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ON THE SYMMETRIES OF SPHERICAL HARMONICS

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CONTENTS

This paper extends the work described in a previous paper by one of the authors (Altmann 1957). The spherical harmonics that belong to the irreducible representations of the cubic groups are now given up to and including $l = 12$. Also, for all point groups the expansions in spherical harmonics that are given belong to the separate columns of the irreducible representations (whereas before they were linear combinations of such functions). Accordingly, full tables for the irreducible representations for all crystallographic point groups are required and are given in the paper. Finally, a technique is described, and used throughout in the tables, to orthogonalize several expansions that belong to the same column of the same irreducible representation. Therefore, the different expansions listed in the tables are always fully orthogonal.

1. Introduction

This paper is a sequel to one of the same title by one of us, (Altmann 1957) henceforth referred to as part I. We shall not, therefore, provide a general introduction: instead we shall describe the position of the subject as it was in part I in order to show how this paper extends and completes our previous work.

In part I, spherical harmonics that belong to the irreducible representations of the crystallographic point groups were constructed by means of the operator

$$\sum_{\mathscr{R}} \chi^i(\mathscr{R})^* \mathscr{R}, \tag{1}$$

where $\chi^i(\mathscr{R})$ is the character of the operation $\mathscr{R}$ in the ith irreducible representation of the group and the summation is over all the operations of the group. This operator is applied on a given spherical harmonic $Y_l^m(\theta, \phi)$, which we call the generator of the expansion, and the terms $\mathscr{R} Y_l^m(\theta, \phi)$ that appear in it are expressed by means of the matrix representations of the rotation group. What appears at first sight to be a formidable task was shown in part I to lead to trivial manipulation for the dihedral and related point groups, and to fairly simple work for the cubic groups. For the latter, however, some auxiliary functions had to be tabulated which required tedious computation for higher values of l. Hence the expansions were obtained for values of l up to and including $l = 6$, for the cubic groups and for all values of l for the remaining groups. In every case all the irreducible representations were treated.

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The present paper extends this work in three ways. First, as reported in the preceding paper (Altmann & Bradley 1962), a new method for the calculation of the auxiliary functions required in the expansions has been developed and a program has been written for an electronic computer to provide them up to values of $l = 20$. As a result, we have extended our tables of the spherical harmonics for the cubic groups up to and including $l = 12$.

The second question is more fundamental. The functions generated by means of the operator (1) form bases that span the irreducible representations of the group, but attention must be called to the fact, which was already stressed in part I, § 6, that any two such bases that belong to the same representation will not necessarily span identical representations but only similar ones. We have shown in part I how to overcome this difficulty, but it is convenient to treat the problem in a more general way and to provide tables where the different bases span always identical irreducible representations.

The reason why this was not the case with the functions generated by the operator (1) is, as is well known, that they are linear combinations of functions that transform like the separate columns of the irreducible representations. This would not have happened if we had used the more powerful operator

$$W^i_{ts} \equiv \frac{l_i}{h} \sum_{\mathscr{R}} D^i(\mathscr{R})^*_{ts} \mathscr{R}, \tag{2}$$

where l_i is the dimension of the ith irreducible representation, h the order of the group, and $D^i(\mathscr{R})^*_{ts}$ the complex conjugate of the ts matrix element of the operation $\mathscr{R}$ in this representation. This operator generates a function that transforms like the t-column of the i-representation. To use it, however, we require the complete matrix representations, rather than their characters. Of course, matrix representations are given in the literature but they depend crucially on the choice of axes (that is of a basis) so that, in order to follow a consistent procedure, we take for each representation the basis of lowest l that is provided by the operators (1). This basis is either listed in part I, or, if the axes are set in a different way, can be obtained most simply by the methods given there. The second step is to form, as explained in part I, § 6, the representation spanned by this basis. Finally, we use this representation to form the operators (2) which in their turn generate the remaining functions. It will be seen that this stepwise application of the operators (1) and (2) makes the use of the latter very much simpler.

Now we come to the third question, which is that of the orthogonality of the expansions. It must not be thought that this follows automatically from the orthogonality of functions of different columns of the irreducible representations or from the properties of the spherical harmonics themselves. This is so because for certain irreducible representations there appear in the *same* column different combinations of the *same* spherical harmonics. This is very inconvenient because, when expansions in spherical harmonics are used in physical problems, one normally requires all the terms in the expansions to be mutually orthogonal. We therefore give in § 3 a method to ensure the orthogonality in the case discussed, and this has been used when necessary in the preparation of the tables. The latter, therefore, provide fully orthogonal expansions.

There is still one last aspect of the formation of symmetry-adapted spherical harmonics that must be mentioned: this is the fact that this work can be made more systematic and less

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laborious by exploiting some properties of the expressions of the point groups as semi-direct products. This question is discussed very fully in the following paper (Altmann 1962*b*) and the present one will be kept as self-contained as possible: we shall refer here to the results of the theory of the semi-direct product only when absolutely necessary.

2. Transformation formulae

The use of the operators (2) rather than (1) requires but small changes in the analysis given in part I. This analysis, as well as the notation of part I, will be followed very closely here. However, we must stress the fact that throughout this paper, unless otherwise stated, we shall use the unnormalized spherical harmonics $\mathscr{Y}_l^m = P_l^m(\cos\theta)\exp(im\phi)$ only. This is so that the coefficients which appear in the expansions can be given exactly in our tables: those using them will therefore be able to write their expansions to whatever accuracy they require.

In order to use the operators (2) we require an expression for $\mathscr{R}\mathscr{Y}_l^m$. This is (cf. (2) of part I)

$$\mathscr{R}\mathscr{Y}_l^m = \sum_{m'} \mathscr{Y}_l^{m'} \mathscr{D}^{(l)}(\mathscr{R})_{m'm}. \tag{3}$$

If $\mathscr{R}$ is an improper rotation, it must be expressed as the product of a proper rotation (which we shall call the associated proper rotation) times the inversion i. In this case the matrix elements of the associated proper rotation must be introduced in the right-hand side of (3) which must also be multiplied by $(-1)^l$.

Once the proper rotation is expressed in terms of its Euler angles α, β, γ (as defined in part I), their matrix elements can be written

$$\mathscr{D}^{(l)}(\mathscr{R})_{m'm} = C_{m'm}\,\mathrm{e}^{\mathrm{i}m'\gamma}\,\mathrm{e}^{\mathrm{i}m\alpha}\,\mathscr{S}^{(l)}_{m'm}(\beta), \tag{4}$$

where

$$C_{m'm} = \mathrm{i}^{|m|'+m'}\,\mathrm{i}^{|m|+m}, \tag{5}$$

and the functions $\mathscr{S}^{(l)}_{m'm}(\beta)$ defined in part I, equation (19) can be obtained from the tables described in Altmann & Bradley (1962).

On introducing (4) into (3), and using the operators (2), we have

$$W^i_{ts}\mathscr{Y}_l^m = \frac{l_i}{h}\sum_{\mathscr{R}} P_{\mathscr{R}} D^{(i)}(\mathscr{R})^*_{ts}\,\mathrm{e}^{\mathrm{i}m\alpha}\sum_{m'} C_{m'm}\,\mathrm{e}^{\mathrm{i}m'\gamma}\,\mathscr{S}^{(l)}_{m'm}(\beta)\,\mathscr{Y}_l^{m'}, \tag{6}$$

where we add over all the operations $\mathscr{R}$ of the group and, when $\mathscr{R}$ is improper, we take in the right-hand side the quantities corresponding to the associated proper rotation. Also, $P_{\mathscr{R}}$ is unity when $\mathscr{R}$ is a proper rotation and $(-1)^l$ when it is improper.

