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Extremal Chemical Graphs of Maximum Degree at Most 3 for 33 Degree–Based Topological Indices

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Abstract

We consider chemical graphs that are defined as connected graphs of maximum degree at most 3.We characterize the extremal ones, that is, those that maximize or minimize 33 degree-based topological indices. This study shows that five graph families are sufficient to characterize the extremal chemical graphs of 29 of these 33 indices. In other words, the extremal properties of this set of degree-based topological indices vary very little.

1 Introduction

Chemical graphs provide a powerful tool for modeling molecular structures. These graphs, where vertices represent atoms and edges represent bonds,

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allow researchers to investigate various chemical and physical properties of molecules through graph-theoretical concepts.

According to Patrick Fowler [21]: "The definition of chemical graphs that is useful depends on context. Two definitions appropriate to different kinds of carbon framework can be found in the literature. The graphs that can be regarded as skeletons of saturated hydrocarbons (such as alkanes), are connected and have maximum degree Δ at most 4. If instead the interest is in (unsaturated) conjugated π systems, such as alkenes, polyenes, benzenoids, and fullerenes, the maximum degree should be at most 3, since a conjugated carbon atom participates in at most three single bonds."

In this paper, we focus on the second definition of chemical graphs (where the maximum degree is at most 3) and explore the bounds on topological indices of such graphs. A topological index, or molecular descriptor, is a graph invariant used to study specific physicochemical properties of molecules. Among the most well-known indices is the Randić index, introduced by Milan Randić [38] in 1975, which has been widely used in quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) studies. Its value $Ra(G)$ for a chemical graph G is defined as

$$Ra(G) = \sum_{vw \in E} \frac{1}{\sqrt{d(v)d(w)}},$$

where $d(v)$ is the degree of vertex v. This is an example of so-called *degree-based* topological index, that is an index computed from the sum of the weights of the edges, each edge vw having a weight defined by a formula using the degrees of v and w.

As stated by Ivan Gutman [24], "Countless topological indices have been and are being proposed so far, in many cases without any examination if these correlate with any of the various physical properties, chemical reactivity or biological activity. To use a mild expression, today we have far too many such descriptors, and there seems to lack a firm criterion to stop or slow down their proliferation."

In this paper, we consider 33 degree-based topological indices that we found in the literature (see Section 2) and whose extremal properties have given rise to scientific publications [1–5, 7–17, 19, 20, 22, 23, 26, 27, 29–35, 37, 39–45]. In the same spirit as Gutman's words, we can wonder whether these indices are very different from each other. We provide a partial answer by analyzing the extremal properties of these indices. We use the word "partial" for several reasons. First, we are only interested in the *extremal* properties of topological indices and it could therefore be that various indices are distinguished by other properties of interest to chemists. Second, we only deal with chemical graphs of maximum degree at most 3. Finally, the list of topological indices studied in this article is not exhaustive, although we have tried to consider the most cited and studied in the scientific literature. Our conclusions will be clear: five families of chemical graphs are sufficient to characterize the vast majority of extremal chemical graphs of degree-based topological indices.

Let $G = (V, E)$ be a graph of *order* $n = |V|$ and *size* $m = |E|$. The maximum degree of a graph G is denoted $\Delta(G)$. An edge with endpoints u and v of degree $d(u) = i$ and $d(v) = j$ is called an (i, j)-edge and is denoted uv. We denote x_{ij} the number of (i, j)-edges in G while n_i is the number of vertices in G of degree i. In what follows, K_n, P_n and C_n denote the complete graph of order n, the path of order n and the cycle of order n, respectively.

In the next section, we give a precise definition of the chemical graphs considered in this paper and we give the list of 33 topological indices whose extremal properties are analyzed. Section 3 is dedicated to defining five families of chemical graphs which are sufficient to characterize the extremal graphs for a large majority of degree-based topological indices. Tools used in our proofs are given in Section 4, and a characterization of extremal chemical graphs for the 33 topological indices is given in Section 5.

2 Preliminaries

As mentioned in the previous section, we are interested in connected graphs of maximum degree at most 3. To avoid border effects, we will not consider small or dense graphs which have only few possible x_{ij} values. This is now explained in detail.

