Lattice Harmonics I. Cubic Groups

S. L. ALTMANN, A. P. CRACKNELL*

Department of Metallurgy, Oxford University, Oxford, England

A review is given of some conventions and definitions required for the derivation of the irreducible representations of the space groups, and of a method to obtain lattice harmonics. These are given for all the irreducible representations of the simple cubic ($Pm3m$), face-centered cubic ($Fm3m$) and body-centered cubic ($Im3m$) space groups for $l \leq 12$. The expansions are given in polar coordinates and care has been taken that different bases corresponding to the same representation span identical, rather than equivalent, representations, which are given in full. Moreover, all the different expansions listed in the tables are fully orthogonal.

1. INTRODUCTION

In many physical problems it is necessary to use linear combinations of spherical harmonics that belong to the irreducible representations of the space group of a crystal. Such expansions were first obtained by von der Lage and Bethe[1] who derived them for the cubic lattice (whence the name of "kubic harmonics" coined by these authors) and applied them for cellular calculations of the band structure in cubic metals. Their use is not, of course, limited to the cellular method. As just one example of a recent application in a different method we mention the work of Ham.[2]

Von der Lage and Bethe did not use the standard form of the spherical harmonics in polar coordinates: they gave instead a method to obtain directly homogeneous polynomials in the Cartesian coordinates x, y, z, with the required symmetry properties. Von der Lage and Bethe's work was extended for other space groups by Bell,[3] who introduced the name lattice harmonics for these polynomials. Bell's work however is rather limited, since the use of Cartesian coordinates becomes extremely difficult for high values of l. Her tables, therefore, did not go further than $l=6$. Moreover, her treatment of the hexagonal close-packed lattice is wrong since no proper account is given of the necessary phase factors that relate the two atoms in the unit cell. Also, the representations that she uses for the top face of the Brillouin zone are incorrect.

No general method was given to symmetry-adapt, in the terminology of Melvin,[4] the spherical harmonics in their usual polar form, until one of us[5] provided a technique for doing so for the point groups. His method and tables have now been extended and improved by Altmann and Bradley.[6] An advantage of this approach is that in many cases the expansions can be given for all orders of l and, where this is not possible, the treatment of large values of l is not difficult. Moreover, Altmann[7] showed how his method could be extended for space groups. The present paper and the following one, to which this section also serves as an introduction, extend this work by making full use of the new results of Altmann and Bradley,[6] to cover all the irreducible representations of the simple, face-centered and body-centered cubic lattices and the hexagonal close-packed lattice. The lattice harmonics for the cubic groups are given for $l \leq 12$ and for all values of l for the hexagonal lattice. It should be noticed that, unlike Bell, we give in full the irreducible representations spanned by our expansions, since such information is important to specify the lattice harmonics unambiguously and is essential in some applications. Also, when two lattice harmonics with the same values of l and m belong to the same column of the same representation, they have been made orthogonal by the technique of Altmann and Bradley.[6]

2. GENERAL THEORY

We give in this section a number of results in great detail which, although well-known in group theory, do appear to cause a certain amount of trouble in solid-state theory.

Symmetry operations in configuration space can be interpreted either as axes transformations (passive interpretation) or as point transformations (active interpretation). We shall represent these with R_p and R_a, respectively, and it is well known that $R_a = R_p^{-1}$. (See, e.g., Altmann.[8]) Such operators induce transformations of functions which we shall designate by operators in script type, such that

$$\mathcal{R} f(x) = f(R^{-1}x). \quad (1)$$

This expression is valid in the active as well as in

* Present address: Department of Physics, University of Singapore, Singapore 10, Malaysia.

1 F. C. von der Lage and H. A. Bethe, Phys. Rev. **71**, 612 (1947).

2 F. S. Ham, Phys. Rev. **128**, 82 (1962).

3 D. G. Bell, Rev. Mod. Phys. **26**, 311 (1954).

4 M. A. Melvin, Rev. Mod. Phys. **28**, 18 (1956).

5 S. L. Altmann, Proc. Cambridge Phil. Soc. **53**, 343 (1957).

6 S. L. Altmann and C. J. Bradley, Phil. Trans. London **A255**, 199 (1963).

7 S. L. Altmann, Proc. Roy. Soc. (London) **A244**, 141 (1958).

8 S. L. Altmann, "Group Theory" in *Quantum Theory*, edited by D. R. Bates (Academic Press Inc., New York, 1962), Vol. II, p. 144.

the passive interpretation and ensures the isomorphism between the script and the roman operators, as shown by Wigner.[9] However, it should be observed that active and passive operators do not multiply in the same manner. For, if $\mathcal{R}_p\mathcal{S}_p=\mathfrak{I}_p$ then, on taking inverses, $\mathcal{S}_p^{-1}\mathcal{R}_p^{-1}=\mathfrak{I}_p^{-1}$, i.e., $\mathcal{S}_a\mathcal{R}_a=\mathfrak{I}_a$.

If we have a representation given by matrix representatives $D(\mathcal{R}_p)$, we obtain one for the active operators by using the rule $D(\mathcal{R}_a)=D(\mathcal{R}_p^{-1})$. For if $\mathcal{R}_p\mathcal{S}_p=\mathfrak{I}_p$, then $\mathcal{S}_a\mathcal{R}_a=\mathfrak{I}_a$ and $D(\mathcal{S}_a)D(\mathcal{R}_a)=D(\mathcal{S}_p^{-1})D(\mathcal{R}_p^{-1})=D[(\mathcal{R}_p\mathcal{S}_p)^{-1}]=D(\mathfrak{I}_p^{-1})=D(\mathfrak{I}_a)$. This new representation is not identical with the original one, but it is nevertheless spanned by the same basis. For if $\mathcal{R}_pf_i=\sum_j f_jD(\mathcal{R}_p)_{ji}$, then $\mathcal{R}_af_i=\mathcal{R}_p^{-1}f_i=\sum_j f_jD(\mathcal{R}_p^{-1})_{ji}=\sum_j f_jD(\mathcal{R}_a)_{ji}$.

In summary, in going from passive to active operators, one applies the rules

$$\mathcal{R}_a\leftrightarrow\mathcal{R}_p^{-1}, \qquad D(\mathcal{R}_a)\leftrightarrow D(\mathcal{R}_p^{-1}), \tag{2}$$

but the multiplication rules are not conserved. Also, the labels of the representations have to be revised with respect to the standard labels given in character tables.

When $\mathcal{R}$ is a space-group operation it includes a translational part $\mathbf{v}$ as well as a rotational part α. The well-known symbol $\{\alpha\mid\mathbf{v}\}$, introduced by Seitz[10] is used to represent such operations. Since it would be too cumbersome to attempt a distinction in this case between the function and configuration-space operators we shall not do so, but it should always be clear from the context which operator is meant. It is traditional in solid-state theory, following Seitz, to multiply the space-group operators as follows

$$\{\alpha\mid\mathbf{v}\}\{\alpha'\mid\mathbf{v}'\}=\{\alpha\alpha'\mid\alpha\mathbf{v}'+\mathbf{v}\}. \tag{3}$$

Nevertheless, it is seldom noticed that this multiplication rule implies the active interpretation for the operators $\{\alpha\mid\mathbf{v}\}$ and that, of course, it is not valid in the passive convention. Since we consider it important to preserve (3), which is much used, we shall always understand the operators $\{\alpha\mid\mathbf{v}\}$ as active.

It is well known that the bases of the representations of space groups are Bloch functions

$$\psi_{\mathbf{k}}(\mathbf{r})=\exp(i\mathbf{k}\cdot\mathbf{r})u_{\mathbf{k}}(\mathbf{r}), \tag{4}$$

where $\mathbf{k}$ is the label of the representation and $u_{\mathbf{k}}(\mathbf{r})$ is periodic in $\mathbf{r}$. We now denote as usual with the symbol $\{E\mid\mathbf{t}\}$ a translation of the translation subgroup $\mathbf{\Gamma}$ of the space group. (E is the identity of the rotation group.) Hence

$$\{E\mid\mathbf{t}\}\psi_{\mathbf{k}}(\mathbf{r})=\psi_{\mathbf{k}}(\mathbf{r}-\mathbf{t})=\exp(-i\mathbf{k}\cdot\mathbf{t})\psi_{\mathbf{k}}(\mathbf{r}), \tag{5}$$

whence

$$D\{E\mid\mathbf{t}\}=\exp(-i\mathbf{k}\cdot\mathbf{t}). \tag{6}$$

[9] E. P. Wigner, *Group Theory* (Academic Press Inc., New York, 1959).
[10] F. Seitz, Ann. Math. **37,** 17 (1936).

