6j symbols and 3jm factors for the group chain D_{4d} contains/implies D_4 contains/implies C_4

1980 J. Phys. A: Math. Gen. 13 781

(http://iopscience.iop.org/0305-4470/13/3/011)

J. Phys. A: Math. Gen. 13 (1980) 781–788. Printed in Great Britain

$6j$ symbols and $3jm$ factors for the group chain $D_{4d} \supset D_4 \supset C_4$

L S R K Prasad and K Bharathi
Department of Applied Mathematics, Andhra University, Waltair, India

Received 12 April 1979, in final form 9 July 1979

Abstract. The complete set of $6j$ symbols for the double point groups D_{4d} and D_4 and the complete set of $3jm$ factors associated with the group chain $D_{4d} \supset D_4 \supset C_4$ are calculated.

1. Introduction

Elementary applications of group theory to a quantum-mechanical system yield qualitative information such as the degeneracies of the states of the system and the selection rules. To obtain quantitative information the well known Wigner–Eckart theorem (Wybourne 1974) must be applied. A knowledge of coupling coefficients is essential for the application of the Wigner–Eckart theorem.

Racah's irreducible tensor method, which was developed for systems with Hamiltonians having full spherical symmetry (such as free atoms), was extended by Griffith (1962) for application to systems having the lower symmetry characteristic of the internal modes of motion of molecules and of the states of ions in solids. Griffith (1962), by analogy with Racah's $\bar{V}$, $\bar{W}$ and X coefficients and Wigner's $3j$, $6j$ and $9j$ symbols, obtained the V, W and X coefficients for the octahedral group and its subgroups and the dihedral groups, considering only their true representations (also known as single-valued representations). Harnung (1973) extended the work of Griffith to the octahedral spinor group and tabulated the 3Γ symbols for this group. His method has revealed symmetries which might otherwise be considered as accidental and has facilitated ligand-field calculations. Golding (1973) obtained the V symmetry-coupling coefficients for the icosahedral double group using the behaviour of a minimum number of $|JM\rangle$ 'ket' vectors, by analogy with the $\bar{V}$ coefficients of Racah. These coupling coefficients are useful in calculations involving systems such as polyhedral conductors and rare-earth double nitrates. Coupling coefficients associated with all the thirty-two crystallographic double point groups were tabulated by Koster *et al* (1963), taking into consideration the time-inversion operator in addition to the spatial operators. Golding and Newmarch (1977) calculated the $\bar{V}$ coupling coefficients for the groups D_n^*, C_n^* and T^* using the fact that they are subgroups of SU(2), the special unitary group in two dimensions, and the earlier method of Golding (1973).

Butler (1975) extended the irreducible tensor theory for arbitrary compact Lie groups (finite or continuous), and their subgroup chains. Butler and Wybourne (1976a) developed a systematic recursive method of computing $6j$ symbols and $3jm$ factors in a group–subgroup chain. Butler (1976) applied this method to SO_3 and was able to rederive all the standard results pertaining to this group. Butler and Wybourne (1976b) applied this recursive method to compute the $6j$ symbols and $3jm$ factors that arise in the group–subgroup chain $SO_3 \supset T \supset C_3 \supset C_1$. The consideration of a group–subgroup chain mainly serves two purposes: it throws light on the structural significance of the system under consideration and, if a suitable chain of groups was chosen, it leads to the elimination of the multiplicity problem, thereby solving the problem of labelling the basis states unambiguously.

In practical applications it is often necessary to consider the coupling of the product of the basis states of three irreducible representations of the symmetry group of the system under consideration. This coupling of the products may be performed in various possible sequences. The various resultant coupled states are related by unitary transformations and the elements of these unitary matrices are known as 'recoupling coefficients'. In practical calculations it is desirable to make use of the highly symmetrical $6j$ symbol which is related to the recoupling coefficient (Butler 1975, equation 9.13). Racah's factorisation lemma states that if the basis states $|\lambda i\rangle$ are chosen to form irreducible spaces of some subgroup $\hat{G}$ of the symmetry group G, then the coupling coefficient of the group G factorises into an isoscalar factor (which is independent of basis labels) and a coupling coefficient of the subgroup $\hat{G}$. The $3jm$ factor is related to the isoscalar factor (Butler 1975, equation 13.8).

The $6j$ symbols and $3jm$ symbols (equivalently the W coefficients and V coefficients) are known only for very few non-crystallographic single and double point groups (Griffith 1962, Golding 1973, Golding and Newmarch 1977). In this paper, the non-crystallographic double point group D_{4d} is taken up and its $6j$ symbols and the $3jm$ factors for the chain $D_{4d} \supset D_4 \supset C_4$ are completely evaluated following the systematic recursive method developed by Butler and Wybourne (1976a). Consideration of this chain eliminates completely the multiplicity problem, thereby solving the problem of unambiguous labelling of the basis states. In this method the calculation of the $6j$ symbols and $3jm$ factors does not require any specific choice of bases for the irreducible representations of the groups considered. Their calculation depends entirely on the characters of the irreducible representations. The sulphur molecule (S_8) having the puckered octagonal structure is a well-known example of a physical system having D_{4d} symmetry. For any physical application one only has to choose suitable bases for the irreducible representations of the lowest group in the chain, namely C_4. Using the resulting coupling coefficients of C_4 and the $3jm$ factors for the chains $D_4 \supset C_4$ and $D_{4d} \supset D_4$ (calculated in this paper), one calculates the coupling coefficients of the largest group in the chain, namely D_{4d}, in a step-by-step fashion.