There are only 10 connected graphs of order n with $1 \leq n \leq 4$, Six of them, namely K_1,K_2,K_3, K_4, P_3 and the diamond (K_4 minus an edge), are the only ones having their order and size. They therefore maximize and minimize any topological index of their order and size. The two pairs (n, m) with $n \leq 4$ that have different chemical graphs of order n and size m are P_4 and the star with 3 branches for $(n, m) = (4, 3)$ and C_4 and a triangle plus a pending vertex for $(n, m) = (4, 4)$. By restricting ourselves to connected graphs of maximum degree at most 3, it is not difficult to show that there are 10 such graphs of order $n = 5$ and 29 ones of order $n = 6$. These can be obtained using *PHOEG* [18], *House of Graphs* [6] or *Nauty's geng* [36]. Hence, given any topological index, it is easy to determine which chemical graph of order $n \leq 6$ has maximum or minimum value. From now on, we will therefore only consider connected graphs G of order at least 7, which implies $x_{11} = 0$ and $2 \leq \Delta(G) \leq 3$.

Definition 1. *A* degree-based topological index *is any function f of the form*

$$f(x_{12}, x_{13}, x_{22}, x_{23}, x_{33}) = c_{12}x_{12} + c_{13}x_{13} + c_{22}x_{22} + c_{23}x_{23} + c_{33}x_{33},$$

where every c_{ij} is a real number.

By abuse of notation, for a graph G, we will write $f(G)$ instead of $f(x_{12}, x_{13}, x_{22}, x_{23}, x_{33})$, where x_{ij} is the number of (i, j)-edges in G. For example, the Randić index (see Section 1) is the degree-based topological index with $c_{ij} = \frac{1}{\sqrt{ij}}$.

Let's focus now on dense graphs. Since we restrict ourselves to graphs G of maximum degree at most 3, the size m of such graphs is at most $\frac{3n}{2}$: if $m = \frac{3n}{2}$, then $x_{33} = m$ (G is 3-regular); if $m = \frac{3n-1}{2}$, then $x_{23} = 2$ and $x_{33} = m - 2$; if $m = \frac{3n-2}{2}$, then there are three possible cases:

- $x_{13} = 1$ and $x_{33} = m - 1$;
- $x_{23} = 4$ and $x_{33} = m - 4$;
- $x_{22} = 1$, $x_{23} = 2$ and $x_{33} = m - 3$.

Hence, given a pair (n, m) with $m \geq \frac{3n-2}{2}$, and given any degree-based topological index f, it is not difficult to determine the x_{ij} values of the connected graphs of order n, size m and maximum degree at most 3 which maximize or minimize f.

From now on, when we talk about chemical graphs, we assume that we are not in the above extreme cases (i.e., very small or very dense graphs). More precisely, here is the definition of the chemical graphs studied in this paper.

Definition 2. *A* chemical graph *is a connected graph of order* $n \geq 7$*, size* $m \leq \frac{3n-3}{2}$ *and maximum degree at most 3.*

It is important to specify here that although the results that we demonstrate are valid for chemical graphs as defined above, it is possible that these results are also valid for some connected graphs of maximum degree at most 3 and of order $n < 7$ or size $m > \frac{3n-3}{2}$.

We found in the literature 33 degree-based topological indices. They are described in Table 1. Most of them, namely 28, appear in [25], the exceptions being ABSC which appears in [5], AG-GA, which appears in [42] and lnZagreb1, lnZagreb2 and lnZagreb3 which can be found in [39]. We are interested in the extremal properties of these indices. More precisely, given a topological index f, we aim to characterize the chemical graphs that maximize f and those that minimize f. For the 33 indices of Table 1, this gives potentially 66 families of chemical graphs. As will be shown, 5 families (instead of 58) are sufficient to characterize the extremal chemical graphs of 29 of the 33 topological indices.

Definition 3. *Given a degree-based topological index* f *defined by* c_{ij} *values, its complement denoted* $\overline{f}$ *is the degree-based topological index defined by* $-c_{ij}$ *values.*

Determining chemical graphs with the *minimum* value for f is thus equivalent to determining chemical graphs with the *maximum* value for $\overline{f}$. In the subsequent proofs, we always aim to maximize the value of a topological index in Table 1 or its complement.

