




The Man Who Knew Symmetry: A Tribute to Ali Reza Ashrafi

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Abstract

Growing up in South Tehran, Ali Reza Ashrafi had a fascination with the application of mathematics in other sciences, particularly the symmetry of molecules, despite having no formal training in the subject. Ashrafi was a prominent mathematician who made significant contributions to the study of symmetry in molecular graphs. His work on this subject has had a profound impact on the field of chemistry, helping chemists to better understand the structure and properties of molecules. With great enthusiasm, Ashrafi explains to his students that the symmetry group plays a significant role in everything and that symmetry can be used to predict or explain many of a molecule's chemical properties.

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1 Introduction

This article outlines the scientific works of Alireza Ashrafi-Qomroodi during his life. Ashrafi was born in 1964 in Tehran, Iran. He was a full professor of pure mathematics and the dean of the nano-computing department at the University of Kashan, where he has been a faculty member since 1996. He has been selected several times as an ISI Highly Cited Researcher and is ranked among the top 1 percent of scientists and scholars worldwide. Also, Ashrafi is widely recognized as one of the top ten scientists in nanotechnology in Iran and was a member of the

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editorial board and a reviewer for many reputable domestic and international journals such as [1, 2]:

1. Editor-in-Chief (2016-2023) *Mathematics Interdisciplinary Research* (University of Kashan, Islamic Republic of Iran).
2. Editorial Board Member (2016 - 2023) *Fuller. Nanotub. Carbon Nanostructures* (Taylor & Francis, UK).
3. Editorial Board Member (2016 - 2023) *Italian Journal of Pure and Applied Mathematics* (Aviani Editore, Italy).
4. Editorial Board Member (2014 - 2023) *Bulletin of the Iranian Mathematical Society* (Iranian Mathematical Society, Islamic Republic of Iran).
5. Editor-in-Chief (2012-2013) *Bulletin of the Iranian Mathematical Society* (Iranian Mathematical Society, Islamic Republic of Iran).
6. Editorial Board Member (2012 - 2023) *International Journal of Group Theory* (University of Isfahan, Islamic Republic of Iran).
7. Editorial Board Member (2012 - 2023) *Transaction on Combinatorics* (University of Isfahan, Islamic Republic of Iran).
8. Editor-in-Chief (2010-2023) *Iranian Journal of Mathematical Chemistry* (University of Kashan, Islamic Republic of Iran).
9. Editorial Board Member (2005 - 2023) *MATCH Communications in Mathematical and in Computer Chemistry* (University of Kragujevac, Serbia).
10. Editorial Board Member (2007 - 2023) *Iranian Journal of Mathematical Sciences and Informatics* (Tarbiat Modares University, Islamic Republic of Iran)
11. Managing Editor (2011) *Bull. Iranian Math. Soc.* (Iranian Mathematical Society, Islamic Republic of Iran).

He has also been a keynote speaker and a reviewer for numerous national and international conferences.

As an accomplished researcher, Ashrafi has published over 300 scientific papers in prestigious journals and has authored 21 international books and 6 Persian books in his specialized field. In addition to being selected as an ISI Highly Cited Researcher, he was a member of the International Academy of Mathematical-Chemistry, a distinguished national researcher in 2009, and a provincial model researcher since 2001 [3, 4]. The objective of this paper is to present the scientific research conducted by Ashrafi on the symmetry group of molecular graphs.

2 Fundamental group theory

Symmetry-centered phenomena are depicted through the lens of group theory, an abstract yet practical model. Despite its abstract foundation, group theory offers valuable methods for quantifying predictions about atomic, molecular, and solid behavior. After grasping the fundamental principles, these techniques can be effortlessly employed using basic arithmetic. Nonetheless, it's crucial not to limit group theory's scope to just geometric symmetry, as it also encompasses ordinary numerical processes.

Definition 2.1. A group is defined as a set, together with an operation called multiplication, that satisfies the following four properties:

1. Closure: When multiplying any two components within the set, the result is also a member of the set.
2. Associativity: $a(bc) = (ab)c$.
3. Existence of an identity element, denoted e , such that $e.a = a.e = a$ for any element of the group.
4. Existence of an inverse element, denoted a^{-1} , for every element a of the group, such that $aa^{-1} = e$. Note that the inverse of the identity element is itself, i.e., $e^{-1} = e$.

