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Unique labelling of symmetry coordinates and cyclic regions in crystals

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Abstract. Earlier work on unique labelling schemes in O_h symmetry is extended to include 48-atom shells and the symmetry coordinates of shells subject to periodicity conditions. A new approach to labelling is introduced based on the concept of cyclic regions in a crystal. These are described by finite factor groups of the crystallographic space group which contain the isogonal group as a subgroup. Some examples are worked out in detail.

1. Introduction

Previous studies by Newman (1981) and Chen and Newman (1982) (denoted henceforth as I and II respectively) were concerned with providing unique group theoretical labels for atomic shell symmetry coordinates and using this scheme as a means of generating the symmetry coordinates explicitly. The approach in I and II differed from the considerable body of work on molecular symmetry coordinates (e.g. see Fieck 1977) in that the labelling problem was seen to be prior to the actual generation of symmetry coordinates. The difference of approach is related to an essential difference between the molecular and crystal problems: in the latter case it is certain, at some distance from the centre of symmetry, that the number of atoms in the shell will equal the number of symmetry operators in the point group, so that their permutations will generate a regular representation. The aim of a labelling scheme is to provide means of distinguishing the repeated (multidimensional) irreducible representations which appear in the regular representation and other representations generated by shells with smaller numbers of atoms.

In the present work we provide an explicit method of generating the symmetry coordinates for the 48-atom shell in O_h symmetry (which generates the regular representation). It will be seen to be advantageous to regard other shells (e.g. with 24 atoms and 12 atoms) as special cases of the 48-atom shell in order to obtain a systematic labelling and method of generating symmetry coordinates.

Following this we investigate the modifications of symmetry coordinates that are necessary when the crystal is divided into regions with periodic boundary conditions. We shall refer to such regions as 'cyclic regions'. Our interest in such regions is that the solutions of vibrational and one-electron problems in cyclic regions correspond to solutions of the same problem in the full crystal for certain points in the Brillouin zone. Lattice impurity effects can then be treated as causing perturbations of this restricted set of solutions.

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The introduction of cyclic regions suggests a new approach to the labelling of lattice distortions near a substituted impurity ion. Instead of using a shell label and a symmetry label for each symmetry coordinate, it is possible to use either space group labels or, more specifically, the labels of the symmetry group describing the cyclic region. Such cyclic region groups (and their character tables) can easily be constructed from space group tabulations (such as Bradley and Cracknell 1972). We give an example of this approach in § 4.

2. Symmetry coordinates for the 48-atom shell

The unique labelling scheme described in I was based on two ideas.

(a) The permutations of atomic positions and rotations of atomic displacements may be associated with separate irreducible representations of the symmetry group G. Symmetry coordinates can be constructed by coupling products of these representations using the Clebsch–Gordan coefficients of G.

(b) If the permutation representation contains repeated representations, these can be distinguished by relating them to representations induced in G from a subgroup describing the spatial symmetry of a subshell of atoms. For the unique labelling of a regular representation it is necessary to choose a subshell corresponding to an Abelian symmetry group.

In II a notation was introduced in which the unique labels were written, for example, as $(E|T_{2u}\otimes T_{1u})A_{2g}$ corresponding to the group structure $(C_{4v}|O_h\otimes O_h)O_h$. The first label (E) corresponds to the subgroup (C_{4v}) representation and serves to distinguish repetitions of the T_{2u} irreducible components in the representation generated by atomic permutations. We shall point out some limitations of this notation in the following discussion.

In order to complete the theory of atom shells in O_h symmetry and to provide a unified labelling for shells with different numbers of atoms, we have determined symmetry coordinates for the (maximal) 48-fold atom shell corresponding to the regular representation of O_h. The unique labelling of this shell has been described in paper I (where three alternative labelling schemes are given in table 2) and can be used to determine explicit symmetry coordinates. The following discussion is based on the atom labelling shown in figure 1.

