$$\langle u_\alpha(^l_\kappa)u_\beta(^l_\kappa)\rangle = \frac{kT}{N}\sum_{\mathbf{k}}(\mathbf{\Phi}^{-1})_{\alpha\beta}(^{\mathbf{k}}_{\kappa\kappa}) + \frac{\hbar^2\delta_{\alpha\beta}}{12kTM_\kappa} - \frac{\hbar^4}{720k^3T_N{}^3M_\kappa^2}\sum_{\mathbf{k}}\Phi_{\alpha\beta}(^{\mathbf{k}}_{\kappa\kappa}),\ T>\Theta_D/2\,. \quad (18)$$

Equation (18) describes the vibration of an atom in a crystal lattice for temperatures above half the Debye temperature of the lattice. From the quantities $\langle u_\alpha(^l_\kappa)u_\beta(^l_\kappa)\rangle$, the anisotropic Debye–Waller B values can be obtained by well known methods (Cruickshank, 1956). At high temperatures, $T>\Theta_D$, only the first term in the right-hand part of equation (18) is of importance, and Debye–Waller B values become independent of the atomic masses.

Two restrictions should be made. Equation (18) has been derived within the harmonic approximation which will certainly be violated at very high temperatures. The second restriction is in dealing with the temperature dependence of the two sums in equation (18). The matrix elements $(\mathbf{\Phi}^{-1})_{\alpha\beta}(^{\mathbf{k}}_{\kappa\kappa})$ and $\Phi_{\alpha\beta}(^{\mathbf{k}}_{\kappa\kappa})$ are temperature dependent, *via* the interatomic forces which depend, for example, on the atomic distances. It is expected, however, that the sums will vary only very little with temperature.

Example

For a cubic lattice, the Debye–Waller B value of the κth atom is obtained from equation (18) as:

$$B_\kappa = 8\pi^2\left[\frac{kT}{N}\sum_{\mathbf{k}}(\mathbf{\Phi}^{-1})_{\alpha\alpha}(^{\mathbf{k}}_{\kappa\kappa}) + \frac{\hbar^2}{12kTM_\kappa} - \frac{\hbar^4}{720k^3T_N{}^3M_\kappa^2}\sum_{\mathbf{k}}\Phi_{\alpha\alpha}(^{\mathbf{k}}_{\kappa\kappa})\right]. \quad (191$$

In the above expression the first term in the right-hand part is independent of the atomic mass. The other two terms are inversely proportional to the atomic mass and to the square of the atomic mass. In general, it is very difficult to evaluate the two sums of equation (19), because, for this, a detailed knowledge of the atomic forces is required. We have determined the two sums by a least-squares fit of equation (19), for 12 temperatures, to KBr B values calculated by Reid & Smith (1970). The Debye temperature of KBr is about 160°K (Reid & Smith, 1970) and the 12 temperatures chosen range from 75°K (about half the Debye temperature) up to 295°K. Results are shown in Table 1.

The results in Table 1 show the various contributions to B_κ at temperatures above the Debye temperature (for KBr 160°K) the main contribution to the Debye–Waller B values comes from the mass-independent term of equation (19). Table 1 also shows that equation (19) describes very well, in a large temperature region, the temperature dependence of both the Debye–Waller B values of KBr.

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The Method of Ascent in Symmetry. I. Theory and Tables

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Supergroup tables are presented whereby a representation of a subgroup can be correlated with those representations of the supergroup which are obtained on ascent in symmetry. The method of derivation is explained and various orientations of the subgroup with respect to the supergroup considered. The tables also include the correlations between the double-valued representations of the corresponding double groups.

Introduction

The well-known process of descent in symmetry allows one to discuss how the representations of a given group decompose into representations of a subgroup. Tables have been constructed to facilitate many such correlations and these are very useful in numerous physical problems, *e.g.* the splitting of atomic energy levels in a crystal field.

The reverse correlation, in which we ascend in symmetry from a group to a supergroup is less well known and supergroup tables have not been published for all the cases of interest. In this series of papers it will be shown that such tables may rigorously be applied to a wide variety of physical problems. These will include the rapid construction of molecular orbitals, the determination of molecular and lattice vibrations, the study of problems concerning electron and nuclear spins and the additivity of the tensorial properties of bonds and atoms, *e.g.* polarizability. The first paper contains the general mathematical theory and the tables which are of use in all the applications.

Theory

Let us consider the ascent in symmetry from the point group C_2 to C_{2v}. The representations of these groups can be specified by considering their behaviour with

Table 1. *Ascent in symmetry from C_{2n+1} groups*

C_1	C_{2p}	C_{2p+1}
A	$A+B+\sum'_{p-1} E_r$	$A+\sum_p E_r$
$B_{1/2}$	$\sum_p E_{(2r-1)/2}$	$B_{(2p+1)/2}+\sum_p E_{(2r-1)/2}$

C_3	C_{6p}	C_{6p+3}	T
A	$A+B+\sum'_{p-1} E_{3r}$	$A+\sum_p E_{3r}$	$A+T$
E	$\sum_p(E_{3r-2}+E_{3r-1})$	$\sum_{p+1} E_{3r-2}+\sum_p E_{3r-1}$	$E+2T$
$B_{3/2}$	$\sum_p E_{(6r-3)/2}$	$B_{(6p+3)/2}+\sum_p E_{(6r-3)/2}$	$G_{3/2}$
$E_{1/2}$	$\sum_p (E_{(6r-5)/2}+E_{(6r-1)/2})$	$\sum_{p+1} E_{(6r-5)/2}+\sum_p E_{(6r-1)/2}$	$2E_{1/2}+G_{3/2}$

