

THE SPHERICAL HARMONICS WITH THE SYMMETRY OF THE ICOSAEDRAL GROUP

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Communicated by C. A. COULSON

Received 25 February 1957

For a long time there has been some interest in obtaining spherical harmonics with the symmetry of the regular polyhedrons, particularly for electrostatic problems involving polyhedral conductors. Work on the icosahedral group has been done, among others, by Meyer (7), Laporte (6), Hodgkinson (3) and Poole (8), apart from the classic work of Klein (4). In the several approaches of these authors, only spherical harmonics for the totally symmetric representation were obtained, the most complete table being that of Laporte who obtained the spherical harmonics up to $l = 21$. New interest in the icosahedral group has arisen in connexion with the structure of some proteins (5), and we obtain here, by the recently developed method of Altmann (1), expansions in spherical harmonics for all the representations of this group. This has been done up to and including $l = 14$. (For the totally symmetric representation we have also included $l = 15$.) In what follows we shall use Altmann's formulae and notation.

We briefly summarize the operational technique given by Altmann. Let α, β and γ be the Euler angles, as defined by Hirschfelder, Curtiss and Bird (2), for the symmetry operations of the group, χ^i the character of the i th irreducible representation and \mathcal{Y}_l^m an unnormalized spherical harmonic, called the generator. Divide the group into subsets $\mathcal{G}^{\beta, \mathcal{C}}$, the elements of which are given as $\mathcal{R}^{\beta, \mathcal{C}_s} t$, where r denotes the β angle, s denotes the class \mathcal{C}_s to which the element belongs and t is a running index over the subset $\mathcal{G}^{\beta, \mathcal{C}}$. Then the expansions in unnormalized spherical harmonics belonging to the i th irreducible representation can be obtained by forming the expression (1) ((32) of reference (1)) for all possible generators \mathcal{Y}_l^m :

$$\sum_r \sum_{m'} \mathcal{S}_{m'm}^{(l)}(\beta_r) \left\{ \sum_s \chi^i(\mathcal{C}_s)^* C_{m'm} \sum_t e^{im'\gamma_t} e^{ima_t} \right\} \mathcal{Y}_l^{m'}. \quad (1)$$

In this expression

$$C_{m'm} = i^{|m|+m} \cdot i^{|m'|+m'},$$

$$\mathcal{S}_{m'm}^{(l)}(\beta) = (l + |m|)! (l - |m'|)! \sum_{r=0}^{r_m} \mathcal{C}_{\mu\nu}^{(l)}(r) \cos^{\nu-\mu+2r} \frac{1}{2}\beta \sin^{2l-(\nu-\mu+2r)} \frac{1}{2}\beta \quad (2)$$

and

$$\mathcal{C}_{\mu\nu}^{(l)}(r) = \frac{(-1)^{\mu-r}}{(\nu - \mu + r)! r! (\mu - r)! (2l - \nu - r)!},$$

where $\mu = \min(l - m', l + m)$, $\nu = \max(l - m', l + m)$, $r_m = \min(\mu, 2l - \nu)$.

The selection of a convenient system of coordinates reduces considerably the work involved in forming (1). In fact, if we choose as z axis one of the twelve five-fold axes†

† This system of axes has been suggested to me by Dr S. L. Altmann.

and as y axis one of the remaining two-fold axes perpendicular to z , the following features appear:

(i) Only two β angles appear in all the operations of the group, apart from 0 and π which are always treated independently. Consequently, expression (2), which is rather heavy to evaluate, will be used only twice for each set of values of l , m and m' .

(ii) The term in curly brackets in (1) (which is independent of l) turns out to be a periodic function of m and m' , that is, the Euler angles α and γ become submultiples of π . It is then a simple matter to obtain the transformation tables (which we define below) which will cover all possible values of m and m' . A number of these values will give zero contributions to the tables so that we shall know immediately those spherical harmonics which will not occur in the expansions.