We shall adopt a rather different approach from that used in I and II, in which there was presumed to be some physical advantage in choosing subshells of neighbouring atoms (Bates 1978). When writing I it was not appreciated just how much freedom exists in the choice of subshells in using the correlation theorem (Wilson *et al* 1955). They can, in fact, be generated from an arbitrary initial atomic position using *any one* of the set of conjugate subgroups to be used in the labelling. In other words, if we wish the labelling to be explicit (as well as unique) in the sense of corresponding to determinate symmetry coordinates, it is necessary to specify the form of the subshells.

Permutation symmetry coordinates have been determined for both the C'_{2v} and D'_{2h} subgroup labelling of the 48-element regular representation. The primes indicate that the principal axis of C'_{2v} is coincident with a C'_2 axis in O_h and $D'_{2h} = C'_{2v}\otimes S_2$ has two C'_2 axes.

We first discuss the C'_{2v} labelling, which was shown in I to be unique. Table 1 shows the irreducible representations of O_h induced by C'_{2v} according to the correlation

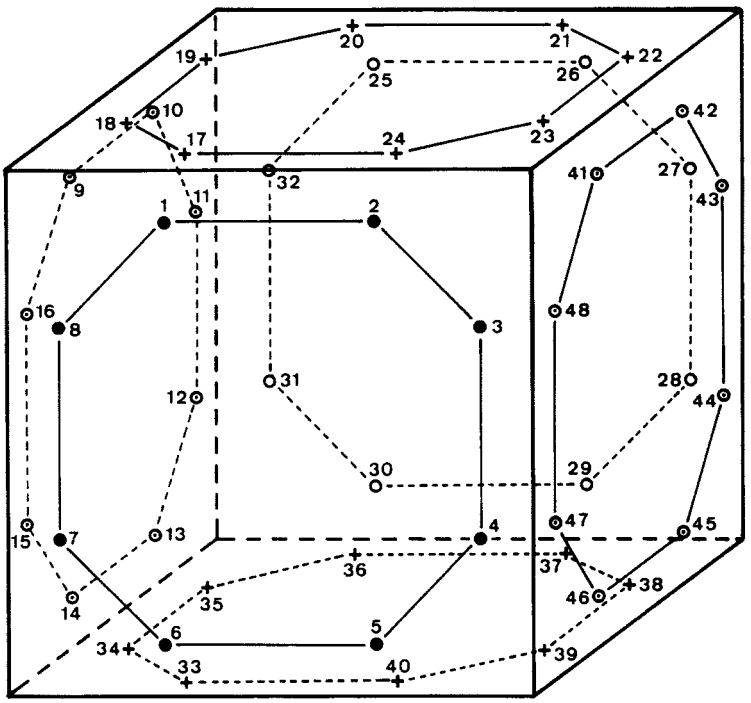

Figure 1. Numbering of the atom positions in a 48-atom shell.

Table 1. Irreducible representation labels of the permutation representations based on C'_{2v} subshells.

C'_{2v}	O_h				
A_1	A_{1g}	E_g	T_{2u}	T_{2g}	T_{1u}
A_2	A_{1u}	E_u	T_{2g}	T_{2u}	T_{1g}
B_1	A_{2g}	E_g	T_{1u}	T_{1g}	T_{2u}
B_2	A_{2g}	E_u	T_{1g}	T_{1u}	T_{2g}

table given in I. Using the labels of figure 1, it is easy to see that a consistent 4-atom C'_{2v} subshell labelling may be achieved as in table 2. The four C'_{2v} modes, in terms of the subshell atom labels shown in the first column in table 2, are given by

$$\begin{aligned}
&A_1: \quad (1)+(2)+(3)+(4) \to A_{1g} \\
&A_2: \quad (1)-(2)+(3)-(4) \to A_{1u} \\
&B_1: \quad (1)-(2)-(3)+(4) \to A_{2g} \\
&B_2: \quad (1)+(2)-(3)-(4) \to A_{2u}
\end{aligned} \tag{2.1}$$

where the signs are determined from the characters shown on the right-hand side of table 2. On the right-hand side we give the irreducible representations of O_h which are induced by assuming that all 12 subshells (as defined in table 2) are associated with the same sign combinations as those given above.