In mathematics, applications of group theory are endless, for example, in physics, in modern physics, etc. In chemistry, group theory is used to describe symmetries of crystal and molecular structures.

Molecular symmetry is based on the idea that a molecule can possess certain symmetrical features that can be used to predict its physical and chemical properties. Symmetry arises from the arrangement of atoms and bonds in a molecule, and it can be described in terms of the spatial orientation of the molecule's parts, [5].

The group of isometries of space induces a group action on objects in it, and the symmetry group $Sym(X)$ consists of those isometries that map X to itself (as well as mapping any further pattern to itself). We say X is invariant under such a mapping, and the mapping is a symmetry of X [6, 7].

The notion of isometry is a general notion commonly accepted in mathematics. The word isometry means "preserving distances". An isometry is a transformation that preserves distance.

Definition 2.2. ([8]). An isometry of \mathbb{R}^n is a function $T : \mathbb{R}^n \rightarrow \mathbb{R}^n$ which preserves the distance, i.e., for every X and Y in \mathbb{R}^n , we have

$$\|T(X) - T(Y)\| = \|X - Y\|.$$

Theorem 2.3. ([8]). The set of all isometries of \mathbb{R}^n forms a group under the function composition.

This group is called the Euclidean group and is denoted by E_n .

Definition 2.4. ([8]). Let F be a set of points in \mathbb{R}^n . The symmetry group of F in \mathbb{R}^n is the set of all isometries of \mathbb{R}^n that carry F onto itself.

Definition 2.5. A polyhedron is a three-dimensional solid which consists of a collection of polygons joined at their edges.

A polyhedron is said to be convex if the planes that bound the solid do not enter its interior.

Definition 2.6. A regular polyhedron is convex with all of its faces congruent regular polygons and with the same number of faces at each vertex.

A group action defines how each element of a group acts like a bijective map or symmetry on some set. To clarify this notion, let G be a group and X be a set. We say that G acts on X when there exists a mapping $\phi : G \times X \rightarrow X$ that satisfies the following conditions for all $x \in X$:

- (i) $\phi(e, x) = x$, where e is the identity element of G ,
and
- (ii) $\phi(g, \phi(h, x)) = \phi(gh, x)$ for all $g, h \in G$.

3 Symmetry group in chemistry

The concept of symmetry group is important in chemistry because it provides a powerful tool for understanding the physical and chemical properties of molecules, and for predicting their behavior in different contexts, such as in spectroscopy, crystallography, and chemical reactions. A symmetry group is a mathematical description of the set of all symmetry operations that can be applied to a molecule without changing its overall shape. This includes rotations, reflections, and inversions, see [9, 10].

For example, a rotation operator might be defined as a mathematical function that rotates the molecule around a certain axis by a certain angle, while leaving its overall shape unchanged. Similarly, a reflection operator might be defined as a mathematical function that reflects the molecule across a certain plane, while again leaving its overall shape unchanged.

The symmetry group of a molecule is typically denoted by a symbol that reflects its point group symmetry, which is based on the arrangement of atoms and bonds in the molecule. For example, the symmetry group of a molecule with a tetrahedral geometry might be denoted as T_d , while the symmetry group of a linear molecule might be denoted as $C_{\infty v}$, see [8, 11].

We demonstrate that the symmetry group of a graph is a subgroup of its automorphism group. The symmetry group consists of all the permutations of vertices that preserve the graph's structure, including rotations, reflections, and combinations thereof. Since the symmetry group captures all the symmetries of the graph, it is a subset or subgroup of the larger automorphism group, which captures all the possible permutations preserving the graph's adjacency relationships. Here are a few examples to illustrate the relationship between symmetry groups and automorphism groups in different types of graphs. Some of the most commonly used symmetry groups for chemical graphs include [11, 12]:

Point groups: Point groups are symmetry groups that describe the arrangement of atoms in space around a central point. Examples of point groups include $C_1, C_2, C_3, C_4, C_5, C_6, C_s, C_i,$ and D_{3h} .

Plane groups: Plane groups are symmetry groups that describe the arrangement of atoms in a two-dimensional plane. Examples of plane groups include $p_1, p_2, p_3, p_4, p_6,$ and p_m .

Space groups: Space groups are symmetry groups that describe the arrangement of atoms in a three-dimensional space.

