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# Enumeration of Heterofullerenes: A Survey

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**Abstract:** 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. Heterofullerenes are fullerene molecules in which one or more carbon atoms are replaced by heteroatoms such as boron or nitrogen. In this paper by using the Pólya's theorem, we compute the number of permutational isomers of some fullerene graphs.

## 1. Introduction

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

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 $G$, 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.

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 co-authors.[1] 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.[2] 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 3 faces and each edge lies in 2 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 having 12 pentagonal and $(n/2 - 10)$ hexagonal faces, where $n \neq 22$ is a natural number equal or greater than 20, see Figure 1. Heterofullerenes 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 Figure 2.

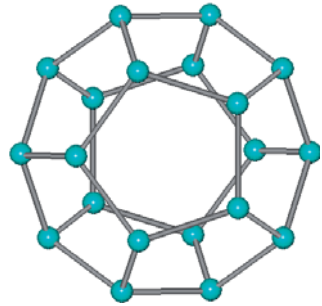


**Figure 1.** 3 –D graph of fullerene $C_{20}$.

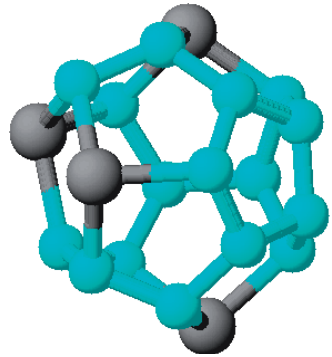


**Figure 2.** 3 –D graph of heterofullerene $C_{16}Br_4$.

Balasubramanian[3-9] has done a lot of work on methods for isomer counting of heterofullerenes 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 heterofullerene. Shao and Jiang[10] discussed hydrogenated $C_{60}$. Furthermore, Zhang[11] also studied the fullerene cages. In [12 – 20] Ghorbani et al. computed the number of permutational isomers of some classes of heterofullerenes.

Detecting symmetry of molecules is a well-studied problem with applications in a large number of areas. Randić[21, 22] and then Balasubramanian considered the Euclidean matrix of a chemical graph to find its symmetry. Here, the Euclidean matrix of a molecular graph $G$ is a matrix $D(G) = [d_{ij}]$, 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 $\sigma$ is a permutation on $n$ atoms of the molecule under consideration. Then, the permutation matrix $P_\sigma$ is defines 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 $\sigma$ and $\tau$ 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 $\sigma$ of the vertices of a graph $G$ belongs to its automorphism group if it satisfies $P_\sigma^t A P_\sigma = A$, where $A$ is the adjacency matrix of $G$. So, for computing the symmetry of a molecule, it is sufficient to solve the matrix equation $P^t E P = E$, 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 $E$.

Symmetry plays an 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 places the molecule in an orientation which appears to be identical to its initial orientation. They 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.

## 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 $\varphi$ 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 $\lambda_1$ orbits of size 1, $\lambda_2$ orbits of size 2, …, and $\lambda_n$ orbits of size $n$. Then the cycle type of $g$ is defined as $1^{\lambda_1}2^{\lambda_2}...n^{\lambda_n}$.

**Example 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 Figure 3 is the same as the second one after rotation through $180^0$.

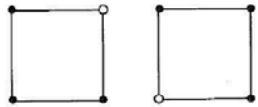


**Figure 3.** Two indistinguishable colorings.

From above, we regard two colorings as being indistinguishable if one is transformed into the other by a 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 Figure 4.

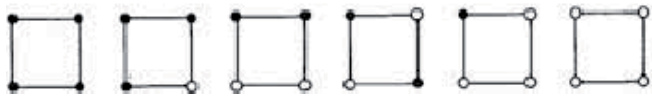


**Figure 4.** The six distinguishable colorings.

Let us here to 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 $Q$ in terms of indeterminates $x_1, x_2, \ldots, x_t$, $t = |X|$, defined by $Z(G, X) = \frac{1}{|G|}\sum_{p\in G}\prod_{i=1}^{t} x_i^{c_i(p)}$, in which $(c_1(p), \cdots, c_t(p))$ is the cycle type of the permutation $p \in G$. The generalized character cycle index is defined as $P_G^{\chi}(x_1, x_2, \ldots, x_t) = \frac{1}{|G|}\sum_{p\in G}\prod_{i=1}^{t}\chi(p)x_i^{c_i(p)}$, where $\chi(g)$ is the linear character of the irreducible representation of $G$. In this paper we use two special cases: One is the anti-symmetric 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 $\chi$ 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:

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

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

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.