In § 2 we calculate the $1j$, $2j$ and $3j$ symbols for the double point groups D_{4d} and D_4. A set of fundamental $6j$ symbols is calculated, and then a complete set of primitive $6j$ symbols is obtained for D_{4d} and D_4 using the orthogonality and Racah back-coupling relations. Using these primitive $6j$ symbols, all the non-trivial inequivalent $6j$ symbols are computed by the recursive method. In § 3 the $2jm$ factors for the chain $D_{4d} \supset D_4$ are suitably fixed. Using these and the orthogonality relations and symmetry properties of $3jm$ factors, a complete set of primitive $3jm$ factors is obtained for the chain $D_{4d} \supset D_4$. The complete set of non-trivial inequivalent $3jm$ factors for the chain $D_{4d} \supset D_4$ is then calculated using a recursion relation. In § 4 the work of § 3 is repeated for the chain $D_4 \supset C_4$. The notation and terminology used in this paper are mostly those of Butler and Wybourne (1976a). The character table and the multiplication table for the double group D_{4d} are taken from Herzberg (1966) and for the double groups D_4 and C_4 we took them from Koster *et al* (1963).

2. $6j$ symbols for the double groups D_{4d} and D_4

The double point groups D_{4d} and D_4 are simply reducible. The symmetric ($\Gamma_i \otimes \{2\}$) and antisymmetric ($\Gamma_i \otimes \{1^2\}$) terms of the Kronecker squares $\Gamma_i^{\times 2}$ of the irreducible representations (irreps) of D_{4d} and D_4 are given respectively in tables 1 and 2.

Table 1.

Γ_i	$\Gamma_i \otimes \{2\}$	$\Gamma_i \otimes \{1^2\}$	ϕ_Γ	Type	Power
$\Gamma_1(A_1)$	Γ_1	—	+1	Orthogonal	2
$\Gamma_2(A_2)$	Γ_1	—	+1	Orthogonal	2
$\Gamma_3(B_1)$	Γ_1	—	+1	Orthogonal	8
$\Gamma_4(B_2)$	Γ_1	—	+1	Orthogonal	8
$\Gamma_5(E_1)$	$\Gamma_1+\Gamma_6$	Γ_2	+1	Orthogonal	2
$\Gamma_6(E_2)$	$\Gamma_1+\Gamma_3+\Gamma_4$	Γ_2	+1	Orthogonal	4
$\Gamma_7(E_3)$	$\Gamma_1+\Gamma_6$	Γ_2	+1	Orthogonal	6
$\Gamma_8(E_{1/2})$	$\Gamma_2+\Gamma_5$	Γ_1	−1	Symplectic	1
$\Gamma_9(E_{3/2})$	$\Gamma_2+\Gamma_7$	Γ_1	−1	Symplectic	3
$\Gamma_{10}(E_{5/2})$	$\Gamma_2+\Gamma_7$	Γ_1	−1	Symplectic	5
$\Gamma_{11}(E_{7/2})$	$\Gamma_2+\Gamma_5$	Γ_1	−1	Symplectic	7

Table 2.

Γ_i	$\Gamma_i \otimes \{2\}$	$\Gamma_i \otimes \{1^2\}$	ϕ_Γ	Type	Power
Γ_1	Γ_1	—	+1	Orthogonal	2
Γ_2	Γ_1	—	+1	Orthogonal	2
Γ_3	Γ_1	—	+1	Orthogonal	4
Γ_4	Γ_1	—	+1	Orthogonal	4
Γ_5	$\Gamma_1+\Gamma_3+\Gamma_4$	Γ_2	+1	Orthogonal	2
Γ_6	$\Gamma_2+\Gamma_5$	Γ_1	−1	Symplectic	1
Γ_7	$\Gamma_2+\Gamma_5$	Γ_1	−1	Symplectic	3

Herzberg's (1966) notation for indicating the irreps of D_{4d} is given inside the parenthesis of the first column of table 1. The irreps of a finite group are classified (Butler and King 1974) into orthogonal, symplectic or complex by the evaluation of Frobenius–Schur invariant C_Γ (Hamermesh 1962) and we assign the $2j$ symbol ϕ_Γ the value of C_Γ in the first two cases.