Table 2. C'_{2v} subshell labelling of the 48-atom shell shown in figure 1. Subshell 1 is used to define the C'_{2v} irreducible representation labels. C'_{2v} representations are shown, together with the induced one-dimensional representations of O_h. Operations relating the atoms in a subshell are also shown.

Atom labels and subgroup operations		Subshell 1	2	3	4	5	6	7	8	9	10	11	12	$A_1(A_{1g})$	$A_2(A_{1u})$	$B_1(A_{2g})$	$B_2(A_{2u})$
(1)	E	2	29	6	25	48	11	44	15	23	38	19	34	+	+	+	+
(2)	σ'_v	3	28	7	32	41	10	45	14	24	37	20	33	+	−	−	+
(3)	C'_2	27	4	31	8	9	42	13	46	40	21	36	17	+	+	−	−
(4)	σ_v	26	5	30	1	16	43	12	47	39	22	35	18	+	−	+	−

Table 3. D'_{2h} subshell labelling corresponding to figure 1. In order to aid comparison with table 2 we have used the same subshell labels and row ordering. The operation C'_2 of table 2 has been rewritten as C''_2 in order to produce a consistent notation for the D'_{2h} operations.

		Subshells 1, 3	2, 4	5, 7	6, 8	9, 11	10, 12	D'_{2h} irreducible representation A_{1g}	B_{1g}	B_{2g}	B_{3g}	A_{1u}	B_{1u}	B_{2u}	B_{3u}
1	E	2	29	48	11	23	38	1	1	1	1	1	1	1	1
2	σ'_v	3	28	41	10	24	37	1	−1	1	−1	−1	1	−1	1
3	$C''_2(x)$	27	4	9	42	40	21	1	−1	−1	1	1	−1	−1	1
4	σ_v	26	5	16	43	39	22	1	1	−1	−1	−1	−1	1	1
5	$C_2(z)$	6	25	44	15	19	34	1	1	−1	−1	1	1	−1	−1
6	σ''_v	7	32	45	14	20	33	1	−1	−1	1	−1	1	1	−1
7	$C'_2(y)$	31	8	13	46	36	17	1	−1	1	−1	1	−1	1	−1
8	i	30	1	12	47	35	18	1	1	1	1	−1	−1	−1	−1

The permutation representations for the 48-fold shell can now be obtained simply by taking the direct product of the matrix of coefficients for a 12-fold shell, which have been given in table 3 of II, with the matrix of coefficients for the C'_{2v} modes shown above. Table 2 defines the atom labels which correspond to these combinations if the numbering $1, \ldots, 12$ is taken to be equivalent to that in table 3 of II. Irreducible representation labels for (C'_{2v}) A_1 modes are determined by associating the 12-fold modes with the top row of O_h representations shown in table 1. Other subshell modes then generate the remaining rows of table 1.

For example, adopting the convention that the atom label in table 3 of II comes first, the 48-element 8, 3 coefficient array (8 corresponding to the η row of T_{2g} in table 3 of II and 3 to the third (or B_1) row of (2.1)) is

$$(0000, +-+-, 0000)\otimes(+--+) =$$

$$0000, 0000, 0000, 0000, +--+, -++-, +--+, -++-,$$

$$0000, 0000, 0000, 0000.$$

In this array the elements correspond sequentially to the atom array 2, 3, 27, 26, 29, 28 etc given in table 2. Using this notation for the coefficient array corresponding to the atom permutation representations it is thus possible, following the method described in II, to use dual labelling (like 8, 3 above) to define the complete set of symmetry coordinates.

The generation of symmetry coordinates then proceeds in the same way as was described in II by reducing the direct products $\Gamma_P \otimes T_{1u}$ where Γ_P is any one of the permutation representations determined above and T_{1u} corresponds to single atom displacements. Following the notation of II we can write such symmetry coordinates in terms of cartesian coordinates with superscripts denoting the array of coefficients and atomic labels generated by the permutation representation. It is not even necessary to write out the full 48×48 table, because, as has been explained above, this is defined by the direct product of the rows of table 3 of II with the numbered rows of the coefficient arrays given in table 2. The dual labels may then be used as superscripts in the description of symmetry coordinates (see II).

