Acta Cryst. (1996). A**52**, 171–175

A Recursive Algorithm for the Generation of Symmetry-Adapted Functions: Principles and Applications to the Icosahedral Group

W. PRANDL, P. SCHIEBEL AND K. WULF

Institut für Kristallographie, Universität Tübingen, Charlottenstrasse 33, D-72070 Tübingen, Germany

(*Received 10 February 1995; accepted 8 September 1995*)

Abstract

Symmetry-adapted functions (SAF's) of order L can be generated recursively from powers of a seed function or from products of SAF's having lower order l. The algorithm uses a symmetry-adapted version of the decomposition of products of spherical harmonic functions *via* Wigner 3-j symbols. The totally symmetric SAF's are calculated for the point group $2/m\bar{3}5$ up to $L = 30$. For $L = 30$, the icosahedral group has two independent SAF's; a simple method is suggested for making a unique choice for these two SAF's.

1. Introduction

The pentagonal symmetry so well established in nature has entered officially into crystallography only recently (Hahn, 1983), and this reserve of our community was justified by the well known fact that fivefold axes just do not comply with a lattice in three dimensions. With the appearance of quasicrystals, this restriction to three-dimensional lattices was dropped and the very existence of the fullerene C_{60} as well as of the long-known metallocene compounds provide strong arguments to accept fivefold symmetry at least locally in a crystal.

The analysis of the orientationally disordered structure of molecules in terms of the molecular orientation probability density $f(\omega)$ [$\omega = (\alpha, \beta, \gamma)$, Euler angles (Press & Hüller, 1973; Prandl, 1981)] requires symmetry-adapted spherical harmonic functions (SAF's), in some cases of high order L. The coefficients that enter into the SAF's are also needed to formulate the symmetry-adapted Wigner functions used in the orientational hindrance potential $V(\omega)$ (James & Keenan, 1959; Vogt & Prandl, 1983; Gerlach, Vogt & Prandl, 1984). SAF's for the icosahedral group have been used so far in the data treatment of the fullerene C_{60} (Michel, Copley & Neumann, 1992; Michel, 1992) and of icosahedral quasicrystals (Elcoro, Perez-Mato & Madariaga, 1994).

So far, only low-order icosahedral SAF's are available in the literature: $L_{MAX} = 6$, 10, 12, 16, respectively, in the monograph by Butler (1981) and in the papers by Laporte (1948), Cohan (1958) and Elcoro, Perez-Mato & Madariaga (1994). Michel (1992) derived SAF's for $L = 6$, 10 in a coordinate system that differs from the other authors' and our choice (see Appendix *A* for comments).

In calculating new SAF's, we avoid the standard algorithm that decomposes reducible representations into irreducible ones by the help of projection operators, since this technique needs matrices of progressively increasing dimensions $(2L + 1)$. The much shorter algorithm we use here starts from a lowest-order seed function determined by the standard method and decomposes powers of this seed function into higher-order SAF's.

The paper is organized in the following way: in §2, we introduce the notation and determine the number $n_\varepsilon(L)$ of SAF's. In §3, we sketch briefly the standard non-recursive procedure. In §4, we describe the new recursive technique and derive the SAF's for $L \leq 30$. §5 contains a short summary. The choice of the coordinate system and a motivation for it are given in Appendix *A*.

2. Preliminaries and notation

Let $Y_{LM}(\theta, \varphi) \equiv Y_{LM}(\mathbf{x})$ be a spherical harmonic function, P a point group, γ one of its irreducible representations and $n_\gamma(L)$ the multiplicity with which the irreducible representation γ occurs among the $Y_{LM}(\mathbf{x})$ for fixed L. An index ε will always refer to a unit irreducible representation. For the $Y_{LM}(\mathbf{x})$, we will use the definition given by *e.g.* Edmonds (1968), Butler (1981) and many other authors, which in particular implies the Condon & Shortley (1935) convention

$$Y^*_{LM}(\mathbf{x}) = (-1)^M Y_{L-M}(\mathbf{x}). \tag{1}$$

We point out here that Altmann (1957), Cohan (1958) and Bradley & Cracknell (1972) do not use the factor $(-1)^M$ given in (1): this has to be taken into account in comparing their tables with those of other authors.