It should be stressed that although (6) would be cumbersome to handle as a primary source of the spherical harmonics, its use is much simpler as a second stage to the work done in part I. This is so because we now know which harmonics appear in each representation (that is the values of l as well as those of m' in the right-hand side of (6)), so that we can choose the appropriate generator in the left-hand side of (6) to provide any desired expansion. Just as in part I, the bases can be obtained at once for all orders of l for all the non-cubic crystallographic point groups.

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3. The orthogonalization of the expansions

We shall describe in this section a method to orthogonalize different expansions of the same spherical harmonics that belong to the same column of the representation (see § 1). In order to do this we require some well-known properties of the symmetrizing operators (2) (see, for example, Altmann 1962*a*):

$$W^j_{tu} W^i_{sr} = W^j_{td}\, \delta_{ij}\, \delta_{us}. \tag{7}$$

Here d can take any of the values $1, 2, \ldots, l_j$, l_j being the dimensionality of the jth representation. Also, as follows from the definition (2) and the unitary property of the matrix representatives,

$$W^{i\dagger}_{ts} = W^i_{st}, \tag{8}$$

where the dagger denotes the adjoint operator.

Let us first consider two expansions, which can be written as $W^i_{ts}\mathscr{Y}^m_l$ and $W^i_{ts}\mathscr{Y}^n_l$ in terms of two different generators. We shall form a linear combination of these two expansions, which we shall make orthogonal to one of them, the first, say. On using the well-known notation $(f, g) \equiv \int f^* g \,d\tau$, we have:

$$\begin{aligned}(W^i_{ts}\mathscr{Y}^m_l, W^i_{ts}\mathscr{Y}^m_l + \lambda W^i_{ts}\mathscr{Y}^n_l) &= (\mathscr{Y}^m_l, W^i_{st}[W^i_{ts}\mathscr{Y}^m_l + \lambda W^i_{ts}\mathscr{Y}^n_l]) \\ &= (\mathscr{Y}^m_l, W^i_{ss}\mathscr{Y}^m_l + \lambda W^i_{ss}\mathscr{Y}^n_l).\end{aligned} \tag{9}$$

Here we have used (8) in the first step and (7) in the second and, for convenience, we have taken in the latter the value of d which equals that of the first suffix. It is now very easy to annihilate the integral in the right-hand side of (9): it is enough to choose λ so that the term that contains $\mathscr{Y}^m_l$ in $W^i_{ss}\mathscr{Y}^m_l + \lambda W^i_{ss}\mathscr{Y}^n_l$ vanishes. It should be noticed that the value of λ thus obtained is independent of t, that is of the particular column considered in the representation. This means that with this value of λ, $W^i_{ts}\mathscr{Y}^m_l + \lambda W^i_{ts}\mathscr{Y}^n_l$ will be orthogonal to $W^i_{ts}\mathscr{Y}^m_l$ for all $t = 1, 2, \ldots, l_i$: we have orthogonalized in one stroke all pairs of functions that correspond to the l_i columns of the given representation.

When three functions belong to the same column we orthogonalize the first two to the third in the manner just described. The two (non-orthogonal) combinations thus obtained can readily be orthogonalized by a simple extension of the same procedure.

All expansions given in the tables have been orthogonalized, when necessary, in this way.

4. The expansions for the dihedral and related point groups

We shall not consider in this paper the cyclic groups: since their representations are all one-dimensional the expansions given in part I are not changed. The basic table of this section is table 3, which gives the expansions themselves. Before these are used, however, they must be referred to the corresponding irreducible representations, which are given in tables 1 and 2. In using these tables of irreducible representations, the symmetry operations must be identified by means of figures 1 and 2. In order to use the tables the following notes are required:

(i) *Notation for the irreducible representations.* It is exactly that used in the character tables given by Margenau & Murphy (1956) or Altmann (1962*a*). It should be noticed, however, that although our notation for the symmetry operations coincides exactly with that of the second reference it differs from the first in the treatment of the secondary binary

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TABLE 1. REPRESENTATIONS FOR THE GROUPS WITH FOURFOLD SYMMETRY

(See notes (iii) and (iv) of this section.)

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

group ...	$\mathbf{D}_4$	$\mathbf{C}_{4v}$	$\mathbf{D}_{2d}$
rep. ...	E	E	E
basis ...	$(\mathscr{Y}_1^{1,c}, \mathscr{Y}_1^{1,s})$	$(\mathscr{Y}_1^{1,c}, \mathscr{Y}_1^{1,s})$	$(\mathscr{Y}_1^{1,c}, \mathscr{Y}_1^{1,s})$
E	ϵ	ϵ	ϵ
C_2	$-\epsilon$	$-\epsilon$	$-\epsilon$
C_4^+	ρ	ρ	—
C_4^-	$-\rho$	$-\rho$	—
C'_{21}	λ	—	λ
C'_{22}	$-\lambda$	—	$-\lambda$
C''_{21}	κ	—	—
C''_{22}	$-\kappa$	—	—
σ_{v1}	—	λ	—
σ_{v2}	—	$-\lambda$	—
σ_{d1}	—	κ	κ
σ_{d2}	—	$-\kappa$	$-\kappa$
S_4^+	—	—	ρ
S_4^-	—	—	$-\rho$

TABLE 2. REPRESENTATIONS FOR THE GROUPS WITH THREEFOLD AND SIXFOLD SYMMETRY

(See notes (iii) and (iv) of this section.)

key: $\epsilon = \begin{bmatrix} 1 & \\ & 1 \end{bmatrix}$ $\alpha = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix}$ $\beta = \begin{bmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix}$ $\lambda = \begin{bmatrix} 1 & \\ & -1 \end{bmatrix}$ $\mu = \begin{bmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & \frac{1}{2} \end{bmatrix}$ $\nu = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & \frac{1}{2} \end{bmatrix}$

group ...	$\mathbf{D}_3$	$\mathbf{C}_{3v}$	$\mathbf{D}_6$		$\mathbf{C}_{6v}$		$\mathbf{D}_{3h}$	
rep. ...	E	E	E_1	E_2	E_1	E_2	E'	E''
basis ...	$(\mathscr{Y}_1^{1,c}, \mathscr{Y}_1^{1,s})$	$(\mathscr{Y}_1^{1,c}, \mathscr{Y}_1^{1,s})$	$(\mathscr{Y}_1^{1,c}, \mathscr{Y}_1^{1,s})$	$(\mathscr{Y}_2^{2,c}, \mathscr{Y}_2^{2,s})$	$(\mathscr{Y}_1^{1,c}, \mathscr{Y}_1^{1,s})$	$(\mathscr{Y}_2^{2,c}, \mathscr{Y}_2^{2,s})$	$(\mathscr{Y}_1^{1,c}, \mathscr{Y}_1^{1,s})$	$(\mathscr{Y}_2^{1,c}, \mathscr{Y}_2^{1,s})$
operation								
E	ϵ	ϵ	ϵ	ϵ	ϵ	ϵ	ϵ	ϵ
C_6^+	—	—	$-\beta$	α	$-\beta$	α	—	—
C_6^-	—	—	$-\alpha$	β	$-\alpha$	β	—	—
C_3^+	α	α	α	β	α	β	α	α
C_3^-	β	β	β	α	β	α	β	β
C_2	—	—	$-\epsilon$	ϵ	$-\epsilon$	ϵ	—	—
C'_{21}	λ	—	λ	λ	—	—	λ	$-\lambda$
C'_{22}	μ	—	μ	ν	—	—	μ	$-\mu$
C'_{23}	ν	—	ν	μ	—	—	ν	$-\nu$
C''_{21}	—	—	$-\lambda$	λ	—	—	—	—
C''_{22}	—	—	$-\mu$	ν	—	—	—	—
C''_{23}	—	—	$-\nu$	μ	—	—	—	—
σ_{v1}	—	λ	—	—	λ	λ	λ	λ
σ_{v2}	—	μ	—	—	μ	ν	μ	μ
σ_{v3}	—	ν	—	—	ν	μ	ν	ν
σ_{d1}	—	—	—	—	$-\lambda$	λ	—	—
σ_{d2}	—	—	—	—	$-\mu$	ν	—	—
σ_{d3}	—	—	—	—	$-\nu$	μ	—	—
σ_h	—	—	—	—	—	—	ϵ	$-\epsilon$
S_3^+	—	—	—	—	—	—	α	$-\alpha$
S_3^-	—	—	—	—	—	—	β	$-\beta$