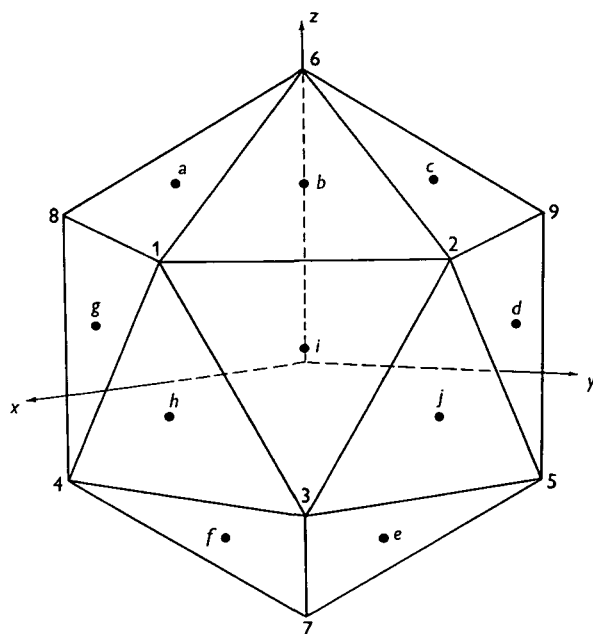


Fig. 1

If, on the other hand, we were to choose as the system of axes the three perpendicular two-fold axes, as has been done sometimes, β has then seven possible values, apart from 0 and π and, owing to the lack of periodicity in m and m' , the transformation tables cease to provide useful information about the form of the expansions.

We have used, therefore, the right-handed system of coordinates shown in Fig. 1.

We adopt the notation of Wilson, Decius and Cross (9) for the classes and irreducible representations of the icosahedral group.† The rotation axes have been denoted in every case by a first subscript, denoting the multiplicity of the axis, and a second one chosen as follows. For the five-fold and three-fold axes it denotes the point, as named in Fig. 1, at which the given axis intersects the surface of the icosahedron. For the

† We have used in the present work the character table for the icosahedral group quoted by Wilson, Decius and Cross. Note, however, the following misprint: the character for the class C_2 in the presentation H should read 1 instead of 0.

two-fold axes we use a double numerical subscript which denotes the end-points of the edge of the icosahedron which they bisect (see Fig. 1). The positive rotations have been chosen to be counter-clockwise.

The Euler angles for the operations of the group are listed, in the above notation, in Table 1.