Given the 48-fold shell symmetry coordinates it is possible to obtain consistent symmetry coordinates for both the 24-fold shell and 12-fold shell symmetry simply by identifying the arrays in different rows of table 2. If we identify rows such that row $1 \equiv$ row 2, row $3 \equiv$ row 4, then we obtain symmetry coordinates of the 24-fold shell with $(p\,p\,q)$ atomic positions. If we identify row $1 \equiv$ row 4 and row $2 \equiv$ row 3 we obtain symmetry coordinates of the 24-fold shell with $(p\,q\,0)$ atomic positions. Identification of all rows of table 2 provides symmetry coordinates for the 12-fold shell.

A defect of the C'_{2v} labelling scheme is that it cannot be applied to the subgroup O of O_h. This suggests that we introduce the Abelian group $D'_{2h} = C'_{2v} \otimes S_2$ to provide an alternative labelling. In this case the labelling has the same pattern if we use D'_2 as a subgroup of O. Table 3 defines the D'_{2h} subshells of O_h and shows that they bear a close relationship to the subshells for C'_{2v}. Table 4 gives the correlation theorem relationships between the irreducible representations of D′ and O. Corresponding relationships between the irreducible representations of D'_{2h} and O_h are obtained by inserting the appropriate subscripts g, u. (Note that D'_2 must not be identified with the *invariant* subgroup of O—in fact six conjugate subgroups are used in this labelling scheme.)

Table 4. Correlation table for O/D_2' representations. Note that D_2' contains two C_2' operations.

D_2'	O
A_1	A_1+E+T_2
B_1	A_2+E+T_1
B_2	T_1+T_2
B_3	T_1+T_2

3. Symmetry coordinates for atom shell displacements on the boundaries of cyclic regions

Cyclic regions in a crystal are regions which reproduce the whole crystal under the operations of a translation group T which is a subgroup of the full Bravais lattice group B. Cyclic region symmetry coordinates satisfy periodic boundary conditions at the surfaces of the region. In this section we shall investigate the effect of such conditions on the symmetry coordinates obtained in II and in the previous section.

The effect of periodic boundary conditions is to constrain sets of atoms on opposite boundaries of a cyclic region to move in the same way. This makes certain symmetry coordinates inoperative. Clearly, the simplest method of imposing such conditions is to relate them to the subshells used to generate the symmetry coordinate labelling. We can achieve this by including pairs of atoms on opposite boundaries in a given subshell.

It is useful, at this point, to introduce a specific example, and we shall consider the 24-fold ($p\,q$ 0) shell for which explicit symmetry coordinates were obtained in II. In order to use the same set of symmetry coordinates as were generated in II with a different definition of the subshells, it is necessary to relabel the atoms as is shown in figure 2. The numbers $\langle n \rangle$ differentiate the six subshells used in a C_{4v} labelling scheme. Periodic boundary conditions identify atoms on opposite faces so that, with the labelling shown, pairs of ions within a subshell are always identified. Considering characters, it is then easy to show that the permutations of a two-atom subshell transform as A_1+B_1 under C_{4v}. It thus follows that all symmetry coordinates labelled E in table 1 of II are eliminated by the cyclic boundary conditions *with the revised labelling of the atoms* shown in figure 2. The allowed permutation labels are thus $A_1|A_{1g}$, $A_1|E_g$, $A_1|T_{1u}$, $B_1|A_{2g}$, $B_1|E_g$ and $B_1|T_{2u}$.

If, on the other hand, we retain the labelling given in II, the effect of cyclic boundary conditions is to identify the subshells in pairs: $\langle 3\rangle \equiv \langle 4\rangle$, $\langle 2\rangle \equiv \langle 5\rangle$, $\langle 1\rangle \equiv \langle 6\rangle$. In this alternative labelling scheme all three C_{4v} labels (A_1, B_1 and E) survive, but each label corresponds to a restricted set of O_h labels. These can be read off table 1 of II by selecting the permutation symmetry coordinates which satisfy the three equivalences set out above. They are $A_1|A_{1g}$, $A_1|E_g$, $B_1|T_{2u}$, $E|T_{1u}$ and $E|T_{2u}$.