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TABLE 3. THE SPHERICAL HARMONICS FOR THE DIHEDRAL AND RELATED POINT GROUPS

(See notes (i) to (vii) of this section.)

$\mathbf{D}_3$	l	m mod $(+6)$	ϕ-dep.	
A_1	0	0	c	z^2
	4	3	s	
	3	3	c	x^3-3y^2x
	7	6	s	
A_2	1	0	c	z; $5z^3-3z$
	3	3	s	$3x^2y-y^3$
	4	3	c	
	6	6	s	
E	1	1	(c, s)	(x, y); $(5z^2x-x, 5z^2y-y)$
	2	1	$(s, -c)$	$(yz, -xz)$
	3	2	(s, c)	(xyz, x^2z-y^2z)
	2	2	$(c, -s)$	$(x^2-y^2, -xy)$
	5	4	$(s, -c)$	
	4	4	(c, s)	
	5	5	$(c, -s)$	
	6	5	(s, c)	

$\mathbf{C}_{3v}$	m mod $(+3)$	ϕ-dep.	
A_1	0	c	z; z^2; $5z^3-3z$, x^3-3y^2x
A_2	3	s	$3x^2y-y^3$
E	1	(c, s)	(x, y); (xz, yz); $(5z^2x-x, 5z^2y-y)$
	2	$(c, -s)$	$(x^2-y^2, -xy)$; $(x^2z-y^2z, -xyz)$

$\mathbf{D}_4$	l	m mod $(+4)$	ϕ-dep.	
E	1	1	(c, s)	(x, y), $(5z^2x-x, 5z^2y-y)$
	2	1	$(s, -c)$	$(yz, -xz)$
	3	3	$(c, -s)$	$(x^3-3y^2x, -3x^2y+y^3)$
	4	3	(s, c)	

$\mathbf{C}_{4v}$	m mod $(+4)$	ϕ-dep.	
E	1	(c, s)	(x, y); (xz, yz); $(5z^2x-x, 5z^2y-y)$
	3	$(c, -s)$	(x^3-3y^2x, y^3-3x^2y)

$\mathbf{D}_{2d}$	l	m mod $(+4)$	ϕ-dep.	
E	1	1	(c, s)	(x, y); $(5z^2x-x, 5z^2y-y)$
	2	1	(s, c)	(yz, xz)
	3	3	$(c, -s)$	(x^3-3y^2x, y^3-3x^2y)
	4	3	$(s, -c)$	

$\mathbf{D}_6$	l	m mod $(+6)$	ϕ-dep.	
E_1	1	1	(c, s)	(x, y); $(5z^2x-x, 5z^2y-y)$
	2	1	$(s, -c)$	$(yz, -xz)$
	5	5	$(c, -s)$	
	6	5	(s, c)	
E_2	2	2	(c, s)	(x^2-y^2, xy)
	3	2	$(s, -c)$	(xyz, y^2z-x^2z)
	4	4	$(c, -s)$	
	5	4	(s, c)	

$\mathbf{C}_{6v}$	m mod $(+6)$	ϕ-dep.	
E_1	1	(c, s)	(x, y); (xz, yz); $(5z^2x-x, 5z^2y-y)$
	5	$(c, -s)$	
E_2	2	(c, s)	(x^2-y^2, xy); (x^2z-y^2z, xyz)
	4	$(c, -s)$	

$\mathbf{D}_{3h}$	l	m mod $(+6)$	ϕ-dep.	
E'	1	1	(c, s)	(x, y); $(5z^2x-x, 5z^2y-y)$
	2	2	$(c, -s)$	$(x^2-y^2, -xy)$
	4	4	(c, s)	
	5	5	$(c, -s)$	
E''	2	1	(c, s)	(xz, yz)
	3	2	$(c, -s)$	$(x^2z-y^2z, -xyz)$
	5	4	(c, s)	
	6	5	$(c, -s)$	

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axes (that is, those perpendicular to the principal axes). Margenau & Murphy use the notation C_2 both for a principal and a secondary axis. The secondary axes in Margenau & Murphy tables can be recognized, however, because they are preceded by a numeral 2 or 3: their symbols C_2 and C_2' are replaced in the present tables, as well as in Altmann (1962*a*) by C_2' and C_2'' respectively (see figures 1 and 2).

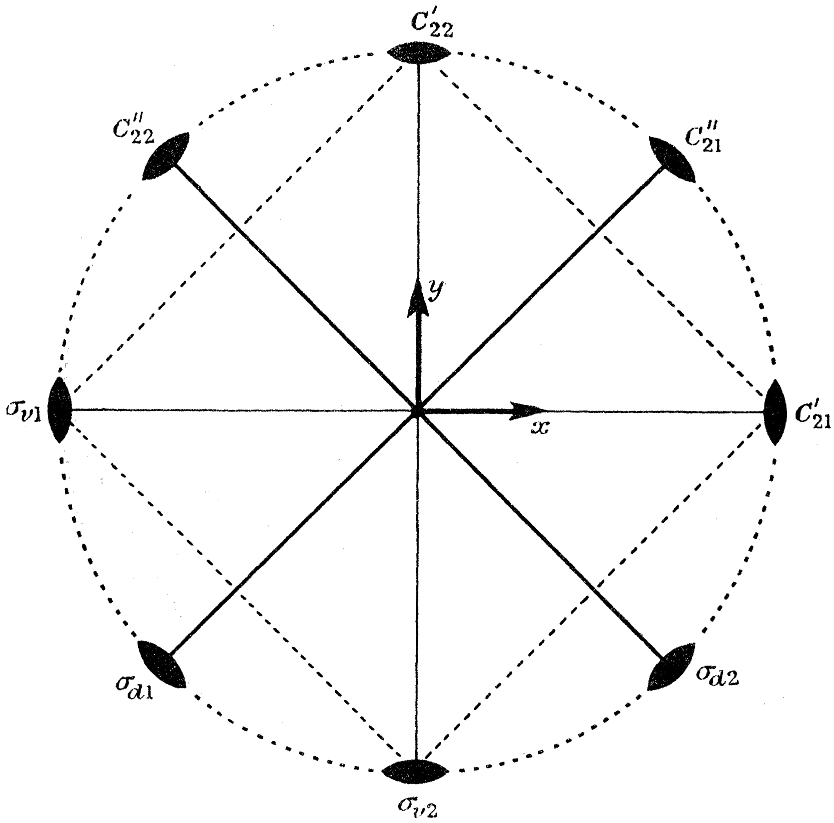

FIGURE 1. Symmetry elements for the groups with fourfold symmetry. Notice that $\sigma_{vr} = iC'_{2s}$ and $\sigma_{dr} = iC''_{2s}$, where $r, s = 1$, 2 and $r \neq s$. x, y, z form a right-handed set.