C_{2p-1}	$C_{(2p-1)h}$
A	$A'+A''$
E_r	$E'_r+E''_r$ $(1\leq r\leq p-1)$
$B_{(2p-1)/2}$	$E_{(2p-1)/2}$
$E_{(2r-1)/2}$	$E_{(2r-1)/2}+E_{(4p-2r-1)/2}$ $(1\leq r\leq p-1)$

C_{2p+1}	$C_{(2p+1)v}$ or D_{2p+1}
A	A_1+A_2
E_r	$2E_r$ $(1\leq r\leq p)$
$B_{(2p+1)/2}$	$E_{(2p+1)/2}$
$E_{(2r-1)/2}$	$2E_{(2r-1)/2}$ $(1\leq r\leq p)$

Table 2. *Ascent in symmetry from C_{2n} groups*

C_2	C_{4p}	C_{4p+2}	$C_2\to C_2^z$* D_2	$C_2\to C_2$ D_{4p+2}	$C_2\to C'_2$† D_{4p+2}
A	$A+B+\sum'_{p-1} E_{2r}$	$A+\sum_p E_{2r}$	$A+B_1$	$A_1+A_2+2\sum_p E_{2r}$	$A_1+B_1+\sum_{2p} E_r$
B	$\sum_p E_{2r-1}$	$B+\sum_p E_{2r-1}$	B_2+B_3	$B_1+B_2+2\sum_p E_{2r-1}$	$A_2+B_2+\sum_{2p} E_r$
$E_{1/2}$	$\sum_{2p} E_{(2r-1)/2}$	$\sum_{2p+1} E_{(2r-1)/2}$	$2E_{1/2}$	$2\sum_{p+1} E_{(2r-1)/2}$	$2\sum_{p+1} E_{(2r-1)/2}$

C_2	D_{2p+1}	$C_2\to C_2$ D_{4p}	$C_2\to C'_2$† D_{4p}
A	$A_1+\sum_p E_r$	$A_1+A_2+B_1+B_2+2\sum'_{p-1} E_{2r}$	$A_1+B_1+\sum_{2p-1} E_r$
B	$A_2+\sum_p E_r$	$2\sum_p E_{2r-1}$	$A_2+B_2+\sum_{2p-1} E_r$
$E_{1/2}$	$E_{(2p+1)/2}+2\sum_p E_{(2p-1)/2}$	$2\sum_{2p} E_{(2r-1)/2}$	$2\sum_{2p} E_{(2r-1)/2}$

C_2	$C_2\to C_2$ D_{2d}	$C_2\to C'_2$ D_{2d}	$C_2\to C_2$ O	$C_2\to C'_2$ O
A	$A_1+A_2+B_1+B_2$	A_1+B_2+E	$A_1+A_2+2E+T_1+T_2$	$A_1+E+T_1+2T_2$
B	$2E$	A_2+B_2+E	$2T_1+2T_2$	$A_2+E+2T_1+T_2$
$E_{1/2}$	$2E_{1/2}+2E_{3/2}$	$2E_{1/2}+2E_{3/2}$	$2E_{1/2}+2E_{5/2}+4G_{3/2}$	$2E_{1/2}+2E_{5/2}+4G_{3/2}$

C_{2p}	S_{4p}	C_{2pv} or D_{2p} (except D_2)
A	$A+B$	A_1+A_2
B	E_p	B_1+B_2
E_r	E_r+E_{2p-r}	$2E_r(1\leq r\leq p-1)$
$E_{(2r-1)/2}$	$E_{(2r-1)/2}+E_{(4p-2r+1)/2}$	$2E_{(2r-1)/2}$ $(1\leq r\leq p)$

* Interchange of $\{C_2^z, C_2^y, C_2^x\}$ in D_2 requires interchange of $\{B_1, B_2, B_3\}$ respectively.
† Interchange of C'_2 and C''_2 in D_{2n+2} requires interchange of B_1 and B_2.

respect to the *generators* of these groups. These are the key elements from which all the others may be derived and will be denoted in braces *e.g.* $\{C_2\}$ and $\{C_2, \sigma_v^{xz}\}$ for the point groups C_2 and C_{2v} respectively. In ascending from C_2 to C_{2v} it is necessary to specify how the representation of C_{2v} obtained will behave with respect to the new generator, σ_v^{xz}. All possibilities must be accounted for and so we obtain the *supergroup table*

C_2	C_{2v}
A	A_1+A_2
B	B_1+B_2

where A and B representations are respectively symmetric and anti-symmetric to the C_2 operation and the subscripts 1 and 2 respectively denote symmetry and anti-symmetry to the σ^{xz} reflexion. If $h_<$ and $h_>$ denote the orders of the sub- and supergroup respectively, the character system of the representation of the supergroup obtained by ascent in symmetry will be such that
(1) for elements in both groups the character will be $h_>/h_<$ times the corresponding character of the representation of the subgroup;
(2) for elements occurring only in the supergroup all characters are zero.