It follows that, in the case of periodic boundary conditions, identical sets of O_h labels will be classified by different C_{4v} labels according to the distribution of atoms in the subshells. Thus the labelling is not explicit unless we adopt a convention such that the subshells always contain equivalent pairs of atoms, if this be possible. In general terms, a labelling must be both unique (distinct labels for all modes) and explicit (specified shells and subshells) to generate a specific set of symmetry coordinates.

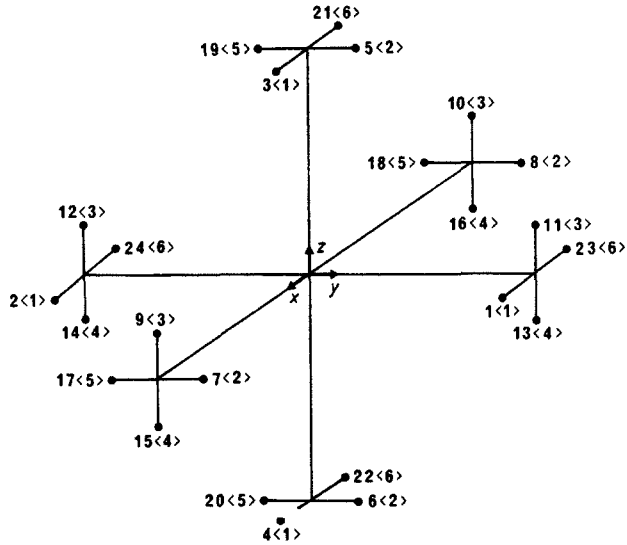

Figure 2. Atom positions in one 24-fold shell.

Periodic boundary conditions can also be applied to the 48-fold shell symmetry coordinates defined in the previous section. They correspond to the row identifications $1 \equiv 4$ and $2 \equiv 3$ in table 2, so that only the A_1, B_1 labelled symmetry coordinates survive. In D'_{2h} labelling periodicity conditions identify rows $1 \equiv 4$, $2 \equiv 3$, $5 \equiv 8$ and $6 \equiv 7$ in table 3, allowing only A_g, B_{1g}, B_{2u} and B_{3u} subshell representations.

4. A cyclic region group

The smallest cyclic region for a face-centred cubic lattice is shown in figure 3. It generates a 192-element group which can be obtained by combining the 24-element group of proper rotations (O) with eight distinct translations. Translations which move atoms to similarly numbered positions in figure 3 are taken to be identical to the identity. An alternative way of expressing this symmetry is to note that it is produced by reducing the operations in the space group O_h^5 modulo T, where T is the translation group produced by doubling the primitive translations of the face-centred cubic Bravais lattice. This produces a group with 384 elements corresponding to the direct product of the group defined by figure 3 with the group (S_2) containing the identity and the inversion. This 384-element group will be denoted $O_h^5/(2FCC)$, indicating that it is the factor (or quotient) group of O_h^5 with respect to the translation group T defined above.

The irreducible representations of $O_h^5/(2FCC)$ are just the irreducible representations of O_h^5 which satisfy the periodic boundary conditions. These are the representations at the Γ, X and L points in the Brillouin zone. There are 13 representations of each parity and hence 26 classes overall. The character table for proper rotations and (cyclic) translations is given in table 5, where we have introduced an alternative notation which links the space group irreducible representations with the Schönflies notation for the group of the $\boldsymbol{k}$ vector.

