\bar{5}),(\bar{1}))\boldsymbol{M}. \tag{4}$$

The corresponding component multiplicities are

$$m^{((\bar{1}),(\bar{1}))}_{(1,\boldsymbol{X})(1,\boldsymbol{X});(\kappa_0,\boldsymbol{GM})} = \begin{cases} 1 & \kappa_0 = 1,2,3 \\ 3 & \kappa_0 = 4 \end{cases} \tag{5a}$$

$$m^{((\bar{1}),(\bar{5}))}_{(1,\boldsymbol{X})(1,\boldsymbol{X});(\kappa_0,\boldsymbol{M})} = m^{((\bar{5}),(\bar{1}))}_{(1,\boldsymbol{X})(1,\boldsymbol{X});(\kappa_0,\boldsymbol{M})} = 1 \qquad \kappa_0 = 1,2,3,4. \tag{5b}$$

Using (I.6), (5a) and (5b), the total multiplicities associated with the vectors $\boldsymbol{GM}$ and $\boldsymbol{M}$ are

$$m_{(1,\boldsymbol{X})(1,\boldsymbol{X});(\kappa_0,\boldsymbol{GM})} = \begin{cases} 1 & \kappa_0 = 1,2,3 \\ 3 & \kappa_0 = 4 \end{cases} \tag{6a}$$

$$m_{(1,\boldsymbol{X})(1,\boldsymbol{X});(\kappa_0,\boldsymbol{M})} = 2 \qquad \kappa_0 = 1,2,3,4. \tag{6b}$$

From (6b) it might appear that non-trivial 'multiplicity problems' exist with regard to calculating the corresponding CG coefficients since the mulitplicities of the unirreps $\Lambda^{(\kappa_0,\boldsymbol{M})}$, $\kappa_0 = 1, 2, 3, 4$, in the Kronecker product $\Lambda^{(1,\boldsymbol{X})}\otimes\Lambda^{(1,\boldsymbol{X})}$ are greater than unity.

However, from (4) and (5*b*) it is clear that these multiplicities greater than unity arise *solely* from the existence of more than one WVSR having identical vectors $\boldsymbol{q}_0$, namely $\boldsymbol{q}_0 = \boldsymbol{M}$. The component multiplicities in (5*b*) are all unity. The orthogonality of the columns of the CG matrix labelled by different WVSR is guaranteed, even when the WVSR have identical vectors $\boldsymbol{q}_0$. Thus, in this Kronecker product, (5) show that the only non-trivial multiplicity problem occurs for $\Lambda^{(4,\boldsymbol{GM})}$ for which the component multiplicity

$$m^{((\bar{1}),(\bar{1}))}_{(1,\boldsymbol{X})(1,\boldsymbol{X});(4,\boldsymbol{GM})} = 3. \tag{7}$$

The little group $\mathrm{G}^{\boldsymbol{GM}} = \mathrm{G}$ and the little groups $\mathrm{G}^{\boldsymbol{X}}$ and $\mathrm{G}^{\boldsymbol{M}}$ are given by

$$\mathrm{G}^{\boldsymbol{X}} = \mathrm{G}^{\boldsymbol{M}} = \{(1), (2,2), (3,3), (4,1)\} \tag{8}$$

together with all possible products with elements of the translation group T. The isogonal point group P and the little co-groups $\mathrm{P}^{\boldsymbol{GM}}$, $\mathrm{P}^{\boldsymbol{X}}$, $\mathrm{P}^{\boldsymbol{M}}$ are given by

$$\mathrm{P} = \mathrm{P}^{\boldsymbol{GM}} = \{(1), (2), (3), (4), (5), (6), (7), (8), (9), (10), (11), (12)\} \tag{9a}$$

$$\mathrm{P}^{\boldsymbol{X}} = \mathrm{P}^{\boldsymbol{M}} = \{(1), (2), (3), (4)\}. \tag{9b}$$