Graph automorphism groups: Graph automorphism groups are symmetry groups that describe the symmetry of a graph under the operation of graph automorphisms. Examples of graph automorphism groups include the full automorphism group, the vertex-transitive group, and the edge-transitive group.

Overall, in all the above definitions, the related groups are based on the number and type of symmetry operations that can be applied to the molecule without changing its overall shape or structure.

In other words, by analyzing the symmetry group of a molecule, chemists can predict a wide range of properties, including spectroscopic behavior, optical activity, chemical reactivity, and crystal structure, [13].

In general, the molecular symmetry group is an important concept in chemistry because it can be used to predict a molecule's properties, such as its dipole moment, reactivity, and spectroscopic behavior. It is also used in the design of new materials and drugs, as well as in the interpretation of experimental data, see [14].

Ashrafi is a mathematician who has made significant contributions to the study of symmetry groups of both rigid and non-rigid molecules. His research has focused on the development of novel computational methods for predicting the symmetry properties of molecules and applying these predictions to a wide range of chemical problems, see [15–19].

3.1 Classifying symmetry operations and group definition

A vital aspect in examining the symmetry of various objects, such as a cube or a water molecule, is the concept of a transformation operation. This operation, known as a covering transformation, alters the geometric structure of an object without changing its outward appearance, as detailed in references [12, 14]. For instance, rotating a water molecule by 180 degrees around an axis bisecting the $H - O - H$ angle interchanges the positions of the two hydrogens, resulting in an identical appearance before and after the rotation, as demonstrated in Figure 1. The comprehensive list of transformation operations accurately represents the symmetry of any object.

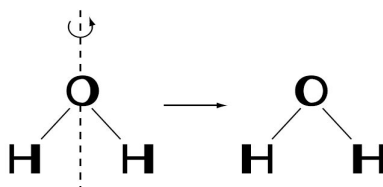


Figure 1: Rotation 180° is a symmetry operation of water molecule.

It is customary to refer to the result of applying two operations consecutively as the product of the two operations. To delve further into whether the products of known covering operations of the water molecule generate any new ones, it is advantageous to construct a complete multiplication table, see [20, 21].

4 Point group versus symmetry group

A point group refers to the symmetry group of a finite object in which its specification completely defines its symmetry. The range of possible types of symmetry that a molecule can exhibit is quite diverse.

4.1 Axes of rotation: C_n

A molecule possesses an axis of rotation of degree n , labeled as C_n , if a rotation by $\frac{1}{n}$ th of a full turn serves as a covering operation. Axes of rotation are a prevalent form of molecular symmetry operation. A single fold axis is equal to the identity, which involves a rotation by a full turn [13, 22].

4.2 Mirror planes

In molecular symmetry, a molecule possesses a plane of symmetry, also known as a mirror plane, if reflecting all atoms in that plane results in a covering operation. While any planar molecule exhibits mirror symmetry since reflection in the molecular plane leaves the positions of all atoms unchanged, a molecule may have multiple mirror planes, such as in the case of water, which is symmetric concerning both the molecular plane and a perpendicular plane, see [10, 13, 22].

4.3 Inversion

In molecular symmetry, the concept of inversion involves moving an atom a certain distance along a line segment that connects it to the origin, then extending the line segment by the same distance and moving the atom to the endpoint of the extended line segment. This results in the atom being as far away from the origin in the opposite direction. A molecule is said to have inversion symmetry, denoted by i , if inverting all of its atoms with respect to the center of gravity of the molecule is a covering operation. While benzene and trans-1,2-dichloroethylene exhibit inversion symmetry, cyclopropane does not, as discussed in references [14] and [10].

4.4 Rotatory reflections, or improper rotations

A twofold rotation followed by a reflection in a plane perpendicular to the molecular axis, denoted by C_2 followed by σ_h , is a covering operation in which its combination with an n -fold rotation yields a rotatory-reflection or improper rotation, symbolized S_n , see [10, 12–14].

5 Ashrafi's scientific papers on symmetry

Here, we used references [23–28]. Ashrafi's first inaugural publication in the field of mathematical chemistry was co-authored with Hamdani and appeared in the journal "Croat. Chem. Acta". The paper, entitled "The full non-rigid group theory for tetraamine platinum(II)," was published in 2003.

