

Appendix : Quasi-Bloch Functions and the Mackey Double Coset Method.

In reducing band representations into irreducible representations of space groups much use was made in the paper of formula (61). The latter was obtained by using the concept of quasi-Bloch functions (Rel. (56)) which lead to the reduction of the infinite-dimensional band representations into finite-dimensional representations of the isotropy groups G_k for the vectors \vec{k} in the Brillouin zone. Formula (61) gives the character $\chi_k^{(q^*, \rho)}$ of the k -component of the band representation induced from the ρ -representation of the isotropy group G_q (\vec{q} is the position in the Wigner-Seitz cell that corresponds to the symmetry center \vec{r} with the isotropy groups G_r ; the connection between G_q and G_r is explained in Section II A). Having the k -component character $\chi_k^{(q^*, \rho)}$ it is easy to find how many times (multiplicity) an irreducible representation $D^{(k, \mu)}$ of G_k is contained in the band representation $D^{(q^*, \rho)}$ (See Formula (62)). An alternative method for calculating this multiplicity was given in the paper (Formula (46)) by using Mackey's double coset expansion (Rel.(43)) The latter method is of very general nature and can be applied each time when we have an induced representation $\text{Ind}_H^G \gamma_H^{(\rho)}$ of the group G from an irreducible representation $\gamma_H^{(\rho)}$ of its subgroup and we are asking for the multiplicity of the induced representation $\text{Ind}_K^G \gamma_K^{(\alpha)}$ of G from an irreducible representation $\gamma_K^{(\alpha)}$ of another subgroup K of G . However, in applying the double coset method one encounters, in general, a decomposition of the group G into double cosets with respect to H and K (Rel. (43)). As a rule, this double coset decomposition is not entirely elementary and it is for this reason that we have preferred the reduction method based on the quasi-Bloch functions (Formula (61)). It should be pointed out that in some cases the double coset expansion reduces to an expansion into single cosets and then the Mackey method becomes very simple. An example of such cases is when $\vec{k} = 0$, because then $G_k = G$ (in the notations of Section II B, $K = G_k = G$) and the general formula

for multiplicities (Formula (44)) goes over into the simple expression (46). A more general example for the double coset expansion to reduce to an expansion in single ones is when G_k is an invariant subgroup of the space group G . This is so because the $Hs G_k$ (we replace K by G_k in Formula (43)) can be rewritten as $HG_k s'$. Also from the invariance property of G_k it follows that HG_k is a subgroup of G and expansion (43) turns therefore into a decomposition in single coset with respect to the subgroup HG_k of G .

Acknowledgements

H. Bacry and J. Zak are grateful for the kind hospitality extended to them at I.H.E.S.

One of the authors (J.Z.) would like to thank Prof. A. Grossmann for very enjoyable discussions on the subject of the manuscript.

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- [16] The concept irreducible-band representation has the meaning of a band irreducible representation, e.g. it is reducible as a representation but irreducible as a band representation. It is for this reason that we connect the words irreducible and band by a hyphen.

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Point Group P	Dimension d of stratum
C_1	3
C_s	2
C_2, C_3, C_4, C_6	1
$C_{2v}, C_{3v}, C_{4v}, C_{6v}$	
The 22 other point groups	0

Table 1. Dimension d of the stratum corresponding to isotropy groups G_r isomorphic to the point group P . The ten point groups which are isotropy groups of a stratum of dimension > 0 (i.e. with non-isolated points) are called polar groups : they leave at least one non-zero vector invariant in their vector representations. The 22 others are called non-polar.

Dimension of Closed Strata	Number of Space Groups	Dimension of Closed Strata	Number of Space Groups
0	104	1 and 2	6
1	61	0 and 2	2
2	5	0 and 1	38
3	13	0,1 and 2	1

Table 2. Statistics of Dimensions of Closed Strata of Space Groups in 3 Dimensions.

Number of Group	International Symbol	Dimension of Stratum	Number of Strata	Little Group	Number of Group	International Symbol	Dimension of Stratum	Number of Strata	Little Group
1	P1	3	1	1	57	Pbcm	0	2	$\bar{1}$
4	P2 ₁	3	1	1			1	1	2
7	Pb	3	1	1					
9	Bb	3	1	1			2	1	m
19	P2 ₁ 2 ₁ 2 ₁	3	1	1	194	P6 ₃ /mmc	0	1	$\bar{3}m$
29	Pca2 ₁	3	1	1			0	3	$\bar{6}m2$
33	Pna2 ₁	3	1	1	221	Pm3m	0	2	m3m
76	P4 ₁	3	1	1			0	2	4/mmm
78	P4 ₃	3	1	1	225	Fm3m	0	2	m3m
144	P3 ₁	3	1	1			0	1	$\bar{4} 3m$
145	P3 ₂	3	1	1			0	1	mmm
169	P6 ₁	3	1	1	227	Fd3m	0	2	$\bar{4} 3m$
170	P6 ₅	3	1	1			0	2	$\bar{3}m$
6	Pm	2	2	m	229	Im3m	0	1	m3m
8	Bm	2	1	m			0	1	4/mmm
26	Pmc2 ₁	2	2	m			0	1	$\bar{3} m$
31	Pmn2 ₁	2	1	m			0	1	$\bar{4}2m$
36	Cmc2 ₁	2	1	m			0	1	

Table 3. Examples of closed strata with their little groups. On the left, in the upper part space groups are listed with 3-dimensional closed strata only. On the left, in the lower part, the same for 2-dimensional closed strata. On the right, in the upper part the space group (# 57) is listed as an exceptional group having 0-, 1- and 2-dimensional closed strata. On the right in lower part some space groups with 0-dimensional closed strata are listed.

