

Review

Counting Polynomials in Chemistry: Past, Present, and Perspectives

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Abstract: Counting polynomials find their way into chemical graph theory through quantum chemistry in two ways: as approximate solutions to the Schrödinger equation or by storing information in a mathematical form and trying to find a pattern in the roots of these expressions. Coefficients count how many times a property occurs, and exponents express the extent of the property. They help understand the origin of regularities in the chemistry of specific classes of compounds. Our objective is to accelerate the research of newcomers into chemical graph theory. One problem in understanding these concepts is in the different approaches and notations of each research study; some researchers provide online tools for computing these mathematical concepts, but these need to be maintained for functionality. We take advantage of similar mathematical aspects of 14 such polynomials that merge theoretical chemistry and pure mathematics; give examples, differences, and similarities; and relate them to recent research.

Keywords: counting polynomials; chemical graph theory; educational research review; Sachs graphs; invariants



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1. Introduction

As Diudea said, a single number, representing a chemical structure in graph-theoretical terms, is called a topological index (TI) [1]. A topological index is a real number related to a molecular graph [2]. Many nanomaterials, drugs, and crystalline materials appear in various industries. Medical behaviour can be studied with TIs, leading to quantitative structure property relationships (QSPR) and quantitative structure activity relationships (QSAR) [3,4]. The first TIs, even before the introduction of the term, are those of Calingaert and Hladky in 1936 [5], Kurtz and Lipkin in 1941 [6], and of Wiener in 1947 [7]. Degree-based TIs are the most studied [8].

Some of the first names to speak about chemical graphs are enumerated by Rouvray [9]: Newton, Macquer, Boscovich, Lomonosov, Cullen, and Higgins. In 1808, Dalton and Wollaston introduced the ball and stick models used in classrooms [10,11]. One of the first chemists to try a prediction of properties was Koop in 1844 [12]. Leading the way into the valence concept, Couper drew the first bond between atoms in 1858, and Frankland had the first idea about valences in 1864. Kekulé's first attempt to depict the tetrahedral carbon followed in 1867 [9]. Cayley, in 1874 [13,14], and Sylvester, in 1875 [15], drew the first chemical graphs. Werner studied complex chemistry in 1893 [9]. During the 1930s many new molecules were synthesized. Chemical graphs became more of a must in order to differentiate this relatively large number of new molecules. In 1937, Polya incorporated the concepts of symmetry classes, permutation groups, and generating functions in his Enumeration Theorem [16] by continuing an earlier work of Cayley [14].

Returning to TIs, two more initial indexes were studied: F by Platt in 1947 [17,18] and N₂ by Scantlebury in 1964 [19], before Hosoya showed that W is the half sum of all

entries in [Di] and afterwards proposed the Z index in 1971 [20], which he first attributed to Wiener. The Zagreb index (M_1) followed in 1975 [21], which can be related to the Platt and Gordon–Scantlebury by: $F=2N_2=M_1-e$. Balaban followed with his Centric index in 1979 [22]. Danail Bonchev, Ovanes Mekenyan, and Milan Randić proposed a generalization of the graph center concept to cyclic graphs in 1980 [23–25]. A way of classifying TIs is the grade of degeneracy, and so we mention another of the first generation, proposed by Schultz in 1989 [26,27]. The beginning of the second generation is marked by the molecular connectivity index of Randić in 1975 [28], which was characterized by a very low degeneracy. To name another few: the high-order molecular connectivity indices studied by Kier and Hall in 1975 [29–32]; the information–theoretic indices of Bonchev and Trinajstić in 1977 [33]; the Merrifield and Simmons indices that were studied in 1980 [34–36]; in an effort to decrease degeneracy, Mekenyan and Trinajstić proposed the topological information superindex in 1981 [37]; in 1982, Balaban modified the Randić formula and gave rise to the average distance-based connectivity index [38]; the information–theoretic indices of Basak and coworkers in 1983 [39]; the orbital information index for graph connections of Bertz in 1988 [40]; or the electrotopological state indices of Kier and Hall in 1990 [41,42]. One important contribution to the idea of using Eigenvalues as TIs was coined by Lovasz and Pelikan in 1973 [43].

The third generation of TIs may be considered to start by defining real-number local vertex invariants (LOVIs) [44], as detailed by Devillers and Balaban in a book chapter [45]. Gutman has summarized the main properties of molecular-graph-based structure descriptors and provided a critical comparative study [46]. Since then, a few indices have been developed: a type of Zagreb index based on degrees of neighbours of vertices [47]; an eccentric atom–bond connectivity index [48]; a Sanskruti index $S(G)$, showing good correlation with entropy of an octane isomer [49]; the multiplicative atom–bond connectivity index [50]; the product connectivity leap index [51]; M_N as a neighbourhood Zagreb index of product graphs [52]; and so on. Many authors have computed indexes for different applications [53–55], or analytical expressions for such indexes [56–60]. A number of TIs are based on polynomial coefficients and can be derived directly or by using integrals or derivatives [54,61].

Haruo Hosoya first introduced a counting polynomial, the Hosoya polynomial (HP), to characterize a graph [20,62]. Counting matrices are the expanded forms of counting polynomials [63], since some distance-related properties can be expressed in the polynomial form with coefficients calculated from matrices [64,65].

Count-polys are very useful for discriminating among similar structures [66]. However, a polynomial is a more general treatment than an index. The advantage of polynomials is the reduction of degeneracy since it is an invariant relative to the numbering of the atoms [66,67]. Degeneracy refers to equal values for different molecules: the molecular weight has high degeneracy since there are many molecules with the same weight; 3D descriptors show low or no degeneracy at all since two molecules with the same weight can have their atoms arranged differently in 3D space. Formulas were obtained for entropies and energies of counting polynomials of some repeated structures f[68].

The overall number of chemicals synthesized, isolated, or marketed increases exponentially. The CAS REGISTRYSM database (www.cas.org, accessed on the 18 August 2023) currently contains almost 200 million entries. However, it would be ideal to know all their properties. During the 1970s, it became obvious it is not feasible to obtain all their properties experimentally. Gutman exemplified, with the aid of maleic anhydride, that a chemical formula is sometimes better represented by a multigraph rather than by a simple graph [69].

Given this, count-polys are molecular descriptors. They should be invariant to all the operations related to molecule manipulation that do not affect the molecular structure. Their number has increased in order to keep pace with large databases, such as CAS, so a few qualities should be sought when choosing descriptors. They should be: invariant to atom labelling and numbering; invariant to the molecule roto-translation; have an

unambiguous algorithm; direct structural interpretation; and be locally defined [61,70]. Even more, they preferably are: theoretical and not based on experimental properties; not trivially related to other descriptors; generalizable to “higher” descriptors; efficient to construct; applicable to a broad class of molecules; interpretative by structure; use familiar structural concepts; change gradually with gradual change in structures; have the correct size dependence, if related to the molecule size; have good correlation with at least one property; and preferably discriminate among isomers.

Coefficients of polynomials and their zeros are of interest in chemistry [69]. Zeros are denoted by “ λ ” or “ x ” and are the same as roots (characteristic values, characteristic roots, latent roots, eigenvalues, proper values, or spectral values) [71]. Since many of the polynomials discussed are derived from matrices, defining the companion matrix is already solved. In other words: say we have an initial polynomial P_i , we require a matrix whose characteristic polynomial (the *ChP* discussed in this text) is the same as P_i ; based on the definition, the roots of this polynomial are identical to the eigenvalues. If one tries to describe the topology of a molecule, one can store information about the adjacencies (the bonds) between atoms as well as the identities (the atoms). Simplifying by disregarding the bond and atom types, the adjacency matrix ($[Ad]$ a matrix of elements $b_{i,j} = 1$ if an edge connects vertices i and j and $b_{i,j} = 0$ otherwise) and the identity matrix ($[Id]$) contain only zeros and ones. Any such or derived square matrix ($[Tm]$) can be used to construct a counting polynomial that carries features of the originating molecule:

$$CoP \stackrel{\text{def}}{=} \sum_{k \geq 0} n \cdot x^k, \quad (1)$$

where “ k ” is any value in $[Tm]$, “ n ” counts the occurrences of “ k ”, $n = \text{count}([Tm]_{i,j} = k)$, and “ x ” represents the roots of the polynomial [66,72]. For example, let there be:

$$[Tm] = [Id] = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Since both “1” and “0” occur two times:

$$CoP_{[Id]} = 2x^1 + 2x^0$$

A procedure is proposed to somehow generalize the use of polynomials in regression analysis [67]. It is used for creating and using a polynomial formula that correlates the structure with a given property through the value of polynomials at one point.

Applications for calculating polynomials can rely on files containing molecular data, such as some gateways of software [73]. These are harder to maintain since there are many file extensions and programs that do not export identical files for the same chemical compound. Also, users should send their contributions if they fix any bugs so that the initial author can implement these improvements. Another way of calculating polynomials can be searched on the Internet, but scripts need to be able to account for symbolic mathematics [74–76].

Rouvray [77,78] attracted attention to the scientific community in 1971 that interdisciplinary studies are indispensable to advance QSAR and QSPR. Today, we can look back at the day where we noticed that experimental studies are too slow to rely on for the discovery of compounds. Now computers are too slow and need to somehow use the advantages of the human mind to take a bigger step into predicting. Recent effort has been initiated to overcome this issue, but we do not know if the approaches are fruitful [79,80]. Machine learning takes some steps into this realm since we program computers to learn patterns we believe will lead to important scientific discoveries [81–83]. It is true that young minds prefer to see fast and easy results before understanding the core of complicated mathematics behind programs.