Definition 4. *A chemical graph* G *is* extremal *for a degree-based topological index* f *if it maximizes* f *or* $\overline{f}$ *over all chemical graphs of the same order and size as* G*.*

Table 1. 33 Degree-based topological indices

Name	Short name	c_{ij}
Atom-bond connectivity index	ABC	$\sqrt{\frac{i+j-2}{ij}}$
Atom-bond sum-connectivity index	ABSC	$\sqrt{\frac{i+j-2}{i+j}}$
Albertson index	Albertson	$\|i-j\|$
Arithmetic-geometric index	AG	$\frac{i+j}{2\sqrt{ij}}$
Difference between AG and GA	AG-GA	$\frac{i+j}{2\sqrt{ij}} - \frac{2\sqrt{ij}}{i+j}$
Extended index	Extended	$\frac{1}{2}(\frac{i}{j} + \frac{j}{i})$
Forgotten index	Forgotten	$i^2 + j^2$
Geometric-arithmetic index	GA	$\frac{2\sqrt{ij}}{i+j}$
First Gourava index	Gourava1	$i + j + ij$
Second Gourava index	Gourava2	$(i + j)ij$
First hyper-Gourava index	hGourava1	$(i + j + ij)^2$
Second hyper-Gourava index	hGourava2	$((i + j)ij)^2$
Gourava sum-connectivity index	GouravaSC	$\frac{1}{\sqrt{i+j+ij}}$
Gourava product-connectivity index	GouravaPC	$\sqrt{ij(i + j)}$
Harmonic index	Harmonic	$\frac{2}{i+j}$
Inverse degree index	InvDeg	$i^{-2} + j^{-2}$
Inverse sum of degree index	InvSumDeg	$\frac{ij}{i+j}$
Randić index	Randić	$\frac{1}{\sqrt{ij}}$
Reciprocal Randić index	rRandić	$\sqrt{ij}$
Sigma index	Sigma	$(i - j)^2$
Sombor index	Sombor	$\sqrt{i^2 + j^2}$
Reduced Sombor index	rSombor	$\sqrt{(i-1)^2 + (j-1)^2}$
Sum connectivity index	SumConn	$\frac{1}{\sqrt{i+j}}$
Reciprocal sum connectivity index	rSumConn	$\sqrt{i + j}$
First Zagreb index	Zagreb1	$i + j$
Second Zagreb index	Zagreb2	ij
Augmented Zagreb index	aZagreb	$(\frac{ij}{i+j-2})^3$
First hyper-Zagreb index	hZagreb1	$(i + j)^2$
Second hyper-Zagreb index	hZagreb2	$(ij)^2$
Nat. log. of the mult. sum Zagreb index	lnZagreb1	$\ln(i + j)$
Nat. log. of the first mult. Zagreb index	lnZagreb2	$2(\frac{\ln(i)}{i} + \frac{\ln(j)}{j})$
Nat. log. of the second mult. Zagreb index	lnZagreb3	$\ln(i) + \ln(j)$
Modified first Zagreb index	mZagreb	$i^{-3} + j^{-3}$

3 Five families of chemical graphs

A chemical graph is characterized by five x_{ij} values, namely, x_{12}, x_{13}, x_{22}, x_{23} and x_{33}. We therefore have:

$$n_1 = x_{12} + x_{13} \tag{1}$$
$$n_2 = \frac{x_{12} + 2x_{22} + x_{23}}{2} \tag{2}$$
$$n_3 = \frac{x_{13} + x_{23} + 2x_{33}}{3} \tag{3}$$
$$n = n_1 + n_2 + n_3 = \frac{3}{2}x_{12} + \frac{4}{3}x_{13} + x_{22} + \frac{5}{6}x_{23} + \frac{2}{3}x_{33} \tag{4}$$
$$m = x_{12} + x_{13} + x_{22} + x_{23} + x_{33}. \tag{5}$$

We now define five families F_1, F_2, F_3, F_4 and F_5 of chemical graphs. As will be shown, these are sufficient to characterize the extremal chemical graphs of 29 topological indices. Fo illustration, examples of chemical graphs belonging to these families are given in Figure 1.

