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# Coupling coefficients for the space group of the hexagonal close-packed structure

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**Abstract.** Vector-coupling or Clebsch-Gordan coefficients for irreducible representations of the space group $D_{6h}^4$ have been calculated at symmetry points of the hexagonal Brillouin zone. All arms of the wavevector stars and all wavevector selection rules are enumerated.

## 1. Introduction

The space group $D_{6h}^4$ ($P6_3/mmc$) of the hexagonal close-packed (HCP) structure is the symmetry group of metals of the second column of the Periodic Table and of graphite (Olbrychski and Gorzkowski 1972). Ice $I_h$ also crystallises in the HCP structure (*Landolt-Börnstein* 1975). It exists over a wide range of temperatures (from about −130 to 0 °C) and over a range of pressures (from 0 to about 2 kbar (Eisenberg and Kauzmann 1969)) and has been studied by several methods (Eisenberg and Kauzmann 1969, *Landolt-Börnstein* 1975). More recently, high-resolution neutron diffraction studies of ice $I_h$ have been performed by Kuhs and Lehmann (1983).

Here we want to give the Clebsch-Gordan coefficients (CGCS) for the irreducible representations of the space group of the HCPS structure.

Birman and Berenson (1974) have shown that the elements of the first-order scattering tensor are precisely CGCS multiplied by certain constants and the elements of the second-order tensor are bilinear sums of CGCS. The matrix elements of the effective Hamiltonian are also products of appropriate CGCS and symmetrised tensorial field quantities (Birman *et al* 1976).

Recently Kotzev and Aroyo (1982) have calculated CGCS for Shubnikov magnetic point groups of the hexagonal structure and Benbow (1980) has published tables of the optical dipole selection rules for Bloch states on the HCP lattice.

The irreducible representations of the space group $D_{6h}^4$ and the selection rules for their products are given by Cracknell *et al* (1979). Leading wavevector selection rules are constructed with the aid of table 5 of Davies and Cracknell (1976) and are the same as those given by Cracknell *et al* (1979).

## 2. Vector-coupling coefficients for the space group

For the irreducible space-group representation $\boldsymbol{k}l$ contained in the direct product of the irreducible representations $\boldsymbol{k}'l'$ and $\boldsymbol{k}''l''$ with wavevectors satisfying the wavevector

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selection rule

$$\varphi_{\sigma'}\boldsymbol{k}' + \varphi_{\sigma''}\boldsymbol{k}'' = \varphi_{\sigma}\boldsymbol{k} \tag{1}$$

the basis functions $\psi^{kl\gamma}_{\sigma\alpha}$ are linear combinations of the basis function products $\psi^{k'l'}_{\sigma'\alpha'}\Phi^{k''l''}_{\sigma''\alpha''}$ with the vector-coupling of Clebsch–Gordan coefficients

$$\psi^{kl\gamma}_{\sigma\alpha} = \sum_{\sigma'\alpha'}\sum_{\sigma''\alpha''}\begin{pmatrix} k'l' & k''l'' & \Big| & kl\gamma \\ \sigma'\alpha' & \sigma''\alpha'' & \Big| & \sigma\alpha \end{pmatrix}\psi^{k'l'}_{\sigma'\alpha'}\Phi^{k''l''}_{\sigma''\alpha''}. \tag{2}$$

Methods of calculation of CGCs have been given by Gard (1973), Sakata (1974), Birman (1974), Berenson and Birman (1975), Berenson *et al* (1975), van den Broek and Cornwell (1978), van den Broek (1979), Dirl (1979), Kunert and Suffczyński (1980), Suffczyński and Kunert (1982) and Kunert (1983). Here we use the method of Berenson and Birman (1975) because in our case the multiplicity index is equal to one.

To compute the CGC

$$\begin{pmatrix} k'l' & k''l'' & \Big| & kl\gamma \\ \sigma'\alpha' & \sigma''\alpha'' & \Big| & \sigma\alpha \end{pmatrix} = U_{\sigma'\alpha'\sigma''\alpha''\sigma\alpha} \tag{3}$$

we decompose the space group G into cosets with respect to the wavevector group, $G(\boldsymbol{k}')$, $G(\boldsymbol{k}'')$ and $G(\boldsymbol{k})$ (see table 2) and we find the coset representatives

$$\{\varphi_{\sigma'}|\boldsymbol{\tau}_{\sigma'}\} \qquad \{\varphi_{\sigma''}|\boldsymbol{\tau}_{\sigma''}\} \qquad \{\varphi_{\sigma}|\boldsymbol{\tau}_{\sigma}\} \tag{4}$$

and the wavevector stars (see tables 1 and 3). Starting from the leading wavevector selection rules

$$\varphi_{\lambda'}\boldsymbol{k}' + \varphi_{\lambda''}\boldsymbol{k}'' = \boldsymbol{k} \tag{5}$$

we construct all wavevector selection rules (1) (see table 4). The principal ($\sigma' = \lambda'$,

**Table 1.** Coordinates of the wavevector stars at the symmetry points of the hexagonal Brillouin zone. $a_L$ and $c_L$ are the hexagonal lattice constants.