Table 1. *Euler angles for the operations of the icosahedral group*

Class	Operation	α	β	γ	Class	Operation	α	β	γ
$12C_5$	$C_{5,2}^+$	0	ω	$\frac{1}{5}\pi$	$12C_5^2$	$C_{5,2}^{2+}$	$\frac{1}{5}\pi$	$\pi - \omega$	$\frac{2}{5}\pi$
	$C_{5,5}^+$	0	ω	$-\frac{1}{5}\pi$		$C_{5,5}^{2+}$	$-\frac{1}{5}\pi$	$\pi - \omega$	$-\frac{2}{5}\pi$
	$C_{5,4}^-$	$\frac{2}{5}\pi$	ω	$-\frac{1}{5}\pi$		$C_{5,1}^{2-}$	$\frac{1}{5}\pi$	$\pi - \omega$	$-\frac{4}{5}\pi$
	$C_{5,3}^+$	$-\frac{2}{5}\pi$	ω	$\frac{1}{5}\pi$		$C_{5,1}^{2+}$	$-\frac{1}{5}\pi$	$\pi - \omega$	$\frac{4}{5}\pi$
	$C_{5,1}^-$	$\frac{2}{5}\pi$	ω	$-\frac{3}{5}\pi$		$C_{5,2}^{2-}$	$\frac{3}{5}\pi$	$\pi - \omega$	$\frac{1}{5}\pi$
	$C_{5,1}^+$	$-\frac{2}{5}\pi$	ω	$\frac{3}{5}\pi$		$C_{5,5}^{2-}$	$-\frac{3}{5}\pi$	$\pi - \omega$	$-\frac{4}{5}\pi$
	$C_{5,2}^-$	$\frac{4}{5}\pi$	ω	$-\pi$		$C_{5,4}^{2-}$	$\frac{3}{5}\pi$	$\pi - \omega$	0
	$C_{5,5}^-$	$-\frac{4}{5}\pi$	ω	π		$C_{5,3}^{2+}$	$-\frac{3}{5}\pi$	$\pi - \omega$	0
	$C_{5,3}^-$	$\frac{4}{5}\pi$	ω	$-\frac{3}{5}\pi$		$C_{5,3}^{2-}$	π	$\pi - \omega$	$-\frac{2}{5}\pi$
	$C_{5,4}^+$	$-\frac{4}{5}\pi$	ω	$\frac{3}{5}\pi$		$C_{5,4}^{2+}$	$-\pi$	$\pi - \omega$	$\frac{2}{5}\pi$
	$C_{5,6}^+$	$\frac{2}{5}\pi$	0	0		$C_{5,6}^{2+}$	$\frac{4}{5}\pi$	0	0
	$C_{5,6}^-$	$-\frac{2}{5}\pi$	0	0		$C_{5,6}^{2-}$	$-\frac{4}{5}\pi$	0	0
Class	Operation	α	β	γ	Class	Operation	α	β	γ
$20C_3$	$C_{3,b}^+$	0	ω	$\frac{3}{5}\pi$	$15C_2$	$C_{2,16}$	0	ω	π
	$C_{3,a}^-$	0	ω	$-\frac{3}{5}\pi$		$C_{2,26}$	$\frac{2}{5}\pi$	ω	$\frac{3}{5}\pi$
	$C_{3,c}^+$	$\frac{2}{5}\pi$	ω	$\frac{1}{5}\pi$		$C_{2,68}$	$-\frac{2}{5}\pi$	ω	$-\frac{3}{5}\pi$
	$C_{3,e}^+$	$-\frac{2}{5}\pi$	ω	$-\frac{1}{5}\pi$		$C_{2,47}$	$\frac{4}{5}\pi$	ω	$\frac{1}{5}\pi$
	$C_{3,b}^-$	$\frac{2}{5}\pi$	ω	π		$C_{2,37}$	$-\frac{4}{5}\pi$	ω	$-\frac{1}{5}\pi$
	$C_{3,a}^+$	$-\frac{2}{5}\pi$	ω	π		$C_{2,12}$	$\frac{1}{5}\pi$	$\pi - \omega$	$\frac{4}{5}\pi$
	$C_{3,f}^-$	$\frac{4}{5}\pi$	ω	$-\frac{1}{5}\pi$		$C_{2,18}$	$-\frac{1}{5}\pi$	$\pi - \omega$	$-\frac{4}{5}\pi$
	$C_{3,f}^+$	$-\frac{4}{5}\pi$	ω	$\frac{1}{5}\pi$		$C_{2,29}$	$\frac{3}{5}\pi$	$\pi - \omega$	$\frac{2}{5}\pi$
	$C_{3,a}^-$	$\frac{4}{5}\pi$	ω	$\frac{3}{5}\pi$		$C_{2,35}$	$-\frac{3}{5}\pi$	$\pi - \omega$	$-\frac{2}{5}\pi$
	$C_{3,e}^-$	$-\frac{4}{5}\pi$	ω	$-\frac{3}{5}\pi$		$C_{2,34}$	π	$\pi - \omega$	0
	$C_{3,d}^+$	$\frac{1}{5}\pi$	$\pi - \omega$	0		$C_{2,25}$	0	π	0
	$C_{3,f}^-$	$-\frac{1}{5}\pi$	$\pi - \omega$	0		$C_{2,13}$	$\frac{1}{5}\pi$	π	π
	$C_{3,g}^-$	$\frac{1}{5}\pi$	$\pi - \omega$	$-\frac{2}{5}\pi$		$C_{2,14}$	$-\frac{1}{5}\pi$	π	π
	$C_{3,i}^+$	$-\frac{1}{5}\pi$	$\pi - \omega$	$\frac{2}{5}\pi$		$C_{2,48}$	$\frac{2}{5}\pi$	π	0
	$C_{3,h}^-$	$\frac{3}{5}\pi$	$\pi - \omega$	$-\frac{2}{5}\pi$		$C_{2,23}$	$-\frac{2}{5}\pi$	π	0
	$C_{3,h}^+$	$-\frac{3}{5}\pi$	$\pi - \omega$	$\frac{2}{5}\pi$					
	$C_{3,i}^-$	$\frac{3}{5}\pi$	$\pi - \omega$	$-\frac{4}{5}\pi$					
	$C_{3,g}^+$	$-\frac{3}{5}\pi$	$\pi - \omega$	$\frac{4}{5}\pi$					
	$C_{3,d}^-$	π	$\pi - \omega$	$\frac{4}{5}\pi$					
	$C_{3,j}^-$	π	$\pi - \omega$	$-\frac{4}{5}\pi$					

From Table 1 we see that, apart from $\beta_r = 0$ and $\beta_r = \pi$, we have two other values, $\beta_r = \omega$ and $\beta_r = \pi - \omega$, where ω is the angle between two nearest five-fold axes. We must now form the transformation tables introduced by Altmann. These are the tables for the expression in curly brackets in (1) for the various subsets of the group defined by a given β_r , and give that part of the general expansion (1) which is independent of l . Tables 2.1 and 2.2 correspond respectively to $\beta_r = \omega$ and $\beta_r = \pi - \omega$. These are simply obtained by forming tables of $\sum e^{im'\gamma_i} \cdot e^{ima_i}$ for each β_r and each \mathcal{C}_s , which are