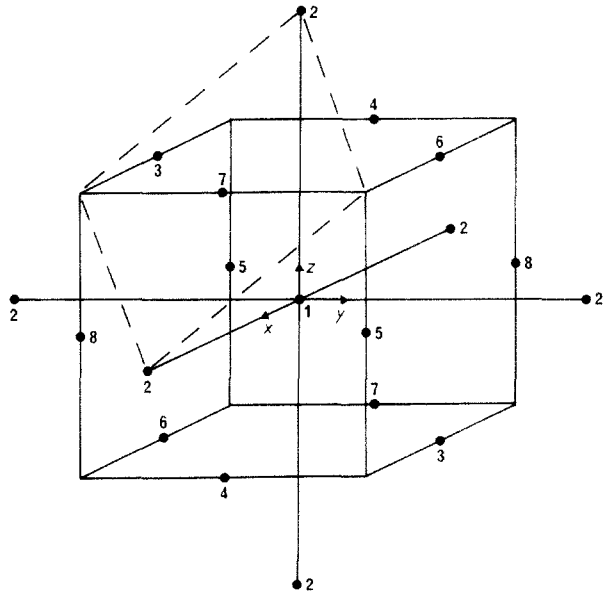

Figure 3. Cyclic region generated by the group $O_h^5/(2FCC)$. We have adopted a scale such that the atoms labelled 5 are at (1 1 0) and (−1 −1 0). Broken lines indicate one surface segment of the region, which has the same form as the BCC Brillouin zone. Repeated labelling is used for equivalent atoms, so that region contains only one distinct atom with each label, or eight in all.

By definition, the atomic positions shown in figure 3 all transform into each other under the operations of $O_h^5/(2FCC)$. This set breaks down into three distinct shells under O_h operations, and may thus be referred to as a *supershell*. By determining how many atoms are invariant under the cyclic group operations it is easy to construct the characters of the supershell permutation representation. (We found that the most reliable way of doing this is to write a computer program.) These are the (000) characters given in table 5. They correspond to the representation $A_{1g}^{\Gamma}+A_{1g}^{X}+A_{1g}^{L}$.

We now develop the model by supposing that figure 3 corresponds to the positive ions in an alkali halide (NaCl structure) lattice. The complementary set of eight negative ions also form a supershell in the positions (001), (010), (100), (−1 00), (0 −10), (00 −1), (111) and (−1 11). The last two atoms each generate sets of four equivalent atom positions on tetrahedra inscribed in the cube shown in figure 3. This supershell is labelled (100) in table 5, and the characters given in the table correspond to $A_{1g}^{\Gamma}+A_{1g}^{X}+A_{2u}^{L}$.

The relations between cyclic region group and point group representations can be obtained from Loudon's (1964, table 1) analysis of the relation between space group and point group representations in cubic crystals. In Schönflies notation we have, for example, that $A_{1g}^{X}\rightarrow A_{1g}+E_g$, $A_{1g}^{L}\rightarrow A_{1g}+T_{2g}$ and $A_{2u}^{L}\rightarrow A_{2u}+T_{1u}$. It follows that cyclic region group irreducible representations provide an alternative to shell labelling in distinguishing (for example) the two occurrences of A_{1g} for the negative ions.

The introduction of larger cyclic region groups, such as $O_h^5/(4FCC)$ with $48\times 64 = 3072$ elements and 64 classes, for labelling purposes may result in a prohibitive amount of effort. Nevertheless there are likely to be advantages in using the group $O_h^5/(2FCC)$

Table 5. Characters of a 192-element group. The classes are partially defined by the cyclic structure of the permutations of the labelled points in figure 3 corresponding to the spatial operations. t denotes translations of the type (1 1 0), and t' denotes (2 0 0) ≡ (0 2 0) ≡ (0 0 2). $t_\perp$ indicates that the translation t is perpendicular to the C_2 axis: the operation $\dot{C}_2 t$ is equivalent to a C_2 rotation about an axis shifted by $\frac{1}{2}t$ from the original axis. Only the thirteen classes of proper rotations are included. The table also includes supershell characters (discussed in the text) and the representations produced by taking direct products of the vector (T_1^Γ) and permutation representations. The number pairs used to denote supershell characters give first the character for the rotation and then the character for the corresponding rotation times the inversion. Littlewood (1958, p 277) gives this character table as a subgroup of the symmetric group S_8.