The first step is to *fix* the left coset representatives $\mathrm{P}:\mathrm{P}^{\boldsymbol{q}}$, $\boldsymbol{q} = \boldsymbol{GM}, \boldsymbol{X}, \boldsymbol{M}$, and these are chosen as follows:

$$\mathrm{P}:\mathrm{P}^{\boldsymbol{GM}} = \{(\bar{1})\} \tag{10a}$$

$$\mathrm{P}:\mathrm{P}^{\boldsymbol{X}} = \mathrm{P}:\mathrm{P}^{\boldsymbol{M}} = \{(\bar{1}), (\bar{5}), (\bar{9})\}. \tag{10b}$$

The allowed matrix unirreps of $\mathrm{G}^{\boldsymbol{GM}}$, $\mathrm{G}^{\boldsymbol{X}}$, $\mathrm{G}^{\boldsymbol{M}}$ are given in CDML but are reproduced here in tables 1, 2 and 3 respectively, for convenience.

In tables 1, 2 and 3, the matrix representing a lattice translation $\boldsymbol{t} \in \mathrm{T}$ is given by $\exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{t})\Gamma^{(\kappa,\boldsymbol{q})}[(1)]$, where $\boldsymbol{q} = \boldsymbol{GM}, \boldsymbol{X}, \boldsymbol{M}$ respectively (see (I.3)).

Table 1. Allowed matrix unirreps $\Gamma^{(\kappa,\boldsymbol{GM})}[g]$, $g \in \mathrm{G}^{\boldsymbol{GM}}$. $\omega = \exp(2\pi\mathrm{i}/3)$.

κ \ g	(1)	(2, 2)	(3, 3)	(4, 1)	(5)	(6, 2)
1	1	1	1	1	1	1
2	1	1	1	1	ω^*	ω^*
3	1	1	1	1	ω	ω
4	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&-1&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}$	$\begin{pmatrix}0&-1&0\\0&0&1\\-1&0&0\end{pmatrix}$

κ \ g	(7, 3)	(8, 1)	(9)	(10, 2)	(11, 3)	(12, 1)
1	1	1	1	1	1	1
2	ω^*	ω^*	ω	ω	ω	ω
3	ω	ω	ω^*	ω^*	ω^*	ω^*
4	$\begin{pmatrix}0&-1&0\\0&0&-1\\1&0&0\end{pmatrix}$	$\begin{pmatrix}0&1&0\\0&0&-1\\-1&0&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$	$\begin{pmatrix}0&0&-1\\1&0&0\\0&-1&0\end{pmatrix}$	$\begin{pmatrix}0&0&-1\\-1&0&0\\0&1&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\-1&0&0\\0&-1&0\end{pmatrix}$

Table 2. Allowed matrix unirrep $\Gamma^{(\kappa,X)}[g]$, $g \in G^X$.

κ \ g	(1)	(2, 2)	(3, 3)	(4, 1)
1	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$

Table 3. Allowed matrix unirreps $\Gamma^{(\kappa,M)}[g]$, $g \in G^M$. $I = \exp(i\pi/2)$.

κ \ g	(1)	(2, 2)	(3, 3)	(4, 1)
1	1	I	$-I$	1
2	1	$-I$	I	1
3	1	I	I	-1
4	1	$-I$	$-I$	-1

As an example of the procedure for solving a non-trivial multiplicity problem, we consider the component multiplicity of $\Lambda^{(4,GM)}$ given in (7). We follow steps (a)-(g) of § 2 of DII.

(a) From the first element in the list (4), we see that

$$\bar{\sigma} = (\bar{1}) \quad (11a)$$

$$\bar{\sigma}' = (\bar{1}) \quad (11b)$$

$$q_0 = \boldsymbol{GM}. \quad (11c)$$

From (II.2) and (9a, b), the triple intersection group

$$P^{q,q';q_0}_{\bar{\sigma},\bar{\sigma}'} = P^{X,X;GM}_{(\bar{1}),(\bar{1})} = \{(1), (2), (3), (4)\}. \quad (12)$$