The negative sign in the exponent should be noted, since in many treatments in solid state it is given as positive. However, this is the only choice compatible with (1) [used in the first step in (5)], (3), and (4). The need to maintain the latter, of course, arises from the physical meaning of $\mathbf{k}$ as a quasimomentum, which would make it unnatural to take a negative exponent in the Bloch function. Confusion in the literature arises from the fact that Bloch used the translations in the *passive* convention: he gave the second term in (5) as $\psi_{\mathbf{k}}(\mathbf{r}+\mathbf{t})$, and this form is still the most commonly used. But this is incompatible with the *active* convention for the Seitz operators implied by (3) and which is entirely standard. We do not give a list of references where such inconsistencies appear since it would be too long. It may suffice to say that of a large number of papers and books that we have surveyed the only fully consistent treatment that we have been able to find is the one given by Herring[11] with whom our conventions and basic expressions agree entirely. It is probable nevertheless that, since Herring did not explain his conventions at all, the whole point has failed to be duly appreciated. Since we shall now use the active convention, whereas in our previous work on point groups we employed the passive one, we shall make the necessary changes, when required, by means of the rules given in (2).

The theory of the space groups given by Seitz[10] and Bouckaert, Smoluchowski, and Wigner[12] is well known.[13–15] An irreducible representation of a space group is fully determined by means of the group of the $\mathbf{k}$ vector, $\mathbf{G}^{\mathbf{k}}$ (the subgroup of operations of the space group that leave $\mathbf{k}$ invariant or transform it into an equivalent vector) and one of its representations. The reduction of the space group is therefore achieved by reducing $\mathbf{G}^{\mathbf{k}}$. The space groups we deal with in this paper are symmorphic, that is they contain no screw axes or glide planes. (Asymmorphic groups are treated in the following paper.) All the operations of the space group can in this case be written as products $\{E\mid\mathbf{t}\}\{\alpha\mid\mathbf{o}\}$, where $\{E\mid\mathbf{t}\}\in\mathbf{\Gamma}$. In the notation of Altmann,[15] $\mathbf{G}^{\mathbf{k}}$ can be expressed as a semidirect product: $\mathbf{G}^{\mathbf{k}}=\mathbf{\Gamma}\wedge G^{\mathbf{k}}$, where $G^{\mathbf{k}}$, the cogroup of $\mathbf{k}$, is the subgroup of operations of the point group that belong to $\mathbf{G}^{\mathbf{k}}$. This simplifies considerably the work required to produce the symmetry-adapted harmonics. They are obtained by using the well-known projection operators (Wigner[9]), which are defined as follows. Consider a group $\mathbf{G}$ of operations $\mathcal{R}$ and assume given an irreducible representation of matrices $D^i(\mathcal{R})$. Then the

[11] C. Herring, J. Franklin Inst. **233,** 525 (1942).
[12] L. P. Bouckaert, R. Smoluchowski, and E. Wigner, Phys. Rev. **50,** 58 (1936).
[13] G. F. Koster, Solid State Phys. **5,** 174 (1957).
[14] D. F. Johnston, Rept. Progr. Phys. **23,** 66 (1960).
[15] S. L. Altmann, Phil. Trans. Roy. Soc. London **A255,** 216 (1963). In this paper the cogroup of $\mathbf{k}$, $G^{\mathbf{k}}$, was denoted with a symbol $\mathbf{G}^{\mathbf{k}}$ with bar. The present change is due to typographical reasons.

projection operator,

$$\sum_{\mathcal{R}\epsilon\mathbf{G}} D^i(\mathcal{R})_{ss}{}^*\mathcal{R}, \tag{7}$$

is such that when applied on any arbitrary function ϕ (called the generator) it will adapt it into a function belonging to the sth column of the ith irreducible representation of $\mathbf{G}$. The generator will always be in our case a spherical harmonic. If $\mathcal{R}$ is a point-group operation, $\mathcal{R}\phi$ can then be evaluated by using the familiar representations of the rotation group, for which it is necessary to express $\mathcal{R}$ in terms of its Euler angles. The representations of the rotation group are complicated and various short-cuts are necessary, which have been fully described.[5,6]

When the properties of the symmorphic groups described above are taken into account, the operator (7) applied on a spherical harmonic takes the form

$$\sum_{\mathbf{\Gamma}} D\{E\mid \mathbf{t}\}^*\{E\mid \mathbf{t}\}\sum_{G^{\mathbf{k}}} D\{\alpha\mid \mathbf{o}\}^*\{\alpha\mid \mathbf{o}\}\, Y_l^m. \tag{8}$$

The summation over the point-group operations can be carried out exactly as in the work of Altmann[5] and Altmann and Bradley[6] and no further description is necessary, except that the appropriate allowance must be made for the active interpretation for α. The result of this summation will be a spherical harmonic of order l, symmetry-adapted to $G^{\mathbf{k}}$, which we call $X_{l\nu}$. This is a linear combination of several Y_l^m with constant l and varying m: the index ν is an arbitrary label to distinguish the various harmonics of the same order that belong to the same representation. We shall always take $X_{l\nu}\equiv X_{l\nu}(\theta, \phi)$ as a function of the polar coordinates around the origin of coordinates for the lattice, $\mathbf{r}=\mathbf{o}$. Let us define ${}^{\mathbf{t}}X_{l\nu}$ as a function identical with $X_{l\nu}$ except that it is centered around the point at the end of the vector $\mathbf{t}$ of the lattice $(\mathbf{r}=\mathbf{t})$. That is

$$\{E\mid \mathbf{t}\}X_{l\nu}={}^{\mathbf{t}}X_{l\nu}. \tag{9}$$

Then, on using (6), (8) gives

$$\sum_{t} \exp\,(i\mathbf{k}\cdot\mathbf{t})\; {}^{\mathbf{t}}X_{l\nu}, \qquad \text{all } \mathbf{t}\in\mathbf{\Gamma}. \tag{10}$$

This multicentered expansion is a lattice harmonic. It should be noticed that it is fully given if we know $X_{l\nu}$ in the unit cell at the origin. The expansion throughout the lattice follows at once, if required, from the Bloch condition, as is apparent from (10). Therefore, it will be enough for symmorphic groups to give the expansions $X_{l\nu}$. The discussion of asymmorphic groups will be left for the following paper.

3. THE METHOD FOR THE CUBIC GROUPS

It follows from Sec. 2 that the problem of obtaining lattice harmonics for the cubic lattices is in principle solved: we must obtain harmonics adapted to the various $G^{\mathbf{k}}$ groups that appear in the lattice. $G^{\mathbf{k}}$ is a point group and clearly also a subgroup of the full cubic group $\mathbf{O}_h$. Therefore the harmonics can be obtained by the use of the techniques of Altmann and Bradley.[6] In fact, for some groups $G^{\mathbf{k}}$ the results can be read off their tables. It should be noticed, nevertheless, that although $G^{\mathbf{k}}$ may be a point group given in the tables referred to, it will often appear in our present work in an orientation that differs from the standard one used by Altmann and Bradley, which causes a drastic change in the harmonics. Rather than repeating their work for these new orientations, the following method yields the results more quickly and in a more convenient form.

Consider the group of operators $G^{\mathbf{k}}$, a subgroup of $\mathbf{O}_h$, and take an irreducible representation of $\mathbf{O}_h$ from the tables, with basis symbolically written as a row vector $\langle\phi\mid$. The matrices of this representation that correspond to the operators of $G^{\mathbf{k}}$ form a representation of $G^{\mathbf{k}}$ which is called a *subduced representation.* This is, in general, reducible. We reduce it under a unitary transformation with a matrix M and we obtain the subduced irreducible representations of $G^{\mathbf{k}}$ that are required. At the same time the new bases are given, as is well known, by $\langle\psi\mid=\langle\phi\mid M$. We therefore have the new symmetry-adapted harmonics as well as the representations that they span.

In order to solve the problem as stated we must find the matrix M that reduces the subduced representation. Most methods given in the literature for this purpose require a knowledge of the irreducible representations that appear under reduction, which would defeat our purpose. Fortunately there is a method that is free from this drawback (Altmann,[8] p. 123). The prescription for it is as follows. Consider a matrix representation to be reduced: take all the matrices of any class and sum them. Find the matrix M that diagonalizes the matrix obtained: this is the matrix that reduces the representation.

It should be noticed that two bases of the same representation may subduce into equivalent rather than identical representations. If this is the case, a similarity transformation is required to make all the bases obtained span the same representation.