| | | |
|---|---|---|
| $\boldsymbol{k}_\Gamma = [0, 0, 0]\pi$ | | |
| $\boldsymbol{k}_A = [0, 0, 1/2c_L]\pi$ | | |
| $\boldsymbol{k}_H = [1/3a_L, 1/3a_L, 1/2c_L]\pi$ | $2\boldsymbol{k}_H = [-1/3a_L, 2/3a_L, 1/2c_L]\pi$ | |
| $\boldsymbol{k}_K = [1/3a_L, 1/3a_L, 0]\pi$ | $2\boldsymbol{k}_K = [-1/3a_L, 2/3a_L, 0]\pi$ | |
| $\boldsymbol{k}_L = [1/2a_L, 0, 1/2c_L]\pi$ | $2\boldsymbol{k}_L = [0, 1/2a_L, 1/2c_L]\pi$ | $3\boldsymbol{k}_L = [-1/2a_L, 1/2a_L, 1/2c_L]\pi$ |
| $\boldsymbol{k}_M = [1/2a_L, 0, 0]\pi$ | $2\boldsymbol{k}_M = [0, 1/2a_L, 1/2c_L]\pi$ | $3\boldsymbol{k}_M = [-1/2a_L, 1/2a_L, 1/2c_L]\pi$ |

**Table 2.** Decompositions of the space group $D^4_{6h}$ into cosets with respect to the wavevector groups $G(\boldsymbol{k}_\Gamma)$, $G(\boldsymbol{k}_A)$, $G(\boldsymbol{k}_H)$, $G(\boldsymbol{k}_K)$, $G(\boldsymbol{k}_L)$ and $G(\boldsymbol{k}_M)$. $\boldsymbol{\tau} = (0, 0, \frac{1}{2})c_L$.

$G = G(\boldsymbol{k}_\Gamma)$
$G = G(\boldsymbol{k}_A)$
$G = G(\boldsymbol{k}_H) + \{2|\boldsymbol{\tau}\}G(\boldsymbol{k}_H)$
$G = G(\boldsymbol{k}_K) + \{2|\boldsymbol{\tau}\}G(\boldsymbol{k}_K)$
$G = G(\boldsymbol{k}_L) + \{2|\boldsymbol{\tau}\}G(\boldsymbol{k}_L) + \{3|\boldsymbol{0}\}G(\boldsymbol{k}_L)$
$G = G(\boldsymbol{k}_M) + \{2|\boldsymbol{\tau}\}G(\boldsymbol{k}_M) + \{3|\boldsymbol{0}\}G(\boldsymbol{k}_M)$

**Table 3.** Coset representatives $\{\varphi_\sigma | \tau_\sigma\}$ and stars of the wavevectors.

| | $\sigma=1$ $\{1\|0\}$ | $\sigma=2$ $\{2\|\boldsymbol{\tau}\}$ | $\sigma=1$ $\{1\|0\}$ | $\sigma=2$ $\{2\|\boldsymbol{\tau}\}$ | $\sigma=1$ $\{1\|0\}$ | $\sigma=2$ $\{2\|\boldsymbol{\tau}\}$ |
|---|---|---|---|---|---|---|
| $\boldsymbol{k}'$ | $\boldsymbol{k}_H, \boldsymbol{k}_K$ | $2\boldsymbol{k}_H, 2\boldsymbol{k}_K$ | $\boldsymbol{k}_H, \boldsymbol{k}_K$ | $2\boldsymbol{k}_H, 2\boldsymbol{k}_K$ | $2\boldsymbol{k}_H, 2\boldsymbol{k}_K$ | $\boldsymbol{k}_H, \boldsymbol{k}_K$ |
| $\boldsymbol{k}''$ | $\boldsymbol{k}_H, \boldsymbol{k}_K$ | $2\boldsymbol{k}_H, 2\boldsymbol{k}_K$ | $2\boldsymbol{k}_H, 2\boldsymbol{k}_K$ | $\boldsymbol{k}_H, \boldsymbol{k}_K$ | $2\boldsymbol{k}_H, 2\boldsymbol{k}_K$ | $\boldsymbol{k}_H, \boldsymbol{k}_K$ |
| $\boldsymbol{k}$ | $\boldsymbol{k}_\Gamma$ | | $\boldsymbol{k}_\Gamma$ | | | |
| $\boldsymbol{k}$ | $\boldsymbol{k}_K$ | $2\boldsymbol{k}_K$ | | | $\boldsymbol{k}_K$ | $2\boldsymbol{k}_K$ |
| | $\sigma=1$ $\{1\|0\}$ | $\sigma=2$ $\{2\|\boldsymbol{\tau}\}$ | $\sigma=3$ $\{3\|0\}$ | $\sigma=1$ $\{1\|0\}$ | $\sigma=2$ $\{2\|\boldsymbol{\tau}\}$ | $\sigma=3$ $\{3\|0\}$ |
| $\boldsymbol{k}'$ | $\boldsymbol{k}_L, \boldsymbol{k}_M$ | $2\boldsymbol{k}_L, 2\boldsymbol{k}_M$ | $3\boldsymbol{k}_L, 3\boldsymbol{k}_M$ | $2\boldsymbol{k}_L, 2\boldsymbol{k}_M$ | $3\boldsymbol{k}_L, 3\boldsymbol{k}_M$ | $\boldsymbol{k}_L, \boldsymbol{k}_M$ |
| $\boldsymbol{k}''$ | $\boldsymbol{k}_L, \boldsymbol{k}_M$ | $2\boldsymbol{k}_L, 2\boldsymbol{k}_M$ | $3\boldsymbol{k}_L, 3\boldsymbol{k}_M$ | $3\boldsymbol{k}_L, 3\boldsymbol{k}_M$ | $\boldsymbol{k}_L, \boldsymbol{k}_M$ | $2\boldsymbol{k}_L, 2\boldsymbol{k}_M$ |
| $\boldsymbol{k}$ | $\boldsymbol{k}_\Gamma$ | | | | | |
| $\boldsymbol{k}$ | $\boldsymbol{k}_M$ | $2\boldsymbol{k}_M$ | $3\boldsymbol{k}_M$ | $\boldsymbol{k}_M$ | $2\boldsymbol{k}_M$ | $3\boldsymbol{k}_M$ |

