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On the relationship between crystal quantum numbers and irreducible representations of point groups

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A classification of all point groups allows us to derive general character tables. The crystal quantum number description of eigenfunctions $|JM\rangle$ is related to the symmetry properties, and general relationships between them are given.

Key words: Crystal field theory — Crystal quantum numbers — Point group representations

1. Introduction

Most of the works using crystal field theory provide eigenfunctions in term of crystal quantum numbers μ as defined by Wybourne [1]. Nevertheless, it is sometimes useful to know the irreducible representations of the crystal field Hamiltonian point group to which the eigenfunctions belong. Moreover, in the absence of an external magnetic field, this latter description of the eigenfunctions leads to maximum decomposition into subsets, whereas the former provides a reducible set. Several partial tables of the irreducible representations already exist (e.g. [1, 2]) but these are only for a few point groups; our purpose is to derive a general method for obtaining this information. The reader not familiar with point group theory is referred to Cotton's book [3].

2. Definitions and notation

Throughout the text, we will use the following notations:
- n is the order of the principal (z) axis.

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– m is an index for the m-th irreducible representation (i.r.) of the group.
– k and k' are integers.
– C_n^α is the α-th power of the operation C_n (rotation of $2\pi/n$ about the principal axis); $\alpha = 1, \ldots, n$.
– β takes the values $1, \ldots, (n-1)/2$ for odd n and $1, \ldots, (n/2)-1$ for even n.
– $|JM\rangle$ is an eigenfunction of the system (or a part eigenfunction in intermediate coupling); for each J value, there are $(2J+1)$ such eigenfunctions.
– μ is a crystal quantum number. It is solution of the equation (see [1])

$$M = kn + \mu \tag{1}$$

This is in fact the formula "dividend = quotient · divisor + remainder" for the division M/n appearing for example in $\exp(i2\pi\alpha M/n)$ (see Eq. 3). μ is thus the remainder upon division of M by n and each M value is related to only one μ value which depends on n.
– $\chi_m(C_n^\alpha)$ is the character associated to the operation C_n^α in the m-th i.r.; an asterisk denotes complex conjugation.
– N is the number of electrons in the system whose eigenfunctions are $|JM\rangle$.
– ε is equal to $\exp(i2\pi/n)$.
– R is the real part of a complex number.

3. A classification of the point groups

Following Prather [4], we can construct a table (Table 1) showing the connections between the different point groups. The generic names of the seven families appearing for even n values and of the five families appearing for odd n values are:

a) C_n This is the cyclic group of order n with operations C_n^α.

b) $C_n \times I$ Holohedric group of order $2n$ with operations C_n^α and $C_n^\alpha I = IC_n^\alpha$ where I is the inversion operator which commutes with C_n^α.

c) $\langle C_n \times I\rangle$ Hemihedric group of order n with operations C_n^α (α even) and $C_n^\alpha I$ (α odd); these groups only exist for even n values.

Table 1. Classification of point groups

$\langle C_n \times I\rangle$ (n)	$C_n \times I$ ($2n$)	C_n (n)	$\{C_nC_2'\}$ ($2n$)	$\{C_nC_2'\} \times I$ ($4n$)	$\langle\{C_nC_2'\} \times I\rangle_a$ ($2n$)	$\langle\{C_nC_2'\} \times I\rangle_b$ ($2n$)	
C_{1h}	C_{2h}	C_2	D_2	D_{2h}	C_{2v}	D_{1h}	order of principal axis n ↓
	S_6	C_3	D_3	D_{3d}	C_{3v}		
S_4	C_{4h}	C_4	D_4	D_{4h}	C_{4v}	D_{2d}	
	S_{10}	C_5	D_5	D_{5d}	C_{5v}		
C_{3h}	C_{6h}	C_6	D_6	D_{6h}	C_{6v}	D_{3h}	
	S_{14}	C_7	D_7	D_{7d}	C_{7v}		
S_8	C_{8h}	C_8	D_8	D_{8h}	C_{8v}	D_{4d}	
⋮	⋮	⋮	⋮	⋮	⋮	⋮	

C_{1h} is sometimes called C_s

d) $\{C_nC'_2\}$ Dihedral group of order $2n$ with operations C_n^α and $C_n^\alpha C'_2$; the operation C'_2 which corresponds to a twofold axis perpendicular to the n-fold one does not commute with the other operations.

e) $\{C_nC'_2\}\times I$ Holohedric group of order $4n$ comprising all operations of $\{C_nC'_2\}$ and the same operations multiplied by the inversion.