4. NORMALIZATION

As follows from Sec. 3, the symmetry-adapted spherical harmonics will be given as linear combinations of those for the cubic groups. The latter are given in Tables 8–11 of Altmann and Bradley.[6] However, in that paper unnormalized spherical harmonics $\mathcal{Y}_l^m=P_l^m(\cos\theta)\exp(im\phi)$ were used to give the necessary coefficients in the $X_{l\nu}$ exact to any number of figures. In practical applications normalized spherical harmonics,

$$Y_l^m(\theta,\phi)=\left[\left(\frac{2l+1}{4\pi}\,\frac{(l-|m|)!}{(l+|m|)!}\right)\right]^{\frac{1}{2}}P_l^m(\cos\theta)\,e^{im\phi}, \tag{11}$$

are required and expansions $X_{l\nu}$ in terms of them were

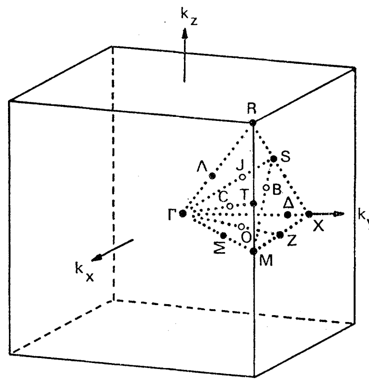

FIG. 1. The first Brillouin zone for the simple cubic lattice. The points marked with open circles belong to planes, but not lines, of symmetry. A is a general point.

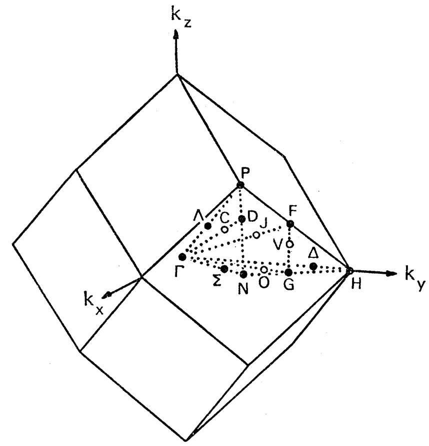

FIG. 2. The first Brillouin zone for the body-centered cubic lattice. The points marked with open circles belong to planes, but not lines, of symmetry. A is a general point.

obtained on a Ferranti Mercury computer and are given in Table I. The coefficients are correct to at least seven significant figures. Various checks and repeated calculation have been used to ensure that these tables are free from error.

TABLE I. The normalized symmetry-adapted harmonics for the cubic groups.

Notes

(*i*) *Representations.* The symmetry-adapted harmonics are the same whether the active or the passive interpretation is used. In the latter case the matrix representatives are identical with those listed by Altmann and Bradley[6] in their Tables 6 and 7. If the active convention is used these matrices can be employed, but for the operation α the matrix corresponding to α^{-1} must be taken. ${}^1E$ and ${}^2E$ are the first and second representation, respectively, in the table for **T** of Altmann[8]. The complete representations of **0**, $\mathbf{0}_h$, and $\mathbf{T}_d$ can be obtained from Tables II and III below.

(*ii*) *Spherical harmonics.* They are

$$Y_l^{m,c}=(Y_l^m+Y_l^{-m})/\sqrt{2}, \tag{12}$$

$$Y_l^{m,s}=-\mathrm{i}(Y_l^m-Y_l^{-m})/\sqrt{2}, \tag{13}$$

where the normalized Y_l^m are defined in (11).

(*iii*) *Bases.* They are understood as *row* vectors. Their transformation properties are obtained by postmultiplying them with the matrix representative: the first function belongs to the first column of the representation, the second to the second, etc.

(*iv*) *Notation of the tables.* A harmonic such as $aY_l^{m,c}+bY_l^{n,c}+cY_l^{p,c}$ is given as follows: the values of l and the superscript c (or s) appear under the headings l and ϕ-dep, respectively. The rest of the expansion appears on the same line in the form $a(m)+b(n)+c(p)$. Degenerate representations are given in several lines, and they must be understood as a row vector, the successive lines corresponding to the successive columns of the vector. In the three-dimensional representations the first two partners are given in one line: the first letter under "ϕ-dep" and the upper sign in the expansion correspond to the first partner.

(*v*) *Orthogonality.* The expansions $X_{l\nu}$ given here are orthonormal for different l or different ν. Also in a multidimensional basis all the partners in the same basis are orthogonal. (See Altmann and Bradley.[6])

TABLE I (a). Harmonics for the one-dimensional representations.

T	$\mathbf{T}_h$	$\mathbf{T}_d$	**0**	$\mathbf{0}_h$	l	ϕ-dep	Spherical harmonic
A	A_g	A_1	A_1	A_{1g}	0	c	1(0)
A	A_u	A_1	A_2	A_{2u}	3	s	1(2)
A	A_g	A_1	A_1	A_{1g}	4	c	0.76376261(0)+0.64549722(4)
A	A_g	A_1	A_1	A_{1g}	6	c	0.35355339(0)−0.93541435(4)
A	A_g	A_2	A_2	A_{2g}	6	c	0.82915619(2)−0.55901699(6)
A	A_u	A_1	A_2	A_{2u}	7	s	0.73598007(2)+0.67700320(6)
A	A_g	A_1	A_1	A_{1g}	8	c	0.71807033(0)+0.38188131(4)+0.58184333(8)
A	A_u	A_1	A_2	A_{2u}	9	s	0.43301270(2)−0.90138782(6)
A	A_u	A_2	A_1	A_{1u}	9	s	0.84162541(4)−0.54006172(8)
A	A_g	A_1	A_1	A_{1g}	10	c	0.41142537(0)−0.58630197(4)−0.69783892(8)
A	A_g	A_2	A_2	A_{2g}	10	c	0.80201569(2)+0.15728822(6)−0.57622153(10)
A	A_u	A_1	A_2	A_{2u}	11	s	0.66536331(2)−0.45927933(6)−0.58851862(10)
A	A_g	A_1	A_1	A_{1g}	12	c	0.69550266(0)+0.31412557(4)+0.34844954(8)+0.54422798(12)
A	A_g	A_1	A_1	A_{1g}	12	c	0.55897937(4)−0.80626751(8)+0.19358400(12)
A	A_g	A_2	A_2	A_{2g}	12	c	0.21040635(2)−0.82679728(6)+0.52166600(10)

TABLE I(b). Harmonics for the complex representations of **T** and $\mathbf{T}_h$. The harmonics of ${}^2E$, ${}^2E_g$, and ${}^2E_u$ are the complex conjugates of the expansions listed in this table. The labels of the representations given are valid *only in the active convention*. If the passive convention is used it is enough to interchange the superscripts 1 and 2 in this table. That is, ${}^1E$ goes into ${}^2E$, etc.

T	$\mathbf{T}_h$	l	ϕ-dep	Spherical harmonic
${}^1E$	${}^1E_g$	2	*c*	0.70710678(0) −0.70710678(2)i
${}^1E$	${}^1E_g$	4	*c*	0.45643546(0) −0.54006172(4) +0.70710678(2)i
${}^1E$	${}^1E_u$	5	*s*	0.70710678(2) −0.70710678(4)i
${}^1E$	${}^1E_g$	6	*c*	0.66143783(0) +0.25(4) −[0.39528471(2) +0.58630196(6)]i
${}^1E$	${}^1E_u$	7	*s*	0.47871355(2) −0.52041650(6) +0.70710678(4)i
${}^1E$	${}^1E_g$	8	*c*	0.49212549(0) −0.27860540(4) −0.42448973(8) +[0.46010167(2) +0.53694176(6)]i
${}^1E$	${}^1E_g$	8	*c*	0.59115342(4) −0.38799180(8) +[0.53694176(2) −0.46010167(6)]i
${}^1E$	${}^1E_u$	9	*s*	0.38188131(4) +0.59511903(8) +[0.63737744(2) +0.30618622(6)]i
${}^1E$	${}^1E_g$	10	*c*	0.64448784(0) +0.18714046(4) +0.22274170(8)
				−[0.31464779(2) +0.34379898(6) +0.53178852(10)]i
${}^1E$	${}^1E_g$	10	*c*	0.54139029(4) −0.45485883(8)
				−[0.28174844(2) −0.60780957(6) +0.22624178(10)]i
${}^1E$	${}^1E_u$	11	*s*	0.52786914(2) −0.28945395(6) −0.37090508(10)
				+[0.35023357(4) +0.61427717(8)]i
${}^1E$	${}^1E_u$	11	*s*	0.55744745(6) −0.43503142(10) +[0.61427717(4) −0.35023357(8)]i
${}^1E$	${}^1E_g$	12	*c*	0.50807284(0) −0.21500378(4) −0.23849688(8) −0.37249777(12)
				+[0.36487352(2) +0.38689303(6) +0.46602693(10)]i
${}^1E$	${}^1E_g$	12	*c*	0.49820374(4) +0.23953507(8) −0.44092628(12)
				+[0.58713874(2) −0.09228708(6) −0.38308119(10)]i

TABLE I(c). Harmonics for the two-dimensional representations of $\mathbf{T}_d$, **0** and $\mathbf{0}_h$.
For the representations marked with an asterisk the partners must be interchanged and the sign of one of them reversed.