A symmetry-adapted spherical harmonic function (SAF) belonging to the irreducible representation γ will be written as

$$P_{L\gamma\mu i}(\mathbf{x}) = \sum_M Y_{LM}(\mathbf{x}) P^L_{M\gamma\mu i}. \tag{2}$$

Here, the index μ counts the 'partners' belonging to γ, and so it runs from 1 to d_γ, the dimension of γ. The characteristic property of the set of d_γ partners is that any one of them is transformed into a linear combination of all of the others by an element $p \in P$. The index i

$= 1, \ldots, n_\gamma(L)$ refers to one of the possibilities that the irreducible representation γ occurs among the $Y_{LM}(\mathbf{x})$. Functions having different i are not transformed into one another by the elements of P.

In the present paper, we are interested only in totally symmetric SAF's of the type ε. Since the unit representation is always one dimensional, the index μ can only be 1, and therefore we will drop it from now on in this paper. We would like to remind the reader, however, that the shortened symbol $P_{L\varepsilon i}(\mathbf{x})$,

$$P_{L\varepsilon i}(\mathbf{x}) = \sum_M Y_{LM}(\mathbf{x}) P^L_{M\varepsilon i}, \tag{3}$$

applies only to one-dimensional representations. The unit representation SAF's can always be chosen as real functions with real coefficients $P^L_{M\varepsilon i}$. This property, together with the Condon & Shortley convention, gives a symmetry relation for the coefficients

$$P^L_{M\varepsilon i} = (-1)^M P^L_{-M\varepsilon i}. \tag{4}$$

The multiplicities $n_\gamma(L)$ given in (5) can be derived from group character tables [*e.g.* Butler (1981) for $P = 2/m\bar{3}\bar{5}$] providing the characters $\chi_\gamma(p)$ and the characters $\chi_L(p)$ are the traces of the matrices $\mathcal{D}^L(p)$ representing an element $p \in P$:

$$n_\gamma(L) = (1/|P|) \sum_{p \in P} \chi_\gamma(p) \chi_L(p). \tag{5}$$

Here, $|P|$ is the order of the group P in question ($|P| = 120$ for $2/m\bar{3}\bar{5}$) and

$$\chi^{\mathrm{PR}}_L(p) = \sin(L + \tfrac{1}{2})\varphi_p / \sin(\varphi_p/2) \tag{6}$$

for proper rotations with the rotation angle φ_p and

$$\chi^{\mathrm{IMPR}}_L(p) = (-1)^L \chi^{\mathrm{PR}}_L(p) \tag{7}$$

if p is an improper rotation expressed as a rotation-inversion axis.

The icosahedral group contains (Ljubarski, 1962) as proper axes the unit operation together with 12 rotations by 72°, 12 by 144°, 20 third-order rotations and 15 by 180°. Another 60 elements are the combinations of the proper axes with the inversion centre.

For the unit representation ε all $\chi_\varepsilon(p)$ are $+1$. From (4) to (6), we obtain multiplicities $n_\varepsilon(L) = 1$ for $L = 0, 6, 10, 12, 16, 18, 20, 22, 24, 26, 28$ and $n_\varepsilon(L) = 2$ for $l = 30$. Since the inversion centre is an element of $2/m\bar{3}\bar{5}$, only even-parity totally symmetric SAF's occur. It is easy to show from (4)–(6) that for orders $L \geq 30$ the $n_\varepsilon(L)$ are given by

$$n_\varepsilon(L + 30m) = n_\varepsilon(L) + m. \tag{8}$$

This means in particular that two unit representations occur for $L = 30, 36, 40, 42, \ldots$. We shall point out a unique way to calculate the corresponding degenerate SAF's.