f) $\langle\{C_nC'_2\}\times I\rangle_a$ Hemihedric group of order $2n$; the set of operations is a restriction of $\{C_nC'_2\}\times I$ where the operations of $\{C_nC'_2\}$ not appearing in C_n and those of $C_n\times I$ not appearing in C_n have been suppressed.

g) $\langle\{C_nC'_2\}\times I\rangle_b$ Hemihedric group of order $2n$; the operations are C_n^α (α even) + operations of $\{C_nC'_2\}$ resulting from C_n^α (α even) + operations of $C_n\times I$ resulting from C_n^α (α odd) + operations of $\{C_nC'_2\}\times I$ resulting from C_n^α (α odd); these groups only exist for even values of n.

4. Relationships between crystal quantum numbers and irreducible representations of the crystal field Hamiltonian point group

It is necessary to derive the correspondence for even N only because when N is odd, Kramers' theorem (see [4, 5]) tells us that, in the absence of an external magnetic field, all the levels are at least doublets. The maximum decomposition is thus already achieved by the crystal quantum number description of eigenfunctions, these numbers being $\mu=\pm(2k+1)/2$ for a system with an odd number of electrons. In what follows, we will thus assume that N is even.

We first show that the separation of the complete set of eigenfunctions into subsets characterized by different μ values corresponds to the symmetry decrease $O_3\rightarrow C_n$; we thus take into account restrictions given by the presence of the principal axis only.

As C_n is abelian, each operation C_n^α forms a class by itself and the i.rs are of dimension one. The character associated with C_n^α in the m-th i.r. is:

$$\chi_m(C_n^\alpha)=\exp\,(i2\pi\alpha m/n) \tag{2}$$

From the definition (1) of μ, we get

$$\begin{aligned} C_n^\alpha|JM\rangle &= \exp\,(i2\pi\alpha M/n)|JM\rangle=\exp\,(i2\pi\alpha(\mu+kn)/n)|JM\rangle \\ &= \exp\,(i2\pi\alpha\mu/n)|JM\rangle. \end{aligned} \tag{3}$$

We see from (2) and (3) that each μ value corresponds to a different i.r. of C_n and thus, classifying M values following μ is equal to decomposing the set of $(2J+1)$ functions $|JM\rangle$ for one J value into subsets transforming like an i.r. of C_n. As

$$\chi_{n-m}(C_n^\alpha)=\exp\,(i2\pi\alpha(n-m)/n)=\exp\,(-i2\pi\alpha m/n)=\chi_m^*(C_n^\alpha)$$

we see that the i.rs. of C_n are conjugated in pairs. It is, however, usually possible to consider these two unidimensional representations as a bidimensional one, this being no longer exact when the perturbation having the studied symmetry is an external magnetic field. As this is precisely the interaction that removes the

Table 2. Character table for C_n (n even)

C_n	C_n^1	C_n^2	...	$C_n^{n/2-2}$	$C_n^{n/2-1}$	$C_n^{n/2}$	$C_n^{n/2+1}$	$C_n^{n/2+2}$	...	C_n^{n-2}	C_n^{n-1}	C_n^n	
$\mu=0$	+1	+1	...	+1	+1	+1	+1	+1	...	+1	+1	+1	A
$\mu=+\beta$	ε^{β}	$\varepsilon^{2\beta}$	...	$-\varepsilon^{*2\beta}$	$-\varepsilon^{*\beta}$	$(-1)^{\beta}$	$-\varepsilon^{\beta}$	$-\varepsilon^{2\beta}$	...	$\varepsilon^{*2\beta}$	$\varepsilon^{*\beta}$	+1	E_β
$\mu=-\beta$	$\varepsilon^{*\beta}$	$\varepsilon^{*2\beta}$	...	$-\varepsilon^{2\beta}$	$-\varepsilon^{\beta}$	$(-1)^{\beta}$	$-\varepsilon^{*\beta}$	$-\varepsilon^{*2\beta}$	...	$\varepsilon^{2\beta}$	ε^{β}	+1	
$\mu=n/2$	−1	+1	...	$(-1)^{n/2-2}$	$(-1)^{n/2-1}$	$(-1)^{n/2}$	$(-1)^{n/2+1}$	$(-1)^{n/2+2}$	...	+1	−1	+1	B

degeneracy of μ values, $\mu=\pm\beta$, we see that this degeneracy is related to time reversal symmetry.