It may be easier to understand these concepts if there was a way of unifying them. One unifying attempt was that of Gutman trees, as pointed out by El-Basil [84]; it applies to very particular cases and cannot be simply extended. We appreciate how these concepts help understand similarities between polynomials. Another, maybe more successful example is the immanantal, which is discussed. We would like to present a few graph-theoretical polynomials in which theoretical chemistry and pure mathematics merge. We expose their differences, similarities, relate them to recent research, and suggest potential new research. They help understand the origin of regularities in chemistry of specific classes of compounds [85].

In our article, when we speak of vertices (denoted by “a”) we refer to atoms and when we speak of edges (denoted by “b”) we refer to bonds. Also, we try to simplify mathematical aspects.

2. Characteristic Polynomial

The characteristic polynomial is certainly the most popular and most extensively studied polynomial in chemical graph theory. It is also found in literature by the terms, secular function or determinantal polynomial, and commonly denoted by ϕ or ChP .

The first use of the ChP in relation with a chemical structure appeared after the discovery of wave-based treatment at the microscopic level. The ChP finds its uses in the topological theory of aromaticity, structure–resonance theory, quantum chemistry, counts of random walks, as well as in eigenvector–eigenvalue problems [86].

Its classic definition is simple:

$$ChP = \det(x \cdot [Id] - [Ad]) = |x \cdot [Id] - [Ad]| \quad (2)$$

Taking methyl-cyclo-butane (Figure 1a, G_1 for example, having 5 vertices/atoms and 5 edges/bonds), $[Id_{G_1}]$ and $[Ad_{G_1}]$ are as follows:

$$[Id_{G_1}] = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$[Ad_{G_1}] = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$ChP_{G_1} = \det \begin{pmatrix} x & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & x & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & x & 0 & 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & x & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & x & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$ChP_{G_1} = \det \begin{pmatrix} x & -1 & -1 & 0 & 0 \\ -1 & x & 0 & -1 & 0 \\ -1 & 0 & x & -1 & 0 \\ 0 & -1 & -1 & x & -1 \\ 0 & 0 & 0 & -1 & x \end{pmatrix}$$

$$ChP_{G_1} = x \cdot \det \begin{pmatrix} x & 0 & -1 & 0 \\ 0 & x & -1 & 0 \\ -1 & -1 & x & -1 \\ 0 & 0 & -1 & x \end{pmatrix} - (-1) \cdot \det \begin{pmatrix} -1 & -1 & 0 & 0 \\ 0 & x & -1 & 0 \\ -1 & -1 & x & -1 \\ 0 & 0 & -1 & x \end{pmatrix} +$$

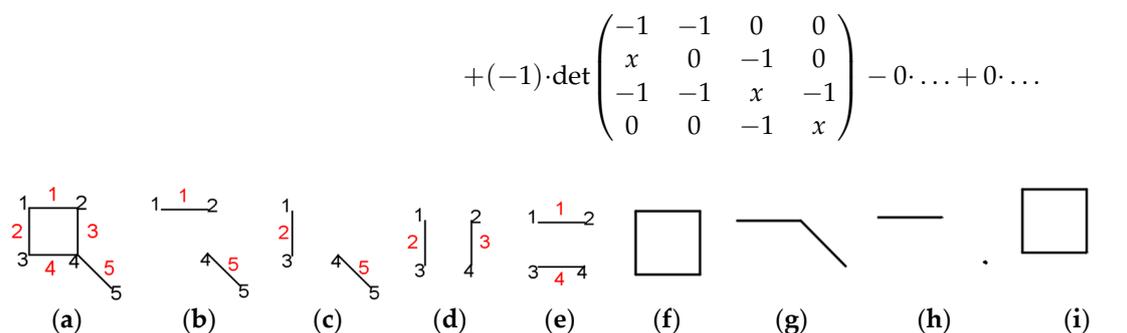


Figure 1. (a) Graph theoretical representation of methyl-cyclo-butane (G_1); (b–e) independent edges (also Sachs graphs); (f) independent ring (also a Sachs graph); (g–i) improper Sachs graphs.

As such:

$$ChP_{G_1} = x^5 - 5 \cdot x^3 + 2 \cdot x$$

An elegant counting method of finding the ChP is that of Sachs [87,88]. A Sachs graph can be composed of isolated edges, rings, or combinations. We denote them with B_2 (“2” being the number of vertices an isolated edge can have) and R_m (“m” being the number of vertices a ring is composed of). The number of isolated edges = o and the number of rings = p . There is one restriction in the definition of a Sachs graph: $2 \cdot o + p \cdot m = k$, where k = the number of vertices. Let S_k be the set of all Sachs subgraphs (s) with “ k ” vertices of any graph G , and “ a ” being the total number of vertices of G . The number of components of the Sachs subgraph is $c(s)$ and the number of rings $r(s)$. The definition of ChP is:

$$ChP_G = \sum_{k \geq 0} \sum_{s \in S_k(G)} (-1)^{c(s)} \cdot 2^{r(s)} \cdot x^{a-k} \quad (3)$$

We thus have:

for $k = 0$, we count the empty Sachs graph with 0 edges and the result is: $1 \cdot (-1)^0 \cdot 2^0 \cdot x^{a-0} = x^a$;

for $k = 1$, there can be no isolated edge with one vertex nor such a ring, and the result is 0.

Taking our example in Figure 1a:

$$ChP_{G_1} = \sum_{k \geq 0} \sum_{s \in S_k(G_1)} (-1)^{c(s)} \cdot 2^{r(s)} \cdot x^{5-k}$$

denoting $q = \sum_{s \in S_k(G_1)} (-1)^{c(s)} \cdot 2^{r(s)} \cdot x^{5-k}$,

for $k = 0$, $q = x^5$;

for $k = 2$, since this is the case where each edge represents a Sachs subgraph, $q = (-1)^1 \cdot 2^0 \cdot x^{5-2} + (-1)^1 \cdot 2^0 \cdot x^{5-2} = 5 \cdot (-1)^1 \cdot 2^0 \cdot x^{5-2} = 5 \cdot (-1) \cdot 1 \cdot x^3 = -5 \cdot x^3$;

for $k = 3$ and $k = 5$, it can be seen in Figure 1g–i that these are not Sachs subgraphs;

for $k = 4$, from each Sachs subgraph in Figure 1b–e $q_{(b)} = q_{(c)} = q_{(d)} = q_{(e)} = (-1)^2 \cdot 2^0 \cdot x^{5-4}$ and in Figure 1f $q_{(f)} = (-1)^1 \cdot 2^1 \cdot x^{5-4}$ (since $c(s)$ counts both edges and rings); as such for $k = 4$ $q = 4 \cdot 1 \cdot 1 \cdot x + 1 \cdot (-1) \cdot 2 \cdot x = 2 \cdot x$.

Summing up the three results, we get: $ChP_{G_1} = x^5 - 5 \cdot x^3 + 2 \cdot x$.

Liu and Zang found that the ChP characterizes paths and even cycles. Those cannot be characterized by the permanental polynomial [89].

The roots of the ChP are obtained by diagonalizing the adjacency matrix [69]. The sum of the w^{th} powers of these roots is equal to the w^{th} spectral moment of a graph. The coefficients of the ChP can be deduced from the spectral moments, and vice versa [61].

Ghosh developed formulas to calculate the coefficients of the ChP quickly and efficiently for the molecules represented by three classes of graphs. Later, they used the ChP

and graph squaring to derive analytical eigenspectra for graphs of linear chains and cycles with alternant edge weights. These methods can be applied to all graphs having unit cells that are repeated along the molecule [90,91].

Mondal and Mandal have made some progress in obtaining the concentration vectors of reaction networks by finding an analytical expression of the *ChP*. They find the recurrence relations among its coefficients. Later, they found that the sum of the coefficients for cycloparaphenylene graphs model physical properties, such as the strain energy and diameter of CPPs [92,93].

Gutman postulated a relation that holds for trees between the *ChP* and the Hosoya index *Z* [94]. Later, Cash extended it to (poly)cyclic graphs by substituting the matching polynomial for the *ChP* [95].

The *ChP* is related to the Laplacian polynomial, which is discussed later [86]. Other modifications of the *ChP* have been put forward, such as the μ -polynomial and the β -polynomial [61].

The *ChP* admits extensions. The Hückel's method of molecular orbital is the first of these. The 'secular determinant' is the determinant of a matrix that is decomposed as $|E \cdot Id - Ad|$ (the energy of the system "E" instead of x). He uses this form to approximate treatment of π electron systems in organic molecules. Hartree and Fock had another direction and ended up with the second extension by approximating treatment of the wave function. It was the same older eigenvector–eigenvalue problem in Slater's treatment of molecular orbitals. Another extension was pursued with the ability to explain area and volume [86].

Since the *ChP* is related to the Hosoya polynomial, it must also be related to the matching polynomial—both are defined by counting independent edges [86]. Among the plethora of other known results, some are stated by Diudea and reveal further deep lying analogies between the characteristic and the matching polynomials. The fundamental difference between *ChP* and *MP* is in the effect of cycles [61].

ChP might be thought of as the determinantal polynomial. One could also construct a permanent polynomial π as the permanent of $(x \cdot [Id] - [Ad])$ [96].

