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Burnside rings: Application to molecules of icosahedral symmetry

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The Burnside ring, $B(G)$, of a group G is the set of isomorphism classes of orbits of G together with the operations of addition and product. The addition is defined as the disjoint union, and the product as the Cartesian product. This paper describes basic facts about this algebraic structure and develops some applications in chemistry, as the labelling of atoms in molecules of high symmetry and the construction of symmetry-adapted functions. For illustrating such applications, the concept of Burnside ring is applied to the icosahedral symmetry. Sets of points which are isomorphic to the orbits of the I group are described and the multiplication table of $B(I)$ is obtained from the table of marks. This multiplication table allows us to obtain an elegant labelling of the atoms of the buckminsterfullerene which is consistent with the icosahedral symmetry. Also, we obtain complete sets of symmetry-adapted functions for the buckminsterfullerene which span the Boyle and Parker's icosahedral representations.

KEY WORDS: Burnside rings, group theory, symmetry-adapted functions, icosahedral group, buckminsterfullerene

1. Introduction

The concept of G-set (a set whose elements are interchanged by the transformations of a group G) is widely applied in several branches of chemistry; for example, construction of symmetry-adapted functions, classification and determination of the symmetric coordinates of a vibrating molecule, enumeration of compounds, etc. One of the first task in working with G-sets is the enumeration of their orbits, i.e., the decomposition of the G-sets into subsets whose elements are equivalent with respect to the group action. The table of marks is an useful tool for decomposing a G-set into orbits since it allows us to know the number and type of orbits which are contained in a G-set starting from the numbers of elements that are invariant with respect to the subgroups of G. A G-set can be considered as the sum of its orbits. The direct product of two orbits is a G-set which can be decomposed into orbits. Thus, we can define the multiplication table of the orbits of a group as that containing the decomposition of the products into orbits. Table of marks is an essential tool for the attainment of such multiplication table.

Burnside ring is an algebraic structure which raises when we introduce the operations of product and sum in the complete set of isomorphism classes of orbits of a

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finite group. It is an interesting concept which until now has not been used beyond the boundaries of pure algebra.

2. Burnside rings

Let G be a finite group. The set S is said to be a G-set if to each $g \in G$ and each $x \in S$ there corresponds an element $gx \in S$, such that $1x = x$ (where 1 is the identity element of G) and $f(hx) = (fh)x$ for all $f, h \in G$ [1]. Two G-sets S and T are isomorphic with respect to the group action (denoted by $S \cong T$) if there exists a bijection $\phi : S \to T$ such that $g\phi(x) = \phi(gx)$ for all $x \in S$ and $g \in G$.

For each element x in S, its orbit $Gx = \{gx\colon\ g \in G\}$ is the smaller G-set containing x. Two elements x and y of S belong to the same orbit if there exists an element g of G such that $y = gx$. Every G-set S can be partitioned into a disjoint union of orbits. A G-set consisting of a single orbit is called transitive.

The stabiliser G_x of an element x of S is the subset of G which fix x, i.e., $G_x = \{g \in G\colon\ gx = x\}$. For any $x \in S$, the stabiliser G_x is a subgroup of G. If x and y are two elements of S belonging to the same orbit, the stabilisers G_x and G_y are conjugated subgroups, $G_y = gG_xg^{-1}$, where $y = gx$. The stabilisers of the elements of an orbit form a complete conjugacy class of subgroups of G.

For any subgroup H of G, the set of left cosets of H in G, given by $G/H = \{gH\colon\ g \in G\}$, is a transitive G-set under the G-action given by $f(gH) = (fg)H$. In this case, the stabiliser of gH is gHg^{-1}. For any element x of a G-set S the orbit of x is isomorphic to G/G_x.

Let H and K be subgroups of G, the sets G/H and G/K are isomorphic G-sets if and only if H and K are conjugated subgroups.

Let $\Re = \{G_1(= \{1\}), G_2, G_3, \ldots, G_s(= G)\}$ be a full set of nonconjugated subgroups of G. The set of transitive G-sets $\{G/G_i\colon\ i = 1, 2, \ldots, s\}$ is a complete set of orbits. This means that every G-set S is isomorphic to a disjoint union of such orbits:

$$S \cong \dot{\bigcup_i} a_i(G/G_i), \tag{1}$$

where G_i ranges over all elements of $\Re$ and a_i is the number of times that the orbit G/G_i appears in the decomposition of S. The coefficients a_i are uniquely determined and can be obtained as solutions of the system of linear equations [2]:

$$\sum_{i=1}^{s} M_{ji} a_i = b_j, \quad j = 1, 2, \ldots, s. \tag{2}$$

Here M_{ji} is the number of elements in G/G_i which are fixed points of the subgroup G_j, and b_j is the number of elements in S which are fixed points of G_j, where both G_i and G_j run through the set $\Re$.