The permutational symmetries of the $3jm$ symbols (Butler 1975) are given by

$$(\lambda_a\lambda_b\lambda_c)_{si_ai_bi_c} = \sum_r \{(\pi)\lambda_1\lambda_2\lambda_3\}_{sr}(\lambda_1\lambda_2\lambda_3)_{ri_1i_2i_3}$$

where 'π' is a permutation of 1, 2, 3. Using the phase convention of Butler (1975), we have

$$\{(\pi)\lambda_1\lambda_2\lambda_3\}_{rs} = \begin{cases} \delta_{rs} & \text{for } \pi \text{ even,} \\ \theta(\lambda_1\lambda_2\lambda_3 r)\delta_{rs} & \text{for } \pi \text{ odd.} \end{cases}$$

where $\theta(\lambda_1\lambda_2\lambda_3 r) = \pm 1$. When two of the three irreps are equal, an inspection of symmetrised Kronecker squares reveals that the value of the $3j$ symbol $\theta(\lambda\lambda\lambda', r)$ is equal to +1 or −1 according to whether the rth term of λ'^{*} occurs in the symmetric or antisymmetric part of the product $\lambda\times\lambda$ respectively. As an example, for the group D_{4d} we have $\theta(\Gamma_5\Gamma_5\Gamma_2, 1) = -1$, $(\Gamma_8\Gamma_8\Gamma_5, 1) = +1$, since $\Gamma_2^{*} = \Gamma_2$ is in the antisymmetric part of $\Gamma_5\times\Gamma_5$ and $\Gamma_5^{*} = \Gamma_5$ is in the symmetric part of $\Gamma_8\times\Gamma_8$. Now we can select a set of $1j$ symbols $(-1)^{\lambda}$ such that

$$\phi_\lambda = (-1)^{2\lambda}$$

and $\theta(\lambda\lambda\lambda', r) = (-1)^{\lambda+\lambda+\lambda'+r-1}$. The remaining $3j$ symbols, when the three irreps are distinct, are calculated from the equation

$$\theta(\lambda_1\lambda_2\lambda_3, r) = (-1)^{\lambda_1+\lambda_2+\lambda_3+r-1}.$$

The groups D_{4d} and D_4 are Kronecker multiplicity free and therefore we drop r throughout. In the present problem the $1j$ symbols for D_{4d} are

$$(-1)^{\Gamma_k} = \begin{cases} +1, & k = 1, 3, 4, 6 \\ -1, & k = 2, 5, 7 \\ +\mathrm{i}, & k = 8, 9, 10, 11 \end{cases}$$

and for D_4 are

$$(-1)^{\Gamma_k} = \begin{cases} +1, & k = 1, 3, 4 \\ -1, & k = 2, 5 \\ +\mathrm{i}, & k = 6, 7. \end{cases}$$

Thus all the $1j$, $2j$ and $3j$ symbols are obtained.

The spin representation Γ_8 of D_{4d} and Γ_6 of D_4 are faithful representations and may be chosen as primitive representations (Butler and Wybourne 1976a). The power of a representation λ is defined as the minimum positive integer l such that $\epsilon^{\times l} \supset \lambda$ or $(\epsilon^{*})^{\times l} \supset \lambda$ where ϵ is the primitive representation. A primitive $6j$ symbol is a $6j$ symbol which contains the primitive irrep at least once as one of its irreps, but does not contain the scalar representation. The trivial $6j$ symbols, being proportional to the $3j$ symbols, are readily determined from equation (17) of Butler and Wybourne (1976a). Using the orthogonality and Racah back-coupling relations (Butler and Wybourne 1976a, equations (25) and (26)), and systematically increasing the power of the largest irrep, all the $6j$ primitives are calculated. The free phases of the $6j$'s are fixed by a subset of primitives known as fundamentals (Butler and Wybourne 1976b). The phases of all the fundamentals for the groups D_{4d} and D_4 are chosen to be +1 for simplicity.

Once the set of primitive $6j$ symbols is obtained, the rest are computed recursively using the modified form of the generalised Biedenharn–Elliott sum rule (Butler and Wybourne 1976a, equation (27)) and the primitives. At this stage no phase freedom exists. The complete sets of non-trivial inequivalent $6j$ symbols of D_{4d} and D_4 are listed in tables 5 and 6 respectively.

3. $3jm$ factors for $D_{4d} \supset D_4$

The branching rules for $D_{4d} \to D_4$ are given in table 3. The first step in calculating the $3jm$ primitives (Butler and Wybourne 1976a) is to fix the $2jm$ factors. We choose

$$(\Gamma_1)_{\gamma_1\gamma_1} = (\Gamma_2)_{\gamma_2\gamma_2} = (\Gamma_3)_{\gamma_1\gamma_1} = (\Gamma_4)_{\gamma_2\gamma_2} = (\Gamma_5)_{\gamma_5\gamma_5} = (\Gamma_6)_{\ 3\ 3} = (\Gamma_6)_{\gamma_4\gamma_4} = (\Gamma_7)_{\gamma_5\gamma_5}$$
$$= (\Gamma_8)_{\gamma_6\gamma_6} = (\Gamma_9)_{\gamma_7\gamma_7} = (\Gamma_{10})_{\gamma_7\gamma_7} = (\Gamma_{11})_{\gamma_6\gamma_6} = +1.$$

Table 3. Branching rules for $D_{4d} \supset D_4$.