**Table 4.** Wavevector selection rules, blocks and symmetry operations $\{\varphi_\Sigma | \boldsymbol{\tau}_\Sigma\}$ for calculating CGCs in $D_{6h}^4$. $N = (1, \{4|\boldsymbol{\tau}\}, 13, \{16|\boldsymbol{\tau}\})$; $\boldsymbol{\tau} = (0, 0, \frac{1}{2})c_L$.

| | | $\boldsymbol{k}'+\boldsymbol{k}''=\boldsymbol{k}$ | | $\boldsymbol{k}'+\boldsymbol{k}''=\boldsymbol{k}$ | $\sigma'$ | $\sigma''$ | $\sigma$ | | $\sigma'$ | $\sigma''$ | $\sigma$ | $\{\varphi_\Sigma \| \boldsymbol{\tau}_\Sigma\}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| LWVSR | $G(\boldsymbol{k}_\Gamma)$ | $\boldsymbol{k}_\Gamma+\boldsymbol{k}_\Gamma=\boldsymbol{k}_\Gamma$ | $G(\boldsymbol{k}_A)$ | $\boldsymbol{k}_A+\boldsymbol{k}_A=\boldsymbol{k}_\Gamma$ | 1 | 1 | 1 | | | | | $\{1\|0\}$ |
| LWVSR | | $\boldsymbol{k}_H+2\boldsymbol{k}_H=\boldsymbol{k}_\Gamma$ | | $\boldsymbol{k}_K+2\boldsymbol{k}_K=\boldsymbol{k}_\Gamma$ | 1 | 2 | 1 | Γ | 1 | 1 | 1 | $\{1\|0\}$ |
| | $G(\boldsymbol{k}_H)$ | $2\boldsymbol{k}_H+\boldsymbol{k}_H=\boldsymbol{k}_\Gamma$ | $G(\boldsymbol{k}_K)$ | $2\boldsymbol{k}_K+\boldsymbol{k}_K=\boldsymbol{k}_\Gamma$ | 2 | 1 | 1 | | 2 | 2 | 1 | $\{2\|\boldsymbol{\tau}\}$ |
| LWVSR | | $2\boldsymbol{k}_H+2\boldsymbol{k}_H=\boldsymbol{k}_K$ | | $2\boldsymbol{k}_K+2\boldsymbol{k}_K=\boldsymbol{k}_K$ | 2 | 2 | 1 | K | 1 | 1 | 1 | $\{1\|0\}$ |
| | $G(\boldsymbol{k}_H)$ | $\boldsymbol{k}_H+\boldsymbol{k}_H=2\boldsymbol{k}_K$ | $G(\boldsymbol{k}_K)$ | $\boldsymbol{k}_K+\boldsymbol{k}_K=2\boldsymbol{k}_K$ | 1 | 1 | 2 | | 2 | 2 | 2 | $\{2\|\boldsymbol{\tau}\}$ |
| LWVSR | | $\boldsymbol{k}_L+\boldsymbol{k}_L=\boldsymbol{k}_\Gamma$ | | $\boldsymbol{k}_M+\boldsymbol{k}_M=\boldsymbol{k}_\Gamma$ | 1 | 1 | 1 | | | | | $\{1\|0\}$ |
| | | $2\boldsymbol{k}_L+2\boldsymbol{k}_L=\boldsymbol{k}_\Gamma$ | | $2\boldsymbol{k}_M+2\boldsymbol{k}_M=\boldsymbol{k}_\Gamma$ | 2 | 2 | 1 | | | | | $\{2\|\boldsymbol{\tau}\}$ |
| | $G(\boldsymbol{k}_L)$ | $3\boldsymbol{k}_L+3\boldsymbol{k}_L=\boldsymbol{k}_\Gamma$ | $G(\boldsymbol{k}_M)$ | $3\boldsymbol{k}_M+3\boldsymbol{k}_M=\boldsymbol{k}_\Gamma$ | 3 | 3 | 1 | | | | | $\{3\|0\}$ |
| LWVSR | | $2\boldsymbol{k}_L+3\boldsymbol{k}_L=\boldsymbol{k}_M$ | | $2\boldsymbol{k}_M+3\boldsymbol{k}_M=\boldsymbol{k}_M$ | 2 | 3 | 1 | M | 1 | 1 | 1 | $\{1\|0\}$ |
| | | $2\boldsymbol{k}_L+\boldsymbol{k}_L=3\boldsymbol{k}_M$ | | $2\boldsymbol{k}_M+\boldsymbol{k}_M=3\boldsymbol{k}_M$ | 2 | 1 | 3 | | 1 | 2 | 3 | $\{7\|0\}$ |
| | | $3\boldsymbol{k}_L+2\boldsymbol{k}_L=\boldsymbol{k}_M$ | | $3\boldsymbol{k}_M+2\boldsymbol{k}_M=\boldsymbol{k}_M$ | 3 | 2 | 1 | | 2 | 3 | 1 | $\{8\|\boldsymbol{\tau}\}$ |
| | | $3\boldsymbol{k}_L+\boldsymbol{k}_L=2\boldsymbol{k}_M$ | | $3\boldsymbol{k}_M+\boldsymbol{k}_M=2\boldsymbol{k}_M$ | 3 | 1 | 2 | | 2 | 2 | 2 | $\{2\|\boldsymbol{\tau}\}$ |
| | | $\boldsymbol{k}_L+3\boldsymbol{k}_L=2\boldsymbol{k}_M$ | | $\boldsymbol{k}_M+3\boldsymbol{k}_M=2\boldsymbol{k}_M$ | 1 | 3 | 2 | | 3 | 1 | 2 | $\{9\|0\}$ |
| | N | $\boldsymbol{k}_L+2\boldsymbol{k}_L=3\boldsymbol{k}_M$ | N | $\boldsymbol{k}_L+2\boldsymbol{k}_L=3\boldsymbol{k}_M$ | 1 | 2 | 3 | | 3 | 3 | 3 | $\{3\|0\}$ |