3. The standard procedure

The standard procedure for generating basis functions belonging to an irreducible representation γ (Altmann, 1957; Cohan, 1958; Bradley & Cracknell, 1972; textbooks of group-representation theory) uses projection operators $\mathcal{P}$, which in the special case of the unit representation are given by

$$\mathcal{P}^L_\varepsilon = (1/|P|) \sum_{p \in P} \mathcal{D}^L_{MM'}(\alpha, \beta, \gamma)_p. \tag{9}$$

The matrices $\mathcal{D}^L$ have the dimension $(2L+1)$ and their elements are the Wigner rotation functions $\mathcal{D}^L_{MM'}(\alpha, \beta, \gamma)_p$, where $(\alpha, \beta, \gamma)_p$ are the Euler angles corresponding to the proper or improper rotation p: these angles, for $2/m\bar{3}\bar{5}$, are listed in the paper by Cohan (1958). So one projection operator consists of 120 matrices $\mathcal{D}^L$ having $(2L+1)^2$ elements each.

We close this short section with two remarks:

(1) The projection-operator technique must be used to obtain at least one non-trivial $P_{L\varepsilon i}(\mathbf{x})$, which can then be used in the recursive algorithm (§4) as a seed. We will use the SAF $P_{6\varepsilon 1}(\mathbf{x})$ as given by Butler (1981), which of course coincides with the corresponding function derived by Cohan (1958) once the Condon & Shortley (1935) convention is applied to the latter function.

(2) The projection-operator technique is non-recursive: SAF's already known for lower l's are not used to calculate higher-L SAF's.

4. Recursive generation of basis functions

The recursive calculation of SAF's, which we apply for the extension of the tables given by, for example, Butler (1981) and Cohan (1958), uses an elementary theorem of group-representation theory, namely that a product of unit-representation basis functions, *i.e.* SAF's, contains only unit-representation basis functions, specifically:

$$P_{L_1\varepsilon i_1}(\mathbf{x}) P_{L_2\varepsilon i_2}(\mathbf{x}) = \sum_{\substack{L = |l_1 - l_2| \\ i = 1, \ldots, n_\varepsilon(L)}}^{|l_1 + l_2|} c_{i_1 i_2 i}(l_1 l_2; L) P_{L\varepsilon i}(\mathbf{x}). \tag{10}$$

In order to perform the multiplication of the l.h.s.of (10), we use the basic definition (3) and the multiplication theorem for spherical harmonic functions (Edmonds, 1968; Lindner, 1984):

$$\begin{aligned} Y_{l_1 m_1}(\mathbf{x}) Y_{l_1 m_2}(\mathbf{x}) &= \sum_{LM} \{[l_1][l_2][L]/4\pi\}^{1/2} \begin{pmatrix} l_1 & l_2 & L \\ 0 & 0 & 0 \end{pmatrix} \\ &\quad \times \begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & -M \end{pmatrix} (-1)^M Y_{LM}(\mathbf{x}) \end{aligned} \tag{11}$$

with the shorthand notation

$$[l] = 2l + 1. \tag{12}$$

The symbols $\begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & M \end{pmatrix}$ in (11) are Wigner coupling coefficients or 3-j symbols, which are non-zero only if the triangular rule $|l_1 - l_2| \leq L \leq |l_1 + l_2|$ is obeyed and if $m_1 + m_2 + M = 0$. From a combination of (10) and (11), we obtain an explicit expression for the recursion from the orders l_1, l_2 to the order L:

$$P^L_{M\varepsilon i} = \gamma_{i_1 i_2 i}(l_1 l_2; L) \sum_m (-1)^M \begin{pmatrix} l_1 & l_2 & L \\ -m & m-M & M \end{pmatrix} \times P^{l_1}_{M\varepsilon i_1} P^{l_2}_{M-m\varepsilon i_2}. \tag{13}$$

The common factor $\gamma_{i_1 i_2 i}(l_1 l_2; L)$ is obtained by normalizing the resulting functions $P_{L\varepsilon i}(\mathbf{x})$. Equation (13) may be used in an obvious way to calculate SAF's with the orders $L = 6$, 10, 12 from one seed function having (see Table 1) $l_1 = l_2 = 6$: the $L = 6$ result serves in this case as a test since it has to reproduce the seed function used.