Symmetry center \vec{q}	Little Group
$\vec{r}_a = (000)$	$T_d = G_a$
$\vec{r}_b = (\frac{a}{2} 00)$	$(E \frac{a}{2} 00) T_d (E \frac{\bar{a}}{2} 00) = G_b$
$\vec{r}_c = (\frac{a}{8} \frac{a}{8} \frac{a}{8})$	$D_{3d}^{(xyz)} = G_c$
$\vec{r}_d = (\frac{a}{8} \frac{a}{8} \frac{3\bar{a}}{8})$	$(E 00 \frac{\bar{a}}{2}) D_{3d}^{(xyz)} (E 00 \frac{a}{2}) = G_d$

Table 4. Symmetry centers \vec{r} of closed strata with their little groups G_r for the diamond structure space group O_h^7 .

O_h	T_d	D_{4h}	D_4
0 1 1 + 6	T 1 1 + 2	C_{4h} 1 1 + 2	C_4 1 1 + 2
2 2 + 7	2 3	2 3 + 4	2 3 + 4
3 3 + 8	3 3	3 5	3 5
4 5 + 10	4 4 + 5	4 5	4 5
5 4 + 9	D_{2d} 1 1 + 3	5 6 + 7	D_2 1 1 + 3
T_d 1 1 + 7	2 5	6 8 + 9	2 5
2 2 + 6	3 2 + 3	7 10	3 5
3 3 + 8	4 4	8 10	4 2 + 4
4 4 + 10	5 4 + 5	D_4 1 1 + 6	D_2' 1 1 + 4
5 5 + 9	C_{3v} 1 1 + 4	2 2 + 7	2 5
T_h 1 1 + 2	2 2 + 5	3 3 + 8	3 5
2 3	3 3 + 4 + 5	4 4 + 9	4 2 + 3
3 3		5 5 + 10	D_{2d}
4 4 + 5	T_h	C_{4v} 1 1 + 7	S_4 1 1 + 2
5 6 + 7	T 1 1 + 5	2 2 + 6	2 3 + 4
6 8	2 2 + 6	3 3 + 9	3 5
7 8	3 3 + 7	4 4 + 8	4 5
8 9 + 10	4 4 + 8	5 5 + 10	D_2 1 1 + 3
D_{4h} 1 1 + 3	D_{2h} 1 1 + 2 + 3	D_{2h} 1 1 + 3	2 5
2 5	2 4	2 5	3 5
3 2 + 3	3 4	3 5	4 2 + 4
4 4	4 4	4 2 + 4	C_{2v} 1 1 + 4
5 4 + 5	5 5 + 6 + 7	5 6 + 8	2 5
6 6 + 8	6 8	6 10	3 2 + 3
7 10	7 8	7 10	4 5
8 7 + 8	8 8	8 7 + 9	C_{4v}
9 9	C_{3i} 1 1 + 4	D_{2h}' 1 1 + 4	C_4 1 1 + 2
10 9 + 10	2 2 + 4	2 5	2 3 + 4
D_{3d} 1 1 + 4	3 3 + 4	3 5	3 5
2 2 + 5	4 5 + 8	4 2 + 3	4 5
3 3 + 4 + 5	5 6 + 8	5 6 + 9	C_{2v} 1 1 + 3
4 7 + 10	6 7 + 8	6 10	2 5
5 6 + 9		7 10	3 2 + 4
6 8 + 9 + 10	T	8 7 + 8	4 5
	D_2 1 1 + 2 + 3	D_{2d}' 1 1 + 8	C_{2v}' 1 1 + 4
0	2 4	2 2 + 9	2 5
T 1 1 + 2	3 4	3 3 + 6	3 2 + 3
2 3	4 4	4 4 + 7	4 5
3 3	C_3 1 1 + 4	5 5 + 10	
4 4 + 5	2 2 + 4	D_{2d}' 1 1 + 9	
D_4 1 1 + 3	3 3 + 4	2 2 + 8	
2 4		3 4 + 6	
3 2 + 3		4 3 + 7	
4 5		5 5 + 10	
5 4 + 5			
D_3 1 1 + 5			
2 2 + 4			
3 3 + 4 + 5			

	D _{6h}	D ₆	D _{3d}
C _{6h}	1 1 + 2 2 9 + 10 3 6 4 6 5 11 6 11 7 7 + 8 8 3 + 4 9 12 10 12 11 5 12 5	C ₆ 1 1 + 2 2 3 + 4 3 6 4 6 5 5 6 5	S ₆ 1 1 + 2 2 <u>3</u> 3 <u>3</u> 4 4 + 5 5 <u>6</u> 6 <u>6</u>
D ₆	1 1 + 7 2 2 + 8 3 3 + 9 4 4 + 10 5 5 + 11	D ₃ 1 1 + 3 2 2 + 4 3 5 + 6	D ₃ 1 1 + 4 2 2 + 5 <u>3 3</u> + <u>6</u>
C _{6v}	6 6 + 12 1 1 + 8 2 2 + 7 3 3 + 10 4 4 + 9 5 5 + 11	D ₃ ' 1 1 + 4 2 2 + 3 3 5 + 6	C _{3v} ' 1 1 + 4 2 2 + 5 <u>3 3</u> + <u>6</u>
D _{3h}	6 6 + 12 1 1 + 9 2 2 + 10 3 6 + 11 4 3 + 7 5 4 + 8	D ₂ 1 1 + 6 2 3 + 5 3 4 + 5 4 2 + 6	C _{2h} 1 1 + <u>3</u> 2 2 + <u>3</u> 3 5 + <u>6</u> 4 4 + <u>6</u>
D _{3h} '	6 5 + 12 1 1 + 10 2 2 + 9 3 6 + 11 4 4 + 7	C _{6v}	D ₃
D _{3h} '	5 3 + 8 6 5 + 12	C ₆ 1 1 + 2 2 3 + 4 3 6 4 6 5 5 6 5	C ₃ 1 1 + 2 2 3 3 3
D _{3d}	1 1 + 3 2 2 + 4 3 5 + 6 4 8 + 10 5 7 + 9	C _{3v} 1 1 + 3 2 2 + 4 3 5 + 6	C ₂ 1 1 + 3 2 2 + 3
D _{3d} '	6 11 + 12 1 1 + 4 2 2 + 3 3 5 + 6 4 8 + 9 5 7 + 10	C _{3v} ' 1 1 + 4 2 2 + 3 3 5 + 6	C _{3v}
D _{2h}	6 11 + 12 1 1 + 6 2 3 + 5 3 4 + 5 4 2 + 6 5 7 + 12 6 9 + 11 7 10 + 11 8 8 + 12	C _{2v} 1 1 + 6 2 3 + 5 3 2 + 6 4 4 + 5	C ₃ 1 1 + 2 2 3 3 3
		D _{3h}	C _s 1 1 + 3 2 2 + 3
		C _{3h} 1 1 + 2 2 <u>3</u> 3 <u>3</u> 4 4 + 5 5 <u>6</u> 6 <u>6</u>	D _{2h}
		D ₃ 1 1 + 4 2 2 + 5 <u>3 3</u> + <u>6</u>	C _{2h} ^z 1 1 + 4 2 2 + 3 3 5 + 8 4 6 + 7
		C _{3v} 1 1 + 5 2 2 + 4 <u>3 3</u> + <u>6</u>	C _i 1 1 + 2 + 3 + 4 2 5 + 6 + 7 + 8
		C _{2v} 1 1 + <u>3</u> 2 2 + <u>3</u> 3 4 + <u>6</u> 4 5 + <u>6</u>	D ₂
			C ₂ ^z 1 1 + 4 2 2 + 3
			C ₂ ^x 1 1 + 2 2 3 + 4
			C _{2v}
			C ₂ 1 1 + 3 2 2 + 4