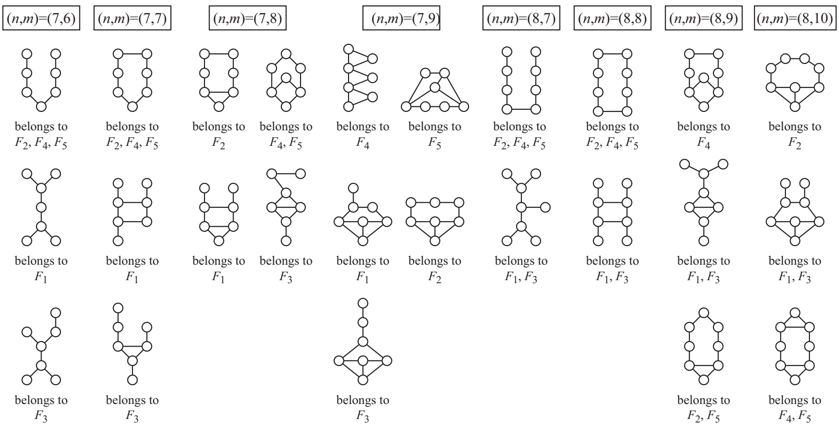

Figure 1. Examples of chemical graphs or order $n \in \{7, 8\}$ and size $m \leq n+2$ belonging to at least one of the families $F_1, \ldots, F_5$.

Definition 5. *F_1 is the set of chemical graphs with the following numbers x_{ij} of (i, j)-edges:*

x_{12}	x_{13}	x_{22}	x_{23}	x_{33}	
0	$\frac{3n-2m}{2}$	0	0	$\frac{4m-3n}{2}$	*if n if even*
0	$\frac{3n-2m-1}{2}$	0	2	$\frac{4m-3n-3}{2}$	*if n if odd*

Definition 6. *F_2 is the set of chemical graphs with the following numbers x_{ij} of (i,j)-edges:*

x_{12}	x_{13}	x_{22}	x_{23}	x_{33}	
2	0	$m-2$	0	0	*if* $m=n-1$
0	0	m	0	0	*if* $m=n$
0	0	$m-5$	4	1	*if* $m=n+1$
0	0	$3n-2m-1$	2	$3m-3n-1$	*if* $n+1<m\leq \frac{3n-3}{2}$

Definition 7. *F_3 is the set of chemical graphs with the following numbers x_{ij} of (i,j)-edges:*

x_{12}	x_{13}	x_{22}	x_{23}	x_{33}	
0	$\frac{3n-2m}{2}$	0	0	$\frac{4m-3n}{2}$	*if* n *if even*
1	$\frac{3n-2m-3}{2}$	0	1	$\frac{4m-3n-1}{2}$	*if* n *if odd*

Definition 8. *F_4 is the set of chemical graphs with the following numbers x_{ij} of (i,j)-edges:*

x_{12}	x_{13}	x_{22}	x_{23}	x_{33}	
2	0	$m-2$	0	0	*if* $m=n-1$
0	0	$6n-5m$	$6m-6n$	0	*if* $n\leq m<\frac{6n}{5}$
0	0	0	$6n-4m$	$5m-6n$	*if* $\frac{6n}{5}\leq m\leq \frac{3n-3}{2}$

Definition 9. *F_5 is the set of chemical graphs with the following numbers x_{ij} of (i,j)-edges:*

x_{12}	x_{13}	x_{22}	x_{23}	x_{33}	
2	0	$m-2$	0	0	*if* $m=n-1$
0	0	m	0	0	*if* $m=n$
0	0	$m-6$	6	0	*if* $m=n+1$
0	0	$m-5$	4	1	
0	0	a	$6n-4m-2a$	$5m-6n+a$	*if* $n+1<m\leq \frac{3n-3}{2}$

where a is any integer such that $\max\{0,6n-5m\}\leq a\leq 3n-2m-1$ *when* $n+1<m\leq \frac{3n-3}{2}$.

It is not difficult to show that for every x_{ij} values of the five families defined above, there is at least one chemical graph having x_{ij} (i,j)-edges.