$\mathbf{T}_d$	0	$\mathbf{0}_h$	l	ϕ-dep	Spherical harmonic
E	*E*	E_g	2	*c*	1(0)
				c	1(2)
E	*E*	E_g	4	*c*	0.64549722(0) −0.76376262(4)
				c	−1(2)
*E**	*E*	E_u	5	*s*	1(4)
				s	−1(2)
E	*E*	E_g	6	*c*	0.93541434(0) +0.35355339(4)
				c	0.55901699(2) +0.82915619(6)
*E**	*E*	E_u	7	*s*	1(4)
				s	0.67700320(2) −0.73598007(6)
E	*E*	E_g	8	*c*	0.69597054(0) −0.39400753(4) −0.60031913(8)
				c	−0.65068202(2) −0.75935032(6)
E	*E*	E_g	8	*c*	0.83601718(4) −0.54870326(8)
				c	−0.11588441(2) +0.99326270(6)
*E**	*E*	E_u	9	*s*	0.54006172(4) +0.84162541(8)
				s	−0.90138782(2) −0.43301270(6)
E	*E*	E_g	10	*c*	0.21628928(0) +0.62804094(4) +0.74751824(8)
				c	0.44497917(2) +0.48620518(6) +0.75206253(10)
E	*E*	E_g	10	*c*	0.76564149(4) −0.64326752(8)
				c	0.39845246(2) −0.85957253(6) +0.31995420(10)
*E**	*E*	E_u	11	*s*	0.49530506(4) +0.86871911(8)
				s	0.74651970(2) −0.40934970(6) −0.52453900(10)
*E**	*E*	E_u	11	*s*	0.86871911(4) −0.49530506(8)
				s	−0.78834975(6) +0.61522733(10)
E	*E*	E_g	12	*c*	0.71852351(0) −0.30406127(4) −0.33728553(8)
					−0.52679140(12)
				c	−0.51600908(2) +0.54714937(6) +0.65906160(10)
E	*E*	E_g	12	*c*	0.70456648(4) +0.33875374(8) −0.62356392(12)
				c	−0.83033957(2) +0.13051364(6) +0.54175861(10)

TABLE I(d). Harmonics for the three-dimensional representations of the five cubic groups.

T	$\mathbf{T}_h$	$\mathbf{T}_d$	**O**	$\mathbf{O}_h$	l	ϕ-dep	Spherical harmonic
T	T_u	T_2	T_1	T_{1u}	1	c, s	1(1)
						c	1(0)
T	T_g	T_2	T_2	T_{2g}	2	s, c	1(1)
						s	1(2)
T	T_u	T_2	T_1	T_{1u}	3	c, s	0.61237243(1)∓0.79056941(3)
						c	−1(0)
T	T_u	T_1	T_2	T_{2u}	3	c, s	∓0.79056941(1)−0.61237243(3)
						c	1(2)
T	T_g	T_2	T_2	T_{2g}	4	s, c	0.35355339(1)∓0.93541435(3)
						s	−1(2)
T	T_g	T_1	T_1	T_{1g}	4	s, c	∓0.93541435(1)−0.35355339(3)
						s	1(4)
T	T_u	T_2	T_1	T_{1u}	5	c, s	0.48412292(1)∓0.52291252(3)+0.70156076(5)
						c	1(0)
T	T_u	T_1	T_2	T_{2u}	5	c, s	±0.66143783(1)−0.30618622(3)∓0.68465320(5)
						c	1(2)
T	T_u	T_2	T_1	T_{1u}	5	c, s	0.57282196(1)±0.79549513(3)+0.19764235(5)
						c	1(4)
T	T_g	T_2	T_2	T_{2g}	6	s, c	0.19764235(1)∓0.56250000(3)+0.80282703(5)
						s	1(2)
T	T_g	T_1	T_1	T_{1g}	6	s, c	±0.43301270(1)−0.68465320(3)∓0.58630197(5)
						s	1(4)
T	T_g	T_2	T_2	T_{2g}	6	s, c	0.87945295(1)±0.46351240(3)+0.10825318(5)
						s	1(6)
T	T_u	T_2	T_1	T_{1u}	7	c, s	0.41339864(1)∓0.42961647(3)+0.47495888(5)∓0.64725985(7)
						c	−1(0)
T	T_u	T_1	T_2	T_{2u}	7	c, s	∓0.57409916(1)+0.41984465(3)∓0.07328775(5)−0.69912054(7)
						c	1(2)
T	T_u	T_2	T_1	T_{1u}	7	c, s	0.53855275(1)±0.10364452(3)−0.78125000(5)∓0.29810600(7)
						c	−1(4)
T	T_u	T_1	T_2	T_{2u}	7	c, s	∓0.45768183(1)−0.79272818(3)∓0.39836090(5)−0.05846340(7)
						c	1(6)
T	T_g	T_2	T_2	T_{2g}	8	s, c	0.13072813(1)∓0.38081430(3)+0.59086470(5)∓0.69912054(7)
						s	−1(2)
T	T_g	T_1	T_1	T_{1g}	8	s, c	∓0.27421764(1)+0.60515364(3)∓0.33802043(5)−0.66658528(7)
						s	1(4)
T	T_g	T_2	T_2	T_{2g}	8	s, c	0.45768183(1)∓0.47134697(3)−0.70883101(5)∓0.25674495(7)
						s	−1(6)
T	T_g	T_1	T_1	T_{1g}	8	s, c	∓0.83560887(1)−0.51633474(3)∓0.18487749(5)−0.03125000(7)
						s	1(8)
T	T_u	T_2	T_1	T_{1u}	9	c, s	0.36685490(1)∓0.37548796(3)+0.39636409(5)∓0.44314853(7) +0.60904939(9)
						c	1(0)
T	T_u	T_1	T_2	T_{2u}	9	c, s	±0.51301422(1)−0.42961647(3)±0.25194555(5)+0.05633674(7) ∓0.69684697(9)
						c	1(2)
T	T_u	T_2	T_1	T_{1u}	9	c, s	0.49435287(1)∓0.13799626(3)−0.39218439(5)±0.67232906(7) +0.36157614(9)
						c	1(4)
T	T_u	T_1	T_2	T_{2u}	9	c, s	±0.45768183(1)+0.29810600(3)∓0.60515365(5)−0.56832917(7) ∓0.11158452(9)
						c	1(6)

TABLE I(d) (*Continued*)

T	$\mathbf{T}_h$	$\mathbf{T}_d$	**0**	$\mathbf{0}_h$	l	ϕ-dep	Spherical harmonic
T	T_u	T_2	T_1	T_{1u}	9	c, s	0.38519666(1) ±0.75268075(3) +0.50931269(5) ±0.15944009(7) +0.01657282(9)
						c	1(8)
T	T_g	T_2	T_2	T_{2g}	10	s, c	0.09472153(1) ∓0.27885263(3) +0.44538102(5) ∓0.57486942(7) +0.62002414(7)
						s	1(2)
T	T_g	T_1	T_1	T_{1g}	10	s, c	±0.19515619(1) −0.48613591(3) ±0.49410588(5) −0.09110862(7) ∓0.68785502(9)
						s	1(4)
T	T_g	T_2	T_2	T_{2g}	10	s, c	0.31049159(1) ∓0.53906250(3) −0.01746928(5) ±0.69255289(7) +0.36479021(9)
						s	1(6)
T	T_g	T_1	T_1	T_{1g}	10	s, c	±0.46456465(1) −0.31560953(3) ∓0.70572436(5) −0.42100605(7) ∓0.09631897(9)
						s	1(8)
T	T_g	T_2	T_2	T_{2g}	10	s, c	0.80044772(1) ±0.54379714(3) +0.24319347(5) ±0.06594509(7) +0.00873464(9)
						s	1(10)
T	T_u	T_2	T_1	T_{1u}	11	c, s	0.33321251(1) ∓0.33846028(3) +0.35033967(5) ∓0.37296506(7) +0.41975833(9) ∓0.57997947(11)
						c	−1(0)
T	T_u	T_1	T_2	T_{2u}	11	c, s	∓0.46765008(1) +0.41655170(3) ∓0.31014124(5) +0.13689999(7) ±0.13594929(9) −0.68875008(11)
						c	1(2)
T	T_u	T_2	T_1	T_{1u}	11	c, s	0.45637974(1) ∓0.23534954(3) −0.13435456(5) ±0.49510852(7) −0.55722625(9) ∓0.40329075(11)
						c	−1(4)
T	T_u	T_1	T_2	T_{2u}	11	c, s	∓0.43552936(1) −0.04764184(3) ±0.52272828(5) −0.32425699(7) ∓0.63603689(9) −0.15847416(11)
						c	1(6)
T	T_u	T_2	T_1	T_{1u}	11	c, s	0.40022386(1) ±0.39401846(3) −0.40784786(5) ∓0.65553754(7) −0.29501240(9) ∓0.03832308(11)
						c	−1(8)
T	T_u	T_1	T_2	T_{2u}	11	c, s	∓0.33485131(1) −0.70641321(3) ∓0.56871666(5) −0.24930093(7) ∓0.05695964(9) −0.00458048(11)
						c	1(10)
T	T_g	T_2	T_2	T_{2g}	12	s, c	0.07271293(1) ∓0.21528718(3) +0.34870256(5) ∓0.46435521(7) +0.54718532(7) ∓0.55833077(11)
						s	−1(2)
T	T_g	T_1	T_1	T_{1g}	12	s, c	∓0.14842465(1) +0.39257812(3) ∓0.48401456(5) +0.34123000(7) ±0.07446249(9) −0.68381274(11)
						s	1(4)
T	T_g	T_2	T_2	T_{2g}	12	s, c	0.23130311(1) ∓0.49003980(3) +0.27404717(5) ±0.30237819(7) −0.58930834(9) ∓0.43879508(11)
						s	−1(6)
T	T_g	T_1	T_1	T_{1g}	12	s, c	∓0.32928552(1) +0.45497333(3) ±0.23408185(5) −0.54296875(7) ∓0.55492127(9) −0.16438770(11)
						s	1(8)
T	T_g	T_2	T_2	T_{2g}	12	s, c	0.46435521(1) ∓0.20164538(3) −0.65705604(5) ∓0.52110934(7) −0.19834078(9) ∓0.03311685(11)
						s	−1(10)
T	T_g	T_1	T_1	T_{1g}	12	s, c	∓0.77144482(1) −0.55833077(3) ∓0.28725881(5) −0.10066650(7) ∓0.02196723(9) −0.00239208(11)
						s	1(12)