The 3-j symbol in (13) becomes algebraically particularly simple if the l_1, l_2, L form a stretched triangle: $L = l_1 + l_2$.

In this case, the $P^{l_1+l_2}_{m\varepsilon i}$ become

$$P^{l_1+l_2}_{m\varepsilon i} = \gamma_{i_1 i_2 i}(l_1 l_2; l_1 + l_2) \sum_m (2l_1)!(2l_2)!(l_1 + l_2 + M)! \times (l_1 + l_2 - M)!\{[2(l_1 + l_2) + 1]!(l_1 + m)! \times (l_1 - m)!(l_2 + m - M)!(l_2 - m + M)!\}^{-1} \times P^{l_1}_{m\varepsilon i_1} P^{l_2}_{M-m\varepsilon i_2}. \tag{14}$$

Starting from the lowest-order non-trivial seed function with $l_1 = 6$, one cannot reach $L = 10$ by using (14), so we apply (13) for this purpose. SAF's for all the other L's given in Table 1 can be generated successively from $l_1 = 6$ and $l_2 = 10$, often in several ways, *e.g.* $16 = 6 + 10$; $18 = 6 + 12$; $26 = 6 + 20 = 10 + 16$; $28 = 6 + 22 = 10 + 18 = 12 + 16$. These multiple possibilities have been used to check the numerical procedures.

As mentioned earlier, the subspace of totally symmetric SAF's becomes two dimensional for $L = 30$, 36, 40, ... and the projection-operator technique does not help in this case to generate a second basis vector once a first vector is known. The recursion formalism (13), (14) gives a unique answer. The recipe is:

(i) for a given L create a normalized $P_{L\varepsilon i}(\mathbf{x})$ having the smallest M_{MAX} possible;

(ii) create a second $\hat{P}_{L\varepsilon 2}(\mathbf{x}) \neq P_{L\varepsilon 1}(\mathbf{x})$. $\hat{P}_{L\varepsilon 2}(\mathbf{x})$ will contain spherical harmonic functions $Y_{LM}(\mathbf{x})$ with $|M| \geq M_{\mathrm{MAX}}$;

(iii) using Schmidt's procedure, calculate from $\hat{P}_{L\varepsilon 2}(\mathbf{x})$ a normalized $P_{L\varepsilon 2}(\mathbf{x})$ that is orthogonal to $P_{L\varepsilon 1}(\mathbf{x})$.

Let us demonstrate the basic idea for the order $L = 30$. The three possible partitions of 30, namely $6 + 24$, $12 + 18$, $10 + 20$, require factor functions, which can be separated into two sets $\{(6, 24), (12, 18)\}$ and $\{(10, 20)\}$. In the first set, the largest values of the indices m obtained in the factor functions is 5 for $l_1 = 6$ and 20 for $l_2 = 24$ or 10 for $l_1 = 12$ and 15 for $l_2 = 18$. If these values are entered into the 3-j symbols of (13) and (14), it becomes immediately obvious that, for the resulting $P_{30\varepsilon 1}(\mathbf{x})$, all $Y_{30M}(\mathbf{x})$ contributing will have $|M| \leq 25$. So, $(l_1, l_2) = (6, 24)$ or (12, 18) lead to one unique SAF $P_{30\varepsilon 1}(\mathbf{x})$. If, on the other hand, we use $(l_1, l_2) = (10, 20)$, then the resulting function $\hat{P}_{L\varepsilon 2}(\mathbf{x})$ will contain $Y_{30M}(\mathbf{x})$ up to $|M| \leq 30$.