The paper outlines a straightforward method for computing character tables for the symmetry group of molecules containing multiple NH_3 groups connected to a rigid framework. The authors investigated the full non-rigid group ("f-NRG") of tetraamine platinum(II) with the C_{2v} symmetry group, establishing that it is a group of order 216 with 27 conjugacy classes. Additionally, they successfully derived the character table for this group.

Although the main thrust of the work concerned the molecular symmetry group, it holds the distinction of being the first mathematical chemistry paper authored by an Iranian mathematician. It is worth noting, however, that chemists had previously published a considerable body of work in this field.

After the publication of this paper, many more papers with Hamdani and Darafsheh were published until 2005. In 2005, Ashrafi published a paper with Ahmadi on the symmetry of molecules titled "New computer program to calculate the symmetry of molecules" in the journal "Central European Journal of Chemistry", which is his first paper that applies a Matlab program for computing the symmetry group, see [29]. In 2006, Ashrafi and Loghman co-authored the first paper on the PI Index of zig-zag polyhex nanotubes in the field of chemical graph theory that did not rely on group theory. This paper, was published in "MATCH Commun. Math. Comput. Chem." was the first to utilize graph theory techniques to calculate topological indices and has since been cited 164 times on Google Scholar [30]. It is worth noting that while subsequent papers authored by Ashrafi with Ahmadi [29] were accepted for publication earlier, this paper stands as a groundbreaking contribution to the field.

Ashrafi was interested in computing the automorphism and symmetry group of molecules. After that, this field became of great interest to many mathematicians and math students in the country. Ashrafi also published papers in this field with Vakili-Nezhaad and Moghani, see [31–39].

It's impressive that Ashrafi has written 47 scientific papers on the topic of "Symmetry" in mathematics. These papers can be found in references [15, 16, 29, 32, 34, 35, 37, 39–58] as well as [17–19, 59–73].

Most of them include the keywords markaracter table of molecular graphs, permutational isomers of fullerenes, and the concept of cycle index. Their joint contributions to this field are undoubtedly valuable and have significantly advanced our understanding of molecular symmetry, see [32, 51, 59–62, 66–68, 71, 72].

5.1 Symmetry Group of Polyhedral Graphs

Fullerenes are a class of carbon molecules that have a unique spherical structure, and the fullerene C_{60} is a particularly well-known example. The symmetry group of C_{60} is a group of transformations that preserve the structure of the molecule, such as rotations and reflections, see [74, 75]. Fullerene graphs are cubic, 3-connected, planar graphs with precisely 12 pentagonal faces, with all other faces being hexagons. These graphs serve as mathematical representations of fullerene molecules, which consist solely of carbon atoms and differ from graphites and diamonds.

As previously mentioned, the initial paper by Ashrafi et al., detailing the symmetry of a specific fullerene, can be traced back to the research conducted by Ashrafi and Ahmadi, titled "New computer program to calculate the symmetry of molecules," published in the "Central European Journal of Chemistry" (see [29]).

In [68, 76], Ashrafi and his colleagues investigated the automorphism group and fixed the number of six families of (3,6)-fullerene graphs. They applied the action of the symmetry group of a fullerene molecule C_{60+12n} on the set of its chemical bonds to calculate the PI index of C_{60+12n} in [55]. This method is efficient and can be used for other classes of fullerenes as well.

The naming convention for ordinary fullerenes is based on their composition of pentagonal and hexagonal faces, denoted as (5,6)-fullerenes. Euler's theorem allows for the construction of (3,6)-fullerenes, but there are no $(r, 6)$ -fullerenes for r greater than or equal to 6.

However, with r equal to 6, one can create various intriguing chemical structures resembling graphene, open nanotubes, and nanotori. In recent years, chemists have been studying (3,6)-fullerenes due to their similarities to ordinary fullerenes. The smallest (3,6)-fullerene is the tetrahedron, and its point group symmetry is isomorphic to the symmetric group T_d .

