Maxima and minima of the Hosoya index and the Merrifield-Simmons index: A survey of results and techniques.

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Abstract

The Hosoya index and the Merrifield-Simmons index are typical examples of graph invariants used in mathematical chemistry for quantifying relevant details of molecular structure. In recent years, quite a lot of work has been done on the extremal problem for these two indices, i. e., the problem of determining the graphs within certain prescribed classes that maximize or minimize the index value. This survey collects and classifies these results, and also provides some useful auxiliary results, tools and techniques that are frequently used in the study of this type of problem.

1 History and chemical background

In 1971 the Japanese chemist Haruo Hosoya introduced a molecular-graph based structure descriptor [34], which he named *topological index* and denoted by Z. He showed that certain physico-chemical properties of alkanes (= saturated hydrocarbons) – in particular, their boiling points – are well correlated with Z. He defined the quantity Z in the following manner.

Let G be a (molecular) graph. Denote by $m(G,k)$ the number of ways in which k mutually independent edges can be selected in G. By definition, $m(G,0) = 1$ for all graphs, and $m(G,1)$ is equal to the number of edges of G. Then

$$Z = Z(G) = \sum_{k \geq 0} m(G,k) \ .$$

In a series of subsequent papers, Hosoya and his coworkers [15, 38, 42, 47, 48, 75, 76, 77] and others [19] showed that the "topological index" Z is related with a variety of physico-chemical properties of alkanes. Another series of researches revealed the applicability of Z in the theory of conjugated π-electron systems [24, 29, 30, 36, 45, 46]. Other applications of Z were also attempted [35].

The molecular structure descriptor Z was soon re-named into *Hosoya index* or *Hosoya topological index*, whereas the name "topological index" is nowadays used for any of the countless graph invariants [28, 95] that are found (or are claimed) to have some chemical applicability.

For a review on the chemical aspects Hosoya–index saga see [37, 39, 40, 41].

The early mathematical investigations [34, 36], related to the Hosoya index were all based on properties of the numbers $m(G,k)$. Recall that if G is a tree (or, more generally, a forest), then its characteristic polynomial is of the form [5, 6]

$$\phi(G;x) = \sum_{k \geq 0} (-1)^k \, m(G,k) \, x^{n-2k} \tag{1}$$

where n stands for the number of vertices. For a general graph G, the right-hand side of Eq. (1) is called *the matching polynomial*. Its theory has been extensively elaborated, see [5]. One of the outstanding algebraic properties of the matching polynomial of any graph is that all its zeros are real [5, 16].

The *energy* $E = E(G)$ of a graph G is, by definition, equal to the sum of absolute values of the eigenvalues of this graph [5, 6, 18, 23, 27, 28]. As a consequence of Eq. (1), the energy of a tree T satisfies the relation [17, 69]

$$E(T) = \frac{2}{\pi} \int_0^{\infty} x^{-2} \, \ln M(T;x^2) \, dx \tag{2}$$

where

$$M(T;x) = \sum_{k \geq 0} m(T,k) \, x^k \ .$$

Note that $Z(T) = M(T;1)$.

Formula (2) has been much used for finding trees of various types, having extremal energies (see the review [27] and the recent works [54, 55, 56, 114]). For this, one can often show that for two trees T_1 and T_2 the inequalities $m(T_1,k) \geq m(T_2,k)$ hold for all k. If so, then from Eq. (2) it follows that $E(T_1) \geq E(T_2)$. In this case, also $Z(T_1) \geq Z(T_2)$. This is also the reason for the fact that in many known instances, the tree within a particular class that maximizes/minimizes the energy is also the one that maximizes/minimizes the Hosoya index [54, 80, 103, 104]. This has even been proven for some non-tree classes, see for instance [49].

From a formal point of view, the definition of the Merrifield-Simmons index is analogous to that of the Hosoya index:

Let G be a (molecular) graph. Denote by $n(G,k)$ the number of ways in which k mutually independent vertices can be selected in G. By definition, $n(G,0) = 1$ for all graphs, and $n(G,1)$ is equal to the number of vertices of G. Then

$$\sigma = \sigma(G) = \sum_{k \geq 0} n(G,k) \ .$$

In spite of the analogy between Z and σ, the way in which the quantity σ was conceived (at least within mathematico-chemical considerations) is quite different. The American chemists Richard E. Merrifield and Howard E. Simmons elaborated a theory aimed at describing molecular structure by means of finite-set topology. Along these lines they published a series of articles [70, 71, 72, 73, 91] and a book [74]. From a present-day's point of view, one can say that their theory was not particularly successful, and certainly was not considered and further extended by later authors. However, one seemingly marginal detail in their topological formalism attracted the attention of colleagues and eventually became known as the Merrifield-Simmons index. This was the *number of open sets of the finite topology*, which the authors immediately recognized to be equal to the number of independent sets of vertices of the graph corresponding to that topology [70]. Already in the first paper [70], the symbol σ was used for this quantity.

Recognizing the analogy between σ and the Hosoya index Z, one of the present authors proposed that the former be called the "*Hosoya index of the second kind*" (in which case Z would be the "*Hosoya index of the first kind*") [26]. In other two early papers [25, 44] (both coauthored by Hosoya), the index σ was not named, but it was only referred to as "proposed by Merrifield and Simmons". The name *Merrifield-Simmons index* seems to be first used by one of the present authors in [20], and then in [21, 22], after which it was accepted by the entire mathematico-chemical community.

The Hosoya index and the Merrifield-Simmons index are typical examples of graph invariants used in mathematical chemistry for quantifying relevant details of molecular structure. In recent years, a lot of work has been done on the *extremal problem* for these two indices, i. e., on determining the graphs within a prescribed class that minimize or maximize the value of the index. The two indices do not only have very similar definitions, they are also quite related in another respect: for most graph classes that have been studied so far, the graph that minimizes the Merrifield-Simmons index is also the one that maximizes the Hosoya index, and vice versa (for a notable exception, see Section 2.3.3). This relation is still not totally understood, as it is not necessarily true that if $\sigma(G_1) > \sigma(G_2)$ for some graphs G_1 and G_2, then also $Z(G_1) < Z(G_2)$. This does not even hold for very restricted graph classes such as trees, see for instance [98]. We will also see that the methods that are usually employed for treating the extremal problem are very similar for the two indices – see Section 3, which gives an overview of important methods and auxiliary results in this context.

In the following, we restrict ourselves to the extremal problem for the Hosoya index and the Merrifield-Simmons index, which has been the topic of many recent papers, and neglect relations to other indices as well as other problems concerning these two indices. The interested reader is referred, however, to other articles [37, 39, 43, 60, 64, 97, 102] and books [28, 74, 96] that treat some of these aspects. The following section discusses known results, i. e., characterizations of graphs that maximize or minimize the two indices within certain prescribed classes of graphs, aiming to give an extensive overview of the progress that has been made since the introduction of the Hosoya index and the Merrifield-Simmons index to the literature.