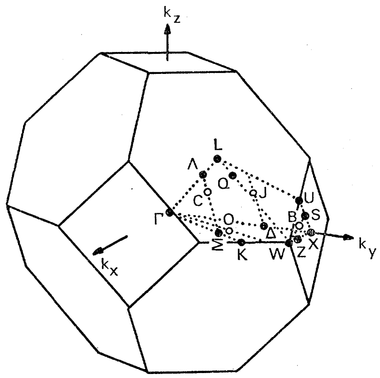

Fig. 3. The first Brillouin zone for the face-centered cubic lattice. The points marked with open circles belong to planes, but not lines, of symmetry. A is a general point.

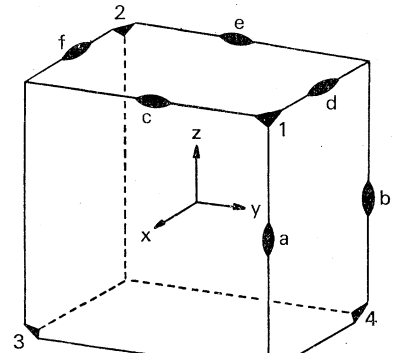

Fig. 4. The symmetry operations of the cubic groups. The σ_m planes ($m=x, y, z$) are perpendicular to the corresponding m axes, and the σ_{dp} planes ($p=a, b, c, d, e, f$) are perpendicular to the C_{2p} axes.

5. RESULTS

We must first identify the cogroups $G^{\mathbf{k}}$ for all the **k** vectors of symmetry in the cubic lattices. The latter are shown in Figs. 1, 2, and 3 in the standard notation of Bouckaert, Smoluchowski, and Wigner.[12] For each **k** the symmetry operations of $G^{\mathbf{k}}$ are obtained in the notation of Fig. 4 (from Altmann and Bradley[6]). The character tables of the corresponding groups are given in Table II, where the actual symmetry operations for each group can be identified from the heading. These tables duplicate to a large extent those given by Bouckaert, Smoluchowski, and Wigner. Nevertheless, they are required here for the following reason. These authors were interested in the characters of the operations only and therefore used the same symbol for

(*Text continues on p. 30*)

Table II. Character tables of the cogroups of the **k** vector for all the **k** vectors of the cubic lattices.

Notes

(*i*) *Points*. The points in **k** space (**k** vectors) should be identified from Figs. 1, 2, and 3.

(*ii*) *Symmetry operations*. They should be identified from Fig. 4. The suffices m, n, p take the following values, with reference to the symmetry operations of Fig. 4: m: x, y, and z; n: 1, 2, 3, and 4; p: a, b, c, d, e, and f. A symbol such as $\sigma_{d(b,e,f)}$ stands for the three operations σ_{db}, σ_{de}, and σ_{df}.

(*iii*) *Direct product groups*. These are recognized in the tables because the names of two representations appear in the column under the name of the point. Also, the operations are listed in two rows linked with braces. For the two representations listed together the characters of the operations in the first row are those given in the table. The characters of the operations in the second row are, for the first representation listed, those in the table and, for the second, their negatives.

(*iv*) *Nomenclature of the irreducible representations*. The names of the representations that correspond to a given point are given in the standard notation for point groups (see, e.g., Altmann,[8] p. 163) under the point symbol underneath, or to the left, of the symbol of the given point. In brackets, underneath the name of the point, we give the suffixes that the corresponding representations carry in the notation of Bouckaert, Smoluchowski, and Wigner. A suffix 1 for Γ, e.g., corresponds to their symbol Γ_1. Except for N, when two representations g and u are listed together we give the Bouckaert, Smoluchowski, and Wigner symbol for g only. That for u is obtained by priming the latter, if unprimed, and vice versa.

	Γ, H, R			{E	$8C_{3n}^{\pm}$	$3C_{2m}$	$6C_{4m}^{\pm}$	$6C_{2p}$
				{i	$8S_{6n}^{\mp}$	$3\sigma_m$	$6S_{4m}^{\mp}$	$6\sigma_{dp}$
			P	E	$8C_{3n}^{\pm}$	$3C_{2m}$	$6S_{4m}^{\pm}$	$6\sigma_{dp}$
$\mathbf{O}_h$		$\mathbf{T}_d$						
A_{1g}, A_{1u}	(1)	A_1	(1)	1	1	1	1	1
A_{2g}, A_{2u}	(2)	A_2	(2)	1	1	1	−1	−1
E_g, E_u	(12)	E	(3)	2	−1	2	0	0
T_{1g}, T_{1u}	(15′)	T_1	(5)	3	0	−1	1	−1
T_{2g}, T_{2u}	(25′)	T_2	(4)	3	0	−1	−1	1

TABLE II (*Continued*)

	Σ, K				E	C_{2a}	σ_z	σ_{db}
		G			E	C_{2b}	σ_{da}	σ_z
		D			E	C_{2z}	σ_{db}	σ_{da}
		S, U			E	C_{2c}	σ_{de}	σ_y
		Z			E	C_{2x}	σ_z	σ_y
				N	$\{E$	C_{2a}	C_{2z}	C_{2b}
					$\{i$	σ_{da}	σ_z	σ_{db}
$\mathbf{C}_{2v}$			$\mathbf{D}_{2h}$					
A_1	(1)	(1)	A_g, A_u	(1, 2′)	1	1	1	1
A_2	(2)	(2)	B_{1g}, B_{1u}	(2, 1′)	1	1	−1	−1
B_1	(4)	(3)	B_{2g}, B_{2u}	(4, 3′)	1	−1	1	−1
B_2	(3)	(4)	B_{3g}, B_{3u}	(3, 4′)	1	−1	−1	1

	T					E	C_{2z}	$C_{4z}^{\pm}$	$\sigma_{(x,y)}$	$\sigma_{d(a,b)}$
	Δ					E	C_{2y}	$C_{4y}^{\pm}$	$\sigma_{(x,z)}$	$\sigma_{d(e,c)}$
			X			$\{E$	C_{2y}	$C_{4y}^{\pm}$	$C_{2(x,z)}$	$C_{2(c,e)}$
						$\{i$	σ_y	$S_{4y}^{\mp}$	$\sigma_{(x,z)}$	$\sigma_{d(c,e)}$
			M			$\{E$	C_{2z}	$C_{4z}^{\pm}$	$C_{2(x,y)}$	$C_{2(a,b)}$
						$\{i$	σ_z	$S_{4z}^{\mp}$	$\sigma_{(x,y)}$	$\sigma_{d(a,b)}$
					W	E	C_{2x}	$S_{4x}^{\pm}$	$C_{2(d,f)}$	$\sigma_{(y,z)}$
$\mathbf{C}_{4v}$		$\mathbf{D}_{4h}$		$\mathbf{D}_{2d}$						
A_1	(1)	A_{1g}, A_{1u}	(1)	A_1	(1)	1	1	1	1	1
A_2	(1′)	A_{2g}, A_{2u}	(4)	A_2	(2)	1	1	1	−1	−1
B_1	(2)	B_{1g}, B_{1u}	(2)	B_1	(1′)	1	1	−1	1	−1
B_2	(2′)	B_{2g}, B_{2u}	(3)	B_2	(2′)	1	1	−1	−1	1
E	(5)	E_g, E_u	(5)	E	(3)	2	−2	0	0	0

	Λ			E	$C_{31}^{\pm}$	$\sigma_{d(b,e,f)}$
	F			E	$C_{34}^{\pm}$	$\sigma_{d(a,d,e)}$
			L	$\{E$	$C_{31}^{\pm}$	$C_{2(b,e,f)}$
				$\{i$	$S_{61}^{\mp}$	$\sigma_{d(b,e,f)}$
$\mathbf{C}_{3v}$		$\mathbf{D}_{3h}$				
A_1	(1)	A_{1g}, A_{1u}	(1)	1	1	1
A_2	(2)	A_{2g}, A_{2u}	(2)	1	1	−1
E	(3)	E_g, E_u	(3)	2	−1	0

V		E	σ_{da}
C		E	σ_{db}
O		E	σ_z
J		E	σ_{de}
B		E	σ_y
	Q	E	C_{2f}
$\mathbf{C}_{1h}$	$\mathbf{C}_2$		
A'	A	1	1
A''	B	1	−1

A	E
$\mathbf{C}_1$	
A	1

TABLE III. The two- and three-dimensional representations of the cogroups of the **k** vectors for all the **k** vectors of the cubic lattices.