Table 2.1. Transformation table for $\beta_r = \omega$

Rep.	$m \backslash m'$	5	4	3	2	1	0	-1	-2	-3	-4	-5
A	0	25					25					-25
F_1	0	c					c					$-c$
	1					e					e	
	-4					$-e$					$-e$	
	4		$-e$					e				
	-1		$-e$					e				
F_2	0	$-c$					$-c$					c
	2				$-b$					b		
	-3				$-b$					b		
	3			b					b			
	-2			$-b$					$-b$			
G	1					$-c$					$-c$	
	-4					c					c	
	2				$-c$					c		
	-3				$-c$					c		
	3			c					c			
	-2			$-c$					$-c$			
	4		c					$-c$				
	-1		c					$-c$				
H	0	-5					-5					5
	1					$-a$					$-a$	
	-4					a					a	
	2				d					$-d$		
	-3				d					$-d$		
	3			$-d$					$-d$			
	-2			d					d			
	4		a					$-a$				
	-1		a					$-a$				

Table 2.1 can be extended as follows:

(i) Coefficients for $m < 0$ and $m' > 0$ are modulo -5 and $+5$ respectively. This means that the coefficient for a value of $m < 0$ and (or) $m' > 0$ will not be altered if m is decreased and (or) m' is increased by $5k$ ($k = 0, 1, 2, \dots$).

(ii) Coefficients for $m > 0$ and $m' < 0$ are modulo $+10$ and -10 respectively. In this case the coefficient for a value of $m > 0$ and (or) $m' < 0$ will not be altered if m is increased and (or) m' is decreased by $5k$ when $k = 0, 2, 4, \dots$, and they will change sign when $k = 1, 3, 5, \dots$.

then multiplied by $C_{m'm}\chi^i(\mathcal{G}_s)^*$ and summed over s . Table 2.3 contains the terms in the summation over r in (1) that correspond to $\beta_r = 0$ and $\beta_r = \pi$ which, being very simple, are conveniently combined in one table. From Tables 2.1, 2.2 and 2.3 we see that the only values of m' that appear are given by

$$m' = m \pm 5k \quad (k = 0, 1, 2, \dots). \quad (3)$$

With the aid of Table 2.3 and by combining the results of Tables 2.1 and 2.2 with auxiliary tables of $\mathcal{S}_{m'm}^0(\beta_r)$ for $\beta_r = \omega$ and $\beta_r = \pi - \omega$ we can obtain expression (1) for all possible generators \mathcal{Y}_l^m .

Table 2.2. Transformation table for $\beta_r = \pi - \omega$

Rep.	$m \backslash m'$	5	4	3	2	1	0	-1	-2	-3	-4	-5
A	0	-25					25					25
F_1	0	c					$-c$					$-c$
	1					b					$-b$	
	-4					b					$-b$	
	4		$-b$					$-b$				
	-1		b					b				
F_2	0	$-c$					c					c
	2				$-e$					$-e$		
	-3				e					e		
	3			e					$-e$			
	-2			e					$-e$			
G	1					c					$-c$	
	-4					c					$-c$	
	2				c					c		
	-3				$-c$					$-c$		
	3			$-c$					c			
	-2			$-c$					c			
	4		$-c$					$-c$				
	-1		c					c				
H	0	5					-5					-5
	1					$-d$					d	
	-4					$-d$					d	
	2				a					a		
	-3				$-a$					$-a$		
	3			$-a$					a			
	-2			$-a$					a			
	4		d					d				
	-1		$-d$					$-d$				

Table 2.2 can be extended similarly to Table 2.1. Rule (i) of Table 2.1 applies now to $m > 0$ and $m' < 0$ and rule (ii) to $m < 0$ and $m' > 0$, that is, the roles of m and m' are interchanged.

In tables 2.1 and 2.2,

$$\begin{aligned} a &= 5(1 - 2 \cos \frac{2}{3}\pi) = 5(3 - \sqrt{5})/2, \\ b &= 5(4 \cos^2 \frac{2}{3}\pi + 1) = 5\sqrt{5}(\sqrt{5} - 1)/2, \\ c &= 5(4 \cos \frac{1}{3}\pi - 1) = 5\sqrt{5}, \\ d &= 5(2 \cos \frac{1}{3}\pi + 1) = 5(3 + \sqrt{5})/2, \\ e &= 5(4 \cos^2 \frac{1}{3}\pi + 1) = 5\sqrt{5}(\sqrt{5} + 1)/2. \end{aligned}$$

and

The task of compiling the auxiliary tables of $\mathcal{S}_{m'm}^{(l)}(\beta_r)$ (see (2)) is rather laborious, especially as the values of l become large. We have, therefore, written a programme to compute $\mathcal{S}_{m'm}^{(l)}(\beta_r)$ for a Ferranti Mark 1* Computer. Floating point arithmetic was used throughout and the final results transformed into floating decimal notation and printed. Given values of l , β_r , and p (p being an integer defined below) the programme computes $\mathcal{S}_{m'm}^{(l)}(\beta_r)$ for all values of l from l down to $l = 0$, all values of m and values of $m' = m \pm p \cdot k$ ($k = 0, 1, 2, \dots$). In view of (3) we have used $p = 5$.