3. Permanent Polynomial

While scarcely used in chemical applications, it is interesting to search for applications of the permanent polynomial (π) related to a more general class of polynomials—the immanatals. Its definition is similar to that of *ChP*:

$$p = \text{per}(xp \cdot p[Id] - [Ad]) \quad (4)$$

For our example in Figure 1a, we can use our matrices $[Id_{G_1}]$ and $[Ad_{G_1}]$:

$$p_{G_1} = \text{per} \begin{pmatrix} x & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & x & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & x & 0 & 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & x & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & x & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$p_{G_1} = \text{per} \begin{pmatrix} x & -1 & -1 & 0 & 0 \\ -1 & x & 0 & -1 & 0 \\ -1 & 0 & x & -1 & 0 \\ 0 & -1 & -1 & x & -1 \\ 0 & 0 & 0 & -1 & x \end{pmatrix}$$

The permanent of a matrix is defined as the unsigned sum of all the permutations.

$$p_{G_1} = x \cdot \text{per} \begin{pmatrix} x & 0 & -1 & 0 \\ 0 & x & -1 & 0 \\ -1 & -1 & x & -1 \\ 0 & 0 & -1 & x \end{pmatrix} - 1 \cdot \text{per} \begin{pmatrix} -1 & -1 & 0 & 0 \\ 0 & x & -1 & 0 \\ -1 & -1 & x & -1 \\ 0 & 0 & -1 & x \end{pmatrix} - \\ - 1 \cdot \text{per} \begin{pmatrix} -1 & -1 & 0 & 0 \\ x & 0 & -1 & 0 \\ -1 & -1 & x & -1 \\ 0 & 0 & -1 & x \end{pmatrix} + 0 \cdot \dots + 0 \cdot \dots$$

As such:

$$p_{G_1} = 1 \cdot x^5 + 5 \cdot x^3 + 6 \cdot x$$

Similar to the counting method of Sachs, but a modification of the theorem [89]:

$$p_G = \sum_{k \geq 0} (-1)^k \cdot x^{a-k} \sum_{s \in S_k(G)} 2^{r(s)} \quad (5)$$

For our example in Figure 1a:

$$p_{G_1} = \sum_{k \geq 0} (-1)^k \cdot x^{a-k} \sum_{s \in S_k(G_1)} 2^{r(s)},$$

denoting $q = (-1)^k \cdot x^{a-k} \sum_{s \in S_k(G_1)} 2^{r(s)}$,

for $k = 0$, $\sum_{k=0} q = x^5$;

for $k = 2$, $\sum_{k=2} q = 5 \cdot x^3$;

for $k = 3$ and $k = 5$, it can be seen in Figure 1g–i that these are not Sachs subgraphs;

for $k = 4$, from each Sachs subgraph in Figure 1b–e $q_{(b)} = q_{(c)} = q_{(d)} = q_{(e)} = x$ and in Figure 1f $q_{(f)} = 2 \cdot x$; as such for $k = 4$ $q = 6 \cdot x$.

Summing up the three results, we get: $p_{G_1} = x^5 + 5 \cdot x^3 + 6 \cdot x$.

DeFord found that the permanent–determinant of a tree is equivalent to the Z–index and can be extended to weighted trees and more general chemical structures [97].

If two chemical structures, say G_1 and G_2 (graph 1 and graph 2), share the same permanental polynomial, then G_1 is a per-cospectral mate of G_2 . A graph G_1 is said to be characterized by its permanental polynomial if all the per-cospectral mates of G_1 have isomorphic graphs to G_1 . Complete graphs, stars, regular complete bipartite graphs, and odd cycles are characterized by their permanental polynomials [89].

Cash developed a computer program for calculating the permanental. He identified some of its properties and uses with respect for unweighted chemical graphs. Additionally, coefficients and zeroes for several representative structures were provided [98].

Li, Qin, and Zhang first studied the coefficients sum of π for hexagonal chains [99]. Li and Wei studied the coefficients sum of π for octagonal chains [100]. Later, they identified among all the phenylene chains all graphs minimizing/maximizing the coefficients sum of π , the spectral radius, the Hosoya index, and the Merrifield–Simmons index [101].

Wu and Lai investigated properties of permanental sums of graphs. They proved recursive formulas to compute the permanental sum, found the ordering of graphs with respect to the sum, and determined the upper and lower bounds of this sum and the corresponding extremal unicyclic graphs [102].

Huo proposed a Fast Fourier Transformation improved method for computing permanental polynomials and applied it to fullerene-type graphs up to C_{56} [103].

π of o-biphenylene is equal to that of 3,3-dimethylhexane divided by x^2 , which is possibly a property of some class of structures [98].

4. Matching Polynomial

The matching polynomial (*MP*) has been independently discovered many times since 1970. It was also called the matching defect polynomial, reference polynomial, and the acyclic polynomial (the latter term has fallen out of use and another polynomial has recycled it [85]). The current name is given by Farrell [104]. It is denoted by “ α ”, M , or *MP*.

MP is a consequence of the topological theory of aromaticity [105]. It is important in both theories of saturated and conjugated hydrocarbons, or in describing the 3D aromaticity of boranes [106]. *MP* is not useful in discriminating if a graph is acyclic or not, nor whether the graph has non-trivial components [107]. Deutsch has shown that degree-based topological indices can be routinely computed from *MP* [108].

Counting independent edges by the general *CoP* (Equation (1)), one can define $n_i(k)$ = the number of possible ways “ k ” edges can be chosen in a molecule (chemical graph) such that no “ k ” (chosen) edges are adjacent:

$$MP = \sum_{k \geq 0} (-1)^k \cdot n_i(k) \cdot x^{a-2k} \quad (6)$$

where “ a ” is the total number of vertices, $a \geq 2 \cdot k$ [109]. If we are talking about an acyclic molecule, it is also equal to the *ChP* [61].

Taking our example in Figure 1a, we can choose:

for $k = 0$, $n_i(k) = 1$, as there is one possibility of choosing zero edges, namely \emptyset ;

for $k = 1$, $n_i(k) = 5$, the number of edges;

and for $k = 2$, $n_i(k) = 4$ possibilities depicted in Figure 1b–e:

Afterwards for $k > 2$, $n_i(k) = 0$. As such:

$$MP_{G_1} = 1 \cdot 1 \cdot x^5 + (-1) \cdot 5 \cdot x^3 + 1 \cdot 4 \cdot x$$

Let us count in a different manner, considering S^0 , acyclic Sachs subgraphs [88]:

$$MP = \sum_{s \in S^0} (-1)^{c(s)} \cdot x^{a-k} \quad (7)$$

Let us repeat the above statement: “If we are talking about an acyclic molecule, it is also equal to the *ChP*”. For our example this is not true, and we can write this mathematically. The only cyclic Sachs subgraph appears in the case of the *ChP* for $k = 4$ in Figure 1f $q_{(f)} = (-1)^1 \cdot 2^1 \cdot x^{5-4} = -2 \cdot x$. As such:

$$MP_{G_1} = ChP_{G_1} - (-2 \cdot x) = x^5 - 5 \cdot x^3 + 4 \cdot x$$

Trying to do the same in comparison to the permanental polynomial, there is a difference in sign. For π , the (-1) term is dependent on k , and for *MP* it is dependent on the number of components. All monomials are positive for π . The only cyclic Sachs subgraph in the case of π for $k = 4$ in Figure 1f $q_{(f)} = (-1)^4 \cdot 2^1 \cdot x^{5-4} = +2 \cdot x$, and it would lead to $MP_{G_1} = p_{G_1} - (+2 \cdot x)$; but we also need to solve the rest of the coefficients, and this makes it easier to write: $pp_{G_1} = |MP_{G_1} + (+2 \cdot x)| = |x^5 - 5 \cdot x^3 + 4 \cdot x + (+2 \cdot x)|$.

Dias used *MP* to find excellent correlations between Dewar resonance structures and some properties: absorption p-band, ionization energies, Hückel HOMO, Aihara’s reduced HOMO-LUMO gap, topological resonance energy (TRE), aromatic stabilization energy (ASE), and the Klein and Randić innate degree of freedom [110].

Munir determined *MP* of some nanostar dendrimers, and then recovered many degree-based topological indices [111]. Ghosh developed very convenient algorithms for calculating *MP* of linear and cylindrical poly(p-phenylene) graphs [109]. Kwun et al. determined general closed forms for *MP* of V-Phylenic nanotubes and nanotori [112]. Later, they computed *MP* for triangular, hourglass, and jagged-rectangle benzenoid systems [113]. Gao computed *MP* of the crystallographic structure of Cu_2O and the crystal structure of

TiF₂ [114], with similar work being done by Moldal et al. [115,116]. Fujita [117] developed a versatile restricted-subduced-cycle-index method for generating *HP* polynomials, as well as the Hosoya indices and *MP*. Ali et al. computed the closed form of *MP* of zigzag and rhombic benzenoid systems and presented graphs of their relations with the parameters of the structures [118]. Later, they calculated some standard polynomials associated with topological indices and some degree-based topological indices of hyaluronic acid–curcumin conjugates by using general inverse sum indeg index [54]. Kürkçü et al. have developed a matrix–collocation method to solve stiff fractional differential equations with cubic non-linearity based on *MP* [119]. Yang derived *MP* for the benzene ring embedded in the P-type surface network in 2D [120]. Mondal et al. obtained the neighborhood *MP* (NMP) of the paraline graph of some convex polytopes [121]. Later, they derived the NMP of 3-layered and 4-layered probabilistic neural networks and some structure property models [122]. Rauf et al. evaluated *MP* and NMP with graphical representations of the structure of graphite carbon nitride [123]. A recent survey can further complete this enumeration [124].