$\sigma''=\lambda''$ and $\sigma=1$) block of CGCs is computed from the small representations $d^{k'l'}$, $d^{k''l''}$ and $d^{kl}$:

$$U_{\lambda' a' \lambda'' a'' 1 a} = \left\{\frac{\dim(l)}{|\bar{G}(\boldsymbol{k})|}\right\}^{1/2} \left(\sum_S d^{\varphi_{\lambda'} k'l'}(S)_{b'b'} d^{\varphi_{\lambda''} k''l''}(S)_{b''b''} d^{kl}(S)^*_{bb}\right)^{-1/2}$$
$$\times \sum_S d^{\varphi_{\lambda'} k'l'}(S)_{a'b'} d^{\varphi_{\lambda''} k''l''}(S)_{a''b''} d^{kl}(S)^*_{ab} \tag{6}$$

by performing summations over the intersection of the three wavevector groups

$$S = \{\varphi_S | \boldsymbol{\tau}_S\} \in N = G(\varphi_{\lambda'}\boldsymbol{k}') \wedge G(\varphi_{\lambda''}\boldsymbol{k}'') \wedge G(\boldsymbol{k}). \tag{7}$$

$|\bar{G}(\boldsymbol{k})|$ is the order of the point group of $G(\boldsymbol{k})$ and $\dim(l)$ is the dimension of the small irreducible representation $d^{kl}$. The indices $b'$, $b''$, $b$ in equation (6) have to be chosen such that the sum with diagonal indices has a non-vanishing value. For each

**Table 5.** CGCs for $\Gamma_n \otimes \Gamma_n$ $(n = 5\pm, 6\pm)$ in $D_{6h}^4$.

| $\Gamma_n \otimes \Gamma_n =$ | | $[\Gamma_{1+}$ | $+\Gamma_{5+}$ | $]$ | $+\Gamma_{2+}$ |
|---|---|---|---|---|---|
| $\alpha$ | $\alpha''$ | $\alpha = 1$ | 1 | 2 | 1 |
| 1 | 1 | 0 | 0 | 1 | 0 |
| 1 | 2 | 1 | 0 | 0 | 1 |
| 2 | 1 | 1 | 0 | 0 | −1 |
| 2 | 2 | 0 | 1 | 0 | 0 |
| | | $\sqrt{2}$ | 1 | | $\sqrt{2}$ |

**Table 6.** CGCs for $A_j \otimes A_j$ $(j = 1, 2)$ in $D_{6h}^4$.

| $A_j \otimes A_j =$ | | $[\Gamma_{1+}$ | $+\Gamma_{3+}$ | $+\Gamma_{4-}]$ | $+\Gamma_{2-}$ |
|---|---|---|---|---|---|
| $\alpha'$ | $\alpha''$ | $\alpha = 1$ | 1 | 1 | 1 |
| 1 | 1 | 0 | 1 | 1 | 0 |
| 1 | 2 | 1 | 0 | 0 | 1 |
| 2 | 1 | 1 | 0 | 0 | −1 |
| 2 | 2 | 0 | 1 | −1 | 0 |
| | | $\sqrt{2}$ | $\sqrt{2}$ | $\sqrt{2}$ | $\sqrt{2}$ |