In order to avoid numerical inaccuracies in the applications by truncation effects, we have calculated the coefficients $P^L_{M\varepsilon i}(\mathbf{x})$ by an integer algorithm using (14) on a PC. It is obvious from (14) that the number of terms to be determined is in any case very small, since all allowed m or M are $m = 0 \bmod 5$.

The results of an application of (13), (14) to the seed function $P_{6\varepsilon 1}(\mathbf{x})$ are given in Table 1. As examples of high-order functions, we show $P_{30\varepsilon 1}(\mathbf{x})$ and $P_{30\varepsilon 2}(\mathbf{x})$: Figs. 1(*a*), (*b*) give a level diagram in a stereographic projection.*

5. Conclusions

We present a recursive algorithm for the extension of tables containing symmetry-adapted functions and use it to derive SAF's of the icosahedral group $2/m\bar{3}\bar{5}$ up to $L = 30$. The algorithm is algebraically particularly simple if the orders l_1, l_2 of the factor functions and the order of the target function are related by $L = l_1 + l_2$ [(14)].

The method given can be generalized for general target representations $\gamma \neq \varepsilon$, for instance by applying the theorem that states that products of arbitrary representations with a unit representation $\gamma \otimes \varepsilon$ contain only functions of the representation γ. Again, one needs only a minimum set of seed functions to reach high-order $P_{l\gamma\mu i}(\mathbf{x})$.

Crystallographic applications of the high-order totally symmetric SAF's include the determination of the orientation probability function $f(\alpha, \beta, \gamma)$ and/or the orientational potential $V(\alpha, \beta, \gamma)$ in orientationally disordered molecular crystals, in particular C_{60} (Schiebel *et al.*, 1996). Further applications may be envisaged in the analysis of scattering data by quasicrystals or by icosahedral biological molecules or assemblies like icosahedral viruses.

* A complete set of contour plots of SAF's with $6 \leq L \leq 30$ has been deposited with the IUCr (Reference: SH0065). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *The coefficients of the symmetry-adapted functions of the icosahedral group in a prime-number representation*

M\L	6	10	12	16	18	20
0	$\sqrt{11}$	$\sqrt{13\cdot19}$	$3\cdot\sqrt{7\cdot17}$	$2^3\cdot\sqrt{5\cdot19\cdot31}$	$\sqrt{5\cdot11\cdot17\cdot23}$	$\sqrt{5\cdot7\cdot23\cdot29}$
±5	$\mp\sqrt{7}$	$\pm\sqrt{3\cdot11\cdot19}$	$\mp\sqrt{2\cdot11\cdot13}$	$\pm\sqrt{3\cdot5\cdot13\cdot17\cdot31}$	$\mp2\cdot3\cdot\sqrt{2\cdot5\cdot19}$	$\pm\sqrt{2\cdot11\cdot17\cdot19\cdot29}$
±10		$\sqrt{11\cdot17}$	$\sqrt{3\cdot13\cdot19}$	$-\sqrt{2\cdot7\cdot17\cdot23\cdot31}$	$\sqrt{3\cdot7\cdot11\cdot19}$	$41\cdot\sqrt{17\cdot19}$
±15				$\mp3\cdot\sqrt{17\cdot23\cdot29}$	$\mp\sqrt{19\cdot29\cdot31}$	$\pm2\cdot\sqrt{2\cdot11\cdot19\cdot31}$
±20						$\sqrt{11\cdot13\cdot31\cdot37}$
Norm	$\frac{1}{5}$	$\frac{1}{5^2\cdot\sqrt{3}}$	$\frac{1}{5^2\cdot\sqrt{5}}$	$\frac{1}{2\cdot5^3\cdot\sqrt{3\cdot5}}$	$\frac{1}{5^3\cdot\sqrt{5}}$	$\frac{1}{5^4\cdot\sqrt{5}}$