One can choose graphs such that their *MP* are the same as several important orthogonal polynomials. For example, the Hermite polynomial is equal to the *MP* of the *n*-vertex complete graph [61].

A combinatorial object, the rook polynomial, which is useful in the study of some classical combinatorial problems, is essentially the *MP* of some bipartite graph [107].

Knop and Trinajstić relate *MP* to *ChP* [85].

MP is essentially the Hosoya polynomial [61]:

$$MP(G, x) = x^a \cdot HP(G, -x^{-2}) \quad (8)$$

5. Hosoya Polynomial

The simplest polynomial is the Hosoya polynomial (Wiener polynomial or *Z*-counting polynomial and denoted by *Q* or *HP*), which is defined only for connected graphs and was invented by Hosoya in 1971 [20]. It is a natural result of the introduction of non-adjacent numbers in the early revival of interest in graph theory. Hosoya named it the Wiener polynomial because of its remarkable property: deriving *HP* once at $x = 1$ leads to the Wiener index [54].

It is used in studying physicochemical properties: boiling point, entropy, heat of vaporization, or conjugated π -electron energy [125], or for classification and coding of hydrocarbons [126]. The correlation between the *Z* topological index and many thermodynamic properties has been thoroughly studied [67].

It is obtained by counting independent edges by the general CoP (Equation (1)). One can define $n_i(k)$ = the number of possible ways “*k*” edges can be chosen in a molecule (chemical graph) such that no “*k*” (chosen) edges are adjacent:

$$HP = \sum_{k \geq 0} n_i(k) \cdot x^k \quad (9)$$

Naturally for $x = 1$, $HP = Z$ topological index [127].

Taking our example in Figure 1a, we can choose:

for $k = 0$, $n_i(k) = 1$, as there is one possibility of choosing zero edges, namely \emptyset ;

for $k = 1$, $n_i(k) = 5$, the number of edges;

and for $k = 2$, $n_i(k) = 4$ possibilities depicted in Figure 1b–e:

Afterwards, for $k > 2$, $n_i(k) = 0$. As such:

$$HP_{G_1} = 1 \cdot x^0 + 5 \cdot x^1 + 4 \cdot x^2$$

Randić proposed the Hosoya matrix and later Plavšić et al. found the relationships between these path numbers and the *Z* index. By choosing every *i, j* pair, excluding the

path ij ; repeating the above counting algorithm; and leaving the diagonal null, one would arrive at the Hosoya matrix, exemplified for G_1 [128].

$$[H_{G_1}] = \begin{pmatrix} 0 & 7 & 7 & 5 & 3 \\ 7 & 0 & 6 & 8 & 5 \\ 7 & 6 & 0 & 8 & 5 \\ 5 & 8 & 8 & 0 & 7 \\ 3 & 5 & 5 & 7 & 0 \end{pmatrix}$$

Recently, Hosoya discovered new features of IS tree graphs from the analysis of isospectrality of conjugated polyenes [129,130].

Hosoya compared correlation between the π -electronic stability and several topological descriptors for isomeric acyclic conjugated hydrocarbons. He discusses the difference in the topological dependency of the HOMO level of these networks. He introduces a method for calculating the Z -index for tree graphs. He also presents some mathematical relations regarding applications of the index [131,132].

Diudea defined HP as a distance-based increasing power sequence [133]. Fujita developed a versatile restricted-subduced-cycle-index method for generating HP , as well as the Hosoya indices and matching polynomials [117]. Yang compared explicit analytical expressions for the expected values of the Hosoya and Merrifield–Simmons indexes of a random polyphenyl chain [134].

Ali et al. found the Hosoya properties of the power graphs of certain finite groups, and illustrated the Z -index of the power graphs of the dihedral and the generalized quaternion groups, respectively [135]. There are several gaps in the determination of the Hosoya characteristics of the power graphs of a finite cyclic group Z_n , the dihedral group D_{2m} , and the generalized quaternion group Q_{4n} . Abbas et al. investigated Hosoya properties of the commuting graph associated with an algebraic structure developed by the symmetries of regular molecular gones [136]. Chen obtained exact formulas for calculating the Hosoya index of dendrimer nanostars [137]. DeFord proved that the permanent–determinant of an $n \times n$ matrix constructed from the adjacency matrix of the tree is equivalent to the Z -index. It can be extended to weighted trees and more general chemical structures [97].

As mentioned before, HP is essentially the same as the matching polynomial (MP):

$$HP(G, x) = (-i\sqrt{x})^a \cdot MP\left(G, \frac{i}{\sqrt{x}}\right) \quad (10)$$

where a is the number of vertices [61,138].

For $x = \sqrt{-1}$, HP is related to the characteristic polynomial (ChP):

$$HP = x^4 \cdot ChP\left(G, \frac{i}{\sqrt{x}}\right) \quad (11)$$

It can also be extended. The sextet polynomial of every unbranched catacondensed benzenoid molecule coincides with the HP of a certain graph (called Gutman tree). Gutman established a relationship between the Coulson function and HP [94].

HP is related to many other counting polynomials. The matching polynomial of several series of graphs is identical to typical orthogonal polynomials, such as Chebyshev, Hermite, and Laguerre polynomials [62]. Wang determined a class of unicyclic graphs and obtained the ordering of their Hosoya and Merrifield–Simmons indexes [139]. It turns out that graphs of minimal Hosoya index coincide with those of maximal Merrifield–Simmons index [125,140,141]. The absolute magnitudes of the coefficients of the HP and the matching polynomial of a caterpillar graph are identical to those of the sextet and resonance polynomials of a benzenoid system. Such coefficients are those of the independence polynomial [105]. The value of the independence polynomial for $x = 1$ is equal to the Merrifield–Simmons index [142]. Gutman and Hosoya found identical HP and independence polynomials for cycles C_n ($n > 2$) [143].

6. Immanantal Polynomials

Most polynomials are not simple because of their non-trivial mathematical nature. At first sight there is a large number of counting polynomials. As such, one may consider that unifying them is the best thing that could happen and solve all problems. Unfortunately, the most that can be said in that direction is “good luck” since there might be one polynomial with hidden features that does just that. Some attempts have been made to unify polynomial concepts. The immanantal polynomial (d_λ , not to be confused with the roots, which are denoted by “ x ” in this chapter) is a natural generalization for the permanent and characteristic polynomials.

Without analysing graph polynomials, collective properties of graph invariant sequences would never be discovered [61]. Some unusual connections between molecular graphs can be determined by using the immanantal polynomial.

Let $M = (m_{ij})$ be a matrix of order “ a ”, and “ χ ” one of the irreducible characters of the symmetric permutation group S_a . The immanant of $[M]$, corresponding to the character “ χ ” of S_a , is defined as:

$$d_c(M) = \sum_{t \in S_a} c(p) \prod_{i=1}^a m_{it(i)} \tag{12}$$

If $\chi(\tau) = \varepsilon(\tau)$ is a character sign, then d_χ is the determinant. If $\chi(\tau) = 1$ for all “ τ ”, then d_χ is the permanent [61]. The immanantal polynomial of $[M]$ is $d_c(x[Id] - [M])$. If $[M]$ is $[Ad]$ (corresponding to a graph G), we call it the immanantal polynomial of graph G .

Just like the last term of $ChP_G = \det(x \cdot [Id] - [Ad])$ is $\det[Ad]$, and the last term of $p_G = per(x \cdot [Id] - [Ad])$ is $per[Ad]$, the last term of the immanantal polynomial is the immanant of $[Ad]$ expressed as $imm_\lambda(x \cdot [Id] - [Ad])$.

For a graph G , “ λ ” refers to a non-decreasing partition of “ a ”. “ τ ” is a permutation of S_a . “ ξ ” is a conjugated class, the set of all “ τ ” for a given “ a ” that has the same cycle structure. The matrix $c = P(a) \times P(a)$ is the matrix of irreducible characters of S_a , where $P(a)$ is the partition function. The elements of “ χ ” are $\chi(\lambda, \xi)$ indexed according to a partition “ λ ” and a conjugated class “ ξ ”. As such:

$$d_\lambda(G, x) = \sum_{i=0}^a \sum_{t(i)} c(\lambda, t) \cdot x^{a-i} \prod_{j=1}^a ([Id] - [Ad])_{j,t(j)} \tag{13}$$

is the immanantal polynomial. For $i = a$ one obtains the immanant $imm_\lambda p([Ad])$.

Let us exemplify how a partition is denoted. For number “6” we can write sums “6 + 0”, “5 + 1”, “4 + 2”, “4 + 1 + 1”, “3 + 2 + 1”, “2 + 2 + 2”, and “1 + 1 + 1 + 1 + 1 + 1”, which are all equal to “6”. Partitions such as {4,1,1} and {2,2,2} are non-increasing and can be written as {4,1²} and {2³}, respectively. In the last variant, it is sufficient to say they are decreasing. For partition {3,2,1} we have prepared an example in Figure 2e, where we have three connected vertices, another two connected vertices, and an independent one. For partitions {6,1⁰}, {5,1¹}, {4,1²}, ... {1⁶}, we could write a general form $\lambda = \{r, 1^{a-r}\}$. In the case of {6,1⁰}, one should not think of 1⁰ = 1, but of 6 vertices and an independent vertex counted zero times (\emptyset). When $r = 1$, the immanant of partition $\lambda_1 = \{1^a\}$ is the determinant of $[Ad]$, and for $r = a$ one obtains $\{a, 1^{a-a}\} = \{a, 1^0\} = \{a\}$, which is the permanent of $[Ad]$.