The square matrix of dimension s formed by the numbers M_{ji} is called the table of marks of the G group. This matrix is nonsingular, hence we can to obtain its inverse M^{-1} which is known as the Burnside matrix. From equation (2) we obtain:

$$a_i = \sum_{j=1}^{s} \left(M^{-1}\right)_{ij} b_j, \quad i = 1, 2, \dots, s, \tag{3}$$

where $(M^{-1})_{ij}$ is the ij entry of M^{-1}.

Let S and T be two G-sets. The Cartesian product of S and T, denoted by $S \times T$, is the set of all ordered pairs (x, y) where $x \in S$ and $y \in T$; i.e., $S \times T = \{(x, y)\colon x \in S, y \in T\}$. The action of G on $S \times T$ is given by $g(x, y) = (g(x), g(y))$, for any $g \in G$ and any $(x, y) \in S \times T$. Since $g(x) \in S$ and $g(y) \in T$, $S \times T$ is a G-set.

The Cartesian product of the G-sets G/G_i and G/G_j is a G-set, then it is isomorphic to a disjoint union of orbits:

$$(G/G_i) \times (G/G_j) \cong \dot{\bigcup_k} n_{ij,k}(G/G_k), \tag{4}$$

where G_k ranges over all elements of $\Re$. If G_l is a subgroup of G the number of fixed points of G_l in G/G_i and G/G_j are M_{li} and M_{lj}, respectively. Then the number of fixed points of G_l in $(G/G_i) \times (G/G_j)$ is $M_{li} M_{lj}$. By applying equation (3), we obtain:

$$n_{ij,k} = \sum_l \left(M^{-1}\right)_{kl} M_{li} M_{lj}. \tag{5}$$

The Burnside ring $B(G)$ of the group G is defined by [3]

$$B(G) = \left\{ \sum_{i=1}^{s} a_i (G/G_i)\colon\ a_i \in \mathbf{Z} \right\}, \tag{6}$$

where $\mathbf{Z}$ is the set of integer numbers. The Burnside ring is a commutative ring with identity G/G_s, where the sum $(G/G_i) + (G/G_j)$ is the disjoint union of G/G_i and G/G_j, and the product $(G/G_i) \cdot (G/G_j)$ is the Cartesian product of G/G_i and G/G_j, i.e.,

$$\begin{aligned} (G/G_i) + (G/G_j) &= (G/G_i) \mathbin{\dot\cup} (G/G_j), \\ (G/G_i) \cdot (G/G_j) &= (G/G_i) \times (G/G_j). \end{aligned} \tag{7}$$

From equations (6), (8) and (9) we conclude that every G-set S is isomorphic to an element of $B(G)$:

$$S \cong \sum_i a_i (G/G_i). \tag{8}$$

3. Representations of the group G generated by G-sets

By the action of the elements of G, a G-set S affords a permutation representation Ω of G. According to equation (1), Ω can be reduced as

$$\Omega = \sum_i a_i \Omega_i, \tag{9}$$

where Ω_i is the transitive permutation representation generated by G/G_i. Each element $g \in G$ is represented in Ω_i by a permutation matrix of dimension $|G|/|G_i|$ whose elements are given by

$$g_{xy}^{(i)} = \begin{cases} 1, & \text{if } gx = y, \\ 0, & \text{if } gx \neq y, \end{cases} \tag{10}$$

for any $x, y \in G/G_i$. The representations Ω_s and Ω_1 are the identity and the regular representations, respectively.

The elements of an orbit G/G_i can be combined linearly in order to obtain basis functions of the irreducible representations (IR) of the group G which are contained in the representation Ω_i. Thus, if the IR Γ is contained in Ω_i, we can write the γ-basis vector of Γ as

$$|\Gamma\gamma\rangle = \sum_x |x\rangle\langle x|\Gamma\gamma\rangle, \tag{11}$$

where the summation extends over all the elements $x \in G/G_i$. Usually the coefficients $\langle x|\Gamma\gamma\rangle$ are obtained by using the projection operator method [4]. However, if the number of elements of G is high, this method is very tedious. In addition, if an IR is contained more than once in Ω_i , the different sets of basis functions of such IR obtained with the projection operator method are, in general, no-orthogonal.

The Cartesian product $(G/G_i) \times (G/G_j)$ affords a representation $\Omega_i \times \Omega_j$, which according to equation (4) can be reduced as

$$\Omega_i \times \Omega_j = \sum_k n_{ij,k} \Omega_k. \tag{12}$$

Each element $g \in G$ is represented in $\Omega_i \times \Omega_j$ by a permutation matrix whose elements are

$$g_{(u,v),(w,x)}^{(i\times j)} = \begin{cases} 1, & \text{if } g(u,v) = (w,x), \\ 0, & \text{if } g(u,v) \neq (w,x), \end{cases} \tag{13}$$

for any $u, w \in G/G_i$ and $v, x \in G/G_j$. According to equation (10), equation (13) is equivalent to

$$g_{(u,v),(w,x)}^{(i\times j)} = \begin{cases} 1, & \text{if } g(u) = w \text{ and } g(v) = x, \\ 0, & \text{if } g(u) \neq w \text{ or } g(v) \neq x. \end{cases} \tag{14}$$

From equations (14) and (10) we obtain:

$$g^{(i\times j)}_{(u,v),(w,x)} = g^{i}_{uw} g^{j}_{vx}. \tag{15}$$

Hence, $\Omega_i \times \Omega_j$ is the Kronecker product of the representations Ω_i and Ω_j [3].