(b) The left coset representatives

$$v_j \in P^{q_0}_{\bar{\sigma},\bar{\sigma}'} : P^{q,q';q_0}_{\bar{\sigma},\bar{\sigma}'} = P^{GM} : P^{X,X;GM}_{(\bar{1}),(\bar{1})}$$

from (9a) and (12) may be chosen to be

$$v_j = (1), (5), (9). \quad (13)$$

(c) Using (11) and (II.3), generate the $|P^{q_0} : P^{q,q';q_0}_{\bar{\sigma},\bar{\sigma}'}| = 3$ pairs of *fixed* left coset representatives $\bar{\sigma}_j$, $\bar{\sigma}'_j$ of P^q, $P^{q'}$ respectively, in P given by

$$\bar{\sigma}_j, \bar{\sigma}'_j = (\bar{1}), (\bar{1}); (\bar{5}), (\bar{5}); (\bar{9}), (\bar{9}). \quad (14)$$

(d) From table 2, the dimension of $\Gamma^{(1,X)}$ is 2, therefore

$$n_\kappa = n_{\kappa'} = 2. \quad (15)$$

From (14) and (15), there is a total of 12 column vectors

$$B^{(\kappa,q)(\kappa',q');(\kappa_0,q_0)(\bar{\sigma}_j,c;\bar{\sigma}'_j,c')}_{\bar{e}a_0} = B^{(1,X)(1,X);(4,GM)(\bar{\sigma}_j,c;\bar{\sigma}'_j,c')}_{\bar{e}a_0} \quad (16)$$

indexed by $\bar{\sigma}_j$, $\bar{\sigma}'_j = (\bar{1}), (\bar{1})$; $(\bar{5}), (\bar{5})$; $(\bar{9}), (\bar{9})$; $c = 1, 2$; $c' = 1, 2$.

(e) The value of a_0 in (16) is fixed at unity, and using (II.5), 6 of the above 12 column vectors have norm $1/\sqrt{2}$ and the remaining 6 have zero norm. The values of $(\bar{\sigma}_j, c; \bar{\sigma}'_j, c')$ of those having non-zero norm are given in table 4.

The dimension of the space spanned by the column vectors of non-zero norm must be equal to the component multiplicity $m^{((\bar{1}),(\bar{1}))}_{(1,X)(1,X);(4,GM)} = 3$ from (7). A 'special solution of the multiplicity problem' is obtained for this component multiplicity if three pairwise orthogonal column vectors can be found.

Table 4. Indices of column vectors of norm $1/\sqrt{2}$. The set of indices $((\bar{1}), 1; (\bar{1}), 1)$ is denoted by a, the set $((\bar{1}), 1; (\bar{1}), 2)$ by b, etc.

	$\bar{\sigma}_j$	c	$\bar{\sigma}'_j$	c'
a	$(\bar{1})$	1	$(\bar{1})$	1
b	$(\bar{1})$	2	$(\bar{1})$	2
c	$(\bar{5})$	1	$(\bar{5})$	2
d	$(\bar{5})$	2	$(\bar{5})$	1
e	$(\bar{9})$	1	$(\bar{9})$	2
f	$(\bar{9})$	2	$(\bar{9})$	1

(f) By using (II.6), it is found that the column vectors in table 4 labelled by a, c, e are pairwise orthogonal.

(g) Thus, the column vectors

$$B^{(1,X)(1,X);(4,GM)(\bar{\sigma}_v,c_v;\bar{\sigma}'_v,c_v)}_{(\bar{1}),1} \qquad v=1,2,3 \tag{17}$$

where

$$\begin{aligned}(\bar{\sigma}_1, c_1; \bar{\sigma}'_1, c'_1) &= ((\bar{1}), 1; (\bar{1}), 1)\\ (\bar{\sigma}_2, c_2; \bar{\sigma}'_2, c'_2) &= ((\bar{5}), 1; (\bar{5}), 2)\\ (\bar{\sigma}_3, c_3; \bar{\sigma}'_3, c'_3) &= ((\bar{9}), 1; (\bar{9}), 2)\end{aligned} \tag{18}$$

are pairwise orthogonal and a 'special solution of the multiplicity problem' exists where the component multiplicity index w is identified with the special column indices in (18):

$$w = (\bar{\sigma}_v, c_v; \bar{\sigma}'_v, c'_v) \qquad v = 1, 2, 3. \tag{19}$$

It is interesting to observe at this point that the 'special solution of the multiplicity problem', given by (18) and (19), is not unique. The row elements of the column vectors are given by (II.4) and are tabulated for those of non-zero norm in table 5.

