

Chapter 16

Enumeration of Hetero-molecules by Using Pólya Theorem

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Abstract A fullerene is any molecule composed entirely of carbon, in the form of a hollow sphere, ellipsoid, or tube. Spherical fullerenes are also called buckyballs and cylindrical ones are called carbon nanotubes or buckytubes. Fullerenes are similar in structure to graphite, which is composed of stacked graphene sheets of linked hexagonal rings; but they may also contain pentagonal rings. Enumeration of chemical compounds has been accomplished by various methods. The Pólya-Redfield theorem has been a standard method for combinatorial enumerations of graphs, polyhedra, chemical compounds, and so forth. Hetero-fullerenes are fullerene molecules in which one or more carbon atoms are replaced by heteroatoms such as boron or nitrogen. In this chapter, by using the Pólya's theorem, we compute the number of permutational isomers of some fullerene graphs.

16.1 Introduction

In this chapter, we introduce some notations which will be kept throughout. A graph is a collection of points and lines connecting them. The points and lines of a graph are also called vertices and edges, respectively. If e is an edge of Γ , connecting the vertices u and v , then we write $e = uv$ and say “ u and v are adjacent.” A connected graph is a graph such that there exists a path between all pairs of vertices. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted.

Group is a set of elements which satisfy the following properties (Trinajstić 1992):

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1. There is an identity element, e , so that $a \cdot e = a$ for any a belonging to the group.
2. The product of two elements is also member of the group, that is, if a and b belong to the group, then $a \cdot b$ will also be a member of the group. It means the group is closed under the given operation.
3. Every element has its inverse as the member of the group, that is, if a belongs to the group, then a^{-1} also belongs to the group. If $a \cdot b = e$, it means a is the inverse of b and vice versa.
4. Group members obey the associative law, that is, $a(b \cdot c) = (a \cdot b)c$.

The order of a group is defined as the number of elements present in the group. The elements of a group can be several things as you define them. It can be integers, vectors, matrices, symmetry operations (elements), etc. One has to define the operation which goes on in the group which can be several things like addition, multiplication, and symmetry operations. There are smaller groups present in the group. They obey all the rules of a group. Their order must divide the order of the group. That is, if you have a group of order seven, then you cannot have any subgroup except a subgroup of order 1 that contains identity only. Similarly, if you have a group of order 12, you should not waste your time in looking for a subgroup of order 5, 7, 8, 9, 10, and 11. Remember there is always a subgroup of order 1. An Abelian group is a group in which every element commutes with every other element, that is, $a \cdot b = b \cdot a$ for every a and b . Cyclic group is a group which is generated by a single element called generator. In other words, if G be a cyclic group, then there is an element g in G where, $G = \{g, g^2, \dots, g^n = 1\}$. The order of this group is n .

A group can be divided into several classes, also called conjugacy classes. The importance of classes will be clear in our later studies. It is time consuming to find out all classes. Choose any element, and perform the so-called similarity transformation, that is, compute $x^{-1}ax$, where x and a belong to the group. For each a , perform this computation with x being all members of the group.

Symmetry plays a central role in the analysis of the structure, bonding, and spectroscopy of molecules. Chemists classify molecules according to their symmetry. The collection of symmetry elements present in a molecule forms a group, typically called a point group. Since all the symmetry elements (points, lines, and planes) will intersect at a single point, so we name it as point group. The symmetry properties of objects (and molecules) may be described in terms of the presence of certain symmetry elements and their associated symmetry operations. Symmetry elements are properties which are related to the structure of the molecule. They include mirror planes, axes of rotation, centers of inversion, and improper axes of rotation (an improper axis of rotation is a rotation followed by a reflection perpendicular to the rotational axis). Symmetry operations are actions which place the molecule in an orientation which appears to be identical to its initial orientation. Symmetry operations include rotation, reflection, inversion, rotation followed by reflection, and identity. The identity operation simply leaves the molecule where it is. All molecules have the identity operation. Certain physical properties of molecules are clearly linked to molecular symmetry. Molecules which are symmetrically bonded to the

same elements will not be polar, due to the canceling dipole moments. Likewise, chirality (left or right handedness) is clearly a symmetry property. Chirality can only be present in molecules which lack an improper axis or rotation. Molecules with a center of inversion or a mirror plane cannot be chiral. The symmetry properties of molecules are tabulated on character tables. A character table lists the symmetry elements of the point group, along with characters which are consistent with the different symmetry operations of the group. The table characterizes how various atomic properties (the symmetry of atomic orbitals, rotations about axes, etc.) are transformed by the symmetry operations of the group.

Character of a symmetry element will be defined as the sum of the diagonal elements in the matrix representing the element. Mathematically, it turns out that representations of a group can be expressed in terms of these characters.

Detecting symmetry of molecules is a well-studied problem with applications in a large number of areas. Randić (1974, 1976) and then Balasubramanian (1980) considered the Euclidean matrix of a chemical graph to find its symmetry. Here the Euclidean matrix of a molecular graph Γ is a matrix $D(\Gamma) = [d_{ij}]$, where for $i \neq j$, d_{ij} is the Euclidean distance between the nuclei i and j . In this matrix d_{ii} can be taken as zero if all the nuclei are equivalent. Otherwise, one may introduce different weights for different nuclei.

Suppose σ is a permutation on n atoms of the molecule under consideration. Then the permutation matrix P_σ is defined as $P_\sigma = [x_{ij}]$, where $x_{ij} = 1$ if $i = \sigma(j)$ and 0 otherwise. It is easy to see that $P_\sigma P_\tau = P_{\sigma\tau}$, for any two permutations σ and τ on n objects, and so, the set of all $n \times n$ permutation matrices is a group isomorphic to the symmetric group S_n on n symbols. It is a well-known fact that a permutation σ of the vertices of a graph Γ belongs to its automorphism group if it satisfies $P_\sigma' A P_\sigma = A$, where A is the adjacency matrix of Γ . So, for computing the symmetry of a molecule, it is sufficient to solve the matrix equation $P' E P = E$, where E is the Euclidean matrix of the molecule under consideration and P varies on the set of all permutation matrices with the same dimension as E .

16.2 Main Results and Discussion

Groups are often used to describe symmetries of objects. This is formalized by the notion of a group action. Let G be a group and X a nonempty set. An action of G on X is denoted by G_X and X is called a G -set. It induces a group homomorphism φ from G into the symmetric group S_X on X , where $\varphi(g)x = gx$ for all $x \in X$. The orbit of x will be denoted by Gx and defines as the set of all $\varphi(g)x$, $g \in G$. The set of all G -orbits will be denoted by $G \backslash X = \{Gx \mid x \in X\}$. Suppose g is a permutation of n symbols with exactly λ_1 orbits of size 1, λ_2 orbits of size 2, ..., and λ_n orbits of size n . Then the cycle type of g is defined as $1^{\lambda_1} 2^{\lambda_2} \dots n^{\lambda_n}$.

A mathematician, namely, Arthur Cayley, has been studying the combinatorial enumeration of rooted trees as models. Pólya's theorem has been widely applied to chemical combinatorics to enumerate objects. In this chapter we will show how

Fig. 16.1 Two indistinguishable colorings

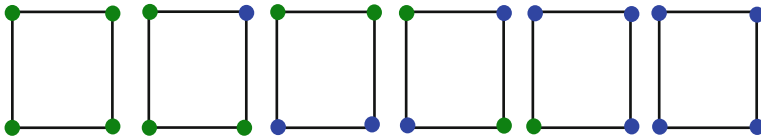
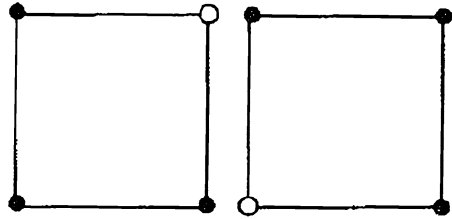


Fig. 16.2 The six distinguishable colorings

Pólya theory can be used in counting objects, which is often the design basis for statistical tests. In other words, Pólya theory determines the number of distinct equivalence classes of objects. It can also give counts for specific types of patterns within equivalence classes.

Example 16.1 As an example, let us consider the number of ways of assigning one of the colors red or white to each corner of a square. Since there are two colors and four corners, there are basically $2^4 = 16$ possibilities. But when we take account of the symmetry of the square, we see that some of the possibilities are essentially the same. For example, the first coloring as in Fig. 16.1 is the same as the second one after rotation through 180° .

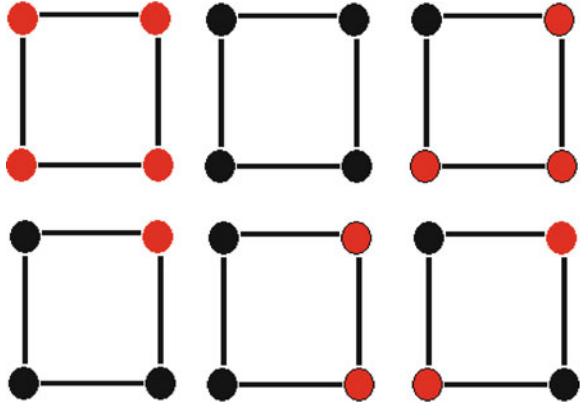
From above, we regard two colorings as being indistinguishable if one is transformed into the other by symmetry of the square. It is easy to find the distinguishable colorings (in this example) by trial and error: there are just six of them, as shown in the Fig. 16.2.

Now consider an n bead necklace. Let each corner of it be colored red or blue. How many different colorings are there? One could argue for 2^n . For example, if $n = 4$ and the corners are numbered 0,1,2,3 in clockwise order around the necklace, then there are only 6 ways of coloring the necklace RRRR, BBBB, RRRB, RBBB, RRBB, and RBRB; see Fig. 16.3.

16.2.1 Pólya's Theorem

We now introduce the notion of cycle index. Let G be a permutation group. The cycle index of G acting on X is the polynomial $Z(G, X)$ over \mathcal{Q} in terms of indeterminates $x_1, x_2, \dots, x_t, t = |X|$, defined by $Z(G, X) =$

Fig. 16.3 Distinguish colorings of four bead necklace



$(1/|G|) \sum_{p \in G} \prod_{i=1}^t x_i^{c_i(p)}$ in which $(c_1(p), \dots, c_t(p))$ is the cycle type of the permutation $p \in G$. The generalized character cycle index is defined as $P_G^\chi(x_1, x_2, \dots, x_t) = (1/|G|) \sum_{p \in G} \prod_{i=1}^t \chi(p) x_i^{c_i(p)}$, where $\chi(g)$ is the linear character of the irreducible representation of G . In this chapter, we use two special cases: one is the antisymmetric representation, that is,

$$\chi(g) = \begin{cases} 1 & \text{if } g \text{ is a proper rotation} \\ -1 & \text{if } g \text{ is an improper rotation} \end{cases}$$

and the other when χ is 1 for all g . Since, all elements of a conjugacy class of a permutation group have the same cycle type, so the cycle index and the generalized character cycle index can be rephrased in the following way:

$$Z(G, x_1, \dots, x_t) = \frac{1}{|G|} \sum_{C \in \text{Conj}(G)} |C| \prod_{i=1}^t x_i^{c_i(g_C)}$$

$$P_G^\chi(x_1, \dots, x_t) = \frac{1}{|G|} \sum_{C \in \text{Conj}(G)} |C| \prod_{i=1}^t \chi(g_C) x_i^{c_i(g_C)}$$

Denote by $C_{m,n}$ the set of all functions $f: \{1, 2, \dots, m\} \rightarrow \{x_1, x_2, \dots, x_n\}$. The action of $p \in S_m$ induced on $C_{m,n}$ is defined by $\hat{p}(f) = f \circ p^{-1}, f \in C_{m,n}$. Treating the colors x_1, x_2, \dots, x_n that comprise the range of $f \in C_{m,n}$ as independent variables, the weight of f is $W(f) = \prod_{i=1}^m f(i)$. Evidently, $W(f)$ is a monomial of (total) degree m . Suppose G is a permutation group of degree m , $\hat{G} = \{\hat{p} : p \in G\}$, \hat{p} is as defined above. Let p_1, p_2, \dots, p_t be representatives of the distinct orbits of \hat{G} . The weight of p_i is the common value of $W(f), f \in p_i$. The sum of the weights of the orbits is the pattern inventory $W_G(x_1, x_2, \dots, x_n) = \sum_{i=1}^t W(p_i)$.

Theorem 16.2 (*Pólya's theorem* (Pólya and Read 1987)) *If G is a subgroup of S_m , the symmetry group on m symbols, then the pattern inventory for the orbits of $C_{m,n}$ modula \hat{G} is*

$$W_G(x_1, x_2, \dots, x_n) = \frac{1}{|G|} \sum_{p \in G} M_1^{C_1(p)} M_2^{C_2(p)} \dots M_m^{C_m(p)},$$

where $M_k = x_1^k + x_2^k + \dots + x_n^k$ is the k th power sum of the x 's.

Theorem 16.3 (*Generalization of Pólya's theorem* (Zhang et al. 1998)) *Substituting M_i for x_i and in the generalized character cycle index, $i = 1, 2, \dots, t$, we get the chiral generating function $\text{CGF} = P_G^X(M_1, \dots, M_k)$.*

16.2.2 Fullerene Graphs

In the past years, nanostructures involving carbon have been the focus of an intense research activity which is driven to a large extent by the quest for new materials with specific applications. Fullerene is one of the main objects of nanostructures. A fullerene is any molecule composed entirely of carbon, in the form of a hollow sphere, ellipsoid, or tube. Spherical fullerenes are also called buckyballs and cylindrical ones are called carbon nanotubes or buckytubes. Fullerenes are similar in structure to graphite, which is composed of stacked graphene sheets of linked hexagonal rings; but they may also contain pentagonal rings. The fullerene era was started in 1985 with the discovery of a stable C_{60} cluster and its interpretation as a cage structure with the familiar shape of a soccer ball, by Kroto and his coauthors (Kroto et al. 1985, 1993). The well-known fullerene, the C_{60} molecule, is a closed-cage carbon molecule with three-coordinate carbon atoms tiling the spherical or nearly spherical surface with a truncated icosahedral structure formed by 20 hexagonal and 12 pentagonal rings. Let p , h , n , and m be the number of pentagons, hexagons, carbon atoms, and bonds between them, in a given fullerene F . Since each atom lies in exactly three faces and each edge lies in two faces, the number of atoms is $n = (5p + 6h)/3$, the number of edges is $m = (5p + 6h)/2 = 3/2n$, and the number of faces is $f = p + h$. By the Euler's formula $n - m + f = 2$, one can deduce that $(5p + 6h)/3 - (5p + 6h)/2 + p + h = 2$, and therefore, $p = 12$, $v = 2h + 20$, and $e = 3h + 30$. This implies that such molecules made up entirely of n carbon atoms and are having 12 pentagonal and $(n/2 - 10)$ hexagonal faces, where $n \neq 22$ is a natural number equal or greater than 20; see Fig. 16.4. Hetero-fullerenes are fullerene molecules in which one or more carbon atoms are replaced by heteroatoms such as boron or nitrogen, whose formation is a kind of "on-ball" doping of the fullerene cage; see Fig. 16.5.