Table 5. Induced representations of Point Groups. On top we list the group for which the representations are induced. In the column on the right-hand side the groups are listed from which we induce the representations. The numbers label the representations of the point groups according to Ref. 15. The induced representations are listed by their contents of irreducible representations of the particular group. Consider as an example the cubic group Q_h . When inducing from representation 1 of O we obtain an induced representation of O_h which contains the irreducible representations 1 and 6 of the latter.

INDUC- TION from T	INDUCED REPS of T _d	INDUC- TION from D _{2d}	INDUCED REPS of T _d	INDUC- TION from C _{3v}	INDUCED REPS of T _d	IRREDUCIBLE INDUCED REPS of T _d
γ ⁽¹⁾	γ ⁽¹⁾ +γ ⁽²⁾	γ ⁽¹⁾	γ ⁽¹⁾ +γ ⁽³⁾	γ ⁽¹⁾	γ ⁽¹⁾ +γ ⁽⁴⁾	γ ⁽¹⁾ +γ ⁽²⁾ , γ ⁽³⁾
γ ⁽²⁾	γ ⁽³⁾	γ ⁽²⁾	γ ⁽²⁾ +γ ⁽³⁾	γ ⁽²⁾	γ ⁽²⁾ +γ ⁽⁵⁾	γ ⁽¹⁾ +γ ⁽³⁾
γ ⁽³⁾	γ ⁽³⁾	γ ⁽³⁾	γ ⁽⁴⁾	γ ⁽³⁾	γ ⁽³⁾ +γ ⁽⁴⁾ +γ ⁽⁵⁾	γ ⁽²⁾ +γ ⁽³⁾
γ ⁽⁴⁾	<u>γ⁽⁴⁾+γ⁽⁵⁾</u>	γ ⁽⁴⁾	γ ⁽⁵⁾			γ ⁽¹⁾ +γ ⁽⁴⁾
		γ ⁽⁵⁾	<u>γ⁽⁴⁾+γ⁽⁵⁾</u>			γ ⁽²⁾ +γ ⁽⁵⁾
						γ ⁽⁴⁾ , γ ⁽⁵⁾

Table 6. Induced representations from maximal subgroups and irreducible-induced representation of T_d. The underlined induced representations are

reducible-induced. Thus,

$$\text{Ind}_T^{T_d} \gamma_T^{(4)} = \gamma_{T_d}^{(4)} + \gamma_{T_d}^{(5)} = \text{Ind}_{D_{2d}}^{T_d} (\gamma_{D_{2d}}^{(3)} + \gamma_{D_{2d}}^{(4)})$$

$$\text{Ind}_{C_{3v}}^{T_d} \gamma_{C_{3v}}^{(3)} = \gamma_{T_d}^{(3)} + \gamma_{T_d}^{(4)} + \gamma_{T_d}^{(5)} = \text{Ind}_T^{T_d} (\gamma_T^{(3)} + \gamma_T^{(4)})$$

INDUCTION from C_{3v}	BAND REPS of T_d	INDUCTION from C_{2v}	BAND REPS of T_d
$\gamma^{(1)}$	$\gamma^{(1)} + \gamma^{(4)}$	$\gamma^{(1)}$	$\gamma^{(1)} + \gamma^{(3)} + \gamma^{(4)}$
$\gamma^{(2)}$	$\gamma^{(2)} + \gamma^{(5)}$	$\gamma^{(2)}$	$\gamma^{(4)} + \gamma^{(5)}$
$\gamma^{(3)}$	$\gamma^{(3)} + \gamma^{(4)} + \gamma^{(5)}$	$\gamma^{(3)}$	$\gamma^{(2)} + \gamma^{(3)} + \gamma^{(5)}$
		$\gamma^{(4)}$	$\gamma^{(4)} + \gamma^{(5)}$

Table 7. Band representations from maximal isotropy subgroups of T_d . They are all irreducible-band representations. Two of them are equivalent

$$\text{Ind}_{C_{2v}}^{T_d} \gamma^{(2)} \sim \text{Ind}_{C_{2v}}^{T_d} \gamma^{(4)} .$$

	a	b		a	b					Number of Groups	a	b
O_h	10	20	D_{4h}	10	30	C_4, S_4	4	2	Cu	5	32	54
O, T_d	5	8	D_4, C_{4v}, D_{2d}	5	7	C_3	3	1	Hex	7	54	101
T_h	8	13	D_3, C_{3v}	3	4	D_{2h}	8	12	Trig.	5	21	33
T	4	5	C_{6h}	12	22	D_2, C_{2v}, C_{2h}	4	6	Tatr.	7	41	67
D_{6h}	12	40	C_6, S_6, C_{3h}	6	5	C_2, C_s, C_i	2	1	Orth.	3	16	24
D_6, C_{6v}	6	12	C_{4h}	8	12	C_1	1		Mon.	3	8	8
D_{3d}, D_{3h}									Tric.	2	3	1

Table 8. Statistics of Irreducible and Irreducible-Induced Representations of Crystallographic point groups in 3 dimensions; a) Inequivalent Irreducible Representations; b) Inequivalent Irreducible-Induced Representations.

