Results of computer programs for determining the reductions of the Kronecker products of the irreducible representations of space groups

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INTRODUCTION

The reduction of the Kronecker product of the irreducible representations $(\Gamma_p^{\underset{\sim}{k}_i} \uparrow \underset{\sim}{G})$ and $(\Gamma_q^{\underset{\sim}{k}_j} \uparrow \underset{\sim}{G})$ of a space group $\underset{\sim}{G}$ into its irreducible component representations $(\Gamma_r^{\underset{\sim}{k}_\ell} \uparrow \underset{\sim}{G})$ is determined by the values of the coefficients $C_{pq,r}^{\underset{\sim}{k}_i\underset{\sim}{k}_j,\underset{\sim}{k}_\ell}$ in the Clebsch-Gordan series expansion

$$(\Gamma_p^{\underset{\sim}{k}_i} \uparrow \underset{\sim}{G}) \boxtimes (\Gamma_q^{\underset{\sim}{k}_j} \uparrow \underset{\sim}{G}) = \sum_\ell \sum_r C_{pq,r}^{\underset{\sim}{k}_i\underset{\sim}{k}_j,\underset{\sim}{k}_\ell} (\Gamma_r^{\underset{\sim}{k}_\ell} \uparrow \underset{\sim}{G}) \tag{1}$$

where $(\Gamma_p^{\underset{\sim}{k}_i} \uparrow \underset{\sim}{G})$ is a (single or double valued) irreducible representation of $\underset{\sim}{G}$ induced from the small representation $\Gamma_p^{\underset{\sim}{k}_i}$ of the little group $\underset{\sim}{G}^{\underset{\sim}{k}_i}$, etc. Computer programs, written in ALGOL 60, have been developed to evaluate the coefficients in equation (1) for any choice of vectors $\underset{\sim}{k}_i$ and $\underset{\sim}{k}_j$ in the representation domain Φ of any of the 230 space groups. The results will be published in two volumes by Plenum Press.

METHOD

The calculation falls naturally into two parts which have been programmed separately. In the first part the wave vector selection rules (WVSRs) are found. The WVSRs determine the allowed values of $\underset{\sim}{k}_\ell$ which can appear on the right hand side of equation (1) and are given by

$$R_\alpha \underset{\sim}{k}_i + R_\beta \underset{\sim}{k}_j \equiv \underset{\sim}{k}_\ell \tag{2}$$

where $\{R_\alpha | \underset{\sim}{v}_\alpha\}$ and $\{R_\beta | \underset{\sim}{v}_\beta\}$ are a very restricted subset of the elements of $\underset{\sim}{G}$. The results of work on the first part, including a description of the WVSR program is given in another contribution to this colloquium [1]. In the second part the WVSRs are used to evaluate the coefficients $C_{pq,r}^{\underset{\sim}{k}_i\underset{\sim}{k}_j,\underset{\sim}{k}_\ell}$ using the Kronecker products (KP) program.

The KP program uses a subgroup method to evaluate the coefficients [2,3]. Given $\underset{\sim}{k}_i$ and $\underset{\sim}{k}_j$ in Φ, the KP program uses the results of the WVSR program to find the allowed values of $\underset{\sim}{k}_\ell$ in Φ together with the corresponding pairs of elements $\{R_\alpha|\underset{\sim}{v}_\alpha\}$ and $\{R_\beta|\underset{\sim}{v}_\beta\}$ in equation (2). The characters $\chi_p^{\underset{\sim}{k}_i}$, $\chi_q^{\underset{\sim}{k}_j}$, $\chi_r^{\underset{\sim}{k}_\ell}$ of the small representations $\Gamma_p^{\underset{\sim}{k}_i}$, $\Gamma_q^{\underset{\sim}{k}_j}$, $\Gamma_r^{\underset{\sim}{k}_\ell}$ are then used in equation (4.7.29) of [3] to evaluate the coefficient $C_{pq,r}^{\underset{\sim}{k}_i \underset{\sim}{k}_j, \underset{\sim}{k}_\ell}$. The character tables we have used are those of [4] as augmented by [5,6]. Profs. S.C. Miller and W.F. Love of the University of Colorado have very generously provided us with a copy of their tables on a magnetic tape which has enormously simplified our data preparation and handling work. These tables only apply to vectors $\underset{\sim}{k}_A$ in the basic domain Ω. It has been shown in [7] that for all space groups except Pa3, the character tables for vectors $\underset{\sim}{k}_B \in \Phi - \Omega$ can be constructed from those for $\underset{\sim}{k}_A \in \Omega$, where $\underset{\sim}{k}_B = R\underset{\sim}{k}_A$ and $\{R|\underset{\sim}{v}_R\} \in \underset{\sim}{G}_o$, $\underset{\sim}{G}$ being an invariant subgroup of $\underset{\sim}{G}_o$. Provision for this is included in the KP program [8].