We now construct the character tables for the different group families and search for the connections between μ and the i.rs. For all families, when n is even, μ values are $0, \pm\beta, (n/2)$ $(\beta=1,\ldots,(n/2)-1)$ and when n is odd, $\mu=0,\pm\beta$ $(\beta=1,\ldots,(n-1)/2)$.

a) C_n

(i) $\mu=0$ always correspond to the totally symmetric i.r. of C_n since, $\exp(i2\pi\alpha 0/n)=+1$ whatever α may be.

(ii) $\chi_\mu(C_n^{n-\alpha})=\chi_\mu^*(C_n^\alpha)$ since, $\exp(i2\pi(n-\alpha)\mu/n)=\exp(-i2\pi\alpha\mu/n)$.

(iii) $\chi_\mu(C_n^n=E)=+1$ for all μ and n.

(iv) When n is even, $\mu=(n/2)$ corresponds to an i.r. with +1 or −1 depending on whether α is even or odd.

(v) When n is even, $\chi_\mu(C_n^{n/2+\alpha})=(-1)^\mu\chi_\mu(C_n^\alpha)$. It is thus possible to study only half of the symmetry operations $C_n^1,\ldots,C_n^{n/2}$ instead of the total set $C_n^1,\ldots,C_n^{n/2},\ldots,C_n^n$.

(vi) When n is even, we get from (ii) and (v) the following result: $(-1)^\mu\chi_\mu(C_n^{n/2+\alpha})=\chi_\mu^*(C_n^{n-\alpha})$.

With all those properties, we are now able to construct general character tables for C_n, when n is even (Table 2) or odd (Table 3). Mulliken's notation for i.rs is indicated on the right of the tables (last column).

b) $C_n\times I$

When n is even, $C_n\times I=C_{nh}$ and when n is odd, $C_n\times I=S_{2n}$ (Schoenflies' notation). In the character table, the i.r. corresponding to $\mu=(n/2)$ only exists for even n values.

Table 3. Character table for C_n (n odd)

C_n	C_n^1	C_n^2	C_n^3	...	C_n^{n-3}	C_n^{n-2}	C_n^{n-1}	C_n^n	
$\mu=0$	+1	+1	+1	...	+1	+1	+1	+1	A
$\mu=+\beta$	ε^{β}	$\varepsilon^{2\beta}$	$\varepsilon^{3\beta}$	...	$\varepsilon^{*3\beta}$	$\varepsilon^{*2\beta}$	$\varepsilon^{*\beta}$	+1	E_β
$\mu=-\beta$	$\varepsilon^{*\beta}$	$\varepsilon^{*2\beta}$	$\varepsilon^{*3\beta}$	...	$\varepsilon^{3\beta}$	$\varepsilon^{2\beta}$	ε^{β}	+1	

On the right of the tables (Table 4 and following), we have indicated what conditions are required for an eigenfunction $|JM\rangle$ to be a basis function of the facing irreducible representation. The conditions noted here are easily found by studying the transformation properties of $|JM\rangle$ under inversion. As $I|JM\rangle = (-1)^J|JM\rangle$, we see that $|JM\rangle$ transforms in an even way when J is even and in an odd way when J is odd.

Important remark. These conditions hold for monoelectronic $|JM\rangle$ functions where J represents a single orbital angular momentum. When dealing with polyelectronic functions, J being either the total or the total orbital angular momentum (usually denoted as J and L respectively), the parity under inversion no longer depends on J but on the sum of all monoelectronic orbital angular momenta $\sum_{i=1}^{N} l_i$. This is also true for $\{C_nC_2'\}\times I$ groups.

c) $\langle C_n \times I\rangle$

These groups only exist when n is even. If $(n/2)$ is even, $\langle C_n\times I\rangle = S_n$ and if $(n/2)$ is odd, $\langle C_n \times I\rangle = C_{n/2h}$. There is an isomorphism between these groups and C_n, so the conclusions found for the latter also apply to $\langle C_n\times I\rangle$. The decomposition of the total set of eigenfunctions into subsets following μ values is, as for C_n, the maximum decomposition (in absence of an external magnetic field).

d) $\{C_nC_2'\}$

In Schoenflies' notation, these are the D_n groups.

A. n odd

(i) C_n^α and $C_n^{n-\alpha}$ belong to the same class because of the presence of the perpendicular binary axes C_2' $(\alpha = 1, 2, \ldots, (n-1)/2)$. We get $(n-1)/2$ such classes.

(ii) E forms a class by itself.