(ii) *Notation for l and m.* By $m = 1$, mod $(+2)$ we mean that 2 can be added, but not subtracted, from $m = 1$. l is always given mod $(+2)$.

(iii) *Spherical harmonics.* The unnormalized spherical harmonics are

$$\mathscr{Y}_l^{m,c}(\theta,\phi) = P_l^m(\cos\theta)\cos m\phi, \tag{10}$$

$$\mathscr{Y}_l^{m,s}(\theta,\phi) = P_l^m(\cos\theta)\sin m\phi. \tag{11}$$

The normalized ones are $Y_l^{m,c}$, $Y_l^{m,s}$, the same as above, multiplied by the factor

$$\surd[(2l+1)\,(l-|m|)!/2\pi(l+|m|)!].$$

In tables 1, 2 and 3 either normalized or unnormalized harmonics can be used. The superscripts c, s of the allowed harmonics appear in table 3 under the heading 'ϕ-dep.' (ϕ-dependence). The symbol (c, s) denotes a degenerate basis $(\mathscr{Y}_l^{m,c}, \mathscr{Y}_l^{m,s})$ (see below). Notice that $(c, -s)$, for instance, means $(\mathscr{Y}_l^{m,c}, -\mathscr{Y}_l^{m,s})$.

(iv) *Bases.* They are given as *row* vectors, such as $(\mathscr{Y}_l^{m,c}, \mathscr{Y}_l^{m,s})$ abbreviated in table 3 with the symbol (c, s). Their transformation properties are given by multiplying them on

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the right by the matrices listed in the tables of the representations: the first function belongs to the first column of the representation and the second to the second column.

(v) *Functions p, d, and f.* In the last column of table 3, we identify explicitly the bases that correspond to the spherical harmonics *p*, *d* and *f*, defined in table 9 of part I. They can be used with or without the normalization factors therein given.

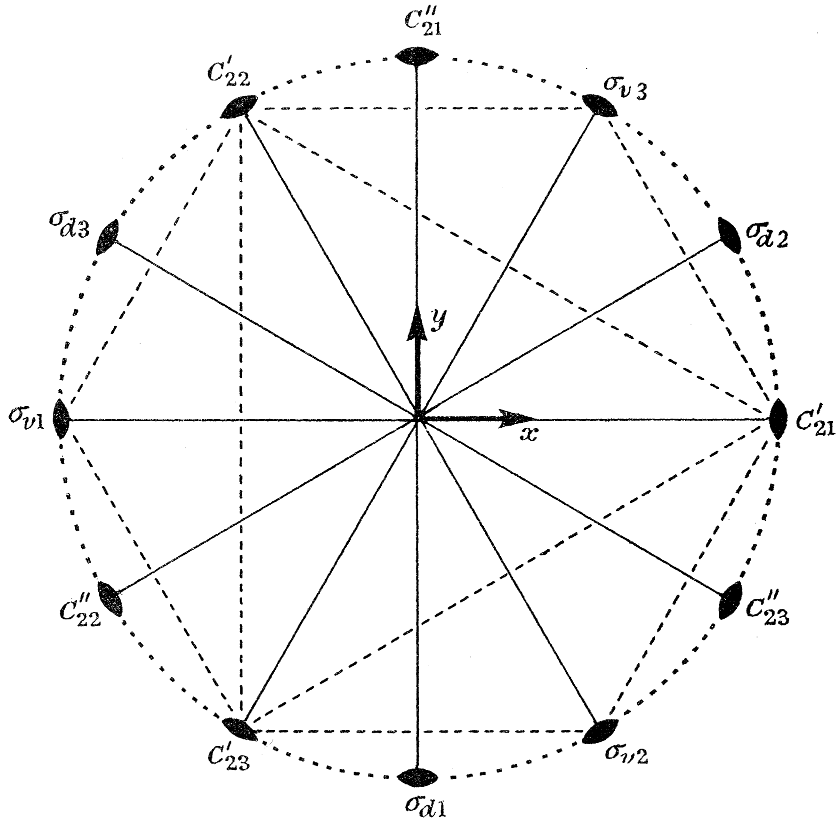

FIGURE 2. Symmetry elements for the groups with threefold and sixfold symmetry. Notice that $\sigma_{vr} = iC''_{2r}$ and $\sigma_{dr} = iC'_{2r}$, where $r = 1, 2, 3$. x, y, z form a right-handed set. Notice also that there is a second setting for the groups with threefold symmetry, where the three symmetry planes (or binary axes) coincide with the σ_d (or the C''_2). This setting was used for $\mathbf{C}_{3v}$ and $\mathbf{D}_3$ in part I but will not be used in this paper.

(vi) *One-dimensional representations and direct product groups.* If required, they must be obtained from the tables in part I, which are not repeated here as they are unchanged, except however those for $\mathbf{C}_{3v}$ and $\mathbf{D}_3$ which are given on account of the different setting now used (see figure 2).

(vii) *Example of the use of the tables.* For the representation E of $\mathbf{D}_{2d}$ the bases

$$(\mathscr{Y}_1^{1,c}, \mathscr{Y}_1^{1,s}), \quad (\mathscr{Y}_3^{1,c}, \mathscr{Y}_3^{1,s}), \quad (\mathscr{Y}_5^{1,c}, \mathscr{Y}_5^{1,s}), \quad (\mathscr{Y}_5^{5,c}, \mathscr{Y}_5^{5,s}), \quad \ldots, \quad (\mathscr{Y}_2^{1,s}, \mathscr{Y}_2^{1,c}), \quad (\mathscr{Y}_4^{1,s}, \mathscr{Y}_4^{1,c}),$$

etc., span the representations listed in table 2.

5. The expansions for the cubic groups

The symmetry operations of the cubic groups are defined by means of figure 3.

They are: the identity E; three binary and six fourfold rotations, C_{2m} and $C_{4m}^{\pm}$ respectively ($m = x, y, z$), around the co-ordinate axes; eight threefold rotations $C_{3n}^{\pm}$ around the

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axes named with $n = 1, 2, 3, 4$ in the figure; six binary rotations C_{2p} around the axes $p = a, b, c, d, e, f$ of the figure. (We always take positive rotations counterclockwise.) Operations that contain the inversion i are named as follows: $\sigma_m = iC_{2m}$, $S^{\pm}_{4m} = iC^{\mp}_{4m}$, $\sigma_{dp} = iC_{2p}$. Other rotary inversions are not named, since they do not appear in $\mathbf{T}$, $\mathbf{O}$ or $\mathbf{T}_d$ (the remaining two groups $\mathbf{T}_h$ and $\mathbf{O}_h$ are direct products and do not require separate treatment).