Since there are quite a few useful auxiliary results that have been used in several contexts, we discuss some of them in Section 3 in more detail and outline the typical techniques that are employed in solving the extremal problem for a given class of graphs. Section 4, which presents some interesting problems for further study, completes this survey.

2 A survey of results

This section is devoted to various results concerning the extremal problem for the Hosoya index and the Merrifield index, most of which have been achieved quite recently. While trying to be as exhaustive as possible, we decided to restrict ourselves as follows: for all the graph classes that will be discussed in the following, we explicitly describe those graphs that maximize/minimize the two indices. In many instances, however, even more is known, such as those graphs that attain the second-largest (-smallest), third-largest (-smallest), etc. values. In such cases, we only give some detail and provide the relevant references for the interested reader. If not mentioned otherwise, the extremal graphs in the following theorems are unique.

2.1 General graphs

It is fairly obvious that, among all graphs of given order n, the complete graph is the one that has the largest number of matchings, namely

$$Z(K_n) = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{n!}{2^k k!(n-2k)!},$$

and the smallest number of independent sets ($n+1$, to be precise), and that the edgeless (empty) graph has the smallest number of matchings (only the empty matching) and the largest number of independent sets (namely 2^n). Generally, it is clear that removing edges decreases the Hosoya index and increases the Merrifield-Simmons index. Things become more interesting if one imposes further restrictions, for instance, if one only considers connected graphs. The complete graph is clearly still extremal, and on the other hand, the aforementioned argument on removing edges shows that the minimum of the Hosoya index and the maximum of the Merrifield-Simmons index must be attained for a tree (see the following section).

A paper by Tichy and one of the present authors [93] goes a little further by characterizing all connected graphs on n vertices whose Merrifield-Simmons is at least $2^{n-2}+5$ and showing that for any integer $s \in \{n+1, n+2, \ldots, 2n\}$, there is a (connected) graph whose Merrifield-Simmons index is s (there are many nonisomorphic graphs in this case, so it is hard to describe them explicitly). Zhao and Liu [120] came to essentially the same result concerning graphs with a large Merrifield-Simmons index with a slightly different approach (they also extended the list further to 2^{n-2}). As a byproduct, one can also determine the connected graph with n vertices and m edges that maximizes the Merrifield-Simmons index, if m is not too large:

Theorem 1 ([120]) For $n-1 \leq m \leq 2n-3$, the maximum value of the Merrifield-Simmons index among all connected graphs with n vertices and m edges is $2^{n-2}+2^{2n-3-m}+1$. It is attained for the graph whose shape is shown in Figure 1, comprising of $m-n+1$ triangles sharing a common edge and $2n-m-3$ edges attached to one of the two endpoints of this edge. This is the unique graphs that maximizes the Merrifield-Simmons index, except when $m = 2n-4$, in which case there is a second graph with this property.

The situation is more involved if the Hosoya index is considered, and one cannot expect to obtain a result that is as strong as that of Zhao and Liu in this case; see [93] for a detailed explanation.

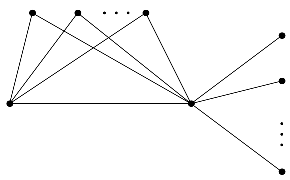


Figure 1: The connected graph that maximizes the Merrifield-Simmons index, given the number of vertices and the number of edges.

Another interesting problem was studied by Bruyère and Mélot in [2]: they consider graphs with a fixed stability number (i.e., the largest size of an independent set) and determine those that maximize the Merrifield-Simmons index. It turns out that the extremal graphs are the well-known Turán graphs that occur frequently in graph theory (see for instance [13]). The Turán graph on n vertices with stability number a consists of a disjoint cliques (complete graphs) of size $\lfloor n/a \rfloor$ or $\lceil n/a \rceil$. This result also appears in a dual version (for cliques instead of independent sets, which is equivalent to considering the complement graph) in an earlier paper by Hedman [31]. Bruyère and Mélot [2] also solve the analogous problem for connected graphs and obtain a similar result: the graph maximizing the Merrifield-Simmons index is the Turán-connected graph that is obtained from a Turán graph (as described above) by connecting one vertex of one of the cliques of size $\lceil n/a \rceil$ with one vertex from each of the other cliques (see Figure 2 for an example with 7 vertices and stability number 3).

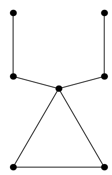


Figure 2: A Turán-connected graph.

On the other hand, the minimum for a given stability number is somewhat easier to obtain and given in [84]: apart from the vertices that form the largest independent set, all vertices are mutually connected in the extremal graph. A very similar problem results if one fixes the size of a maximum matching; Yu and Tian [111] consider this in even more generality: in addition to the order n of the graph and its edge-independence number m (i.e., the size of a maximum matching), the cyclomatic number t is fixed (this is equivalent to prescribing the number of edges, which is equal to $n + t - 1$). Trees correspond to the case that the cyclomatic number is 0, see Section 2.2.4. If the cyclomatic number is less than the edge-independence number, then the maximum of the Merrifield-Simmons index and the minimum of the Hosoya index are attained for a graph that consists of t triangles, $m - t - 1$ paths of length 2 and $n - 2m + 1$ single edges attached to a common center (see

Figure 3 for an example).

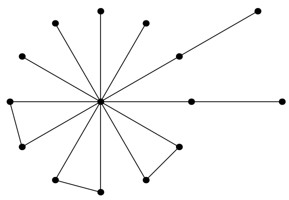


Figure 3: The graph that maximizes the Merrifield-Simmons index and minimizes the Hosoya index among all graphs with 15 vertices, cyclomatic number 3 and edge-independence number 6.

2.2 Trees

Probably the earliest account of our two indices in the mathematical literature is a short paper by Prodinger and Tichy [86], in which they prove, among other things, that the star is the tree that maximizes the Merrifield-Simmons index, and that the path is the tree that minimizes it (see Figure 4). It is easy to see, by means of a recursion, that the Merrifield-Simmons index of a path is exactly a Fibonacci number, a result that has been used frequently as an auxiliary tool. This fact was also the reason why they called the number of independent sets of a graph the *Fibonacci number* of a graph—the work of Merrifield and Simmons [70, 71, 72, 73, 74], which led to the name that is now most frequently used, was published around the same time.

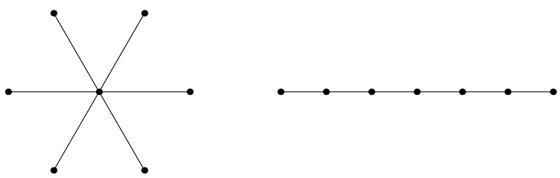


Figure 4: The star and the path on 7 vertices.

As in most other instances, the situation for the Hosoya index is absolutely analogous. The star minimizes the Hosoya index, while the path maximizes it, see [17, 28]. Let us summarize this as a single statement:

Theorem 2 Among all trees with a given number of vertices n, the star S_n maximizes the Merrifield-Simmons index ($\sigma(S_n) = 2^{n-1} + 1$) and minimizes the Hosoya index ($Z(S_n) = n$), while the path P_n minimizes the Merrifield-Simmons index ($\sigma(S_n) = F_{n+2}$, where F_n denotes the Fibonacci numbers throughout this paper, defined by $F_0 = 0$, $F_1 = 1$ and $F_{n+1} = F_n + F_{n-1}$) and maximizes the Hosoya index ($Z(P_n) = F_{n+1}$).