Table 5. Row elements of column vectors in table 4. The indices $(\bar{\sigma}_j, c_j; \bar{\sigma}'_j, c'_j)$ labelling the column vectors of non-zero norm are abbreviated to a, b, c, d, e, f (see table 4). For all column vectors, the row elements other than those labelled by a, b, c, d, e, f are zero.

	a	b	c	d	e	f
a	$\frac{1}{2}$	$-\frac{1}{2}$	0	0	0	0
b	$-\frac{1}{2}$	$\frac{1}{2}$	0	0	0	0
c	0	0	$\frac{1}{2}$	$\frac{1}{2}$	0	0
d	0	0	$\frac{1}{2}$	$\frac{1}{2}$	0	0
e	0	0	0	0	$\frac{1}{2}$	$-\frac{1}{2}$
f	0	0	0	0	$-\frac{1}{2}$	$\frac{1}{2}$

From table 5 it is clearly seen that there are, in fact, $2^3 = 8$ triples of pairwise orthogonal column vectors, namely ((a or b), (c or d), (e or f)). Thus, there are 8 different 'special solutions of the multiplicity problem' for this case.

From (5), all remaining component multiplicities are unity and therefore, for each of these, it is only necessary to select one column vector of non-zero norm. The 'special solutions of the multiplicity problem' in terms of the indices of the chosen column vectors and their norms, for all component multiplicities in (5), are given in table 6.

Table 6. Special solutions of the multiplicity problem $w=(\bar{\sigma}_v, c_v;\ \bar{\sigma}'_v, c'_v)$.

κ_0	$(\bar{\sigma}, \bar{\sigma}')\boldsymbol{q}_0$	$w=(\bar{\sigma}_v, c_v;\ \bar{\sigma}'_v, c'_v)$	v	Norm
1	$((\bar{1}), (\bar{1}))\boldsymbol{GM}$	$((\bar{1}), 1; (\bar{1}), 1)$	1	$1/\sqrt{6}$
2	$((\bar{1}), (\bar{1}))\boldsymbol{GM}$	$((\bar{1}), 1; (\bar{1}), 1)$	1	$1/\sqrt{6}$
3	$((\bar{1}), (\bar{1}))\boldsymbol{GM}$	$((\bar{1}), 1; (\bar{1}), 1)$	1	$1/\sqrt{6}$
4	$((\bar{1}), (\bar{1}))\boldsymbol{GM}$	$((\bar{1}), 1; (\bar{1}), 1)$	1	$1/\sqrt{2}$
4	$((\bar{1}), (\bar{1}))\boldsymbol{GM}$	$((\bar{5}), 1; (\bar{5}), 2)$	2	$1/\sqrt{2}$
4	$((\bar{1}), (\bar{1}))\boldsymbol{GM}$	$((\bar{9}), 1; (\bar{9}), 2)$	3	$1/\sqrt{2}$
1	$((\bar{1}), (\bar{5}))\boldsymbol{M}$	$((\bar{1}), 1; (\bar{5}), 1)$	1	$\frac{1}{2}$
2	$((\bar{1}), (\bar{5}))\boldsymbol{M}$	$((\bar{1}), 1; (\bar{5}), 1)$	1	$\frac{1}{2}$
3	$((\bar{1}), (\bar{5}))\boldsymbol{M}$	$((\bar{1}), 1; (\bar{5}), 1)$	1	$\frac{1}{2}$
4	$((\bar{1}), (\bar{5}))\boldsymbol{M}$	$((\bar{1}), 1; (\bar{5}), 1)$	1	$\frac{1}{2}$
1	$((\bar{5}), (\bar{1}))\boldsymbol{M}$	$((\bar{5}), 1; (\bar{1}), 1)$	1	$\frac{1}{2}$
2	$((\bar{5}), (\bar{1}))\boldsymbol{M}$	$((\bar{5}), 1; (\bar{1}), 1)$	1	$\frac{1}{2}$
3	$((\bar{5}), (\bar{1}))\boldsymbol{M}$	$((\bar{5}), 1; (\bar{1}), 1)$	1	$\frac{1}{2}$
4	$((\bar{5}), (\bar{1}))\boldsymbol{M}$	$((\bar{5}), 1; (\bar{1}), 1)$	1	$\frac{1}{2}$

Using the special solutions of the multiplicity problem in table 6, all the columns of the CG matrix may be calculated using (1) and the allowed matrix unirreps in tables 1, 2 and 3.