Table 9

α	E	C_3^{xyz}	C_3^{2xyz}	$C_3^{\bar{xyz}}$	$C_3^{2\bar{xyz}}$	$C_3^{x\bar{yz}}$	$C_3^{2x\bar{yz}}$
χ							
$\chi^{(a^*,1)}(\alpha, \vec{k})$	2	2	2	$1+\delta\epsilon$	$1+\gamma\epsilon$	$1+\delta\gamma$	$1+\delta\epsilon$
$\chi^{(b^*,1)}(\alpha, \vec{k})$	2	$\delta\gamma^*+\delta^*\gamma$	$\delta\epsilon^*+\delta^*\epsilon$	$\delta\gamma^*+\gamma\epsilon$	$\delta\epsilon+\delta^*\epsilon$	$1+\delta\gamma$	$1+\delta\gamma$
α							
χ	$C_3^{xy\bar{z}}$	$C_3^{2xy\bar{z}}$	C_2^x	C_2^y	C_2^z	σ^{xy}	$\sigma^{\bar{x}y}$
$\chi^{(a^*,1)}(\alpha, \vec{k})$	$1+\gamma\epsilon$	$1+\delta\gamma$	$1+\gamma\epsilon$	$1+\delta\epsilon$	$1+\delta\gamma$	$1+\delta\gamma$	2
$\chi^{(b^*,1)}(\alpha, \vec{k})$	$\delta\gamma+\delta^*\epsilon$	$\delta\epsilon^*+\gamma\epsilon$	$1+\gamma\epsilon$	$\delta^2+\delta^*\epsilon$	$\delta^2+\delta^*\gamma$	$1+\delta\epsilon$	$\delta\gamma^*+\delta^*\gamma$
α							
χ	σ^{xz}	$\sigma^{\bar{x}z}$	σ^{yz}	$\sigma^{\bar{y}z}$	S_4^x	S_4^{3x}	S_4^y
$\chi^{(a^*,1)}(\alpha, \vec{k})$	$1+\delta\epsilon$	2	$1+\gamma\epsilon$	2	$1+\delta\gamma$	$1+\delta\epsilon$	$1+\gamma\epsilon$
$\chi^{(b^*,1)}(\alpha, \vec{k})$	$1+\delta\epsilon$	$\gamma\epsilon^*+\delta^*\epsilon$	$1+\gamma\epsilon$	2	$\delta^2+\delta^*\gamma$	$\delta^2+\delta^*\epsilon$	$\delta\epsilon+\delta^*\gamma$
α							
χ	S_4^{3y}	S_4^z	S_4^{3z}				
$\chi^{(a^*,1)}(\alpha, \vec{k})$	$1+\delta\gamma$	$1+\delta\epsilon$	$1+\gamma\epsilon$				
$\chi^{(b^*,1)}(\alpha, \vec{k})$	$\delta\epsilon^*+\gamma\epsilon$	$\delta\gamma^*+\gamma\epsilon$	$\delta\gamma+\delta^*\epsilon$				
α							
χ	E	C_3^{xyz}	C_3^{2xyz}	$C_2^{\bar{xy}}$	$C_2^{\bar{xz}}$	$C_2^{\bar{yz}}$	I
$\chi^{(c^*,1)}(\alpha, \vec{k})$	4	1	1	$1+\delta^*\gamma^*$	$1+\delta\epsilon$	$1+\gamma\epsilon$	$1+\gamma\epsilon+$ $+\delta^*\gamma^*+\delta\epsilon$
$\chi^{(d^*,1)}(\alpha, \vec{k})$	4	$\delta\epsilon^*$	$\gamma\epsilon^*$	$(\epsilon^*)^2+(\delta\gamma\epsilon^2)^*$	$1+\delta^*\epsilon^*$	$1+\gamma^*\epsilon^*$	$(\epsilon^*)^2+\gamma\epsilon^*+$ $+(\delta\gamma\epsilon^2)^*+\delta\epsilon^*$
α							
χ	S_6^{xyz}	S_6^{5xyz}	$\sigma^{\bar{xy}}$	$\sigma^{\bar{xz}}$	$\sigma^{\bar{yz}}$	$C_3^{2x\bar{yz}}$	C_3^{xyz}
$\chi^{(c^*,1)}(\alpha, \vec{k})$	1	1	2	2	$2\gamma\epsilon^*$	$\delta\epsilon$	$\delta\gamma$
$\chi^{(d^*,1)}(\alpha, \vec{k})$	$\delta^*\epsilon^*$	$\gamma^*\epsilon^*$	2	$2\delta\epsilon^*$	$2\gamma\epsilon^*$	$\delta\gamma$	$\delta\epsilon^*$

Table 9 (Cont.)

α	C_2^{xy}	C_2^{xz}	$S_6^{5x\bar{y}z}$	$S_6^{x\bar{y}z}$	σ^{xy}	σ^{xz}	$C_3^{\bar{xy}z}$	$C_3^{2\bar{xy}z}$	
$\chi^{(c^*,1)}(\alpha, \vec{k})$	$\delta^*\epsilon + \gamma^*\epsilon$	$\delta^*\gamma + \delta^*\gamma^*$	$\delta^*\gamma$	$\delta^*\epsilon$	$2\delta\gamma$	$1 + \delta\epsilon$	1	1	
$\chi^{(d^*,1)}(\alpha, \vec{k})$	$\delta^*\epsilon^* + \gamma^*\epsilon^*$	$\gamma\epsilon^* + \gamma^*\epsilon$	$\delta^*\epsilon^*$	1	$2\delta\gamma$	$1 + \delta^*\epsilon^*$	$\delta^*\epsilon^*$	$\gamma^*\epsilon^*$	