Since trees are quite natural objects from a chemical point of view (acyclic systems), it is not surprising that trees have been investigated further in the literature. Therefore, of course, much more than Theorem 2 is known by now:

Two different groups (Knopfmacher et al. [53] and Li et al. [61]) obtained essentially the same results (among others) in their respective papers: they characterized all trees on n vertices whose Merrifield-Simmons index is between $2^{n-2}+6$ and $2^{n-1}+1$ ([61] goes a little further, namely to 2^{n-2}). It turns out that all such trees have diameter ≤ 4. Both were unaware of an earlier paper by Lin and Lin [63], in which the same result appears. This is a typical example that illustrates why many results have been obtained independently by different groups: these papers use three different names for the same thing (the number of independent sets of a graph). Nevertheless, it is interesting to see how three slightly different approaches end up with the same result.

On the other hand, a lot is known about trees with small Merrifield-Simmons index as well: the aforementioned paper of Lin and Lin [63] also gives the tree with second-smallest Merrifield-Simmons index, and the third-smallest was determined by Zhao and Li [119]. Building up on their ideas, it was shown in [98] that all trees on n vertices whose Merrifield-Simmons index is less than $18F_{n-5} + 21F_{n-6}$ or whose Hosoya index is greater than $16F_{n-5}$ (F_n denoting Fibonacci numbers as above) are tripodes, i.e., trees with exactly three leaves (equivalently, exactly one vertex whose degree is 3, while all other vertices have degree 1 or 2) or paths. Interestingly, the sum of Merrifield-Simmons index and Hosoya index of these trees is constant (equal to F_{n+3}), which implies that their orders with respect to the two indices are the same.

A few further things about trees with small Hosoya index are known as well, but no result that is as extensive as those in [61] or [98]; in the aforementioned paper [17], one of the earliest references in this context, the trees with second-smallest and third-smallest Hosoya index are determined (as well as the tree with second-largest Hosoya index). Hou [50] also gives the tree with second-smallest Hosoya-index (as a byproduct of a more general result).

Once one can solve the extremal problem for general trees, it is quite natural to impose additional restrictions, such as fixing the number of leaves, the diameter or the maximum degree. The following pages provide an overview over results that have been obtained in this direction.

2.2.1 Trees with fixed number of leaves

This is another instance of a class of graphs for which the extremal graphs for the two indices coincide:

Theorem 3 ([82, 110]) Among all trees with n vertices and k leaves (also known as pendant vertices), the tree that maximizes the Merrifield-Simmons index and minimizes the Hosoya index is the broom, i.e., the tree that results from identifying the center of a star S_k with one end of a path of length $n-k$, see Figure 5. Its Merrifield-Simmons index is $2^{k-1}F_{n-k+2} + F_{n-k+1}$, its Hosoya index is $kF_{n-k+1} + F_{n-k}$.

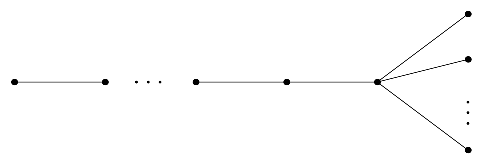


Figure 5: The broom.

This theorem was proven by Pan et al. [82] and independently by Yu and Lv [110], and extended by Wang et al. [101] for the Merrifield-Simmons index (they also provide the trees with second-largest Merrifield-Simmons index) as well as Lv et al. [67] (second-largest Merrifield-Simmons index and second-smallest Hosoya index). The problem seems to be much more complicated if one asks for the minimum Merrifield-Simmons index or maximum Hosoya index; Yan and Ye [103] (for the Hosoya index) and Deng and Guo [12] (for the Merrifield-Simmons index) provide partial (yet interesting) results in this direction for trees with many leaves (trees with n vertices and at least $\lfloor \frac{n}{2} + 1 \rfloor$ leaves).

2.2.2 Trees with fixed diameter

Let us consider trees with fixed diameter now. This problem is closely related to the one in the previous subsection: note that if the diameter is large, the number of leaves can be expected to be small, and vice versa. Therefore, it is also not surprising that the broom (Figure 5) occurs once again:

Theorem 4 ([4, 53, 61, 82, 85, 104]) Among all trees with n vertices and diameter d, the broom is the tree that maximizes the Merrifield-Simmons index and minimizes the Hosoya index.

This theorem occurs in several papers by different authors (for the Merrifield-Simmons index in [53, 61, 85] and for the Hosoya index in [4, 82, 104]), partly as auxiliary result (as in [53]) or corollary to a more general theorem (see for instance [104], where minimality of the energy is established and minimality of the Hosoya index is stated as a byproduct). This theorem was greatly extended for both indices by Liu et al. [66]: they determine a complete list of $\lfloor \frac{d}{2} \rfloor + 1$ trees (with largest, second-largest, third-largest, ... Merrifield-Simmons index as well as smallest, second-smallest, third-smallest, ... Hosoya index) for arbitrary diameter d between 3 and $n - 4$.

Again things seem to be much harder if the minimum Merrifield-Simmons index or the maximum Hosoya index are considered, and results are only available for trees with very short diameter (up to at most 5), see [53, 80] for details.

2.2.3 Trees with fixed maximum degree

Since the path and the star, the two extremal trees with respect to our two indices, are also extremal when it comes to the maximum degree, one might ask what happens if the maximum degree is fixed. From a chemical point of view, it is also very natural to study trees with restrictions on their degrees; in particular, chemical trees (all degrees less than or equal to 4, see [14]) have been of interest.

The trees that maximize the Hosoya index and minimize the Merrifield-Simmons index among all trees with given maximum degree are essentially generalized stars:

Theorem 5 ([98]) Given the number n of vertices and the maximum degree d, the tree that maximizes the Hosoya index and minimizes the Merrifield-Simmons index is a d-pode, i.e., a tree that is obtained from a collection of d paths by attaching one endpoint of each path to a common center. The lengths of the rays depend on d as follows:

- If $d \geq \frac{n-1}{2}$, then there are $n-1-d$ rays of length 2 and $2d-n+1$ rays of length 1 (Figure 6, left). The Merrifield-Simmons index of the resulting tree is $3^{n-d-1}2^{2d-n+1} + 2^{n-d-1}$, the Hosoya index is $2^{n-d-2}(3d-n+3)$.
- If $d < \frac{n-1}{2}$, then there are $d-1$ rays of length 2 and one ray of length $n-2d+1$ (Figure 6, right). The Merrifield-Simmons index of the resulting tree is $3^{d-1}F_{n-2d+3} + 2^{d-1}F_{n-2d+2}$, the Hosoya index is $2^{d-2}((d+1)F_{n-2d+2} + 2F_{n-2d+1})$.