Notes

All the matrices correspond to operators in their active interpretation.

TABLE III(a). The two-dimensional representations. Key:

$$\epsilon = \begin{bmatrix} 1 & \\ & 1 \end{bmatrix} \quad \lambda = \begin{bmatrix} 1 & \\ & -1 \end{bmatrix} \quad \kappa = \begin{bmatrix} & 1 \\ 1 & \end{bmatrix} \quad \rho = \begin{bmatrix} & 1 \\ -1 & \end{bmatrix}$$

$$\alpha = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix} \quad \beta = \begin{bmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix} \quad \mu = \begin{bmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & \frac{1}{2} \end{bmatrix} \quad \nu = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & \frac{1}{2} \end{bmatrix}.$$

For the representations E, the matrices listed in the left (right) column under E correspond to the operations listed in the first (last) column of the table. For the points that admit representations E_g, E_u, both operations which are on the same row and are in the first and last columns of the table belong to the group. Only the matrices for the operations in the first column are given. Those for the corresponding operations of the last column, are, for the E_g representations, the same and for the E_u representations the same matrices multiplied by -1. For typographical reasons the negatives of the matrices listed in the key are printed with a bar above the corresponding symbol.

	Γ, H, R	Δ	T	Λ	F	P	X	M	W	L	
	E_g E_u	E	E	E	E	E	E_g E_u	E_g E_u	E	E_g E_u	
E	ϵ ···	ϵ ···	ϵ ···	ϵ ···	ϵ ···	ϵ ···	ϵ ···	ϵ ···	ϵ ···	ϵ ···	i
C_{31}^+	β ···			β ···		β ···				β ···	S_{61}^-
C_{31}^-	α ···			α ···		α ···				α ···	S_{61}^+
C_{32}^+	β ···					β ···					S_{62}^-
C_{32}^-	α ···					α ···					S_{62}^+
C_{33}^+	β ···					β ···					S_{63}^-
C_{33}^-	α ···					α ···					S_{63}^+
C_{34}^+	β ···				β ···	β ···					S_{64}^-
C_{34}^-	α ···				α ···	α ···					S_{64}^+
C_{2x}	ϵ ···	··· κ	··· λ			ϵ ···	κ ···	λ ···	$\bar{\epsilon}$ ···		σ_x
C_{2y}	ϵ ···	$\bar{\epsilon}$ ···	··· $\bar{\lambda}$			ϵ ···	$\bar{\epsilon}$ ···	$\bar{\lambda}$ ···	··· λ		σ_y
C_{2z}	ϵ ···	··· $\bar{\kappa}$	$\bar{\epsilon}$ ···			ϵ ···	$\bar{\kappa}$ ···	$\bar{\epsilon}$ ···	··· $\bar{\lambda}$		σ_z
C_{4x}^+	μ ···					··· μ			··· $\bar{\rho}$		S_{4x}^-
C_{4x}^-	μ ···					··· μ			··· ρ		S_{4x}^+
C_{4y}^+	ν ···	$\bar{\rho}$ ···				··· ν	$\bar{\rho}$ ···				S_{4y}^-
C_{4y}^-	ν ···	ρ ···				··· ν	ρ ···				S_{4y}^+
C_{4z}^+	λ ···		ρ ···			··· λ		ρ ···			S_{4z}^-
C_{4z}^-	λ ···		$\bar{\rho}$ ···			··· λ		$\bar{\rho}$ ···			S_{4z}^+
C_{2a}	λ ···		··· $\bar{\kappa}$		··· λ	··· λ		$\bar{\kappa}$ ···			σ_{da}
C_{2b}	λ ···		··· κ	··· λ		··· λ		κ ···		λ ···	σ_{db}
C_{2c}	ν ···	··· λ				··· ν	λ ···				σ_{dc}
C_{2d}	μ ···				··· μ	··· μ			$\bar{\kappa}$ ···		σ_{dd}
C_{2e}	ν ···	··· $\bar{\lambda}$		··· ν	··· ν	··· ν	$\bar{\lambda}$ ···			ν ···	σ_{de}
C_{2f}	μ ···			··· μ		··· μ			κ ···	μ ···	σ_{df}

TABLE III(b). The three-dimensional representations.

Notes

The matrices of the operations listed in column (1) are those printed on the right of the symbol for the operation, for all the representations of Γ, H, R, and P.

The matrices for the operations listed under column (2) are obtained by postmultiplying the matrix printed on the left of the symbol of the operation with the following matrices:

for T_{1g}, T_{1u} of Γ, H, R and T_1 of P: $\begin{bmatrix} & 1 & \\ 1 & & \\ & & -1 \end{bmatrix}$,

for T_{2g}, T_{2u} of Γ, H, R and T_2 of P: $\begin{bmatrix} & -1 & \\ -1 & & \\ & & 1 \end{bmatrix}$.

For the operations in the columns (1′) and (2′) obtain first the matrices of the corresponding operations in the columns (1) and (2), respectively, by means of the above-given prescriptions. Then multiply the matrices thus obtained with **1** for T_{1g}, T_{2g} and **−1** for T_{1u}, T_{2u}.

Γ, H R, P (1)	Γ, H R (1′)		Γ, H R (2)	Γ, H R (2′)	P (2)	Γ, H R, P (1)	Γ, H R (1′)		Γ, H R (2)	Γ, H R (2′)	P (2)
E	i	$\begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix}$	C_{2a}	σ_{da}	σ_{da}	C_{33}^-	S_{63}^+	$\begin{bmatrix} & -1 & \\ & & 1 \\ -1 & & \end{bmatrix}$	C_{2f}	σ_{df}	σ_{df}
C_{31}^+	S_{61}^-	$\begin{bmatrix} & & 1 \\ 1 & & \\ & 1 & \end{bmatrix}$	C_{4y}^-	S_{4y}^+	S_{4y}^+	C_{34}^+	S_{64}^-	$\begin{bmatrix} & & 1 \\ -1 & & \\ & -1 & \end{bmatrix}$	C_{2e}	σ_{de}	σ_{de}
C_{31}^-	S_{61}^+	$\begin{bmatrix} & 1 & \\ & & 1 \\ 1 & & \end{bmatrix}$	C_{4x}^+	S_{4x}^-	S_{4x}^-	C_{34}^-	S_{64}^+	$\begin{bmatrix} & -1 & \\ & & -1 \\ 1 & & \end{bmatrix}$	C_{2d}	σ_{dd}	σ_{dd}
C_{32}^+	S_{62}^-	$\begin{bmatrix} & & -1 \\ 1 & & \\ & -1 & \end{bmatrix}$	C_{4y}^+	S_{4y}^-	S_{4y}^-	C_{2x}	σ_x	$\begin{bmatrix} 1 & & \\ & -1 & \\ & & -1 \end{bmatrix}$	C_{4z}^-	S_{4z}^+	S_{4z}^+
C_{32}^-	S_{62}^+	$\begin{bmatrix} & 1 & \\ & & -1 \\ -1 & & \end{bmatrix}$	C_{4x}^-	S_{4x}^+	S_{4x}^+	C_{2y}	σ_y	$\begin{bmatrix} -1 & & \\ & 1 & \\ & & -1 \end{bmatrix}$	C_{4z}^+	S_{4z}^-	S_{4z}^-
C_{33}^+	S_{63}^-	$\begin{bmatrix} & & -1 \\ -1 & & \\ & 1 & \end{bmatrix}$	C_{2c}	σ_{dc}	σ_{dc}	C_{2z}	σ_z	$\begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix}$	C_{2b}	σ_{db}	σ_{db}

different operations that have the same characters. On the other hand, since we want to specify the full representations we must identify the operations explicitly. As an example, for the point Σ Bouckaert, Smoluchowski, and Wigner list two operations, given in their notation as C_2 and JC_2, respectively (J is the inversion). However, the binary rotations are around *different* axes. We name our representations in the standard notation for point groups and, therefore, we give in Table II the correlation with Bouckaert, Smoluchowski, and Wigner's notation.