To enumerate all possibilities of the hetero-fullerene structures, we have to consider the rotation group of the fullerene and its whole automorphism group to

Fig. 16.4 3-D graph of fullerene C_{20}

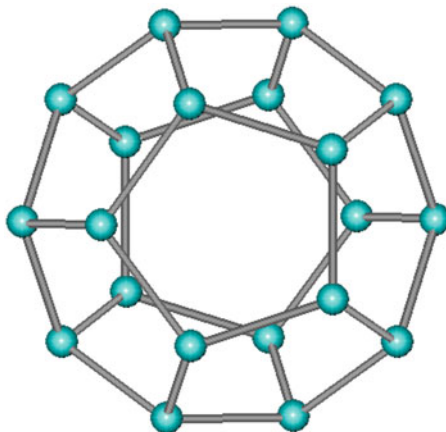
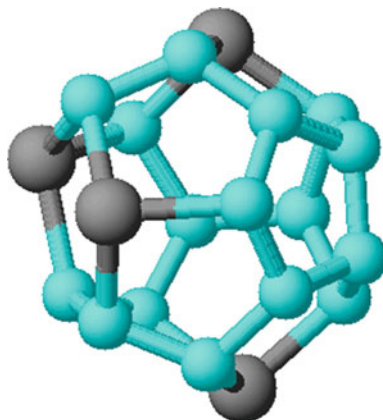


Fig. 16.5 3-D graph of hetero-fullerene $C_{16}Br_4$



enumerate the number of chiral isomers. Friperinger (Friperinger 1996) computed the symmetry of some fullerenes and then applied SYMMETRICA to calculate the number of $C_{60}H_kCl_{60-k}$ molecules, and Balasubramanian computed the number of $C_{60}H_{36}$ isomers. (Zhang et al. 1998), for calculating the possibilities of different positional isomers, used the Pólya's counting theorem. He also applied the generalization of the Pólya's theorem to compute the number of chiral isomers.

Balasubramanian (1981, 1984, 1995a, b, 2004a, b) has done a lot of work on methods for isomer counting of hetero-fullerenes and of poly-substituted fullerenes, especially, using the generalized character cycle index. Mathematically the isomer counting of poly-substituted fullerene is essentially the same as that of hetero-fullerene. Shao and Jiang (1995) discussed hydrogenated C_{60} . Furthermore, (Zhang et al. 1998) also studied the fullerene cages. In Ghorbani et al. (2006a, b, 2009, 2011, 2012), Ashrafi and Ghorbani (2010) and Faghani and Ghorbani (2011), the number of permutational isomers of some classes of hetero-fullerenes is computed.

Fig. 16.6 2-D graph of zigzag nanotube $T_z[6, p]$, for $p = 5$ and its Clar structures

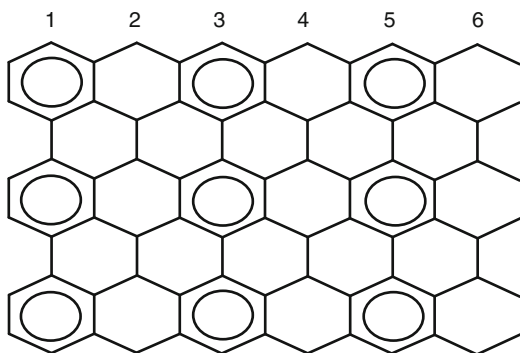
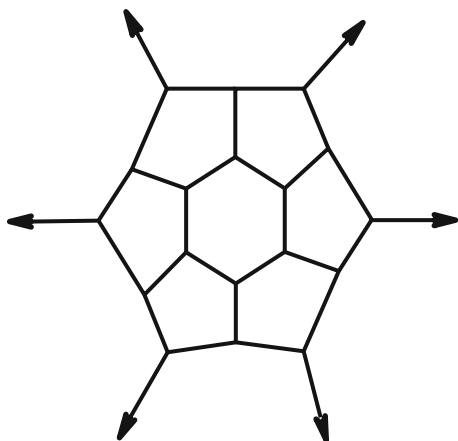


Fig. 16.7 Caps B



16.2.3 Construction of Infinite Classes of Fullerenes

In Ghorbani et al. (2011), a method is described to obtain a fullerene graph from a zigzag or armchair nanotubes. Here by continuing his method, we construct an infinite class of fullerenes. Denoted by $T_z[q, p]$ means a zigzag nanotube with p rows and q columns of hexagons; see Fig. 16.6. Combining a nanotube $T_z[6, p]$ with two copies of caps B (Fig. 16.7) as shown in Fig. 16.8, the resulted graph is a non-IPR fullerene, which has $12p$ vertices and $6p - 10$ hexagonal faces.

Now, combine a nanotube $T_z[5, p]$ (Fig. 16.9) with two copies of caps C (Fig. 16.10) as shown in Fig. 16.11. The resulted graph is a non-IPR fullerene, which has $10p$ vertices and $5p - 10$ hexagonal faces.

Finally, we can construct a fullerene with $12n + 30$ vertices (Fig. 16.12), by combining a $T_z[6, p]$ nanotube and two caps E (see Fig. 16.13) added to its inside and its outside. In this chapter, we will construct some infinite classes of fullerene graphs and then compute the number of their chiral isomers.

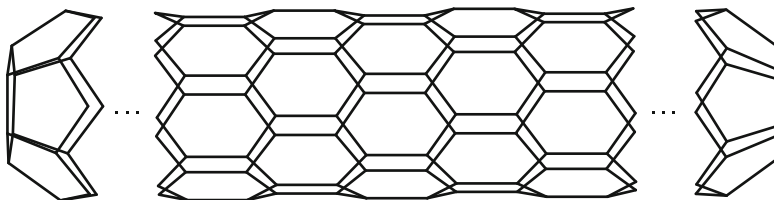


Fig. 16.8 Fullerene C_{12p} constructed by combining two copies of caps B and the zigzag nanotube $T_z[6, p]$

Fig. 16.9 2-D graph of zigzag nanotube $T_z[6, p]$, for $p = 5$ and its Clar structures

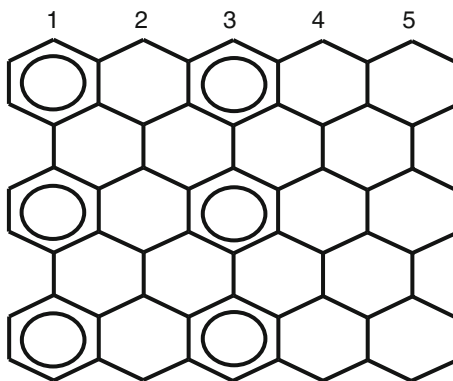


Fig. 16.10 Caps C

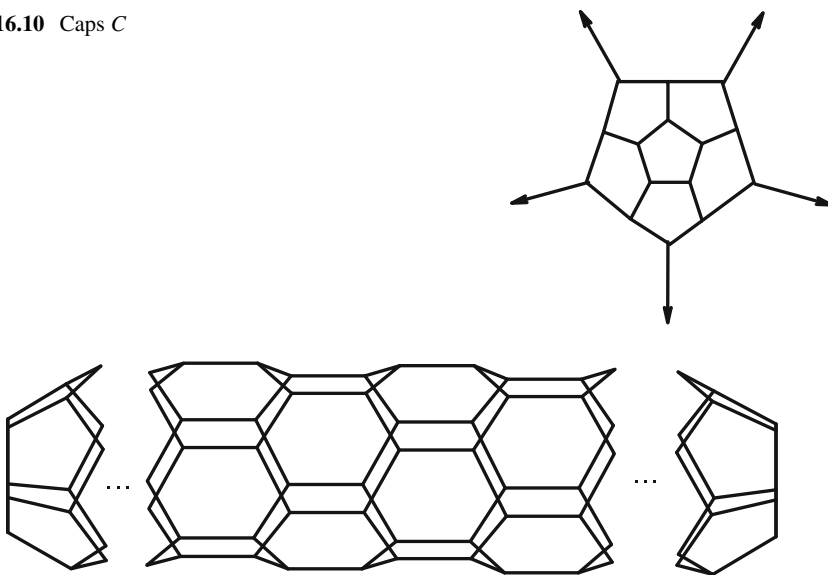


Fig. 16.11 Fullerene C_{10p} constructed by combining two copies of caps C and the zigzag nanotube $T_z[5, p]$

Fig. 16.12 2-D graph of fullerene C_{12n+30}

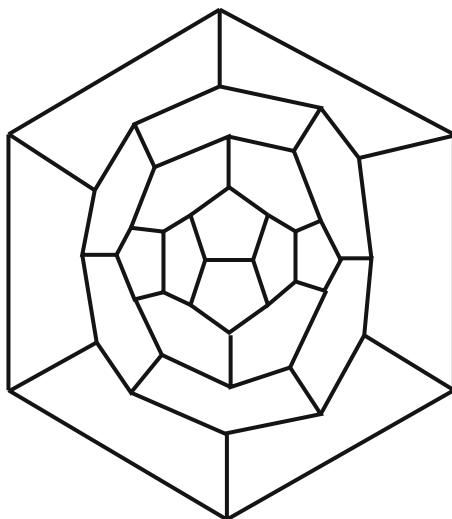
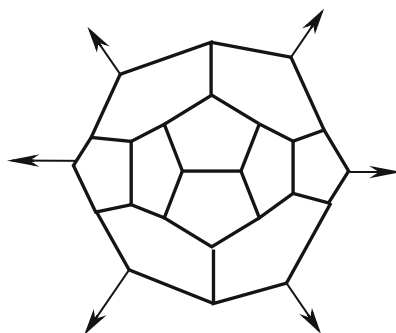


Fig. 16.13 Caps E



16.2.4 Leapfrog Fullerenes

A method (Fowler et al. 1986, 1987) has been described on how to construct a fullerene C_{3n} from a fullerene C_n having the same or even a bigger symmetry group as C_n . This method is called the Leapfrog principle. If one starts with a C_n cluster with icosahedral symmetry, all the new clusters will be of the same symmetry, since this is the biggest symmetry group in 3-dimensional space. In the first step, an extra vertex has to be put into the center of each face of C_n . Then, these new vertices have to be connected with all the vertices surrounding the corresponding face. Then, the dual polyhedron is again a fullerene having $3n$ vertices, 12 pentagonal, and $(3n/2) - 10$ hexagonal faces. From Fig. 16.14, it can be seen that $Le(C_{20}) = C_{60}$.

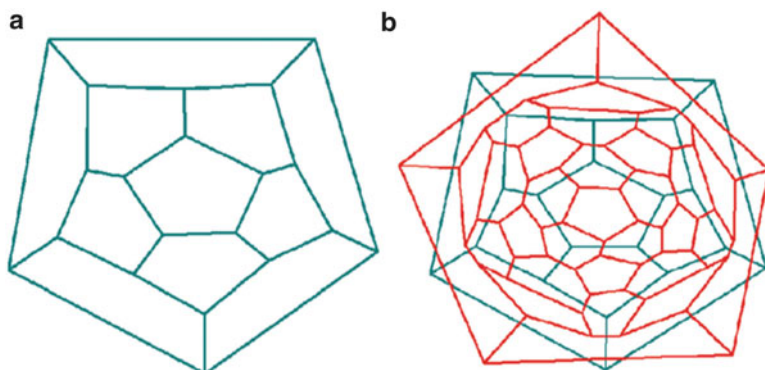


Fig. 16.14 The fullerene C_{20} (a) and $Le(C_{20})$ (b)

16.3 Enumeration of Nanostructures

Enumeration of chemical compounds has been accomplished by various methods. The Polya-Redfield theorem has been a standard method for combinatorial enumerations of graphs, polyhedra, chemical compounds, and so forth. Combinatorial enumerations have found a wide-ranging application in chemistry, since chemical structural formulas can be regarded as graphs or three-dimensional objects. The aim of this section is to enumerate the number of permutational isomers of hetero-fullerenes, see Appendix 16.B.

16.3.1 Hetero-Fullerenes with Small Number of Vertices

To demonstrate our method, we should compute the number of permutational isomers of some well-known fullerenes. In this section, we enumerate hetero-fullerenes $C_{n-k}B_k$ for $n = 24, 80, 84,$ and 150 . Consider at first the molecular graph of the fullerene C_{24} , shown in Fig. 16.15. In Ghorbani et al. (2006b), the symmetry group of C_{24} is computed, and it is isomorphic with the group $Z_2 \times S_4$. So, we have the following theorem without proof:

Theorem 16.4

$$Z(C_{24}, X) = \frac{x_1^{24} + 16x_2^{12} + 8x_3^8 + 12x_4^6 + 8x_6^4 + 3x_1^8x_2^8}{48}.$$

Consider now the molecular graph of the fullerene C_{80} , Fig. 16.16. We have the following theorem:

Fig. 16.15 3-D graph of fullerene C_{24}

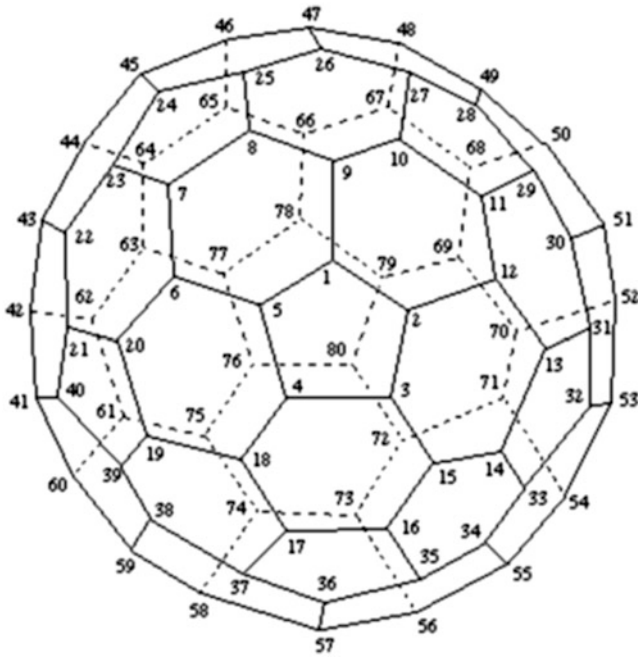
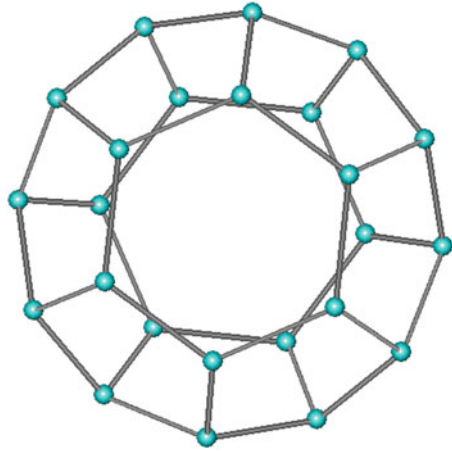


Fig. 16.16 3-D graph of fullerene C_{80}

Theorem 16.5

$$Z(C_{80}, X) = \frac{x_1^{80} + 4x_5^{16} + 6x_2^{40} + 4x_{10}^8 + 5x_1^4x_2^{38}}{20}.$$

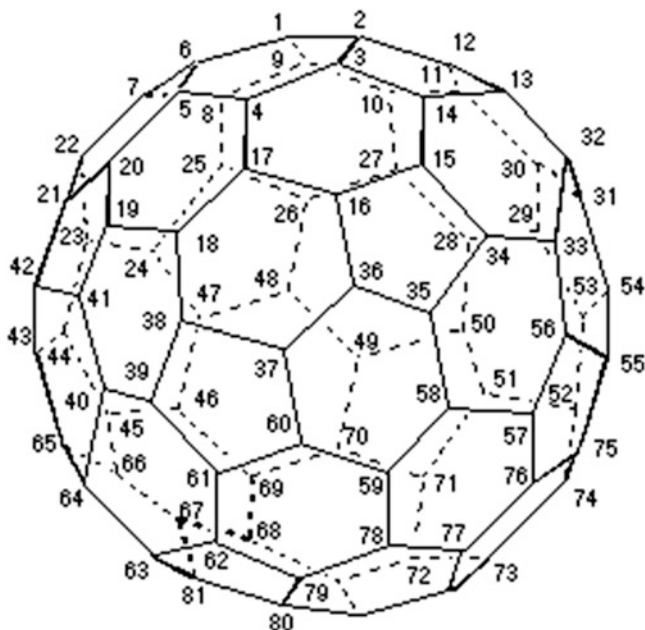


Fig. 16.17 2-D graph of fullerene C_{84}

Proof By using concept of symmetry, one can see that the generators of fullerene graph C_{80} are as follows:

$X = (2,16)(4,14)(5,18)(6,17)(7,20)(8,19)(9,36)(10,35)(11,34)(12,33)(13,49)(15,51)(21,24)(22,23)(25,37)(26,52)(27,39)(28,50)(29,54)(30,53)(31,56)(32,55)(38,40)(41,42)(43,44)(45,60)(46,59)(47,58)(48,57)(62,67)(63,66)(65,77)(68,80)(69,73)(70,79)(71,78)(72,76)(74,75);$

$Y = (1,65)(2,66)(3,68)(4,67)(5,48)(6,45)(7,46)(8,47)(9,42)(10,43)(11,44)(12,41)(13,69)(14,70)(15,72)(16,71)(17,36)(18,33)(19,34)(20,35)(21,30)(22,31)(23,32)(24,29)(25,73)(26,74)(27,76)(28,75)(37,77)(38,78)(39,80)(40,79)(49,61)(50,62)(51,64)(52,63)(53,60)(54,57)(55,58)(56,59).$

By using GAP (The GAP Team 1995) program, one can see that $X^2 = Y^2 = (XY)^{10} = 1$ and $X^{-1}(XY)X = (XY)^{-1}$, and so, this symmetry group is isomorphic with a dihedral group of order 20, namely, D_{20} . Now by using definition of the cycle index, the proof is completed, see Appendix 16.A.