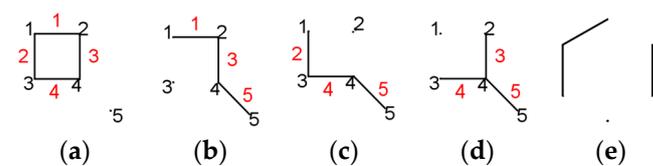


Figure 2. Representation of partition {4,1} of (G_1) : (a) vertex “5” is independent and the rest are connected (bonded); (b) “3” is independent; (c) “2” is independent; (d) “1” is independent; and (e) a representation of partition {3,2,1} from the example with 6 vertices, here benzene.

Next, we will take our graph G_1 (Figure 1a), for example, which has 5 vertices ($a = 5$). The non-increasing partitions of 5 are $\{5\}$, $\{4,1\}$, $\{3,2\}$, $\{3,1,1\}$ (denoted $\{3,1^2\}$), $\{2,2,1\}$ (denoted $\{2^2,1\}$), $\{2,1,1,1\}$ (denoted $\{2,1^3\}$), and $\{1,1,1,1,1\}$ (denoted $\{1^5\}$), totalling 7 partitions. Therefore, G_1 will have a family of 7 immanantal polynomials, one for each partition.

For partition $\{5\}$, ChP is obtained, and for partition $\{1^5\}$, π is obtained—both presented in Chapter 2 and 3, respectively.

We will determine the immanantal polynomial for partition $\lambda = \{4,1\}$, which are exemplified in Figure 2a–d:

Denoting $[Ad]$ of the subgraph in Figure 2a as just $[Ad_{(a)}]$, we have:

$$[Ad_{(a)}] = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\det(x[Id] - [Ad_{(a)}]) = \det \begin{pmatrix} x & -1 & -1 & 0 & 0 \\ -1 & x & 0 & -1 & 0 \\ -1 & 0 & x & -1 & 0 \\ 0 & -1 & -1 & x & 0 \\ 0 & 0 & 0 & 0 & x \end{pmatrix} = x \cdot \det \begin{pmatrix} x & -1 & -1 & 0 \\ -1 & x & 0 & -1 \\ -1 & 0 & x & -1 \\ 0 & -1 & -1 & x \end{pmatrix} =$$

$$= x \left(x \cdot \det \begin{pmatrix} x & 0 & -1 \\ 0 & x & -1 \\ -1 & -1 & x \end{pmatrix} + (-1) \cdot (-1)^3 \cdot \det \begin{pmatrix} -1 & 0 & -1 \\ -1 & x & -1 \\ 0 & -1 & x \end{pmatrix} + (-1) \cdot (-1)^4 \cdot \det \begin{pmatrix} -1 & x & -1 \\ -1 & 0 & -1 \\ 0 & -1 & x \end{pmatrix} \right) = x^5 - 4x^3$$

For Figure 2b we have:

$$[Ad_{(b)}] = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\det(x[Id] - [Ad_{(b)}]) = \det \begin{pmatrix} x & -1 & 0 & 0 & 0 \\ -1 & x & 0 & -1 & 0 \\ 0 & 0 & x & 0 & 0 \\ 0 & -1 & 0 & x & -1 \\ 0 & 0 & 0 & -1 & x \end{pmatrix} = x \cdot \det \begin{pmatrix} x & -1 & 0 & 0 \\ -1 & x & -1 & 0 \\ 0 & -1 & x & -1 \\ 0 & 0 & -1 & x \end{pmatrix} = x^5 - 3x^3 + x$$

For Figure 2c we have:

$$[Ad_{(c)}] = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\det(x[Id] - [Ad_{(c)}]) = \det \begin{pmatrix} x & 0 & -1 & 0 & 0 \\ 0 & x & 0 & 0 & 0 \\ -1 & 0 & x & -1 & 0 \\ 0 & 0 & -1 & x & -1 \\ 0 & 0 & 0 & -1 & x \end{pmatrix} = x \cdot \det \begin{pmatrix} x & -1 & 0 & 0 \\ -1 & x & -1 & 0 \\ 0 & -1 & x & -1 \\ 0 & 0 & -1 & x \end{pmatrix} = x^5 - 3x^3 + x$$

For Figure 2d we have:

$$[Ad_{(d)}] = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\det(x[Id] - [Ad_{(d)}]) = \det \begin{pmatrix} x & 0 & 0 & 0 & 0 \\ 0 & x & 0 & -1 & 0 \\ 0 & 0 & x & -1 & 0 \\ 0 & -1 & -1 & x & 0 \\ 0 & 0 & 0 & -1 & x \end{pmatrix} = x \cdot \det \begin{pmatrix} x & 0 & -1 & 0 \\ 0 & x & -1 & 0 \\ -1 & -1 & x & 0 \\ 0 & 0 & -1 & x \end{pmatrix} = x^5 - 3x^3$$

Summing up the four results, we get:

$$d_{\{4,1\}}(G_1, x) = 4x^5 - 13x^3 + 2x.$$

According to Botti and Merris, two graphs are isomorph if and only if they share a complete set of immanantal polynomials [144].

Cash generalises the matching polynomial to a class of acyclic immanantal polynomials; generalises the Sachs theorem to immanantal polynomials; and gives relations between immanants and other graph properties [96].

7. Laplacian Polynomial

The matrix $[La] = [Dg] - [Ad]$ is sometimes called the Kirchhoff matrix of G (see the Matrix-Tree Theorem usually attributed to Kirchhoff), or the matrix of admittance [145]. $[Dg]$ (from vertex degree) simply counts the number of edges (the atom’s bonds–valencies) on the main diagonal [86]. The Laplacian polynomial (LaP), called the Laplacian characteristic polynomial, is trivially $ChP[La]$. The set of eigenvalues is referred to as the spectrum of $[La]$ of a graph G or the Laplacian spectrum of G [146]. The spectrum is useful for calculating the Wiener number [61].

The Laplacian polynomial is defined as:

$$LaP = |x \cdot [Id] - [Dg] + [Ad]| \tag{14}$$

For our example in Figure 1a:

$$LaP_{G_1} = \left| \begin{pmatrix} x & 0 & 0 & 0 & 0 \\ 0 & x & 0 & 0 & 0 \\ 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & 0 \\ 0 & 0 & 0 & 0 & x \end{pmatrix} - \begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \right|$$

$$\begin{aligned}
 &= \begin{vmatrix} x-2 & 1 & 1 & 0 & 0 \\ 1 & x-2 & 0 & 1 & 0 \\ 1 & 0 & x-2 & 1 & 0 \\ 0 & 1 & 1 & x-3 & 1 \\ 0 & 0 & 0 & 1 & x-1 \end{vmatrix} \\
 &= x^5 - 10 \cdot x^4 + 34 \cdot x^3 - 46 \cdot x^2 + 20 \cdot x
 \end{aligned}$$

Oliveira et al. showed some general results about the coefficients of LaP [147].

While some authors have stated that the Laplacian spectrum is much more natural and more important than the adjacency matrix spectrum, it could be studied more intensively [145,146].

8. Zagreb Polynomials

Although the Zagreb index is much older, the first Zagreb polynomial was introduced in 2009 [148,149]. They are useful for: surveying nanotube structure; the study of anti-inflammatory activities; modelling the fraction bound and clearance of cephalosporins in humans; or total π -electron energy [150–152]. They can be obtained by taking into account each edge “e” = “uv” and counting the number “n” of adjacent (neighbouring) edges (valencies, or degrees of vertices “u” and “v”) for each vertex “u” and “v”:

$$ZgP_1 = \sum_{k>0} x^{n_u(k)+n_v(k)} \tag{15}$$

$$ZgP_2 = \sum_{k>0} x^{n_u(k) \cdot n_v(k)} \tag{16}$$

$$ZgP_3 = \sum_{k>0} x^{|n_u(k)-n_v(k)|} \tag{17}$$

$$ZgP_4 = \sum_{k>0} x^{n_u(k) \cdot (n_u(k)+n_v(k))} \tag{18}$$

$$ZgP_5 = \sum_{k>0} x^{n_v(k) \cdot (n_u(k)+n_v(k))} \tag{19}$$

For example, G_1 in Figure 1a, having 5 edges, we take edge “1”; in this case $u = 1$ and $v = 2$. For vertex $u = 1$, it can be seen in Figure 3a that there are two adjacent edges “1” and “2”. For $v = 2$ in Figure 3b there are also two adjacent edges, “1” and “3”.

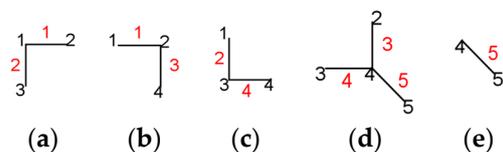


Figure 3. (a–e) Vertex degrees in G_1 .

