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Clebsch–Gordan coefficients for the space group of garnets

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Abstract. Based on the published reduction of Kronecker products, the Clebsch-Gordan coefficients for irreducible representations of the non-symmorphic space group of garnets at the symmetry points in the representation domain are calculated.

1. Introduction

Garnets are composite oxides with the general formula $C_3A_2D_3O_{12}$ where C is a cation on a pseudo-dodecahedral c site, A is a cation on an octahedral a-site and D is a cation on a tetrahedral d site. The site preference for the different cations in the lattice is essentially determined by their ionic radius. The c sites are occupied by large ions, a sites by ions of intermediate radii and the smallest ions are located on d sites. A typical garnet is calcium aluminium orthosilicate, $Ca_3Al_2(SiO_4)_3$. In the primitive cubic unit cell it contains four molecular constituents: 12 Ca, 8 Al, 12 Si and 48 O atoms while in the unit cell of the body-centred cubic lattice it contains two molecular constituents (Slater 1965). Table 1 describes the garnet structure (Geller 1967).

Table 1. Description of garnet structure.

Point symmetry				
international	222	$\bar{3}$	$\bar{4}$	1
Schoenflies	D_2	C_{3i}	S_4	C_1
Space-group position	24*c*	16*a*	24*d*	96*h*
Site coordinates	$\frac{1}{8}0\frac{1}{4}$	000	$\frac{3}{8}0\frac{1}{4}$	*xyz*
Typical ideal formula	Ca_3	Al_2	Si_3	O_{12}
Coordinatation to oxygen	8	6	4	
Type of polyhedron	dodecahedron (distorted cube)	octahedron	tetrahedron	

The class of crystals with garnet structure has become increasingly important over the last few decades. During this period a number of refinements to the structure of garnets have been carried out, for instance by Prandl (1966) and by Plumier and Sougi (1979). The crystal chemistry of garnets has been reviewed by Geller (1967) and the crystal chemistry of antiferromagnetic garnets has been reviewed by Belov and Sokolov (1977). Magnetic iron garnets in particular have important technological uses. They can be paramagnetic, antiferromagnetic or ferrimagnetic crystalline materials. Their

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lattice allows a broad variety of substitutions; in particular, oxygen can be substituted by fluorine. The literature of recent years is full of papers on studies of garnets from various points of view, as evidenced, for example, by the volume *Garnets and Perovskites* of the *Landolt-Börnstein New Series* (1978).

The non-symmorphic space group $O_h^{10}(Ia3d)$ of the garnet structure is one of the most complicated space groups and is probably the most difficult one to handle from the point of view of representation theory.

Selection rules for the holosymmetric space groups based on the body-centred cubic Bravais lattice have been published by Cracknell *et al* (1979) while the irreducible representations and the reduction of Kronecker products for space groups, and thus also for the garnet space group, have been listed in the *Kronecker Product Tables* of Cracknell *et al* (1979-80), hereafter referred to as KPT. The magnetic basis vectors in the garnet structure have been calculated by Prandl (1976) to test the consistency of the magnetic structures determined experimentally.

In the present paper we report a computation, based on the published selection rules, of the Clebsch-Gordan coefficients (CGCs) for the unitary irreducible representations of the space group of garnets using the method given by Koster (1958) and developed by Berenson and Birman (1975), Berenson *et al* (1975), van den Broek (1979) and Dirl (1979a, b, c).

The CGCs allow the basis functions of representations contained in the Kronecker product of two irreducible representations to be constructed (Berenson *et al* 1975, Kunert and Suffczyński 1980). The CGC can be used to determine matrix elements of the effective mass Hamiltonian (Birman *et al* 1976, Dirl 1979c). The elements of the scattering tensors for scattering of light by elementary excitations in a crystal are a prescribed linear combination of CGC (Birman and Berenson 1974, Berenson 1981).