The expansions in spherical harmonics are tabulated in Table 3 for the totally symmetric representation A , in 4.1 and 4.2 for the triply degenerate representation

F_1 , in 5·1 and 5·2 for the triply degenerate representation F_2 , in 6·1 and 6·2 for the four-fold degenerate representation G and in 7·1, 7·2 and 7·3 for the five-fold degenerate representation H . In these tables the expansions are given in terms of

$$\mathcal{Y}_l^{m,c} = \frac{1}{2}(\mathcal{Y}_l^m + \mathcal{Y}_l^{-m})$$

(in the tables denoted as ϕ dependence: cos) and

$$\mathcal{Y}_l^{m,s} = \frac{1}{2}i(\mathcal{Y}_l^m - \mathcal{Y}_l^{-m})$$

(in the tables denoted as ϕ dependence: sin). In fact, for $m \neq \pm 5k$ ($k = 0, 1, 2, \dots$) we

Table 2.3. $\beta_r = 0$ and $\beta_r = \pi$

Rep.	$m' \backslash m$	5	4	3	2	1	0	-1	-2	-3	-4	-5
A	0						$5 + (-1)^l \times 5$					
	5	5										$(-1)^l \times 5$
F_1	0						$5 - (-1)^l \times 5$					
	1					5						
	4		5									
	5	5										$(-1)^{l+1} \times 5$
F_2	0						$5 - (-1)^l \times 5$					
	2				5							
	3			5								
	5	5										$(-1)^{l+1} \times 5$
G	1					5						
	2				5							
	3			5								
	4		5									
H	0						$5 + (-1)^l \times 5$					
	1					5						
	2				5							
	3			5								
	4		5									
	5	5										$(-1)^l \times 5$

In Table 2.3 for values of m and $m' \neq 5k$ ($k = 0, 1, 2, \dots$) the only coefficients different from zero are those for $m = m'$, and they are modulo 5. For m and $m' = \pm 5k$ ($k = 0, 1, 2, \dots$) the only coefficients different from zero correspond to $m = m'$ and $m = -m'$. Coefficients for $m > 0$ and $m' > 0$ are modulo +5 and those for $m < 0$ and $m' < 0$ are modulo -5.

Table 3. Spherical harmonics for the totally symmetric representation A

ϕ dep. ...		cos								sin							
$l \backslash m$	p	0		5		10		15		5		10		15			
		p	A	p	A	p	A	p	A	p	A	p	A	p	A		
0	0	1.00															
6	3	3.9600		0	1.00												
10	8	8.96313600		4	-2.73600	0	1.00										
12	10	1.4250297600		4	5.54400	0	1.00										
15										10	3.630614400	3	-6.26400	0	-1.00		

Table 4.1. *Spherical harmonics for the triply degenerate representation F_1*

ϕ dep. ...		cos						sin			
l	m	0		5		10		5		10	
		p	A	p	A	p	A	p	A	p	A
1	0	1.00									
5	3	2.1600		0	1.00						
6								0	1.00		
7	4	1.38600		0	1.00						
9	4	2.18400		0	-1.00						
10											
11	9	8.226489600		3	-2.1600	0	1.00	4	1.36800	0	-1.00
	9	3.11351043600		6	-1.1228400	0	-1.00				
12											
13	10	6.17512896		5	1.478400	0	1.00	4	2.77200	0	1.00
14								5	4.636800	0	-1.00

Table 4.2. *Spherical harmonics for the triply degenerate representation F_1*

ϕ dep. ...		cos											
l	m	1		4		6		9		11		14	
		p	A	p	A	p	A	p	A	p	A	p	A
1	0	1.00											
5	1	7.200		0	-1.00								
6	3	7.9200		1	-2.200	0	1.00						
7	3	7.9200		0	-6.00	0	1.00						
9	6	4.7174400		4	1.51200	1	-7.200	0	-1.00				
10	7	8.96313600		5	1.231200	3	-1.36800	0	-1.00				
11	9	5.276275200		5	-9.676800	4	-1.65600	1	-6.200	0	1.00		
	9	1.98132480		6	3.4423200	4	-3.90600	1	6.300	0	1.00		
12	10	2.8500595200		6	-7.5398400	4	5.54400	1	-6.600	0	1.00		
13	10	2.8500595200		6	-3.9916800	4	5.54400	1	-1.200	0	1.00		
14				10	1.585785600	7	-4.1731200	4	-4.3200	1	-7.200	0	-1.00