A large number of checks are incorporated in the KP program but the following three are the most important ones.

1) The $C_{pq,r}^{\underset{\sim}{k}_i \underset{\sim}{k}_j, \underset{\sim}{k}_\ell}$ must be positive integers.

2) If d_p^i, d_q^j, d_r^ℓ are the dimensions of $(\Gamma_p^{\underset{\sim}{k}_i} \uparrow \underset{\sim}{G})$, $(\Gamma_q^{\underset{\sim}{k}_j} \uparrow \underset{\sim}{G})$, $(\Gamma_r^{\underset{\sim}{k}_\ell} \uparrow \underset{\sim}{G})$ respectively then

$$d_p^i d_q^j = \sum_\ell \sum_r C_{pq,r}^{\underset{\sim}{k}_i \underset{\sim}{k}_j, \underset{\sim}{k}_\ell} d_r^\ell . \quad (3)$$

3) If $d_p^i \geq d_q^j$ then $d_r^\ell \geq d_p^i / d_q^j$, for all ℓ, r in equation (3).

RESULTS

The KP program has been run successfully for more than 150 groups and we expect to finish the remainder by the end of August, 1977. On the DEC system 10 computer the time taken for the reduction of all the Kronecker products for all the points, lines and planes of symmetry in Φ for Fm3m, Fm3c, Fd3m and Fd3c is approximately 6 minutes each, contrasting with I23 and $I2_13$ which take about 2 minutes each. In Table 1 the reductions for $\underset{\sim}{k}_i = \underset{\sim}{DT}$, $\underset{\sim}{k}_j = \underset{\sim}{P}$, $\underset{\sim}{k}_\ell = \underset{\sim}{D}$ ($R_\alpha = 10$, $R_\beta = 1$) for the groups I23 and $I2_13$ are displayed in the notation of [4]. (N.B. The coordinate parameters of $\underset{\sim}{k}$ vectors on lines or planes of symmetry were given definite values.) The upper and lower entries refer to I23 and $I2_13$ respectively, e.g. in I23 (= $\underset{\sim}{G}$), DT2 ⊠ P4 = 2D1 + D2 where DT2 stands for (DT2 ↑ $\underset{\sim}{G}$), etc. In $I2_13$ however, DT2 ⊠ P4 = D4. The above product is an example where only one pair (R_α, R_β) is associated with $\underset{\sim}{k}_\ell$. However, for $\underset{\sim}{k}_i = \underset{\sim}{N} = \underset{\sim}{k}_j$, $\underset{\sim}{k}_\ell = \underset{\sim}{G}M, \underset{\sim}{H}, \underset{\sim}{N}$ and the corresponding sets of pairs (R_α, R_β) are (1,1), (1,2), [(5,11), (9,6)] respectively. The products Np ⊠ Nq are identical for I23 and $I2_13$ and the reductions are given in Table 2.

If any worker would like some particular results for any space group before our work is published then we shall be glad to supply them.

Table 1

	P1	P2	P3	P4	P5	P6	P7
DT1	1 1 + 2	1 1 + 2	1 1 + 2	1 + 2 + 2 3	3 + 4 3	3 + 4 3	3 + 4 3 + 4 + 4
DT2	2 1 + 2	2 1 + 2	2 1 + 2	1 + 1 + 2 4	3 + 4 4	3 + 4 4	3 + 4 3 + 3 + 4
DT3	3 3 + 4	3 3 + 4	3 3 + 4	3 + 4 + 4 2	1 + 2 2	1 + 2 2	1 + 2 1 + 1 + 2
DT4	4 3 + 4	4 3 + 4	4 3 + 4	3 + 3 + 4 1	1 + 2 1	1 + 2 1	1 + 2 1 + 2 + 2

Table 2

N1 ⊠ N1 = N2 ⊠ N2 = GM1 + GM2 + GM3 + GM4 + H1 + H2 + H3 + H4 + 2N1 + 2N2 .

N1 ⊠ N2 = 2GM4 + 2H4 + 2N1 + 2N2 .

N1 ⊠ N3 = N1 ⊠ N4 = N2 ⊠ N3 = N2 ⊠ N4 = GM5 + GM6 + GM7 + H5 + H6 + H7 + 2N3 + 2N4.

N3 ⊠ N3 = N4 ⊠ N4 = 2GM4 + H1 + H2 + H3 + H4 + 2N1 + 2N2 .

N3 ⊠ N4 = GM1 + GM2 + GM3 + GM4 + 2H4 + 2N1 + 2N2 .

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