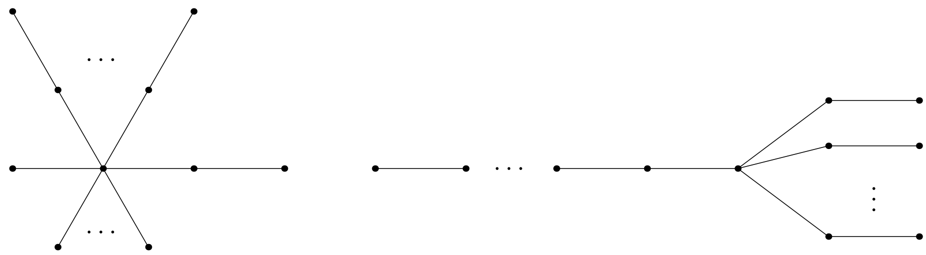
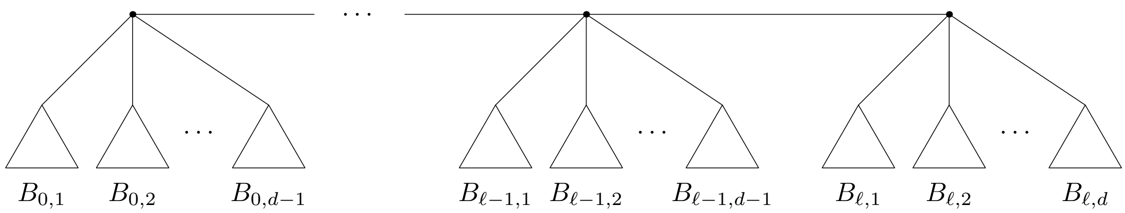


Figure 6: The trees described in Theorem 5: $d \geq \frac{n-1}{2}$ (left), $d < \frac{n-1}{2}$ (right).

Note that the vertex of maximum degree is unique, while all other vertices have degree 1 or 2, so as to make the tree as "path-like" as possible. The result for the minimum Hosoya index and maximum Merrifield-Simmons index appears to be much less intuitive: a partial solution to this problem was found by Lv and Yu [68] for trees with large maximum degree (at least one third of the number of vertices), the general problem was settled by Heuberger and one of the authors of this survey [32]:

Theorem 6 ([32]) Given the number n of vertices and the maximum degree $d \geq 3$, the tree that minimizes the Hosoya index and maximizes the Merrifield-Simmons index has the following shape:



with $B_{k,1}, \ldots, B_{k,d-1} \in \{C_k, C_{k+2}\}$ for $0 \leq k < \ell$ and

- either $B_{\ell,1} = \cdots = B_{\ell,d} = C_{\ell-1}$
- or $B_{\ell,1} = \cdots = B_{\ell,d} = C_\ell$
- or $B_{\ell,1}, \ldots, B_{\ell,d} \in \{C_\ell, C_{\ell+1}, C_{\ell+2}\}$, where at least two of $B_{\ell,1}, \ldots, B_{\ell,d}$ equal $C_{\ell+1}$.

Here, C_k denotes a complete $(d-1)$-ary tree of height $k-1$ (C_0 is an empty tree, C_1 is a single vertex, and C_k is obtained by attaching $d-1$ copies of C_{k-1} to a common root). See Figure 7 for an example.

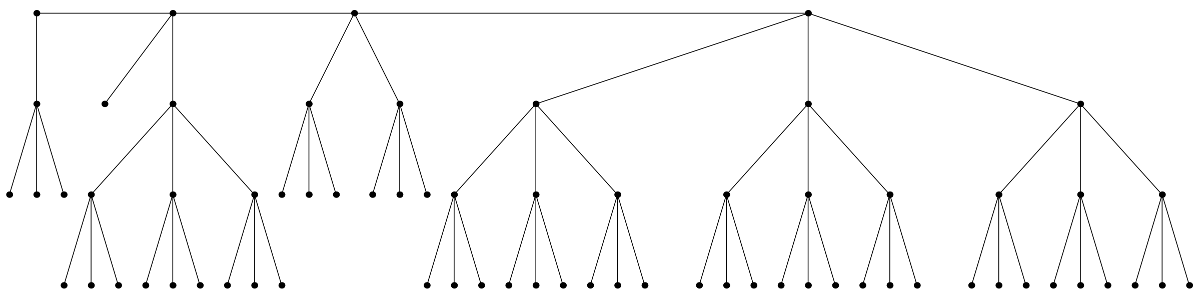


Figure 7: The tree described in Theorem 6 for $d = 4$ and $n = 69$.

There is no simple closed formula for either the Merrifield-Simmons index or the Hosoya index of the tree described in Theorem 6. For a more precise description, further discussion of the properties and construction of the trees described in Theorem 6, see [33]. For trees with more general degree restrictions, [94] provides an algorithmic approach.

2.2.4 Trees with matchings of a given size or given bipartition

It is clear that any graph with a matching M of size m has at least 2^m matchings (all subsets of M). Hence it is natural to expect that a tree with a large matching has large Hosoya index. Note also that the star, which minimizes the Hosoya index, only has matchings of size at most 1, while the path has a perfect matching (if the number of vertices is even). These observations led Hou to investigate the class of trees with n vertices and a matching of size (at least) m: in his paper [50], he characterizes the trees within this class with smallest and second-smallest Hosoya index; interestingly, the minimum is attained for the d-pode (called a "spur" by Hou) that also occurs in Theorem 5:

Theorem 7 ([50]) Among all trees with n vertices and an m-matching ($1 \leq m \leq \frac{n}{2}$), the minimum of the Hosoya index, which is $2^{m-2}(2n-3m+3)$, is attained for the $(n-m)$-pode with $m-1$ rays of length 2 and $n-2m+1$ rays of length 1 (see Figure 6, left).

This result was extended by Ye et al., who determined the trees with third-smallest [107], fourth-smallest and fifth-smallest [106] Hosoya index. On the other hand, one can ask the analogous question how large the Hosoya index of a tree can be if the tree does not have a large matching. A result in this direction is due to Ou [78], characterizing trees without a perfect matching that maximize the Hosoya index: they are essentially paths with an additional edge attached in the middle.

Finally, let us mention a somewhat isolated result by Ye and Chen [108] that characterizes the trees with smallest and second-smallest Hosoya index among all trees with a given bipartition (i.e., the sizes of the two color classes in the unique 2-coloring of a tree).

2.3 Treelike graphs

Many of the methods that can be applied to the study of trees work just as well for graphs that are similar to trees in a certain respect. Therefore it is not surprising that treelike graphs have been investigated quite extensively in the literature.

2.3.1 Forests

The connected components of a forest are trees, and so the methods for trees apply quite directly. While forests might be a very natural generalization of trees from a graph-theoretical point of view, they are less important in chemistry, where typically only connected structures are considered. The only reference in the literature where forests have been treated explicitly is the paper by Lin and Lin [63] (see Section 2.2), in which all forests on n vertices with Merrifield-Simmons index $\geq 2^{n-1}+1$ are determined (either one star and an arbitrary number of isolated vertices or two isolated edges and an arbitrary number of isolated vertices). It is not difficult to see that any graph that contains a cycle has Merrifield-Simmons index $\leq 2^{n-1}$, and so these forests are also extremal among arbitrary graphs of order n.