The doubly and triply degenerate representations of the cubic groups can be obtained from tables 6 and 7. In order to simplify the tables we make use of the fact that $\mathbf{T}$ is a subgroup of both $\mathbf{O}$ and $\mathbf{T}_d$: it is then convenient to expand the latter groups in their cosets with respect to $\mathbf{T}$. We can write, in an obvious notation, $\mathbf{O} = \mathbf{T} + \mathbf{T}C_{2a}$, $\mathbf{T}_d = \mathbf{T} + \mathbf{T}\sigma_{da}$. Therefore, in order to get the full representations for $\mathbf{O}$ and $\mathbf{T}_d$ it is enough to have the

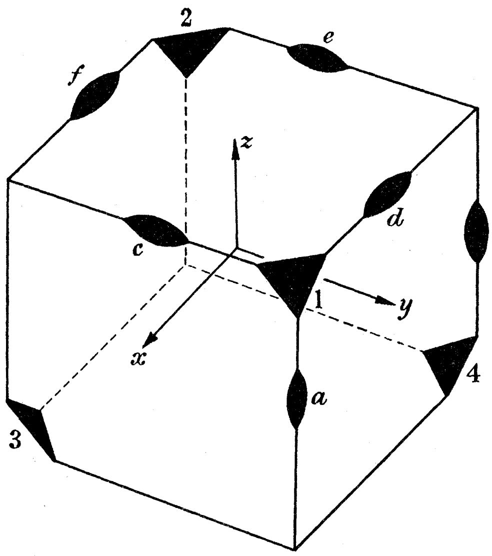

FIGURE 3. The symmetry operations of the cubic groups. Notice that the σ_{dp} planes ($p =$ a, b, c, d, e, f) are perpendicular to the C_{2p} axes.

matrices of $\mathbf{T}$ and multiply them by the matrices that correspond to C_{2a} and σ_{da}. In order to do this, careful correspondence must be established between the operations of the coset $\mathbf{T}C_{2a}$, say, and those of $\mathbf{O}$. This can be found from table 7, where the operations listed under $\mathbf{O}$ are the product of the operation listed under $\mathbf{T}$ times C_{2a}†. The same remark is valid for $\mathbf{T}_d$ with respect to the operation σ_{da}.

The relation between $\mathbf{O}$ and $\mathbf{T}_d$ and their subgroup $\mathbf{T}$ is in fact stronger than the one just given. $\mathbf{T}$ is clearly an invariant subgroup of both groups and these can be written as a semi-direct product (see, for example, Altmann 1962*b*) of $\mathbf{T}$ with $\mathbf{C}_2$ for $\mathbf{O}$ and $\mathbf{T}$ with $\mathbf{C}_s$ for $\mathbf{T}_d$‡. This results allows us to obtain very simply all the expansions for $\mathbf{O}$ and $\mathbf{T}_d$ in terms of those of $\mathbf{T}$, as we shall see. We give elsewhere (Altmann 1962*b*) the full theory of the representations of the semi-direct products and its application to the derivation of

† In checking these products, attention must be paid to the fact that we always use our transformations as *passive*, that is, as transformations of the axes and not of the points.

‡ It is important to realize, for future reference, that $\mathbf{C}_2$ and $\mathbf{C}_s$ are described in a different setting from the usual one for these groups (as, for instance, given in part I): C_2 lies in the x, y plane and σ is perpendicular to it.

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symmetry-adapted spherical harmonics, and we shall only quote here such results as are important in the derivation of the expansions.

First, the representations of **O** and $\mathbf{T}_d$ are related to those of **T** as shown in the following scheme:

T		**O**, $\mathbf{T}_d$
A	<	A_1, A_2
${}^1E$, ${}^2E$	—	E
T	<	T_1, T_2

A basis of A will span one of the two irreducible representations of $\mathbf{C}_2$ and $\mathbf{C}_s$: those that span the totally symmetrical ones belong to A_1 of **O** and $\mathbf{T}_d$, the others to A_2. Secondly, the general theory shows that the only values of l that appear in the expansions for A of **T** are those listed in table 4, and that for each value of l the linear combination that forms any expansion can contain only the spherical harmonics with the values of m and ϕ-dependence given in the table. In order to see how these bases go over to bases of **O** and **T**, it is enough to find the representations of $\mathbf{C}_2$ and $\mathbf{C}_s$ (expressed in the appropriate setting) to which they belong. This we do by means of table 12 in the appendix, which provides the assignments given in the columns 5 and 6 of table 4. The assignments for **O** and $\mathbf{T}_d$, given in the last two columns follow immediately, and they are embodied in table 8.

Table 4. The splitting up of the functions belonging to A

T	l mod (+2)	m mod (+4)	ϕ-dep.	$\mathbf{C}_2$	$\mathbf{C}_s$	**O**	$\mathbf{T}_d$
A	0	0	c	A	A'	A_1	A_1
	6	2	c	B	A''	A_2	A_2
	3	2	s	B	A'	A_2	A_1
	9	4	s	A	A''	A_1	A_2

For the doubly degenerate representations the result is that the bases of ${}^1E$ and ${}^2E$ of **T** (these being the first and second representations, respectively, listed by Margenau & Murphy 1956 and Altmann 1962*a*) will go over unchanged into bases (in complex form) of E for both **O** and $\mathbf{T}_d$. When these bases are taken into real form, as in our tables, small changes are required in the bases of $\mathbf{T}_d$, as explained in the note at the head of table 10.

For the triply degenerate representations the result is that a basis of T of **T** can always be chosen so that one of its three functions will belong to one of the irreducible representations of $\mathbf{C}_2$ and $\mathbf{C}_s$. We have chosen this function to be the third one of the basis: when it belongs to A of $\mathbf{C}_2$ or A' of $\mathbf{C}_s$, the whole basis belongs to T_2 of **O** or $\mathbf{T}_d$ (notice that this is the representation for which the characters of the secondary binary axes or mirror planes are +1). Otherwise the basis belongs to T_1. The values of l, m, and ϕ-dependence for this

Table 5. The splitting up of the functions belonging to T

T	l mod (+2)	m mod (+4)	ϕ-dep.	$\mathbf{C}_2$	$\mathbf{C}_s$	**O**	$\mathbf{T}_d$
T (3rd column)	1	0	c	B	A'	T_1	T_2
	2	2	s	A	A'	T_2	T_2
	3	2	c	A	A''	T_2	T_1
	4	4	s	B	A''	T_1	T_1

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third function of the representation T of $\mathbf{T}$ are predicted by the theory to be those given in table 5. The assignments for $\mathbf{C}_2$ and $\mathbf{C}_s$ are obtained from table 12 in the appendix, and those for $\mathbf{O}$ and $\mathbf{T}_d$ follow; they have been included in table 11 that gives the expansions in full.

Notes to tables 6 *to* 11

(i) *Notation for the irreducible representations.* In order to use the tables of Margenau & Murphy (1956) or Altmann (1962*a*), note the following changes of notation: In the first, for $\mathbf{T}$, $4C_3$ and $4C_3'$ correspond to our $4C_3^+$ and $4C_3^-$, respectively; for $\mathbf{O}$, $6C_2$ correspond to our C_{2p} ($p = a, b, c, d, e, f$) and, for $\mathbf{T}_d$, $6\sigma_d$ correspond to our σ_{dp}. In Altmann's table for $\mathbf{O}$, $6C_2'$ correspond to our C_{2p} and for $\mathbf{T}_d$, $6\sigma_d$ to our σ_{dp}. We use the symbols ${}^1E$ and ${}^2E$ for the

Table 6. The doubly degenerate representations, E, of the cubic groups

The basis of the representations is $(2\mathcal{Y}_2^0, \tfrac{1}{2}\sqrt{3}\,\mathcal{Y}_2^{2,c})$.