The CG matrix $C^{(1,\boldsymbol{X})(1,\boldsymbol{X})}$ in table 7 will reduce the Kronecker product $\Lambda^{(1,\boldsymbol{X})}[g]\otimes\Lambda^{(1,\boldsymbol{X})}[g]$, for all $g\in G=P2_13$, into block diagonal form. As an example, consider $g=(4,1)$. The allowed matrices $\Gamma^{(\kappa_0,\boldsymbol{GM})}[(4,1)]$, $\Gamma^{(\kappa_0,\boldsymbol{X})}[(4,1)]$, $\Gamma^{(\kappa_0,\boldsymbol{M})}[(4,1)]$, $\kappa_0=1$, 2, 3, 4, are given in tables 1, 2 and 3 respectively. Using (I.5) and tables (3.2a) and (3.6) of CDML, the matrices $\Lambda^{(\kappa_0,\boldsymbol{GM})}[(4,1)]$, $\Lambda^{(\kappa_0,\boldsymbol{X})}[(4,1)]$, $\Lambda^{(\kappa_0,\boldsymbol{M})}[(4,1)]$, $\kappa_0=1$, 2, 3, 4, may be constructed and are given in table 8.

The Kronecker product matrix $\Lambda^{(1,\boldsymbol{X})}[(4,1)]\otimes\Lambda^{(1,\boldsymbol{X})}[(4,1)]$ is a 36×36 matrix given by the block matrix

$$\Lambda^{(1,\boldsymbol{X})}[(4,1)]\otimes\Lambda^{(1,\boldsymbol{X})}[(4,1)]=\begin{pmatrix} X & 0 & 0 & 0 & 0 & 0\\ 0 & -X & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & X & 0 & 0\\ 0 & 0 & X & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & -X\\ 0 & 0 & 0 & 0 & X & 0 \end{pmatrix} \tag{20}$$

where the matrix X is given by

$$X=\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0\\ 0 & -1 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & -1\\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}. \tag{21}$$

The rows and columns of $\Lambda^{(1,\boldsymbol{X})}[(4,1)]\otimes\Lambda^{(1,\boldsymbol{X})}[(4,1)]$ are indexed lexicographically by $\bar{\tau}$, d; $\bar{\tau}'$, d' where $\bar{\tau}\in\{(\bar{1}),(\bar{5}),(\bar{9})\}$, $d=1,2$, $\bar{\tau}'\in\{(\bar{1}),(\bar{5}),(\bar{9})\}$, $d'=1,2$. It may be verified that the CG matrix $C^{(1,\boldsymbol{X})(1,\boldsymbol{X})}$ in table 7, when substituted into (I.10) (with $(\kappa,\boldsymbol{q})=(\kappa',\boldsymbol{q}')=(1,\boldsymbol{X})$, and the component multiplicities $m^{(\bar{\sigma},\bar{\sigma}')}_{(\kappa,\boldsymbol{q})(\kappa',\boldsymbol{q}');(\kappa_0,\boldsymbol{q}_0)}$ are given by (5), reduces the Kronecker product $\Lambda^{(1,\boldsymbol{X})}[(4,1)]\otimes\Lambda^{(1,\boldsymbol{X})}[(4,1)]$ into block diagonal

Table 7. CG matrix $C^{(1,X)(1,X)}$ for the reduction of $\Lambda^{(1,X)}\otimes\Lambda^{(1,X)}$. $\omega=\exp(2i\pi/3)$, $I=\exp(i\pi/2)$, $a=\sqrt{2}$, $b=2$, $c=\sqrt{6}$. The indexing of the rows and columns is explained by (1.11) *et seq.* The number at the base of each column divides each element of that column. The asterisk * denotes the complex conjugate.