In reference [68], the authors demonstrated that for a (3,6)-fullerene graph F , the order of the automorphism group $|Aut(F)|$ divides 24. Additionally, they put forward the conjecture that $Aut(F)$ is isomorphic to a subgroup of T_d that is isomorphic to one of the following groups:

$$C_s, C_2, C_3, D_2, C_{2v}, C_{3v}, D_{2d}, S_4, T.$$

Lemma 5.1. (Cauchy–Frobenius Lemma) For the action G on Ω , the number of orbits is

$$\frac{1}{|G|} \sum_{g \in G} |fix(g)|.$$

A polyhedral graph is a 3-vertex-connected, planar graph. Cubic polyhedra are extensions of the classical fullerenes with face sizes restricted to 3, 4, 5, and 6. In general, there are 19 classes of cubic polyhedra of positive curvature, each corresponding to a unique face-signature (t, s, p) , as detailed in [77]. Moreover, in the same reference, the authors derived the list of allowed symmetry groups for each class and constructed the smallest polyhedron for each allowed symmetry, as documented in [74, 78, 79]. Here is an example to illustrate how the automorphism group of a polyhedral graph can be computed.

Example 5.2. Consider a polyhedral graph with 96 vertices denoted by F_{96} as depicted in Figure 2. Suppose $G = Aut(F_{96})$, it can be seen that if α denotes the rotation through an angle

of 60° around an axis through the midpoints of the front and back faces, then one of orbits of $\langle \alpha \rangle$ containing vertex 1 is $\{1, 2, 3, 4, 5, 6\}$. Now, consider the axis symmetry line β which is colored by blue, then $G = \langle \alpha, \beta \rangle \cong D_{12}$.

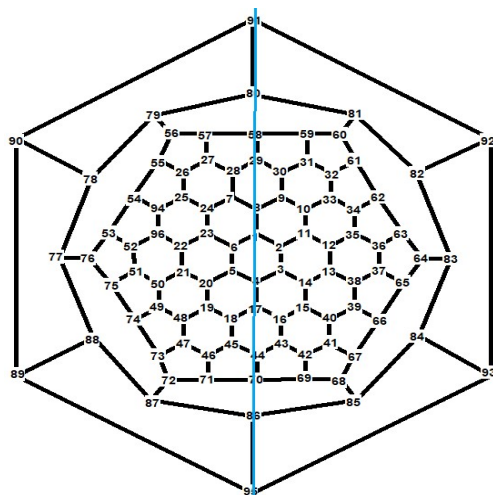


Figure 2: The polyhedral graph F_{96} .

In [47], Ashrafi et al. investigated the symmetry properties of several large carbon molecules, while in [54], they studied the symmetry structure of different types of graphene lattices. The obtained symmetry information was then used to compute well-known distance-based topological indices for these lattices. In addition, they addressed several topology-related problems for graphene-like structures using polynomial approaches and computed the limiting behavior of the associated counting polynomial as the number of carbon atoms tends to infinity. This method enables the identification of symmetries in large systems of nanostructures.

In [64], the authors employed operations on maps to solve the equivalence classes of substructures of multi-shell clusters with icosahedral and octahedral symmetry. They used a topological index of centrality, computed on the layer matrix of rings surrounding the vertices in the molecular graph, to compare with the results of matrix permutation. The study also provides a centrality order of vertices in multi-shell clusters.

5.2 Mark table and markaracter table

The notion of the table of marks of a finite group was first introduced by William Burnside, one of the pioneers of finite groups, in the second edition of his classical book, see [80]. Shinsaku Fujita on the other hand, introduced the term "markaracter" to describe a unified framework for understanding marks of permutation representations and characters of linear representations on a common basis. The markaracter table, therefore, is a table that contains information about the marks and characters of a finite group, presented consistently. In other words, the markaracter table of G is obtained by selecting rows and columns from $M(G)$ corresponding to cyclic subgroups of G , see [59, 67, 71, 72, 81, 82].

In contrast, the table of marks introduced by Burnside only describes the marks of a finite group's permutation representations. Fujita's markaracter table extends Burnside's table of marks to include both permutation and linear representations of a finite group. This unified

framework provides a more comprehensive understanding of the structure of finite groups and their representations, see [81–92].

The table of marks of a finite group is a compact way to describe the subgroup lattice of a finite group G . It characterizes the permutation representations of G by certain numbers of fixed points and provides a detailed partially ordered set of all conjugacy classes of subgroups of G . The table is constructed by considering the set of all subgroups of G , denoted as $\Gamma_G = \{U : U \leq G\}$, and the G -action on Γ_G by conjugation. The G -orbits of subgroups in Γ_G form a partially ordered set, where the incidence relation is given by $[U] \leq [V]$ if $U \leq V^g$ for some $g \in G$.