$\mathbf{O}, \mathbf{T}_d$: $E, C_{2x}, C_{2y}, C_{2z}$	$\begin{bmatrix} 1 & \\ & 1 \end{bmatrix}$	$\mathbf{O}$: $C_{2a}, C_{4z}^+, C_{4z}^-, C_{2b}$ $\mathbf{T}_d$: $\sigma_{da}, S_{4z}^-, S_{4z}^+, \sigma_{db}$	$\begin{bmatrix} 1 & \\ & -1 \end{bmatrix}$
$\mathbf{O}, \mathbf{T}_d$: $C_{31}^+, C_{32}^+, C_{33}^+, C_{34}^+$	$\begin{bmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix}$	$\mathbf{O}$: $C_{4x}^-, C_{4x}^+, C_{2f}, C_{2d}$ $\mathbf{T}_d$: $S_{4x}^+, S_{4x}^-, \sigma_{df}, \sigma_{dd}$	$\begin{bmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & \frac{1}{2} \end{bmatrix}$
$\mathbf{O}, \mathbf{T}_d$: $C_{31}^-, C_{32}^-, C_{33}^-, C_{34}^-$	$\begin{bmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{bmatrix}$	$\mathbf{O}$: $C_{4y}^+, C_{4y}^-, C_{2c}, C_{2e}$ $\mathbf{T}_d$: $S_{4y}^-, S_{4y}^+, \sigma_{dc}, \sigma_{de}$	$\begin{bmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & \frac{1}{2} \end{bmatrix}$

Table 7. The triply degenerate representations of the cubic groups

Given a representation of $\mathbf{O}$ or $\mathbf{T}_d$, the representatives for the operations of these groups that do not belong to $\mathbf{T}$, which are listed under the headings $\mathbf{O}$ and $\mathbf{T}_d$ in the first part of the table, are obtained as follows: take the corresponding matrix from the first part of the table and post-multiply it with the matrix that appears under the representation chosen at the bottom of the table.

The bases of the representations are

for T of $\mathbf{T}$, T_1 of $\mathbf{O}$, T_2 of $\mathbf{T}_d$: $(\mathcal{Y}_1^{1,c}, \mathcal{Y}_1^{1,s}, \mathcal{Y}_1^0)$;
for T_2 of $\mathbf{O}$: $(\mathcal{Y}_2^{1,s}, \mathcal{Y}_2^{1,c}, \tfrac{1}{2}\mathcal{Y}_2^{2,s})$;
for T_1 of $\mathbf{T}_d$: $(-10\mathcal{Y}_3^{1,c} - \mathcal{Y}_3^{3,c}, 10\mathcal{Y}_3^{1,s} - \mathcal{Y}_3^{3,s}, 4\mathcal{Y}_3^{2,c})$

$\mathbf{T}, \mathbf{O}, \mathbf{T}_d$	$\mathbf{O}$	$\mathbf{T}_d$		$\mathbf{T}, \mathbf{O}, \mathbf{T}_d$	$\mathbf{O}$	$\mathbf{T}_d$	
E	C_{2a}	σ_{da}	$\begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix}$	C_{33}^+	C_{2f}	σ_{df}	$\begin{bmatrix} & -1 & \\ & & 1 \\ -1 & & \end{bmatrix}$
C_{2x}	C_{4z}^+	S_{4z}^-	$\begin{bmatrix} 1 & & \\ & -1 & \\ & & -1 \end{bmatrix}$	C_{34}^+	C_{2d}	σ_{dd}	$\begin{bmatrix} & -1 & \\ & & -1 \\ 1 & & \end{bmatrix}$
C_{2y}	C_{4z}^-	S_{4z}^+	$\begin{bmatrix} -1 & & \\ & 1 & \\ & & -1 \end{bmatrix}$	C_{31}^-	C_{4y}^+	S_{4y}^-	$\begin{bmatrix} & & 1 \\ 1 & & \\ & 1 & \end{bmatrix}$
C_{2z}	C_{2b}	σ_{db}	$\begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix}$	C_{32}^-	C_{4y}^-	S_{4y}^+	$\begin{bmatrix} & & -1 \\ 1 & & \\ & -1 & \end{bmatrix}$
C_{31}^+	C_{4x}^-	S_{4x}^+	$\begin{bmatrix} & 1 & \\ & & 1 \\ 1 & & \end{bmatrix}$	C_{33}^-	C_{2c}	σ_{dc}	$\begin{bmatrix} & & -1 \\ -1 & & \\ & 1 & \end{bmatrix}$
C_{32}^+	C_{4x}^+	S_{4x}^-	$\begin{bmatrix} & 1 & \\ & & -1 \\ -1 & & \end{bmatrix}$	C_{34}^-	C_{2e}	σ_{de}	$\begin{bmatrix} & & 1 \\ -1 & & \\ & -1 & \end{bmatrix}$

$\mathbf{O}$	$\mathbf{T}_d$	T_1	T_2
C_{2a}	σ_{da}	$\begin{bmatrix} & 1 & \\ 1 & & \\ & & -1 \end{bmatrix}$	$\begin{bmatrix} & -1 & \\ -1 & & \\ & & 1 \end{bmatrix}$

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TABLE 8. HARMONICS FOR THE SINGLY DEGENERATE REPRESENTATIONS OF **T**, **O** AND $\mathbf{T}_d$

(See notes (i) to (iii) of this section and note (iv) of §4.)

T	**O**	$\mathbf{T}_d$	l	ϕ-dep.	spherical harmonic
A	A_1	A_1	0	—	1(0)
	A_2	A_1	3	s	1(2)
	A_1	A_1	4	c	168(0) + 1(4)
	A_1	A_1	6	c	360(0) − 1(4)
	A_2	A_2	6	c	792(2) − 1(6)
	A_2	A_1	7	s	1 560(2) + 1(6)
	A_1	A_1	8	c	3 991 680(0) + 672(4) + 1(8)
	A_2	A_1	9	s	2 520(2) − 1(6)
	A_1	A_2	9	s	4 080(4) − 1(8)
	A_1	A_1	10	c	23 587 200(0) − 4 320(4) − 1(8)
	A_2	A_2	10	c	19 918 080(2) + 456(6) − 1(10)
	A_2	A_1	11	s	61 689 600(2) − 3 240(6) − 1(10)
	A_1	A_1	12	c	711 796 377 600(0) + 19 958 400(4) + 1 584(8) + 1(12)
	A_1	A_1	12	c	99 845 760(4) − 10 304(8) + 1(12)
	A_2	A_2	12	c	61 689 600(2) − 12 600(6) + 1(10)

TABLE 9. HARMONICS FOR THE REPRESENTATIONS E OF **T**

The expansions given belong to ${}^1E$. Those for ${}^2E$ are just the complex conjugates of the expansions in this table. The real part of the expansion is given in every case in the first line and the complex part, which should be multiplied by the coefficient provided, in the second line. See notes (i) to (iii) of this section for the notation.