This can be proved in several ways. The first approach is to use the necessary and sufficient conditions provided in Hansen *et al.* [28] for the existence of a simple connected graph with given x_{ij} values. These conditions for chemical graphs can be written as follows:

$$\begin{aligned}
x_{33} &\le \tfrac{n_3(n_3-1)}{2} && \text{if } n_3 = 1, 2 \text{ or } 3, && (6)\\
x_{22} &\le \tfrac{n_2(n_2-1)}{2} && \text{if } n_2 = 1 \text{ or } 2, && (7)\\
x_{23} &\le n_2 n_3 && \text{if } n_2 = 1 \text{ or } 2 \text{ and } n_3 = 1, && (8)\\
x_{23} &\ge \delta(n_2) + \delta(n_3) - 1, && && (9)\\
x_{23} + x_{33} &\ge n_3 + \delta(n_2) - 1, && && (10)\\
x_{22} + x_{23} &\ge n_2 + \delta(n_3) - 1, && && (11)\\
x_{22} + x_{23} + x_{33} &\ge n_2 + n_3 - 1. && && (12)
\end{aligned}$$

where

$$\delta(x) = \begin{cases} 1 & \text{if } x \ge 1, \\ 0 & \text{otherwise.} \end{cases}$$

Condition (12) is equivalent to $m - x_{12} - x_{13} \ge n - x_{12} - x_{13} - 1$, which is equivalent to $m \ge n - 1$. In summary, given a pair (n, m) of integers such that $n \ge 7$ and $n - 1 \le m \le \frac{3n-3}{2}$, and given x_{ij} values that satisfy conditions (1)-(5), we can state that there is a chemical graph of order n and size m with x_{ij} (i, j)-edges if and only if conditions (6)-(11) are satisfied. This is now illustrated with family F_1.

Given x_{ij} values as in Definition 5, Equations (1), (2) and (3) give

$$\begin{cases} n_1 &= \frac{3n-2m-(n \bmod 2)}{2}, \\ n_2 &= n \bmod 2, \\ n_3 &= \frac{2m-n-(n \bmod 2)}{2}. \end{cases}$$

Clearly, $n = n_1 + n_2 + n_3$ and $m = x_{12} + x_{13} + x_{22} + x_{23} + x_{33}$, which means that conditions (1)-(5) are satisfied. Let's now prove that Constraints (6)-(11) are also satisfied. Note first that $n \ge 7$ implies $m \ge n - 1 \ge 6$. Since $3n_3 = m + x_{33}$, we have $n_3 \ge 2$.

- If $n_3 = 2$ then $6 = m + x_{33} \ge 6 + x_{33}$ implies $x_{33} < 1 = \frac{n_3(n_3-1)}{2}$; if $n_3 = 3$, then $9 = m + x_{33} \ge 6 + x_{33}$ implies $x_{33} \le 3 = \frac{n_3(n_3-1)}{2}$.

Hence, Constraint (6) is satisfied.

- Since $x_{22} = 0 \leq \frac{n_2(n_2-1)}{2}$ for $n_2 = 1$ and 2, Constraint (7) is satisfied.
- As mentioned above, $n_3 \geq 2$ which implies that there is no Constraint (8).
- If n is even, then $x_{23} = n_2 = \delta(n_2) = 0$. Therefore,
  - $x_{23} = 0 \geq \delta(n_2) + \delta(n_3) - 1$;
  - Since $m \geq n-1$, we have $2x_{33} = 4m - 3n \geq m - 3$. Hence, $m - 3 + x_{33} \leq 3x_{33}$ which implies $x_{23} + x_{33} = x_{33} \geq \frac{m+x_{33}-3}{3} = n_3 - 1 = n_3 + \delta(n_2) - 1$;
  - $x_{22} + x_{23} \geq n_2 + \delta(n_3) - 1$.

  Hence, Constraints (9)-(11) are satisfied.
- If n is odd, then, $x_{23} = 2$ and $n_2 = \delta(n_2) = 1$. Therefore,
  - $x_{23} = 2 > \delta(n_2) + \delta(n_3) - 1$.
  - Since $m \geq n-1$, we have $2x_{33} = 4m - 3n - 3 \geq m - 6$. Hence, $m - 6 + x_{33} \leq 3x_{33}$ which implies $x_{23} + x_{33} = 2 + x_{33} \geq \frac{m+x_{33}}{3} = n_3 = n_3 + \delta(n_2) - 1$.
  - $x_{22} + x_{23} = 2 > n_2 + \delta(n_3) - 1$.

  Hence, Constraints (9)-(11) are satisfied.