2. Clebsch–Gordan coefficients for space-group representations

We consider an irreducible space-group representation labelled by $\boldsymbol{k}l$, and contained $m_{l'l'',l}$ times in the direct product of the irreducible representations labelled by $\boldsymbol{k}'l'$ and $\boldsymbol{k}'l''$, respectively. We decompose the space group G into cosets with respect to the wavevector group $G(\boldsymbol{k})$ (Gard 1973):

$$G = \sum_{\sigma=1}^{c_k} \{R_\sigma|\boldsymbol{v}_\sigma\}G(\boldsymbol{k}). \tag{1}$$

The number c_k of the left coset representatives $\{R_\sigma|\boldsymbol{v}_\sigma\}$, and thus of the arms $\boldsymbol{k}_\sigma = R_\sigma\boldsymbol{k}$ of the $\boldsymbol{k}$ wavevector star, is equal to $|\bar{G}|/|\bar{G}(\boldsymbol{k})|$, the order of the point group of G divided by the order of the point group of $G(\boldsymbol{k})$. We find $c_{k'}$ and $c_{k''}$ arms of the $\boldsymbol{k}'$ and $\boldsymbol{k}''$ wavevector stars, respectively. From the arms we compose all wavevector selection rules

$$\boldsymbol{k}'_{\sigma'} + \boldsymbol{k}''_{\sigma''} = \boldsymbol{k}_\sigma. \tag{2}$$

We choose one leading wavevector selection rule (WVSR)

$$R_{\lambda'}\boldsymbol{k}' + R_{\lambda''}\boldsymbol{k}'' = \boldsymbol{k} \tag{3}$$

with two space-group operations $\{R_{\lambda'}|\boldsymbol{v}_{\lambda'}\}$ and $\{R_{\lambda''}|\boldsymbol{v}_{\lambda''}\}$.

The small irreducible representations $d^{\boldsymbol{k}'l'}$, $d^{\boldsymbol{k}''l''}$ and $d^{\boldsymbol{k}l}$ of dimension $\dim(l')$, $\dim(l'')$ and $\dim(l)$, respectively, are tabulated for the first arm of the wavevector star.

Therefore we have to transform

$$d^{R_{\lambda'},k'l'}(\{R_S|\boldsymbol{v}_S\}) = d^{k'l'}(\{R_{\lambda'}|\boldsymbol{v}_{\lambda'}\}^{-1}\{R_S|\boldsymbol{v}_S\}\{R_{\lambda'}|\boldsymbol{v}_{\lambda'}\})$$
$$d^{R_{\lambda''},k''l''}(\{R_S|\boldsymbol{v}_S\}) = d^{k''l''}(\{R_{\lambda''}|\boldsymbol{v}_{\lambda''}\}^{-1}\{R_S|\boldsymbol{v}_S\}\{R_{\lambda''}|\boldsymbol{v}_{\lambda''}\}). \tag{4}$$

The principal, or $\sigma' = \lambda'$, $\sigma'' = \lambda''$, $\sigma = 1$, block of CGCS is computed from the unitary small representations

$$U^{\gamma}_{\lambda'a'\lambda''a''1a} = \left(\frac{\dim(l)}{|\bar{G}(\boldsymbol{k})|}\right)^{1/2}\left(\sum_S d^{R_{\lambda'},k'l'}(S)_{b'b'}d^{R_{\lambda''},k''l''}(S)_{b''b''}d^{kl}(S)^*_{bb}\right)^{-1/2}$$
$$\times\sum_S d^{R_{\lambda'},k'l'}(S)_{a'b'}d^{R_{\lambda''},k''l''}(S)_{a''b''}d^{kl}(S)^*_{ab} \tag{5}$$

by performing summations over the space-group elements $S = \{R_S|\boldsymbol{v}_S\}$ belonging to the intersection of the wavevector groups

$$S = \{R_S|\boldsymbol{v}_S\} \in G(R_{\lambda'}\boldsymbol{k}') \wedge G(R_{\lambda''}\boldsymbol{k}'') \wedge G(\boldsymbol{k})/T \tag{6}$$

Table 2. Coordinates of the wavevector stars at the symmetry points of the Brillouin zone of the body-centred cubic lattice. a_L is the cubic lattice constant.