The two- and three-dimensional representations that appear under subduction are given in Table III and the symmetry-adapted harmonics in Table IV. A complete table of compatibilities between the representations is given in Table V.

(*Text continues on p. 32*)

Table IV. The symmetry-adapted harmonics for the cubic groups.

Notes

(*i*) *Representations.* The representations spanned by the bases given here are obtained from Table II (one dimensional) and Table III (two and three dimensional). Although these representations correspond to active operators, the bases listed here are also correct for the representations that correspond to passive operators (Altmann and Bradley[6]).

(*ii*) *Notation.* The symmetry-adapted harmonics are given as linear combinations of the bases that span the representations of 0_h (point Γ). These are obtained from Table I. The successive partners of a multidimensional basis of 0_h in Table I are identified with superscripts 1, 2, etc. The symmetry-adapted harmonics that span a multidimensional basis are linked together with braces. The resulting bases should be understood as row vectors.

To simplify the printing, *all symmetry-adapted harmonics which are given as a sum of two or three terms have been denormalized.* To normalize them one must therefore divide the functions concerned by the square root of the sum of the squares of the coefficients; thus $T_{2u}^1+T_{2u}^2-2T_{2u}^3$ should be read as $(T_{2u}^1+T_{2u}^2-2T_{2u}^3)/\sqrt{6}$.

The suffix s (t) in the body of the tables must be given successively the values g, u (u, g), which correspond, respectively, to the first and second representations given.

(*iii*) *Example.* The normalized harmonics up to $l=2$ that are obtained from those listed for A_1 of Δ are: Y_1^0, $\frac{1}{2}Y_2^0+\frac{1}{2}\sqrt{3}\ Y_2^{2,c}$, $Y_1^{1,s}$.

(*iv*) *Uses of the tables.* Although the symmetry-adapted harmonics given here are such that, on using (10), they generate immediately all the lattice harmonics for all the cubic groups, they can also be used as symmetry-adapted harmonics for the point groups listed in Table II, if the special setting therein used, rather than that chosen by Altmann and Bradley[6] is required.

Γ, H, R

Identical with those of 0_h

P

$A_1,\ A_2$	$A_{1s},\ A_{2t}$
E	$\{E_g^1,\ E_g^2\},\ \{E_u^2,\ -E_u^1\}$
$T_1,\ T_2$	$\{T_{1s}^1,\ T_{1s}^2,\ T_{1s}^3\},\ \{T_{2t}^1,\ T_{2t}^2,\ T_{2t}^3\}$

Σ, K

$A_1,\ A_2$	$A_{1s},\ E_s^1,\ T_{2s}^3,\ T_{2t}^1-T_{2t}^2,\ T_{1t}^1+T_{1t}^2$
$B_1,\ B_2$	$A_{2s},\ E_s^2,\ T_{1s}^3,\ T_{2t}^1+T_{2t}^2,\ T_{1t}^1-T_{1t}^2$

G

$A_1,\ A_2$	$A_{1s},\ E_s^1,\ T_{2s}^3,\ T_{2t}^1+T_{2t}^2,\ T_{1t}^1-T_{1t}^2$
$B_1,\ B_2$	$A_{2t},\ E_t^2,\ T_{1t}^3,\ T_{2s}^1-T_{2s}^2,\ T_{1s}^1+T_{1s}^2$

D

$A_1,\ A_2$	$A_{1s},\ A_{2t},\ E_s^1,\ E_t^2,\ T_{2s}^3,\ T_{1t}^3$
$B_1,\ B_2$	$T_{2s}^1+T_{2s}^2,\ T_{1s}^1-T_{1s}^2,\ T_{2t}^1-T_{2t}^2,\ T_{1t}^1+T_{1t}^2$

S, U

$A_1,\ A_2$	$A_{1s},\ E_s^1+3^{\frac{1}{2}}\ E_s^2,\ T_{2s}^2,\ T_{2t}^1-T_{2t}^3,\ T_{1t}^1+T_{1t}^3$
$B_1,\ B_2$	$A_{2t},\ -3^{\frac{1}{2}}\ E_t^1+E_t^2,\ T_{1t}^2,\ T_{2s}^1+T_{2s}^3,\ T_{1s}^1-T_{1s}^3$

Z

$A_1,\ A_2$	$A_{1s},\ A_{2s},\ E_s^1,\ E_2^2,\ T_{2t}^1,\ T_{1t}^1$
$B_1,\ B_2$	$T_{2s}^3,\ T_{1s}^3,\ T_{2t}^2,\ T_{1t}^2$

N

$A_g,\ A_u$	$A_{1s},\ E_s^1,\ T_{2s}^3$
$B_{1g},\ B_{1u}$	$T_{2s}^1-T_{2s}^2,\ T_{1s}^1+T_{1s}^2$
$B_{2g},\ B_{2u}$	$A_{2s},\ E_s^2,\ T_{1s}^3$
$B_{3g},\ B_{3u}$	$T_{2s}^1+T_{2s}^2,\ T_{1s}^1-T_{1s}^2$

T

$A_1,\ A_2$	$A_{1s},\ E_s^1,\ T_{1t}^3$
$B_1,\ B_2$	$A_{2s},\ E_s^2,\ T_{2t}^3$
E	$\{T_{2g}^1,\ T_{2g}^2\},\ \{T_{1g}^1,\ -T_{1g}^2\},\ \{T_{2u}^2,\ -T_{2u}^1\},\ \{T_{1u}^2,\ T_{1u}^1\}$

Δ

$A_1,\ A_2$	$A_{1s},\ E_s^1+3^{\frac{1}{2}}E_s^2,\ T_{1t}^2$
$B_1,\ B_2$	$A_{2s},\ -3^{\frac{1}{2}}E_s^1+E_s^2,\ T_{2t}^2$
E	$\{T_{2g}^1-T_{2g}^3,\ T_{2g}^1+T_{2g}^3\},\ \{T_{1g}^1+T_{1g}^3,\ T_{1g}^1-T_{1g}^3\},$ $\{-T_{2u}^1-T_{2u}^3,\ T_{2u}^1-T_{2u}^3\},$ $\{-T_{1u}^1+T_{1u}^3,\ T_{1u}^1+T_{1u}^3\}$

X

$A_{1g},\ A_{1u}$	$A_{1s},\ E_s^1+3^{\frac{1}{2}}E_s^2$
$A_{2g},\ A_{2u}$	T_{1s}^2
$B_{1g},\ B_{1u}$	$A_{2s},\ -3^{\frac{1}{2}}E_s^1+E_s^2$
$B_{2g},\ B_{2u}$	T_{2s}^2
$E_g,\ E_u$	$\{T_{2s}^1-T_{2s}^3,\ T_{2s}^1+T_{2s}^3\},\ \{T_{1s}^1+T_{1s}^3,\ T_{1s}^1-T_{1s}^3\}$

TABLE IV (*Continued*)