In continuing consider the molecular graph of fullerene C_{84} , Fig. 16.17. We prove that the symmetry group of the C_{84} fullerene is isomorphic to the group S_4 . To do this, suppose G is the symmetry group of this fullerene. Then $G = \langle X, Y \rangle$, where X and Y are the following permutations:

$X = (1, 2)(3, 4)(5, 8)(6, 80)(7, 81)(9, 18)(10, 19)(11, 20)(12, 78)(14, 83)(15, 82)(17, 84)(21, 54)(22, 77)(23, 55)(24, 79)(25, 76)(26, 27)(28, 59)(29, 60)(30, 57)(31, 58)(32, 66)(33, 70)(34, 72)(35, 67)(36, 64)(37, 65)(38, 74)(39, 73)(40, 75)(41, 56)(42, 51)(43, 53)(44, 52)(45, 48)(46, 49)(47, 50)(61, 71)(62, 63)(68, 69),$

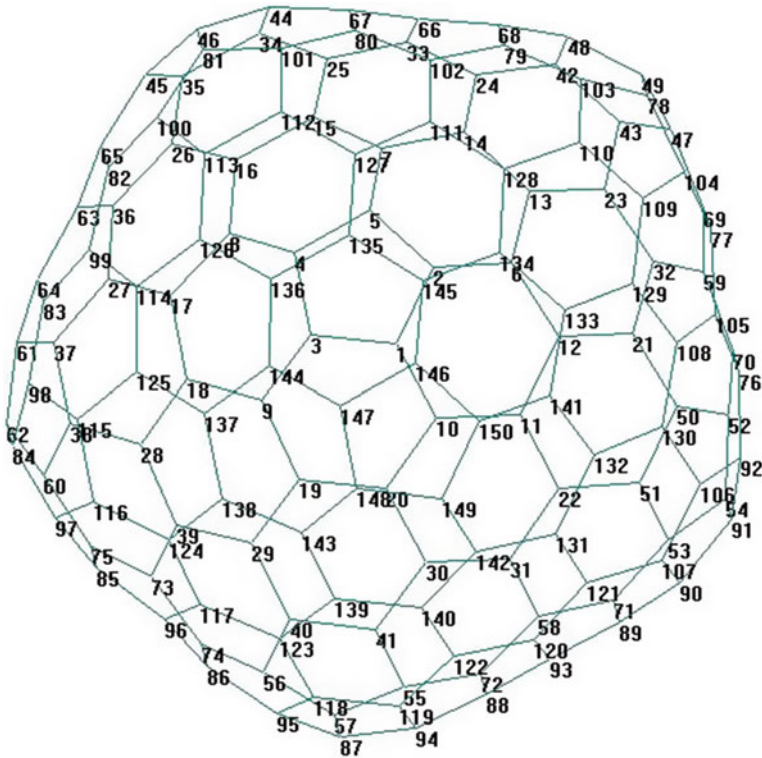


Fig. 16.18 3-D graph of fullerene C_{150}

$Y = (1,76,31,69) (2,59,30,40) (3,79,28,68) (4,58,29,39) (5,51,35,17) (6,84,49,66) (7,83,48,65) (8,80,41,71) (9,77,42,61) (10,78,43,62) (11,81,44,63) (12,82,45,64) (13,55,27,33) (14,20,53,36) (15,19,52,37) (16,54,26,34) (18,56,32,38) (21,72,23,70) (22,74,46,67) (24,73,50,57) (25,75,47,60).$

By using GAP software one can see that this group is isomorphic with S_4 . Thus, the cycle index of G is as follows:

Theorem16. 6

$$Z(C_{84}, X) = \frac{(x_1^{84} + 3x_2^{42} + 8x_3^{28} + 6x_4^{21} + 6x_1^2x_2^{41})}{24}.$$

Proof By means of group action, one can see that the number of conjugacy classes of symmetric group S_4 , on the set of vertices of C_{84} , is 5. The cycle types of its elements are $1^{84}, 2^{42}, 3^{28}, 4^{21}$, and $1^2 2^{41}$, respectively. This completes the proof.

Now consider the molecular graph of the fullerene C_{150} , Fig. 16.18. In Ghorbani et al. (2006b), the symmetry group of C_{150} is computed, and it is isomorphic with dihedral group D_{20} . On the other hand, the 3-dimensional cycle index of C_{150} is computed, and so, we have

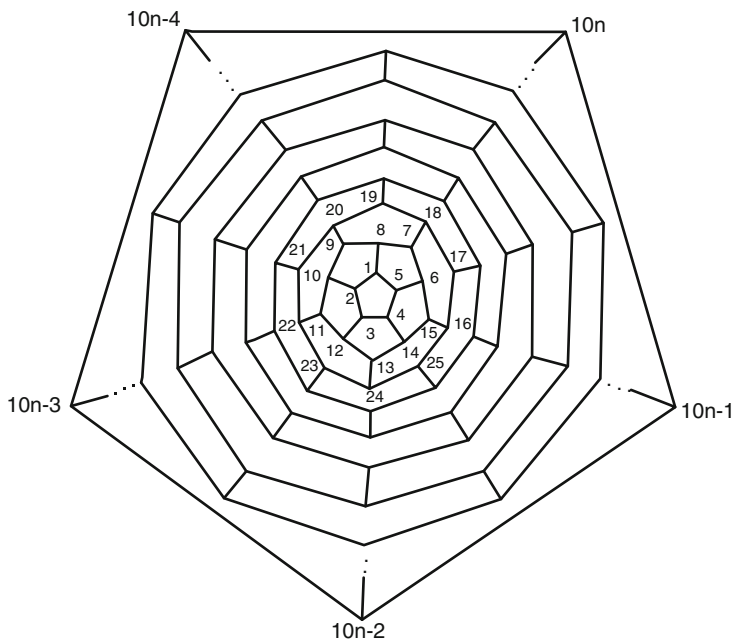


Fig. 16.19 The Schlegel diagram of C_{10n}

Theorem 16.7

$$Z(C_{150}, X) = \frac{(x_1^{150} + 5x_2^{75} + 4x_5^{30} + 5x_1^8x_2^{71} + 4x_5^2x_{10}^{14} + x_1^{10}x_2^{70})}{20}$$

16.3.2 Enumeration of Infinite Classes of Hetero-fullerenes

In this section, we enumerate the number of infinite families of hetero-fullerenes, namely, C_{10n} , C_{12n} , C_{12n+6} , C_{24n} , and C_{40n} fullerenes. Many properties of these classes of fullerenes are studied in Fowler et al. (1995, 2007), Ashrafi et al. (2008a, b, c, 2009), Ashrafi and Ghorbani (2010), Ghorbani (2011, 2012), Ghorbani and Naserpour (2011) and Ghorbani and Ashrafi (2012).

16.3.2.1 C_{10n} Fullerene

This class of fullerenes has exactly $10n$ carbon atoms ($n \geq 2$). That’s why we denote this class of fullerenes by C_{10n} ; see Fig. 16.19. The first member of this class of fullerenes can be obtained by putting $n = 2$, for example, C_{20} . Our problem is reduced to the coloring of the corresponding fullerene graph with $10n$ vertices. By

considering a labeling of its vertices as we did in Fig. 16.19, it is easy to see that the generators of this group are

$$\begin{aligned} \sigma &= (2, 5)(3, 4)(6, 10)(7, 9)(11, 15)(12, 14) \dots (10n - 4, 10n)(10n - 3, 10n - 1), \\ \tau &= (1, 10n - 4, 2, 10n - 3, 3, 10n - 2, 4, 10n - 1, 5, 10n) \dots \\ &\quad (7, 10n - 6, 9, 10n - 14, 11, 10n - 12, 13, 10n - 10, 15, 10n - 8), \end{aligned}$$

where σ fixes elements $1, 8, 19, 30, \dots, 11i - 3, 11i + 2, \dots, 10n - 2, i = 1, 2, \dots, n - 1$ and τ does not have fixed points.

Since $\sigma^2 = \tau^{10} = \text{identity}$ and $\sigma^{-1}\tau\sigma = \tau^{-1}$, the symmetry group G of these fullerenes is isomorphic to the dihedral group of order 20. In the following table the cycle types of elements of G are computed:

Fullerene	Cycle type	#Permutations
C_{10n}	$1^{10n\#}$	1#
	$1^{2n}2^{4n\#}$	5#
	5^{2n}	4#
	2^{5n}	6#
	10^n	4

Thus, the cycle index of G is computed as

$$Z(G, X) = \frac{x_1^{10n} + 5x_1^{2n}x_2^{4n} + 4x_5^{2n} + 6x_2^{5n} + 4x_{10}^n}{20}.$$

16.3.2.2 C_{12n} Fullerene

Now consider the graph of fullerene C_{12n} ($n \geq 2$), Fig. 16.20. This class of fullerenes has exactly $12n$ carbon atoms, and the first member of this class of fullerenes can be obtained by putting $n = 2$, for example, C_{24} . Again our problem is reduced to the coloring of the corresponding fullerene graph with $12n$ vertices. By using the labeling of its vertices, similar to the last example, one can see that the generators of this group are as follows:

$$\begin{aligned} \sigma &= (1, 12n - 5)(2, 12n - 4)(3, 12n - 3) \dots (12n - 24, 12n - 18) \\ &\quad \times (12n - 22, 12n - 19)(12n - 21, 12n - 20), \\ \tau &= (1, 12n - 5, 2, 12n, 3, 12n - 1, 4, 12n - 2, 5, 12n - 3, 6, 12n - 4) \dots \\ &\quad \times (12n - 29, 12n - 25, 12n - 26, 12n - 18, 12n - 20, 12n - 19, 12n - 22, \\ &\quad \times 12n - 21, 12n - 24, 12n - 23, 12n - 28, 12n - 27). \end{aligned}$$

Since $\sigma^2 = \tau^{10} = \text{identity}$ and $\sigma^{-1}\tau\sigma = \tau^{-1}$, the symmetry group G of these fullerenes is isomorphic to the dihedral group of order 24. In the following table, the cycle types of elements of G are computed:

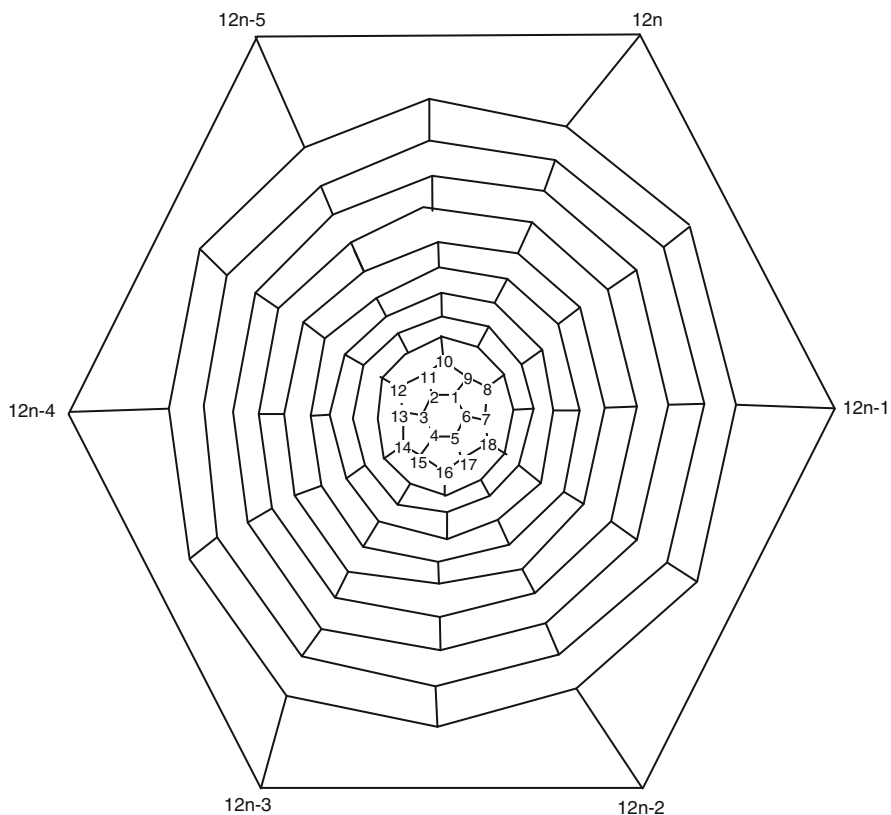


Fig. 16.20 The Schlegel diagram of C_{12n}

Fullerene	Cycle type	#Permutations
C _{12n}	1 ²⁰ⁿ	1
	1 ²ⁿ 2 ⁹ⁿ	5
	2 ¹⁰ⁿ	6
	10 ²ⁿ	4
	5 ⁴ⁿ	4

Thus, the cycle index of G is

$$Z(G, X) = \frac{x_1^{12n} + 6x_1^{2n}x_2^{5n} + 2x_6^{2n} + 2x_3^{4n} + 7x_2^{6n} + 4x_{12}^n + 2x_4^{3n}}{24}$$