**Table 7.** CGCs for $A_3 \otimes A_3$ in $D_{6h}^4$.

| $A_3 \otimes A_3 =$ | | $[\Gamma_{1\mp} +$ | $\Gamma_{3+}$ | $+\Gamma_{4-}$ | $+\Gamma_{5+}$ | | $+\Gamma_{6\pm}$ | $]$ | $+\Gamma_{2\mp}$ | $+\Gamma_{3-}$ | $+\Gamma_{4+}$ | $+\Gamma_{5-}$ | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $\alpha'$ | $\alpha''$ | $\alpha = 1$ | 1 | 1 | 1 | 2 | 1 | 2 | 1 | 1 | 1 | 1 | 2 |
| 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 |
| 1 | 2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 |
| 1 | 3 | 0 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 0 | 0 |
| 1 | 4 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 1 |
| 2 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | −1 | 0 | 0 | 0 | 0 |
| 2 | 2 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 2 | 3 | 0 | 0 | 0 | −1 | 0 | 0 | 0 | 0 | 0 | 0 | −1 | 0 |
| 2 | 4 | 0 | −1 | 1 | 0 | 0 | 0 | 0 | 0 | −1 | 1 | 0 | 0 |
| 3 | 1 | 0 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | −1 | −1 | 0 | 0 |
| 3 | 2 | 0 | 0 | 0 | −1 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 |
| 3 | 3 | 0 | 0 | 0 | 0 | 0 | ∓1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | 4 | ±1 | 0 | 0 | 0 | 0 | 0 | 0 | ∓1 | 0 | 0 | 0 | 0 |
| 4 | 1 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | −1 |
| 4 | 2 | 0 | −1 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | −1 | 0 | 0 |
| 4 | 3 | ±1 | 0 | 0 | 0 | 0 | 0 | 0 | ±1 | 0 | 0 | 0 | 0 |
| 4 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | ∓1 | 0 | 0 | 0 | 0 | 0 |
| | | 2 | 2 | 2 | $\sqrt{2}$ | | $\sqrt{2}$ | | 2 | 2 | 2 | $\sqrt{2}$ | |

wavevector selection rule of equation (1) we compute one symmetry operation $\{\varphi_\Sigma | \boldsymbol{\tau}_\Sigma\}$ which rotates the principal block into the $\sigma'\sigma''\sigma$ block:

$$\varphi_\Sigma \varphi_{\lambda'} \boldsymbol{k}' = \boldsymbol{k}'_{\sigma'} \qquad \varphi_\Sigma \varphi_{\lambda''} \boldsymbol{k}'' = \boldsymbol{k}''_{\sigma''} \qquad \varphi_\Sigma \boldsymbol{k} = \boldsymbol{k}_{\sigma} \tag{8}$$

The $\sigma'\sigma''\sigma$ block is computed from the principal block by matrix multiplication:

$$\begin{aligned} U_{\sigma'\alpha'\sigma''\alpha''\sigma\alpha} = \sum_{a'=1}^{\dim(l')} \sum_{a''=1}^{\dim(l'')} \sum_{a=1}^{\dim(l)} & d^{\varphi_{\lambda'}\boldsymbol{k}'l'}(\{\varphi_{\lambda'}|\boldsymbol{\tau}_{\lambda'}\}\{\varphi_{\sigma'}|\boldsymbol{\tau}_{\sigma'}\}^{-1}\{\varphi_\Sigma|\boldsymbol{\tau}_\Sigma\})_{\alpha'a'} \\ & \times d^{\varphi_{\lambda''}\boldsymbol{k}''l''}(\{\varphi_{\lambda''}|\boldsymbol{\tau}_{\lambda''}\}\{\varphi_{\sigma''}|\boldsymbol{\tau}_{\sigma''}\}^{-1}\{\varphi_\Sigma|\boldsymbol{\tau}_\Sigma\})_{\alpha''a''} U_{\lambda'a'\lambda''a''1a} \\ & \times d^{\boldsymbol{k}l}(\{\varphi_\sigma|\boldsymbol{\tau}_\sigma\}^{-1}\{\varphi_\Sigma|\boldsymbol{\tau}_\Sigma\})^{-1}_{a\alpha}. \end{aligned} \tag{9}$$

**Table 8.** CGCs for $H_j \otimes H_j$ ($j = 1, 2$) and $K_n \otimes K_n$ ($n = 5, 6$) in $D_{6h}^4$. The channel Γ.

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $H_j \otimes H_j =$ | | | | $[\Gamma_{1+}$ | $+\Gamma_{4-}$ | $+\Gamma_{6+}$ | $]$ | $+\Gamma_{2+}$ | $+\Gamma_{3-}$ | $+\Gamma_{5-}$ | |
| $K_n \otimes K_n =$ | | | | $\Gamma_{2+}$ | $+\Gamma_{3-}$ | $+\Gamma_{6-}$ | | $+[\Gamma_{1+}$ | $+\Gamma_{4-}$ | $+\Gamma_{5+}$ | $]$ |
| | | | | | | $\sigma = 1$ | | | | | |
| $\sigma'$ | $\sigma''$ | $\alpha'$ | $\alpha''$ | $\alpha = 1$ | 1 | 1 | 2 | 1 | 1 | 1 | 2 |
| 1 | 2 | 1 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 |
| | | 1 | 2 | 1 | 1 | 0 | 0 | 1 | 1 | 0 | 0 |
| | | 2 | 1 | $-\bar{w}$ | $\bar{w}$ | 0 | 0 | $\bar{w}$ | $-\bar{w}$ | 0 | 0 |
| | | 2 | 2 | 0 | 0 | $\mp w$ | 0 | 0 | 0 | $\mp w$ | 0 |
| 2 | 1 | 1 | 1 | 0 | 0 | 0 | $-\bar{w}$ | 0 | 0 | 0 | $\bar{w}$ |
| | | 1 | 2 | 1 | $-1$ | 0 | 0 | 1 | $-1$ | 0 | 0 |
| | | 2 | 1 | $-\bar{w}$ | $-\bar{w}$ | 0 | 0 | $\bar{w}$ | $\bar{w}$ | 0 | 0 |
| | | 2 | 2 | 0 | 0 | $\pm\bar{w}$ | 0 | 0 | 0 | $\mp\bar{w}$ | 0 |
| | | | | 2 | 2 | $\sqrt{2}$ | | 2 | 2 | $\sqrt{2}$ | |