If the orbit G/G_k is contained in the product $(G/G_i) \times (G/G_j)$ we can obtain symmetry-adapted functions for G/G_k by coupling the symmetry-adapted functions for G/G_i and G/G_j. In fact, let Γ, Γ' and Γ'' be irreducible representation of G such that $\Gamma \in \Omega_k$, $\Gamma' \in \Omega_i$, $\Gamma'' \in \Omega_j$ and $\Gamma \in \Gamma' \times \Gamma''$, then the γ-basis vector of Γ can be written as

$$\left|\Gamma\gamma; \Gamma', \Gamma''\right\rangle = \sum_{\gamma',\gamma''} \sum_{x,y} \left|(x, y)\right\rangle\left\langle x\middle|\Gamma'\gamma'\right\rangle\left\langle y\middle|\Gamma''\gamma''\right\rangle\left\langle\Gamma'\gamma'\Gamma''\gamma''\middle|\Gamma\gamma\right\rangle, \tag{16}$$

where x and y run over the elements of G/G_i and G/G_j, respectively, and $\langle\Gamma'\gamma'\Gamma''\gamma''|\Gamma\gamma\rangle$ are Clebsch–Gordan coefficients.

4. Orbits of the icosahedral rotation group (I)

Figure 1 shows the subgroup lattice for the I group. As we see, there exist nine icosahedral orbits. In order to simplify the notation, the icosahedral orbit I/G_k (where G_k is a subgroup of I) will be denoted as (G_k). The icosahedral orbits are isomorphic to I-sets which can be obtained from a regular icosahedron (see table 1). The orbits (D_2), (D_3), (D_5) and (T) cannot be isomorphic to sets containing single elements [5] and, hence, for such orbits we have used I-sets whose elements are sets containing more than one element. Figures 2 and 3 show the orbits (C_5) and (T), respectively.

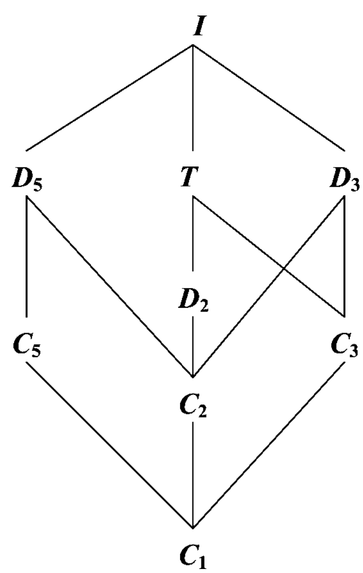

Figure 1. Subgroup lattice of the I group.

Table 1
Orbits of the I group.

Orbit	Description
(I)	A single point in the origin of coordinates
(T)	The set of three orthogonal pairs of antipodal edge midpoints of the icosahedron
(D_5)	The set of pairs of antipodal vertices of the icosahedron
(D_3)	The set of pairs of antipodal face midpoints of the icosahedron
(D_2)	The set of pairs of antipodal edge midpoints of the icosahedron
(C_5)	The set of vertices of the icosahedron
(C_3)	The set of face midpoints of the icosahedron
(C_2)	The set of edge midpoints of the icosahedron
(C_1)	The set of vertices of a truncated icosahedron

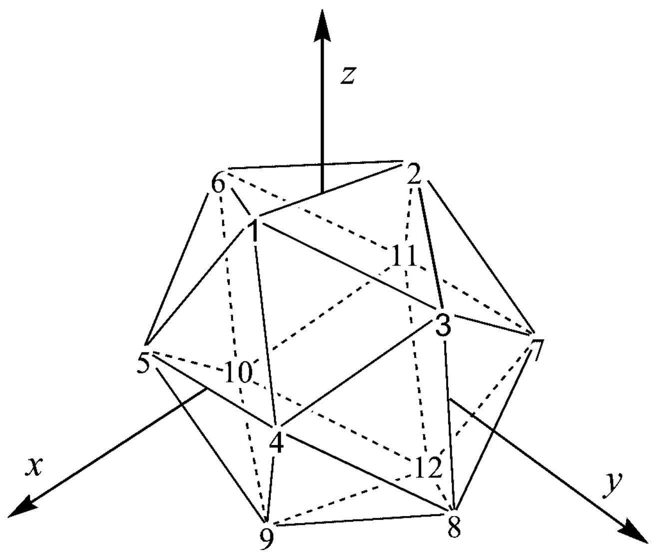

Figure 2. Numbering of the icosahedral vertices.