D_{4d}	D_4
Γ_1	γ_1
Γ_2	γ_2
Γ_3	γ_1
Γ_4	γ_2
Γ_5	γ_5
Γ_6	$\gamma_3+\gamma_4$
Γ_7	γ_5
Γ_8	γ_6
Γ_9	γ_7
Γ_{10}	γ_7
Γ_{11}	γ_6

Table 4. Branching rules for $D_4 \supset C_4$.

D_4	C_4
Γ_1	γ_1
Γ_2	γ_1
Γ_3	γ_2
Γ_4	γ_2
Γ_5	$\gamma_3+\gamma_4$
Γ_6	$\gamma_5+\gamma_6$
Γ_7	$\gamma_7+\gamma_8$

Table 5. Non-trivial inequivalent $6j$ symbols for the group D_{4d}.

(2 3 4/2 3 4) = +1	(2 3 4/6 6 6) = $+2^{-1/2}$	(3 5 7/9 11 8) = $-\frac{1}{2}$	(3 5 7/9 9 10) = $+\frac{1}{2}$
(2 3 4/5 7 7) = $+2^{-1/2}$	(2 3 4/7 5 5) = $+2^{-1/2}$	(3 5 7/10 10 9) = $+\frac{1}{2}$	(3 5 7/10 8 11) = $-\frac{1}{2}$
(2 3 4/8 11 11) = $-2^{-1/2}$	(2 3 4/9 10 10) = $+2^{-1/2}$	(3 5 7/11 9 10) = $-\frac{1}{2}$	†(3 5 7/11 8 11) = $+\frac{1}{2}$
(2 3 4/10 9 9) = $-2^{-1/2}$	†(2 3 4/11 8 8) = $+2^{-1/2}$	(3 6 6/4 6 6) = $-\frac{1}{2}$	(3 6 6/3 6 6) = $+\frac{1}{2}$
(2 5 5/2 5 5) = $+\frac{1}{2}$	(2 5 5/3 7 7) = $+\frac{1}{2}$	(3 6 6/9 8 11) = $+\frac{1}{2}$	†(3 6 6/8 9 10) = $+\frac{1}{2}$
(2 5 5/4 7 7) = $+\frac{1}{2}$	(2 5 5/5 6 6) = $+\frac{1}{2}$	(3 6 6/11 9 10) = $+\frac{1}{2}$	(3 6 6/10 8 11) = $-\frac{1}{2}$
(2 5 5/6 5 5) = $+\frac{1}{2}$	(2 5 5/6 7 7) = $-\frac{1}{2}$	(3 8 11/4 8 11) = $+\frac{1}{2}$	(3 8 11/3 8 11) = $-\frac{1}{2}$
(2 5 5/7 6 6) = $-\frac{1}{2}$	†(2 5 5/8 8 8) = $+\frac{1}{2}$	†(3 8 11/5 11 8) = $+\frac{1}{2}$	(3 8 11/5 10 9) = $+\frac{1}{2}$
(2 5 5/8 9 9) = $-\frac{1}{2}$	(2 5 5/9 8 8) = $-\frac{1}{2}$	(3 8 11/6 10 9) = $-\frac{1}{2}$	(3 8 11/6 9 10) = $+\frac{1}{2}$
(2 5 5/9 10 10) = $+\frac{1}{2}$	(2 5 5/10 9 9) = $-\frac{1}{2}$	†(3 8 11/7 9 10) = $+\frac{1}{2}$	(3 8 11/7 8 11) = $+\frac{1}{2}$
(2 5 5/10 11 11) = $-\frac{1}{2}$	(2 5 5/11 10 10) = $-\frac{1}{2}$	(3 9 10/4 9 10) = $+\frac{1}{2}$	(3 9 10/3 9 10) = $-\frac{1}{2}$
(2 5 5/11 11 11) = $+\frac{1}{2}$	(2 6 6/2 6 6) = $+\frac{1}{2}$	(3 9 10/7 10 9) = $+\frac{1}{2}$	(3 9 10/5 9 10) = $+\frac{1}{2}$
(2 6 6/3 6 6) = $+\frac{1}{2}$	(2 6 6/4 6 6) = $+\frac{1}{2}$	(4 5 7/5 6 6) = $+\frac{1}{2}$	(4 5 7/4 5 7) = $+\frac{1}{2}$
(2 6 6/5 7 7) = $+\frac{1}{2}$	(2 6 6/7 7 7) = $-\frac{1}{2}$	(4 5 7/6 7 5) = $+\frac{1}{2}$	(4 5 7/6 5 7) = $+\frac{1}{2}$
(2 6 6/8 9 9) = $-\frac{1}{2}$	(2 6 6/8 10 10) = $+\frac{1}{2}$	†(4 5 7/8 11 8) = $+\frac{1}{2}$	(4 5 7/7 6 6) = $-\frac{1}{2}$
†(2 6 6/9 8 8) = $+\frac{1}{2}$	(2 6 6/9 11 11) = $-\frac{1}{2}$	(4 5 7/9 9 10) = $+\frac{1}{2}$	†(4 5 7/8 10 9) = $+\frac{1}{2}$
(2 6 6/10 8 8) = $-\frac{1}{2}$	(2 6 6/10 11 11) = $+\frac{1}{2}$	(4 5 7/10 8 11) = $-\frac{1}{2}$	(4 5 7/9 11 8) = $+\frac{1}{2}$
(2 6 6/11 9 9) = $+\frac{1}{2}$	(2 6 6/11 10 10) = $-\frac{1}{2}$	(4 5 7/11 8 11) = $-\frac{1}{2}$	(4 5 7/10 10 9) = $-\frac{1}{2}$