$(\bar\sigma,\bar\sigma')\mathbf{q}_0$				$((\bar1),(\bar1))GM$											
			κ_0	1	2	3	4								
			v	1	1	1	1			2			3		
			$\bar\sigma_0$	$(\bar1)$	$(\bar1)$	$(\bar1)$	$(\bar1)$			$(\bar1)$			$(\bar1)$		
			j	1	1	1	1	2	3	1	2	3	1	2	3
$\bar\tau$	d	$\bar\tau'$	d'												
$(\bar1)$	1	$(\bar1)$	1	1	1	1	1								
			2								1				1
		$(\bar5)$	1												
			2												
		$(\bar9)$	1												
			2												
	2	$(\bar1)$	1								1				−1
			2	1	1	1	−1								
		$(\bar5)$	1												
			2												
		$(\bar9)$	1												
			2												
$(\bar5)$	1	$(\bar1)$	1												
			2												
		$(\bar5)$	1	1	ω	ω^*			1						
			2							1				1	
		$(\bar9)$	1												
			2												
	2	$(\bar1)$	1												
			2												
		$(\bar5)$	1							1				−1	
			2	1	ω	ω^*			−1						
		$(\bar9)$	1												
			2												
$(\bar9)$	1	$(\bar1)$	1												
			2												
		$(\bar5)$	1												
			2												
		$(\bar9)$	1	1	ω^*	ω		1							
			2									1	1		
	2	$(\bar1)$	1												
			2												
		$(\bar5)$	1												
			2												
		$(\bar9)$	1									1	−1		
			2	1	ω^*	ω		−1							
$\bar\tau$	d	$\bar\tau'$	d'	c	c	c	a	a	a	a	a	a	a	a	a

$(\bar\sigma,\bar\sigma')\mathbf{q}_0$				$((\bar1),(\bar5))M$											
			κ_0	1			2			3			4		
			v	1			1			1			1		
			$\bar\sigma_0$	$(\bar1)$	$(\bar5)$	$(\bar9)$	$(\bar1)$	$(\bar5)$	$(\bar9)$	$(\bar1)$	$(\bar5)$	$(\bar9)$	$(\bar1)$	$(\bar5)$	$(\bar9)$
			j	1	1	1	1	1	1	1	1	1	1	1	1
$\bar\tau$	d	$\bar\tau'$	d'												
$(\bar1)$	1	$(\bar1)$	1												
			2												
		$(\bar5)$	1	1			1			1			1		
			2	1			1			−1			−1		
		$(\bar9)$	1												
			2												
	2	$(\bar1)$	1												
			2												
		$(\bar5)$	1	I			−I			−I			I		
			2	−I			I			−I			I		
		$(\bar9)$	1												
			2												
$(\bar5)$	1	$(\bar1)$	1												
			2												
		$(\bar5)$	1												
			2												
		$(\bar9)$	1		1			1			1			1	
			2		1			1			−1			−1	
	2	$(\bar1)$	1												
			2												
		$(\bar5)$	1												
			2												
		$(\bar9)$	1		I			−I			I			I	
			2		−I			I			−I			I	
$(\bar9)$	1	$(\bar1)$	1			1			1			1			1
			2			1			1			−1			−1
		$(\bar5)$	1												
			2												
		$(\bar9)$	1												
			2												
	2	$(\bar1)$	1			I			−I			−I			I
			2			−I			I			−I			I
		$(\bar5)$	1												
			2												
		$(\bar9)$	1												
			2												
$\bar\tau$	d	$\bar\tau'$	d'	b	b	b	b	b	b	b	b	b	b	b	b