Table 2 contains the characters of the representations of the icosahedral group generated by the above orbits and the reductions into irreducible representations. The permutation representation of the generators of the I group which are spanned by the orbits (T) and (C_5) are shown in table 3.

From the table of marks for the I group [6] and its inverse, shown in tables 4 and 5, respectively, and using equations (4) and (5), we have obtained the multiplication table for the icosahedral Burnside ring $B(I)$ shown in table 6.

A simple application of such multiplication table is the labelling of elements of I-sets. For example, $(T) \cdot (T) \cong (T) + (C_3)$, where it is evident that

$$(T) \cong \{(a, a)\colon\ a \in (T)\},$$
$$(C_3) \cong \{(a, b)\colon\ a \neq b; a, b \in (T)\}.$$

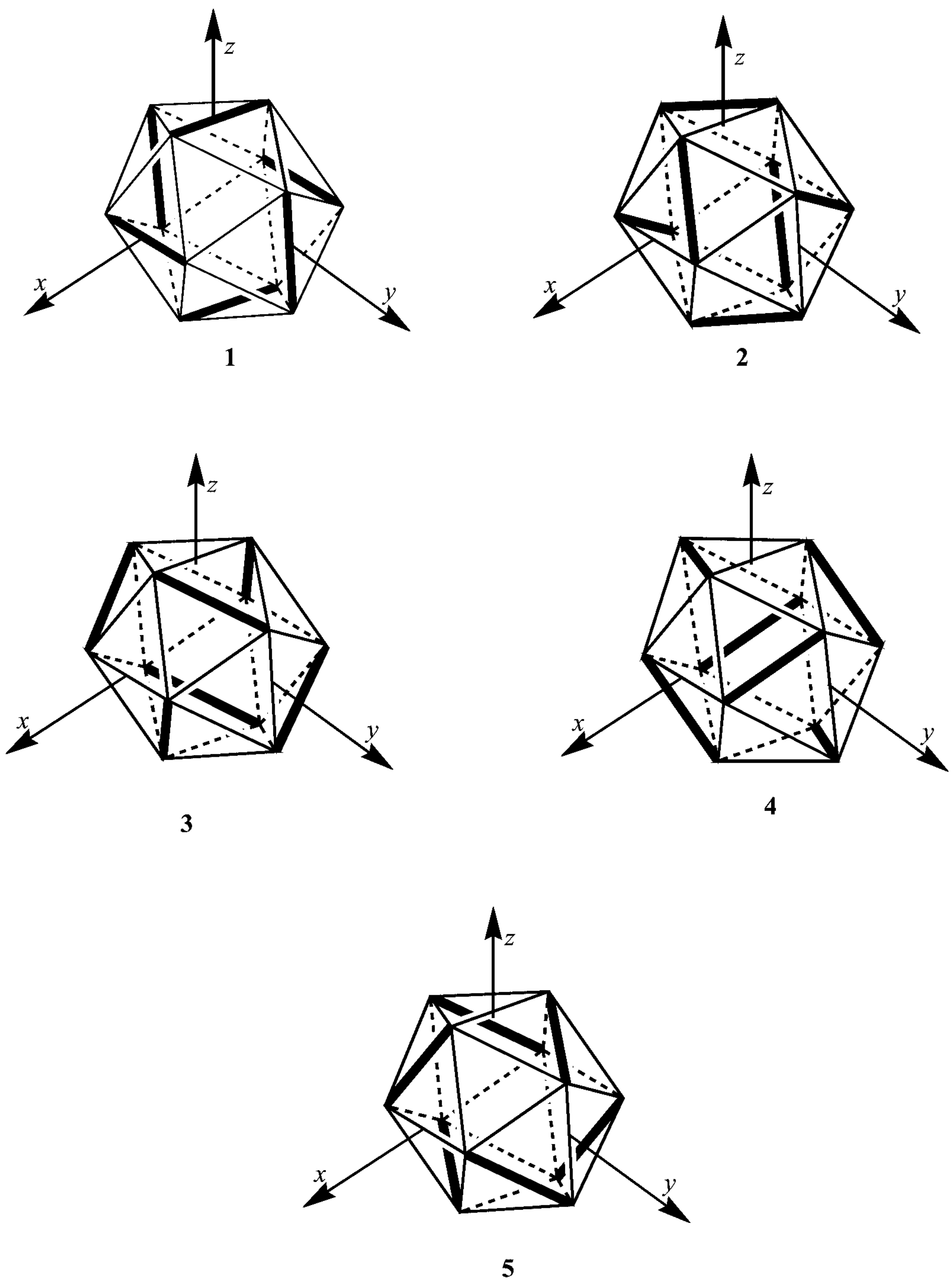

Figure 3. Elements of the orbit (T).

Table 2
Characters and reduction of the transitive permutation representations of the I group.