(iii) The n C_2' belong to the same class because it is possible to obtain one from another through the C_n^α operations.

We thus have a total of $(n+3)/2$ classes and irreducible representations. The complex conjugated representations of C_n collapse into bidimensional ones whose characters are the sums of the characters of the two components.

Table 4. Character table for $C_n \times I$

$C_n \times I$	C_n^α	$C_n^\alpha I$		
$\mu = 0$ $\mu = \pm\beta$ $\mu = n/2$	+Table for C_n	+Table for C_n	A_g $E_{\beta g}$ B_g	even J values[a]
$\mu = 0$ $\mu = \pm\beta$ $\mu = n/2$	+Table for C_n	−Table for C_n	A_u $E_{\beta u}$ B_u	odd J values[a]

[a] See remark in Sect. 4b

Because of the introduction of binary axes, we must find new basis functions for spanning the i.rs of these groups, since, $C_2'|JM\rangle=(-1)^{J+M}|J-M\rangle$. C_2' does preserve the functions:

$$\begin{cases} |JM\rangle^+ = \dfrac{1}{\sqrt{2}}(|J-M\rangle + (-1)^M|JM\rangle) \\ \\ |JM\rangle^- = \dfrac{1}{\sqrt{2}}(|J-M\rangle - (-1)^M|JM\rangle) \end{cases} \tag{4}$$

corresponding to the tesseral harmonics of first and second kind respectively. With these new functions we get

$$C_2'\begin{pmatrix}|JM\rangle^+\\|JM\rangle^-\end{pmatrix} = (-1)^J\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}\begin{pmatrix}|JM\rangle^+\\|JM\rangle^-\end{pmatrix}.$$

If one of the functions transforms in a symmetrical way under C_2', the other one will transform antisymmetrically.

We now search for the transformation properties of these new functions under all other operations C_n^α, S_n^α, I, σ_h, σ_v and C_2'', σ_d for even n values.

$$C_n^\alpha\begin{pmatrix}|JM\rangle^+\\|JM\rangle^-\end{pmatrix} = \begin{pmatrix}\cos(2\pi\alpha M/n) & -i\sin(2\pi\alpha M/n)\\-i\sin(2\pi\alpha M/n) & \cos(2\pi\alpha M/n)\end{pmatrix}\begin{pmatrix}|JM\rangle^+\\|JM\rangle^-\end{pmatrix}. \tag{5}$$

The conditions for the functions to transform in an independent manner is $\sin(2\pi\alpha M/n)=0$, i.e. $2\alpha M=kn$. This is in fact the condition for M to be associated with an unidimensional i.r. ($\mu=0$ for odd n values and $\mu=0$ and $\mu=n/2$ for even n values).

$$I\begin{pmatrix}|JM\rangle^+\\|JM\rangle^-\end{pmatrix} = (-1)^J\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}\begin{pmatrix}|JM\rangle^+\\|JM\rangle^-\end{pmatrix}$$

$$\sigma_h\begin{pmatrix}|JM\rangle^+\\|JM\rangle^-\end{pmatrix} = (-1)^{J+M}\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}\begin{pmatrix}|JM\rangle^+\\|JM\rangle^-\end{pmatrix}$$

$$\sigma_v\begin{pmatrix}|JM\rangle^+\\|JM\rangle^-\end{pmatrix} = (-1)^M\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}\begin{pmatrix}|JM\rangle^+\\|JM\rangle^-\end{pmatrix}$$

$$S_n^\alpha\begin{pmatrix}|JM\rangle^+\\|JM\rangle^-\end{pmatrix} = (-1)^{J+M}\begin{pmatrix}\cos(2\pi\alpha M/n) & -i\sin(2\pi\alpha M/n)\\-i\sin(2\pi\alpha M/n) & \cos(2\pi\alpha M/n)\end{pmatrix}\begin{pmatrix}|JM\rangle^+\\|JM\rangle^-\end{pmatrix}$$

$$C_2''\begin{pmatrix}|JM\rangle^+\\|JM\rangle^-\end{pmatrix} = (-1)^J\begin{pmatrix}\cos(2\pi\alpha M/n) & -i\sin(2\pi\alpha M/n)\\i\sin(2\pi\alpha M/n) & -\cos(2\pi\alpha M/n)\end{pmatrix}\begin{pmatrix}|JM\rangle^+\\|JM\rangle^-\end{pmatrix}$$

$$\sigma_d\begin{pmatrix}|JM\rangle^+\\|JM\rangle^-\end{pmatrix} = (-1)^M\begin{pmatrix}\cos(2\pi\alpha M/n) & -i\sin(2\pi\alpha M/n)\\i\sin(2\pi\alpha M/n) & -\cos(2\pi\alpha M/n)\end{pmatrix}\begin{pmatrix}|JM\rangle^+\\|JM\rangle^-\end{pmatrix}.$$

The transformation properties of $|J0\rangle$ are those of $|JM\rangle^+$ with $M=0$. The character table for $\{C_nC_2'\}$ with n odd is presented in Table 5.