$\boldsymbol{k} = (0, 0, 0)\pi/a_L$		
$\boldsymbol{k}_H = (0, 2, 0)\pi/a_L$		
$\boldsymbol{k}_P = (1, 1, 1)\pi/a_L$	$13\boldsymbol{k}_P = (-1, -1, -1)\pi/a_L$	
$\boldsymbol{k}_N = (1, 1, 0)\pi/a_L$	$2\boldsymbol{k}_N = (1, -1, 0)\pi/a_L$	$5\boldsymbol{k}_N = (1, 0, 1)\pi/a_L$
$6\boldsymbol{k}_N = (1, 0, -1)\pi/a_L$	$9\boldsymbol{k}_N = (0, 1, 1)\pi/a_L$	$11\boldsymbol{k}_N = (0, 1, -1)\pi/a_L$

Table 3. Wavevector selection rules, block indices and the symmetry operations $\{R_{\sigma\Sigma}|\boldsymbol{v}_{\sigma\Sigma}\}$ at the symmetry point P.

$R_{\sigma'}\boldsymbol{k}' + R_{\sigma''}\boldsymbol{k}'' = \boldsymbol{k}_\sigma$	σ'	σ''	σ	$R_{\lambda'\sigma'\Sigma}$	$R_{\lambda''\sigma''\Sigma}$	$\{R_{\sigma\Sigma}\|\boldsymbol{v}_{\sigma\Sigma}\}^{-1}$
$\boldsymbol{k}_P + 13\boldsymbol{k}_P = \boldsymbol{k}_\Gamma$	1	1	1	1	1	$\{1\|0\}$
$13\boldsymbol{k}_P + \boldsymbol{k}_P = \boldsymbol{k}_\Gamma$	2	2	1	1	1	$\{13\|\boldsymbol{v}_4\}$
$\boldsymbol{k}_P + \boldsymbol{k}_P = \boldsymbol{k}_H$	1	1	1	1	1	$\{1\|0\}$
$13\boldsymbol{k}_P + 13\boldsymbol{k}_P = \boldsymbol{k}_H$	2	2	1	1	1	$\{13\|\boldsymbol{v}_4\}$
$\boldsymbol{v}_4 = (\frac{1}{4}, \frac{1}{4}, \frac{1}{4})a_L$						

Table 4. Clebsch-Gordan coefficients of the space group O_h^{10} for $H_j \times H_j$ ($j = 1, 2, 3$).

$H_1 \times H_1 =$		$\Gamma_{1+} + \Gamma_{2+} + \Gamma_{1-} + \Gamma_{2-}$				$H_2 \times H_2 =$		$\Gamma_{1-} + \Gamma_{2-} + \Gamma_{3+}$				$H_3 \times H_3 =$		$\Gamma_{1-} + \Gamma_{2-} + \Gamma_{3+}$			
α'	α''	$\alpha = 1$	1	1	1	α'	α''	$\alpha = 1$	1	1	2	α'	α''	$\alpha = 1$	1	1	2
1	1	1	1	0	0	1	1	0	0	0	1	1	1	0	0	1	0
1	2	0	0	1	1	1	2	1	1	0	0	1	2	1	1	0	0
2	1	0	0	1	−1	2	1	1	−1	0	0	2	1	1	−1	0	0
2	2	1	−1	0	0	2	2	0	0	1	0	2	2	0	0	0	1
		$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$			$\sqrt{2}$	$\sqrt{2}$	1				$\sqrt{2}$	$\sqrt{2}$	1	

Table 5. Clebsch-Gordan coefficients of the space group O_h^{10} for $H_4 \times H_4$.