I	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	Reduction
Ω_I	1	1	1	1	1	A
Ω_T	5	0	0	2	1	$A+G$
Ω_{D_5}	6	1	1	0	2	$A+H$
Ω_{D_3}	10	0	0	1	2	$A+G+H$
Ω_{D_2}	15	0	0	0	3	$A+G+2H$
Ω_{C_5}	12	2	2	0	0	$A+T_1+T_2+H$
Ω_{C_3}	20	0	0	2	0	$A+T_1+T_2+2G+H$
Ω_{C_2}	30	0	0	0	2	$A+T_1+T_2+2G+3H$
Ω_{C_1}	60	0	0	0	0	$A+3T_1+3T_2+4G+5H$

Table 3
Permutation representations Ω_{C_5} and Ω_T for the generators of the I group.

	Ω_{C_5}	Ω_T
$C_5^{1,12}$	(1)(2 6 5 4 3)(7 11 10 9 8 7)	(1 4 5 2 3)
$C_3^{1,4,3}$	(1 4 3)(2 5 8)(6 9 7)(10 12 11)	(1)(2 4 3)(5)
$C_2^{1,2}$	(1 2)(3 6)(4 11)(5 7)(8 10)(9 12)	(1)(2 3)(4 5)

Table 4
Table of marks of the I group.

	(I)	(T)	(D_5)	(D_3)	(C_5)	(D_2)	(C_3)	(C_2)	(C_1)
I	1	0	0	0	0	0	0	0	0
T	1	1	0	0	0	0	0	0	0
D_5	1	0	1	0	0	0	0	0	0
D_3	1	0	0	1	0	0	0	0	0
C_5	1	0	1	0	2	0	0	0	0
D_2	1	1	0	0	0	3	0	0	0
C_3	1	2	0	1	0	0	2	0	0
C_2	1	1	2	2	0	3	0	2	0
C_1	1	5	6	10	12	15	20	30	60

This means that each face of the icosahedron can be labelled by (a, b), where $a \neq b$, $1 \leqslant a \leqslant 5$ and $1 \leqslant b \leqslant 5$ (see figure 4).

According to table 6, the triple product of $(T) \cdot (T) \cdot (T)$ can be decomposed into five orbits: $(T) \cdot (T) \cdot (T) \cong (T) + 3(C_3) + (C_1)$, where it is easy to see that

$$(T) \cong \{(a, a, a)\colon\ a \in (T)\},$$
$$(C_3) \cong \{(a, a, b)\colon\ a \neq b;\ a, b \in (T)\},$$
$$(C_3) \cong \{(a, b, a)\colon\ a \neq b;\ a, b \in (T)\},$$

Table 5
Inverse matrix of the table of marks of the I group.

	I	T	D_5	D_3	C_5	D_2	C_3	C_2	C_1
(I)	1	0	0	0	0	0	0	0	0
(T)	−1	1	0	0	0	0	0	0	0
(D_5)	−1	0	1	0	0	0	0	0	0
(D_3)	−1	0	0	1	0	0	0	0	0
(C_5)	0	0	−1/2	0	1/2	0	0	0	0
(D_2)	0	−1/3	0	0	0	1/3	0	0	0
(C_3)	1	−1	0	−1/2	0	0	1/2	0	0
(C_2)	2	0	−1	−1	0	−1/2	0	1/2	0
(C_1)	−1	1/3	1/2	1/2	−1/10	1/6	−1/6	−1/4	1/60

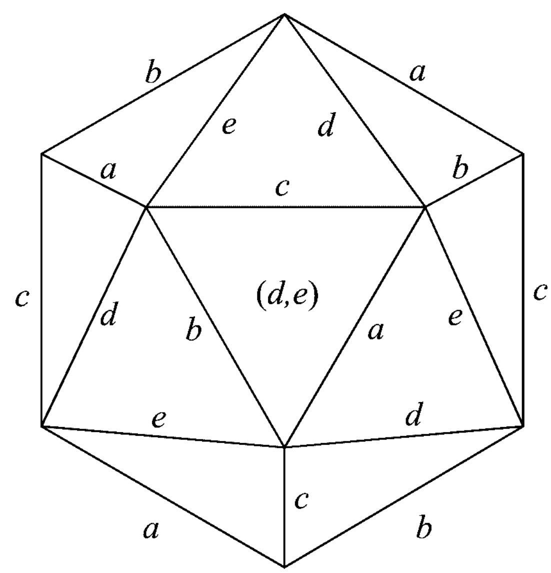

Figure 4. Labelling of the faces of the icosahedron.

$$(C_3) \cong \{(b,a,a)\colon\ a \neq b;\ a,b \in (T)\},$$
$$(C_1) \cong \{(a,b,c)\colon\ a \neq b \neq c;\ a \neq c;\ a,b,c \in (T)\}.$$

Thus, each vertex of the truncated icosahedron can be labelled by (a,b,c), where $a \neq b \neq c$, $a \neq c$, $1 \leqslant a \leqslant 5$, $1 \leqslant b \leqslant 5$ and $1 \leqslant c \leqslant 5$ (see figure 5). According to this, the regular representation of I, Ω_{C_1} can be obtained from Ω_T.