The i.r. $\mu=0$ of C_n gives rise to two i.rs. for $\{C_nC_2'\}$, one for which the basis function does not change sign under C_2' and one for which it does. We have

Table 5. Character table for $\{C_nC_2'\}$ (n odd)

$\{C_nC_2'\}$	E	$2C_n^1$	$2C_n^2$	...	$2C_n^{(n-1)/2}$	nC_2'		
$\mu=0$	$+1$	$+1$	$+1$	...	$+1$	$+1$	A_1	J even: $\|JM\rangle^+$ J odd: $\|JM\rangle^-$
								$2\alpha M = kn$
$\mu=0$	$+1$	$+1$	$+1$	...	$+1$	-1	A_2	J even: $\|JM\rangle^-$ J odd: $\|JM\rangle^+$
$\mu=\pm\beta$	$+2$	$2R(\varepsilon^{\beta})$	$2R(\varepsilon^{2\beta})$	...	$2R(\varepsilon^{((n-1)/2)\beta})$	0	E_β	

written on the right of the table the conditions for a given function to be a basis function of the facing i.r. For bidimensional i.rs $\mu=\pm\beta$, $|JM\rangle^+$ and $|JM\rangle^-$ together are basis functions. For example, in D_3 symmetry, the functions $|00\rangle^+$, $|20\rangle^+$, $|33\rangle^-$, $|43\rangle^+$, $|53\rangle^-$, $|63\rangle^+$, $|66\rangle^+, \ldots$ with $\mu=0$, will span the i.r. A_1.

B. n even

(i) C_n^α and $C_n^{n-\alpha}$ belong to the same class ($\alpha=1,2,\ldots,(n/2)-1$). We get $(n/2)-1$ such classes.

(ii) E forms a class by itself.

(iii) $C_n^{n/2}=C_2$ forms a class by itself.

(iv) We have two classes of binary axes C_2' and C_2'' each containing $n/2$ operations.

We thus have a total of $(n/2)+3$ classes and irreducible representations. The two supplementary conditions on the extreme right of Table 6 are given by the transformation properties of $|JM\rangle^+$ and $|JM\rangle^-$ under C_n^α operations (Eq. (5)). The matrix is diagonal if $2\alpha M=kn$ which is the condition for $|JM\rangle^+$ or $|JM\rangle^-$ to be a basis function for a unidimensional i.r. If this condition is fulfilled, $\cos(2\pi\alpha M/n)=+1$ or -1 respectively for k even or odd; the function will span one of the two $\mu=0$ i.rs in the first case and one of the two $\mu=n/2$ i.rs in the second case.

e) $\{C_nC_2'\}\times I$

When n is even, these groups are D_{nh} and when n is odd, these are D_{nd} in Schoenflies' notation.

The character table has the same form as the table for $C_m\times I$. The irreducible representations $\mu=n/2$ only exist for even n values.

f) $\langle\{C_nC_2'\}\times I\rangle_a$

In Schoenflies' notation, these are the C_{nv} groups.

There is an isomorphism between these groups and $\{C_nC_2'\}$ so the conclusions are identical.

g) $\langle\{C_nC_2'\}\times I\rangle_b$

These groups only exist when n is even.

If $n/2$ is even, $\langle\{C_nC_2'\}\times I\rangle_b=D_{n/2d}$ and if $n/2$ is odd, $\langle\{C_nC_2'\}\times I\rangle_b=D_{n/2h}$. These are also isomorphic with $\{C_nC_2'\}$ so the same conclusions apply. However,

Table 6. Character table for $\{C_nC_2'\}$ (n even)