This is a mathematical process by which all supergroup tables may be obtained, but it is much quicker to take advantage of the subgroup tables, many of which have already been published. The basis for this is that if two representations are related by descent in symmetry, they must also be related by ascent in symmetry. The subgroup table $C_{2v} \to C_2$ shows that the A representations of C_2 are only obtained from A_1 and A_2 representations of C_{2v} so we should expect the supergroup table $C_2 \to C_{2v}$ to contain the entry $A \to A_1+A_2$. In applying this method, two points must be taken into account in more difficult cases:

Table 3. *Ascent in symmetry from $C_{(2n-1)h}$ groups*

C_{1h}	$C_{(2p+1)h}$	$\sigma \to \sigma_h$ $D_{(2p+1)h}$	$\sigma \to \sigma_v$ $D_{(2p+1)h}$	$\sigma \to \sigma_v$† C_{2pv}	$\sigma \to \sigma^{xy}$‡ D_{2h}
A'	$A'+\sum_p E'_r$	$A'_1+A'_2+2\sum_p E'_r$	$A'_1+A''_2+\sum_p \{E'_r+E''_r\}$	$A_1+B_1+\sum'_{p-1} E_r$	$A_g+B_{1g}+B_{2u}+B_{3u}$
A''	$A''+\sum_p E''_r$	$A''_1+A''_2+2\sum_p E''_r$	$A''_1+A'_2+\sum_p \{E'_r+E''_r\}$	$A_2+B_2+\sum'_{p-1} E_r$	$A_u+B_{1u}+B_{2g}+B_{3g}$
$E_{1/2}$	$\sum_{2p+1} E_{(2r-1)/2}$	$2\sum_{2p+1} E_{(2r-1)/2}$	$2\sum_{2p+1} E_{(2r-1)/2}$	$2\sum_p E_{(2r-1)/2}$	$2E_{1/2g}+2E_{1/2u}$

C_{1h}	$\sigma \to \sigma_h$ D_{4ph}	$\sigma \to \sigma_v$ † D_{4ph}
A'	$A_{1g}+A_{2g}+B_{1g}+B_{2g}+2\sum_p E_{(2r-1)u}+2\sum'_{p-1} E_{2rg}$	$A_{1g}+A_{2u}+B_{1g}+B_{2u}+\sum_{2p-1} \{E_{rg}+E_{ru}\}$
A''	$A_{1u}+A_{2u}+B_{1u}+B_{2u}+2\sum_p E_{(2r-1)g}+2\sum'_{p-1} E_{2ru}$	$A_{1u}+A_{2g}+B_{1u}+B_{2g}+\sum_{2p-1} \{E_{rg}+E_{ru}\}$
$E_{1/2}$	$2\sum_{2p} \{E_{(2r-1)/2g}+E_{(2r-1)/2u}\}$	$2\sum_{2p} \{E_{(2r-1)/2g}+E_{(2r-1)/2u}\}$

C_{1h}	$\sigma \to \sigma_h$ $D_{(4p+2)h}$	$\sigma \to \sigma_v$† $D_{(4p+2)h}$
A'	$A_{1g}+A_{2g}+B_{1u}+B_{2u}+2\sum_p \{E_{(2r-2)u}+E_{2rg}\}$	$A_{1g}+A_{2u}+B_{1u}+B_{2g}+\sum_{2p} \{E_{rg}+E_{ru}\}$
A''	$A_{1u}+A_{2u}+B_{1g}+B_{2g}+2\sum_p \{E_{(2r-2)g}+E_{2ru}\}$	$A_{1u}+A_{2g}+B_{1g}+B_{2u}+\sum_{2p} \{E_{rg}+E_{ru}\}$
$E_{1/2}$	$2\sum_{2p+1} \{E_{(2r-1)/2g}+E_{(2r-1)/2u}\}$	$2\sum_{2p+1} \{E_{(2r-1)/2g}+E_{(2r-1)/2u}\}$

C_{1h}	$\sigma \to \sigma_h$ O_h	$\sigma \to \sigma_d$ O_h
A'	$A_{1g}+A_{2g}+2E_g+T_{1g}+2T_{1u}+T_{2g}+2T_{2u}$	$A_{1g}+A_{2u}+E_g+E_u+T_{1g}+2T_{1u}+2T_{2g}+T_{2u}$
A''	$A_{1u}+A_{2u}+2E_u+2T_{1g}+T_{1u}+2T_{2g}+T_{2u}$	$A_{1u}+A_{2g}+E_g+E_u+2T_{1g}+T_{1u}+T_{2g}+2T_{2u}$
$E_{1/2}$	$2E_{1/2g}+2E_{1/2u}+2E_{5/2g}+2E_{5/2u}+4G_{3/2g}+4G_{3/2u}$	$2E_{1/2g}+2E_{1/2u}+2E_{5/2g}+2E_{5/2u}+4G_{3/2g}+4G_{3/2u}$

$C_{(2p-1)h}$	$C_{(4p-2)h}$	
A'	A_g+B_u	
A''	A_u+B_g	
E'_{2r-1}	$E_{(2r-1)u}+E_{(2p-2r)g}$	$(1 \le r \le p-1)$
E''_{2r-1}	$E_{(2r-1)g}+E_{(2p-2r)u}$	$(1 \le r \le p-1)$
E'_{2r}	$E_{2rg}+E_{(2p-2r-1)u}$	$(1 \le r \le p-2)$
E''_{2r}	$E_{2ru}+E_{(2p-2r-1)g}$	$(1 \le r \le p-2)$
$E_{(2r-1)/2}$	$E_{(2r-1)/2g}+E_{(2r-1)/2u}$	$(1 \le r \le 2p-1)$

$C_{(2p+1)h}$	$D_{(2p+1)h}$	
A'	$A'_1+A'_2$	
A''	$A''_1+A''_2$	
E'_r	$2E'_r$	$(1 \le r \le p)$
E''_r	$2E''_r$	$(1 \le r \le p)$
$E_{(2r-1)/2}$	$2E_{(2r-1)/2}$	$(1 \le r \le 2p+1)$

$C_{1h} \to C_{(2p+1)v}$: This Table is identical with that for $C_2 \to D_{2p+1}$ if the A and B representations of C_2 are replaced by A' and A'' respectively.