As such:

- for $k = 1, n_u(k) = 2, n_v(k) = 2;$
- for $k = 2, n_u(k) = 2, n_v(k) = 2;$
- for $k = 3, n_u(k) = 2, n_v(k) = 3;$
- for $k = 4, n_u(k) = 2, n_v(k) = 3;$
- and for $k = 5, n_u(k) = 3, n_v(k) = 1.$

Rewriting Equations (15)–(19):

$$ZgP_{1G_1} = x^{2+2} + x^{2 \cdot 2} + x^{2+3} + x^{2 \cdot 3} + x^{3+1}$$

$$ZgP_{2G_1} = x^{2 \cdot 2} + x^{2 \cdot 2} + x^{2 \cdot 3} + x^{2 \cdot 3} + x^{3 \cdot 1}$$

$$ZgP_{3G_1} = x^{|2-2|} + x^{|2-2|} + x^{|2-3|} + x^{|2-3|} + x^{|3-1|}$$

$$ZgP_{4G_1} = x^{2 \cdot (2+2)} + x^{2 \cdot (2+2)} + x^{2 \cdot (2+3)} + x^{2 \cdot (2+3)} + x^{3 \cdot (3+1)}$$

$$ZgP_{5G_1} = x^{2 \cdot (2+2)} + x^{2 \cdot (2+2)} + x^{3 \cdot (2+3)} + x^{3 \cdot (2+3)} + x^{1 \cdot (3+1)}$$

Bindusree et al. investigated relations between Zagreb polynomials of a graph G and a graph obtained by applying the $S(G)$, $R(G)$, and $Q(G)$ operators [153]. Farooq found general 5th M_1 and general 5th M_2 Zagreb polynomials for Dyck-56 Networks [154]. Maji and Ghorai determined the Zagreb polynomials, its copolynomials, and their complement for the w^{th} generalized transformation graphs [155]. First and second Zagreb indexes are found by differentiating their polynomials at $x = 1$ [54]. Due to the good correlation between Zagreb indices and chemical properties, a considerable effort has been observed in computing Zagreb polynomials since the first ZgP was defined. This effort can be visualized in Table 1:

Table 1. Chemical structures for which Zagreb polynomials have been computed.

Structure Name	Author/s	Reference
families of nanotubes	Farahani	[150,156,157]
Capra-Designed Planar Benzenoid Series	Farahani and Vlad	[158]
nanostar dendrimers	Husin et al., Siddiqui et al. and Kang et al.	[159–161]
zigzag, rhombic, triangular, hourglass and jagged-rectangle benzenoid systems; Silicon Carbide structures	Kwun et al.	[162,163]
hetrofunctional dendrimers, triangular benzenoids, and nanocones	Gao et al.	[151]
the generalized class of carbon nanocones	Noreen and Mahmood	[164]
some nanostructures	Rehman and Khalid	[165]
perylene-diimide-cored dendrimers	Iqbal et al.	[166]
Cu_2O and TiF_2	Yang et al.	[167]
some dendrimers and polyomino chains	Farooq et al.	[168]
Sierpiński graphs	Siddiqui	[169]
remdesivir, chloroquine, hydroxychloroquine and theaflavin	Virk	[170]
benzene ring implanted in P -type surface structure	Sarkar and Pal	[171]
hexagonal network HX_n , the honeycomb network HC_n , the silicate sheet network SL_n and the oxide network OX_n	Salman et al.	[172]
benzenoid Triangular system and benzenoid Hourglass system	Chu et al.	[173]
Silicate Network and Silicate Chain Network	Ghani et al.	[174]

Zagreb polynomials could be further studied for their applicability of deriving multiple linear regression models [165].

9. Sextet Polynomial

The sextet polynomial (denoted by SP or σ) reflects the combinatorial description of both Kekulé structures and Clar's concept of the aromatic sextet. It finds its uses in the calculation of the resonance energy of benzenoid hydrocarbons, or enumeration of Kekulé structures of catafusenes.

Counting disconnected (non-adjacent) but resonant sextets by the general CoP (Equation (1)), one can define $n_r(k)$ is the so called "resonant sextet number", the number of possible ways "k" mutually resonant sextets can be chosen in a molecule (chemical graph):

$$SP = \sum_{k \geq 0} n_r(k) \cdot x^k \quad (20)$$

Our most used example in Figure 1a is not suitable for this purpose, and benzo[p,q,r]tetraphene (G_4) in Figure 4a will take its place.

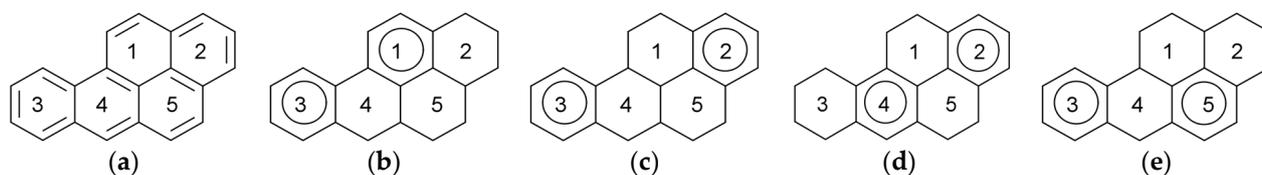


Figure 4. (a) benzo[p,q,r]tetraphene (G_4); (b–e) possibilities of choosing two mutually resonant sextets.

We can choose:

for $k = 0$, $n_r(k) = 1$, as there is one possibility of choosing zero sextets, namely \emptyset ;

for $k = 1$, $n_r(k) = 5$, the number of benzene rings;

and for $k = 2$, $n_r(k) = 4$, possibilities depicted in Figure 4b–e:

As such:

$$SP_{G_4} = 1 \cdot x^0 + 5 \cdot x^1 + 4 \cdot x^2$$

Gutman et al. pointed out a combinatorial polynomial (Zhang–Zhang) from which Kekulé structures, Clar number, Clar formulas, and SP can be directly deduced [175]. Gutman and Borovičanić detailed some applications for the Zhang–Zhang polynomial (ζ) and showed its relation to SP for some structures [176]:

$$SP = \zeta(x - 1)$$

SP is also related to the resonance polynomial (AP) of Aihara by the relation [105,177]:

$$SP = x^{a-2b} \cdot AP,$$

where $a =$ vertices and $b =$ edges.

Shiu et al. have obtained the SP for buckminsterfullerene [178]. Wang et al. defined a new ordering of benzenoid chains and cyclo-polyphenacenes [179]. Yan and Zhang have obtained the SP of boron–nitrogen fullerenes, which were anomalously stable [180,181]. Ye et al. computed the SP of 3-resonant fullerene graphs [182]. Sereni and Stehlík showed that the sextet pattern count of every fullerene is strictly smaller than the Kekulé structure count [183]. Balasubramanian showed computational symmetry techniques that can be applied to SP [184]. Li et al. investigated analytic properties of sextet polynomials of hexagonal systems [185]. A review presenting the SP, Clar polynomial, and Clar-covering polynomial may further complete this enumeration [186].

The sextet polynomial extends Hosoya's non-adjacent concept to aromatic sextets, and it was extended to the R and cell polynomials [85,105,187]. It is related to Clar, independence, king, color, and star polynomials [188].

10. Independence Polynomial

The independence polynomial is defined first by Gutman and Harary [189,190], and is closely related to HP and MP. It can be found as I, IP, the independent set polynomial, the Fibonacci polynomial, or the stable set polynomial [191]. It can be found by counting sets of k independent vertices by the general CoP (Equation (1)):

$$IP = \sum_{k \geq 0} n_{ia}(k) \cdot x^k \quad (21)$$

For our example in Figure 1a, we can choose:

for $k = 0$, $n_{ia}(k) = 1$, as there is one case of which zero independent vertices, namely \emptyset ;

for $k = 1$, $n_{ia}(k) = 5$, the number of vertices;

and for $k = 2$, $n_{ia}(k) = 5$ sets of two independent vertices (1,4; 1,5; 2,3; 2,5; 3,5).

As such:

$$IP_{G_1} = 1 + 5 \cdot x + 5 \cdot x^2$$

Rosenfeld found formulae expressing IPs of two sorts of the rooted product of graphs [192]. Song et al. determined IPs of several classes of k-tree related graphs [191]. Sreeja investigated IP of Fibonacci trees [138].

To further illustrate how this polynomial relates to chemistry, a starting point is the Merrifield–Simmons index—the number of independent vertex subsets of G , including \emptyset [140,193]. Many properties of IP and HP are fully analogous. In the same manner that IP is analogous to MP, other attempts have been made in the discovery of new polynomials. One example is the sextet polynomial in the theory of benzenoid hydrocarbons. King, color, and star polynomials are also related to IP [61].

The opposite polynomial that would count dependent (adjacent) vertices is the clique polynomial [140]. Hoede has defined a clique polynomial and found that it is essentially the same as the dependence polynomial [194,195].

Other polynomials have been stated to be independence polynomials, such as HP, clique, or SP [61].

11. King and Domino Polynomials

The king polynomial (KP) was proposed for enumerating the number of ways for arranging non-taking kings on a given polyomino (or chessboard) of an arbitrary size and shape [196]. As a hexagonal analog of polyomino one could choose some polycyclic aromatic hydrocarbons. The king and domino polynomials could be used for correlating lattice problems. We will propose anthracene and its polyomino analogue in Figure 5a, respectively Figure 5b, for depicting ways of arranging kings and dominoes:

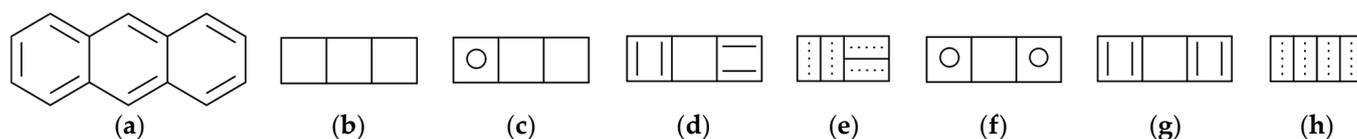


Figure 5. (a) anthracene; (b) its polyomino analogue (G_5); (c) one way of arranging a single king; (d) Kekulé pattern corresponding to (c); (e) domino pattern corresponding to (c); (f) the only way one can arrange two non-taking kings; (g) Kekulé pattern corresponding to (f); (h) domino pattern corresponding to (f).