Denote by $C_{m,n}$ the set of all functions $f$: $\{1, 2, \ldots, m\} \rightarrow \{x_1, x_2, ..., x_n\}$. The action of $p \in S_m$ induced on $C_{m,n}$ is defined by $\hat{p}(f) = fop^{-1}$, $f \in C_{m,n}$. Treating the colors $x_1, x_2, \ldots, x_n$ 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 $p_1, p_2, \ldots, p_t$ 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 $W_G(x_1, x_2, \ldots, x_n) = \sum_{i=1}^{t} W(p_i)$.

**Theorem 1 (Pólya's Theorem [23]).** 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

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

where $M_k = x_1^k + x_2^k + \ldots + x_n^k$ is the $k^{\text{th}}$ power sum of the $x_i$'s.

**Theorem 2 (Generalization of Pólya's Theorem [11]).** Substituting $M_i$ for $x_i$ and in the generalized character cycle index, $i$ = 1, 2, **…**, t, we get the chiral generating function $CGF = P_G^z(M_1, \ldots, M_k)$.

To enumerate all possibilities of the heterofullerene structures, we have to consider the whole automorphism group to enumerate the number of permutational isomers. Balasubramanian in one of his paper[6] computed the number of isomers of substituted fullerene cages $C_{20} - C_{50}$. For example, in table 1 one can find these values for fullerene graph $C_{20}$. In tables [2 – 4] the number of $C_{n-k}B_k$ molecules are reported for $n$ = 24, 30 and 34, respectively. Fripertinger[24] computed the symmetry of some fullerenes and then applied SYMMETRICA[25] to calculate the number of $C_{60}H_kCl_{60-k}$ molecules and Balasubramanian computed the number of $C_{60}H_{36}$ isomers, see table 5. In table 6 the number of orbits under whole point group of $C_{72-k}B_k$ is reported. Finally, in tables [7 - 9] the number of $C_{n-k}B_k$ molecules respectively for $n$ = 80, 84 and 150 are reported. The aim of this paper is to explain how we computed the number of permutational isomers of heterofullerenes.

| $k$, 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 1.** The number of $C_{20-k}B_k$ molecules.

| $k$, 24 -$k$ | $_{24-k}B_k$ 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 2.** Number of $C_{24-k}B_k$ 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 3.** Number of $C_{30-k}B_k$ 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 4.** Number of $C_{34-k}B_k$ molecules.

| $k$, 60 -$k$ | $_{60-k}B_k$ 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 | 194877752875260 |
| 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 5** The Number of $C_{60-k}B_k$ 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 6** The Number of $C_{72-k}B_k$ Molecules.

| Number of Orbits under Whole Point Group $I_h$ |
|---|
| 0 |
| 0 |
| 14 |
| 274 |
| 4046 |
| 45312 |
| 417006 |
| 3216564 |
| 21319974 |
| 123181170 |
| 628272150 |
| 2855775000 |
| 11661270420 |
| 43056957720 |
| 144548950080 |
| 443283298844 |
| 1246735824660 |
| 3226845176280 |
| 7708578047670 |
| 17040013308780 |
| 34932033844650 |
| 66537204375780 |
| 117952327562160 |
| 194877752875260 |
| 300436550914530 |
| 432628623838260 |
| 582384704656986 |
| 733373318297492 |
| 864332859447352 |
| 953746586743696 |
| 985538158387164 |

Continuing of Table 6.

| $k$, 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 7.** The number of $C_{80-k}B_k$ molecules.

| $k$, 84 -$k$ | Number of $C_{84-k}B_k$ molecules for Symmetry Group |
|---|---|
| 0, 84 | |
| 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 8.** The number of $C_{84-k}B_k$ molecules.