2.3.2 Unicyclic graphs

Apart from trees, unicyclic graphs have certainly received most attention in the literature, which is a consequence of the fact that they are very similar to trees (a unicyclic graph is obtained from a tree by adding an edge), and many useful auxiliary results and methods can still be used. As in the case of trees, several additional restrictions have been considered as well (e.g., unicyclic graphs with fixed diameter). A particularly interesting additional parameter that does not exist for trees is the girth, i.e., the length of the (unique) cycle. The following theorem (or parts thereof) occurs in several papers:

Theorem 8 ([10, 79, 81, 83, 99, 100, 109]) Among all unicyclic graphs of order n and girth r, the maximum of the Merrifield-Simmons index (which is $2^{n-r}F_{r+1} + F_{r-1}$) and the minimum of the Hosoya index (which is $(n-r+1)F_r + 2F_{r-1}$) are attained by the graph that results from attaching $n-r$ leaves to a single vertex of a cycle C_r (see Figure 8, left). Similarly, the maximum of the Hosoya index (which is $F_{n-r+2}F_r + 2F_{n-r+1}F_{r-1}$) and the minimum of the Merrifield-Simmons index (which is $F_{n-r+2}F_{r+1} + F_{n-r+1}F_{r-1}$) are attained by the graph that results from identifying one end of a path of length $n-r$ ($n-r+1$ vertices) with one of the vertices of a cycle C_r (see Figure 8, right).

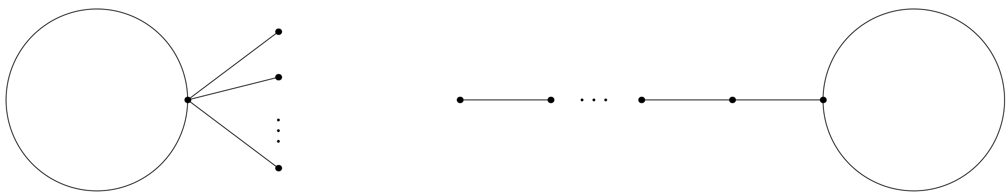


Figure 8: The graphs described in Theorem 8.

Second- and third-smallest or (-largest) and even further values have been determined as well in some of the cases: see [10, 79, 81, 99] and in particular the paper by Ye et al. [109], in which the first $\approx \frac{r}{2}$ unicyclic graphs of given order n and girth r with respect to the Merrifield-Simmons index (i.e., the graphs with largest, second largest, ... Merrifield-Simmons index) are characterized as well as the last $\approx \frac{r}{2}$ with respect to the Hosoya index; the two lists essentially coincide. From Theorem 8, it is not difficult to deduce the following result:

Theorem 9 ([10, 79, 81, 83]) Among all unicyclic graphs of order n, the maximum of the Merrifield-Simmons index and the minimum of the Hosoya index (which are $3 \cdot 2^{n-3} + 1$ and $2n-2$ respectively) are attained for the graph that results from attaching $n-3$ leaves to a triangle (the only exception being $n = 4$, in which case the cycle C_4 also maximizes the Merrifield-Simmons index). On the other hand, the maximum of the Hosoya index and the minimum of the Merrifield-Simmons index ($F_{n+1} + F_{n-1}$ in both cases) is attained for the cycle C_n; in the case of the Merrifield-Simmons index, the graph that results from attaching a path to a triangle attains the maximum as well.

For the maximum of the Merrifield-Simmons index and the minimum of the Hosoya index, this was also obtained by Yan et al. [105] as a corollary of a slightly different result: in their paper, unicyclic graphs with a given number k of leaves are studied. It turns out that under this restriction, the extremal graph is also the one that is shown in Figure 8, obtained by attaching k leaves to a cycle. This is further generalized for the minimum of the Hosoya index by Hua [51], who considers the number of leaves and the girth as two simultaneous parameters. Theorem 9 itself has also been extended further, in particular for the minimum of the Hosoya index: up to the sixth-smallest value, see [58]. Yet another problem regarding unicyclic graphs was studied by Li and Zhu:

Theorem 10 ([59]) Among all unicyclic graphs with order n and diameter $d \geq 4$, the graph that maximizes the Merrifield-Simmons index is obtained by attaching a path of length $d-3$ to one of the vertices of a 4-cycle C_4 and $n-d-1$ leaves to the opposite vertex of this cycle (see Figure 9). Its Merrifield-Simmons index is $2^{n-d-1}(2F_{d-1}+F_{d+1})+F_d$.

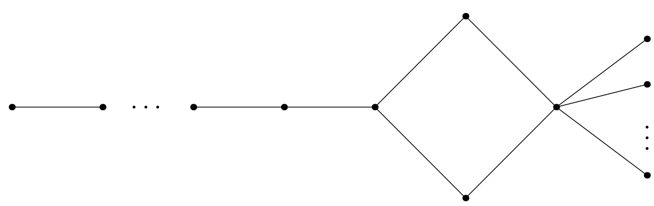


Figure 9: The graph described in Theorem 10.

For $d = 3$, the graph described in Theorem 10 is still extremal, but not unique any longer. Finally, let us mention a result by Hua [52], who considers "fully loaded" unicyclic graphs (i.e., every vertex of the cycle has degree ≥ 3): the minimum Hosoya index within this class is attained for a graph that results from a 3-cycle C_3 by attaching $n-5$ leaves to one of the three vertices of the cycle and one leaf to each of the two others.

Finally, a result by Pedersen and Vestergaard [84] deserves to be mentioned: if the girth r and the maximum distance h of a vertex from the unique cycle are fixed, the maximum of the Merrifield-Simmons index is attained for a graph that results from attaching $n-r-h$ single edges as well as a path of length h to one of the vertices of a cycle C_r.

2.3.3 Bicyclic graphs

Bicyclic graphs or $(n, n+1)$-graphs (i.e., graphs whose cyclomatic number is 2, so that the number of edges is exactly the number of vertices plus one) have been the object of study of a series of articles by Deng and coauthors [7, 8, 9, 11]; the collected main results of these four papers read as follows:

Theorem 11 ([7, 8, 9, 11]) The maximum of the Merrifield-Simmons index among all $(n, n+1)$-graphs is $5 \cdot 2^{n-4} + 1$, and it is attained for a graph that results from a star by connecting one of the leaves to two other leaves (see Figure 10). The same graph minimizes the Hosoya index (with a value of $3n - 4$). On the other hand, the minimum of the Merrifield Simmons is attained for a graph that consists of two 3-cycles, connected by a path of length $n - 5$ (the Merrifield-Simmons index of this graph, shown in Figure 11, left, is $5F_{n-2}$), while the graph that maximizes the Hosoya index results from identifying two edges of a cycle of length 4 and a cycle of length $n - 2$ respectively (Figure 11, right). Its Hosoya index is $F_{n+1} + F_{n-1} + 2F_{n-3}$.