$(\bar\sigma,\bar\sigma')\mathbf{q}_0$				$((\bar5),(\bar1))M$											
			κ_0	1			2			3			4		
			v	1			1			1			1		
			$\bar\sigma_0$	$(\bar1)$	$(\bar5)$	$(\bar9)$	$(\bar1)$	$(\bar5)$	$(\bar9)$	$(\bar1)$	$(\bar5)$	$(\bar9)$	$(\bar1)$	$(\bar5)$	$(\bar9)$
			j	1	1	1	1	1	1	1	1	1	1	1	1
$\bar\tau$	d	$\bar\tau'$	d'												
$(\bar1)$	1	$(\bar1)$	1												
			2												
		$(\bar5)$	1												
			2												
		$(\bar9)$	1			1			1			1			1
			2			I			−I			−I			I
	2	$(\bar1)$	1												
			2												
		$(\bar5)$	1												
			2												
		$(\bar9)$	1			1			1			−1			−1
			2			−I			I			−I			I
$(\bar5)$	1	$(\bar1)$	1	1			1			1			1		
			2	I			−I			−I			I		
		$(\bar5)$	1												
			2												
		$(\bar9)$	1												
			2												
	2	$(\bar1)$	1	1			1			−1			−1		
			2	I			I			−I			I		
		$(\bar5)$	1												
			2												
		$(\bar9)$	1												
			2												
$(\bar9)$	1	$(\bar1)$	1												
			2												
		$(\bar5)$	1		1			1			1			1	
			2		I			−I			−I			I	
		$(\bar9)$	1												
			2												
	2	$(\bar1)$	1												
			2												
		$(\bar5)$	1		1			1			−1			−1	
			2		−I			I			−I			I	
		$(\bar9)$	1												
			2												
$\bar\tau$	d	$\bar\tau'$	d'	b	b	b	b	b	b	b	b	b	b	b	b

Table 8. Induced matrices $\Lambda^{(\kappa,q)}[(4,1)]$. The rows and columns of $\Lambda^{(\kappa,q)}[(4,1)]$ for $q = X$, M are labelled by the *fixed* left coset representatives $(\bar{1})$, $(\bar{5})$, $(\bar{9})$ of P^X, P^M in P.

$$I = \exp(i\pi/2),\ A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},\ B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ C = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

κ	q	$\Lambda^{(\kappa,q)}[(4,1)]$
1	***GM***	1
2	***GM***	1
3	***GM***	1
4	***GM***	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
1	***X***	$\begin{pmatrix} A & 0 & 0 \\ 0 & B & 0 \\ 0 & 0 & C \end{pmatrix}$
1	***M***	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & -I \end{pmatrix}$
2	***M***	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -I & 0 \\ 0 & 0 & I \end{pmatrix}$
3	***M***	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{pmatrix}$
4	***M***	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -I & 0 \\ 0 & 0 & -I \end{pmatrix}$

form given by:

$$\mathrm{diag}\{1, 1, 1, J, J, J, K, L, M, N, K, L, M, N\} \tag{22}$$

where

$$J = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad K = \begin{pmatrix} 1 & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & -I \end{pmatrix}$$

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -I & 0 \\ 0 & 0 & I \end{pmatrix} \qquad M = \begin{pmatrix} -1 & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{pmatrix} \qquad N = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -I & 0 \\ 0 & 0 & -I \end{pmatrix}.$$

From (5) and table 8, it is verified that (22) gives the correct block diagonal form.

5. Conclusion

The purpose of this paper is to report that a computer program has been written, based on the method of Dirl (1979), to calculate CG coefficients for the reduction of Kronecker products of Miller and Love (1967) matrix unirreps (as extended by Cracknell *et al* 1979) in any of the 230 (single or double) crystallographic space groups. The program uses WVSR and multiplicities previously computed (Davies and Cracknell 1979, Cracknell and Davies 1979) and the 'special solutions of the multiplicity problem' reported in DI and DII. The method is ideally suited for computer application, since a crucial feature, with respect to obtaining an efficient computer program, is that all elements of the CG matrix can be computed using a single, explicit formula (equation (1)) in terms of the allowed matrix unirreps of the little groups occurring in the Kronecker product. No solving of simultaneous equations is required as in, for example, Chen *et al* (1983).

The method is attractive for its elegance and essential simplicity. Once the rather complicated (but necessary) notation was mastered, it was straightforward to program. It is our intention to make available, in an appropriate form through Plenum Press, the CG matrices for the Kronecker products tabulated in Davies and Cracknell (1979, 1980) and Cracknell and Davies (1979).

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