$H_4 \times H_4 =$		$\Gamma_{1+}+\Gamma_{2+}$	$\Gamma_{1-}+\Gamma_{2-}+\Gamma_{3+}$		$+\Gamma_{3+}$		$+\Gamma_{3-}$		$+\Gamma_{3-}$		$+\Gamma_{4+}$			$+\Gamma_{4+}$			$+\Gamma_{4-}$			$+\Gamma_{4-}$		
α'	α''	$\alpha=1$	1	1	2	1	2	1	2	1	2	1	2	3	1	2	3	1	2	3	1	2	3
1	1	1	0	1		1	0		0														
1	2														0	1	0						
1	3											1	0	0									
1	4																	1	0	0			
1	5																				0	1	0
1	6	0	1	0		0	1		−1														
2	1											0	1	0									
2	2	1	0	$\bar{w}$		w	0																
2	3														0	0	1						
2	4																				0	0	1
2	5	0	1	0		0	$\bar{w}$		$-w$														
2	6																	0	1	0			
3	1														1	0	0						
3	2											0	0	1									
3	3	1	0	w		$\bar{w}$	0		0														
3	4	0	1	0		0	w		$-\bar{w}$														
3	5																	0	0	1			
3	6																				1	0	0
4	1																	∓1	0	0			
4	2																				0	0	∓1
4	3	0	±1		0	0		−1	1														
4	4	±1	0		1	1		0	0														
4	5														0	0	∓1						
4	6											∓1	0	0									
5	1																				0	∓1	0
5	2	0	±1		0	0		$-\bar{w}$	w														
5	3																	0	0	∓1			
5	4											0	0	∓1									
5	5	±1	0		$\bar{w}$	w		0	0														
5	6														0	∓1	0						
6	1	0	±1		0	0		$-w$	$\bar{w}$														
6	2																	0	∓1	0			
6	3																				∓1	0	0
6	4														∓1	0	0						
6	5											0	∓1	0									
6	6	±1	0		w	$\bar{w}$		0	0														
		$\sqrt{6}$	$\sqrt{6}$	$\sqrt{3}$		$\sqrt{3}$		$\sqrt{3}$	$\sqrt{3}$			$\sqrt{2}$			$\sqrt{2}$			$\sqrt{2}$			$\sqrt{2}$	

where T is the primitive translations subgroup of G. The column indices b', b'', b in equation (5) have to be chosen such that the sum with diagonal indices has a non-vanishing value.

For each wavevector selection rule of equation (2) we compute one space-group operation $\{R_\Sigma|v_\Sigma\}$ which rotates the principal block into the $\sigma'\sigma''\sigma$ block

$$R_\Sigma R_{\lambda'} k' = k'_{\sigma'} \qquad R_\Sigma R_{\lambda''} k'' = k''_{\sigma''} \qquad R_\Sigma k = k_\sigma. \tag{7}$$

In the transformation

$$\{R_{\lambda'\sigma'\Sigma}|v_{\lambda'\sigma'\Sigma}\} = \{R_{\sigma'}|v_{\sigma'}\}^{-1}\{R_\Sigma|v_\Sigma\}\{R_{\lambda'}|v_{\lambda'}\} \tag{8}$$

Table 6. Clebsch-Gordan coefficients of the space group O_h^{10} for $P_j \times P_j$ $(j = 1, 2)$.

$P_j \times P_j =$					Γ_{1-}	$+\Gamma_{2+}$	$+\Gamma_{4-}$			$+\Gamma_{5+}$		
σ'	σ''	σ	α'	α''	$\alpha = 1$	1	1	2	3	1	2	3
1	1	1	1	1	1	1	1			1		
			1	2				i	1		i	1
			2	1				1	i		1	i
			2	2	i	i	−i			−i		
2	2	1	1	1	1	−1	−1			1		
			1	2				−1	−i		1	i
			2	1				−i	−1		i	1
			2	2	i	−i	i			−i		
					2	2	2			2		

$P_j \times P_j =$						H_1		$+H_4$					
σ'	σ''	σ	α'	α''	$\alpha =$	1	2	1	2	3	4	5	6
1	1	1	1	1				1		i	1		−i
			1	2		1	i		−i			−1	
			2	1		−1	−i		−i			−1	
			2	2				1		−i	−1		−i
2	2	1	1	1				1		−i	1		i
			1	2		−i	−1		−1			−i	
			2	1		i	1		−1			−i	
			2	2				−1		−i	1		−i
						2		2					

Table 7. Clebsch-Gordan coefficients of the space group O_h^{10} for $P_3 \times P_3 = \Gamma$.