| $k$, 150 - $k$ | Number of $C_{150-k}B_k$ |
|---|---|
| | 10 |
| | 608 |
| | 27762 |
| | 1015132 |
| | 29587626 |
| | 714908767 |
| | 14705679304 |
| | 262861756418 |
| | 4147359263564 |
| | 58477733568550 |
| | 744261878846444 |
| | 8621033058155532 |
| | 91515579793041740 |
| | 895545312914462338 |
| | 8119610820294861024 |
| | 68509216265755052423 |
| | 540013822200718017274 |
| | 3990102130481989637532 |
| | 2772070953720633767248 2 |
| | 1815706474672560322862 70 |
| | 1124008770030069888944122 |
| | 6590778696986152507958223 |
| | 3667911622667656153042156 8 |
| | 1940936566994534391468657 12 |
| | 9782320297651025843068313 60 |
| | 4703038604639712304854528992 |
| | 2159914025834470550337413 6608 |
| | 9488193756344193998758012 2208 |
| | 3991584959565462273165077 06912 |
| | 1609939267024733028272418627950 |
| | 6232022969127988937630220494912 |
| 32,118 | 2317533541644469654927078126 5772 |
| 33,117 | 8286938118607494122725703257 4344 |
| 34,116 | 2851681646697284333944962233 05568 |
| 35,115 | 9451287743339569833338541595 48184 |
| 36,114 | 3019161362455695793849475118 633168 |
| 37,113 | 9302280954593224550068789712 330120 |
| 38,112 | 2766204599655353580671997589 1990092 |
| 39,111 | 7943972183625630704855831840 5485664 |
| 40,110 | 2204452280956112511230484655 78384610 |
| 41,109 | 5914384168418838421303093877 14175824 |
| 42,108 | 1534923510375365207042049180 063976208 |
| 43,107 | 3855156723733475398082512651 736762064 |
| 44,106 | 9375040214533678803733124039 197920912 |
| 45,105 | 2208342806090155450273572094 5545628656 |

**Table 9.** The number of $C_{150-k}B_k$ molecules.

| $k$, 150 - $k$ | Number of $C_{150-k}B_k$ molecules for Symmetry Group |
|---|---|
| 46,104 | 504078249216231135277096226862903363 12 |
| 47,103 | 111540718975506463949387235122286925152 |
| 48,102 | 23934779280160762053597045378435114 7068 |
| 49,101 | 49823418093395872024638667121562724 7400 |
| 50,100 | 10064330454865966148568902567327354997 06 |
| 51,99 | 19733981284050914015820187016276875304 40 |
| 52,98 | 37570464367712317067878581555031422135 36 |
| 53,97 | 69469915245958624010596939036263110244 24 |
| 54,96 | 12478855146033308386976398312593227196124 |
| 55,95 | 21781274436712683729716490061393340262312 |
| 56,94 | 36950376276566159898459691595847481631824 |
| 57,93 | 60935708245565246147909753636832722794208 |
| 58,92 | 97707256324785653305903584594286513690016 |
| 59,91 | 15235707765898779837469214663007573402620 8 |
| 60,90 | 23107490111613149420133221097656562962147 0 |
| 61,89 | 34093018197462023734539672849880849505148 8 |
| 62,88 | 48939977735066453425355697231207014351598 4 |
| 63,87 | 68360603820410284149597905602452588104672 0 |
| 64,86 | 92927695818370230015828574395252013728038 6 |
| 65,85 | 12295048985199753509774062210736194432202 68 |
| 66,84 | 15834532783969379520161164757987830211399 36 |
| 67,83 | 19852250057513848950635985754688588909765 08 |
| 68,82 | 24231422864318374454451794688703457726151 44 |
| 69,81 | 28796763403972560945859896940179956056916 4 |
| 70,80 | 33321969081739677665920279417215406059940 00 |
| 71,79 | 37545880655481326947502207599888131945244 64 |
| 72,78 | 41196174608097567067402128190655909644823 16 |
| 73,77 | 44017830403172742893924630275009469099025 36 |
| 74,76 | 45802337041139205443685027506266984892949 84 |
| 75,75 | 46413034868354394849591457185689238954584 72 |

Continuing of Table 9.

In [26 – 32] Ghorbani and his coauthors studied some properties of fullerene graphs. A coloring of the vertices, edges or faces of a fullerene with $k$ colors can be interpreted as a function from the set of all vertices, edges or faces into the set of $k$ colors. Two colorings are called different if and only if the corresponding functions lie in different orbits of the symmetry group acting on the set of all these functions in a natural way. This means that the group is acting on the domain of these functions. From the cycle indices above you can compute the number of different colorings using $k$ colors via Pólya - theory by replacing each variable $x_i$ in the cycle index by $k$. We mention here

that our computations of symmetry properties and cycle indices of fullerenes were carried out with the use of GAP[33]. This software was constructed by the GAP team in Aachen. The Pólya theorem says that the number of $C_{n-k}B_k$ molecules is given as the coefficient of $x_k$ in the expansion of the cycle index of the symmetry group acting on the set of vertices when all the indeterminates $x_i$ are replaced by $1+x^i$.