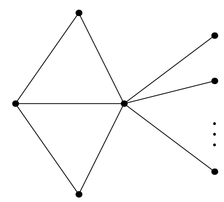


Figure 10: One of the graphs described in Theorem 11.

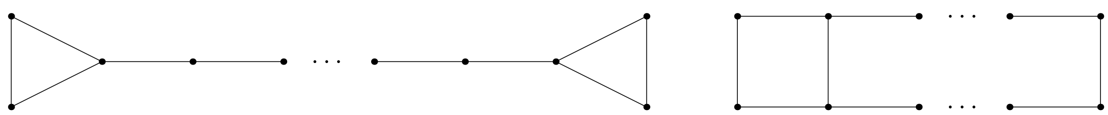


Figure 11: Two of the graphs described in Theorem 11.

It is quite notable that the graphs that maximize the Hosoya-index and minimize the Merrifield-Simmons index do not coincide in this case, as opposed to all other examples we have encountered so far. Very similar results were obtained by Startek et al. [92], who studied graphs with two elementary (disjoint) cycles.

2.3.4 Quasi-trees

Quasi-trees are obtained by adding a single vertex to a tree and connecting it to some of the vertices of the tree. This produces another possible generalization of unicyclic graphs. Quasi-trees are studied at length in a recent paper by Li et al. [57]: it turns out that the minimum of the Merrifield-Simmons index and the maximum of the Hosoya index are attained for the fan, a graph that results from connecting an additional vertex to all vertices of a path; see Figure 12. If the number of vertices is n, the respective values are $F_{n+1}+1$ (Merrifield-Simmons index) and $\frac{(n+4)F_n+2nF_{n-1}}{5}$ (Hosoya index). The maximum of the Merrifield-Simmons index and the minimum of the Hosoya index, on the other hand, are obtained for the star yet again. If the degree of the added vertex is assumed to be ≥ 2, the extemal graph is the same as for unicyclic graphs (compare Theorem 9).

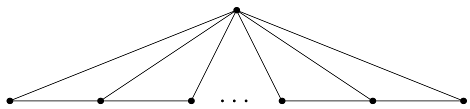


Figure 12: The extremal quasi-tree.

2.4 Hexagonal chains and general polygonal chains

Hexagonal systems play an important role in mathematical chemistry as natural representations of benzenoid hydrocarbons. In particular, hexagonal chains have been treated in the literature. The first main result concerning the extremal problem for the class of hexagonal chains occurs in a paper by one of the present authors [22]:

Theorem 12 ([22]) Among all hexagonal chains consisting of n hexagons, the linear chain (Figure 13) maximizes the Merrifield-Simmons index and minimizes the Hosoya index.

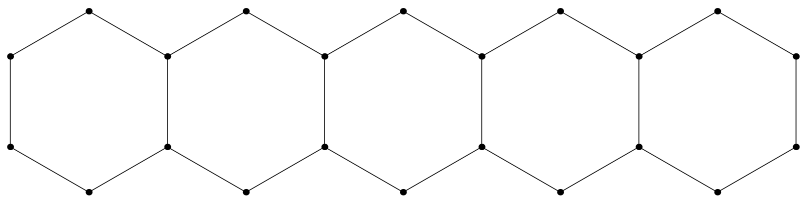


Figure 13: The linear hexagonal chain of length 5.

The analogous result for the minimum of the Merrifield-Simmons index and the maximum of the Hosoya index was conjectured by one of the authors of this survey in [22] and proven by Zhang [115]:

Theorem 13 ([115]) Among all hexagonal chains consisting of n hexagons, the zigzag chain (Figure 14) maximizes the Merrifield-Simmons index and minimizes the Hosoya index.

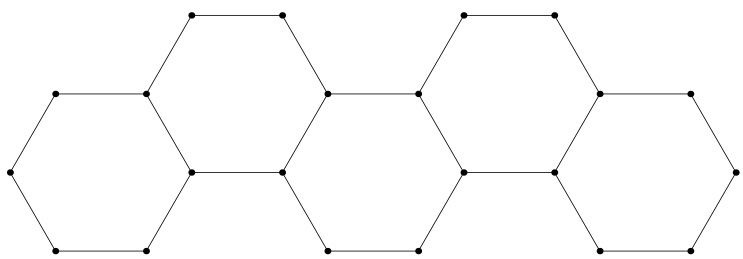


Figure 14: The zigzag chain of length 5.

These results were further generalized in various directions: the second-smallest (-largest) values were determined [116] as well as the corresponding extremal chains, and it was shown that the linear chain is still optimal if catacondensed benzenoids are considered (which allow branching, as opposed to chains), see [117]. A very surprising result due to Zhang and Zhang [118] states that the linear chain and the zigzag chain are even extremal if the number of independent sets or edges of any fixed size k (and not just the sum over all k) are considered.

Further generalizations include those by Shiu et al. [90], who consider k^*-cycle resonant hexagonal chains: in the recursive construction of hexagonal chains, a new hexagon is attached in one of three possible positions—left, middle, right—to the last hexagon of an existing chain; k^*-cycle resonant hexagonal chains are essentially those for which only "left" or "right" is allowed. The linear chain does not belong to this class, its place is taken over by the helicene chain ("left" at every step or "right" at every step).

Shiu [89] considers hexagonal spiders (which consist of a central hexagon to which three chains are attached), and Ren and Zhang [87, 88] generalize the above results to double hexagonal chains. Chains comprising of other types of polygons (such as squares, pentagons or octagons rather than hexagons are perhaps a little less natural from a chemical point of view; however, analogous results hold, see [3, 112, 113] for details.

2.5 Other classes of graphs

From a purely graph-theoretical point of view, but perhaps also considering chemical applications, there are many other classes of graphs that can be studied. One such example is a paper by Alameddine [1], in which maximum and minimum of the Merrifield-Simmons index are determined for maximal outerplanar graphs (which are equivalent to triangulations of polygons). Various classes of graphs are studied by Pedersen and Vestergaard in [84], for instance connected bipartite graphs: the maximum and minimum of the Merrifield-Simmons index are obtained for the star and the complete bipartite graph whose two parts are equal in size (or differ at most by one if the total number of vertices is odd). Another remarkable result proven in [84] is the fact that the maximum of the Merrifield-Simmons index for connected claw-free graphs is attained for the path (note that one the other hand, the path minimizes the Merrifield-Simmons index within the class of trees).

3 Useful auxiliary results and methods

There are various helpful lemmas and auxiliary results that occur frequently in the literature and can be applied to several different problems, usually even for both the Merrifield-Simmons index and the Hosoya index, and sometimes even for other indices (see [62], [65] for notable contributions towards a unified theory). This section is devoted to some of the most important techniques that have been used to obtain the results described in the preceding section. At the end of this section, a general approach that has proven useful in many instances is described.

3.1 Explicit and recusive formulas

The Hosoya index of a graph G can be written as the permanent of the matrix $I + A$, where A is the adjacency matrix of G and I the identity matrix. While permanents are not particularly convenient for computational purposes, they often serve as auxiliary tools, for instance to obtain recursive relations for the Hosoya index, see [49, 51, 52, 78, 79, 80, 81, 103, 106, 107].