Let $G_1 (= 1), G_2, \dots, G_r (= G)$ represent the conjugacy classes of subgroups of G . Then $\Gamma_G/G = \{[G_i], i = 1, 2, \dots, r\}$. For each subgroup $U \leq G$, the group G acts transitively on the set $U/G = \{Ug : g \in G\}$ of right cosets of U in G . Conversely, every transitive G -set X is isomorphic to a G -set U/G where U is a point stabilizer of X in G . For every $g \in G$, the G -set U^g/G is isomorphic to U/G . Therefore, every transitive G -set is isomorphic to G_i/G for some $i \leq r$.

Definition 5.3. For the finite group G with G -set X and $U \leq G$, the mark $\beta_X(U)$ of U on X is

$$\beta_X(U) = |\text{Fix}_X(U)|,$$

where $\text{Fix}_X(U) = \{x \in X : x.u = x, \forall u \in U\}$.

The table of marks $M(G)$ is a square matrix

$$M(G) = (\beta_{G_j/G}(G_i))_{j,i},$$

where G_i and G_j run through of non-conjugated subgroups of G .

The paper [59] describes a straightforward computational method for calculating the mark-character tables of finite groups. With this method, the authors were able to compute the mark-character table of a dihedral group of order $2n$, as well as several abelian groups. The paper also includes a GAP program that is effective for calculating mark-character tables of groups with order $d \leq 10000$. Using this program, the mark-character table of the I_h point group symmetry was calculated.

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

$$Z(G, X) = \frac{1}{|G|} \sum_{g \in G} \prod_{i=1}^t x_i^{c_i(p)},$$

in which $(c_1(p), \dots, c_t(p))$ is the cycle type of the permutation $p \in G$. All elements of a conjugacy class have the same cycle type, so the cycle index can be rephrased in the following way:

$$Z(G, X) = \frac{1}{|G|} |C| \sum_{c \in C} \prod_{i=1}^t x_i^{c_i(gc)},$$

where C is the set of all conjugacy classes of G with representatives $gc \in C$.

In papers [71, 72], Ashrafi et al. calculated the mark-character table of generalized quaternion groups and finite groups of order pqr , where p, q , and r are prime numbers and $p \geq q \geq r$.

In [66, 67] they computed the $USCI$ table and cycle index of some classes of fullerene graphs. The concept of unit subduces cycle indices (USCIs) is a mathematical tool used in the study of symmetry groups and their actions on sets of objects. USCIs are polynomial expressions

that encode the symmetry properties of a finite group and are used to calculate the number of fixed points and cycles under group actions. More specifically, USCIs are derived from the cycle index polynomial of a finite group, which is a polynomial expression that encodes the group's permutation action on a set of labeled objects.

The cycle index polynomial can be used to count the number of permutations that leave a set of objects invariant, as well as the number of permutations that have a given cycle structure.

The USCIs are obtained by taking the unit subductions of the cycle index polynomial, which involves substituting certain variables in the cycle index polynomial with unity. The resulting polynomial expresses the number of fixed points and cycles of the group action on subsets of the original set of objects.

The concept of USCIs is closely related to the Polya enumeration theorem, which is a mathematical theorem used to count the number of orbits of a finite group on a set of objects. The USCIs can be used in conjunction with the Polya enumeration theorem to systematically count the number of isomers of chemical compounds based on their underlying symmetry groups. The use of USCIs has important applications in the fields of chemistry and materials science, as it provides a systematic and efficient way to predict and enumerate the structural isomers of compounds and materials based on their underlying symmetry groups.

The main content of the paper [93] is an analysis of the cycle index of the symmetry group of C_{60} . The cycle index is a mathematical tool used to describe the cycle structure of a permutation group, which is a group of transformations that rearrange a set of objects.

In the paper [93], Fripertinger derives an explicit formula for the cycle index of the symmetry group of C_{60} , which allows for a detailed analysis of the group's cycle structure. This analysis provides insights into the geometric and chemical properties of the molecule, such as its bond lengths, bond angles, and electronic structure.

The paper also includes several examples and applications of the cycle index formula, demonstrating its usefulness for predicting and analyzing various properties of C_{60} and related fullerene structures. Overall, the paper represents an important contribution to the field of mathematical chemistry and demonstrates the power of group theory and other mathematical tools for understanding the properties of complex molecular structures.