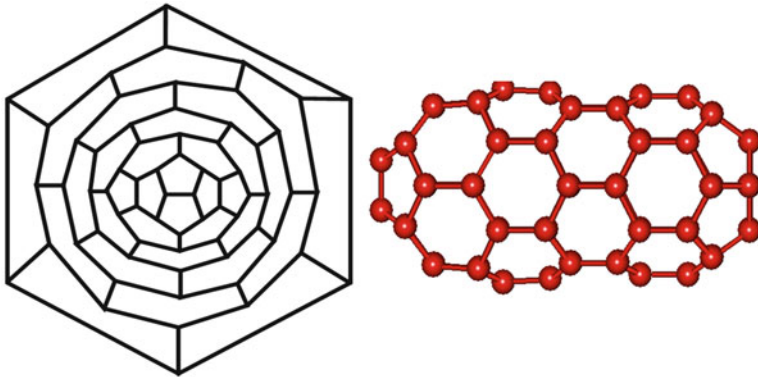


Fig. 16.21 2-D and 3-D graphs of fullerene C_{12n+6} , for $n = 3$

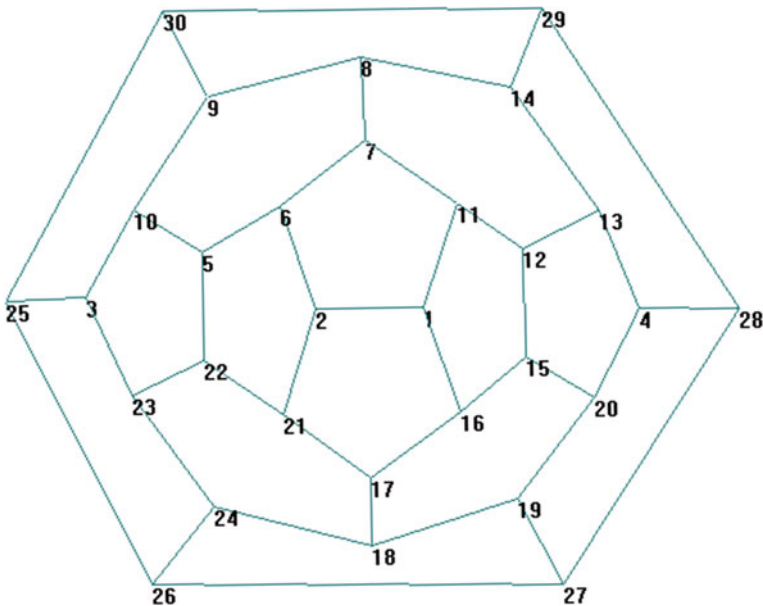


Fig. 16.22 Labeling of fullerene C_{30}

16.3.2.3 C_{12n+6} Fullerene

In this section consider a fullerene graph C_{12n+6} ($n \geq 2$) with $12n + 6$ carbon atoms, Fig. 16.21. As we know from the last discussions, our problem is reduced to the coloring of the corresponding fullerene graph with $12n + 6$ vertices. Consider the labeling of the molecular graph C_{12n+6} , as depicted in Fig. 16.22. The generators of its symmetry group will be indicated by a and b , whereas a stands for a reflection. In the first step, we consider the labeling of vertices of the fullerene C_{30} (the first

member of this class) indicated in Fig. 16.12. The permutation representation of generators of symmetry group acting on the set of vertices is given by

$$a := (29, 30) (9, 14) (10, 13) (6, 11) (5, 12) (1, 2) (22, 15) (21, 16) (19, 24) (26, 27) \\ (20, 23) (3, 4) (25, 28) ;$$

$$b := (26, 30) (10, 23) (5, 22) (6, 21) (7, 17) (8, 18) (9, 24) (11, 16) (12, 15) (14, 19) \\ (13, 20) (27, 29) .$$

The generators satisfy in the following relations:

$$a^2 = b^2 = 1 \quad \text{and} \quad ab = ba.$$

This implies that the symmetry group of fullerene C_{30} is isomorphic with Abelian group $Z_2 \times Z_2$. So its cycle index is as follows:

$$Z(C_{30}, X) = \frac{x_1^{30} + x_1^6 x_2^{12} + x_1^4 x_2^{13} + 4x_2^{15}}{4}.$$

By using GAP [37], one can see that the symmetry group of C_{12n+6} fullerenes has two generators a, b of order 2, satisfying in the following relations:

$$a^2 = b^2 = 1 \quad \text{and} \quad ab = ba.$$

Further, this group is isomorphic to the Abelian group $Z_2 \times Z_2$ of order 4, and the cycle types of elements of S are as in the following table:

Fullerene	Cycle type	#Permutations
C_{12n+6}	$1^{12n+6}\#$	1#
	$1^4 2^{6n+1}$	1
	$1^6 2^{6n}$	1
	2^{6n+3}	1

Thus, the cycle index of symmetry group is computed as

$$Z(G, S) = \frac{x_1^{12n+6} + x_1^4 x_2^{6n+1} + x_1^6 x_2^{6n} + x_2^{6n+3}}{4}.$$

16.3.2.4 C_{24n} Fullerene

In this section we enumerate the number of hetero-fullerenes C_{24n} ($n \geq 3$), Fig. 16.23. The first member of this family of fullerenes is C_{72} , obtained by putting $n = 3$. By considering the molecular graph of the fullerene C_{24n} , one can see that the generators of its symmetry group will be indicated by a and b , whereas a stands for a reflection. In the first step, consider the labeling of vertices of the fullerene

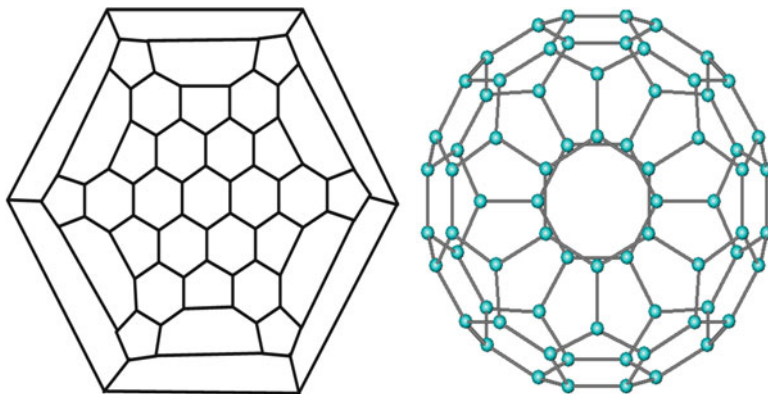
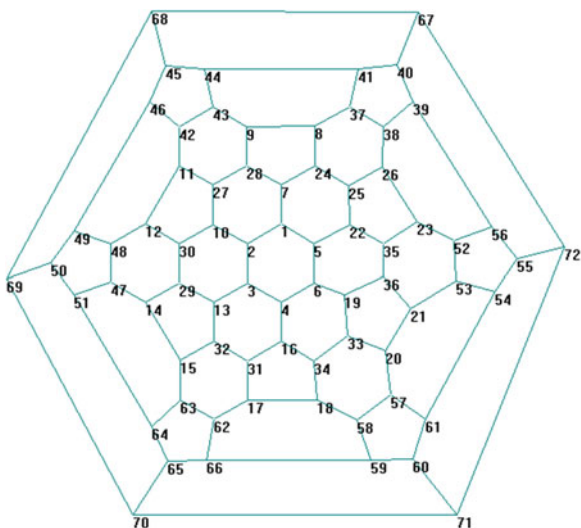


Fig. 16.23 2-D and 3-D graphs of fullerene C_{24n} , for $n = 3$

Fig. 16.24 Labeling of fullerene C_{72}



C_{72} as is indicated in Fig. 16.24, the permutation representation of generators of symmetry group S acting on the set of vertices is given by

$$a = (1,28,31,54,43,64,50,56,39,30,13,25)(2,24,10,44,51,70,59,65,49,37,16,21) \\ (3,9,32,52,60,69,68,66,48,27,19,17)(4,23,42,61,62,72,67,57,38,22,14,8)(5,34,41,63, \\ 53,71,58,47,20,26,7,18)(6,35,11,45,33,55,40,46,15,36,12,29);$$

$$b = (1,25)(2,18)(3,8)(4,17)(5,21)(6,29)(7,24)(9,14)(10,26)(11,36)(12,35)(13,28) \\ (15,45)(16,34)(19,23)(20,44)(22,32)(27,42)(30,31)(33,46)(37,41)(38,52)(39,54)(40, \\ 55)(43,56)(47,51)(48,61)(49,63)(50,64)(53,65)(57,60)(58,70)(59,71)(62,66)(67,69) \\ (68,72).$$

The generators satisfy in the following relations:

$$a^{12} = b^2 = 1 \text{ and } bab = a^{11} = a^{-1}.$$

This implies that the symmetry group of fullerene C_{72} is isomorphic with dihedral group D_{24} . However, by using GAP, one can see that the symmetry group of this family of fullerenes is isomorphic to the dihedral group D_{24} of order 24, and the cycle types of elements of S are as in the following table:

Fullerene	Cycle type	#Permutations
C_{24n}	$1^{24n\#}$	1#
	$1^4 2^{12n-2}$	6
	2^{12n}	7
	3^{8n}	2
	4^{6n}	2
	6^{4n}	2
	12^{2n}	4

Thus, the cycle index of symmetry group S is computed as

$$Z(G, S) = \frac{x_1^{24n} + 7x_2^{12n} + 6x_1^4 x_2^{12n-2} + 2x_3^{8n} + 2x_4^{6n} + 2x_6^{4n} + 4x_{12}^{2n}}{24}.$$

It is easy to see that the generators of the rotational group of fullerene C_{72} are

$$a = (1,2,3,4,5,6)*(7,10,13,16,19,22)*(29,31,33,35,25,27)*(30,32,34,36,26,28)*(8,11,14,17,20,23)*(62,57,52,47,42,37)*(63,58,53,48,43,38)*(12,15,18,21,24,9)*(66,61,56,51,46,41)*(65,60,55,50,45,40)*(64,59,54,49,44,39)*(69,70,71,72,67,68);$$

$$b = (68,69)*(47,53)*(40,65)*(39,66)*(62,38)*(41,64)*(37,63)*(9,8)*(29,28)*(23,12)*(27,30)*(10,22)*(11,24)*(44,61)*(2,6)*(5,3)*(25,32)*(20,15)*(42,58)*(46,59)*(45,60)*(67,70)*(13,19)*(36,33)*(21,14)*(52,48)*(17,18)*(34,35)*(57,43)*(49,56)*(50,55)*(51,54)*(72,71)*(26,31).$$

By using GAP, it is not difficult to see that $a^6 = b^2 = 1$ and $bab = a^5 = a^{-1}$. Hence, this group is isomorphic with dihedral group D_{12} . In general, the cycle types of elements of rotational group R of C_{24n} are as in the following table:

Fullerene	Cycle type of rotational subgroup	#Permutations
C_{24n}	$1^{24n\#}$	1#
	2^{12n-2}	6
	2^{12n}	1
	6^{4n}	2
	3^{8n}	2

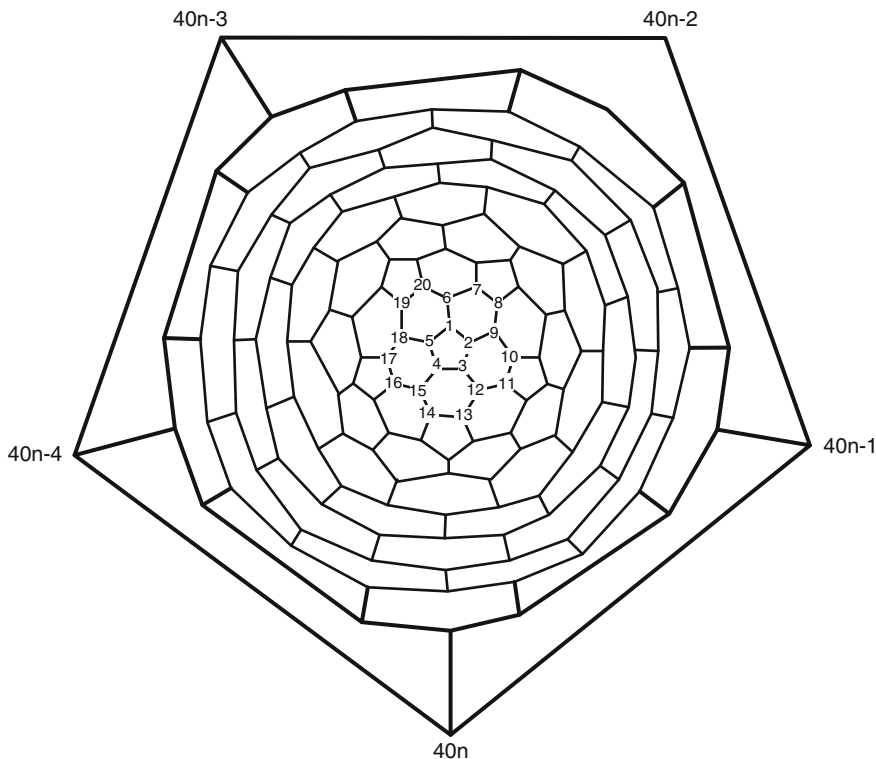


Fig. 16.25 The Schlegel diagram of C_{40n}

This implies that the cycle index of rotational group R is as follows:

$$Z(G, R) = \frac{x_1^{24n} + x_2^{12n} + 6x_1^4 x_2^{12n-2} + 2x_3^{8n} + 2x_6^{4n}}{12}.$$

16.3.2.5 C_{40n} Fullerene

In this section, we consider an infinite class C_{40n} ($n \geq 2$) of fullerene molecules with $40n$ carbon atoms as shown in Fig. 16.25. To compute the number of isomers of these fullerenes, we first compute a permutation representation for the symmetry group of these fullerenes. Consider the graph of fullerene C_{40n} . The generators of this group are

$$\begin{aligned} \sigma &= (2, 5)(3, 4)(7, 10) \dots (10n - 10, 10n - 7)(10n - 4, 10n - 2)(10n - 1, 10n), \\ \tau &= (1, 10n - 4, 3, 10n - 1, 5, 10n - 3, 2, 10n, 4, 10n - 2) \dots \\ &\quad \times (10n - 44, 10n - 36, 10n - 41, 10n - 38, 10n - 43, 10n - 39, \\ &\quad \times 10n - 40, 10n - 37, 10n - 42, 10n - 32). \end{aligned}$$

Since $\sigma^2 = \tau^{10} = \text{identity}$ and $\sigma^{-1}\tau\sigma = \tau^{-1}$, the symmetry group G of these fullerenes is isomorphic to the dihedral group D_{20} of order 20. In the following table, the cycle types of elements of G are computed:

Fullerene	Cycle type	#Permutations
C_{40n}	1^{40n}	1
	$1^{4n}2^{18n}$	5
	2^{20n}	6
	10^{4n}	4
	5^{8n}	4

Thus, the cycle index of G is computed as

$$Z(G, X) = \frac{x_1^{40n} + 5x_1^{4n}x_2^{18n} + 6x_2^{20n} + 4x_{10}^{4n} + 4x_5^{8n}}{20}.$$

16.3.3 Fullerenes Constructed by Leapfrog Operation

Knowing the 3-dimensional cycle index of $S(C_n)$ acting on the sets of vertices, edges, and faces, it is very easy to compute the cycle index for the induced action of $S(C_n)$ on the set of vertices of C_{3n} . We just have to identify the vertices of C_n with the n new hexagonal faces of C_{3n} .