(2 7 7/2 7 7) = $+\frac{1}{2}$	(2 7 7/6 7 7) = $+\frac{1}{2}$	(4 6 6/4 6 6) = $+\frac{1}{2}$	(4 5 7/11 9 10) = $+\frac{1}{2}$
(2 7 7/8 10 10) = $+\frac{1}{2}$	(2 7 7/8 11 11) = $-\frac{1}{2}$	(4 6 6/9 8 11) = $+\frac{1}{2}$	(4 6 6/8 9 10) = $-\frac{1}{2}$
(2 7 7/9 9 9) = $-\frac{1}{2}$	(2 7 7/9 11 11) = $+\frac{1}{2}$	(4 6 6/11 9 10) = $-\frac{1}{2}$	†(4 6 6/10 8 11) = $+\frac{1}{2}$
†(2 7 7/10 8 8) = $+\frac{1}{2}$	(2 7 7/10 10 10) = $-\frac{1}{2}$	(4 8 11/5 10 9) = $+\frac{1}{2}$	(4 8 11/4 8 11) = $-\frac{1}{2}$
(2 7 7/11 8 8) = $-\frac{1}{2}$	(2 7 7/11 9 9) = $+\frac{1}{2}$	(4 8 11/6 9 10) = $+\frac{1}{2}$	(4 8 11/5 11 8) = $-\frac{1}{2}$
(2 8 8/2 8 8) = $-\frac{1}{2}$	(2 8 8/3 11 11) = $+\frac{1}{2}$	(4 8 11/7 8 11) = $+\frac{1}{2}$	(4 8 11/6 10 9) = $+\frac{1}{2}$
(2 8 8/4 11 11) = $+\frac{1}{2}$	(2 8 8/5 8 8) = $+\frac{1}{2}$	(4 9 10/4 9 10) = $-\frac{1}{2}$	(4 8 11/7 9 10) = $-\frac{1}{2}$
†(2 8 8/5 9 9) = $+\frac{1}{2}$	(2 8 8/6 9 9) = $+\frac{1}{2}$	(4 9 10/7 10 9) = $-\frac{1}{2}$	(4 9 10/5 9 10) = $+\frac{1}{2}$
†(2 8 8/6 10 10) = $+\frac{1}{2}$	(2 8 8/7 10 10) = $+\frac{1}{2}$	(5 5 6/5 7 6) = $+\frac{1}{2}$	(5 5 6/5 5 6) = 0
†(2 8 8/7 11 11) = $+\frac{1}{2}$	(2 9 9/2 9 9) = $+\frac{1}{2}$	†(5 5 6/9 8 8) = $+\frac{1}{2}$	(5 5 6/7 7 6) = 0
(2 9 9/3 10 10) = $+\frac{1}{2}$	(2 9 9/4 10 10) = $+\frac{1}{2}$	(5 5 6/11 9 10) = $+\frac{1}{2}$	(5 5 6/10 8 9) = $+\frac{1}{2}$
(2 9 9/5 10 10) = $+\frac{1}{2}$	(2 9 9/6 11 11) = $+\frac{1}{2}$	(5 6 7/5 6 7) = 0	(5 5 6/11 10 11) = $-\frac{1}{2}$
(2 9 9/7 9 9) = $-\frac{1}{2}$	(2 9 9/7 11 11) = $+\frac{1}{2}$	†(5 6 7/8 10 9) = $+\frac{1}{2}$	(5 6 7/7 6 7) = $+\frac{1}{2}$
(2 10 10/2 10 10) = $+\frac{1}{2}$	(2 10 10/7 10 10) = $+\frac{1}{2}$	(5 6 7/9 9 8) = $-\frac{1}{2}$	(5 6 7/8 11 10) = $-\frac{1}{2}$
(2 10 10/6 11 11) = $+\frac{1}{2}$	(2 10 10/5 11 11) = $+\frac{1}{2}$	(5 6 7/10 8 8) = $+\frac{1}{2}$	(5 6 7/9 11 11) = $-\frac{1}{2}$
(2 11 11/5 11 11) = $+\frac{1}{2}$	(2 11 11/2 11 11) = $-\frac{1}{2}$	(5 6 7/11 8 9) = $-\frac{1}{2}$	(5 6 7/10 10 11) = $-\frac{1}{2}$
(3 5 7/4 5 7) = $-\frac{1}{2}$	(3 5 7/3 5 7) = $+\frac{1}{2}$	(5 8 8/5 8 8) = 0	(5 6 7/11 9 10) = $+\frac{1}{2}$
(3 5 7/6 5 7) = $+\frac{1}{2}$	(3 5 7/5 6 6) = $+\frac{1}{2}$	†(5 8 8/6 9 10) = $+\frac{1}{2}$	(5 8 8/5 8 9) = $-\frac{1}{2}$
(3 5 7/7 6 6) = $+\frac{1}{2}$	(3 5 7/6 7 5) = $-\frac{1}{2}$	(5 8 8/7 11 11) = 0	†(5 8 8/7 10 11) = $+\frac{1}{2}$
(3 5 7/8 11 8) = $+\frac{1}{2}$	(3 5 7/8 10 9) = $-\frac{1}{2}$	(5 8 9/5 10 9) = $-\frac{1}{2}$	(5 8 9/5 8 9) = 0