Table 5.1. *Spherical harmonics for the triply degenerate representation F_2*

ϕ dep. ...		cos						sin			
l	m	0		5		10		5		10	
		p	A	p	A	p	A	p	A	p	A
3	0	1.00									
5	1	8.400		0	-1.00						
7	3	8.6400		0	-1.00						
8								0	1.00		
9	4	8.31600		0	1.00						
10								4	1.63200	0	1.00
11	9	3.113510400		3	2.1600	0	-1.00	5	2.872800	0	-1.00
12											
13	10	6.17512895		5	-5.084100	0	1.00				
	10	6.2988710400		5	-1.478400	0	1.00				
14								5	1.663200	0	1.00

Table 5.2. Spherical harmonics for the triply degenerate representation F_2

ϕ dep. ...		cos											
l	m	2		3		7		8		12		13	
		p	A	p	A	p	A	p	A	p	A	p	A
3	0	3.00		0	1.00								
5	0	6.00		0	-1.00								
7	3	1.6800		3	1.17600	0	-1.00						
8	5	1.029600		3	-4.6800	0	-3.00	0	-1.00				
9	5	1.612800		4	1.00800	0	6.00	0	1.00				
10	5	6.364800		4	9.79200	0	-78/7	0	-1.00				
11	6	1.3910400		4	-6.04800	0	8.00	0	-1.00				
12	9	2.344204800		8	-4.688409600	4	-1.34400	3	2.85600	0	-1.00		
13	11	1.45829376		10	3.61005119	5	-4.53600	4	8.0800	0	-46/3	0	1.00
	10	3.86394624		10	-1.47365567	5	-5.083200	4	-6.81600	1	1.00	0	1.00
14	11	7.7358758400		10	-1.137628800	5	5.54400	4	-3.600	0	-6.00	0	-1.00

Table 6.1. Spherical harmonics for the four-fold degenerate representation G

ϕ dep. ...		cos											
l	m	1		4		6		9		11		14	
		p	A	p	A	p	A	p	A	p	A	p	A
3	0	1.00											
4	1	4.200		0	1.00								
6	3	2.8800		1	1.200	0	-1.00						
7	4	2.80800		2	1.5600	0	-1.00						
8	4	1.84800		1	-2.800	0	-1.00						
9	7	5.41094400		4	-2.68800	2	5.2800	0	-1.00				
	6	1.05705600		3	9.3800	2	3.4700	0	1.00				
10	7	2.83046400		3	2.8800	2	1.6800	0	1.00				
11	8	8.01964800		6	-2.0563200	4	-1.94400	1	1.200	0	-1.00		
12	10	1.0817452800		6	1.6934400	3	9.3600	1	3.600	0	-1.00		
	9	7.82369282		7	3.23114400	5	1.083600	2	-1.1400	0	-1.00		
13	11	4.12580043		8	1.59727680	5	-6.014400	2	7.1200	0	-1.00		
	10	4.78887552		7	1.46923200	5	-4.185600	0	-734/7	0	1.00		
14	13	2.011327718400		9	7.58419200	7	-6.4310400	4	-2.8200	1	4.200	0	1.00
	13	4.08181213		9	2.56524141	7	-7.05066352	4	-3.99352941	2	-2.09470588	0	1.00

Table 6.2. Spherical harmonics for the four-fold degenerate representation G

ϕ dep. ...		cos											
l	m	2		3		7		8		12		13	
		p	A	p	A	p	A	p	A	p	A	p	A
3	0	2.00		0	-1.00								
4	1	1.400		0	-1.00								
6	0	3.00		0	-1.00								
7	3	4.6800		2	-6.2400	0	-1.00						
8	4	5.54400		4	1.00800	0	-2.00	0	1.00				
9	5	4.132800		4	4.60800	1	-1.900	0	1.00				
	5	3.6495529		4	1.2155294	0	-3.0588235	0	-1.00				
10	6	1.5724800		4	-1.00800	1	2.100	0	-1.00				
11	5	2.570400		5	1.285200	0	-9/2	0	-1.00				
12	9	2.944771200		8	9.091958400	4	3.65400	3	-2.01600	0	1.00		
	8	5.40970339		8	5.2293799	4	-2.7193846	2	-4.7630769	0	-1.00		
13	12	1.06828762		10	-5.06515680	6	1.544400	0	-1511400/7	0	-873/14	0	1.00
	11	1.10512512		9	-9.2093760	5	-5.74200	0	310200/7	0	1.00	0	-27/14
14	12	1.54717516		10	-8.342611200	6	-8.038800	5	1.69200	1	1.400	0	-1.00
	11	6.69813640		10	3.30189823	5	-9.53297561	5	1.06068293	0	-2.41463415	0	1.00