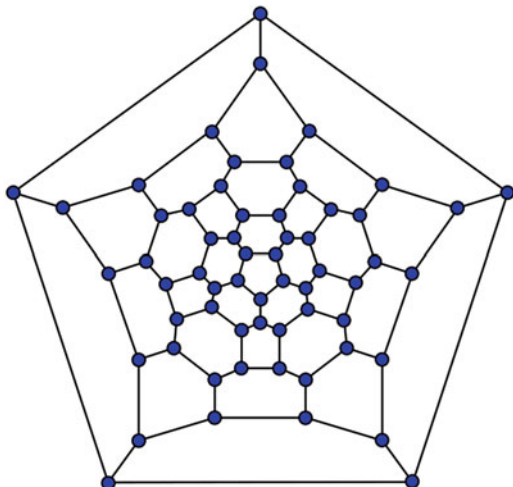
Here, we enumerate the number of hetero-fullerenes of two series of fullerenes constructed by Leapfrog, for example, $C_{3^n \times 20}$ and two classes of $C_{3^n \times 34}$ ($n \geq 0$). From the above discussion our problem is reduced to the coloring of the corresponding fullerene graph with $3^n \times m$ vertices ($m \in \{20, 34\}$).

16.3.3.1 $C_{3^n \times 20}$ Fullerene

Consider the molecular graph of the fullerene $C_{3^n \times 20}$ as depicted in Fig. 16.26. The first member of this class is C_{20} , obtained by putting $n = 0$. It is well-known fact that the symmetry group of C_{20} is isomorphic to the non-Abelian group $I_h = Z_2 \times A_5$ of order 120. So, according to the Leapfrog principle, the symmetry group G of these fullerenes is again isomorphic to the group I_h , and the cycle types of elements of G are as follows:

Fullerene	Cycle type	#Permutations
$C_{3^n \times 20}$	$1^{3^n \times 20}$	1
	$2^{3^n \times 10}$	16
	$1^{3^n-1 \times 4} 2^{3^n-1 \times 28}$	15
	$3^{3^n-1 \times 20}$	20
	$5^{3^n \times 4}$	24
	$6^{3^n-1 \times 10}$	20
	$10^{3^n \times 2}$	24

Fig. 16.26 The Schlegel diagram of $C_{3^n \times 20}$, for $n = 2$



This implies that the cycle index of G can be computed as

$$Z(G, X) = \left(x_1^{20 \times 3^n} + 20(x_3^{20 \times 3^{n-1}} + x_6^{10 \times 3^{n-1}}) + 24(x_5^{4 \times 3^n} + x_{10}^{2 \times 3^n}) \right. \\ \left. + 15x_1^{4 \times 3^{n-1}} x_2^{28 \times 3^{n-1}} + 16x_2^{10 \times 3^n} \right).$$

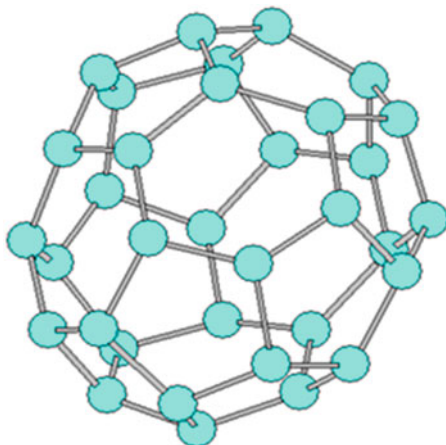
But from the cycle indices, one can compute the number of possible positional isomers, the number of chiral isomers, and the number of orbits under the whole point group I_h . For the number of orbits under the whole point group I_h , we simply note that $Z_{I_h} - P_{I_h}^X = P_{I_h}^1$. We use from this relation and then we obtain the number of $C_{72-k}B_k$ molecules for both symmetry group and rotational group.

16.3.3.2 $C_{3^n \times 34}$ Fullerene

In this section, we compute the number of permutational isomers of a class of fullerenes with $3^n \times 34$ vertices ($n = 0, 1, \dots$); see Fig. 16.27. The symmetry group of the first member of this class of fullerenes, namely, C_{34} , is isomorphic with the non-Abelian group S_3 of order 6. From Leapfrog principle, the symmetry group G of $C_{3^n \times 34}$ fullerene is isomorphic to S_3 , and so, the cycle types of elements of G are as in the following table:

Fullerene	Cycle type	# Permutations
$C_{3^n \times 34}$	$1^{3^n \times 34}$	1
	$1^{6n} 2^{17 \times 3^n - 3n}$	3
	$3^{3^{n-1} \times 34}$	2

Fig. 16.27 3-D graph of fullerene $C_{3^n \times 34}$, $n = 1$



Hence, the cycle index of G is computed as [25]

$$Z(G, X) = \frac{x_1^{34 \times 3^n} + 3x_1^{6n}x_2^{17 \times 3^n - 3n} + 2x_3^{34 \times 3^{n-1}}}{6}.$$

16.3.3.3 $F_{3^n \times 34}$ Fullerene

Finally, we enumerate the number of hetero-fullerenes in a new series of fullerenes constructed by Leapfrog. This class of fullerenes has again $3^n \times 34$ vertices, and we denote this class of fullerenes by $F_{3^n \times 34}$; see Figs. 16.28 and 16.29. Similar to the last discussion, our problem is reduced to the coloring of the corresponding fullerene graph with $3^n \times 34$ vertices. The symmetry group of this fullerene is isomorphic with cyclic group of order 2, namely, Z_2 . From Leapfrog principle, one can see that the symmetry group G of these fullerenes is isomorphic to the group Z_2 of order 2, and the cycle types of elements of G are as in the following table:

Fullerene	Cycle type#	Cycle type#	#Permutations
	n is even	n is odd	
$F_{3^n \times 34}$	$1^{34 \times 3^n \#}$	$1^{34 \times 3^n \#}$	1
	$1^{6 \times 3^{n/2}} 2^{34 \times 3^n - 6 \times 3^{n/2}}$	$1^{4 \times 3^{(n-1)/2}} 2^{34 \times 3^n - 4 \times 3^{(n-1)/2}}$	1

This implies that the cycle index of G is computed as

$$Z(G, X) = \begin{cases} \frac{1}{2} \left(x_1^{34 \times 3^n} + x_1^{6 \times 3^{n/2}} x_2^{17 \times 3^n - 3 \times 3^{n/2}} \right) & 2|n \\ \frac{1}{2} \left(x_1^{34 \times 3^n} + x_1^{4 \times 3^{(n-1)/2}} x_2^{17 \times 3^n - 2 \times 3^{(n-1)/2}} \right) & 2 \nmid n \end{cases}.$$

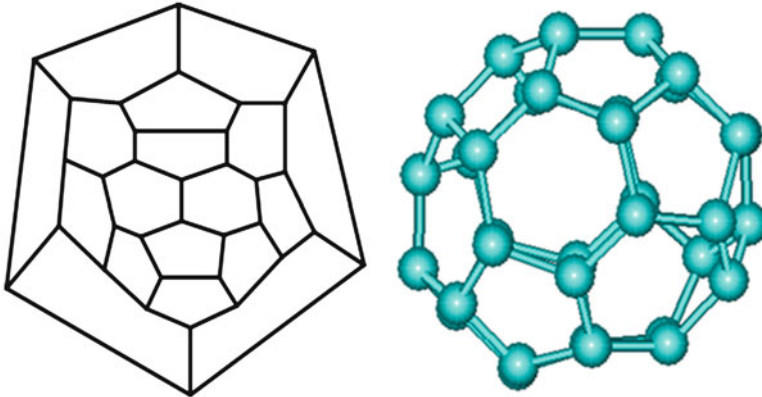


Fig. 16.28 2-D and 3-D graphs of fullerene $C_{3^n \times 34}$, $n = 1$

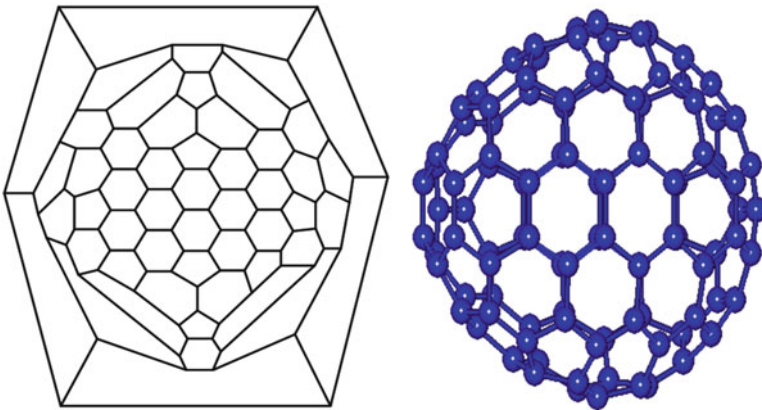


Fig. 16.29 2-D and 3-D graphs of fullerene $C_{3^n \times 34}$, $n = 2$

We can also apply our GAP program to compute the number of hetero-fullerenes $F_{3^n \times 34-k} B_k$.

16.4 Other Structures

Carbon exists in several forms in nature. One is the so-called nanotube which was discovered for the first time in 1991. Unlike carbon nanotubes, carbon nanohorns can be made simply without the use of a catalyst [38, 39]. The tips of these short nanotubes are capped with pentagonal faces; see Fig. 16.30a. Let p , h , n ,

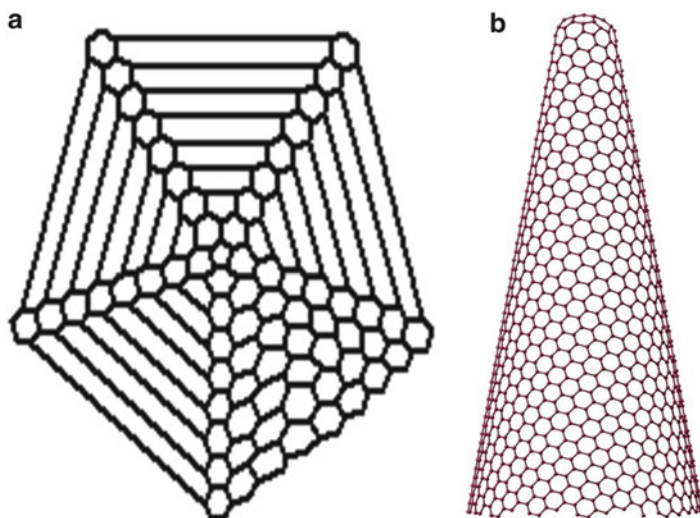


Fig. 16.30 2-D and 3-D graphs of nanohorn H

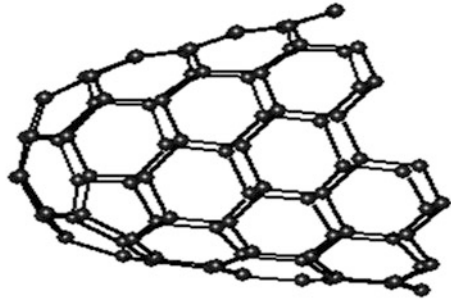
and m be the number of pentagons, hexagons, carbon atoms, and bonds between them, in a given nanohorn H . Then one can see that $n = r^2 + 22r + 41$, $m = \frac{3r^2 + 65r + 112}{2}$ ($r = 0, 1, \dots$), and the number of faces is $f = p + h$. By the Euler's formula $n - m + f = 2$, one can deduce that $p = 5$ and $h = \frac{r^2 + 21r + 40}{2}$, $r = 1, 2, \dots$. From the above discussion our problem is reduced to the coloring of the corresponding nanohorn graph with $n = r^2 + 22r + 41$ vertices. Consider the molecular graph of the nanohorn H ; see Fig. 16.30 for the case of $r = 8$. By using GAP software, one can see that the symmetry group H of these fullerenes is isomorphic to the group C_2 of order 2. Thus, the cycle index of H is computed as

$$Z(H, X) = \frac{\left(x_1^{r^2 + 22r + 41} + x_1^{1+r} x_2^{(r^2 + 21r + 40)/2} \right)}{2}.$$

But from the cycle indices, one can compute the number of possible positional isomers and the number of chiral isomers under the symmetry group C_2 .

In what follows we prepare a GAP program to compute the number of possible positional isomers for H . We mention here that our computations of symmetry properties and cycle indices of molecules were carried out with the use of GAP. In Table 16.14 (Appendix 16.B), we apply this program to compute the number of possible positional isomers for the case of $r = 4$, Fig. 16.31.

Fig. 16.31 Nanohorn H for the case of $r = 4$



16.5 USCI Table

The concept of the table of marks of a finite group was introduced by one of the pioneers of finite groups, William Burnside, in the second edition of his classical book (Burnside 1897). This table describes a characterization of the permutation representations of a group G by certain numbers of fixed points and in some detail the partially ordered set of all conjugacy classes of subgroups of G .

Shinsaku Fujita in some of his leading papers introduced the term markaracter to discuss marks for permutation representations and characters for linear representations in a common basis. To explain, we assume that G is a finite group and M is the mark table of G . By considering the rows and columns of $M(G)$ corresponding to cyclic subgroups of G , a new table $MC(G)$ is obtained. Fujita named this table as markaracter table of G (Fujita 1988a, b, c, d, e, 1999a, b, c, 2000, 2001; El-Basil 2002; Ashrafi and Ghorbani 2008). So, it is a modification of the classical notion of mark table. A dominant markaracter for a cyclic subgroup is defined as a row vector appearing in the resulting markaracter table.

A permutation representation (PR) of a finite group G is produced when the group G acts on a finite set $X = \{x_1, x_2, \dots, x_k\}$. The PR(P_G) is a set of permutations (P_g) on X , each of which is associated with an element $g \in G$. Let H be a subgroup of G . The set of cosets of H in G provides a partition of G , that is, $G = Hg_1 + Hg_2 + \dots + Hg_m$, where $g_1 = I$ (identity) and $g_i \in G$. Consider the set of cosets $\{Hg_1, Hg_2, \dots, Hg_m\}$. For any $g \in G$, the set of permutations of degree m ,

$$(G/H)_g = \begin{pmatrix} Hg_1 & Hg_2 & \dots & Hg_m \\ Hg_1g & Hg_2g & \dots & Hg_mg \end{pmatrix},$$

constructs a permutation representation of G , which is called a coset representation (CR) of G by H and notified as G/H . The degree of G/H is $m = |G|/|H|$, where $|G|$ is the number of elements in G . Obviously, the coset representation G/H is transitive and, in other words, has one orbit.

The Burnside's theorem states that any permutation representation P_G of a finite group G acting on X can be reduced into transitive CRs in accord with equation

$P_G = \sum_{i=1}^s \alpha_i G/G_i$, wherein the multiplicity α_i is a nonnegative integer, where α_i is obtained by solving

$$\mu_j = \sum_{i=1}^s \alpha_i M_{ij} \quad (1 \leq j \leq s) \quad (16.1)$$

where μ_j is the number of fixed points of G_j in P_G , mark of G_j , and the symbol M_{ij} denotes the mark of G_j in G/G_i . Following Burnside, the matrix $M(G) = [M_{ij}]$ is called the table of mark or mark table of G . If we restrict such elements within those of $G_j \leq G$, we have a permutation representation of the subgroup G_j . We call this permutation representation a subduced representation of G/G_i by G_j and designate this by the symbol $G/G_i \downarrow G_j$. According to $P_G = \sum_{i=1}^s \alpha_i G/G_i$, we arrive at a definition of the subduced representation, $G/G_i \downarrow G_j = \{\pi_g | g \in G_j\}$. Since this permutation representation is transitive in general, it can be reduced to a sum of CRs of the group G_j . Then the subduced representation (Fujita 2001) is represented by

$$G/G_i \downarrow G_j = \sum_{k=1}^{v_j} \beta_k^{(ij)} G/G_k^{(j)}, \quad 1 \leq i, j \leq s,$$

where the $\beta_k^{(ij)}$ multiplicity is obtained by solving $\mu_l^{(j)} = \sum_{k=1}^{v_j} \beta_k^{(ij)} m_{kl}^{(j)}$, $1 \leq l \leq v_j$ and $\mu_l^{(j)}$ is the mark of $G_l^{(j)}$ in $G/G_i \downarrow G_j$. A unit-subduced cycle index (USCI) is defined by

$$Z(G/G_i \downarrow G_j; s_d) = Z(G/G_i \downarrow G_j; s_d) = \prod_{k=1}^{v_j} s_{d_{jk}} \beta_k^{(ij)},$$

for each $G/G_i \downarrow G_j$, where the subscript d_{jk} is expressed by $d_{jk} = |G_j| / |G_k^{(j)}|$.