α	C_2^{yz}	$S_6^{\bar{xy}z}$	$S_6^{5\bar{xy}z}$	σ^{yz}	$C_3^{2xy\bar{z}}$	$C_3^{xy\bar{z}}$	$S_6^{5xy\bar{z}}$	$S_6^{xy\bar{z}}$	Oth- ers
$\chi^{(c^*,1)}(\alpha, \vec{k})$	$\delta^*\gamma^* + \delta\gamma^*$	$\delta^*\gamma^*$	$\delta^*\gamma^*$	$1 + \gamma\epsilon$	$\delta\gamma$	$\gamma\epsilon$	$\gamma^*\epsilon$	$\delta\gamma^*$	0
$\chi^{(d^*,1)}(\alpha, \vec{k})$	$\delta^*\epsilon^* + \delta\epsilon^*$	$\gamma^*\epsilon^*$	$\delta^*\epsilon^*$	$1 + \gamma^*\epsilon^*$	$\delta\epsilon^*$	$\delta\gamma$	1	$\gamma^*\epsilon^*$	0

Table 9. Characters of the k-components of all the irreducible band representations for the diamond structure space group O_h^7 . a,b,c,d are the different symmetry centers of the closed strata. The characters are listed for the band representation that is induced from the unit representation of the little group. All other characters are obtained according to the formula

$$\chi^{(r,\rho)}(\alpha, \vec{k}) = \chi^{(r,1)}(\alpha) \times D^{(\rho)}(\alpha) . \text{ For } r = a,b, \rho = 1,2,3,4,5 ; \text{ for } r = c,d, \rho = 1,2,3,4,5,6. \delta = \exp\left(\frac{i}{2} k_x a\right) ; \gamma = \exp\left(\frac{i}{2} k_y a\right) ; \epsilon = \exp\left(\frac{i}{2} k_z a\right) :$$

SPACE GROUPS

EQUIVALENT BAND REPRESENTATIONS

	2	<u>89</u>	D_4^1		$D_4(a,5)$	$D_4(b,5)$	$C_4(g,3)$
	2				$D_4(c,5)$	$D_4(d,5)$	$C_4(h,3)$
	2	<u>97</u>	D_4^9		$D_4(a,5)$	$D_4(b,5)$	$C_4(e,3)$
$P4_2cm$	1	101	C_{4v}^3		$C_{2v}(a,2)$	$C_{2v}(a,4)$	
	1				$C_{2v}(b,2)$	$C_{2v}(b,4)$	
$P4cc$	1	103	C_{4v}^5		$C_4(a,3)$	$C_4(a,4)$	
	1				$C_4(b,3)$	$C_4(b,4)$	
$P4_2mc$	1	105	C_{4v}^7		$C_{2v}(a,2)$	$C_{2v}(a,4)$	
	1				$C_{2v}(b,2)$	$C_{2v}(b,4)$	
$I4cm$	1	108	C_{4v}^{10}		$C_4(a,3)$	$C_4(a,4)$	
	2	<u>111</u>	D_{2d}^1 $P\bar{6}3m$		$D_{2d}(a,5)$	$D_{2d}(c,5)$	$C_{2v}(g,2)$
	2				$D_{2d}(b,5)$	$D_{2d}(d,5)$	$C_{2v}(h,2)$
	2	<u>115</u>	D_{2d}^5 $P\bar{6}3m$		$D_{2d}(a,5)$	$D_{2d}(d,5)$	$C_{2v}(e,2)$
	2				$D_{2d}(b,5)$	$D_{2d}(c,5)$	$C_{2v}(f,2)$
	2	<u>119</u>	D_{2d}^9 $I\bar{4}3m$		$D_{2d}(a,5)$	$D_{2d}(b,5)$	$C_{2v}(e,2)$
	2				$D_{2d}(c,5)$	$D_{2d}(d,5)$	$C_{2v}(f,2)$
	2	<u>121</u>	D_{2d}^{11} $I\bar{4}3m$		$D_{2d}(a,5)$	$D_{2d}(b,5)$	$C_{2v}(e,2)$
	3	124	D_{4h}^2		$D_4(a,5)$	$C_{4h}(b,3+7)$	$C_4(g,3)$
	3				$D_4(c,5)$	$C_{4h}(d,3+7)$	$C_4(h,3)$
	2	125	D_{4h}^3		$D_4(a,5)$	$D_4(b,5)$	$C_4(g,3)$
	2				$D_{2d}(c,5)$	$D_{2d}(d,5)$	$C_{2v}(h,2)$
	3	126	D_{4h}^4		$D_4(a,5)$	$D_4(b,5)$	$C_4(e,3)$
	3	129	D_{4h}^7		$D_{2d}(a,5)$	$D_{2d}(b,5)$	$C_{2v}(f,2)$
$P4_1nc$	1	130	D_{4h}^8		$C_4(c,3)$	$C_4(c,4)$	
	3	131	D_{4h}^9		$D_{2d}(e,5)$	$D_{2h}(a,2+7)$	$C_{2v}(g,2)$
	3				$D_{2d}(f,5)$	$D_{2h}(b,2+7)$	$C_{2v}(h,2)$
	3	132	D_{4h}^{10}		$D_{2d}(b,5)$	$D_{2h}(a,2+7)$	$C_{2v}(g,2)$