* In the group C_{2v}, take $\sigma^{xz}=\sigma_v$ and $\sigma^{yz}=\sigma_d$.
† For σ_d instead of σ_v, interchange B_1 and B_2, parity labels being unchanged where relevant.
‡ Permutation of $\{\sigma^{xy}, \sigma^{xz}, \sigma^{yz}\}$ implies a corresponding permutation of $\{B_1, B_2, B_3\}$ irrespective of the parity label.

Table 4. *Ascent in symmetry from C_{2nv} groups*

C_{2v}	$\sigma_v \to \sigma_v$* C_{4pv}	$\sigma^{xz} \to \sigma_v$*† $C_{(4p+2)v}$
A_1	$A_1+B_1+\sum'_{p-1} E_{2r}$	$A_1+\sum_p E_{2r}$
A_2	$A_2+B_2+\sum'_{p-1} E_{2r}$	$A_2+\sum_p E_{2r}$
B_1	$\sum_p E_{2r-1}$	$B_1+\sum_p E_{2r-1}$
B_2	$\sum_p E_{2r-1}$	$B_2+\sum_p E_{2r-1}$
$E_{1/2}$	$\sum_{2p} E_{(2r-1)/2}$	$\sum_{2p+1} E_{(2r-1)/2}$

C_{2v}	$\sigma^{xz} \to \sigma^{xz}$† $C_2 \to C_2^z$‡ D_{2h}	$2\sigma_v \to 2\sigma_v$* D_{4h}	$\sigma^{xz} \to \sigma_h$; $\sigma^{yz} \to \sigma_v$*† D_{4h}
A_1	A_g+B_{1u}	$A_{1g}+A_{2u}+B_{1g}+B_{2u}$	$A_{1g}+B_{1g}+E_u$
A_2	A_u+B_{1g}	$A_{1u}+A_{2g}+B_{1u}+B_{2g}$	$A_{1u}+B_{1u}+E_g$
B_1	$B_{2g}+B_{3u}$	E_g+E_u	$A_{2g}+B_{2g}+E_u$
B_2	$B_{2u}+B_{3g}$	E_g+E_u	$A_{2u}+B_{2u}+E_g$
$E_{1/2}$	$E_{1/2g}+E_{1/2u}$	$E_{1/2g}+E_{1/2u}+E_{3/2g}+E_{3/2u}$	$E_{1/2g}+E_{1/2u}+E_{3/2g}+E_{3/2u}$

C_{2v}	$C_2 \to C_2$; $\sigma^{xz} \to \sigma_v$*† D_{6h}	$C_2 \to C_2'$; $\sigma^{xz} \to \sigma_h$†§ D_{6h}
A_1	$A_{1g}+A_{2u}+E_{2g}+E_{2u}$	$A_{1g}+B_{1u}+E_{1u}+E_{2g}$
A_2	$A_{1u}+A_{2g}+E_{2g}+E_{2u}$	$A_{1u}+B_{1g}+E_{1g}+E_{2u}$
B_1	$B_{1u}+B_{2g}+E_{1g}+E_{1u}$	$A_{2g}+B_{2u}+E_{1u}+E_{2g}$
B_2	$B_{1g}+B_{2u}+E_{1g}+E_{1u}$	$A_{2u}+B_{2g}+E_{1g}+E_{2u}$
$E_{1/2}$	$E_{1/2g}+E_{1/2u}+E_{3/2g}+E_{3/2u}+E_{5/2g}+E_{5/2u}$	$E_{1/2g}+E_{1/2u}+E_{3/2g}+E_{3/2u}+E_{5/2g}+E_{5/2u}$

C_{2v}	$\sigma^{xz} \to \sigma_h$† $D_{(2p+1)h}$	D_{2pd}
A_1	$A_1'+\sum_p E_r'$	$A_1+B_2+\sum'_{p-1} E_{2r}$
A_2	$A_1''+\sum_p E_r''$	$A_2+B_1+\sum'_{p-1} E_{2r}$
B_1	$A_2'+\sum_p E_r'$	$\sum_p E_{2p-1}$
B_2	$A_2''+\sum_p E_r''$	$\sum_p E_{2p-1}$
$E_{1/2}$	$\sum_{2p+1} E_{(2r-1)/2}$	$\sum_{2p} E_{(2r-1)/2}$