It is well – known fact that the dihedral group $D_{2n}$ is the symmetry group of an $n$-sided regular polygon for $n > 1$. These groups are one of the most important classes of finite groups currently applicable in chemistry. For example $D_6$, $D_8$, $D_{10}$ and $D_{12}$ point groups are dihedral groups. One group presentation for $D_{2n}$ is $\langle x,y \mid x^n = y^2 = e, yxy = x^{-1}\rangle$. This means that $D_{2n}$ is generated by a two elements set $\{x, y\}$ with the following condition

$$x^n = y^2 = e \text{ and } yxy = x^{-1}.$$

This presentation will be used in the next section for computing the symmetry group of fullerenes.

## 2.1. Enumeration of heterofullerenes with small number of vertices

To demonstrate our method we should to compute number of permutational isomers of some well – known fullerenes. In this section we enumerate heterofullerenes $C_{n-k}B_k$ for n = 24, 80, 84 and 150. Consider at first the molecular graph of the fullerene $C_{24}$, shown in Figure 5. In [26] 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 3.**

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

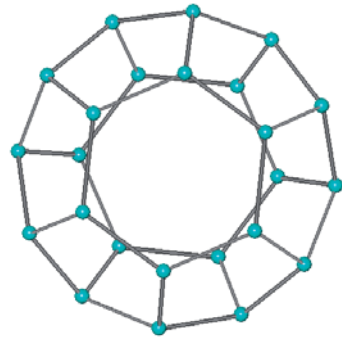


**Figure 5.** 3 - *D* graph of fullerene $C_{24}$.

Consider now the molecular graph of the fullerene $C_{80}$, Figure 6. We have the following Theorem:

**Theorem 4.**

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

**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 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.

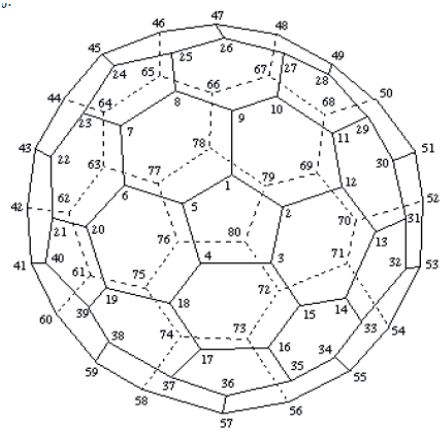



**Figure 6.** 3 - *D* graph of fullerene $C_{80}$.

In continuing consider the molecular graph of fullerene $C_{84}$, Figure 7. 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),

$Y$ = (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:

**Theorem 5.**

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

**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 five. The cycle type of its elements are $1^{84}$, $2^{42}$, $3^{28}$, $4^{21}$ and $1^2 2^{41}$, respectively. This completes the proof.

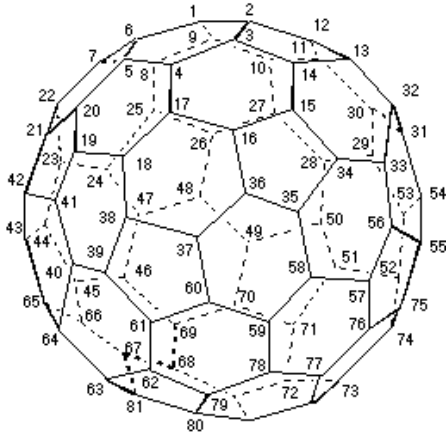


**Figure 7.** 2 - $D$ graph of fullerene $C_{84}$.

Now consider the molecular graph of the fullerene $C_{150}$, Figure 8. In [26] the symmetry group of $C_{150}$ is computed and it is isomorphic with Dihedral group $D_{20}$. On the other hand, in [26] the 3 - dimentional cycle index of $C_{150}$ is computed. Thus

**Theorem 6.**

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

**Proof.** Use from definition of the cycle index and the main Theorem of [26].

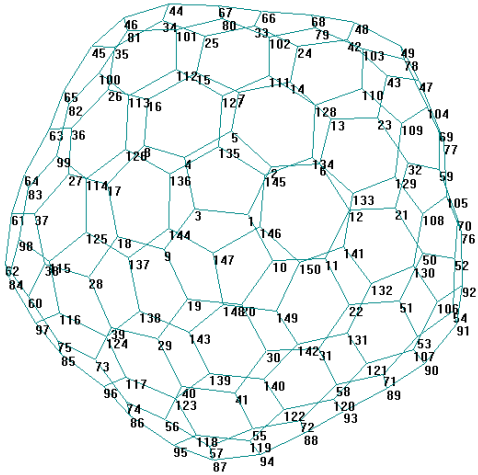


**Figure 8.** 3 - *D* graph of fullerene $C_{150}$.

## 2.2. Enumeration of infinite classes of heterofullerenes

In this section we enumerate the number of infinite families of heterofullerenes, namely $C_{10n}$, $C_{12n}$, $C_{12n+6}$, $C_{24n}$ and $C_{40n}$ fullerenes. Many properties of these classes of fullerenes are studied in [12 – 20, 26 – 33].