16.5.1 Markaracter Table

In this section we obtain some results about markaracter table. We also use of these results in the next section to compute the markaracter table of symmetry group of icosahedral fullerenes. Suppose the set of fixed points of the subgroup U in the action of G on X is $\text{Fix}_X(U) = \{x \in X : x.u = x; \forall u \in U\}$. Then the ij th entry of mark table of G is as follows:

$$M_{ij}(G) = |\text{Fix}_{G/G_j}(G_i)|.$$

Let also U and V be subgroups of G and $v_G(V, U) = |\{U^g : g \in G, U^g \leq V\}|$; thus, we have

Lemma 16.8 (Pfeiffer 1997)

$$|\text{Fix}_{G/V}(U)| = [G : V]v_G(V, U)/v_G(G, U).$$

Theorem 16.9 *Let G be a finite group and G_1, G_2, \dots, G_s be all nonconjugated subgroups of G in which $|G_1| \leq |G_2| \leq \dots \leq |G_s|$. Then the matrix $M(G)$ is a lower triangular matrix and for all $1 \leq i, j \leq s, M_{ij}|M_{1j}$.*

Proof For the first claim use definition of markaracter table and for the second part use Lemma 16.8.

Lemma 16.10 *Let G be a finite group and $G_i \leq G$ be a subgroup. Then*

$$M_{ii} = (N_G(G_i) : G_i).$$

Proof By using definition of mark table, we have

$$\begin{aligned} M_{ii} &= |\{gG_i : \forall x \in G_i, x.gG_i = gG_i\}| \\ &= |\{gG_i : \forall x \in G_i, g^{-1}xgG_i = G_i\}| \\ &= |\{gG_i : \forall x \in G_i, x \in gG_i g^{-1}\}| \\ &= |\{gG_i : G_i = gG_i g^{-1}\}|. \end{aligned}$$

Corollary 16.11 *If G_j be a normal subgroup of G ($1 \leq j \leq s$), then*

$$M_{ij} = \begin{cases} |G|/|G_j| & G_i \subseteq G_j \\ 0 & \text{otherwise} \end{cases}.$$

Proof Similar to proof of Lemma 16.10, it is easy to see that $M_{ij} = |\{gG_j : G_i \subseteq g^{-1}G_jg\}|$. Since G_j is normal, then $g^{-1}G_jg = G_j$. This completes the proof.

Theorem 16.12 *Table of marks of a non-Abelian group of order pq ($p > q$), where p and q are prime numbers, is as follows:*

Mark table	G_1	G_2	G_3	G_4
G/G_1	pq	0	0	0
G/G_2	p	1	0	0
G/G_3	q	0	q	0
G/G_4	1	1	1	1

Proof It is easy to see that all nonconjugated subgroups of G are $G_1 = ()$, $G_2 = Q$, $G_3 = P$, and $G_4 = G$, in which $|Q| = q$ and $|P| = p$. By Sylow theorem, one can see that $P \triangleleft G$. So, by using Lemma 16.10, we have $M_{12} = p$, $M_{22} = 1$, and $M_{32} = M_{42} = 0$. On the other hand, $Q \not\triangleleft G$, because G is non-Abelian; hence, $M_{23} = M_{43} = 0$ and $M_{13} = M_{33} = 0$.

Fig. 16.32 The skeleton of naphthalene

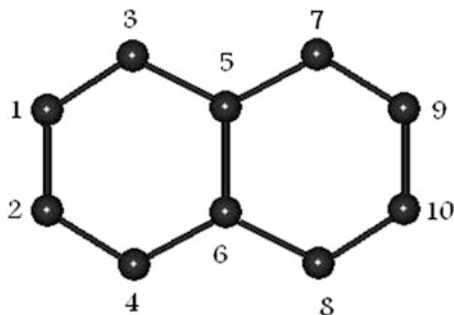


Table 16.1 Mark table of the point group $Z_2 \times Z_2$

Mark table	G_1	G_2	G_3	G_4	G_5
$G/(G_1)$	4	0	0	0	0
$G/(G_2)$	2	2	0	0	0
$G/(G_3)$	2	0	2	0	0
$G/(G_4)$	2	0	0	2	0
$G/(G_5)$	1	1	1	1	1

Table 16.2 Markcharacter table of the point group $Z_2 \times Z_2$

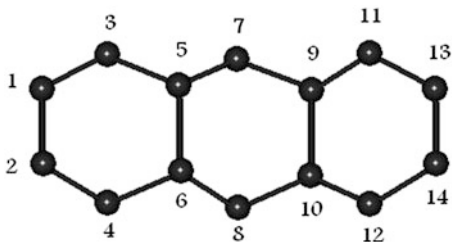
Mark table	G_1	G_2	G_3	G_4
$G/(G_1)$	4	0	0	0
$G/(G_2)$	2	2	0	0
$G/(G_3)$	2	0	2	0
$G/(G_4)$	2	0	0	2

16.5.2 Benzenoid Chains

Consider the skeleton of naphthalene, Fig. 16.32. Generators of its symmetry group are λ and ω , where $\lambda = (1, 9)(2, 10)(3, 7)(4, 8)$ and $\omega = (1, 2)(3, 4)(5, 6)(7, 8)(9, 10)$. The subgroups of G are $G_1 = \langle () \rangle$, $G_2 = \langle \lambda \rangle$, $G_3 = \langle \omega \rangle$, $G_4 = \langle \lambda\omega \rangle$, and $G_5 = G$. This group is isomorphic with $Z_2 \times Z_2$, where Z_2 is a group of order 2. Since every group of order 4 is Abelian and then $Z_2 \times Z_2$, by using Corollary 16.11, for any subgroup G_i of $Z_2 \times Z_2$, $M_{ij} = 0$ or $|Z_2 \times Z_2|/|G_i|$. But for pure subgroup H of $Z_2 \times Z_2$, $|H| = 2$. This implies that the entries of mark table are 1, 2, and 4. By Theorem 16.9, $M_{11} = 4$ and $M_{i1} = 0$ for $2 \leq i \leq 4$. Also $M_{4j} = 1$ for $1 \leq j \leq 4$. Since all subgroups in Abelian group are normal, by using Lemma 16.10, we have $M_{12} = M_{22} = 2$ and $M_{32} = M_{42} = 0$. Using again Lemma 16.10, it is easy to see that $M_{13} = M_{33} = 2$ and $M_{23} = M_{43} = 0$. In Tables 16.1 and 16.2, the mark table and markcharacter table of this group are computed. On the other hand, the number of (μ_j) of fixed points is obtained by a geometrical examination of Eq. (16.1):

$$(10, 2, 0, 0, 0) = (\alpha_{G_1}, \alpha_{G_2}, \alpha_{G_3}, \alpha_{G_4}, \alpha_{G_5}) \times \begin{pmatrix} 4 & 0 & 0 & 0 \\ 2 & 2 & 0 & 0 \\ 2 & 0 & 2 & 0 \\ 2 & 0 & 0 & 2 \\ 1 & 1 & 1 & 1 \end{pmatrix}.$$

Fig. 16.33 The skeleton of anthracene



So, $\alpha_{G_5} = \alpha_{G_4} = \alpha_{G_3} = 0$, $\alpha_{G_1} = 2, \alpha_{G_2} = 1$, and $P_G = 2G (/G_1) + G (/G_2)$. This implies that sub-orbits of X are

$$X_{11} = \{1, 2, 9, 10\}, X_{21} = \{5, 6\}, X_{12} = \{3, 4, 7, 8\}.$$

With a similar discussion, the generators of the point group of anthracene skeleton (Fig. 16.33) are δ and γ , where

$$\begin{aligned} \gamma &= (1, 13)(2, 14)(3, 11)(4, 12)(5, 9)(6, 10), \\ \eta &= (1, 2)(3, 4)(5, 6)(7, 8)(9, 10)(11, 12)(13, 14). \end{aligned}$$

The subgroups of G are $G_1 = \langle () \rangle$, $G_2 = \langle \gamma \rangle$, $G_3 = \langle \eta \rangle$, $G_4 = \langle \gamma\eta \rangle$, and $G_5 = G$. Also, the mark table and markaracter table of this group are the same of naphthalene. The number of (μ_j) of fixed points is

$$(10, 2, 0, 0, 0) = (\alpha_{G_1}, \alpha_{G_2}, \alpha_{G_3}, \alpha_{G_4}, \alpha_{G_5}) \times \begin{pmatrix} 4 & 0 & 0 & 0 & 0 \\ 2 & 2 & 0 & 0 & 0 \\ 2 & 0 & 2 & 0 & 0 \\ 2 & 0 & 0 & 2 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix}.$$

Hence, $\alpha_{G_5} = \alpha_{G_4} = \alpha_{G_3} = 0$, $\alpha_{G_2} = 1$, $\alpha_{G_1} = 2$, and then by the similar way, one can see that $P_G = 2G (/G_1) + G (/G_2)$. Thus, the sub-orbits of X are $X_{11} = \{1, 2, 13, 14\}$, $X_{21} = \{7, 8\}$, $X_{22} = \{5, 6, 9, 10\}$, and $X_{12} = \{3, 4, 11, 12\}$.

In generally, consider the graph of benzenoid chain with exactly n hexagons, Fig. 16.34. Its point group is isomorphic with group $Z_2 \times Z_2$ generated by α and β where

$$\begin{aligned} \alpha &= (1, 3)(2, 4) \cdots (4n - 4, 4n - 2)(4n - 3, 4n - 1), \\ \beta &= (1, 2)(3, 4) \cdots (4n - 1, 4n)(4n + 1, 4n + 2). \end{aligned}$$

This implies the mark table and markaracter table of a benzenoid chain with exactly n hexagons are similar to anthracene and naphthalene; see Ghorbani et al. (2012) for more details.

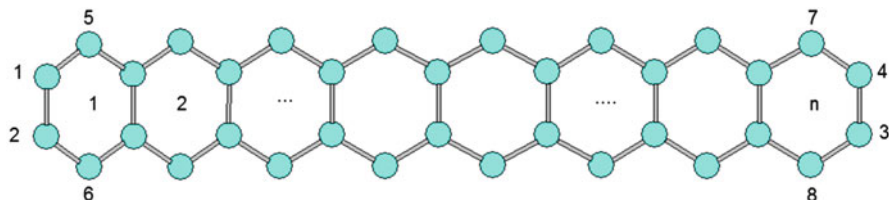
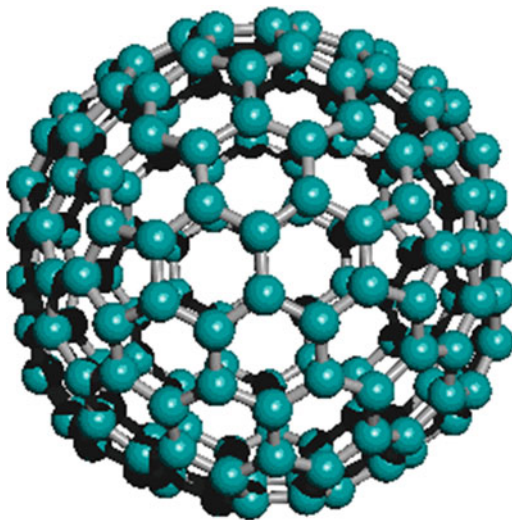


Fig. 16.34 The skeleton of a benzenoid chain with n hexagons

Fig. 16.35 The fullerene $C_{3^n \times 20}$ for $n = 2$



Now is the time to compute the markaracter table and then *USCI* table of fullerenes in a series of fullerenes constructed by Leapfrog. From the above discussion, the problem is reduced to compute the markaracter table and *USCI* table of the corresponding fullerene graph with 20 vertices. Consider the molecular graph of the fullerene $C_{3^n \times 20}$, Fig. 16.35. From the Leapfrog principle, it can be seen that the symmetry group G of these fullerenes is isomorphic to the group $I_h = Z_2 \times A_5$ of order 120, where A_5 is an alternating group on five symbols. Consider the fullerene graph C_{20} , depicted in Fig. 16.36, with symmetry group $Z_2 \times A_5$. By using computer algebra system GAP, one can see that this group has exactly 22 conjugacy classes of subgroups and the generators of its symmetry group

```
gap > List(ConjugacyClassesSubgroups(G), x -> Elements(x)); z := Length(aa);
```

Hence, this group has eight nonconjugated cyclic subgroups as follows:

$$G_1 = \langle () \rangle,$$

$$G_2 = \langle (1,9)(2,16)(3,10)(4,13)(5,17)(6,14)(7,15)(8,18)(11,20)(12,19) \rangle,$$

$$G_3 = \langle (1,3)(2,18)(4,15)(5,17)(6,14)(7,13)(8,16)(9,10)(11,19)(12,20) \rangle,$$

$$G_4 = \langle (2,4)(5,6)(7,8)(11,19)(12,20)(13,16)(14,17)(15,18) \rangle,$$

Fig. 16.36 The fullerene C_{20}

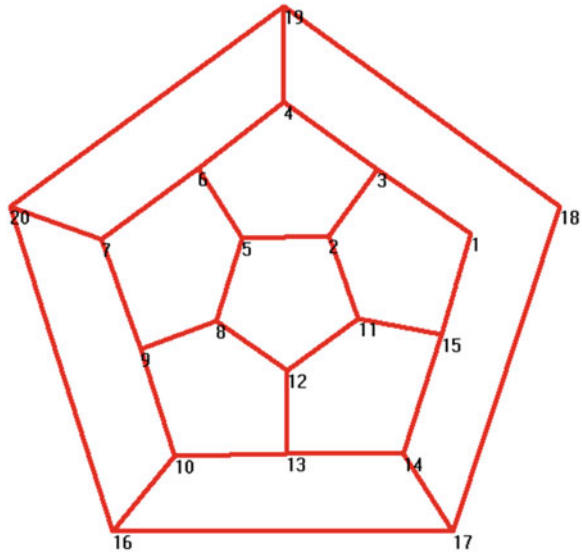


Table 16.3 Mark table of the symmetry group $Z_2 \times A_5$

Markaracter table	G_1	G_2	G_3	G_4	G_5	G_6	G_7	G_8
G/G_1	120	0	0	0	0	0	0	0
G/G_2	60	60	0	0	0	0	0	0
G/G_3	60	0	4	0	0	0	0	0
G/G_4	60	0	0	4	0	0	0	0
G/G_5	40	0	0	0	4	0	0	0
G/G_6	24	0	0	0	0	4	0	0
G/G_7	20	20	0	0	2	0	2	0
G/G_8	12	12	0	0	0	2	0	2

$$G_5 = \langle (2,14,19)(3,15,18)(4,11,17)(5,13,20)(6,12,16)(7,8,10) \rangle,$$

$$G_6 = \langle (1,2,8,10,17)(3,5,9,16,18)(4,6,7,20,19)(11,12,13,14,15) \rangle,$$

$$G_7 = \langle (2,14,19)(3,15,18)(4,11,17)(5,13,20)(6,12,16)(7,8,10), (1,9)(2,16)(3,10)(4,13)(5,17)(6,14)(7,15)(8,18)(11,20)(12,19) \rangle,$$

$$G_8 = \langle (1,2,8,10,17)(3,5,9,16,18)(4,6,7,20,19)(11,12,13,14,15), (1,9)(2,16)(3,10)(4,13)(5,17)(6,14)(7,15)(8,18)(11,20)(12,19) \rangle$$

By considering the rows and columns of $M(Z_2 \times A_5)$ corresponding to cyclic subgroups of $Z_2 \times A_5$, the markaracter table is obtained as follows (Table 16.3).