Quite frequently, recursive formulas for the Merrifield-Simmons index or the Hosoya index are needed in order to determine explicit formulas for specific graphs. The most important recursive properties of the two indices are summarized in the following theorem.

Theorem 14 If $G_1, G_2, \ldots, G_r$ are the connected components of a graph G, then

$$\sigma(G) = \prod_{i=1}^{r} \sigma(G_i)$$

and

$$Z(G) = \prod_{i=1}^{r} Z(G_i).$$

Furthermore, the following recursive formulas hold:

1. $$\sigma(G) = \sigma(G \setminus v) + \sigma(G \setminus N[v]),$$

   where $N[v]$ denotes the closed neighborhood of a vertex v (v together with all its neighbors),

2. $$Z(G) = Z(G \setminus v) + \sum_{w \sim v} Z(G \setminus \{v, w\}),$$

   where the sum is taken over all neighbors w of v,

3. $$\sigma(G) = \sigma(G \setminus e) - \sigma(G \setminus (N[v] \cup N[w])),$$

   where v and w are the ends of an edge e,

4. and

   $$Z(G) = Z(G \setminus e) + Z(G \setminus \{v, w\})$$

   where v and w are the ends of an edge e.

See [28] for a standard reference. Even though the recursive formulas are easy to prove (to obtain 1., for instance, distinguish between independent sets that contain v and those that do not contain v), they are crucial in the proofs of most of the results presented in the preceding section. Quite often, these formulas together with elementary methods such as induction or the trivial fact that deleting edges results in a decrease of the Hosoya index and an increase of the Merrifield-Simmons index are sufficient, if applied in the right way (see [1, 3, 4, 7, 8, 9, 10, 11, 12, 22, 32, 51, 52, 53, 57, 59, 61, 63, 65, 67, 68, 82, 84, 85, 86, 87, 89, 90, 92, 93, 98, 99, 100, 101, 103, 105, 109, 110, 111, 112, 115, 116, 117, 119, 120] for various examples). They are also frequently used to determine explicit formulas for the Merrifield-Simmons index or Hosoya index of specific graphs. It should finally be mentioned that analogous formulas even hold more generally for associated polynomials (such as the matching polynomial, see [16]).

3.2 Replacing parts of a graph

The path and the star are the extremal trees with respect to both indices, as stated in Section 2.2. However, an even stronger theorem holds, which plays a major role in the analysis of treelike graphs. It can be stated as follows:

Theorem 15 Suppose that G is a connected graph and T an induced subgraph of G such that T and G only share a cut vertex v and T is a tree. If G_1 and G_2 are the graphs that result from replacing T by a star and a path respectively (see Figure 15), then the inequalities

$$\sigma(G_1) \geq \sigma(G) \geq \sigma(G_2)$$

and

$$Z(G_2) \leq Z(G) \leq Z(G_2)$$

hold. Both inequalities are strict unless G is isomorphic to either G_1 or G_2.

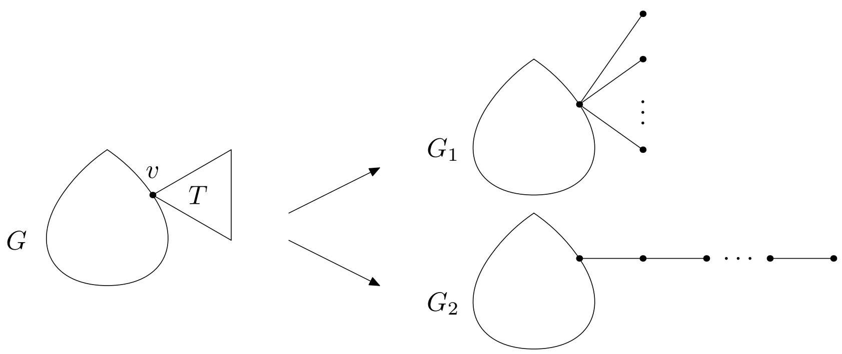


Figure 15: Replacing a tree by a star or a path.

This theorem is very useful to reduce the set of potentially extremal graphs considerably, see [4, 7, 8, 9, 10, 11, 52, 53, 59, 66, 98, 100, 101, 105, 109, 119] for various applications. Note also that those graphs within a given class of trees or treelike graphs that maximize the Merrifield-Simmons index or minimize the Hosoya index typically contain large stars (see Sections 2.2 and 2.3). Analogously, the minimum of the Merrifield-Simmons index and the maximum of the Hosoya index are typically attained for graphs that contain long paths. Things tend to become much harder if one imposes restrictions that do not allow for large stars or long paths (e.g. degree restrictions, as in Section 2.2.3, or restricted diameter, as in Section 2.2.2). The notion of so-called α-optimal trees introduced in [94] is an attempt to extend Theorem 15 to such cases.

3.3 Moving parts of a graph

Another typical auxiliary result considers the case that parts of a graph (typically, trees attached to a cut vertex) are moved from one place to another. The following theorem provides information on the behavior of the Merrifield-Simmons index and the Hosoya index under such transformations:

Theorem 16 Suppose G is a connected graph and H_1, H_2 are (nonempty) induced subgraphs that only share a cut vertex (v_1 resp. v_2) with the rest of the graph. Let G_1 denote the graph that results from moving H_1 from v_1 to v_2, and let G_2 denote the graph that results from moving H_2 from v_2 to v_1 (see Figure 16). Then the following statements hold:

- Either $\sigma(G_1) > \sigma(G)$ or $\sigma(G_2) > \sigma(G)$.
- Either $Z(G_1) < Z(G)$ or $Z(G_2) < Z(G)$.

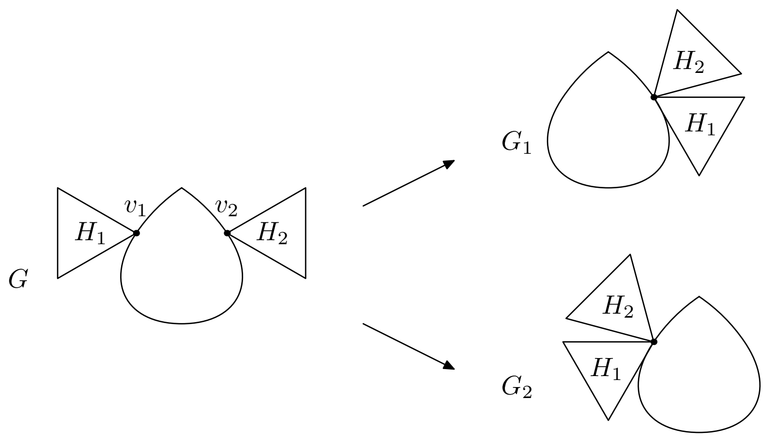


Figure 16: Moving parts of a graph.

A proof that even includes other indices is given in [65]. In the literature, this theorem appears in various variants and special cases (for example in the case that H_1 and H_2 are stars [8, 11, 66, 67, 109, 110]). See also [57, 59, 94, 105] for applications of this "transfer theorem", which is usually used to rule out specific substructures in extremal graphs. A related result that is specifically geared towards trees with fixed maximum degree can be found in [32].