M\L	22	24	26	28
0	$2\cdot\sqrt{3\cdot5\cdot11\cdot19\cdot31\cdot37}$	$7\cdot\sqrt{5\cdot13\cdot23\cdot29}$	$2\cdot3\cdot\sqrt{3\cdot13\cdot29\cdot31\cdot41}$	$2^4\cdot3\cdot\sqrt{7\cdot31\cdot37\cdot43}$
±5	$\pm\sqrt{7\cdot13\cdot23\cdot31\cdot37}$	$\mp2\cdot59\cdot\sqrt{2\cdot3\cdot11}$	$\pm23\cdot\sqrt{5\cdot7\cdot11\cdot23\cdot41}$	$\pm\sqrt{5\cdot11\cdot13\cdot29\cdot37\cdot43}$
±10	$-\sqrt{2\cdot7\cdot17\cdot23\cdot29\cdot37}$	$19\cdot\sqrt{2\cdot19\cdot31}$	$2^3\cdot\sqrt{2\cdot5\cdot7\cdot19\cdot23\cdot41}$	$-\sqrt{2\cdot3\cdot5\cdot13\cdot17\cdot23\cdot29\cdot43}$
±15	$\pm103\cdot\sqrt{23\cdot29}$	$\mp2\cdot3\cdot\sqrt{11\cdot31\cdot37}$	$\mp139\cdot\sqrt{3\cdot5\cdot23\cdot37}$	$\pm29\cdot\sqrt{2\cdot5\cdot23\cdot29\cdot41}$
±20	$\sqrt{13\cdot19\cdot23\cdot29\cdot41}$	$\sqrt{31\cdot37\cdot41\cdot43}$	$-89\cdot\sqrt{5\cdot37\cdot43}$	$-2^2\cdot3\cdot\sqrt{2\cdot5\cdot13\cdot29\cdot41\cdot47}$
±25			$\mp7\cdot\sqrt{2\cdot17\cdot37\cdot43\cdot47}$	$\mp\sqrt{7\cdot17\cdot29\cdot41\cdot47\cdot53}$
Norm	$\frac{1}{5^5\cdot\sqrt{2\cdot3}}$	$\frac{1}{5^5}$	$\frac{1}{5^6\cdot\sqrt{2\cdot3}}$	$\frac{1}{2\cdot5^6\cdot\sqrt{3}}$