C_{2v}	$2\sigma_v \to 2\sigma_h$ O_h	$2\sigma_v \to 2\sigma_d$ O_h	$\sigma^{xz} \to \sigma_h$; $\sigma^{yz} \to \sigma_d$† O_h
A_1	$A_{1g}+A_{2g}+2E_g+T_{1u}+T_{2u}$	$A_{1g}+A_{2u}+E_g+E_u+T_{1u}+T_{2g}$	$A_{1g}+E_g+T_{1u}+T_{2g}+T_{2u}$
A_2	$A_{1u}+A_{2u}+2E_u+T_{1g}+T_{2g}$	$A_{1u}+A_{2g}+E_g+T_{2u}+E_u+T_{1g}$	$A_{1u}+E_u+T_{1g}+T_{2g}+T_{2u}$
B_1	$T_{1g}+T_{1u}+T_{2g}+T_{2u}$	$T_{1g}+T_{1u}+T_{2g}+T_{2u}$	$A_{2g}+E_g+T_{1g}+T_{1u}+T_{2u}$
B_2	$T_{1g}+T_{1u}+T_{2g}+T_{2u}$	$T_{1g}+T_{1u}+T_{2g}+T_{2u}$	$A_{2u}+E_u+T_{1g}+T_{1u}+T_{2g}$
$E_{1/2}$	$E_{1/2g}+E_{1/2u}+E_{5/2g}+E_{5/2u}+2G_{3/2g}$ $+2G_{3u/2}$	$E_{1/2g}+E_{1/2u}+E_{5/2g}+E_{5u/2}+2G_{3/2g}$ $+2G_{3/2u}$	$E_{1/2g}+E_{1/2u}+E_{3/2g}+E_{3/2u}+2G_{3/2g}$ $+2G_{3u/2}$

C_{2pv}	D_{2pd}
A_1	A_1+B_2
A_2	A_2+B_1
B_1, B_2	E_p
E_r	E_r+E_{2p-r} $(1 \le r \le p-1)$
$E_{(2r-1)/2}$	$E_{(2r-1)/2}+E_{(4p-2r+1)/2}$ $(1 \le r \le p)$

C_{4pv}	$\sigma_v \to \sigma_v$* D_{4ph}
A_1	$A_{1g}+A_{2u}$
A_2	$A_{1u}+A_{2g}$
B_1	$B_{1g}+B_{2u}$
B_2	$B_{1u}+B_{2g}$
E_r	$E_{rg}+E_{ru}$ $(1 \le r \le 2p-1)$
$E_{(2r-1)/2}$	$E_{(2r-1)/2g}+E_{(2r-1)/2u}$ $(1 \le r \le 2p)$

$C_{(4p+2)v}$	$\sigma_v \to \sigma_v$* $D_{(4p+2)h}$
A_1	$A_{1g}+A_{2u}$
A_2	$A_{1u}+A_{2g}$
B_1	$B_{1u}+B_{2g}$
B_2	$B_{1g}+B_{2u}$
E_r	$E_{rg}+E_{ru}$ $(1 \le r \le 2p)$
$E_{(2r-1)/2}$	$E_{(2r-1)/2g}+E_{(2r-1)/2u}$ $(1 \le r \le 2p+1)$

* For σ_d instead of σ_v in the supergroup, interchange B_1 and B_2 (irrespective of any parity label) on the right-hand side of the Table.

† For σ^{yz} instead of σ^{xz} in C_{2v} interchange B_1 and B_2 on the left-hand side of the Table.

‡ Permutation of $\{C_2^z, C_2^y, C_2^x\}$ in D_{2h} implies a corresponding permutation of $\{B_1, B_2, B_3\}$, irrespective of the parity label, on the right-hand side of the Table.

§ For C_2'' instead of C_2', proceed as footnote marked*.

(1) if on descent in symmetry, an irreducible representation of the subgroup occurs more than once, then on ascent in symmetry that number of the representation of the supergroup will be obtained from the representation of the subgroup, *except when*

(2) the representation of the supergroup is degenerate and *separable*, *i.e.* it consists of a complex conjugate pair of representations, in which case each member of the pair should be treated separately.

The separable representations are the doubly-degenerate representations of the point groups C_n, C_{nh} (both for $n \geq 3$), $S_{2n} (n \geq 2)$, T and T_h, the doubly degenerate representations of the double groups $C'_n (n \geq 3)$, $C'_{nh} (n \geq 1)$, $S'_{2n} (n \geq 2)$, the $E_{n/2}$ representations of C'_{nv} and D'_n (both for $n = 3, 5, 7, \ldots$), the $E_{n/2g}$ and $E_{n/2u}$ representations of $D'_{nd} (n = 3, 5, 7, \ldots)$, and the fourfold degenerate representations of T' and T'_h.

Differences in orientation

In many cases where the subgroup contains fewer twofold axes and/or reflexion planes than the supergroup, it is possible to ascend in more than one way according to which axes or planes of the supergroup correspond to those of the subgroup. Different supergroup tables then arise when at least one of the following conditions is fulfilled.

Table 5. *Ascent in symmetry from $C_{(2n+1)v}$ groups*

	$\sigma_v \to \sigma_v$*		$\sigma_v \to \sigma_v$*	
C_{3v}	C_{6pv}	$C_{(6p+3)v}$	D_{6h}	T_d
A_1	$A_1 + B_1 + \sum'_{p-1} E_{3r}$	$A_1 + \sum_p E_{3r}$	$A_{1g} + A_{2u} + B_{1u} + B_{2g}$	$A_1 + T_2$
A_2	$A_2 + B_2 + \sum'_{p-1} E_{3r}$	$A_2 + \sum_p E_{3r}$	$A_{1u} + A_{2g} + B_{1g} + B_{2u}$	$A_2 + T_1$
E	$\sum_p (E_{3r-2} + E_{3r-1})$	$\sum_{p+1} E_{3r-2} + \sum_p E_{3r-1}$	$E_{1g} + E_{1u} + E_{2g} + E_{2u}$	$E + T_1 + T_2$
$E_{1/2}$	$\sum_p (E_{(6r-5)/2} + E_{(6r-1)/2})$	$\sum_{p+1} E_{(6r-5)/2} + \sum_p E_{(6r-1)/2}$	$E_{1/2g} + E_{1/2u} + E_{5/2g} + E_{5/2u}$	$E_{1/2} + E_{5/2} + G_{3/2}$
$E_{3/2}$	$2 \sum_p E_{(6r-3)/2}$	$E_{(6r+3)/2} + 2 \sum_p E_{(6r-3)/2}$	$2E_{3/2g} + 2E_{3/2u}$	$2G_{3/2}$