According to Fujita’s theorem for computing the $USCI$ table of group $G = Z_2 \times A_5$, it is enough to compute the inverse of markaracter table of every subgroup H , and then $M(G)M^{-1}(H)$ results the corresponded column of $USCI$ table. For example, if $H = G_2$, then the mark table and its inverse are as follows (Table 16.4):

Table 16.4 Mark table and its inverse of group Z_2

$M(G)$	G_1	G_2		$M^{-1}(G)$	G_1	G_2
G/G_1	2	0	\Rightarrow	G/G_1	1/2	0
G/G_2	1	1		G/G_2	-1/2	1

So, the entries of the second column of *USCI* table are as follows:

$$\begin{pmatrix} 120 & 0 \\ 60 & 60 \\ 60 & 0 \\ 60 & 0 \\ 40 & 0 \\ 30 & 0 \\ 30 & 0 \\ 30 & 30 \\ 24 & 0 \\ 20 & 0 \\ 20 & 0 \\ 20 & 20 \\ 15 & 15 \\ 12 & 0 \\ 12 & 0 \\ 12 & 12 \\ 10 & 0 \\ 10 & 10 \\ 6 & 6 \\ 5 & 5 \\ 2 & 0 \\ 1 & 1 \end{pmatrix} \times \begin{pmatrix} 1/2 & 0 \\ -1/2 & 1 \end{pmatrix} = \begin{pmatrix} S_2 & S_1 \\ 60 & 0 \\ 0 & 60 \\ 30 & 0 \\ 30 & 0 \\ 20 & 0 \\ 15 & 0 \\ 15 & 0 \\ 0 & 30 \\ 12 & 0 \\ 10 & 0 \\ 10 & 0 \\ 0 & 20 \\ 0 & 15 \\ 6 & 0 \\ 6 & 0 \\ 0 & 12 \\ 5 & 0 \\ 0 & 10 \\ 0 & 6 \\ 0 & 5 \\ 1 & 0 \\ 0 & 1 \end{pmatrix} \Rightarrow \text{USCI}(G)_j \begin{pmatrix} S_2^{60} \\ S_1^{60} \\ S_2^{30} \\ S_2^{30} \\ S_2^{20} \\ S_2^{15} \\ S_2^{15} \\ S_1^{30} \\ S_2^{12} \\ S_2^{10} \\ S_2^{10} \\ S_1^{20} \\ S_1^{15} \\ S_2^6 \\ S_2^6 \\ S_1^{12} \\ S_2^5 \\ S_1^{10} \\ S_1^6 \\ S_1^5 \\ S_2 \\ S_1 \end{pmatrix}$$

It should be noted that we use from GAP software to compute the mark table of the group $G = Z_2 \times A_5$ by the following function:

```
gap> Display(TableOfMarks(DirectProduct(CyclicGroup(2),AlternatingGroup(5)))).
```

By a similar method, one can compute the whole of *USCI* table. This table is reported in the Appendix 16.C.

Appendices

Appendix 16.A: GAP Programs

This software was constructed by the GAP team in Aachen. GAP is a system for computational discrete algebra, with particular emphasis on computational group theory. GAP provides a programming language, a library of thousands of functions implementing algebraic algorithms written in the GAP language as well as large data libraries of algebraic objects. GAP is used in research and teaching for studying groups and their representations, rings, vector spaces, algebras, combinatorial structures, and more; see The GAP Team (1995).

A GAP Program for Enumerating the Hetero-fullerenes

```

h:=function (f,g)
  local t,i,tt;
    Print("Coefficients of f are:", "\n");
    t:=CoefficientsofLaurentPolynomial(f);
    for i in t[1] do
      Print(i, "\n");
    od;
    Print("Coefficients of g are:", "\n");
    tt:=CoefficientsofLaurentPolynomial(g);
  for i in tt[1] do
    Print(i, "\n");
  od;
  return();
end;

```

A Gap Program for Counting the Number of Nanohorn H

```

f:=function (n)
  locals,i,f,x,t;
    x:=Indeterminate(Rationals, "x");
    f:=((1+x)^(89)+(1+x)^5*(1+x^2)^(42))/2;
    t:= CoefficientsOfLaurentPolynomial(f);
  Print("*****", "\n");
  Print("\n");
  Print("Number of Molecules for Symmetry Group =", "\n");
  for i in t[1] do
    Print(i, "\n");
  od;
  Print("*****", "\n");
  return;end;

```

Appendix 16.B: Number of Permutational Isomers**Table 16.5** The number of $C_{20-k}B_k$ molecules

$k, 20 - k$	Number of $C_{20-k}B_k$ molecules for symmetry group
0,20	1
1,19	1
2,18	12
3,17	51
4,16	265
5,15	931
6,14	2972
7,13	7365
8,12	15730
9,11	27582
10,10	41544

Table 16.6 Number of $C_{24-k}B_k$ molecules

$k, 24 - k$	Number of $C_{24-k}B_k$ molecules for symmetry group	Number of $C_{24-k}B_k$ molecules for rotational group
0,24	1	1
1,23	2	2
2,22	19	30
3,21	96	170
4,20	489	924
5,19	1826	3542
6,18	5775	11350
7,17	14586	28842
8,16	31034	61578
9,15	54814	108968
10,14	82358	163900
11,13	104468	208012
12,12	113434	225898

Table 16.7 Number of $C_{30-k}B_k$ molecules

$k, 30 - k$	Number of $C_{30-k}B_k$ molecules for symmetry group	Number of $C_{30-k}B_k$ molecules for rotational group
0,30	1	1
1,29	3	3
2,28	51	33
3,27	406	226
4,26	2793	1467
5,25	14253	7287
6,24	59605	30173
7,23	203580	102468
8,22	585975	294255
9,21	1430715	717299
10,20	3006009	1506051
11,19	5462730	2735358
12,18	8651825	4331275
13,17	11975985	5994081
14,16	14545485	7279821
15,15	15511760	7762876

Table 16.8 Number of $C_{34-k}B_k$ molecules

$k, 34 - k$	Number of $C_{34-k}B_k$ molecules for symmetry group
0,34	1
1,33	6
2,32	102
3,31	1001
4,30	7801
5,29	46376
6,28	224509
7,27	896621
8,26	3027224
9,25	8741931
10,24	21857839
11,23	47682960
12,22	91398638
13,21	154664070
14,20	232005664
15,19	309328074
16,18	367339214
17,17	388934370

Table 16.9 The number of $C_{60-k}B_k$ molecules

$k, 60 - k$	Number of $C_{60-k}B_k$ molecules for rotational group	Number of $C_{60-k}B_k$ molecules for symmetry group	Number of orbits under whole point group I_h
0,60	1	1	0
1,59	1	1	0
2,58	23	37	14
3,57	303	577	274
4,56	4190	8236	4046
5,55	45718	91030	45312
6,54	418470	835476	417006
7,53	3220218	6436782	3216564
8,52	21330558	42650532	21319974
9,51	123204921	246386091	123181170
10,50	628330629	1256602779	628272150
11,49	2855893755	5711668755	2855775000
12,48	11661527055	23322797475	11661270420
13,47	43057432740	86114390460	43056957720
14,46	144549869700	289098819780	144548950080
15,45	443284859624	886568158468	443283298844
16,44	1246738569480	2493474394140	1246735824660
17,43	3226849468425	6453694644705	3226845176280
18,42	7708584971055	15417163018725	7708578047670
19,41	17040023323785	34080036632565	17040013308780
20,40	34932048763560	69864082608210	34932033844650
21,39	66537224405790	133074428781570	66537204375780
22,38	117952355252550	235904682814710	117952327562160
23,37	194877787472550	389755540347810	194877522875260
24,36	300436595453640	600873146368170	300436550914530
25,35	432628675734195	865257299572455	432628623838260
26,34	582384767014701	1164769471671687	582384704656986
27,33	733373386161407	1466746704458899	733373318297492
28,32	864332935668892	1728665795116244	864332859447352
29,31	953746664302456	1907493251046152	953746586743696
30,30	985538239868528	1971076398255692	985538158387164

Table 16.10 The number of $C_{72-k}B_k$ molecules

$k, 72 - k$	Number of $C_{72-k}B_k$ molecules for rotational group	Number of $C_{72-k}B_k$ molecules for symmetry group
0,72	1	1
1,71	4	8
2,70	127	236
3,69	2522	5044
4,68	43243	86168
5,67	583576	1167152
6,66	6514407	13025244
7,65	61386116	122772232
8,64	498746918	997464358
9,63	3546427742	7092855484
10,62	22342414424	44684640352
11,61	125928884480	251857768960
12,60	640138180164	1280275386294
13,59	2954479373440	5908958746880
14,58	12451019242744	24902034311648
15,57	48143925115958	96287850231916
16,56	171512731027768	343025446924856
17,55	564983065793776	1129966131587552
18,54	1726337142727692	3452674238383744
19,53	4906431753373920	9812863506747840
20,52	13002044149467636	26004088171840416
21,51	32195537606713866	64391075213427732
22,50	74635109937400116	149270219574397584
23,49	162250238419042800	324500476838085600
24,48	331260903551195565	662521806476549181
25,47	636020933801574048	1272041867603148096
26,46	1149730149855983496	2299460298556572192
27,45	1958799512979179380	3917599025958358760
28,44	3148070646470848632	6296141291043543360
29,43	4776383047609873920	9552766095219747840
30,42	6846149035990297176	13692298069196643072
31, 41	9275427723456099744	18550855446912199488
32, 40	11884141772331102516	23768283541008261684
33, 39	14405020327110683172	28810040654221366344
34,38	16523405671536565290	33046811338774382280
35,37	17939697583328247888	35879395166656495776
36,36	18438022518784399786	36876045033031223812

Table 16.11 The number of $C_{80-k}B_k$ molecules

$k, 80 - k$	Number of $C_{80-k}B_k$ molecules for symmetry group
0,80	1
1,79	5
2,78	181
3,77	4147
4,76	79546
5,75	1202745
6,74	15031147
7,73	158844959
8,72	1449435558
9,71	11595097111
10,70	82325041251
11,69	523884428977
12,68	3012334769066
13,67	15756817617163
14,66	75407624568509
15,65	331793506218077
16,64	1347911111443259
17,63	5074488744913588
18,62	17760710591159316
19,61	57956002543262252
20,60	176765807739834016
21,59	505045163808913156
22,58	1354439302981356268
23,57	3415542587404475164
24,56	8111913645381087112
25,55	18170686559985988028
26,54	38437990801023264444
27,53	76875981591517458868
28,52	145515250872462217832
29,51	260923898098627253308
30,50	443570626773816168644
31,49	715436494770338700580
32,48	1095512132628624165470
33,47	1593472192879288312630
34,46	2202740972528516942390
35,45	2895030992423701444170
36,44	3618788740556990692460
37,43	4303424448183910977070
38,42	4869664507190697241610
39,41	5244254084621907482050
40,40	5375360436777969680320

Table 16.12 The number of $C_{84-k}B_k$ molecules

$k, 84 - k$	Number of $C_{84-k}B_k$ molecules for symmetry group
0,84	1
1,83	4
2,82	161
3,81	4000
4,80	80724
5,79	1286744
6,78	16941162
7,77	188728904
8,76	1816506426
9,75	15339084436
10,74	115043064318
11,73	773924297744
12,72	4708039172851
13,71	26075285193864
14,70	132238945055628
15,69	617115040987920
16,68	2661308609905260
17,67	10645234310343900
18,66	39623927700233625
19,65	137641011605240660
20,64	447333287699520054
21,63	1363301447106388504
22,62	3903999598530800496
23,61	10523825001987843104
24,60	26748055213518461739
25,59	64195332506438811392
26,58	145674023765218737768
27,57	312929384372799539932
28,56	637034818189367985288
29,55	1230136200620880101792
30,54	2255249701142983248018
31,53	3928499479377611057376
32,52	6506577262729079657604
33,51	10252788413950491335316
34,50	15379182620943916403538
35,49	21970260887002103927160
36,48	29903966207337904208345
37,47	38794334539178147226960
38,46	47982466403762890020840
39,45	56594703963337371170880
40,44	63669041958809577715404
41,43	68327752345967341397280
42,42	69954603592363988835420

Table 16.13 The number of $C_{150-k}B_k$ molecules

$k, 150 - k$	Number of $C_{150-k}B_k$ molecules for symmetry group
0,150	1
1,149	10
2,148	608
3,147	27762
4,146	1015132
5,145	29587626
6,144	714908767
7,143	14705679304
8,142	262861756418
9,141	4147359263564
10,140	58477733568550
11,139	744261878846444
12,138	8621033058155532
13,137	91515579793041740
14,136	895545312914462338
15,135	8119610820294861024
16,134	68509216265755052423
17,133	540013822200718017274
18,132	3990102130481989637532
19,131	27720709537206337672482
20,130	181570647467256032286270
21,129	1124008770030069888944122
22,128	6590778696986152507958223
23,127	36679116226676561530421568
24,126	194093656699453439146865712
25,125	978232029765102584306831360
26,124	4703038604639712304854528992
27,123	21599140258344705503374136608
28,122	94881937563441939987580122208
29,121	399158495956546227316507706912
30,120	1609939267024733028272418627950
31,119	6232022969127988937630220494912
32,118	23175335416444696549270781265772
33,117	82869381186074941227257032574344
34,116	285168164669728433394496223305568
35,115	945128774333956983333854159548184
36,114	3019161362455695793849475118633168
37,113	9302280954593224550068789712330120
38,112	27662045996553535806719975891990092
39,111	79439721836256307048558318405485664
40,110	220445228095611251123048465578384610
41,109	591438416841883842130309387714175824
42,108	1534923510375365207042049180063976208
43,107	3855156723733475398082512651736762064
44,106	9375040214533678803733124039197920912
45,105	22083428060901554502735720945545628656

(continued)

Table 16.13 (continued)

$k, 150 - k$	Number of $C_{150-k}B_k$ molecules for symmetry group
46,104	50407824921623113527709622686290336312
47,103	111540718975506463949387235122286925152
48,102	239347792801607620535970453784351147068
49,101	498234180933958720246386671215627247400
50,100	1006433045486596614856890256732735499706
51,99	1973398128405091401582018701627687530440
52,98	3757046436771231706787858155503142213536
53,97	6946991524595862401059693903626311024424
54,96	12478855146033308386976398312593227196124
55,95	21781274436712683729716490061393340262312
56,94	36950376276566159898459691595847481631824
57,93	60935708245565246147909753636832722794208
58,92	97707256324785653305903584594286513690016
59,91	152357077658987798374692146630075734026208
60,90	231074901116131494201332210976565629621470
61,89	340930181974620237345396728498808495051488
62,88	489399777350664534253556972312070143515984
63,87	683606038204102841495979056024525881046720
64,86	929276958183702300158285743952520137280386
65,85	1229504898519975350977406221073619443220268
66,84	1583453278396937952016116475798783021139936
67,83	1985225005751384895063598575468858890976508
68,82	2423142286431837445445179468870345772615144
69,81	2879676340397256094585598969401799560569164
70,80	3332196908173967766592027941721540605994000
71,79	3754588065548132694750220759988813194524464
72,78	4119617460809756706740212819065590964482316
73,77	4401783040317274289392463027500946909902536
74,76	4580233704113920544368502750626698489294984
75,75	4641303486835439484959145718568923895458472