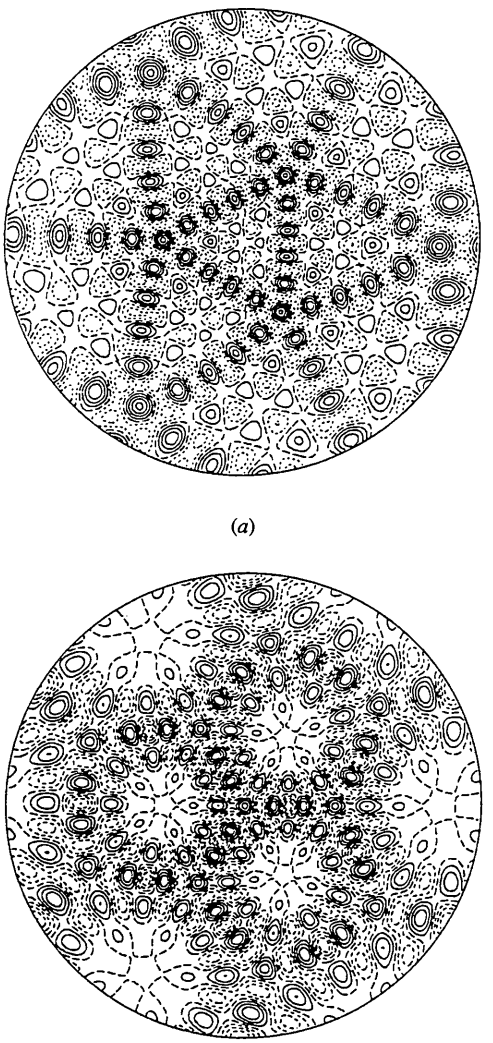
M\L	30 – 1	30 – 2
0	$3\cdot12251\cdot\sqrt{11\cdot13\cdot23\cdot29}$	$2^3\cdot\sqrt{17\cdot19\cdot31\cdot37\cdot41\cdot43\cdot47\cdot53\cdot59}$
±5	$\mp2\cdot5\cdot4639\cdot\sqrt{3\cdot17\cdot23\cdot31}$	$\pm2\cdot3\cdot\sqrt{3\cdot11\cdot13\cdot19\cdot29\cdot37\cdot41\cdot43\cdot47\cdot53\cdot59}$
±10	$2^3\cdot17\cdot\sqrt{5\cdot7\cdot11\cdot13\cdot17\cdot19\cdot31\cdot37}$	$3^2\cdot41\cdot\sqrt{5\cdot7\cdot23\cdot29\cdot41\cdot43\cdot47\cdot53\cdot59}$
±15	$\mp241\cdot\sqrt{3\cdot5\cdot13\cdot31\cdot37\cdot41\cdot43}$	$\pm2^4\cdot31\cdot\sqrt{3\cdot5\cdot11\cdot17\cdot19\cdot23\cdot29\cdot47\cdot53\cdot59}$
±20	$2\cdot5\cdot\sqrt{2\cdot7\cdot11\cdot23\cdot31\cdot37\cdot41\cdot43\cdot47}$	$3\cdot2161\cdot\sqrt{2\cdot7\cdot13\cdot17\cdot19\cdot29\cdot53\cdot59}$
±25	$\mp\sqrt{2\cdot3\cdot13\cdot17\cdot23\cdot31\cdot37\cdot41\cdot43\cdot47\cdot53}$	$\pm2\cdot101\cdot151\cdot\sqrt{2\cdot3\cdot11\cdot19\cdot29\cdot59}$
±30		$71\cdot233\cdot4793\cdot\sqrt{7\cdot11}$
Norm	$\frac{1}{5^5\cdot\sqrt{71\cdot233\cdot4793}}$	$\frac{1}{2\cdot5^7\cdot\sqrt{3\cdot71\cdot233\cdot4793}}$

We acknowledge the support of this investigation by the DFG (project PR-44/7-1) and by the BMFT (project 03-PR3TUE-0).

APPENDIX *A*
The choice of the coordinate system

The icosahedral groups contain two-, three- and five-fold axes. Since the $P_{L\varepsilon i}(\mathbf{x})$ are composed of spherical harmonic functions $Y_{LM}(\mathbf{x})$, all the M in (2) or (3) must be multiples of two, three or five if the 2, 3 or 5 axis is chosen as the z axis. Clearly, selecting $\mathbf{z}\|5$ introduces the smallest number of terms in the $P_{L\varepsilon i}(\mathbf{x})$, namely $2[L/5]+1$, where $[L/5]$ means the smallest integer less than or equal to $L/5$. A further simplification arises if we choose the xz plane as a mirror plane, since then all φ-dependent terms in (2) and (3) are $\sim\cos(5\mu\varphi)$ with $\mu = 0, 1, \ldots, [L/5]$. In this case, $\mathbf{y}$ is parallel to one of the twofold axes in $2/m\bar{3}\bar{5}$. This choice of the coordinate system is distinguished among