	M
A_{1g}, A_{1u}	A_{1s}, E_s^1
A_{2g}, A_{2u}	T_{1s}^3
B_{1g}, B_{1u}	A_{2s}, E_s^2
B_{2g}, B_{2u}	T_{2s}^3
E_g, E_u	$\{T_{2s}^1, T_{2s}^2\}$, $\{T_{1s}^1, -T_{1s}^2\}$
	W
A_1, B_1	A_{1s}, T_{2t}^1, $E_s^1-3^{\frac{1}{2}}E_s^2$
A_2, B_2	A_{2t}, T_{1s}^1, $3^{\frac{1}{2}}E_t^1+E_t^2$
E	$\{T_{2g}^2, T_{2g}^3\}$, $\{T_{1g}^2, -T_{1g}^3\}$, $\{T_{2u}^3, T_{2u}^2\}$, $\{-T_{1u}^3, T_{1u}^2\}$
	Λ
A_1, A_2	A_{1s}, A_{2t}, $T_{2s}^1+T_{2s}^2+T_{2s}^3$, $T_{1t}^1+T_{1t}^2+T_{1t}^3$
E	$\{E_g^1, E_g^2\}$, $\{-E_u^2, E_u^1\}$, $\{T_{1g}^1-T_{1g}^2, T_{1g}^1+T_{1g}^2-2T_{1g}^3\}$, $\{T_{2u}^1-T_{2u}^2, T_{2u}^1+T_{2u}^2-2T_{2u}^3\}$, $\{-T_{2g}^1-T_{2g}^2+2T_{2g}^3, T_{2g}^1-T_{2g}^2\}$, $\{-T_{1u}^1-T_{1u}^2+2T_{1u}^3, T_{1u}^1-T_{1u}^2\}$
	F
A_1, A_2	A_{1s}, A_{2t}, $T_{2s}^1-T_{2s}^2+T_{2s}^3$, $T_{1t}^1-T_{1t}^2+T_{1t}^3$
E	$\{E_g^1, E_g^2\}$, $\{E_u^1, E_u^2\}$, $\{T_{2g}^1-T_{2g}^2-2T_{2g}^3, -T_{2g}^1-T_{2g}^2\}$, $\{T_{1u}^1-T_{1u}^2-2T_{1u}^3, -T_{1u}^1-T_{1u}^2\}$, $\{T_{1g}^1+T_{1g}^2, T_{1g}^1-T_{1g}^2-2T_{1g}^3\}$, $\{T_{2u}^1+T_{2u}^2, T_{2u}^1-T_{2u}^2-2T_{2u}^3\}$
	L
A_{1g}, A_{1u}	A_{1s}, $T_{2s}^1+T_{2s}^2+T_{2s}^3$
A_{2g}, A_{2u}	A_{2s}, $T_{1s}^1+T_{1s}^2+T_{1s}^3$
E_g, E_u	$\{E_s^1, E_s^2\}$, $\{T_{2s}^1+T_{2s}^2-2T_{2s}^3, T_{2s}^1-T_{2s}^2\}$, $\{T_{1s}^1-T_{1s}^2, T_{1s}^1+T_{1s}^2-2T_{1s}^3\}$
	V
A', A''	A_{1s}, A_{2t}, E_s^1, E_t^2, T_{2s}^3, T_{1t}^3, $T_{1s}^1+T_{1s}^2$, $T_{2s}^1-T_{2s}^2$, $T_{2t}^1+T_{2t}^2$, $T_{1t}^1-T_{1t}^2$
	C
A', A''	A_{1s}, A_{2t}, E_t^2, E_s^1, T_{2s}^3, T_{1t}^3, $T_{2s}^1+T_{2s}^2$, $T_{1s}^1-T_{1s}^2$, $T_{2t}^1-T_{2t}^2$, $T_{1t}^1+T_{1t}^2$
	O
A', A''	A_{1s}, A_{2s}, E_s^1, E_s^2, T_{2t}^1, T_{2t}^2, T_{1t}^1, T_{1t}^2, T_{2s}^3, T_{1s}^3
	J
A', A''	A_{1s}, A_{2t}, $E_s^1+3^{\frac{1}{2}}E_s^2$, $-3^{\frac{1}{2}}E_t^1+E_t^2$, $T_{2s}^1+T_{2s}^3$, T_{2s}^2, $T_{1s}^1-T_{1s}^3$, $T_{2t}^1-T_{2t}^3$, $T_{1t}^1+T_{1t}^3$, T_{1t}^2
	B
A', A''	A_{1s}, A_{2s}, E_s^1, E_s^2, T_{2s}^2, T_{1s}^2, T_{2t}^1, T_{2t}^3, T_{1t}^1, T_{1t}^3
	A
A	All harmonics of Γ.

TABLE V. Compatibility conditions.

Notes

The compatibility conditions are given along lines in the Brillouin zones. The three points of a line have to be chosen from the appropriate column (or columns) to the left of the table, with the condition that no more than one of the points listed in brackets can be used for any one line. All the representations listed in each of the columns corresponding to a line are compatible.

Γ	R	A_{1g}, E_g, T_{1u}	T_{1g}, A_{1u}, E_u	A_{2g}, E_g, T_{2u}	T_{2g}, A_{2u}, E_u	T_{2g}, T_{1g}, T_{2u}, T_{1u}
Δ	T	A_1	A_2	B_1	B_2	E
(H)		A_{1g}, E_g, T_{1u}	T_{1g}, A_{1u}, E_u	A_{2g}, E_g, T_{2u}	T_{2g}, A_{2u}, E_u	T_{2g}, T_{1g}, T_{2u}, T_{1u}
(X)	M	A_{1g}, A_{2u}	A_{2g}, A_{1u}	B_{1g}, B_{2u}	B_{2g}, B_{1u}	E_g, E_u
	Γ	A_{1g}, E_g, T_{2g}, T_{2u}, T_{1u}	T_{2g}, T_{1g}, A_{1u}, E_u, T_{2u}	A_{2g}, E_g, T_{1g}, T_{2u}, T_{1u}	T_{2g}, T_{1g}, A_{2u}, E_u, T_{1u}	
	Σ	A_1	A_2	B_1	B_2	
	(N)	A_g, B_{1u}	B_{1g}, A_u	B_{2g}, B_{3u}	B_{3g}, B_{2u}	
	(K)	A_1	A_2	B_1	B_2	
	(M)	A_{1g}, B_{2g}, E_u	A_{1u}, B_{2u}, E_g	A_{2g}, B_{1g}, E_u	A_{2u}, B_{1u}, E_g	
Γ	H	A_{1g}, T_{2g}, A_{2u}, T_{1u}	A_{2g}, T_{1g}, T_{2u}, A_{1u}	E_g, T_{2g}, T_{1g}, E_u, T_{2u}, T_{1u}		
Λ	F	A_1	A_2	E		
(P)	P	A_1, T_2	A_2, T_1	E, T_1, T_2		
(L)		A_{1g}, A_{2u}	A_{2g}, A_{1u}	E_g, E_u		
(R)		A_{1g}, T_{2g}, A_{2u}, T_{1u}	A_{2g}, T_{1g}, T_{2u}, A_{1u}	E_g, T_{2g}, T_{1g}, E_u, T_{2u}, T_{1u}		

TABLE V (*Continued*)

H	R	$A_{1g}, E_g, T_{2g}, T_{2u}, T_{1u}$	$T_{2g}, T_{1g}, A_{1u}, E_u, T_{2u}$	$T_{2g}, T_{1g}, A_{2u}, E_u, T_{1u}$	$A_{2g}, E_g, T_{1g}, T_{2u}, T_{1u}$
G	S	A_1	A_2	B_1	B_2
N		A_g, B_{3u}	B_{3g}, A_u	B_{1g}, B_{2u}	B_{2g}, B_{1u}
	X	A_{1g}, B_{2g}, E_u	E_g, A_{1u}, B_{2u}	E_g, A_{2u}, B_{1u}	A_{2g}, B_{1g}, E_u
	P	A_1, E, T_2	A_2, E, T_1	T_1, T_2	T_1, T_2
	D	A_1	A_2	B_1	B_2
	N	A_g, B_{2u}	A_u, B_{2g}	B_{3g}, B_{1u}	B_{3u}, B_{1g}
	X	A_{1g}, B_{1g}, E_u	E_g, A_{1u}, B_{1u}	E_g, A_{2u}, B_{2u}	A_{2g}, B_{2g}, E_u
	Z	A_1	A_2	B_1	B_2
	(W)	A_1, B_2	A_2, B_1	E	E
	(M)	A_{1g}, B_{1g}, E_u	E_g, A_{1u}, B_{1u}	E_u, A_{2g}, B_{2g}	A_{2u}, B_{2u}, E_g
	K	A_1, B_1	A_2, B_2		
	O	A'	A''		
	W	A_1, B_2, E	A_2, B_1, E		
	L	A_{1g}, A_{2u}, E_g, E_u	A_{2g}, A_{1u}, E_g, E_u		
	C	A'	A''		
	K	A_1, B_2	A_2, B_1		
	L	A_{1g}, A_{2u}, E_g, E_u	A_{2g}, A_{1u}, E_g, E_u		
	J	A'	A''		
	U	A_1, B_1	A_2, B_2		
	X	A_{1g}, B_{2g}, E_u	E_g, A_{1u}, B_{2u}	E_g, A_{2u}, B_{1u}	A_{2g}, B_{1g}, E_u
	S	A_1	A_2	B_1	B_2
	U	A_1	A_2	B_1	B_2
	W	A_1, B_2, E	A_2, B_1, E		
	B	A'	A''		
	U	A_1, B_2	A_2, B_1		
	L	A_{1g}, A_{1u}, E_g, E_u	A_{2g}, A_{2u}, E_g, E_u		
	Q	A	B		
	W	A_1, B_1, E	A_2, B_2, E		

ACKNOWLEDGMENTS

This work was supported by a grant from the U.K.A.E.A. which is gratefully acknowledged. We are grateful to Professor L. Fox for the grant of computing time on the Oxford University Computer. One of us (A. P. C.) would like to acknowledge a D.S.I.R. Studentship and the other (S. L. A.) useful correspondence with Professor R. McWeeny. We are indebted to Dr. C. J. Bradley for useful discussion and much help and to Dr. J. E. Jeacocke for help in checking some of the results.