T	l	ϕ-dep.	coeff.	spherical harmonic
${}^1E$	2	c		6(0)
		c	i $\sqrt{3}$	1(2)
	4	c		120(0) − 1(4)
		c	−i $\sqrt{3}$	8(2)
	5	s		36(2)
		s	i $\sqrt{3}$	1(4)
	6	c		2 520(0) + 1(4)
		c	i $\sqrt{3}/12$	360(2) + 1(6)
	7	s		1 320(2) − 1(6)
		s	−i $\sqrt{3}$	24(4)
	8	c		3 749 760(0) − 672(4) − 1(8)
		c	−16i $\sqrt{3}$	2 520(2) + 1(6)
	8	c		1 560(4) − 1(8)
		c	−15i $\sqrt{3}$	3 432(2) − 1(6)
	9	s		1 680(4) + 1(8)
		s	−12i $\sqrt{3}$	10 920(2) + 1(6)
	10	c		2 315 174 400(0) + 86 400(4) + 20(8)
		c	i $\sqrt{3}$	8 467 200(2) + 1 080(6) + 1(10)
	10	c		587 520(4) − 96(8)
		c	i $\sqrt{3}$	17 821 440(2) − 4 488(6) + 1(10)
	11	s		77 656 320(2) − 3 240(6) − 1(10)
		s	−48i $\sqrt{3}$	5 040(4) + 1(8)
	11	s		15 960(6) − 3(10)
		s	−70i $\sqrt{3}$	15 504(4) − 1(8)
	12	c		759 696 537 600(0) − 19 958 400(4) − 1 584(8) − 1(12)
		c	−24i $\sqrt{3}$	119 750 400(2) + 6 600(6) + 1(10)
	12	c		117 210 240(4) + 4 032(8) − 3(12)
		c	−10i $\sqrt{3}$	1 172 102 400(2) − 9 576(6) − 5(10)

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first and second representations respectively given under E for **T** in both tables. For the two- and three-dimensional representations no ambiguity can arise as they are fully listed in tables 6 and 7.

(ii) *Normalization.* The expansions are given in terms of the unnormalized harmonics defined by (10) and (11). They can be normalized by means of the relations given in p. 361 of part I.

Table 10. Harmonics for the doubly degenerate representations of **O** and $\mathbf{T}_d$

The expansions given belong to E of **O**. Those for E of $\mathbf{T}_d$ are obtained as follows: for even l they are the expansions listed; for odd l, the partners must be interchanged and the sign of one of them reversed. In all cases, multiply the second partner listed by the coefficient provided. See notes (i) to (iii) of this section and note (iv) of §4 for the notation.

O	l	ϕ-dep.	coeff.	spherical harmonic
E	2	—		1(0)
		c	$\sqrt{3}/6$	1(2)
	4	c		120(0) − 1(4)
		c	$-\sqrt{3}/6$	48(2)
	5	s		1(4)
		s	$-\sqrt{3}/6$	72(2)
	6	c		5040(0) + 2(4)
		c	$\sqrt{3}/6$	360(2) + 1(6)
	7	s		12(4)
		s	$\sqrt{3}/6$	1320(2) − 1(6)
	8	c		3749760(0) − 672(4) − 1(8)
		c	$-\sqrt{3}/6$	241920(2) + 96(6)
	8	c		1560(4) − 1(8)
		c	$-\sqrt{3}/6$	30880(2) − 90(6)
	9	s		1680(4) + 1(8)
		s	$-\sqrt{3}/6$	786240(2) + 72(6)
	10	c		231517440(0) + 86400(4) + 20(8)
		c	$\sqrt{3}/6$	50803200(2) + 6480(6) + 6(10)
	10	c		587520(4) − 96(8)
		c	$\sqrt{3}/6$	106928640(2) − 26928(6) + 6(10)
	11	s		120960(4) + 24(8)
		s	$\sqrt{3}/6$	77656320(2) − 3240(6) − 1(10)
	11	s		542640(4) − 35(8)
		s	$-\sqrt{3}/6$	15960(6) − 3(10)
	12	c		759696537600(0) − 19958400(4) − 1584(8) − 1(12)
		c	$-\sqrt{3}/6$	17244057600(2) − 950400(6) − 144(10)
	12	c		39070080(4) + 1344(8) − 1(12)
		c	$-\sqrt{3}/6$	23442048000(2) − 191520(6) − 100(10)

(iii) *Notation of the tables.* A combination of the form $a\mathscr{Y}_l^{m,c}+b\mathscr{Y}_l^{n,c}+c\mathscr{Y}_l^{p,c}$ is given as follows: the values of l and the superscript c (or s) appear under the headings l and ϕ-dep., respectively. (Notice that now, of course, l should *not* be understood mod + 2). The rest of the expansion appears on the same line in the form $a(m)+b(n)+c(p)$. Degenerate representations are given in two or three lines, and they must be understood as a row vector, the successive lines corresponding to the successive columns of the vector.

Example (see table 8): for $l = 8$ the spherical harmonic that belongs to A of **T**, A_1 of **O** and A_1 of $\mathbf{T}_d$ is

$$3991680\,\mathscr{Y}_8^0+672\,\mathscr{Y}_8^{4,c}+\mathscr{Y}_8^{8,c}.$$

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TABLE 11. HARMONICS FOR THE TRIPLY DEGENERATE REPRESENTATION OF **T**, **O** AND $\mathbf{T}_d$

(See notes (i) to (iii) of this section and note (iv) of §4.)

T	**O**	$\mathbf{T}_d$	l	ϕ-dep.	spherical harmonic
T	T_1	T_2	1	c	1(1)
				s	1(1)
				—	1(0)
	T_2	T_2	2	s	2(1)
				c	2(1)
				s	1(2)
	T_1	T_2	3	c	6(1) − 1(3)
				s	6(1) + 1(3)
				—	−24(0)
	T_2	T_1	3	c	−10(1) − 1(3)
				s	10(1) − 1(3)
				c	4(2)
	T_2	T_2	4	s	6(1) − 1(3)
				c	6(1) + 1(3)
				s	−4(2)
	T_1	T_1	4	s	−42(1) − 1(3)
				c	42(1) − 1(3)
				s	1(4)
	T_1	T_2	5	c	240(1) − 10(3) + 1(5)
				s	240(1) + 10(3) + 1(5)
				—	1920(0)
	T_2	T_1	5	c	336(1) − 6(3) − 1(5)
				s	−336(1) − 6(3) + 1(5)
				c	96(2)
	T_1	T_2	5	c	1008(1) + 54(3) + 1(5)
				s	1008(1) − 54(3) + 1(5)
				c	16(4)
	T_2	T_2	6	s	240(1) − 18(3) + 1(5)
				c	240(1) + 18(3) + 1(5)
				s	192(2)
	T_1	T_1	6	s	720(1) − 30(3) − 1(5)
				c	−720(1) − 30(3) + 1(5)
				s	8(4)
	T_2	T_2	6	s	23760(1) + 330(3) + 3(5)
				c	23760(1) − 330(3) + 3(5)
				s	8(6)
	T_1	T_2	7	c	25200(1) − 504(3) + 14(5) − 1(7)
				s	25200(1) + 504(3) + 14(5) + 1(7)
				—	−322560(0)
	T_2	T_1	7	c	−32400(1) + 456(3) − 2(5) − 1(7)
				s	32400(1) + 456(3) + 2(5) − 1(7)
				c	7680(2)
	T_1	T_2	7	c	71280(1) + 264(3) − 50(5) − 1(7)
				s	71280(1) − 264(3) − 50(5) + 1(7)
				c	−384(4)
	T_2	T_1	7	c	−308880(1) − 10296(3) − 130(5) − 1(7)
				s	308880(1) − 10296(3) + 130(5) − 1(7)
				c	64(6)
	T_2	T_2	8	s	25200(1) − 1080(3) + 30(5) − 1(7)
				c	25200(1) + 1080(3) + 30(5) + 1(7)
				s	−23040(2)
	T_1	T_1	8	s	−55440(1) + 1800(3) − 18(5) − 1(7)
				c	55440(1) + 1800(3) + 18(5) − 1(7)
				s	384(4)