all others by its mathematical economy, *i.e.* by the minimum of non-zero coefficients in the SAF's: it was therefore recommended by Cohan (1958) and applied also by Butler (1981), who gives the $P_{6\varepsilon 1}(\mathbf{x})$, which we use as a seed function, and by Elcoro, Perez-Mato & Madariaga (1994). Michel, Copley & Neumann (1992) and Michel (1992) use a coordinate system with **x**, **y** and **z** parallel to three of the twofold axes in $2/m\bar{3}5$, and they derive SAF's for $L = 6$, 10 by an algorithm that is tightly connected to the geometry of the C_{60} molecule. With this choice, the number of independent coefficients in the SAF's increases appreciably, in particular for larger L, *e.g.* for $P_{30\varepsilon 2}(\mathbf{x})$ to 16 as compared to 7 for Cohan's choice. In all practical applications, whether with quasicrystals or with fullerenes, one uses series expansions of the relevant quantities in terms of orthonormal SAF's, in which the expansion coefficients are, of course, independent of the choice of the axes x, y and z as long as the objects, *e.g.* experimental densities, and the SAF's are referred to the same symmetry-adapted coordinate system. In some cases, one might wish to rotate the object by arbitrary axes in crystal space. This is for instance the case in visualizations of the rotational potential written in terms of symmetry-adapted Wigner functions (Vogt & Prandl, 1983). The algorithm for the determination of the Euler angles (α, β, γ) needed for this purpose from the rotation angle ϕ about an axis n is given in Altmann (1986).



(*a*)

(*b*)

Fig. 1. Density contour lines of the functions (*a*) $P_{30\varepsilon 1}(\mathbf{x})$ and (*b*) $P_{30\varepsilon 2}(\mathbf{x})$ looking down a threefold axis in a stereographic projection. Positive and negative densities are marked by full and dotted lines, respectively.

References

Altmann, S. L. (1957). *Proc. Cambridge Philos. Soc.* **53**, 343–367.

Altmann, S. L. (1986). *Rotations, Quaternions, and Double Groups*. Oxford: Clarendon Press

Bradley, C. J. & Cracknell, A. P. (1972). *The Mathematical Theory of Symmetry in Solids*. Oxford: Clarendon Press

Butler, P. H. (1981). *Point Group Symmetry Applications*. New York: Plenum Press

Cohan, N. V. (1958). *Proc. Cambridge Philos. Soc.* **54**, 28–38.

Condon, E. U. & Shortley, G. H. (1935). *The Theory of Atomic Spectra*. Cambridge University Press

Edmonds, A. R. (1968). *Angular Momentum in Quantum Mechanics*. Princeton University Press

Elcoro, L., Perez-Mato, J. M. & Madariaga, G. (1994). *Acta Cryst.* A**50**, 182–193.

Gerlach, P., Vogt, K. & Prandl, W. (1984). *Mol. Phys.* **52**, 383–397.

Hahn, T. (1983). Editor. *International Tables for Crystallography*, Vol. A. Dordrecht: Kluwer.

James, H. M. & Keenan, T. A. (1959). *J. Chem. Phys.* **31**, 12–41.

Laporte, O. (1948). *Z. Naturforsch. Teil A*, **3**, 447–456.

Lindner, A. (1984). *Drehimpulse in der Quantenmechanik*. Stuttgart: Teubner.

Ljubarski, G. J. (1962). *Anwendungen der Gruppentheorie in der Physik*. Berlin: Deutscher Verlag der Wissenschaften.

Michel, K. H. (1992). *Z. Phys.* B**88**, 71–78.

Michel, K. H., Copley, J. R. D. & Neumann, D. A. (1992). *Phys. Rev. Lett.* **68**, 2929–2932.

Prandl, W. (1981). *Acta Cryst.* A**37**, 811–818.

Press, W. & Hüller, A. (1973). *Acta Cryst.* A**29**, 252–259.

Schiebel, P., Wulf, K., Prandl, W., Heger, G., Papoular, R. J. & Paulus, W. (1996). *Acta Cryst.* A**52**, 176–188.

Vogt, K. & Prandl, W. (1983). *J. Phys. C*, **16**, 4753–4768.