$P_3 \times P_3 =$		Γ_{1+}^{2+}	$+\Gamma_{1-}^{2-}$	$+\Gamma_{3+}^{3-}$		$+\Gamma_{4+}^{5+}$			$+\Gamma_{4+}^{5+}$			$+\Gamma_{4-}^{5-}$			$+\Gamma_{4-}^{5-}$		
		$\sigma' = 1,\ \sigma'' = 1,\ \sigma = 1$															
α'	α''	$\alpha = 1$	1	1	2	1	2	3	1	2	3	1	2	3	1	2	3
1	1	1	1			1	0	0				1	0	0			
1	2					0	i	1				0	i	1			
1	3								0	$-w$	$\bar{u}$				0	$-w$	$\bar{u}$
1	4			1	0				1	0	0				1	0	0
2	1					0	1	i				0	1	i			
2	2	i	i			−i	0	0				−i	0	0			
2	3			−1	0				1	0	0				1	0	0
2	4								0	w	$\bar{u}$				0	w	$\bar{u}$
3	1								0	$\mp\bar{u}$	$\pm w$				0	$\pm\bar{u}$	$\mp w$
3	2			0	1				∓ 1	0	0				± 1	0	0
3	3	$\pm$i	$\mp$i			$\mp$i	0	0				$\pm$i	0	0			
3	4					0	$\mp$i	± 1				0	$\pm$i	∓ 1			
4	1			0	−1				∓ 1	0	0				± 1	0	0
4	2								0	$\mp\bar{u}$	$\mp w$				0	$\pm\bar{u}$	$\pm w$
4	3					0	± 1	$\mp$i				0	∓ 1	$\pm$i			
4	4	∓ 1	± 1			∓ 1	0	0				± 1	0	0			

Table 7. (continued).

$P_3 \times P_3 =$		Γ_{1+}^{2+}	$+\Gamma_{1-}^{2-}$	$+\Gamma_{3+}^{3+}$		$+\Gamma_{4+}^{5+}$			$+\Gamma_{4+}^{5+}$			$+\Gamma_{4-}^{5-}$			$+\Gamma_{4-}^{5-}$		
		$\sigma'=2,\ \sigma''=2,\ \sigma=1$															
α'	α''	$\alpha=1$	1	1	2	1	2	3	1	2	3	1	2	3	1	2	3
1	1	± 1	± 1			∓ 1	0	0				∓ 1	0	0			
1	2					0	∓ 1	$\mp i$				0	∓ 1	$\mp i$			
1	3								0	$\mp\bar{u}$	$\pm w$				0	$\mp\bar{u}$	$\pm w$
1	4			0	± 1				∓ 1	0	0				∓ 1	0	0
2	1					0	$\mp i$	∓ 1				0	$\mp i$	∓ 1			
2	2	$\pm i$	$\pm i$			$\pm i$	0	0				$\pm i$	0	0			
2	3			0	∓ 1				∓ 1	0	0				∓ 1	0	0
2	4								0	$\mp\bar{u}$	$\mp w$				0	$\mp\bar{u}$	$\mp w$
3	1								0	$-w$	$\bar{u}$				0	w	$-\bar{u}$
3	2			± 1	0				1	0	0				-1	0	0
3	3	i	$-i$			i	0	0				$-i$	0	0			
3	4					0	-1	i				0	1	$-i$			
4	1			∓ 1	0				1	0	0				-1	0	0
4	2								0	w	$\bar{u}$				0	$-w$	$-\bar{u}$
4	3					0	i	-1				0	$-i$	1			
4	4	$\frac{-1}{\sqrt{8}}$	$\frac{1}{\sqrt{8}}$	2		$\frac{1}{\sqrt{8}}$	0	0	$\sqrt{8}$			$\frac{-1}{\sqrt{8}}$	0	0	$\sqrt{8}$		

a primitive translation may appear in $\boldsymbol{v}_{\lambda'\sigma'\Sigma}$. This is also to be observed for $\{R_{\sigma''}|\boldsymbol{v}_{\sigma''}\}$ and $\{R_\sigma|\boldsymbol{v}_\sigma\}$, and in equations (4).