Table 5. (continued).

(5 8 9/6 11 10) = $-\frac{1}{2}$	(5 8 9/6 8 9) = $+\frac{1}{2}$	†(6 8 9/7 9 11) = $+\frac{1}{2}$	(6 8 9/6 11 10) = 0
(5 8 9/7 11 10) = 0	†(5 8 9/7 9 10) = $+\frac{1}{2}$	(6 8 10/6 8 10) = 0	(6 8 9/7 11 10) = $+\frac{1}{2}$
(5 9 10/5 9 10) = 0	†(5 8 9/7 11 11) = $+\frac{1}{2}$	(6 8 10/7 8 10) = $+\frac{1}{2}$	(6 8 10/6 11 10) = $-\frac{1}{2}$
(5 9 10/6 11 11) = $-\frac{1}{2}$	(5 9 10/5 11 10) = $-\frac{1}{2}$	(6 9 11/6 9 11) = 0	(6 8 10/7 10 11) = $+\frac{1}{2}$
(5 9 10/7 10 11) = $+\frac{1}{2}$	(5 9 10/7 10 9) = 0	(6 9 11/7 9 11) = $+\frac{1}{2}$	(6 9 11/6 10 11) = $-\frac{1}{2}$
(5 10 11/5 11 11) = $-\frac{1}{2}$	(5 10 11/5 10 11) = 0	(7 8 10/7 8 10) = 0	(6 10 11/6 10 11) = 0
(5 11 11/5 11 11) = 0	(5 10 11/6 10 11) = $+\frac{1}{2}$	(7 8 10/7 10 10) = $-\frac{1}{2}$	(7 8 10/7 8 11) = $-\frac{1}{2}$
†(6 7 7/8 10 11) = $+\frac{1}{2}$	(6 7 7/6 7 7) = 0	(7 8 11/7 9 11) = $-\frac{1}{2}$	(7 8 11/7 8 11) = 0
†(6 7 7/10 8 10) = $+\frac{1}{2}$	(6 7 7/9 9 11) = $-\frac{1}{2}$	(7 9 9/7 9 11) = $-\frac{1}{2}$	(7 9 9/7 9 9) = 0
(6 8 9/6 8 9) = 0	†(6 7 7/11 8 9) = $+\frac{1}{2}$	(7 10 10/7 10 10) = 0	(7 9 11/7 9 11) = 0
(6 8 9/6 11 9) = $-\frac{1}{2}$	(6 8 9/6 8 10) = $-\frac{1}{2}$		

† These $6j$ symbols are fundamentals

$$(ijk/qrs)_{r_1r_2r_3r_4} = \begin{Bmatrix} \Gamma_i & \Gamma_j & \Gamma_k \\ \Gamma_q & \Gamma_r & \Gamma_s \end{Bmatrix}_{r_1r_2r_3r_4}.$$

For the group under consideration the Kronecker multiplicities are 1 and hence r_1, r_2, r_3, and r_4 are suppressed. The same notation is adapted in table 6.

Table 6. Non-trivial inequivalent $6j$ symbols for the group D_4.