**Table 9.** CGCs for $H_j \otimes H_j$ ($j = 1, 2$) and $K_n \otimes K_n$ ($n = 5, 6$) in $D_{6h}^4$. The channel K.

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $H_j \otimes H_j =$ | | | | $[K_2$ | | $+K_5$ | | | $]$ | $+K_3$ | |
| $K_n \otimes K_n =$ | | | | $[K_1$ | | $+K_5$ | | | $]$ | $+K_4$ | |
| | | | | $\sigma = 1$ | 2 | 1 | 1 | 2 | 2 | 1 | 2 |
| $\sigma'$ | $\sigma''$ | $\alpha'$ | $\alpha''$ | $\alpha = 1$ | 1 | 1 | 2 | 1 | 2 | 1 | 1 |
| 1 | 1 | 1 | 1 | | 0 | | | 0 | 1 | | 0 |
| | | 1 | 2 | | 1 | | | 0 | 0 | | 1 |
| | | 2 | 1 | | 1 | | | 0 | 0 | | $-1$ |
| | | 2 | 2 | | 0 | | | $\bar{w}$ | 0 | | 0 |
| 2 | 2 | 1 | 1 | 0 | | 0 | 1 | | | 0 | |
| | | 1 | 2 | 1 | | 0 | 0 | | | 1 | |
| | | 2 | 1 | 1 | | 0 | 0 | | | $-1$ | |
| | | 2 | 2 | 0 | | $\bar{w}$ | 0 | | | 0 | |
| | | | | $\sqrt{2}$ | | 1 | | | | $\sqrt{2}$ | |

## 3. Description of tables

Tables 1-4 give details which are needed in the calculation of the CGCs. The canonical wavevector, numbering of symmetry operations, labels and generators of the irreducible representations are as given in the tables of Miller and Love (1967). The principal blocks of CGCs have been computed with the aid of the computer program given by Kowalczyk *et al* (1980). The wavevector group intersections are also indicated in table 4. On the right-hand side of table 4 we give a column with an additional description of the blocks such that the block corresponding to the leading wavevector selection rules (LWVSR) in both channels Γ and K or Γ and M has the indices 111 which facilitates the calculation of the other blocks of CGCs. This column is connected with the right-hand sides, after the vertical rules, of table 3.

**Table 10.** CGCs for $H_3 \otimes H_3$in $D_{6h}^4$. The channel Γ.

| $H_3 \otimes H_3 =$ | | | | $[\Gamma_{1+}$ | $+\Gamma_{3+}$ | $+\Gamma_{4\pm}]$ | $+\Gamma_{1-}$ | $+\Gamma_{2\pm}$ | $+\Gamma_{3-}$ |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | $\sigma = 1$ | | | | |
| $\sigma'$ | $\sigma''$ | $\alpha'$ | $\alpha''$ | $\alpha = 1$ | 1 | 1 | 1 | 1 | 1 |
| 1 | 2 | 1 | 1 | 0 | 0 | 1 | 0 | 1 | 0 |
| | | 1 | 2 | 1 | 1 | 0 | 1 | 0 | 1 |
| | | 2 | 1 | −1 | 1 | 0 | 1 | 0 | −1 |
| | | 2 | 2 | 0 | 0 | ±1 | 0 | ∓1 | 0 |
| 2 | 1 | 1 | 1 | 0 | 0 | −1 | 0 | 1 | 0 |
| | | 1 | 2 | 1 | −1 | 0 | 1 | 0 | −1 |
| | | 2 | 1 | −1 | −1 | 0 | 1 | 0 | 1 |
| | | 2 | 2 | 0 | 0 | ∓1 | 0 | ∓1 | 0 |
| | | | | 2 | 2 | 2 | 2 | 2 | 2 |

**Table 11.** CGCs for $H_3 \otimes H_3$ in $D_{6h}^4$. The channel K.

| $H_3 \otimes H_3 =$ | | | | $[K_1$ | | $+K_2$ | | $+K_4$ | $]$ | $+K_3$ | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | $\sigma = 1$ | 2 | 1 | 2 | 1 | 2 | 1 | 2 |
| $\sigma'$ | $\sigma''$ | $\alpha'$ | $\alpha''$ | $\alpha = 1$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 1 | 1 | 1 | 1 | | 1 | | 1 | | 0 | | 0 |
| | | 1 | 2 | | 0 | | 0 | | 1 | | 1 |
| | | 2 | 1 | | 0 | | 0 | | 1 | | −1 |
| | | 2 | 2 | | 1 | | −1 | | 0 | | 0 |
| 2 | 2 | 1 | 1 | 1 | | 1 | | 0 | | 0 | |
| | | 1 | 2 | 0 | | 0 | | 1 | | 1 | |
| | | 2 | 1 | 0 | | 0 | | 1 | | −1 | |
| | | 2 | 2 | 1 | | −1 | | 0 | | 0 | |
| | | | | $\sqrt{2}$ | | $\sqrt{2}$ | | $\sqrt{2}$ | | $\sqrt{2}$ | |

For the one-dimensional representations $\Gamma_m$, $m = 1\pm, 2\pm, 3\pm, 4\pm$, in $D_{6h}^4$, the Clebsch-Gordan matrices for $\Gamma_m \otimes \Gamma_m = \Gamma_{1+}$ are one dimensional with a single element equal to unity.