Finally, in [67] the authors generalized Fripertinger's method to compute the three-dimensional Polya cycle indices for the natural actions of the symmetry group on the set of vertices, edges, and faces of the small fullerene C_{24} and the big fullerene C_{150} .

5.3 Permutational isomers of fullerenes

The Polya Enumeration Theorem provides a powerful tool for counting the number of objects (such as colorings) that can be formed subject to certain symmetries. The theorem is named after the Hungarian mathematician George Polya, who developed the theory in the early 20th century, see [81–92].

The basic idea of the theorem is to use group theory to exploit the symmetries of the objects being counted. In the case of counting colorings with k colors, the relevant symmetry group is the group of permutations of the n objects being colored (where n is the number of regions in the object being colored). The cycle index of this group captures the relevant information about the symmetries of the object and can be used to derive a formula for the number of colorings.

To apply the Polya Enumeration Theorem to the problem of counting colorings, one replaces each variable x_i in the cycle index with $1 + x^i$, where x is a formal variable representing the color, and i ranges over the positive integers. The resulting polynomial can then be evaluated at $x = k$ to obtain the number of colorings using k colors, see [61].

Hetero fullerenes are a class of fullerenes that contain atoms other than carbon. In [93], Friperinger utilized SYMMETRICA to develop codes for computing the number of $C_{60-k}B_k$ molecules, where B represents a hetero-atom, such as S_i .

Ashrafi and Ghorbani computed the numbers of hetero-fullerenes for various infinite families of fullerenes in a series of related works [61, 94–96]. To accomplish this task, they utilized the computer algebra system GAP. Furthermore, the authors used GAP to calculate the number of permutational isomers of hetero-fullerenes in the C_{60} fullerene with I_h point group symmetry.

The Polya-Redfield theorem is a standard method for enumerating of chemical compounds polyhedra, hetero-fullerenes and other structures.

In [59–62, 95, 97] Ghorbani by using Polya's theorem, enumerated the permutational isomers of several infinite families of fullerenes, namely C_{10n} , C_{12n} , C_{12n+6} , C_{24n} and C_{40n} . As a result, it is shown that, for example, the number of $C_{75}B_{75}$ molecules are

$$"4641303486835439484959145718568923895458472",$$

where B denotes the boron atom.

The hues of large fullerenes have been scrutinized using a combination of methods derived from Sheehan's adaptation of Polya's theorem, the Möbius inversion technique, and character cycle indices. In reference [98], the authors employed these techniques to examine various giant fullerenes, such as icosahedral C_{80} featuring a chamfered dodecahedron structure, chiral fullerene C_{140} , icosahedral C_{180} , and C_{240} with a chamfered truncated icosahedron geometry. These methods are utilized to produce both achiral and chiral face colorings in four distinct situations: (1) coloring only pentagons while painting all hexagons white, (2) coloring hexagonal faces with all pentagons painted white, (3) both pentagons and hexagons painted with variable colors from a single set, and (4) both pentagons and hexagons painted with variable colors but chosen from two different sets.

For the icosahedral fullerenes with I_h symmetry group, it has been shown that at least two black colors are needed, along with the remaining white, to produce chiral colorings when both pentagons and hexagons are varied. The results provide new insights into facial labeling and facial dynamics of fullerenes. The techniques used in [98] are fully prepared to be inscribed in the new so-called neutrosophical science (of carbon) nano-structural physical chemistry.

5.4 Topological indices and symmetry group

The initial investigations of the Wiener index were conducted by Harold Wiener in 1947. He discovered correlations between the boiling points of paraffin and the molecular structure, as detailed in reference [99]. Wiener noted in his article that the boiling point (t_B) can be closely approximated by the formula $t_B = aw + bp + c$, where w represents the Wiener index, p denotes the polarity number, and a , b , and c are constants specific to a given isomeric group. Since then, the Wiener index has become one of the most commonly used topological indices in chemistry, particularly for modeling molecules as undirected graphs, especially trees, see [100–103]. For example, in 1994, Gutman et al. [104] conducted numerical testing and proposed the conjecture that there exists a bound $M \in \mathbb{N}$, such that for all $w \geq M$, a tree T with $W(T) = w$ can be found. Further examination of all possible trees with 20 or fewer vertices revealed that out of all natural numbers up to 1206, only 49 numbers are not Wiener indices of trees (refer to [105]). Consequently, in [105], the conjecture was put forth that all natural numbers, except for these 49, are Wiener indices of trees, see [106–114].