(2 3 4/2 3 4) = +1	(2 3 4/5 5 5) = $+2^{-1/2}$
†(2 3 4/6 7 7) = $+2^{-1/2}$	(2 3 4/7 6 6) = $-2^{-1/2}$
(2 5 5/2 5 5) = $+\frac{1}{2}$	(2 5 5/3 5 5) = $+\frac{1}{2}$
(2 5 5/4 5 5) = $+\frac{1}{2}$	†(2 5 5/6 6 6) = $+\frac{1}{2}$
(2 5 5/6 7 7) = $-\frac{1}{2}$	(2 5 5/7 6 6) = $-\frac{1}{2}$
(2 5 5/7 7 7) = $+\frac{1}{2}$	(2 6 6/2 6 6) = $-\frac{1}{2}$
(2 6 6/3 7 7) = $+\frac{1}{2}$	(2 6 6/4 7 7) = $+\frac{1}{2}$
(2 6 6/5 6 6) = $+\frac{1}{2}$	†(2 6 6/5 7 7) = $+\frac{1}{2}$
(2 7 7/2 7 7) = $-\frac{1}{2}$	(2 7 7/5 7 7) = $+\frac{1}{2}$
(3 5 5/3 5 5) = $+\frac{1}{2}$	(3 5 5/4 5 5) = $-\frac{1}{2}$
†(3 5 5/6 6 7) = $+\frac{1}{2}$	(3 5 5/7 6 7) = $+\frac{1}{2}$
(3 6 7/3 6 7) = $-\frac{1}{2}$	(3 6 7/4 6 7) = $+\frac{1}{2}$
(3 6 7/5 6 7) = $+\frac{1}{2}$	†(3 6 7/5 7 6) = $+\frac{1}{2}$
(4 5 5/4 5 5) = $+\frac{1}{2}$	†(4 5 5/6 6 7) = $+\frac{1}{2}$
(4 5 5/7 6 7) = $-\frac{1}{2}$	(4 6 7/4 6 7) = $-\frac{1}{2}$
(4 6 7/5 6 7) = $+\frac{1}{2}$	(4 6 7/5 7 6) = $-\frac{1}{2}$
(5 6 6/5 6 6) = 0	(5 6 6/5 6 7) = $-\frac{1}{2}$
(5 6 6/5 7 7) = 0	(5 6 7/5 6 7) = 0
(5 6 7/5 7 7) = $-\frac{1}{2}$	(5 7 7/5 7 7) = 0

The trivial $3jm$ factors follow immediately (Butler and Wybourne 1976a, equation (29)) from the equation

$$\begin{pmatrix} \lambda & \lambda^* & 1 \\ a\sigma & a'\sigma' & 1 \end{pmatrix} = \langle 1|\lambda a\sigma; \lambda^* a'\sigma'\rangle = |\lambda|^{-1/2}|\sigma|^{1/2}(\lambda)_{a\sigma,a'\sigma'}.$$

The magnitudes of the primitive $3jm$ factors are obtained using the orthogonality relations (equations (35) and (36) of Butler and Wybourne 1976a). Choosing the relative phases from the orthogonality relations and systematically increasing the power of the largest irrep, we obtain nine independent and two dependent primitive $3jm$ factors of $D_{4d} \supset D_4$. The non-trivial non-primitive inequivalent $3jm$ factors for $D_{4d} \supset$

D_4 are calculated recursively using equation (41) of Butler and Wybourne (1976a), $3jm$ primitives of $D_{4d} \supset D_4$, and primitive $6j$ symbols of D_{4d}. The complete set of non-trivial inequivalent $3jm$ factors of $D_{4d} \supset D_4$ is listed in table 7.

Table 7. Non-trivial inequivalent $3jm$ factors for $D_{4d} \supset D_4$.

$(2\,3\,4/2\,1\,2) = +1$	$(2\,5\,5/2\,5\,5) = +1$
$(2\,6\,6/2\,3\,4) = -2^{-1/2}$	$(2\,7\,7/2\,5\,5) = -1$
$(2\,8\,8/2\,6\,6) = +1$	$(2\,9\,9/2\,7\,7) = +1$
$(2\,10\,10)/2\,7\,7) = +1$	$(2\,11\,11/2\,6\,6) = +1$
$(3\,5\,7/1\,5\,5) = +1$	$(3\,6\,6/1\,3\,3) = -2^{-1/2}$
$(3\,6\,6/1\,4\,4) = +2^{-1/2}$	$(3\,8\,11/1\,6\,6) = +1$
$(3\,9\,10/1\,7\,7) = -1$	$(4\,5\,7/2\,5\,5) = -1$
$(4\,6\,6/2\,3\,4) = +2^{-1/2}$	$(4\,8\,11/2\,6\,6) = +1$
$(4\,9\,10/2\,7\,7) = -1$	$(5\,5\,6/5\,5\,3) = +2^{-1/2}$
$(5\,5\,6/5\,5\,4) = +2^{-1/2}$	$(5\,6\,7/5\,3\,5) = +2^{-1/2}$
$(5\,6\,7/5\,4\,5) = -2^{-1/2}$	$(5\,8\,8/5\,6\,6) = +1$
$(5\,8\,9/5\,6\,7) = +1$	$(5\,9\,10/5\,7\,7) = +1$
$(5\,10\,11/5\,7\,6) = -1$	$(5\,11\,11/5\,6\,6) = +1$
$(6\,7\,7/3\,5\,5) = -2^{-1/2}$	$(6\,7\,7/4\,5\,5) = -2^{-1/2}$
$(6\,8\,9/3\,6\,7) = +2^{-1/2}$	$(6\,8\,9/4\,6\,7) = +2^{-1/2}$
$(6\,8\,10/3\,6\,7) = +2^{-1/2}$	$(6\,8\,10/4\,6\,7) = -2^{-1/2}$
$(6\,9\,11/3\,7\,6) = -2^{-1/2}$	$(6\,9\,11/4\,7\,6) = +2^{-1/2}$
$(6\,10\,11/3\,7\,6) = -2^{-1/2}$	$(6\,10\,11/4\,7\,6) = -2^{-1/2}$
$(7\,8\,10/5\,6\,7) = +1$	$(7\,8\,11/5\,6\,6) = +1$
$(7\,9\,9/5\,7\,7) = -1$	$(7\,9\,11/5\,7\,6) = -1$
$(7\,10\,10/5\,7\,7) = -1$	