### 2.2.1 $C_{10n}$ 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 Figure 9. The first member of this class of fullerenes can be obtained by putting $n = 2$, e. g. $C_{20}$. 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 Figure 9, it is easy to see that the generators of this group are:

$$\sigma = (2,5)(3,4)(6,10)(7,9)(11,15)(12,14)...(10n-4,10n)(10n-3,10n-1),$$

$$\tau = (1,10n-4,2,10n-3,3,10n-2,4,10n-1,5,10n)\ ...$$
$$(7,10n-6,9,10n-14,11,10n-12,13,10n-10,15,10n-8),$$

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

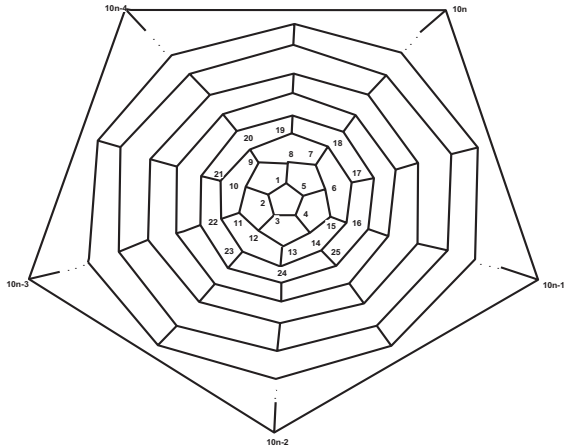



**Figure 9**. The Schlegel diagram of $C_{10n}$.

Since $\sigma^2 = \tau^{10}$ = 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** | | **#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:

$$Z(G,X) = (x_1^{10n} + 5x_1^{2n}x_2^{4n} + 4_5^{2n} + 6x_2^{5n} + 4x_{10}^{n})/20 .$$

**2. 2. 2 $C_{12n}$ fullerene**

Now consider the graph of fullerene $C_{12n}$ ($n \geq 2$), Figure 10. This class of fullerenes has exactly 12$n$ carbon atoms and the first member of this class of fullerenes can be obtained by putting $n$ = 2, e. g. $C_{24}$. Again our problem is reduced to the

coloring of the corresponding fullerene graph with 12*n* 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:

σ=(1,12n-5)(2,12n-4)(3,12n-3)...(12n-24,12n-18)(12n-22,12n-19)(12n-21,12n-20),

τ=(1,12n-5,2,12n,3,12n-1,4,12n-2,5,12n-3,6,12n-4)...(12n-29,12n-25,12n-26,12n-18,12n-20,12n-19,12n-22,12n-21,12n-24,12n-23,12n-28,12n-27).

Since $\sigma^2 = \tau^{10}$ = 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:

| Fullerene | Cycle type | #Permutations |
|---|---|---|
| | | 1 |
| | | 5 |
| $C_{12n}$ | $2^{10n}$ | 6 |
| | $10^{2n}$ | 4 |
| | $5^{4n}$ | 4 |

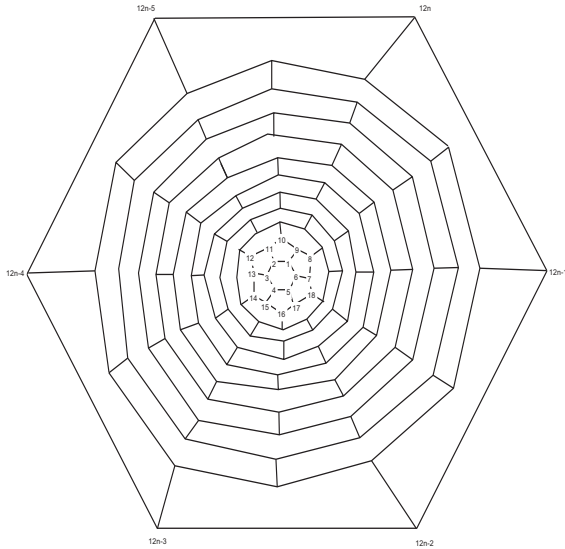



**Figure 10.** The Schlegel diagram of $C_{12n}$.

Thus, the cycle index of $G$ is:

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

**2. 2. 3 $C_{12n+6}$ fullerene**

In this section consider a fullerene graph $C_{12n+6}$ ($n \geq 2$) with $12n + 6$ carbon atoms, Figure 11. 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 Figure 12. 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 Figures 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:

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

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:

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

By using GAP, 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:

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

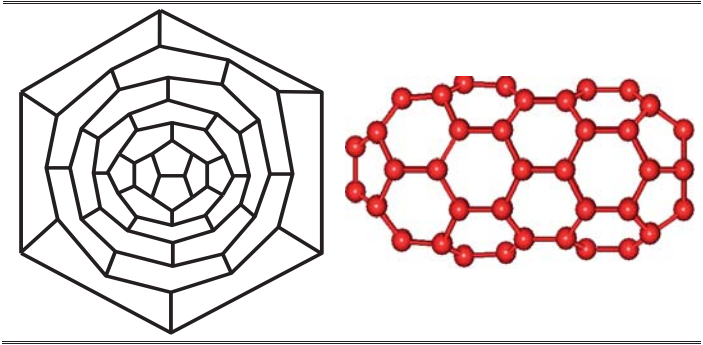


**Figure 11.** 2 – $D$ and 3 – $D$ graph of fullerene $C_{12n+6}$, for $n = 3$.

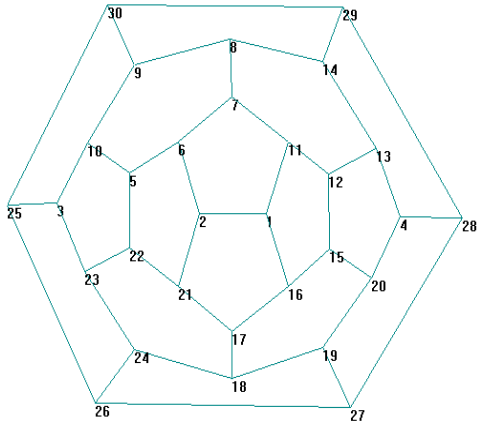



**Figure 12.** Labling of fullerene $C_{30}$.

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:

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

**2. 2. 4 $C_{24n}$ fullerene**

In this section we enumerate the number of heterofullerenes $C_{24n}$ ($n \geq 3$), Figure 13. 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 $C_{72}$ as is indicated in Figure 14 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:

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

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);

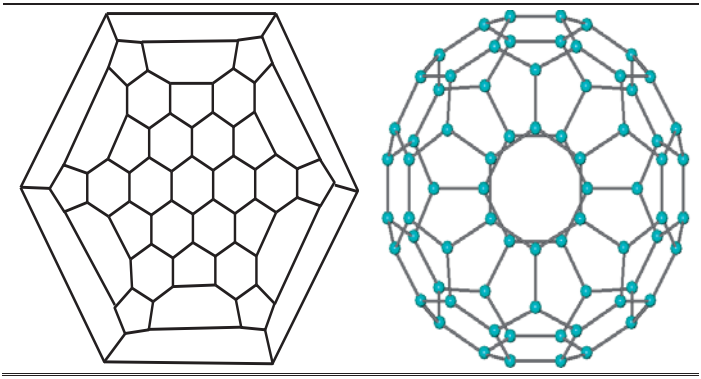


**Figure 13.** 2 – D and 3 – D graph of fullerene $C_{24n}$, for $n = 3$.

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 generally, the cycle types of elements of rotational group $R$ of $C_{24n}$ are as in the following table:

| **Fullerene** | | **#Permutations** |
|---|---|---|
| $C_{24n}$ | $1^{24n}$ | 1 |
| | $2^{12n-2}$ | 6 |
| | $2^{12n}$ | 1 |
| | $6^{4n}$ | 2 |
| | $3^{8n}$ | 2 |

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

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

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 $Z_{I_h} - P_{I_h}^{\chi} = P_{I_h}^{1}$. 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 of $C_{24n}$.

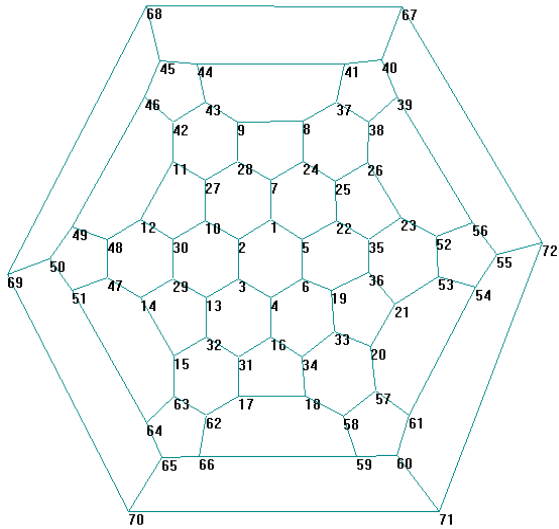



**Figure 14**. Labling of fullerene $C_{72}$.

**2. 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 Figure 15. 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:

σ=(2,5)(3,4)(7,10)...(10n-10,10n-7)(10n-4,10n-2)(10n-1,10n),

τ=(1,10n-4,3,10n-1,5,10n-3,2,10n,4,10n-2)...(10n-44,10n-36,10n-41,10n-38,10n-43, 10n-39,10n-40,10n-37,10n-42,10n-32).