The Graovac-Pisanski index, also known as the GP index [115], is a modified version of the Wiener index that takes into account the symmetries of a given graph. Since there have been many generalizations of the Wiener index and multiple of them are called modified Wiener index,

we refer to this generalization as modified version of the Wiener index. This comprehensive measure considers both the distances between atoms or nodes and the overall symmetry of the system, allowing for a more accurate analysis of molecular or network structure.

One key advantage of this index, as opposed to other distance-based indices, lies in its ability to account for the symmetries present within a graph. This is particularly important as the symmetries of a molecule can significantly impact its properties [116].

Recent research has further demonstrated the significance of the Graovac-Pisanski index in chemistry, as evidenced by publications such as [117], [118], and [119]. This underscores its importance as a tool for analyzing chemical properties and molecular structures.

The Graovac-Pisanski index of a graph G with vertex set $V(G)$ and the automorphism group $Aut(G)$ is denoted as $GP(G)$ and is defined as

$$GP(G) = \frac{|V(G)|}{2|Aut(G)|} \sum_{v \in V(G)} \sum_{\alpha \in Aut(G)} d(v, \alpha(v)).$$

The Graovac-Pisanski index has been widely used as a topological index in quantitative structure-property relationship studies of organic molecules. After its introduction, the GP index received almost no attention, but in the last years the situation has been completely different, see [119–123]. Also, in [78] the author interested the inverse problem for the GP index. In general, the inverse problem asks, for a given (chemical) graph invariant TI and a given value k , find (chemical) graphs G for which $TI(G) = k$, cf. [124–127].

In [53], Ashrafi et al. proved that for every graph G , the class function

$$\delta = \frac{1}{|Aut(G)| \times |V(G)|} \sum_{u \in V(G)} \sum_{\alpha \in Aut(G)} d(u, \alpha(u)),$$

can be expressed as a rational combination of the trivial character χ_1 and, at most, two other irreducible characters of the automorphism group of G .

In related work, Ashrafi et al. [57] proposes a novel graph invariant that captures both the distance and symmetry properties of the studied molecules. The study presented in [118] computed the symmetry groups and Graovac-Pisanski index of certain linear polymers, and in [128], they extended this analysis to compute the GP index of some classes of fullerenes and fullerene-like molecules. Furthermore, in [46], three infinite classes of (3,6)-fullerenes were studied, and upper and lower bounds for the proposed graph invariant were presented in [53]. In [58], the GP index was computed for both armchair and zig-zag polyhex carbon nanotubes, and the relative stability of these structures and the effects of edge states were investigated.

Ashrafi et al. used the wreath product of two graphs to compute the symmetry group of a molecule made from cycloalkynes by replacing hydrogen atoms with alkyl groups in [54]. This method is a general approach that can be useful for such computations. In addition, they calculated the symmetry of several types of carbon nanotubes and nanotori, including series of armchair polyhex, zig-zag polyhex, and $C_4C_8(R/S)$ nanotubes, in [129]. They also examined the topological properties of these nanostructures.

6 Conclusion

The symmetry group of a molecular graph is a group of transformations that preserve the structure of the molecule. The study of the symmetry group of molecular graphs is an important area of research in the field of mathematical chemistry, which involves the application of mathematical concepts and methods to the study of chemical structures and properties. By analyzing

the symmetry group of a molecule, researchers can gain insights into its physical properties, such as its stability, reactivity, and spectroscopic behavior.

Ashrafi's research focused on developing mathematical techniques for computing the symmetry group of molecular graphs, as well as analyzing the properties of these groups. He developed new algorithms for determining the symmetry group of large, complex molecular structures, and explored the relationship between the symmetry group and other mathematical properties of the molecule, such as its graph theory and topological properties.

The insights gained from this research have important applications in fields such as drug design and materials science. For example, understanding the symmetry properties of a molecule can help researchers design more effective drugs by identifying structural features that are more likely to interact with specific biological targets. Similarly, knowledge of the symmetry properties of materials can be used to design new materials with specific mechanical, electrical, or optical properties.

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

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