Tables 5-15 give the CGCs for $\Gamma \otimes \Gamma$, $A \otimes A$, $H \otimes H$, $K \otimes K$, $L \otimes L$ and $M \otimes M$ in $D_{6h}^4$. In these tables we use $w = \exp(\frac{2}{3}i\pi)$ and an overbar denotes complex conjugate. The number at the bottom of each representation column divides each element of that representation column. The entries not written explicitly are zero.

In tables 7, 10, 13 and 14 the upper signs refer to the upper and the lower signs to the lower signs of the representations. In tables 8 and 15 the upper signs refer to the representations indicated by index $j$ and the lower signs refer to the ones indicated by index $n$. In the tables labels of representations that contribute to the symmetrised square are enclosed in square brackets.

**Table 12.** CGCs for $K_j \otimes K_j$ ($j = 1, 2, 3, 4$) in $D_{6h}^4$.

| $K_j \otimes K_j =$ | | | | $[\Gamma_{1+}]$ | $+\Gamma_{3-}$ | $+[K_1$ | $]$ |
|---|---|---|---|---|---|---|---|
| | | | | $\sigma = 1$ | 1 | 1 | 2 |
| $\sigma'$ | $\sigma''$ | $\alpha'$ | $\alpha''$ | $\alpha = 1$ | 1 | 1 | 1 |
| 1 | 1 | 1 | 1 | 0 | 0 | 0 | 1 |
| 1 | 2 | 1 | 1 | 1 | 1 | 0 | 0 |
| 2 | 1 | 1 | 1 | 1 | −1 | 0 | 0 |
| 2 | 2 | 1 | 1 | 0 | 0 | 1 | 0 |
| | | | | $\sqrt{2}$ | $\sqrt{2}$ | 1 | |

**Table 13.** CGCs for $L_j \otimes L_j$ ($j = 1, 2$) in $D_{6h}^4$. The channel $\Gamma$.

| $L_j \otimes L_j =$ | | | | $[\Gamma_{1+}$ | $+\Gamma_{3+}$ | $+\Gamma_{1}$ | $+\Gamma_{5-}$ | | $+\Gamma_{6\pm}$ | $]$ | $+\Gamma_{2-}$ | $+\Gamma_{5-}$ | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | $\sigma = 1$ | | | | | | | | | |
| $\sigma'$ | $\sigma''$ | $\alpha'$ | $\alpha''$ | $\alpha = 1$ | 1 | 1 | 1 | 2 | 1 | 2 | 1 | 1 | 2 |
| 1 | 1 | 1 | 1 | 0 | 1 | 1 | 0 | 0 | 1 | $\pm\bar{w}$ | 0 | 0 | 0 |
| | | 1 | 2 | 1 | 0 | 0 | 1 | $\bar{w}$ | 0 | 0 | 1 | 1 | $-\bar{w}$ |
| | | 2 | 1 | 1 | 0 | 0 | 1 | $\bar{w}$ | 0 | 0 | −1 | −1 | $\bar{w}$ |
| | | 2 | 2 | 0 | 1 | −1 | 0 | 0 | ±1 | $\bar{w}$ | 0 | 0 | 0 |
| 2 | 2 | 1 | 1 | 0 | −1 | −1 | 0 | 0 | $-w$ | $\mp w$ | 0 | 0 | 0 |
| | | 1 | 2 | 1 | 0 | 0 | $w$ | $w$ | 0 | 0 | 1 | $w$ | $-w$ |
| | | 2 | 1 | 1 | 0 | 0 | $w$ | $w$ | 0 | 0 | −1 | $-w$ | $w$ |
| | | 2 | 2 | 0 | −1 | 1 | 0 | 0 | $\mp w$ | $-w$ | 0 | 0 | 0 |
| 3 | 3 | 1 | 1 | 0 | 1 | 1 | 0 | 0 | $\bar{w}$ | ±1 | 0 | 0 | 0 |
| | | 1 | 2 | 1 | 0 | 0 | $\bar{w}$ | 1 | 0 | 0 | 1 | $\bar{w}$ | −1 |
| | | 2 | 1 | 1 | 0 | 0 | $\bar{w}$ | 1 | 0 | 0 | −1 | $-\bar{w}$ | 1 |
| | | 2 | 2 | 0 | 1 | −1 | 0 | 0 | $\pm\bar{w}$ | 1 | 0 | 0 | 0 |
| | | | | $\sqrt{6}$ | $\sqrt{6}$ | $\sqrt{6}$ | $\sqrt{6}$ | | $\sqrt{6}$ | | $\sqrt{6}$ | $\sqrt{6}$ | |