SPACE GROUPS		EQUIVALENT BAND REPRESENTATIONS		
		$D_{2d}(d,5)$	$D_{2h}(c,2+7)$	$C_{2v}(h,2)$
134	D_{4h}^{12}	$D_{2d}(a,5)$	$D_{2d}(b,5)$	$C_{2v}(g,2)$
137	D_{4h}^{15}	$D_{2d}(a,5)$	$D_{2d}(b,5)$	$C_{2v}(d,2)$
		$C_{2v}(d,2)$	$C_{2v}(d,4)$	
138	D_{4h}^{16}	$C_{2v}(e,2)$	$C_{2v}(e,4)$	
139	D_{4h}^{17}	$D_{2d}(d,5)$	$D_{2h}(c,2+7)$	$C_{2v}(g,2)$
140	D_{4h}^{18}	$D_4(a,5)$	$C_{4h}(c,3+7)$	$C_4(f,3)$
		$D_{2d}(b,5)$	$D_{2h}(d,2+7)$	$C_{2v}(g,2)$
141	D_{4h}^{19}	$D_{2d}(a,5)$	$D_{2d}(b,5)$	$C_{2v}(e,2)$
149	D_3^1	$D_3(a,3)$	$D_3(b,3)$	$C_3(g,2)$
		$D_3(c,3)$	$D_3(d,3)$	$C_3(h,2)$
		$D_3(e,3)$	$D_3(f,3)$	$C_3(i,2)$
150	D_3^2	$D_3(a,3)$	$D_3(b,3)$	$C_3(c,2)$
155	D_3^7	$D_3(a,3)$	$D_3(b,3)$	$C_3(c,2)$
158	C_{3v}^3	$C_3(a,2)$	$C_3(a,3)$	
		$C_3(b,2)$	$C_3(b,3)$	
		$C_3(c,2)$	$C_3(c,3)$	
159	C_{3v}^4	$C_3(a,2)$	$C_3(a,3)$	
161	C_{3v}^6	$C_3(a,2)$	$C_3(a,3)$	
162	D_{3d}^1	$D_3(c,3)$	$D_3(d,3)$	$C_3(h,2)$
163	D_{3d}^2	$D_3(a,3)$	$C_{3i}(b,2+5)$	$C_3(e,2)$
		$D_3(c,3)$	$D_3(d,3)$	$C_3(f,2)$
165	D_{3d}^4	$D_3(a,3)$	$C_{3i}(b,2+5)$	$C_3(c,2)$
167	D_{3d}^6	$D_3(a,3)$	$C_{3i}(b,2+5)$	$C_3(c,2)$
177	D_6^1	$D_6(a,5)$	$D_6(b,5)$	$C_6(e,3)$
		$D_6(a,b)$	$D_6(b,6)$	$C_6(e,5)$
		$D_3(c,3)$	$D_3(d,3)$	$C_3(h,2)$

SPACE GROUPS		EQUIVALENT BAND REPRESENTATIONS		
182	D_6^6	$D_3(a,3)$	$D_3(b,3)$	$C_3(e,2)$
		$D_3(c,3)$	$D_3(d,3)$	$C_3(f,2)$
188	D_{3h}^2	$D_3(a,3)$	$C_{3h}(b,2+5)$	$C_3(g,2)$
		$D_3(c,3)$	$C_{3h}(d,2+5)$	$C_3(h,2)$
		$D_3(e,3)$	$C_{3h}(f,2+5)$	$C_3(i,2)$
190	D_{3h}^4	$D_3(a,3)$	$C_{3h}(b,2+5)$	$C_3(e,2)$
192	D_{6h}^2	$D_6(a,5)$	$C_{6h}(b,5+11)$	$C_6(e,5)$
		$D_6(a,6)$	$C_{6h}(b,3+9)$	$C_6(e,3)$
		$D_3(c,3)$	$C_{3h}(d,2+5)$	$C_3(h,2)$
193	D_{6h}^3	$D_3(d,3)$	$C_{3h}(c,2+5)$	$C_3(h,2)$
207	O^1	$D_4(c,5)$	$O(b,4+5)$	$C_4(f,3)$
208	O^2	$D_3(b,3)$	$T(a,2+4)$	$C_3(g,2)$
		$D_3(c,3)$	$T(a,2+4)$	$C_3(g,2)$
		$D_3(b,3)$	$D_3(c,3)$	$C_3(g,2)$
210	O^4	$D_3(c,3)$	$T(a,2+4)$	$C_3(e,2)$
		$D_3(d,3)$	$T(a,2+4)$	$C_3(e,2)$
		$D_3(c,3)$	$D_3(d,3)$	$C_3(e,2)$
211	O^5	$D_3(c,3)$	$O(a,3+4+5)$	$C_3(f,2)$
212	O^6	$D_3(a,3)$	$D_3(b,3)$	$C_3(c,2)$
213	O^7	$D_3(a,3)$	$D_3(b,3)$	$C_3(c,2)$
214	O^8	$D_3(a,3)$	$D_3(b,3)$	$C_3(e,2)$
215	T_d^1	$D_{2d}(d,5)$	$T_d(a,4+5)$	$C_{2v}(f,2)$
		$D_{2d}(c,5)$	$T_d(b,4+5)$	$C_{2v}(g,2)$
222	O_h^2	$D_4(b,5)$	$O(a,4+5)$	$C_4(e,3)$
223	O_h^3	$D_{2d}(c,5)$	$D_{2h}(b,2+7)$	$C_{2v}(g,2)$
		$D_{2d}(d,5)$	$D_{2h}(b,2+7)$	$C_{2v}(h,2)$
		$D_{2d}(c,5)$	$D_{2d}(d,5)$	$C_{2v}(g,2)$
		$D_3(e,3)$	$T_h(a,2+7)$	$C_3(i,2)$

SPACE GROUPS		EQUIVALENT BAND REPRESENTATIONS		
3	224 O_h^4	$D_{2d}(d,5)$	$T_d(a,4+5)$	$C_{2v}(g,2)$
3	226 O_h^6	$D_{2d}(c,5)$	$T_h(b,4+8)$	$C_{2v}(e,2)$
3	228 O_h^8	$D_3(b,3)$	$T(a,3+4)$	$\{C_3(e,2)$ $\{C_3(e,2+5)$
3	229 O_h^9	$D_{2d}(d,5)$	$D_{4h}(b,5+10)$	$C_{2v}(g,2)$
3	230 O_h^{10}	$D_3(b,3)$	$C_{3i}(a,2+5)$	$C_3(e,2)$

Table 10. List of equivalent band representations (also called exceptional ones) induced by maximal finite subgroups. We give an example of using this Table (in addition to the examples in the Summary Section) :

Space group 89 (D_4^1) . From Ref. 13 we learn that there exist six closed Wyckoff positions a,b,c,d,e,f. The band representations obtained from them are $D_4(a,i)$, $D_4(b,i)$, $D_4(c,i)$, $D_4(d,i)$, $D_2(e,j)$, $D_2(f,j)$ where i runs from 1 to 5 and j from 1 to 4 since D_4 has five irreducible representations and D_2 four. This leads to $4 \times 5 + 2 \times 4 = 28$ band representations. From the Table we see that there are two pairs of equivalent representations among them. They correspond to inductions from one-dimensional representations of a non-maximal isotropy group given in the third column. We are left with $28-2 = 26$ non equivalent irreducible-band representations. When a band representation is equivalent to a direct sum of induced representations (first example appears for group 124) it is, of course, a reducible-band representation.