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

$$\begin{pmatrix} \boldsymbol{k}'l' & \boldsymbol{k}''l'' \\ \sigma'\alpha' & \sigma''\alpha'' \end{pmatrix} \Bigg| \begin{matrix} kl\gamma \\ \sigma\alpha \end{matrix} = U^{\gamma}_{\sigma'\alpha'\sigma''\alpha''\sigma\alpha} = \sum_{a'=1}^{\dim(l')} \sum_{a''=1}^{\dim(l'')} \sum_{a=1}^{\dim(l)} \times d^{\boldsymbol{k}'l'}(\{R'_{\lambda'\sigma'\Sigma}|\boldsymbol{v}_{\lambda'\sigma'\Sigma}\})_{\alpha'a'} d^{\boldsymbol{k}''l''}(\{R_{\lambda''\sigma''\Sigma}|\boldsymbol{v}_{\lambda''\sigma''\Sigma}\})_{\alpha''a''} U^{\gamma}_{\lambda'a'\lambda''a''1a} \times d^{kl}(\{R_{\sigma\Sigma}|\boldsymbol{v}_{\sigma\Sigma}\})^{-1}_{a\alpha}. \tag{9}$$

In the case that the multiplicity $m_{l'l'',l}$ is greater than one, or the multiplicity index $\gamma \geqslant 1$, we have, by appropriate choice of the diagonal indices $b'b''b$ of equation (5), to find CGCS for all $\gamma \leqslant m_{l'l'',l}$ and ensure orthonormalisation of columns and rows of the CGCS square matrix of dimension

$$c_{\boldsymbol{k}'} \dim(l') c_{\boldsymbol{k}''} \dim(l'') = c_{\boldsymbol{k}} \sum_l m_{l'l'',l} \dim(l). \tag{10}$$

3. Description of tables

Table 2 lists the wavevector stars at the symmetry points of the Brillouin zone of the body-centred cubic lattice. The first, or canonical, wavevector at each symmetry point is given as in the KPT. We use the numbering of symmetry operations and the multiplication tables as given for cubic groups in tables 3.1 and 3.2, respectively, of the KPT. We use the fractional translations of the non-symmorphic space group

Table 8. Clebsch-Gordan coefficients of the space group O_h^{10} for $P_3 \times P_3 = H$.

$P_3 \times P_3 =$		H_1		$+H_1$		$+H_2$		$+H_3$		$+H_4$						$+H_4$						$+H_4$						$+H_4$					
α'	α''	$\alpha=1$	2	1	2	1	2	1	2	1	2	3	4	5	6	1	2	3	4	5	6	1	2	3	4	5	6	1	2	3	4	5	6
1	1	0		0		0		0		1	0	$\bar{u}$																			−1	0	$-u$
1	2	0		0		1		−1		0	u	0																			0	$\bar{w}$	0
1	3	1		−i		0		0								0	1	0							0	−1	0						
1	4	0		0		0		0								1	0	i							−i	0	−1						
2	1	0		0		−1		1		0	u	0																			0	$\bar{w}$	0
2	2	0		0		0		0		1	0	$-\bar{u}$																			1	0	$-u$
2	3	0		0		0		0								i	0	1							−1	0	−i						
2	4	i		1		0		0								0	−i	0							0	i	0						
3	1		−i	1			0		0										0	−i	0	0	−i	0									
3	2		0	0			0		0										−i	0	1	1	0	−i									
3	3		0	0			0		0				1	0	$\bar{u}$													1	0	u				
3	4		0	0			1		1				0	u	0													0	$-\bar{w}$	0				
4	1		0	0			0		0										1	0	−i	−i	0	1									
4	2		1	i			0		0										0	−1	0	0	−1	0									
4	3		0	0			−1		−1				0	u	0													0	$-\bar{w}$	0				
4	4		0	0			0		0				1	0	$-\bar{u}$													−1	0	u				

Table 8. (continued).

$P_1 \times P_3 =$	H_1	$+H_1$	$+H_2$	$+H_3$	$+H_4$	$+H_4$	$+H_4$	$+H_4$	H_4
	$\sigma' = 2,\ \sigma'' = 2,\ \sigma = 1$								
α' α''	$\alpha = 1$ 2	1 2	1 2	1 2	1 2 3 4 5 6	1 2 3 4 5 6	1 2 3 4 5 6	1 2 3 4 5 6	1 2 3 4 5 6
1 1	0	0	0	0	1 0 $\bar{u}$				−1 0 $-u$
1 2	0	0	−1	1	0 u 0				0 $\bar{w}$ 0
1 3	−1	i	0	0		0 1 0	0 −1 0		
1 4	0	0	0	0		1 0 i	−i 0 −1		
2 1	0	0	1	−1	0 u 0				0 $\bar{w}$ 0
2 2	0	0	0	0	1 0 $-\bar{u}$				1 0 $-u$
2 3	0	0	0	0		i 0 1	−1 0 −i		
2 4	−i	−1	0	0		0 −i 0	0 i 0		
3 1	i	−1 0	0			0 −i 0		0 −i 0	
3 2	0	0 0	0			−i 0 1		1 0 −i	
3 3	0	0 0	0	1 0 $\bar{u}$					1 0 u
3 4	0	0 −1	−1	0 u 0					0 $-\bar{w}$ 0
4 1	0	0 0	0			1 0 −i		−i 0 1	
4 2	−1	−i 0	0			0 −1 0		0 −1 0	
4 3	0	0 1	1	0 u 0					0 $-\bar{w}$ 0
4 4	0	0 0	0	1 0 $-\bar{u}$					−1 0 u
	2	2	2	2		2	2		2