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TABLE 11 (*cont.*)

T	**O**	$\mathbf{T}_d$	l	ϕ-dep.	spherical harmonic
T	T_2	T_2	8	s	720720(1) − 10920(3) − 294(5) − 3(7)
				c	720720(1) + 10920(3) − 294(5) + 3(7)
				s	− 64(6)
	T_1	T_1	8	s	− 3603600(1) − 32760(3) − 210(5) − 1(7)
				c	3603600(1) − 32760(3) + 210(5) − 1(7)
				s	8(8)
	T_1	T_2	9	c	5080320(1) + 60480(3) + 864(5) − 18(7) + 1(9)
				s	5080320(1) + 60480(3) + 864(5) + 18(7) + 1(9)
				—	92897280(0)
	T_2	T_1	9	c	6209280(1) − 60480(3) + 480(5) + 2(7) − 1(9)
				s	− 6209280(1) − 60480(3) − 480(5) + 2(7) + 1(9)
				c	1290240(2)
	T_1	T_2	9	c	11531520(1) − 37440(3) − 1440(5) + 46(7) + 1(9)
				s	11531520(1) + 37440(3) − 1440(5) − 46(7) + 1(9)
				c	30720(4)
	T_2	T_1	9	c	34594560(1) + 262080(3) − 7200(5) − 126(7) − 1(9)
				s	− 34594560(1) + 262080(3) + 7200(5) − 126(7) + 1(9)
				c	1536(6)
	T_1	T_2	9	c	196035840(1) + 4455360(3) + 40800(5) + 238(7) + 1(9)
				s	196035840(1) − 4455360(3) + 40800(5) − 238(7) + 1(9)
				c	256(8)
	T_2	T_2	10	s	5080320(1) − 141120(3) + 2400(5) − 42(7) + 1(9)
				c	5080320(1) + 141120(3) + 2400(5) + 42(7) + 1(9)
				s	5160960(2)
	T_1	T_1	10	s	9434880(1) − 221760(3) + 2400(5) − 6(7) − 1(9)
				c	− 9434880(1) − 221760(3) − 2400(5) − 6(7) + 1(9)
				s	46080(4)
	T_2	T_2	10	s	28304640(1) − 463680(3) − 160(5) + 86(7) + 1(9)
				c	28304640(1) + 463680(3) − 160(5) − 86(7) + 1(9)
				s	1024(6)
	T_1	T_1	10	s	160392960(1) − 1028160(3) − 24480(5) − 198(7) − 1(9)
				c	− 160392960(1) − 1028160(3) + 24480(5) − 198(7) + 1(9)
				s	64(8)
	T_2	T_2	10	s	15237331200(1) + 97675200(3) + 465120(5) + 1710(7) + 5(9)
				c	15237331200(1) − 97675200(3) + 465120(5) − 1710(7) + 5(9)
				s	128(10)
	T_1	T_2	11	c	1676505600(1) − 13305600(3) + 118800(5) − 1320(7) + 22(9) − 1(11)
				s	1676505600(1) + 13305600(3) + 118800(5) + 1320(7) + 22(9) + 1(11)
				—	− 40874803200(0)
	T_2	T_1	11	c	− 1981324800(1) + 13789440(3) − 88560(5) + 408(7) + 6(9) − 1(11)
				s	1981324800(1) + 13789440(3) + 88560(5) + 408(7) − 6(9) − 1(11)
				c	371589120(2)
	T_1	T_2	11	c	3302208000(1) − 13305600(3) − 65520(5) + 2520(7) − 42(9) − 1(11)
				s	3302208000(1) + 13305600(3) − 65520(5) − 2520(7) − 42(9) + 1(11)
				c	− 5160960(4)
	T_2	T_1	11	c	− 8019648000(1) − 6854400(3) + 648720(5) − 4200(7) − 122(9) − 1(11)
				s	8019648000(1) − 6854400(3) − 648720(5) − 4200(7) + 122(9) − 1(11)
				c	122880(6)

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TABLE 11 (*cont.*)

T	**O**	$\mathbf{T}_d$	l	ϕ-dep.	spherical harmonic
T	T_1	T_2	11	c	30474662400(1) + 234420480(3) − 2093040(5) − 35112(7) − 234(9) − 1(11)
				s	30474662400(1) − 234420480(3) − 2093040(5) + 35112(7) − 234(9) + 1(11)
				c	−6144(8)
	T_2	T_1	11	c	−213322636800(1) − 3516307200(3) − 24418800(5) − 111720(7) − 378(9) − 1(11)
				s	213322636800(1) − 3516307200(3) + 24418800(5) − 111720(7) + 378(9) − 1(11)
				c	1024(10)
	T_2	T_2	12	s	1676505600(1) − 32659200(3) + 378000(5) − 4200(7) + 54(9) − 1(11)
				c	1676505600(1) + 32659200(3) + 378000(5) + 4200(7) + 54(9) + 1(11)
				s	−1857945600(2)
	T_1	T_1	12	s	−2794176000(1) + 48625920(3) − 428400(5) + 2520(7) + 6(9) − 1(11)
				c	2794176000(1) + 48625920(3) + 428400(5) + 2520(7) − 6(9) − 1(11)
				s	1032170(4)
	T_2	T_2	12	s	6785856000(1) − 94590720(3) + 378000(5) + 3480(7) − 74(9) − 1(11)
				c	6785856000(1) + 94590720(3) + 378000(5) − 3480(7) − 74(9) + 1(11)
				s	−122880(6)
	T_1	T_1	12	s	−25786252800(1) + 234420480(3) + 861840(5) − 16680(7) − 186(9) − 1(11)
				c	25786252800(1) + 234420480(3) − 861840(5) − 16680(7) + 186(9) − 1(11)
				s	3072(8)
	T_2	T_2	12	s	902518848000(1) − 2578625280(3) − 60041520(5) − 397320(7) − 1650(9) − 5(11)
				c	902518848000(1) + 2578625280(3) − 60041520(5) + 397320(7) − 1650(9) + 5(11)
				s	−1024(10)
	T_1	T_1	12	s	−12454760102400(1) − 59308381440(3) − 218045520(5) − 637560(7) − 1518(9) − 3(11)
				c	12454760102400(1) − 59308381440(3) + 218045520(5) − 637560(7) + 1518(9) − 3(11)
				s	256(12)

APPENDIX. THE GROUP $\mathbf{C}_2$ IN THE HORIZONTAL SETTING AND THE GROUP $\mathbf{C}_s$ IN THE VERTICAL SETTING

The operations C_2 and σ of these groups coincide with C''_{21} and σ_{d1} of figure 1 respectively. See notes (i) to (iv) of §4 for the notation. In these tables $c \pm s$ means the combination $Y_l^{m,c} \pm Y_l^{m,s}$.

$\mathbf{C}_2$	l	m mod (+4)	ϕ-dep.		l	m mod (+4)	ϕ-dep.
A	0	0	c	B	1	0	c
	2	1	$c-s$		2	1	$c+s$
	1	1	$c+s$		1	1	$c-s$
	2	2	s		2	2	c
	3	2	c		3	2	s
	4	3	$c+s$		4	3	$c-s$
	3	3	$c-s$		3	3	$c+s$
	5	4	s		4	4	s

$\mathbf{C}_s$	m	ϕ-dep.		m	ϕ-dep.
A'	0	c	A''	1	$c+s$
	1	$c-s$		2	c
	2	s		3	$c-s$
	3	$c+s$		4	s

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