Table 11. Continuity Chords of Irreducible Band Representations for 2-Dimensional Space Groups. The symmetry points in the Brillouin zone and their symmetry groups are given in Table 12. The irreducible representations for the non-symmorphic space groups are presented in Table 13.

OBLIQUE

p2 N°2

	(a,1)	(a,2)	(b,1)	(b,2)	(c,1)	(c,2)	(d,1)	(d,2)
Γ	Γ_1	Γ_2	Γ_1	Γ_2	Γ_1	Γ_2	Γ_1	Γ_2
X	X_1	X_2	X_1	X_2	X_2	X_1	X_2	X_1
Y	Y_1	Y_2	Y_2	Y_1	Y_1	Y_2	Y_2	Y_1
R	R_1	R_2	R_2	R_1	R_2	R_1	R_1	R_2

RECTANGULAR

plml N°3

	(a,1)	(a,2)	(b,1)	(b,2)
Γ	Γ_1	Γ_2	Γ_1	Γ_2
X	X_1	X_2	X_2	X_1

plgl N°4

	(a,1)
Γ	Γ_1, Γ_2
X	X_1, X_2

clml N°5*

	(a,1)	(a,2)	(b,1)	(b,2)
Γ	Γ_1	Γ_2	Γ_1	Γ_2
X	X_1	X_2	X_2	X_1

* The symmetry center $b \frac{a}{2} y$ is missing in Ref. 13.

p2mm N°6

	(a,1)	(a,2)	(a,3)	(a,4)	(b,1)	(b,2)	(b,3)	(b,4)
Γ	Γ_1	Γ_3	Γ_2	Γ_4	Γ_1	Γ_3	Γ_2	Γ_4
X	X_1	X_3	X_2	X_4	X_1	X_3	X_2	X_4
Y	Y_1	Y_3	Y_2	Y_4	Y_3	Y_1	Y_4	Y_2
R	R_1	R_3	R_2	R_4	R_3	R_1	R_4	R_2

	(c,1)	(c,2)	(c,3)	(c,4)	(d,1)	(d,2)	(d,3)	(d,4)
Γ	Γ_1	Γ_3	Γ_2	Γ_4	Γ_1	Γ_3	Γ_2	Γ_4
X	X_4	X_2	X_3	X_1	X_4	X_2	X_3	X_1
Y	Y_1	Y_3	Y_2	Y_4	Y_3	Y_1	Y_4	Y_2
R	R_4	R_2	R_3	R_1	R_2	R_4	R_1	R_3

p2mg N°7

	(a,1)	(a,2)	(b,1)	(b,2)	(c,1)	(c,2)
Γ	$\Gamma_1\Gamma_2$	$\Gamma_3\Gamma_4$	$\Gamma_1\Gamma_2$	$\Gamma_3\Gamma_4$	$\Gamma_1\Gamma_3$	$\Gamma_2\Gamma_4$
X	X_1	X_1	X_1	X_1	X_1	X_1
Y	Y_1Y_2	Y_3Y_4	Y_3Y_4	Y_1Y_2	Y_1Y_3	Y_2Y_4
R	R_1	R_1	R_1	R_1	R_1	R_1

p2gg N°8

	(a,1)	(a,2)	(b,1)	(b,2)
Γ	$\Gamma_1\Gamma_2$	$\Gamma_3\Gamma_4$	$\Gamma_1\Gamma_2$	$\Gamma_3\Gamma_4$
X	X_1	X_1	X_1	X_1
Y	Y_1	Y_1	Y_1	Y_1
R	R_1R_2	R_3R_4	R_3R_4	R_1R_2

HEXAGONAL

p3 N°13

	(a,1)	(a,2)	(a,3)	(b,1)	(b,2)	(b,3)	(c,1)	(c,2)	(c,3)
Γ	Γ_1	Γ_2	Γ_3	Γ_1	Γ_2	Γ_3	Γ_1	Γ_2	Γ_3
M	M_1	M_2	M_3	M_3	M_1	M_2	M_2	M_3	M_1
N	N_1	N_2	N_3	N_2	N_3	N_1	N_3	N_1	N_2

p3m1 N°14

	(a,1)	(a,2)	(a,3)	(b,1)	(b,2)	(b,3)	(c,1)	(c,2)	(c,3)
Γ	Γ_1	Γ_2	Γ_3	Γ_1	Γ_2	Γ_3	Γ_1	Γ_2	Γ_3
M	M_1	M_2	M_3	M_3	M_1	M_2	M_2	M_3	M_1
N	N_1	N_2	N_3	N_2	N_3	N_1	N_3	N_1	N_2

p31m N°15

	(a,1)	(a,2)	(a,3)	(b,1)	(b,2)	(b,3)
Γ	Γ_1	Γ_2	Γ_3	$\Gamma_1\Gamma_2$	Γ_3	Γ_3
M	M_1	M_2	M_3	M_3	M_1M_2	M_3
N	N_1	N_2	N_3	N_3	N_3	N_1N_2