**Table 14.** CGCs for $L_j \otimes L_j (j = 1, 2)$ in $D^4_{6h}$. The channel M.

| $L_j \otimes L_j =$ | | | | $[M_{1\pm}$ | | | $+M_{3+}$ | | | $+M_{4-}$ | | $]$ | $+M_{2+}$ | | | $+M_{3-}$ | | | $+M_{4+}$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | $\sigma = 1$ | 2 | 3 | 1 | 2 | 3 | 1 | 2 | 3 | 1 | 2 | 3 | 1 | 2 | 3 | 1 | 2 | 3 |
| $\sigma'$ | $\sigma''$ | $\alpha'$ | $\alpha''$ | $\alpha = 1$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 1 | 2 | 1 | 1 | | | 0 | | | 1 | | | 1 | | | 0 | | | 1 | | | 1 |
| | | 1 | 2 | | | 1 | | | 0 | | | 0 | | | 1 | | | 0 | | | 0 |
| | | 2 | 1 | | | ∓1 | | | 0 | | | 0 | | | ∓1 | | | 0 | | | 0 |
| | | 2 | 2 | | | 0 | | | −1 | | | 1 | | | 0 | | | 1 | | | −1 |
| 1 | 3 | 1 | 1 | | 0 | | | −1 | | | −1 | | | 0 | | | 1 | | | 1 | |
| | | 1 | 2 | | ±1 | | | 0 | | | 0 | | | ∓1 | | | 0 | | | 0 | |
| | | 2 | 1 | | −1 | | | 0 | | | 0 | | | 1 | | | 0 | | | 0 | |
| | | 2 | 2 | | 0 | | | 1 | | | −1 | | | 0 | | | 1 | | | −1 | |
| 2 | 1 | 1 | 1 | | | 0 | | | −i | | | −i | | | 0 | | | i | | | i |
| | | 1 | 2 | | | ±i | | | 0 | | | 0 | | | ∓i | | | 0 | | | 0 |
| | | 2 | 1 | | | i | | | 0 | | | 0 | | | −i | | | 0 | | | 0 |
| | | 2 | 2 | | | 0 | | | −i | | | i | | | 0 | | | −i | | | i |
| 2 | 3 | 1 | 1 | 0 | | | 1 | | | 1 | | | 0 | | | 1 | | | 1 | | |
| | | 1 | 2 | 1 | | | 0 | | | 0 | | | 1 | | | 0 | | | 0 | | |
| | | 2 | 1 | ∓1 | | | 0 | | | 0 | | | ∓1 | | | 0 | | | 0 | | |
| | | 2 | 2 | 0 | | | −1 | | | 1 | | | 0 | | | 1 | | | −1 | | |
| 3 | 1 | 1 | 1 | | 0 | | | 1 | | | 1 | | | 0 | | | 1 | | | 1 | |
| | | 1 | 2 | | 1 | | | 0 | | | 0 | | | 1 | | | 0 | | | 0 | |
| | | 2 | 1 | | ∓1 | | | 0 | | | 0 | | | ∓1 | | | 0 | | | 0 | |
| | | 2 | 2 | | 0 | | | −1 | | | 1 | | | 0 | | | 1 | | | −1 | |
| 3 | 2 | 1 | 1 | 0 | | | −i | | | −i | | | 0 | | | i | | | i | | |
| | | 1 | 2 | ∓i | | | 0 | | | 0 | | | ±i | | | 0 | | | 0 | | |
| | | 2 | 1 | −i | | | 0 | | | 0 | | | i | | | 0 | | | 0 | | |
| | | 2 | 2 | 0 | | | −i | | | i | | | 0 | | | −i | | | i | | |
| | | | | 2 | | | | 2 | | | 2 | | | 2 | | | 2 | | | 2 | |

**Table 15.** CGCs for $M_j \otimes M_j$ $(j = 1\pm, 2\pm)$ and $M_n \otimes M_n$ $(n = 3\pm, 4\pm)$ in $D^4_{6h}$.

| $M_j \otimes M_j =$<br>$M_n \otimes M_n =$ | | | | $[\Gamma_{1+} + \Gamma_{5+}$<br>$[\Gamma_{1+} + \Gamma_{5+}$ | | | $+M_{1-}$<br>$+M_{1+}$ | | $]$<br>$]$ | $+M_{2+}$<br>$+M_{2+}$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | $\sigma = 1$ | 1 | 1 | 1 | 2 | 3 | 1 | 2 | 3 |
| $\sigma'$ | $\sigma''$ | $\alpha'$ | $\alpha''$ | $\alpha = 1$ | 1 | 2 | 1 | 1 | 1 | 1 | 1 | 1 |
| 1 | 1 | 1 | 1 | 1 | 1 | $\bar{w}$ | 0 | 0 | 0 | 0 | 0 | 0 |
| 1 | 2 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 1 |
| 1 | 3 | 1 | 1 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | −1 | 0 |
| 2 | 1 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | ±1 | 0 | 0 | ∓1 |
| 2 | 2 | 1 | 1 | 1 | $w$ | $w$ | 0 | 0 | 0 | 0 | 0 | 0 |
| 2 | 3 | 1 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 1 | 0 | 0 |
| 3 | 1 | 1 | 1 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 1 | 0 |
| 3 | 2 | 1 | 1 | 0 | 0 | 0 | ±1 | 0 | 0 | ∓1 | 0 | 0 |
| 3 | 3 | 1 | 1 | 1 | $\bar{w}$ | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| | | | | $\sqrt{3}$ | $\sqrt{3}$ | | $\sqrt{2}$ | | | $\sqrt{2}$ | | |

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