Counting the number of ways of arranging non-taking kings (nk) by the general CoP (Equation (1)), one can define $n_{nk}(k)$ = the number of possible ways k non-taking kings can be arranged in a molecule (chemical graph):

$$KP = \sum_{k \geq 0} n_{nk}(k) \cdot x^k \quad (22)$$

We can thus choose:

for $k = 0$, $n_{nk}(k) = 1$, as there is one possibility of arranging zero kings—Figure 5b;

for $k = 1$, $n_{nk}(k) = 3$, the number of cells;

and for $k = 2$, $n_{nk}(k) = 1$ possibility depicted in Figure 5f:

$$KP_{G_5} = 1 \cdot x^0 + 3 \cdot x^1 + 1 \cdot x^2$$

KP is related to independence and the rook polynomial [188,197].

The domino polynomial is almost the same. One needs to count: improper patterns = improper kings = ik = king patterns that do not have Kekulé correspondents; and degenerate patterns = degenerate kings = dk = king patterns with two Kekulé correspondents.

$$DP = KP - ik + dk \quad (23)$$

Balasubramanian and Ramaraj developed a program for generating king and color polynomials [198].

12. Cluj Polynomial

Diudea proposed the Cluj polynomial in 2007 after first publishing an interpretation indirectly related to counting content [188]. The Cluj polynomial counts the vertex proximities in a connected graph. It is formed by choosing two initial vertices and counting the number of vertices that are closer to each of the initial two.

Descriptors related to this polynomial are useful for predicting the boiling point, chromatographic retention index, resonance energy for some planar polyhex compounds, and the toxicity of a number of dibenzofurans.

Using the general CoP (Equation (1)), we can write:

$$CjP = \sum_{k>0} n_{kp} \cdot x^k, \quad (24)$$

where “ n ” counts the number of times “ k ” vertices are closer to another (or in other words the vertex proximity of the vertex “ i ” with respect to any vertex “ j ”).

For our example in Figure 1a, we can choose two vertices, find the shortest path between them, and exclude the vertices of that path. Choosing vertices “1” and “2”, we need to delete edge “1”, as depicted in Figure 6b. It can be seen that there are two vertices closer to “1”, and those are vertices “1” and “3”. There are three vertices closer to “2”: vertices “2”, “4”, and “5”. We can create matrix $[Cj_{G_1}]$ in order to store this information:

$$[Cj_{G_1}] = \begin{pmatrix} 0 & 2 & & & \\ 3 & 0 & & & \\ & & 0 & & \\ & & & 0 & \\ & & & & 0 \end{pmatrix}$$

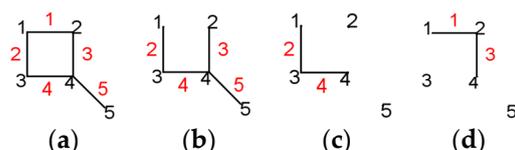


Figure 6. (a) Figure 1a (G_1); (b) what remains after deleting the path between vertices “1” and “2”; (c,d) what remains after deleting paths between vertices “1” and “5”.

Taking the shortest path between vertices “1” and “5”, for example, we have two cases. This would pose some problems in some chemical structures, but we will come back to that. In our structure, one case depicted in Figure 6c would be path 1, 2, 4, and 5, leaving two vertices—“1” and “3”, which are closer to “1”. The second case depicted in Figure 6d would be path 1, 3, 4, and 5, leaving two vertices—“1” and “2”, closer to “1”. We have the

same number so we have no additional problems in constructing our matrix. Only vertex “5” is closer to “5”. As such we can further complete our matrix:

$$[Cj_{G_1}] = \begin{pmatrix} 0 & 2 & 2 & 1 & 2 \\ 3 & 0 & 1 & 2 & 3 \\ 3 & 1 & 0 & 2 & 3 \\ 2 & 3 & 3 & 0 & 4 \\ 1 & 1 & 1 & 1 & 0 \end{pmatrix}$$

Counting the occurrence of each character:

for $k = 1, n_{k\ at} = 7$, counting how many times “1” appears in our matrix;
 for $k = 2, n_{k\ at} = 6$, counting how many times “2” appears in our matrix;
 for $k = 3, n_{k\ at} = 6$, counting how many times “3” appears in our matrix;
 for $k = 4, n_{k\ at} = 1$, since “4” appears once,

as such:

$$CjP_{G_1} = 1 \cdot x^4 + 6 \cdot x^3 + 6 \cdot x^2 + 7 \cdot x$$

We return to the problematic case where there is more than one shortest path between two vertices. We have to check if the results are the same for each case (methylcyclobutane showed to have no problem in that regard). If results differ we need to bring to mind that there are more kinds of Cluj polynomials. The one we have calculated takes into account shortest paths, and it can be denoted by p: $Cj_{G_{1p}}$. Another polynomial that solves the problem with more than one shortest path can be formulated if we take into account only edges: $Cj_{G_{1b}}$ (usually referred to as $Cj_{G_{1e}}$). We have matrix $[Cj_{G_{1b}}]$:

$$Cj_{G_{1b}} = \begin{pmatrix} 0 & 2 & 2 & 0 & 0 \\ 3 & 0 & 0 & 2 & 0 \\ 3 & 0 & 0 & 2 & 0 \\ 0 & 3 & 3 & 0 & 4 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

And the corresponding polynomial:

$$CjP_{G_{1b}} = 1 \cdot x^4 + 4 \cdot x^3 + 4 \cdot x^2 + 1 \cdot x$$

There are also two other Cluj polynomials that count longest paths (detours). Now we need to specify this: $CjDe_{G_{1b}}$ and $CjDe_{G_{1p}}$, where De stands for detour. The polynomials we calculated above are $CjDi_{G_{1b}}$ and $CjDi_{G_{1p}}$, where Di stands for distance (shortest).

Diudea et al. published aspects related to the Cluj polynomials, including: a method for calculating the polynomial by orthogonal edge cuts of the $CjDi$ matrix; some analytical formulas for calculating the Cluj and related polynomials; basic definitions and properties of the Cluj matrices and corresponding polynomials; relations of Cluj polynomials with Ω -type polynomials; meaning of Cluj descriptors as vertex proximity descriptors; and the relation of Cluj polynomials with the Π and Π polynomials. [188,199]

Cluj and related polynomials (Π_v vertex-PadmakarIvan—a pairwise summation; Cluj-Sum; and Cluj-Product—pair-wise product or also Szeged) are derived for tori [200].

Analytical formulas and some examples are also given for polynomials and for a single-edge pairwise product polynomial (called Wiener) of the classical diamond D6 and two related structures [201].

These polynomials are later computed for several 3D nanostructures and crystal networks [202].

13. Omega Polynomial

Another counting polynomial was proposed by Diudea to account for the opposite cuts in a bipartite lattice [203,204]. It is useful in the topological description of benzenoid structures, of tubular nanostructures, as well as in counting TIs [72].

First, we need to define codistance for naphthalene in Figure 7. Edges b_5 (between vertex “3” and vertex “6”) and b_6 (between vertex “4” and vertex “7”) are called codistant (briefly: $b_5 \text{ co } b_6$) if the distances d between vertices satisfy:

$$\begin{cases} d(3,4) = d(6,7) = m; \\ d(3,7) = d(6,4) = m + 1. \end{cases} \text{ or } \begin{cases} d(3,4) = d(6,7) = m + 1; \\ d(3,7) = d(6,4) = m. \end{cases}$$

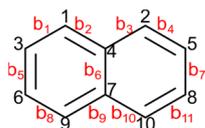


Figure 7. Graph theoretical representation of naphthalene (G_7).

Let $CO_{(5)} = (b_1, b_2, \dots, b_p)$ be (in general) the set of all edges codistant to b_5 . If all elements of $CO_{(5)}$ also satisfy:

$$\begin{cases} b_i \text{ co } b_i \\ b_i \text{ co } b_j \iff b_j \text{ co } b_i \\ b_i \text{ co } b_j \iff b_j \text{ co } b_h \iff b_i \text{ co } b_h \end{cases}, \tag{25}$$

then $CO_{(5)}$ is an orthogonal cut (oc) of G_7 . We have, in particular, these oc’s: $CO_{(5)} = (b_5, b_6, b_7)$, $CO_{(1)} = (b_1, b_9)$, $CO_{(2)} = (b_2, b_8)$, $CO_{(3)} = (b_3, b_{11})$, $CO_{(4)} = (b_4, b_{10})$, $CO_{(6)} = (b_5, b_6, b_7)$, $CO_{(7)} = (b_5, b_6, b_7)$, $CO_{(8)} = (b_2, b_8)$, $CO_{(9)} = (b_1, b_9)$, $CO_{(10)} = (b_4, b_{10})$, and $CO_{(11)} = (b_3, b_{11})$.