$C_{(2p+1)v}$	$D_{(2p+1)d}$	$D_{(2p+1)h}$
A_1	$A_{1g} + A_{2u}$	$A'_1 + A''_2$
A_2	$A_{1u} + A_{2g}$	$A''_1 + A'_2$
E_r	$E_{rg} + E_{ru}$	$E'_r + E''_r \; (1 \leq r \leq p)$
$E_{(2r-1)/2}$	$E_{(2r-1)/2g} + E_{(2r-1)/2u}$	$E_{(2r-1)/2} + E_{(4p-2r+3)/2} \; (1 \leq r \leq p)$
$E_{(2p+1)/2}$	$E_{(2p+1)/2g} + E_{(2p+1)/2u}$	$2E_{(2p+1)/2}$

* For σ_d instead of σ_v in the supergroup, interchange B_1 and B_2 (irrespective of any parity label) on the right-hand side of the Table.

Table 6. *Ascent in symmetry from D_{2n} groups*

	$3C_2 \to C_2 + 2C'_2$; $C_2^z \to C_2^z$*	$C_2^z \to C_2$; $C_2^y \to C'_2$†
D_2	D_{4p}	D_{4p+2}
A	$A_1 + B_1 + \sum'_{p-1} E_{2r}$	$A_1 + \sum_p E_{2r}$
B_1	$A_2 + B_2 + \sum'_{p-1} E_{2r}$	$A_2 + \sum_p E_{2r}$
B_2	$\sum_p E_{2r-1}$	$B_1 + \sum_p E_{2r-1}$
B_3	$\sum_p E_{2r-1}$	$B_2 + \sum_p E_{2r-1}$
$E_{1/2}$	$\sum_{2p} E_{(2r-1)/2}$	$\sum_{2p+1} E_{(2r-1)/2}$

		$C_2^z \to C_2$; $C_2^x + C_2^y \to 2C'_2$*	$3C_2 \to 3C_2$	$C_z^2 \to C_2$*
D_2	T	O	O	D_{2pd}
A	$A + E$	$A_1 + E + T_2$	$A_1 + A_2 + 2E$	$A_1 + B_1 + \sum'_{p-1} E_{2r}$
B_1	T	$A_2 + E + T_1$	$T_1 + T_2$	$A_2 + B_2 + \sum'_{p-1} E_{2r}$
B_2, B_3	T	$T_1 + T_2$	$T_1 + T_2$	$\sum_p E_{2r-1}$
$E_{1/2}$	$E_{1/2} + G_{3/2}$	$E_{1/2} + E_{5/2} + 2G_{3/2}$	$E_{1/2} + E_{5/2} + 2G_{3/2}$	$\sum_{2p} E_{(2r-1)/2}$

D_{2p+2}	$D_{(2p+2)d}$
A_1	$A_1 + B_1$
A_2	$A_2 + B_2$
B_1, B_2	E_{p+1}
E_r	$E_r + E_{2p+2-r} \; (1 \leq r \leq p)$
$E_{(2r-1)/2}$	$E_{(2r-1)/2} + E_{(4p-2r+5)/2} \; (1 \leq r \leq p+1)$

	$C'_2 \to C'_2$‡
D_4	O
A_1	$A_1 + E$
A_2	T_1
B_1	T_2
B_2	$A_2 + E$
E	$T_1 + T_2$
$E_{1/2}$	$E_{1/2} + G_{3/2}$
$E_{3/2}$	$E_{5/2} + G_{3/2}$

* Permutation of $\{C_2^z, C_2^y, C_2^x\}$ in D_2 implies a corresponding permutation of $\{B_1, B_2, B_3\}$ on the left-hand side of the Table.
† For C''_2 instead of C'_2, interchange B_1 and B_2 on the right-hand side of the Table
‡ For C''_2 instead of C'_2 in D_4, interchange B_1 and B_2 on the left-hand side of the Table.

(1) A twofold axis in the subgroup correlates with *either* the principal axis *or* a subsidiary twofold axis of the axial point groups D_{2nd} and $D_{2nh}(n \geq 1)$ or the cubic groups O and O_h.
(2) A set of three twofold axes in the subgroup correlates with *either* the three principal *or* one principal and two subsidiary twofold axes in the cubic point groups O and O_h.
(3) A reflexion plane in the subgroup correlates with *either* the horizontal (σ_h) *or* a vertical plane in a $D_{nh}(n \geq 2)$ supergroup.
(4) A set of reflexion planes in the subgroup correlates with *either* only vertical planes *or* vertical plane(s) and the horizontal plane in a $D_{nh}(n \geq 2)$ supergroup.
(5) The supergroup contains representations which are geometrically equivalent, *i.e.* differences in character systems arise only for classes of geometrically equivalent elements such that the systems can be considered as permutation variants. In practice such representations are all the B-type representations of the point groups C_{2nv}, D_{2n} and $D_{2nh}(n \geq 1)$.