Table 16.14 The number of $H_{89-k}B_k$ molecules

$k, 89 - k$	Number of $H_{89-k}B_k$ molecules for symmetry group
0,89	1
1,88	47
2,87	1984
3,86	56892
4,85	1221456
5,84	20756184
6,83	290563644
7,82	3445167312
8,81	35312741949
9,80	317813975539

(continued)

Table 16.14 (continued)

$k, 89 - k$	Number of $H_{89-k}B_k$ molecules for symmetry group
10,79	2542510116752
11,78	18259840795912
12,77	118688954831096
13,76	703003784422072
14,75	3816306205549832
15,74	19081530912625424
16,73	88252080242700895
17,72	378964814703449873
18,71	1515859257963982160
19,70	5664526699240696204
20,69	19825843444588399064
21,68	65142057027473837360
22,67	201348176258905833868
23,66	586535991698093381120
24,65	1612973977150092969259
25,64	4193732340560438311493
26,63	10323033453643439331136
27,62	24087078058438832974432
28,61	53335672843599223614176
29,60	112188829084695301825888
30,59	224377658169237491264096
31,58	427041349418676753435712
32,57	774012445821111101559914
33,56	1336930588236176461627382
34,55	2202003321800426034874816
35,54	3460290934257434856293432
36,53	5190436401385740907480896
37,52	7434949439822385325514640
38,51	10174141338703878921425976
39,50	13304646365996955576915552
40,49	16630807957495803542747490
41,48	19875843656519036615151870
42,47	22715249893164345209272800
43,46	24828296394853866796169520
44,45	25956855321892585506612240

Appendix 16.C

USCI table of the point group $Z_2 \times A_5$

$\downarrow G_{11}$	$\downarrow G_{10}$	$\downarrow G_9$	$\downarrow G_8$	$\downarrow G_7$	$\downarrow G_6$	$\downarrow G_5$	$\downarrow G_4$	$\downarrow G_3$	$\downarrow G_2$	$\downarrow G_1$	USCI table
S_6^{20}	S_6^{20}	S_5^{24}	S_4^{30}	S_4^{30}	S_4^{30}	S_2^{40}	S_2^{60}	S_2^{60}	S_2^{60}	S_1^{120}	G/G ₁
S_6^{10}	S_6^{10}	S_5^{12}	S_2^{30}	S_4^{15}	S_4^{15}	S_3^{20}	S_2^{30}	S_2^{30}	S_1^{60}	S_1^{60}	G/G ₂
S_6^{10}	$S_6^8 S_3^4$	S_5^{12}	$S_4^{14} S_2^2$	$S_4^{13} S_3^4$	S_4^{15}	S_3^{20}	S_2^{30}	$S_2^{28} S_1^4$	S_2^{30}	S_1^{60}	G/G ₃
$S_6^8 S_3^4$	S_6^{10}	S_5^{12}	$S_4^{14} S_2^2$	$S_4^{14} S_2^2$	$S_4^{12} S_2^6$	S_3^{20}	$S_2^{28} S_1^4$	S_2^{30}	S_2^{30}	S_1^{60}	G/G ₄
$S_6^6 S_2^2$	$S_6^6 S_2^2$	S_5^8	S_4^{10}	S_4^{10}	S_4^{10}	$S_3^{12} S_1^4$	S_2^{20}	S_2^{20}	S_2^{20}	S_1^{40}	G/G ₅
$S_6^2 S_3^6$	S_6^5	S_5^6	$S_4^6 S_2^3$	$S_4^6 S_2^3$	$S_4^6 S_1^6$	S_3^{10}	$S_2^{12} S_1^6$	S_2^{15}	S_2^{15}	S_1^{30}	G/G ₆
$S_6^4 S_3^2$	$S_6^3 S_3^4$	S_5^6	$S_4^6 S_2^3$	$S_4^6 S_2^4$	$S_4^6 S_2^3$	S_3^{10}	$S_2^{14} S_1^2$	$S_2^{13} S_1^4$	S_2^{15}	S_1^{30}	G/G ₇
$S_6^4 S_3^2$	$S_6^4 S_3^2$	S_5^6	$S_2^{14} S_1^2$	$S_4^6 S_2^3$	$S_4^6 S_2^3$	S_3^{10}	$S_2^{14} S_1^2$	$S_2^{14} S_1^2$	S_1^{30}	S_1^{30}	G/G ₈
S_6^4	S_6^4	$S_5^4 S_1^4$	S_4^6	S_4^6	S_4^6	S_3^8	S_2^{12}	S_2^{12}	S_2^{12}	S_1^{24}	G/G ₉
$S_6^3 S_2$	$S_6^2 S_3^2 S_1^2$	S_5^4	$S_4^4 S_2^2$	$S_4^3 S_3^4$	S_4^5	$S_3^6 S_1^2$	S_2^{10}	$S_2^8 S_1^4$	S_2^{10}	S_1^{20}	G/G ₁₀
$S_6^2 S_3^2 S_1^2$	$S_6^3 S_2$	S_5^4	$S_4^4 S_2^2$	$S_4^4 S_2^2$	$S_4^2 S_2^6$	$S_3^6 S_1^2$	S_2^{10}	S_2^{10}	S_2^{10}	S_1^{20}	G/G ₁₁
$S_6^3 S_2$	$S_6^3 S_2$	S_5^4	S_2^{10}	S_4^5	S_4^5	$S_3^6 S_1^2$	S_2^{10}	S_2^{10}	S_2^{20}	S_1^{20}	G/G ₁₂
$S_6^3 S_3$	$S_6^3 S_3$	S_5^3	$S_2^6 S_1^3$	$S_4^3 S_1^3$	$S_4^3 S_1^3$	S_3^5	$S_2^6 S_1^3$	$S_2^6 S_1^3$	S_1^{15}	S_1^{15}	G/G ₁₃
S_3^4	S_6^2	$S_5^2 S_1^2$	$S_4^2 S_2^2$	$S_4^2 S_2^2$	S_2^6	S_3^4	$S_2^4 S_1^4$	S_2^6	S_2^6	S_1^{12}	G/G ₁₄
S_6^2	S_3^4	$S_5^2 S_1^2$	$S_4^2 S_2^2$	$S_4^2 S_2^2$	S_4^3	S_3^4	S_2^6	$S_2^4 S_1^4$	S_2^6	S_1^{12}	G/G ₁₅
S_6^2	S_6^2	$S_5^2 S_1^2$	S_3^6	S_4^3	S_4^3	S_3^4	S_2^6	$S_2^4 S_1^4$	S_2^6	S_1^{12}	G/G ₁₆
$S_3^2 S_2^2$	$S_6^2 S_2^2$	S_5^2	$S_4^2 S_2$	$S_4^2 S_2$	$S_4^2 S_1^2$	$S_3^2 S_1^4$	$S_2^4 S_1^2$	S_2^6	S_2^5	S_1^{10}	G/G ₁₇
$S_6^5 S_3 S_1$	$S_6^5 S_3 S_1$	S_5^2	$S_2^4 S_1^2$	$S_4 S_2^3$	$S_4 S_2^3$	$S_3^2 S_1^4$	$S_2^4 S_1^2$	$S_2^4 S_1^2$	S_1^{10}	S_1^{10}	G/G ₁₈
S_3^2	S_3^2	$S_5 S_1$	$S_2^2 S_1^2$	S_2^3	S_2^3	S_3^2	$S_2^2 S_1^2$	$S_2^2 S_1^2$	S_1^6	S_1^6	G/G ₁₉
$S_3 S_2$	$S_3 S_2$	S_5	$S_2^2 S_1$	$S_4 S_1$	$S_4 S_1$	$S_3 S_1^2$	$S_2^2 S_1$	$S_2^2 S_1$	S_1^5	S_1^5	G/G ₂₀
S_1^2	S_2	S_1^2	S_2	S_2	S_1^2	S_1^2	S_1^2	S_2	S_2	S_1^2	G/G ₂₁
S_1	S_1	S_1	S_1	S_1	S_1	S_1	S_1	S_1	S_1	S_1	G/G ₂₂

$\downarrow G_{22}$	$\downarrow G_{21}$	$\downarrow G_{20}$	$\downarrow G_{19}$	$\downarrow G_{18}$	$\downarrow G_{17}$	$\downarrow G_{16}$	$\downarrow G_{15}$	$\downarrow G_{14}$	$\downarrow G_{13}$	$\downarrow G_{12}$	USCI table
S ₁₂₀	S ₆₀ ²	S ₂₄ ⁵	S ₁₂ ¹⁰	S ₁₂ ¹⁰	S ₁₂ ¹⁰	S ₁₀ ¹²	S ₁₀ ¹²	S ₁₀ ¹²	S ₈ ¹⁵	S ₆ ²⁰	G/G ₁
S ₆₀	S ₆₀	S ₁₂ ⁵	S ₆ ¹⁰	S ₆ ¹⁰	S ₁₂ ⁵	S ₅ ¹²	S ₁₀ ⁶	S ₁₀ ⁶	S ₄ ¹⁵	S ₃ ²⁰	G/G ₂
S ₂₄	S ₆₀	S ₂₄ ² S ₆	S ₁₂ ⁴ S ₆ ²	S ₁₂ ⁴ S ₆ ²	S ₁₂ ⁵	S ₁₀ ⁶	S ₁₀ ⁴ S ₅ ⁴	S ₁₀ ⁶	S ₆ ⁸ S ₄ ³	S ₆ ¹⁰	G/G ₃
S ₂₀	S ₁₂ ²	S ₂₄ ² S ₈	S ₁₂ ⁴ S ₆ ²	S ₁₂ ⁴ S ₆ ²	S ₁₂ ⁴ S ₄ ²	S ₁₀ ⁶	S ₁₀ ⁶	S ₁₀ ⁴ S ₅ ⁴	S ₈ ⁶ S ₄ ³	S ₆ ¹⁰	G/G ₄
S ₁₂	S ₁₀ ²	S ₂₄ S ₄ ²	S ₁₂ ³ S ₄	S ₁₂ ³ S ₄	S ₁₂ ² S ₃ ⁴	S ₁₀ ⁴	S ₁₀ ⁴	S ₁₀ ⁴	S ₈ ⁵	S ₆ ⁶ S ₂ ²	G/G ₅
S ₁₂	S ₆ ²	S ₂₄ S ₄	S ₁₂ S ₆ ³	S ₁₂ S ₆ ³	S ₁₂ ² S ₂ ²	S ₁₀ ³	S ₁₀ ³	S ₅ ⁶	S ₈ ³ S ₂ ³	S ₆ ⁵	G/G ₆
S ₁₀	S ₁₂	S ₂₄ S ₃	S ₁₂ S ₆ S ₆ ²	S ₁₂ S ₆ S ₆ ²	S ₁₂ ² S ₄	S ₁₀ ³	S ₁₀ S ₅ ⁴	S ₁₀ ² S ₂ ²	S ₈ ³ S ₂ ⁴	S ₆ ⁵	G/G ₇
S ₁₀	S ₁₂	S ₁₂ ² S ₄	S ₆ ⁴ S ₃ ²	S ₆ ⁴ S ₃ ²	S ₁₂ ² S ₄	S ₅ ⁶	S ₁₀ ² S ₅ ²	S ₁₀ ² S ₅ ²	S ₄ ⁶ S ₂ ³	S ₃ ¹⁰	G/G ₈
S ₁₀	S ₅ ²	S ₂₄	S ₁₂ ²	S ₁₂ ²	S ₁₂ ²	S ₁₀ ² S ₂ ²	S ₁₀ ² S ₂ ²	S ₁₀ ² S ₅ ²	S ₈ ³	S ₆ ⁴	G/G ₉
S ₈	S ₁₀	S ₆ S ₄	S ₁₂ S ₆ S ₂	S ₁₂ S ₆ S ₂	S ₁₂ S ₃ ²	S ₁₀ ²	S ₅ ⁴	S ₁₀ ²	S ₈ S ₄ ³	S ₆ ³ S ₂	G/G ₁₀
S ₆	S ₄ ²	S ₈ S ₄	S ₁₂ S ₆ S ₂	S ₁₂ S ₆ S ₂	S ₄ ² S ₃ ²	S ₁₀ ²	S ₁₀ ²	S ₅ ⁴	S ₈ S ₄ ³	S ₆ ³ S ₂	G/G ₁₁
S ₆	S ₁₀	S ₁₂ S ₂ ²	S ₆ ³ S ₂	S ₆ ³ S ₂	S ₁₂ S ₃ ²	S ₅ ⁴	S ₁₀ ²	S ₁₀ ²	S ₄ ⁵	S ₃ ⁶ S ₁ ²	G/G ₁₂
S ₆	S ₆	S ₁₂ S ₂	S ₆ S ₃ ³	S ₆ S ₃ ³	S ₁₂ S ₂	S ₅ ³	S ₅ ³	S ₅ ³	S ₃ ⁵ S ₁ ³	S ₅ ⁵	G/G ₁₃
S ₅	S ₃ ²	S ₈	S ₆ ²	S ₆ ²	S ₄ ²	S ₁₀ S ₂	S ₁₀ S ₂	S ₅ ² S ₁ ²	S ₃ ³	S ₆ ²	G/G ₁₄
S ₄	S ₅	S ₆	S ₆ ²	S ₆ ²	S ₁₂	S ₁₀ S ₂	S ₅ ² S ₁ ²	S ₁₀ S ₂	S ₄ ³	S ₆ ²	G/G ₁₅
S ₄	S ₅	S ₁₂	S ₆ ²	S ₆ ²	S ₁₂	S ₅ ² S ₁ ²	S ₁₀ S ₂	S ₁₀ S ₂	S ₄ ³	S ₃ ⁴	G/G ₁₆
S ₄	S ₂ ²	S ₄ S ₂	S ₆ S ₄	S ₆ S ₄	S ₃ ² S ₁ ²	S ₁₀	S ₁₀	S ₅ ²	S ₈ S ₂	S ₆ S ₂ ²	G/G ₁₇
S ₃	S ₄ S ₂	S ₄ S ₂	S ₆ S ₃ S ₁	S ₆ S ₃ S ₁	S ₄ S ₃	S ₅ ²	S ₅ ²	S ₅ ²	S ₄ S ₂ ³	S ₃ ³ S ₁	G/G ₁₈
S ₂	S ₃	S ₄	S ₂ ²	S ₃ ²	S ₄	S ₅ S ₁	S ₅ S ₁	S ₅ S ₁	S ₂ ³	S ₃ ²	G/G ₁₉
S ₂	S ₂	S ₂ S ₁	S ₃ S ₂	S ₃ S ₂	S ₃ S ₁	S ₅	S ₅	S ₅	S ₄ S ₁	S ₃ S ₁ ²	G/G ₂₀
S ₂	S ₁ ²	S ₂	S ₂	S ₂	S ₁ ²	S ₂	S ₂	S ₁ ²	S ₂	S ₂	G/G ₂₁
S ₁	S ₁	S ₁	S ₁	S ₁	S ₁	S ₁	S ₁	S ₁	S ₁	S ₁	G/G ₂₂

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