At last, the orbit (C_1) is isomorphic to the product $(T) \cdot (C_5)$. Then, since $(T) \cdot (C_5) = \{(a,b)\colon\ a \in (T), b \in (C_5)\}$, every vertex of a truncated icosahedron can be labelled by (a,b), where $1 \leqslant a \leqslant 5$ and $1 \leqslant b \leqslant 12$ (see figure 6).

Table 6
Multiplication table of the Burnside ring $\Omega(I)$.

	(I)	(T)	(D_5)	(D_3)	(C_5)	(D_2)	(C_3)	(C_2)	(C_1)
(I)	(I)	(T)	(D_5)	(D_3)	(C_5)	(D_2)	(C_3)	(C_2)	(C_1)
(T)		$(T)+(C_3)$	(C_2)	$(C_3)+(C_2)$	(C_1)	$(D_2)+(C_1)$	$2(C_3)+(C_1)$	$(C_2)+2(C_1)$	$5(C_1)$
(D_5)			$(D_5)+(C_2)$	$2(C_2)$	$(C_5)+(C_1)$	$3(C_2)$	$2(C_1)$	$2(C_2)+2(C_1)$	$6(C_1)$
(D_3)				$(D_3)+(C_2)+(C_1)$	$2(C_1)$	$3(C_2)+(C_1)$	$(C_3)+3(C_1)$	$2(C_2)+4(C_1)$	$10(C_1)$
(C_5)					$2(C_5)+2(C_1)$	$3(C_1)$	$4(C_1)$	$6(C_1)$	$12(C_1)$
(D_2)						$3(D_2)+3(C_1)$	$5(C_1)$	$3(C_2)+6(C_1)$	$15(C_1)$
(C_3)							$2(C_3)+6(C_1)$	$10(C_1)$	$20(C_1)$
(C_2)								$2(C_2)+14(C_1)$	$30(C_1)$
(C_1)									$60(C_1)$

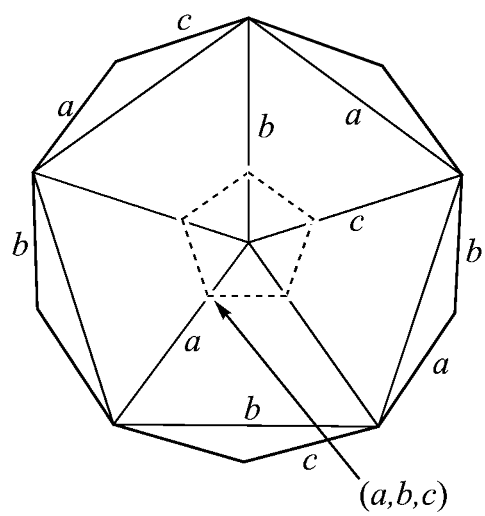

Figure 5. Labelling of the elements of (C_1) by using the elements of (T).

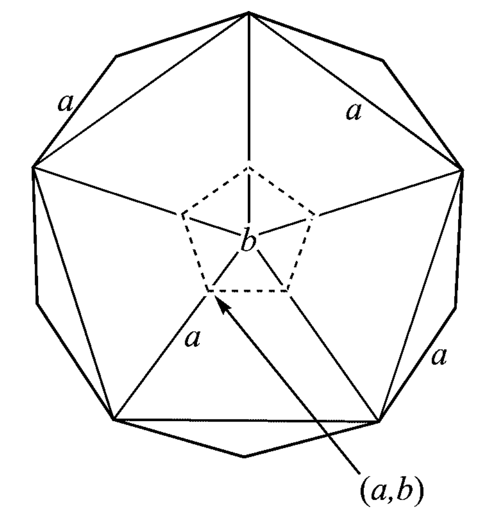

Figure 6. Labelling of the elements of (C_1) by using the elements of (C_5) and (T).

5. Symmetry-adapted functions for the C_{60} molecule

Because of the high order of the icosahedral group I, the attainment of icosahedral symmetry-adapted functions by direct application of the projection operators method is a laborious task. Therefore, any alternative method introducing some simplification is well received. Here we show how the symmetry-adapted functions for the C_{60} molecule can be obtained by using the concepts developed in the above sections.

Table 7
Symmetry-adapted functions for the orbit (C_5).