"Sliding along a path" is another recurring aspect that deserves to be mentioned. The following theorem appears in [119] for the Merrifield-Simmons index, and the (almost completely analogous) proof can be found in [98]; see also [7, 9, 10, 99] for further applications.

Theorem 17 Let G be a connected graph with at least two vertices, and choose a vertex $u \in V(G)$. $P(n,k,G,u)$ then denotes the graph that results from identifying u with the vertex v_k of a simple path $v_1,\ldots,v_n$ (Figure 17). Write n as $n = 4m+i$, $i \in \{1,2,3,4\}$, $m \geq 0$. Then the inequalities

$$\begin{aligned} &Z(P(n,2,G,u)) < Z(P(n,4,G,u)) < \ldots < Z(P(n,2m+2l,G,u)) < \\ &\quad Z(P(n,2m+1,G,u)) < \ldots < Z(P(n,3,G,u)) < Z(P(n,1,G,u)) \end{aligned}$$

and

$$\begin{aligned} &\sigma(P(n,2,G,u)) > \sigma(P(n,4,G,u)) > \ldots > \sigma(P(n,2m+2l,G,u)) > \\ &\quad \sigma(P(n,2m+1,G,u)) > \ldots > \sigma(P(n,3,G,u)) > \sigma(P(n,1,G,u)), \end{aligned}$$

hold, where $l = \lfloor \frac{i-1}{2} \rfloor$.

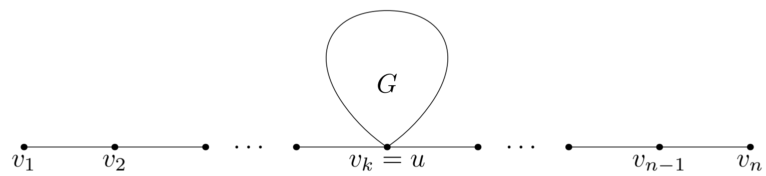


Figure 17: Sliding along a path.

As in the case of the previous theorem, some variants and related results exist, see for instance [67, 99, 105, 110]. In particular, the following result was repeatedly used by Deng et al. [7, 9, 10] in their study of $(n,n+1)$-graphs (for convenience, we use a slightly different notation):

Theorem 18 Let G be a connected graph with at least three vertices, and choose two vertices $u_1,u_2 \in V(G)$ that are not neighbors in G. $P(n,k,l,G,u_1,u_2)$ then denotes the graph that results from identifying u_1 with the vertex v_k and u_2 with the vertex v_l of a simple path $v_1, \ldots, v_n$ (Figure 18). For any $1 < k < l < n$, at least one of the inequalities

$$\sigma(P(n,k,l,G,u_1,u_2)) > \sigma(P(n,1,l-k+1,G,u_1,u_2)),$$
$$\sigma(P(n,k,l,G,u_1,u_2)) > \sigma(P(n,n+k-l,n,G,u_1,u_2))$$

and at least one of the inequalities

$$Z(P(n,k,l,G,u_1,u_2)) < Z(P(n,1,l-k+1,G,u_1,u_2)),$$
$$Z(P(n,k,l,G,u_1,u_2)) < Z(P(n,n+k-l,n,G,u_1,u_2))$$

must hold.

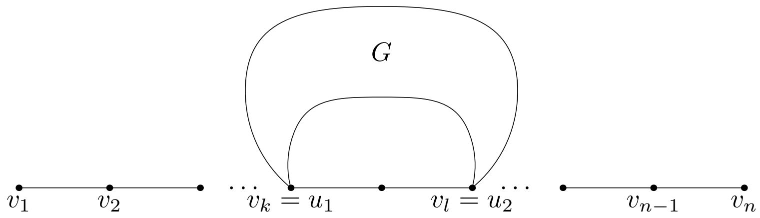


Figure 18: Sliding along a path, second part.

3.4 Outline of a general approach

Let us finally describe the approach that is typically followed in order to obtain the results described in Section 2. It is only a rough outline, of course, but it applies to most of the cases that have been treated in the literature, and we believe that many other problems of a similar flavor can be solved along these lines.

- Aim to rule out certain substructures and generally reduce the set of potentially extremal graphs within the prescribed class. The auxiliary results presented in the Section 3.2 and 3.3 often prove useful in this regard.

- Once the set of candidates has been reduced to a simpler class (or classes) of graphs, one can often establish explicit formulas (depending on one or two parameters) for the Merrifield-Simmons index or the Hosoya index of the remaining cases to be considered. The recursive relations presented in Section 3.1 are usually used for this purpose.

- Determine the maximum or minimum from these explicit formulas. This process can often be rather technical and frequently involves identities for Fibonacci numbers (since they occur in the formulas for Merrifield-Simmons index and Hosoya index of paths and cycles).

- At this stage, the remaining number of candidate graphs should be reduced considerably, so that only a few different graphs need to be compared. This yields the graph within the originally prescribed class of graphs that maximizes (minimizes) the Merrifield-Simmons (Hosoya) index, and in some cases also the graph with second-largest (-smallest) index value or even more.

4 Open problems

In spite of the fact that there is a substantial amount of literature on the topic of maximizing or minimizing the Merrifield-Simmons index and the Hosoya index (as can be seen from this survey), there are still many interesting open questions for further study. Let us mention the following problems:

- It seems to be difficult to obtain results analogous to Theorems 3 and 4 for the minimum of the Merrifield-Simmons index and the maximum of the Hosoya index among trees with a given number of leaves or given diameter. However, partial results are available, so the problem might not be totally intractable, and results in this direction would definitely be interesting.

- Little is also known about the case that two restrictions are imposed at the same time (e.g. fixed diameter and fixed number of leaves), so this might be another worthwhile problem to study.

- While the main questions are settled for trees with prescribed maximum degree (Section 2.2.3), it is also natural to consider other degree restrictions. It might even be possible to characterize the trees with a prescribed degree sequence that maximize or minimize the two indices.

- If the aforementioned questions can be answered for trees, then it is also natural to consider the analogous questions for treelike graphs (such as unicyclic graphs).

- While hexagonal chains have been studied quite extensively (see Section 2.4), not much is known about hexagonal systems that are not necessarily chains. If hexagons are allowed to "cluster", new phenomena might arise.

- At least from a purely graph-theoretical point of view, there are many other classes of graphs to be studied, even if they are perhaps not chemically relevant. For instance, nothing seems to be known about general planar graphs (even though there exists a result for the special subclass of outerplanar graphs, see Section 2.5).

- In several instances, it has been shown that the extremal graphs within a given class are even extremal with respect to the number of independent sets (or matchings) of any fixed size, which is a much stronger property. For some cases, this has been conjectured, but not proven (for instance the trees described in Theorem 6, see [33]).

Of course this list only contains some interesting problems for further study, and there might be many other worthwhile questions to consider. The Merrifield-Simmons index and the Hosoya index have been the focus of many interesting articles in the past, and will certainly also lead to further interesting investigations in the future.

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