Table 7.1. *Spherical harmonics for the five-fold degenerate representation H*

ϕ dep. ...		cos						sin			
l	m	0		5		10		5		10	
		p	A	p	A	p	A	p	A	p	A
2	0	1.00									
4	0	1.00									
5								0	1.00		
6	3	5.0400		0	-1.00			0	1.00		
7								0	1.00		
8	0	1.00									
9				0	1.00						
10	9	5.907686400		4	2.73600	0	-1.00	0	1.00		
	8	8.96313600		0	149040/11	0	1.00				
11								0	1.00		
12	10	2.7329702400		4	-5.54400	0	-1.00			0	1.00
	10	1.42502976		5	-2.47444615	0	1.00				
13								0	1.00		
14	0	1.00								0	1.00
				0	1.00						
						0	1.00				

Table 7.2. *Spherical harmonics for the five-fold degenerate representation H*

ϕ dep. ...		cos											
l	m	1		4		6		9		11		14	
		p	A	p	A	p	A	p	A	p	A	p	A
2	0	1.00											
4	1	4.800		0	-1.00								
5	2	1.6800		0	1.00								
6	2	7.200		1	1.800	0	1.00						
7	4	1.18800		1	-2.400	0	-1.00						
8	4	4.45200		1	2.800	0	1.00						
	4	1.84800		2	1.2200	0	-1.00						
9	6	5.7657600		3	1.6800	2	-1.6800	0	1.00				
10	7	3.88281600		4	-2.80800	1	7.200	0	-1.00				
	8	1.839801600		5	-3.160800	3	-2.32800	0	-1.00				
11	10	1.7077132800		6	3.3868800	4	4.53600	2	1.0200	0	-1.00		
	10	1.1227507200		6	-1.3708800	4	3.86400	1	9.800	0	1.00		
12	9	7.74385919		6	5.3049600	4	-3.81600	0	258/7	0	1.00		
	11	3.27078259		8	1.08984960	6	-3.3981600	3	-1.10600	0	1.00		
13	10	5.97155326		7	-7.82611200	5	-1.646400	2	1.5200	0	-1.00		
	10	2.57862527		7	5.63068800	5	1.923600	2	-2.4800	0	-1.00		
14	14	1.91422914		11	1.02255830	7	-9.32156689	5	3.42786207	3	-1.39200	0	-1.00
	13	7.81368004		10	-2.24323222	7	2.96630603	4	-4.64890595	2	9.91877159	0	-1.00
	13	1.18884398		9	-1.82114581	7	-7.50823269	3	4.35981491	2	1.30543883	0	-1.00

only tabulate the expansions in terms of $\mathcal{Y}_l^{m,c}$ because in these cases for each expansion in the spherical harmonics $\mathcal{Y}_l^{m,c}$ there corresponds another expansion in the $\mathcal{Y}_l^{m,s}$ with the same coefficients but with different signs for alternate elementary spherical harmonics. It is therefore unnecessary to duplicate the tables so as to include the

expansions in the $\mathcal{Y}_l^{m,s}$. For $m = \pm 5k$ ($k = 0, 1, 2, \dots$) the only expansions that appear are those listed. In tables 3–7·3 the coefficients are given as $A \times 10^p$. In many cases we have been able to determine the coefficients exactly; to indicate this we either terminate the mantissas A with two zeros or express them as fractional numbers. Otherwise 8 significant figures can be assured.

 Table 7·3. Spherical harmonics for the five-fold degenerate representation H

ϕ dep. ...		cos											
l	m	2		3		7		8		12		13	
		p	A	p	A	p	A	p	A	p	A	p	A
2	0	1·00											
4	0	1·00		0	1·00								
5	0	4·00		0	1·00								
6	1	1·200		0	1·00								
7	3	7·9200		2	2·6400	0	1·00						
8	5	1·202400		3	−6·1200	1	1·300	0	1·00				
	5	8·517600		0	229320/11	0	1207/11	0	−1·00				
9	5	2·620800		4	−6·55200	0	−4·00	0	1·00				
10	5	5·443200		4	−4·03200	0	−6·00	0	1·00				
	5	5·896800		5	−1·329300	0	−51/4	0	−1·00				
11	5	4·233600		5	1·180800	1	1·200	0	1·00				
	6	4·1126400		5	−5·140800	1	−8·700	0	−1·00				
12	10	4·4656012800		9	2·1148646400	5	1·713600	3	9·57600	0	−1·00		
	9	1·110412800		8	2·097446400	4	3·63600	2	5·7600	0	−1·00		
13	11	5·1572505600		9	5·86051200	6	1·058400	4	5·2800	1	1·800	0	1·00
	10	2·344204800		9	5·86051200	5	1·00800	4	3·00	0	8/11	0	1·00
14	12	2·32076273		11	−2·76823008	7	1·0072800	5	8·56800	1	8·600	0	1·00
	11	2·16863465		10	2·62273419	5	−8·28120502	5	−1·98346444	−1	2·25941423	0	1·00
	12	4·98370810		11	1·48016705	6	9·03412016	4	−2·45566541	2	1·7889227	0	−1·00