Tables specifying the orientation of the point groups at Wyckoff sites within the point group of a crystal (*i.e.* the crystal class) have been published earlier (Boyle, 1971).

The tables

In order to minimize the area of these tables (Tables 1 to 11), it was necessary to restrict the ascents to those in which there is no intermediate subgroup, *e.g.* $C_2 \rightarrow C_{2v}$, $C_3 \rightarrow T$, other ascents being attained by a multi-stage process, *e.g.* $C_{4v} \rightarrow D_{4h} \rightarrow O_h$. Some useful diagrams for finding some such routes have been given by Boyle (1969). Where significant orientational differences occur, changes in notation and the need for working with representations of unconventional point groups (*e.g.* where the z axis is *not* chosen as the principal axis) make the calculation quite difficult for anyone not completely familiar with the elements of point groups, so that all such ascents have been included. It has been possible to incorporate many as footnotes giving instructions for altering a given table. All the point groups appearing in the tables are conventional, so that local frames of axes are used in the context of molecules or crystals. Not all of the orientational variants are represented crystallographically since some of the differences are merely ones of labelling of equivalent planes or axes so that geometrically the ascents are identical. However, when relative differences in labelling can be distinguished geometrically, these may occur crystallographically.

When a centre of symmetry is present in both subgroup and supergroup, the ascent between the corresponding uncentrosymmetric groups should be used, the subscripts g or u being added as required. Ascents involving addition of a centre of symmetry only have not been tabulated (with the sole exception of $T_d \rightarrow O_h$ to avoid notational complications) since each representation gives one *gerade* and one *ungerade* without other change of notation. The group products useful for these cases are: $C_{2p-1} \times S_2 = S_{4p-2}$; $C_{2p} \times S_2 = C_{2ph}$; $C_{(2p-1)h} \times S_2 = C_{(4p-2)h}$; $C_{2pv} \times S_2 = D_{2ph}$; $C_{(2p+1)v} \times S_2 = D_{(2p+1)d}$; $D_{2p} \times S_2 = D_{2ph}$; $D_{2p+1} \times S_2 = D_{(2p+1)d}$; $D_{2pd} \times S_2 = D_{4ph}$; $I \times S_2 = I_h$; $O \times S_2 = O_h$; $S_{4p} \times S_2 = C_{4ph}$; $T \times S_2 = T_h$.

Where feasible, general tables have been produced using the variable p, which consistently takes integral values greater than or equal to one. However, such general tables have been restricted to those involving a constant subgroup, or those in which the ratio $h_>/h_<$ is constant. To simplify printing the summations over the dummy index r have been abbreviated so that

$\sum_{r=1}^{r=p}$ becomes $\sum_p$ and $\sum_{r\geq 1}^{r\leq p-1}$ becomes $\sum'_{p-1}$. This latter type of summation has no terms unless both conditions on r are met, which is the case in this paper when $p \geq 2$. If a group has only one doubly-degenerate (single-valued) representation, then the E_1 generated by the general formulae should be read E. The point groups which are still occasionally known as C_s, C_i and C_{3i} have been written C_{1h}, S_2 and S_6 and thus fitted into the corresponding families of groups.

Finally, the ascents in symmetry for the double groups have been condensed into the same table as those for the corresponding ordinary point groups, the correlations between the double-valued representations

Table 7. *Ascent in symmetry from D_{2n+1} groups*

D_3	O	I
A_1	A_1+T_2	$A+G+H$
A_2	A_2+T_1	T_1+T_2+G
E	$E+T_1+T_2$	T_1+T_2+G+2H
$E_{1/2}$	$E_{1/2}+E_{5/2}+G_{3/2}$	$E_{1/2}+E_{7/2}+G_{3/2}+2I_{5/2}$
$E_{3/2}$	$2G_{3/2}$	$2G_{3/2}+2I_{5/2}$

D_5	I
A_1	$A+H$
A_2	T_1+T_2
E_1	T_1+G+H
E_2	T_2+G+H
$E_{1/2}$	$E_{1/2}+G_{3/2}+I_{5/2}$
$E_{3/2}$	$E_{3/2}+G_{3/2}+I_{5/2}$
$E_{5/2}$	$2I_{5/2}$

D_{2p+1}	$C_2' \rightarrow C_2'$* D_{4p+2}
A_1	A_1+B_1
A_2	A_2+B_2
E_r	E_r+E_{2p-r+1} $(1 \leq r \leq p)$
$E_{(2r-1)/2}$	$E_{(2r-1)/2}+E_{(4p-2r+3)/2}$ $(1 \leq r \leq p)$
$E_{(2p+1)/2}$	$2E_{(2p+1)/2}$

$D_{2p+1} \rightarrow D_{(2p+1)h}$: This Table is identical with that for $C_{(2p+1)v} \rightarrow D_{(2p+1)h}$.

* For C_2'' instead of C_2' in D_{4p+2}, interchange B_1 and B_2 on the right-hand side of the Table.