Since $\sigma^2 = \tau^{10}$ = 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 |
| | | 5 |
| | $2^{20n}$ | 6 |
| | $10^{4n}$ | 4 |
| | $5^{8n}$ | 4 |

Thus the cycle index of $G$ is computed as

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

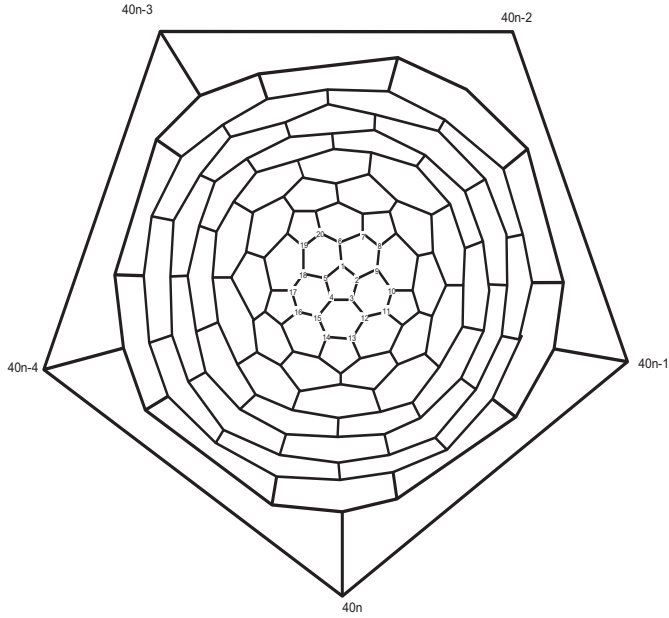
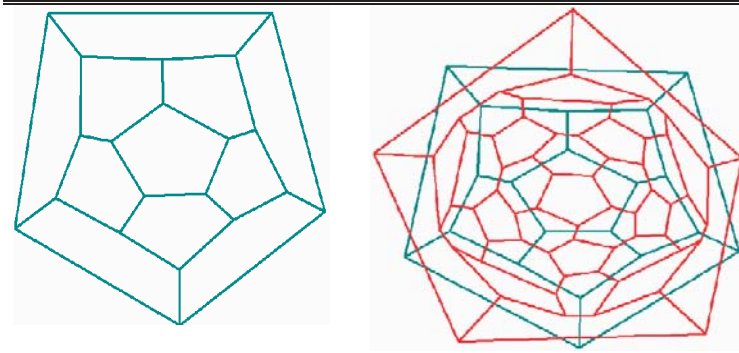



**Figure 15.** The Schlegel diagram of $C_{40n}$.

## 2.3. Fullerenes constructed by Leapfrog operation

In this section, we enumerate the number of heterofullerenes constructed by a new method. In other words, in [34] and [35] a method is described 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 we are starting 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 you have to put an extra vertex into the centre of each face of $C_n$. Then connect these new vertices 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. 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 $C_{3n}$. From Figure 16, one can see that $Le(C_{20}) = C_{60}$.



$C_{20}$ Fullerene $Le(C_{20}) = C_{60}$

**Figure 16.** The Fullerene $C_{20}$ and $Le(C_{20})$**.**

Here, we enumerate the number of heterofullerenes of two series of fullerenes constructed by Leapfrog, e. g. $C_{3^n\times 20}$ 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 ( $m \in \{20,34\}$ ).