Table 9. Clebsch–Gordan coefficients of the space group O_h^{10} for $N_j \times N_j$ ($j = 1, 2$).

$N_j \times N_j =$					H_1		$+H_2$		$+H_3$		$+H_4$						$+H_4$						$+H_4$					
σ'	σ''	σ	α'	α''	$\alpha = 1$	2	1	2	1	2	1	2	3	4	5	6	1	2	3	4	5	6	1	2	3	4	5	6
1	2	1	1	1	1	−1	1	−1	1	−1							0	1	0	0	1	0						
			1	2							1	0	0	1	0	0							0	0	1	0	0	1
			2	1							1	0	0	−1	0	0							0	0	1	0	0	−1
			2	2	−1	−1	−1	−1	−1	−1							0	1	0	0	−1	0						
2	1	1	1	1	−1	1	−1	1	−1	1							0	1	0	0	1	0						
			1	2							1	0	0	−1	0	0							0	0	−1	0	0	1
			2	1							1	0	0	1	0	0							0	0	−1	0	0	−1
			2	2	1	1	1	1	1	1							0	1	0	0	−1	0						
3	4	1	1	1	1	−1	$\bar{w}$	$-w$	w	$-\bar{w}$							0	0	1	1	0	0						
			1	2							0	1	0	0	0	1							1	0	0	0	1	0
			2	1							0	−1	0	0	0	1							−1	0	0	0	1	0
			2	2	1	1	$\bar{w}$	w	w	$\bar{w}$							0	0	−1	1	0	0						
4	3	1	1	1	−1	1	$-\bar{w}$	w	$-w$	$\bar{w}$							0	0	1	1	0	0						
			1	2							0	1	0	0	0	−1							−1	0	0	0	1	0
			2	1							0	−1	0	0	0	−1							1	0	0	0	1	0
			2	2	−1	−1	$-\bar{w}$	$-w$	$-w$	$-\bar{w}$							0	0	−1	1	0	0						
5	6	1	1	1	1	−1	w	$-\bar{w}$	$\bar{w}$	$-w$							1	0	0	0	0	1						
			1	2							0	0	1	0	1	0							0	1	0	1	0	0
			2	1							0	0	1	0	−1	0							0	1	0	−1	0	0
			2	2	−1	−1	$-w$	$-\bar{w}$	$-\bar{w}$	$-w$							1	0	0	0	0	−1						
6	5	1	1	1	−1	1	$-w$	$\bar{w}$	$-\bar{w}$	w							1	0	0	0	0	1						
			1	2							0	0	−1	0	1	0							0	1	0	−1	0	0
			2	1							0	0	−1	0	−1	0							0	1	0	1	0	0
			2	2	$\frac{1}{\sqrt{12}}$	1	$\frac{w}{\sqrt{12}}$	$\bar{w}$	$\frac{\bar{w}}{\sqrt{12}}$	w	2						2						2					

$O_h^{10}(Ia3d)$ and the labels and generators of the irreducible representations of the KPT. The representation matrices and the principal blocks of CGCs have been computed with the aid of the computer program of Kowalczyk *et al* (1980).

Table 3 presents the wavevector selection rules of the group O_h^{10} for P×P. For each wavevector selection rule we give the indices $\sigma'\sigma''\sigma$ of the corresponding block of CGC and the symmetry operation $\{R_{\sigma\Sigma}|\boldsymbol{v}_{\sigma\Sigma}\}$ which rotates the principal block into the $\sigma'\sigma''\sigma$ block.