Table 8. *Ascent in symmetry from the group D_{2d}*

	$\sigma_d \to \sigma_d$*			$\sigma_d \to \sigma_h$	$\sigma_d \to \sigma_d$
D_{2d}	D_{4h}	D_{6d}	T_d	O_h	O_h
A_1	$A_{1g}+B_{1u}$	A_1+E_4	A_1+E	$A_{1g}+E_g+T_{2u}$	$A_{1g}+A_{2u}+E_g+E_u$
A_2	$A_{2g}+B_{2u}$	A_2+E_4	T_1	$A_{2u}+E_u+T_{1g}$	$T_{1g}+T_{2u}$
B_1	$A_{1u}+B_{1g}$	B_1+E_2	A_2+E	$A_{1u}+E_u+T_{2g}$	$A_{1u}+A_{2g}+E_g+E_u$
B_2	$A_{2u}+B_{2g}$	B_2+E_2	T_2	$A_{2g}+E_g+T_{1u}$	$T_{1u}+T_{2g}$
E	E_g+E_u	$E_1+E_3+E_5$	T_1+T_2	$T_{1g}+T_{1u}+T_{2g}+T_{2u}$	$T_{1g}+T_{1u}+T_{2g}+T_{2u}$
$E_{1/2}$	$E_{1/2}+E_{7/2}$	$E_{1/2}+E_{5/2}+E_{9/2}$	$E_{1/2}+G_{3/2}$	$E_{1/2g}+E_{1/2u}+G_{3/2g}+G_{3/2u}$	$E_{1/2g}+E_{1/2u}+G_{3/2g}+G_{3/2u}$
$E_{3/2}$	$E_{3/2}+E_{5/2}$	$E_{3/2}+E_{7/2}+E_{11/2}$	$E_{5/2}+G_{3/2}$	$E_{1/2g}+E_{1/2u}+G_{3/2g}+G_{3/2u}$	$E_{1/2g}+E_{1/2u}+G_{3/2g}+G_{3/2u}$

* For σ_v instead of σ_d in the supergroup, interchange B_1 and B_2 (irrespective of the parity label) on the right-hand side of the Table.

being separated from those between the single-valued representations by a horizontal line. Orientational differences are not relevant to ascents between double groups since the characters of the double-valued representations are all zero for the relevant reflexions and twofold rotations. The notation used for the double-valued representations is that of Herzberg (1966) with analogous extensions to cover the groups he does not describe. In order to avoid the use of inconveniently small type in subscripts, $\frac{1}{2}$, $\frac{3}{2}$ *etc.* have been printed as 1/2, 3/2 *etc.*; representations such as $E_{1/2g}$ and $G_{3/2u}$ are thus to be read as $E_{\frac{1}{2}g}$ and $G_{\frac{3}{2}u}$.

The tables have not been restricted to crystallographic groups but they are only complete for point groups containing proper axes of symmetry of order up to six and improper axes of order up to twelve. In practice many other groups can be reached using the general formulae where these have been given.

Table 9. *Ascent in symmetry from the group D_{3h}*

	$\sigma_v \to \sigma_v$*
D_{3h}	D_{6h}
A_1'	$A_{1g}+B_{1u}$
A_1''	$A_{1u}+B_{1g}$
A_2'	$A_{2g}+B_{2u}$
A_2''	$A_{2u}+B_{2g}$
E'	$E_{1u}+E_{2g}$
E''	$E_{1g}+E_{2u}$
$E_{1/2}$	$E_{1/2g}+E_{1/2u}$
$E_{3/2}$	$E_{3/2g}+E_{3/2u}$
$E_{5/2}$	$E_{5/2g}+E_{5/2u}$

* For σ_v instead of σ_d in the supergroup interchange B_1 and B_2 (irrespective of the parity label) on the right-hand side of the Tabel.

Table 10. *Ascent in symmetry from S_{4n} groups*

S_4	S_{12}
A	$A+E_4$
B	$B+E_2$
E	$E_1+E_3+E_5$
$E_{1/2}$	$E_{1/2}+E_{5/2}+E_{9/2}$
$E_{3/2}$	$E_{3/2}+E_{7/2}+E_{11/2}$

S_{4p}	C_{4ph}	D_{2pd}
A	A_g+B_u	A_1+A_2
B	A_u+B_g	B_1+B_2
E_r	$E_{rg}+E_{ru}$	$2E_r$ $(1\le r\le 2p-1)$
$E_{(2r-1)/2}$	$E_{(2r-1)/2g}+E_{(2r-1)/2u}$	$2E_{(2r-1)/2}$ $(1\le r\le 2p)$

Table 11. *Ascent in symmetry from the groups T and T_d*

T	T_d	O	I
A	A_1+A_2	A_1+A_2	$A+G$
E	$2E$	$2E$	$2H$
T	T_1+T_2	T_1+T_2	T_1+T_2+G+H
$E_{1/2}$	$E_{1/2}+E_{5/2}$	$E_{1/2}+E_{5/2}$	$E_{1/2}+E_{7/2}+I_{5/2}$
$G_{3/2}$	$2G_{3/2}$	$2G_{3/2}$	$2G_{3/2}+2I_{5/2}$

T_d	O_h
A_1	$A_{1g}+A_{2u}$
A_2	$A_{1u}+A_{2g}$
E	E_g+E_u
T_1	$T_{1g}+T_{2u}$
T_2	$T_{1u}+T_{2g}$
$E_{1/2}$	$E_{1/2g}+E_{1/2u}$
$E_{5/2}$	$E_{5/2g}+E_{5/2u}$
$G_{3/2}$	$G_{3/2g}+G_{3/2u}$

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