$\psi_{Aa} = (1/2\sqrt{3})(v_1 + v_2 + v_3 + v_4 + v_5 + v_6 + v_7 + v_8 + v_9 + v_{10} + v_{11} + v_{12})$
$\psi_{T_1x} = (1/2\sqrt{\Phi+2})(v_1 - v_2 + \Phi v_4 + \Phi v_5 - \Phi v_7 + v_9 - \Phi v_{11} - v_{12})$
$\psi_{T_1y} = (1/2\sqrt{\Phi+2})(\Phi v_3 + v_4 - v_5 - \Phi v_6 + v_7 + \Phi v_8 - \Phi v_{10} - v_{11})$
$\psi_{T_1z} = (1/2\sqrt{\Phi+2})(\Phi v_1 + \Phi v_2 + v_3 + v_6 - v_8 - \Phi v_9 - v_{10} - \Phi v_{12})$
$\psi_{T_2x} = (1/2\sqrt{\Phi+2})(\Phi v_1 - \Phi v_2 - v_4 - v_5 + v_7 + \Phi v_9 + v_{11} - \Phi v_{12})$
$\psi_{T_2y} = (1/2\sqrt{\Phi+2})(-v_3 + \Phi v_4 - \Phi v_5 + v_6 + \Phi v_7 - v_8 + v_{10} - \Phi v_{11})$
$\psi_{T_2z} = (1/2\sqrt{\Phi+2})(-v_1 - v_2 + \Phi v_3 + \Phi v_6 - \Phi v_8 + v_9 - \Phi v_{10} + v_{12})$
$\psi_{H\vartheta} = (1/2\sqrt{2})(v_1 + v_2 - v_3 - v_6 - v_8 + v_9 - v_{10} + v_{12})$
$\psi_{H\varepsilon} = (1/2\sqrt{6})(-v_1 - v_2 - v_3 + 2v_4 + 2v_5 - v_6 + 2v_7 - v_8 - v_9 - v_{10} + 2v_{11} - v_{12})$
$\psi_{Hx} = (1/2)(v_3 - v_6 - v_8 + v_{10})$
$\psi_{Hy} = (1/2)(v_1 - v_2 - v_9 + v_{12})$
$\psi_{Hz} = (1/2)(v_4 - v_5 - v_7 + v_{11})$

Note. $\Phi = (1+\sqrt{5})/2$ is the golden number.

Table 8
Symmetry-adapted functions for the orbit (T).

$\varphi_{Aa} = (1/\sqrt{5})(v^1 + v^2 + v^3 + v^4 + v^5)$
$\varphi_{Ga} = (1/2\sqrt{5})(4v^1 - v^2 - v^3 - v^4 - v^5)$
$\varphi_{Gx} = (1/2)(v^2 - v^3 + v^4 - v^5)$
$\varphi_{Gy} = (1/2)(-v^2 + v^3 + v^4 - v^5)$
$\varphi_{Gz} = (1/2)(v^2 + v^3 - v^4 - v^5)$

Using equation (16) and bearing in mind the relation $(T) \cdot (C_5) \cong (C_1)$ (see table 6) we can obtain mutually orthogonal symmetry-adapted functions for (C_1) by coupling the symmetry-adapted functions of (T) and (C_5). For this purpose we have obtained symmetry-adapted functions for (T) and (C_5) by using the results obtained by Boyle and Parker in their paper on a vibrating icosahedral cage [7] (see tables 7 and 8). In order to use equation (16) we have employed the coupling coefficients which were obtained by Fowler and Ceulemans [8] for the single-valued irreducible representations of the I group based on the symmetry functions of Boyle and Parker. The symmetry functions for the C_{60} molecule thus obtained are basis functions of the matrix representation of the I group given in the appendix to the work by Boyle and Parker [7]. Table 9 contains the functions for the representation H obtained by coupling the symmetry-adapted functions for (C_5) and (T) which are base of the representations T_1 and G, respectively. By reasons of space the resting functions are not shown in this paper, but are available upon request.

Bearing in mind the relation $(T) \cdot (T) \cdot (T) \cong (T) + 3(C_3) + (C_1)$, where $(C_1) \cong \{(a,b,c)\colon\ a \neq b \neq c; a \neq c; a,b,c \in (T)\}$, we could obtain symmetry-adapted functions for (C_1) from those of (T). However, the functions thus obtained have the disadvantage that, as occurs with the projection operator method, the different sets of functions belonging to the same irreducible representation are non-orthogonal.

Table 9
Functions $|H\gamma;\, H, G\rangle$, $\gamma = \vartheta, \varepsilon, x, y, z$.