p6 N°16

	(a,1)	(a,2)	(a,3)	(a,4)	(a,5)	(a,6)	(b,1)	(b,2)	(b,3)	(c,1)	(c,2)
Γ	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	$\Gamma_1\Gamma_2$	$\Gamma_4\Gamma_5$	$\Gamma_3\Gamma_6$	$\Gamma_1\Gamma_3\Gamma_4$	$\Gamma_2\Gamma_5\Gamma_6$
M	M_1	M_1	M_3	M_2	M_2	M_3	M_2M_3	M_1M_3	M_1M_2	$M_1M_2M_3$	$M_1M_2M_3$
N	N_1	N_1	N_3	N_2	N_2	N_3	N_2N_3	N_1N_3	N_1N_2	$N_1N_2N_3$	$N_1N_2N_3$
X	X_1	X_2	X_1	X_1	X_2	X_2	X_1X_2	X_1X_2	X_1X_2	$X_1^2X_2$	$(2X_1)X_2$
Y	Y_1	Y_2	Y_1	Y_1	Y_2	Y_2	Y_1Y_2	Y_1Y_2	Y_1Y_2	$Y_1^2Y_2$	$(2Y_1)Y_2$
R	R_1	R_2	R_1	R_1	R_2	R_2	R_1R_2	R_1R_2	R_1R_2	$R_1^2R_2$	$(2R_1)R_2$

p6mm N°17

	(a,1)	(a,2)	(a,3)	(a,4)	(a,5)	(a,6)	(b,1)	(b,2)	(b,3)	(c,1)	(c,2)	(c,3)	(c,4)
Γ	Γ_1	Γ_2	Γ_3	Γ_4	Γ_6	Γ_5	$\Gamma_1\Gamma_3$	$\Gamma_2\Gamma_4$	$\Gamma_5\Gamma_6$	$\Gamma_1\Gamma_5$	$\Gamma_3\Gamma_6$	$\Gamma_2\Gamma_5$	$\Gamma_4\Gamma_6$
M	M_1	M_2	M_1	M_2	M_3	M_3	M_3	M_3	$M_1M_2M_3$	M_1M_3	M_2M_3	M_2M_3	M_1M_3
N	N_1	N_2	N_1	N_2	N_3	N_3	N_3	N_3	$N_1N_2N_3$	N_1N_3	N_2N_3	N_2N_3	N_1N_3
X	X_1	X_2	X_3	X_4	X_3X_4	X_1X_2	X_1X_3	X_2X_4	$X_1X_2X_3X_4$	$X_1X_3X_4$	$X_1X_2X_3$	$X_2X_3X_4$	$X_1X_2X_4$
Y	Y_1	Y_2	Y_3	Y_4	Y_3Y_4	Y_1Y_2	Y_1Y_3	Y_2Y_4	$Y_1Y_2Y_3Y_4$	$Y_1Y_3Y_4$	$Y_1Y_2Y_3$	$Y_2Y_3Y_4$	$Y_1Y_2Y_4$
R	R_1	R_2	R_3	R_4	R_3R_4	R_1R_2	R_1R_3	R_2R_4	$R_1R_2R_3R_4$	$R_1R_3R_4$	$R_1R_2R_3$	$R_2R_3R_4$	$R_1R_2R_4$

1. OBLIQUE

WAVE VECTOR	SYMMETRY
$\Gamma = (0,0)$	C_2
$X = \frac{\vec{k}_1}{2}$	C_2
$Y = \frac{\vec{k}_2}{2}$	C_2
$R = \frac{1}{2} (\vec{k}_1 + \vec{k}_2)$	C_2

2. RECTANGULAR (SIMPLE)

WAVE VECTOR	SYMMETRY
$\Gamma = (0,0)$	C_{2v}
$X = \frac{\vec{k}_1}{2}$	C_{2v}
$Y = \frac{\vec{k}_2}{2}$	C_{2v}
$R = \frac{1}{2} (\vec{k}_1 + \vec{k}_2)$	C_{2v}

3. RECTANGULAR (CENTERED)

WAVE VECTOR	SYMMETRY
$\Gamma = (0,0)$	C_{2v}
$Y = \frac{\vec{k}_2}{2}$	C_{2v}
$R = \frac{1}{2} (\vec{k}_1 + \vec{k}_2)$	C_2

4. SQUARE

WAVE VECTOR	SYMMETRY
$\Gamma = (0,0)$	C_{4v}
$R = \frac{1}{2} (\vec{k}_1 + \vec{k}_2)$	C_{4v}
$X = \frac{\vec{k}_1}{2}$	C_{2v}

5. HEXAGONAL

WAVE VECTOR	SYMMETRY
$\Gamma = (0,0)$	C_{6v}
$M = \frac{1}{3} (\vec{k}_1 + \vec{k}_2)$	C_{3v}
$N = \frac{2}{3} (\vec{k}_1 + \vec{k}_2)$	C_{3v}
$X = \frac{\vec{k}_1}{2}$	C_{2v}
$Y = \frac{\vec{k}_2}{2}$	C_{2v}
$R = \frac{1}{2} (\vec{k}_1 + \vec{k}_2)$	C_{2v}

Table 12. Symmetry points in the Brillouin zone and their isotropy groups for 2-dimensional space groups.

1. RECTANGULAR

p1g1 (N°4) :

X	E	σ^x
X_1	1	δ
X_2	1	$-\delta$

$$\delta = \exp(i \frac{k_y b}{2})$$

p2mg (N°7) :

X,R	E	C_2	σ^x	σ^y
1	2		0	

Y like Γ

pgg (N°8) :

X,Y	E	C_2	σ^x	σ^y
1	2		0	

R	E	C_2	σ^x	σ^y
R_1	1	1	i	i
R_2	1	1	i	$-i$
R_3	1	-1	i	$-i$
R_4	1	-1	$-i$	i

2. SQUARE

p4gm (N°12) :

R	E	C_4	C_4^2	C_4^3	σ^{xy}	$\overline{\sigma^{xy}}$	σ^x	σ^y
R_1	1	i	-1	$-i$	1	-1	i	$-i$
R_2	1	i	-1	$-i$	-1	1	$-i$	i
R_3	1	$-i$	-1	i	$+1$	-1	$-i$	i
R_4	1	$-i$	-1	i	-1	1	i	$-i$
R_5	2	0	2	0	0	0	0	0

X	E	C_2	σ^x	σ^y
X_1	2		0	

Table 13. Irreducible representations of non-symmetric groups for points on the surface of the Brillouin zone.