The wavevector selection rules for N×N have been given explicitly by Suffczyński and Kunert (1982) and the CGCs for N×N = Γ by Kunert (1983).

Tables 4 and 5 present the computed CGCs for H×H and tables 6–8 for P×P. Table 9 presents CGCs for N×N = H and table 10 the principal block of CGCs for

Table 10. Principal block of Clebsch-Gordan coefficients of the space group O_h^{10} for $N_j \times N_j$ ($j=1,2$).

$N_j \times N_j =$	N_1		$+N_1$		$+N_1$		$+N_1$		$+N_2$		$+N_2$		$+N_2$		$+N_2$	
α' α''	$\alpha=1$	2	1	2	1	2	1	2	1	2	1	2	1	2	1	2
1 1	1	0					0	−1	1	0					0	−1
1 2			1	0	0	−1					1	0	0	−1		
2 1			0	−1	1	0					0	−1	1	0		
2 2	0	−1					1	0	0	−1					1	0
	2		2		2		2		2		2		2		2	

Table 11. The diagonal indices $b'b''b$ and the phase factors of the Clebsch-Gordan coefficients proportional to those printed in tables 5, 7 and 8. The phase factor is omitted if it is equal to one. For each representation the columns corresponding to consecutive values of the multiplicity index are arranged in the same order as in tables 5, 7 and 8.

$H_4 \times H_4 =$	Γ_{3+}				$+\Gamma_{3-}$			
	111		441		161		431	
	221	w	551	$\bar{w}$	251	w	521	$\bar{w}$
	331	$\bar{w}$	661	w	351	$\bar{w}$	611	w

$H_4 \times H_4 =$	Γ_{4+}				$+\Gamma_{4-}$				$+\Gamma_{5+}$				$+\Gamma_{5-}$			
	131		311		141		361		131		311		141		361	
	431	−1	641	−1	411	−1	631	−1	461		641		411		631	

$P_3 \times P_3 =$	Γ_{4-}				$+\Gamma_{5+}$				$+\Gamma_{4-}$				$+\Gamma_{5-}$			
	111		141		111		141		111		141		111		141	
	221	i	231		221	i	231		221	i	231		221	i	231	
	331	i	321	−1	331	−i	321		331	−i	321		331	i	321	−1
	441	−1	411	−1	441		411		441		411		441	−1	411	−1

$P_3 \times P_3 =$	H_1				$+H_4$							
	131		311		111		141		321		331	
	241	−i	421	−i	221		231	−i	411	i	441	−i

$N \times N = N$. In the tables of CGCs we use the symbols

$$u = \exp(i\pi/6) \qquad w = \exp(\tfrac{2}{3}i\pi)$$

and an overbar stands for complex conjugate. Empty entries correspond to zero elements. The number at the bottom of each representation column divides each element of that column for normalisation. In tables 5 and 7 the upper signs refer to the upper and the lower signs to the lower description line of the table, respectively.

The CGC for $P_3 \times P_3$ in tables 7 and 8 agree with those published by Davies and Dirl (1984). This provides a good cross-check of work performed independently.

Since our program prints all non-vanishing CGCs of the principal block we can give a few details concerning the case of multiplicity greater than one. In table 11, below the representation symbol, we give in the first line the sets of diagonal indices $b'b''b$ of equation (5) for which the CGCs are given in tables 5, 7 and 8. The subsequent lines give the sets of diagonal indices for which the CGCs are proportional to those of the first set, with the phase factor given on the right. This phase factor is omitted if it is equal to one.

4. Conclusions

In contrast to the case of crystal point groups (Kotzev and Aoryo 1982a, b) the tables of CGCs for space groups have not been published extensively until now. We have computed the CGCs of the non-symmorphic space group of garnets for the unsymmetrised squares of the single-valued representations of Cracknell *et al* (1979-80). The computation of CGCs for the complicated space group of garnets with the aid of the computer program of Kowalczyk *et al* (1980) was a test of the program's capabilities. The presentation of CGCs for the space group of garnets, apart from its intrinsic value, may be useful for comparison of future results of more extended and more automatic programs.

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