The graph G_7 is called a cograph if and only if the edge set $B(G_7)$ is the union of disjoint oc(G_7): $CO_1 \cup CO_2 \cup \dots \cup CO_p = B$ and $CO_i \cap CO_j = \emptyset$ for $i \neq j, i, j = 1, 2, \dots, p$. CO_{1-5} satisfy these requirements. If any two consecutive edges of such a sequence are codistant (satisfying (25)) and belong to the same face of the covering, the sequence is called a quasi-orthogonal cut “qoc” strip. Our explanation is somewhat shorter and may not cover all possibilities, but the original one can be found in Ref. [203]. A note for non-chemical structures: any other graph taken into consideration needs to be a connected graph.

Counting $n_{qoc}(k) =$ the number of qoc’s of length “ k ”:

$$\Omega = \sum n_{qoc}(k) \cdot x^k, \tag{26}$$

in our example of naphthalene (G_7), taking into account disjoint oc’s CO_{1-5} :

- for $k = 0, n_{qoc}(k) = 0$;
- for $k = 1, n_{qoc}(k) = 0$;
- for $k = 2, n_{qoc}(k) = 4, CO_{1-4}$;
- for $k = 3, n_{qoc}(k) = 1, CO_5$.

$$\Omega_{G_7} = 4x^2 + x^3$$

Diudea led most of the research with various groups: in 2009, he proved Ω to be a useful description of polyhedral coverings appearing in nanostructures [72]; later, he described dendritic polymers by composing the large molecule from its monomer(s) [205]; networks related to the Dyck graph using Ω and Padmakar–Ivan (PI) polynomials [206,207] and the topology of diamond-like networks [208]; two linearly periodic BTX-networks [209]; three benzene-based infinite networks [210,211]; studied the properties and computed Ω for polycyclic aromatic hydrocarbons and fullerenes [212]; and described rhombellane-related crystal networks [213]. Ghorbani and Ghazi computed Ω and PI polynomials for some classes of 8-cycle graphs [214,215]. Saheli et al. used closed formulas of Ω to describe the topology

of a new graphene pattern, called CorSu [216,217]. Gao et al. calculated Ω , Theta, Sadhana, and PI polynomials of a benzene ring embedded in the P-type surface on 2-Dnetworkandn-phenylene [218]. Gayathri et al. calculated the Ω , Theta, PI, and Sadhana polynomials, and subsequent indices of convex benzenoid system [219]. Arulperumjothi et al. found the Theta, Omega, PI, and Sadhana polynomials of hexa-peri-hexabenzocoronene, hexa-cata-hexabenzocoronene, and dodeca-benzo-circumcoronene [220]. These more detailed studies may complete ours [207,221–224]. Diudea et al. derived a relation between the Sadhana polynomial (SdP) and Ω [225,226]:

$$SdP(G) = SdP'(G,1) = \Omega'(G,1)(\Omega(G,1) - 1)$$

14. Wheland Polynomial

The Wheland polynomial counts canonical structures for each degree of excitation in an unsaturated or aromatic hydrocarbon. It is not an invariant [227], however it can be generalized to count all valence structures, which makes it an invariant [228]. It associates a polynomial to each molecule or grouping of atoms where “ n ” is the number of structures of the k^{th} degree of excitation.

$$WP = \sum_{k \geq 0} n_k \cdot x^k, \quad (27)$$

We will start with some simple examples. For small linear chains, $WP(L_0) = WP(L_1) = 1$; 1,3-butadiene in Figure 8a is an example of a linear chain with two double bonds:

$$WP(L_2) = 1 + x$$

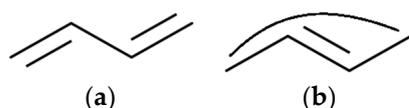


Figure 8. (a) the only structure with no degree of excitation; (b) the only structure with degree of excitation one.

For a linear chain with three double bonds, we shall use 1,3,5-hexatriene in Figure 9a:

$$WP(L_3) = 1 + 3 \cdot x + x^2$$

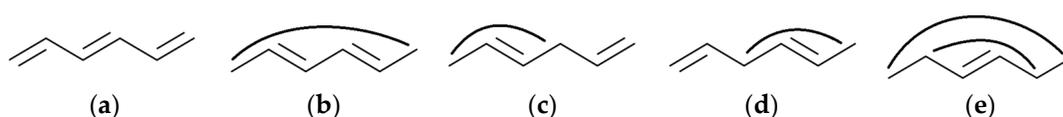


Figure 9. (a) the only structure with no degree of excitation; (b–d) three structures with degree of excitation one; (e) the only structure with degree of excitation two.

For larger structures, Wheland has provided a way of computing WP :

$$WP(L_k) = \sum_{j=0}^{k-1} \frac{k! \cdot (k-1)!}{j! \cdot (j+1)! \cdot (k-j)! \cdot (k-j-1)!} \cdot x^j \quad (28)$$

For example:

$$WP(L_4) = 1 + 6 \cdot x + 6 \cdot x^2 + x^3$$

$$WP(L_5) = 1 + 10 \cdot x + 20 \cdot x^2 + 10 \cdot x^3 + x^4$$

For rings with two double bonds, $WP(R_2) = 2$. Benzene in Figure 10a is an example of a ring with three double bonds:

$$WP(R_3) = 2 + 3 \cdot x$$

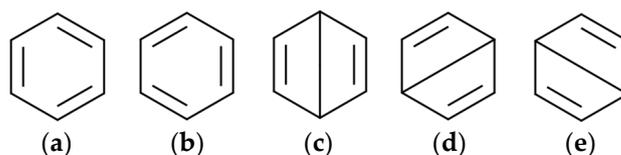


Figure 10. (a,b) the two structures with no degree of excitation; (c–e) three structures with degree of excitation one.

For larger structures there is also a way of computing them:

$$WP(R_k) = WP(L_k) + (1 - x) \cdot WP(L_{k-1}) \quad (29)$$

For example:

$$WP(R_4) = 2 + 8 \cdot x + 4 \cdot x^2$$

$$WP(R_5) = 2 + 15 \cdot x + 20 \cdot x^2 + 5 \cdot x^3$$

Now we shall speak about the case of more complex structures. There is another rule that states: if G_i differs from G_j by having a single additional line, and if this line together with its end points divides G_i into G_{i1} and G_{i2} , then:

$$WP(G_i) = WP(G_j) + (1 - x) \cdot WP(G_{i1}) \cdot WP(G_{i2}) \quad (30)$$

For this we shall take naphthalene as an example and use it without double bonds (G_{11} in Figure 11b):

$$WP(G_{11}) = WP(G_{12}) + (1 - x) \cdot WP(G_{13}) \cdot WP(G_{14})$$

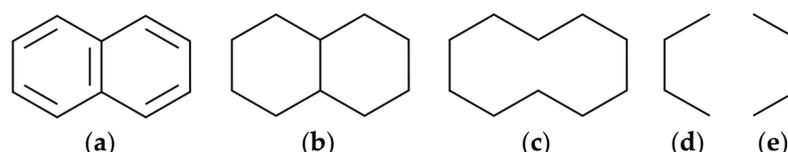


Figure 11. (a) similar graph theoretical representation of naphthalene (G_7) to Figure 7; (b) graph theoretical representation of naphthalene without double bonds (G_{11}); (c) what remains after removing a convenient edge in order to apply Equation (30) (G_{12}); (d,e) result of dividing G_{11} in order to apply Equation (30) (G_{13} and G_{14}).

G_{12} is a ring that can be populated with 5 double bonds. Since G_{13} in Figure 11d is equivalent to G_{14} in Figure 11e in terms of the Wheland polynomial:

$$WP(G_{11}) = WP(R_5) + (1 - x) \cdot WP(L_2)^2$$

Wheland went even further as to define this polynomial for the case of structures with an unpaired electron. WP along with ChP , MP , HP , SP , and a cyclic polynomial are closely related to the π -electron energy of conjugated systems. These polynomials and their properties can be used to predict the stability of such a system [85].

15. Discussion

It was well said by Clerk Maxwell: “For the sake of persons of different types of mind, scientific truth should be presented in different forms, and should be regarded as equally scientific whether it appears in the robust form and coloring of a physical illustration, or in the tenuity and paleness of a symbolical expression”. From N. V. Sidgwick’s Presidential Address to the Chemical Society, London, 1937

Interest for polynomials related to chemistry is steadily growing. For example, isospectral graphs [229] (that supply valuable information in physics and chemistry [230], such as those covered by the collection [231]) were recently brought to light by molecular partition methods. This is done by dividing the wave function in Hilbert space (e.g., the orbital-based approaches of Mulliken), or by dividing a molecular descriptor in real space (e.g., the electron-density-based approaches of Politzer [232]). Another two recent examples of visual representations are inducted: by the partition of a graph [233], and by a case study related to utilizing a program dedicated to molecular dynamics and to fragments [234].

Readers are one step closer to starting their research after understanding similar mathematical aspects of polynomials, such as the general counting Equation (1) or Sachs's theorem. In the past these similarities have been used to unify polynomial concepts. Differences are equally important since they help point out how one polynomial is unique. This helps memorizing a larger number of mathematical aspects. We share the opinion of Knop and Trinajstić that "there are many more properties of these polynomials which remain to be discovered . . . there may be as yet unknown or unappreciated polynomials" [85]. We hope we did not miss the "best" polynomial in our short enumeration. Several polynomials were not covered in this review for various reasons. The most important being the authors' experience with them and the ability to provide links to chemistry. We are constantly making improvements to explanations of polynomial concepts such as: β , F , μ , Chromatic, Tutte and those already mentioned in the text. Any contributions or new authors in joining the effort for our continuous search that will be illustrated in future papers are welcomed.

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