Cyclic structure		$(1)^8$	$(1)^4(2)^2$	$(2)^4$					$(4)^2$				$(2)(6)$	$(1)^2(2)(4)$	$(1)^2(3)$	
Classes		E	$6C_2$	$12C_2'$	$6t$	$6C_2t_\perp$	$12C_2't'$	t'	$12C_2t$	$24C_4t$	$24C_2't$	$32C_3t$	$24C_4$		$32C_3$	$\otimes T_1^\Gamma$
Γ_1	A_1^Γ	1	1	1	1	1	1	1	1	1	1	1	1		1	T_1^Γ
Γ_2	A_2^Γ	1	1	−1	1	1	−1	1	1	−1	−1	1	−1		1	T_2^Γ
Γ_{12}	E^Γ	2	2	0	2	2	0	2	2	0	0	−1	0		−1	$T_1^\Gamma+T_2^\Gamma$
Γ'_{25}	T_1^Γ	3	−1	−1	3	−1	−1	3	−1	1	−1	0	1		0	$A_1^\Gamma+E^\Gamma+T_1^\Gamma+T_2^\Gamma$
Γ'_{15}	T_2^Γ	3	−1	1	3	−1	1	3	−1	−1	1	0	−1		0	$A_2^\Gamma+E^\Gamma+T_1^\Gamma+T_2^\Gamma$
X_1	A_1^X	3	3	1	−1	−1	1	3	−1	−1	−1	0	1		0	$A_2^X+E^X$
X_2	A_2^X	3	−1	−1	−1	3	−1	3	−1	−1	1	0	1		0	$A_1^X+E^X$
X_3	B_1^X	3	3	−1	−1	−1	−1	3	−1	1	1	0	−1		0	$B_2^X+E^X$
X_4	B_2^X	3	−1	1	−1	3	1	3	−1	1	−1	0	−1		0	$B_1^X+E^X$
X_5	E^X	6	−2	0	−2	−2	0	6	2	0	0	0	0		0	$A_1^X+A_2^X+B_1^X+B_2+E^X$
L_1	A_1^L	4	0	2	0	0	−2	−4	0	0	0	−1	0		1	$A_2^L+E^L$
L_2	A_2^L	4	0	−2	0	0	2	−4	0	0	0	−1	0		1	$A_1^L+E^L$
L_3	E^L	8	0	0	0	0	0	−8	0	0	0	1	0		−1	$A_1^L+A_2^L+2E^L$
(0 0 0)		8, 8	4, 4	4, 4									2, 2		2, 2	
(1 0 0)		8, 0	4, 4	0, 4			4, 0	0, 8				0, 2	2, 2		2, 0	
$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$		16, 0		0, 8						0, 4					4, 0	
$(\frac{1}{2}0\,0)$		48, 0	8, 16	0, 8		8, 0							4, 0			
$(\frac{1}{2}\frac{1}{2}0)$		48, 0	0, 8	4, 8	0, 8	8, 0	4, 0									

in problems concerning the cyclic *region* generated from the unit cell by $O_h^5/(4FCC)$. Note that $O_h^5/(2FCC)$ is a factor group of $O_h^5/(4FCC)$, not a subgroup.

In order to illustrate the application of factor groups of cyclic region groups we have determined the characters for intervening supershells of atoms generated from atoms in the positions $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$, $(\frac{1}{2}\frac{1}{2}0)$ and $(\frac{1}{2}00)$ in figure 3. These supershells are described in table 6 and their characters are given in table 5. They correspond to the following irreducible representations:

$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$: $A_{1g}^{\Gamma}+A_{2u}^{\Gamma}+A_{2u}^{X}+B_{2g}^{X}+A_{1g}^{L}+A_{2u}^{L}$

$(\frac{1}{2}\frac{1}{2}0)$: $A_{1g}^{\Gamma}+E_g^{\Gamma}+T_{2g}^{\Gamma}+A_{1g}^{X}+E_u^{X}+B_{2g}^{X}+B_{2u}^{X}+A_{2u}^{X}+A_{1g}^{L}+A_{2u}^{L}+E_g^{L}+E_u^{L}$

$(\frac{1}{2}00)$: $A_{1g}^{\Gamma}+E_g^{\Gamma}+T_{1u}^{\Gamma}+2A_{1g}^{X}+B_{1g}^{X}+A_{2u}^{L}+E_u^{L}+A_{1g}^{L}+A_{2u}^{L}+E_g^{L}+E_u^{L}$.

Note that A_{1g}^{X} is repeated in the $(\frac{1}{2}00)$ permutation representation, showing the need to use the correlation theorem (or some other method) to distinguish the symmetry coordinates in this case.