### 2. 3. 1 $C_{3^n\times 20}$ fullerene

Consider the molecular graph of the fullerene $C_{3^n\times 20}$ as depicted in Figure 17. 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[35], 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 |

This implies the cycle index of $G$ can be computed as[18]

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

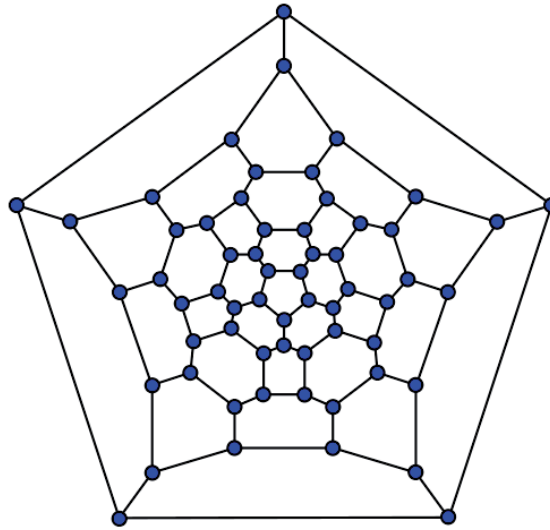


**Figure 17.** The Schlegel diagram of $C_{3^n\times 20}$, for $n = 2$.

### 2. 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 ($n = 0, 1, \ldots$), see Figure 18. 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.[35] 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 |

Hence, the cycle index of $G$ is computed as[19]:

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

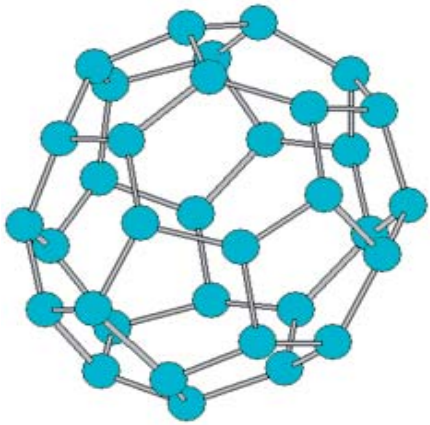


**Figure 18.** 3 – $D$ graph of fullerene $C_{3^n\times 34}$, $n = 1$.

### 2. 3. 3 $F_{3^n\times 34}$ fullerene

Finally, we enumerate the number of heterofullerenes 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 Figures 19, 20. 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 $Z_2$.[35] 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:

| | Cycle type<br>***n* is even** | Cycle type<br>***n* is odd** | #Permutations |
|---|---|---|---|
| $F_{3^n\times 34}$ | $1^{34\times 3^n}$ | $1^{34\times 3^n}$ | 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

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

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

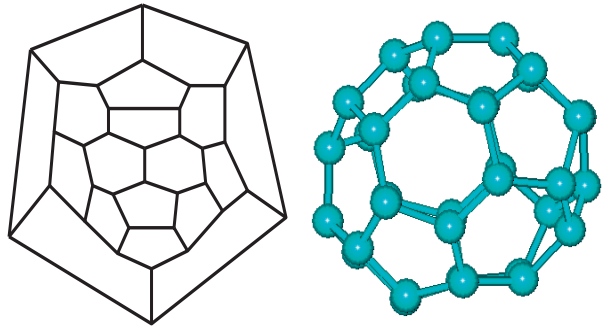


**Figure 19.** 2 – D and 3 – D graphs of fullerene $C_{3^n\times 34}$, $n = 1$.

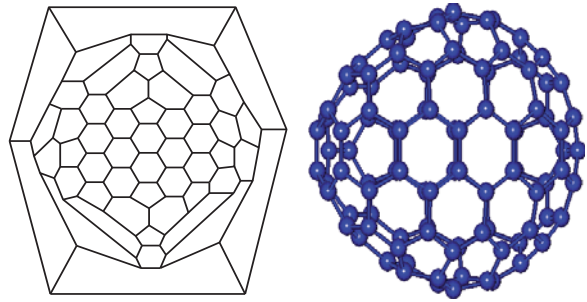


**Figure 20.** 2 – *D* and 3 – *D* graphs of fullerene $C_{3^n\times 34}$, $n = 2$.

**A GAP Program for Enumerating the Heterofullerenes**

```
h:=function(f, g)
        local t,i,tt;
             Print("Coefficients of f are:", "\n");
                  t:=Coefficients of LaurentPolynomial(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;
```

#Notice that in above program *f* and *g* denote to the symmetry group and rotational group, respectively.

## 3. Conclusions

In this paper, an efficient method is presented which is useful for computing permutational isomers of heterofullerenes. We applied our method on some classes of fullerenes and we computed the number of such isomers. We mention here that our computations of symmetry properties and cycle indices of fullerenes were carried out with the use of GAP. The study of IPR fullerene is very important, that's why some classes of fullerenes studied in this paper are IPR fullerenes. Among all classes of fullerene graphs, IPR fullerenes (fullerenes with isolated pentagons) are more stable. For this, we also computed the number of chiral isomers of these fullerenes.

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