Note that

$$(ijk/(a)l(b)m(c)n)^r_s = \begin{pmatrix} \Gamma_i & \Gamma_j & \Gamma_k \\ (a)\gamma_l & (b)\gamma_m & (c)\gamma_n \end{pmatrix}^r_s$$

where a, b and c are the branching multiplicities of γ_l, γ_m and γ_n. The group under consideration is branching multiplicity free and hence a, b and c are suppressed. The same notation is adapted in table 8.

4. $3jm$ factors for $D_4 \supset C_4$

The branching rules for $D_4 \to C_4$ are given in table 4. Choosing

$$(\Gamma_1)_{\gamma_1\gamma_1} = (\Gamma_3)_{\gamma_2\gamma_2} = (\Gamma_5)_{\gamma_3\gamma_4} = (\Gamma_6)_{\gamma_5\gamma_6} = (\Gamma_7)_{\gamma_7\gamma_8} = +1$$

and

$$(\Gamma_2)_{\gamma_1\gamma_1} = (\Gamma_4)_{\gamma_2\gamma_2} = -1,$$

equation (31) of Butler and Wybourne (1976a) gives

$$(\Gamma_5)_{\gamma_4\gamma_3} = +1, \qquad (\Gamma_6)_{\gamma_6\gamma_5} = (\Gamma_7)_{\gamma_8\gamma_7} = -1,$$

where we have used the $2j$ symbols of the groups D_4 and C_4. For Abelian groups all irreps are orthogonal or quasi-orthogonal (Butler and Wybourne 1976a), giving $\phi_{\gamma_k} = +1$. Here Γ refers to irreps of D_4 and γ refers to irreps of C_4. Certain $2jm$ factors are chosen to be -1 to make all the $3jm$ factors real. Proceeding as in § 3 we obtain four independent and one dependent $3jm$ primitives. The $6j$ symbols of C_4 may be taken to be $+1$. The complete set of non-trivial inequivalent $3jm$ factors of $D_4 \supset C_4$ is listed in table 8.

Table 8. Non-trivial inequivalent $3jm$ factors for $D_4 \supset C_4$.

$(2\,3\,4/1\,2\,2) = -1$
$(2\,5\,5/1\,3\,4) = +2^{-1/2}$
$(2\,6\,6/1\,5\,6) = +2^{-1/2}$
$(2\,7\,7/1\,7\,8) = +2^{-1/2}$
$(3\,5\,5/2\,3\,3) = +2^{-1/2}$
$(3\,6\,7/2\,5\,8) = +2^{-1/2}$
$(4\,5\,5/2\,3\,3) = +2^{-1/2}$
$(4\,6\,7/2\,5\,8) = +2^{-1/2}$
$(5\,6\,6/3\,6\,6) = +2^{-1/2}$
$(5\,6\,7/3\,5\,7) = +2^{-1/2}$
$(5\,7\,7/3\,8\,8) = +2^{-1/2}$

Acknowledgments

We are grateful to the referees for their constructive suggestions. Our thanks are due to Professor T S G Krishnamurty for his sustained interest in this work. One of the authors (KB) is grateful to the Council of Scientific and Industrial Research, Government of India, for the award of a Junior Research Fellowship.

References

Butler P H 1975 *Trans. R. Soc.* (London) A **277** 545–85
—— 1976 *Int. J. Quantum Chem.* **10** 599–614
Butler P H and King R C 1974 *Can. J. Math.* **26** 328–39
Butler P H and Wybourne B G 1976a *Int. J. Quantum Chem.* **10** 581–98
—— 1976b *Int. J. Quantum Chem.* **10** 615–28
Golding R M 1973 *Molec. Phys.* **26** 661–72
Golding R M and Newmarch J D 1977 *Molec. Phys.* **33** 1301–18
Griffith J S 1962 *The Irreducible Tensor Method for Molecular Symmetry Groups* (Englewood Cliffs, NJ: Prentice–Hall)
Hamermesh M 1962 *Group theory and its applications to physical problems* (Reading, MA: Addison–Wesley) p 142
Harnung S E 1973 *Molec. Phys.* **26** 473–502
Herzberg G 1966 *Molecular Spectra and Molecular Structure, III Electronic Spectra and Electronic Structure of Polyatomic Molecules* (NY: Van Nostrand) pp 566, 572
Koster G F, Dimmock J O, Wheeler R G and Statz H 1963 *Properties of the thirty-two point groups* (Cambridge, MA: MIT Press)
Wybourne B G 1974 *Classical groups for physicists* (NY: Wiley)