Table 6. Supershells in the region $O_h^5/(4FCC)$ of the NaCl structure with respect to the operations of the group $O_h^5/(2FCC)$. See figure 3 for atomic positions.

Ionic charge	Supershell label	O_h shells (number of atoms)
+	000	000 (1), 110 (6), 200 (1)
+	100	100 (6), 111 (2)
−	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ (8), $\frac{3}{2}\frac{1}{2}\frac{1}{2}$ (8)
+	$\frac{1}{2}\frac{1}{2}0$	$\frac{1}{2}\frac{1}{2}0$ (12), $1\frac{1}{2}\frac{1}{2}$ (24), $\frac{3}{2}\frac{1}{2}0$ (12)
−	$\frac{1}{2}00$	$\frac{1}{2}00$ (6), $1\frac{1}{2}0$ (24), $11\frac{1}{2}$ (12), $\frac{3}{2}00$ (6)

It is, in fact, possible to apply the correlation theorem in two stages using the subgroup sequence $O_h^5/(2FCC) \supset O_h \supset D_{2h}$. Note that O_h is not an invariant subgroup of $O_h^5/(2FCC)$. There are four conjugate O_h groups, each leaving one of the pairs of atoms (1, 2), (3, 6), (4, 7) or (5, 8) of figure 3 in fixed positions. The relations between $O_h^5/(2FCC)$ and O_h irreducible representations may be deduced from the pure rotation characters in table 5 or read directly from Loudon (1964, table 1).

As we have stated previously, the solutions of one-electron problems and (pure) lattice vibration problems for a cyclic region form a subset of the full lattice solutions. Hence no advantages accrue from using cyclic region group labelling rather than the full space group labelling. Cyclic region solutions are only important when the finite size of the region can be used to advantage. One example of this occurs in finding exact many-electron solutions when correlation terms (such as the Hubbard term) are present in the Hamiltonian. Small region solutions (e.g. see Rössler *et al* 1981) can then be related to, but are not equivalent to, the full lattice solutions (D J Newman and Betty Ng, unpublished).

This series of papers was originally stimulated by the need to develop a formalism to describe local distortions and local strain effects in the neighbourhood of isolated substituted ions. At some level of approximation the form of solution of such problems in the immediate neighbourhood of quasi-isolated substituted ions (i.e. a substituted ion in each cyclic region) will be the same as that for an isolated substituted ion. If, for example, we consider the case of a single substituted ion at the centre of the region

with symmetry group $O_h^5/(4FCC)$, the symmetry of the cyclic region will be reduced to O_h. On the other hand the group $O_h^5/(2FCC)$ describes a system with substituted ions at all points on the supershell shown in figure 3. We would expect the displacements of the nearest neighbours of the substituted ions to be similar in both cases. Approximate $O_h^5/(4FCC)$ region solutions can then be constructed from the $O_h^5/(2FCC)$ region solutions using the decoupling transformation method described by Newman (1973a, b). We shall not go into the details of this here, but just point out that it should be possible to refine such solutions by a perturbation approach.

Finally, we should note that certain formal problems remain to be solved. In particular, cyclic region groups are not in general simply reducible (e.g. see the result for $E^L \otimes T_1^\Gamma$ in table 5), so that further separation criteria are necessary when symmetry coordinates are constructed from direct products of the vector and permutation representations.

5. Discussion

We have described three distinct developments of the work in papers I and II. A consistent scheme for labelling and generating symmetry coordinates for the 48-fold, 24-fold and 12-fold shells of atoms in O_h symmetry using the set of conjugate C'_{2v} subgroups has been described. This was then related to an alternative scheme using the set of conjugate D'_{2h} subgroups. Secondly the effect of using periodic boundary conditions defining cyclic regions has been investigated. Finally, we have introduced an entirely different approach to the labelling of symmetry coordinates in cyclic regions, indicating certain advantages that this may have over point group shell labelling. In particular, we have suggested that cyclic region group symmetry coordinates may be useful in the solution of correlated electron problems as well as local distortion and local strain effects in crystals.

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