In Tables 3–7·3 the coefficients are given as $A \times 10^p$. Values of A that have been exactly determined are either terminated with two zeros or expressed as fractional numbers.

As an example of the use of the tables we list the expansions for the F_2 representation and $l = 13$, which form two sets of triply degenerate functions:

$$6·17512895 \times 10^{10} \mathcal{Y}_{13}^0 - 5·084100 \times 10^5 \mathcal{Y}_{13}^{5,c} + \mathcal{Y}_{13}^{10,c};$$

$$6·2988710400 \times 10^{10} \mathcal{Y}_{13}^0 - 1·478400 \times 10^5 \mathcal{Y}_{13}^{5,c} + \mathcal{Y}_{13}^{10,c};$$

$$1·45829376 \times 10^{11} \mathcal{Y}_{13}^{2,c} + 3·61005119 \times 10^{10} \mathcal{Y}_{13}^{3,c} - 4·53600 \times 10^5 \mathcal{Y}_{13}^{7,c} \\ + 8·0800 \times 10^4 \mathcal{Y}_{13}^{8,c} - \frac{4}{3} \mathcal{Y}_{13}^{12,c} + \mathcal{Y}_{13}^{13,c};$$

$$1·45829376 \times 10^{11} \mathcal{Y}_{13}^{2,s} - 3·61005119 \times 10^{10} \mathcal{Y}_{13}^{3,s} - 4·53600 \times 10^5 \mathcal{Y}_{13}^{7,s} \\ - 8·0800 \times 10^4 \mathcal{Y}_{13}^{8,s} - \frac{4}{3} \mathcal{Y}_{13}^{12,s} - \mathcal{Y}_{13}^{13,s};$$

$$3·86394624 \times 10^{10} \mathcal{Y}_{13}^{2,c} - 1·47365567 \times 10^{10} \mathcal{Y}_{13}^{3,c} - 5·083200 \times 10^5 \mathcal{Y}_{13}^{7,c} \\ - 6·81600 \times 10^4 \mathcal{Y}_{13}^{8,c} + 10 \mathcal{Y}_{13}^{12,c} + \mathcal{Y}_{13}^{13,c};$$

$$3·86394624 \times 10^{10} \mathcal{Y}_{13}^{2,s} + 1·47365567 \times 10^{10} \mathcal{Y}_{13}^{3,s} - 5·083200 \times 10^5 \mathcal{Y}_{13}^{7,s} \\ + 6·81600 \times 10^4 \mathcal{Y}_{13}^{8,s} + 10 \mathcal{Y}_{13}^{12,s} - \mathcal{Y}_{13}^{13,s}.$$

We have also obtained the partition table (Table 8) up to $l = 15$, which is very useful for checking purposes. Each of the expansions given in Tables 3–7·3 has been checked either by using more than one generator to obtain it, or, as in many cases for the

degenerate representations, by obtaining more expansions than the number of independent ones (which is known from the partition table) and proving that the extra ones are linear combinations of those chosen as independent.

Table 8. *Partition table for the spherical harmonics of the icosahedral group*

l	A	F_1	F_2	G	H
0	1				
1		1			
2					1
3			1	1	
4				1	1
5		1	1		1
6	1	1		1	1
7		1	1	1	1
8			1	1	2
9		1	1	2	1
10	1	1	1	1	2
11		2	1	1	2
12	1	1	1	2	2
13		1	2	2	2
14		1	1	2	3
15	1	2	2	2	2

I would like to thank Dr S. L. Altmann for suggesting the problem and providing me with the manuscript of his paper. I am also very grateful to him for his valuable comments and advice and for introducing me to the techniques of electronic computing. I would also like to thank Dr A. Klug for correspondence and Prof. C. A. Coulson, Dr S. L. Altmann and Mr V. W. Maslen for comments on the manuscript.

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