$$
\begin{aligned}
|H_\vartheta;\, H, G\rangle = {} & (1/8\sqrt{15})(-6v_1^1 - v_1^2 + 4v_1^3 + 4v_1^4 - v_1^5 - 6v_2^1 + 4v_2^2 - v_2^3 - v_2^4 + 4v_2^5 + 6v_3^1 \\
& + v_3^2 - 4v_3^3 + v_3^4 - 4v_3^5 - 5v_4^2 - 5v_4^3 + 5v_4^4 + 5v_4^5 + 5v_5^2 + 5v_5^3 - 5v_5^4 - 5v_5^5 \\
& + 6v_6^1 - 4v_6^2 + v_6^3 - 4v_6^4 + v_6^5 + 5v_7^2 + 5v_7^3 - 5v_7^4 - 5v_7^5 + 6v_8^1 - 4v_8^2 + v_8^3 - 4v_8^4 \\
& + v_8^5 - 6v_9^1 + 4v_9^2 - v_9^3 - v_9^4 + 4v_9^5 + 6v_{10}^1 + v_{10}^2 - 4v_{10}^3 + v_{10}^4 - 4v_{10}^5 - 5v_{11}^2 \\
& - 5v_{11}^3 + 5v_{11}^4 + 5v_{11}^5 - 6v_{12}^1 - v_{12}^2 + 4v_{12}^3 + 4v_{12}^4 - v_{12}^5) \\
|H\varepsilon;\, H, G\rangle = {} & (1/8\sqrt{5})(2v_1^1 - 3v_1^2 + 2v_1^3 + 2v_1^4 - 3v_1^5 + 2v_2^1 + 2v_2^2 - 3v_2^3 - 3v_2^4 + 2v_2^5 + 2v_3^1 \\
& - 3v_3^2 + 2v_3^3 - 3v_3^4 + 2v_3^5 - 4v_4^1 + v_4^2 + v_4^3 + v_4^4 + v_4^5 - 4v_5^1 + v_5^2 + v_5^3 + v_5^4 + v_5^5 \\
& + 2v_6^1 + 2v_6^2 - 3v_6^3 + 2v_6^4 - 3v_6^5 - 4v_7^1 + v_7^2 + v_7^3 + v_7^4 + v_7^5 + 2v_8^1 + 2v_8^2 - 3v_8^3 \\
& + 2v_8^4 - 3v_8^5 + 2v_9^1 + 2v_9^2 - 3v_9^3 - 3v_9^4 + 2v_9^5 + 2v_{10}^1 - 3v_{10}^2 + 2v_{10}^3 - 3v_{10}^4 + 2v_{10}^5 \\
& - 4v_{11}^1 + v_{11}^2 + v_{11}^3 + v_{11}^4 + v_{11}^5 + 2v_{12}^1 - 3v_{12}^2 + 2v_{12}^3 + 2v_{12}^4 - 3v_{12}^5) \\
|H_x;\, H, G\rangle = {} & (1/4\sqrt{30})(-5v_1^3 + 5v_1^4 + 5v_2^2 - 5v_2^5 + 4v_3^1 - v_3^2 - v_3^3 - v_3^4 - v_3^5 - 5v_4^4 + 5v_4^5 \\
& - 5v_5^2 + 5v_5^3 - 4v_6^1 + v_6^2 + v_6^3 + v_6^4 + v_6^5 - 5v_7^2 + 5v_7^3 - 4v_8^1 + v_8^2 + v_8^3 + v_8^4 + v_8^5 \\
& + 5v_9^2 - 5v_9^5 + 4v_{10}^1 - v_{10}^2 - v_{10}^3 - v_{10}^4 - v_{10}^5 - 5v_{11}^4 + 5v_{11}^5 - 5v_{12}^3 + 5v_{12}^4) \\
|H_y;\, H, G\rangle = {} & (1/4\sqrt{30})(4v_1^1 - v_1^2 - v_1^3 - v_1^4 - v_1^5 - 4v_2^1 + v_2^2 + v_2^3 + v_2^4 + v_2^5 - 5v_3^3 + 5v_3^5 - 5v_4^2 \\
& + 5v_4^3 + 5v_5^4 - 5v_5^5 + 5v_6^2 - 5v_6^4 + 5v_7^4 - 5v_7^5 + 5v_8^2 - 5v_8^4 - 4v_9^1 + v_9^2 + v_9^3 + v_9^4 \\
& + v_9^5 - 5v_{10}^3 + 5v_{10}^5 - 5v_{11}^2 + 5v_{11}^3 + 4v_{12}^1 - v_{12}^2 - v_{12}^3 - v_{12}^4 - v_{12}^5) \\
|H_z;\, H, G\rangle = {} & (1/4\sqrt{30})(-5v_1^2 + 5v_1^5 - 5v_2^3 + 5v_2^4 + 5v_3^2 - 5v_3^4 + 4v_4^1 - v_4^2 - v_4^3 - v_4^4 - v_4^5 - 4v_5^1 \\
& + v_5^2 + v_5^3 + v_5^4 + v_5^5 + 5v_6^3 - 5v_6^5 - 4v_7^1 + v_7^2 + v_7^3 + v_7^4 + v_7^5 + 5v_8^3 - 5v_8^5 - 5v_9^3 \\
& + 5v_9^4 + 5v_{10}^2 - 5v_{10}^4 + 4v_{11}^1 - v_{11}^2 - v_{11}^3 - v_{11}^4 - v_{11}^5 - 5v_{12}^2 + 5v_{12}^5)
\end{aligned}
$$

6. Supplementary material

A print-out of the complete symmetry-adapted functions for the C_{60} molecule is available upon request.

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