$\{C_nC_2'\}$	E	$2C_n^1$	$2C_n^2$	...	$2C_n^{n/2-2}$	$2C_n^{n/2-1}$	C_2	$n/2C_2'$	$n/2C_2''$			
$\mu=0$	+1	+1	+1	...	+1	+1	+1	+1	+1	A_1	J even: $\lvert JM\rangle^+$; J odd: $\lvert JM\rangle^-$	$M=2k'(n/2)$
$\mu=0$	+1	+1	+1	...	+1	+1	+1	−1	−1	A_2	J even: $\lvert JM\rangle^-$; J odd: $\lvert JM\rangle^+$	
$\mu=n/2$	+1	−1	+1	...	$(-1)^{n/2-2}$	$(-1)^{n/2-1}$	$(-1)^{n/2}$	+1	−1	B_1	J even: $\lvert JM\rangle^+$; J odd: $\lvert JM\rangle^-$	$M=(2k'+1)(n/2)$
$\mu=n/2$	+1	−1	+1	...	$(-1)^{n/2-2}$	$(-1)^{n/2-1}$	$(-1)^{n/2}$	−1	+1	B_2	J even: $\lvert JM\rangle^-$; J odd: $\lvert JM\rangle^+$	
$\mu=\pm\beta$	+2	$2R(\varepsilon^{\beta})$	$2R(\varepsilon^{2\beta})$	...	$-2R(\varepsilon^{2\beta})$	$-2R(\varepsilon^{\beta})$	$2(-1)^{\beta}$	0	0	E_β		

Table 7. Character table for $\{C_nC_2'\}\times I$

$\{C_nC_2'\}\times I$	$\{C_nC_2'\}$	$\{C_nC_2'\}I$				
$\mu=0$			A_{1g}	$\|JM\rangle^+$	$M=2k'(n/2)$	even J values[a]
$\mu=0$			A_{2g}	$\|JM\rangle^-$		
$\mu=\pm\beta$	+Table for $\{C_nC_2'\}$	+Table for $\{C_nC_2'\}$	$E_{\beta g}$			
$\mu=n/2$			B_{1g}	$\|JM\rangle^+$	$M=(2k'+1)(n/2)$	
$\mu=n/2$			B_{2g}	$\|JM\rangle^-$		
$\mu=0$			A_{1u}	$\|JM\rangle^-$	$M=2k'(n/2)$	odd J values[a]
$\mu=0$			A_{2u}	$\|JM\rangle^+$		
$\mu=\pm\beta$	+Table for $\{C_nC_2'\}$	−Table for $\{C_nC_2'\}$	$E_{\beta u}$			
$\mu=n/2$			B_{1u}	$\|JM\rangle^-$	$M=(2k'+1)(n/2)$	
$\mu=n/2$			B_{2u}	$\|JM\rangle^+$		

[a] See remark in Sect. 4b

there is a slight difference in the correspondence with Mulliken's notations when $n/2$ is odd, i.e. for $D_{n/2h}$ groups.

A_1 is replaced by A_1', A_2 by A_2', B_1 by A_1'', B_2 by A_2'' and E_β by $E^{(\beta')}$.

h) *High symmetries*

We will consider these groups as special cases of lower symmetry ones. The lower symmetry crystal field Hamiltonian will contain additional information about the actual symmetry through the conditions on the B_q^k imposed by the high symmetry.

These are, for example, for the cubic group O_h:

$$B_0^2=0 \qquad B_4^4=\sqrt{\tfrac{5}{14}}B_0^4 \qquad B_4^6=-\sqrt{\tfrac{7}{2}}B_0^6$$

when O_h is viewed as a special case of D_4

$$B_0^2=0 \qquad B_3^4=-\sqrt{\tfrac{10}{7}}B_0^4 \qquad B_3^6=\tfrac{\sqrt{210}}{24}B_0^6 \qquad B_6^6=\tfrac{\sqrt{231}}{24}B_0^6$$

when O_h is viewed as a special case of C_{3v}

$$B_0^2=0 \qquad B_2^2=0 \qquad B_2^4=-\sqrt{10}B_0^4 \qquad B_4^4=-\tfrac{3}{14}\sqrt{70}B_0^4 \qquad B_2^6=\tfrac{\sqrt{105}}{26}B_0^6$$
$$B_4^6=-\tfrac{5}{26}\sqrt{14}B_0^6 \qquad B_6^6=\tfrac{\sqrt{231}}{26}B_0^6$$

when O_h is viewed as a special case of C_{2v}.

The resulting energies will appear degenerate and with the help of correlation tables, it will be rather easy to assign all the eigenfunctions to the right i.r. of the high symmetry point group. In the difficult case where some accidental degeneracy remains, a detailed study of the degenerate set of levels must be performed to avoid mistakes.

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