Another way of proving that a chemical graph exists for given x_{ij} values is to give an explicit construction for such a graph. For family F_1, for an even order $n \geq 7$ and for $m \geq n$, one can for example consider the following construction (a similar one can be given for odd values of n and for $m = n - 1$):

1. Construct a cycle on vertices $v_1, v_2, \ldots, v_{m-\frac{n}{2}}$, with edges $v_i v_{i+1}$ $(1 \leq i \leq m - \frac{n}{2} - 1)$ and $v_1 v_{m-\frac{n}{2}}$.
2. Add a matching with the $m - n$ edges $v_i v_{\lceil \frac{2m-n}{4} \rceil + i}$ $(1 < i \leq m - n)$. Let W be the set of endpoints of these edges.
3. For each $v_i \notin W$, add a pending vertex w_i adjacent to v_i.

The resulting graph belongs to F_1. Indeed, every v_i has degree 3 and every w_i has degree 1. We thus have $x_{12} = x_{22} = x_{23} = 0$. Moreover, $x_{13} = m - \frac{n}{2} - |W| = \frac{3n-2m}{2}$ and $x_{33} = m - \frac{n}{2} + |W| = \frac{4m-3n}{2}$.

In summary, it is tedious but easy to check that given x_{ij} values of one of the five graph families defined above, there is at least one chemical graph with x_{ij} (i,j)-edges. Therefore, from now on, we assume that this is true for the five families $F_1, \ldots, F_5$.

4 Tools used to characterize extremal chemical graphs

Given a set of x_{ij} values, we consider transformations which generate x'_{ij} values having specific properties.

Definition 10. *Let $A = (a_{12}, a_{13}, a_{22}, a_{23}, a_{33})$ be a vector with integer coefficients.*

- *Given any integer k, the (A,k)-transform of a vector $(x_{12}, x_{13}, x_{22}, x_{23}, x_{33})$ is the vector $(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33})$ such that $x'_{ij} = x_{ij} + ka_{ij}$.*
- *We say that A is (n,m)-preserving if it satisfies the two following equations:*

$$\frac{3}{2}a_{12} + \frac{4}{3}a_{13} + a_{22} + \frac{5}{6}a_{23} + \frac{2}{3}a_{33} = 0; \qquad (13)$$

$$a_{12} + a_{13} + a_{22} + a_{23} + a_{33} = 0. \qquad (14)$$

The idea behind these definitions is that if $(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33})$ is the (A,k)-transform of $(x_{12}, x_{13}, x_{22}, x_{23}, x_{33})$ and if A is (n,m)-preserving, then

$$\frac{3}{2}x_{12}+\frac{4}{3}x_{13}+x_{22}+\frac{5}{6}x_{23}+\frac{2}{3}x_{33} = \frac{3}{2}x'_{12}+\frac{4}{3}x'_{13}+x'_{22}+\frac{5}{6}x'_{23}+\frac{2}{3}x'_{33} \quad \text{and}$$

$$x_{12} + x_{13} + x_{22} + x_{23} + x_{33} = x'_{12} + x'_{13} + x'_{22} + x'_{23} + x'_{33}.$$

Hence, the values of n and m derived from Equations (4) and (5) are the same, whether calculated using x_{ij} or x'_{ij} values.

Let G be a chemical graph of order n and size m that maximizes the value of a topological index f over all chemical graphs of same order and same size as G. We now study the impact on the x_{ij} values of G if some of the four following values are strictly positive:

$$V_1 = c_{13} - c_{22} + \min_{i=1,2,3}(c_{3i} - c_{2i}) + \min_{j=2,3}(c_{3j} - c_{2j}),$$
$$V_2 = c_{13} - c_{12} + \min_{i=2,3}(c_{2i} - c_{3i}),$$
$$V_3 = c_{22} - c_{13} + \min_{i=1,2,3}(c_{2i} - c_{3i}) + \min_{j=2,3}(c_{2j} - c_{3j}),$$
$$V_4 = 2c_{22} - c_{12} - c_{23} + 2\min_{i=1,2,3}(c_{2i} - c_{3i}).$$

Lemma 1. *Let f be a degree-based topological index such that $V_1 > 0$. A chemical graph G that maximizes f over all chemical graphs of the same order and size as G has no (2,2)-edge.*

Proof. Assume G contains an edge uv with both endpoints of degree 2.

- If u and v have no common neighbor, then let x be the second neighbor of u and let y be the second neighbor of v. At least one of x, y, say y, has degree at least two, else G has order 4. We can then obtain a chemical graph G' by replacing ux by vx. Let $i \in \{1, 2, 3\}$ be the degree of x and $j \in \{2, 3\}$ the degree of y. The graph G' contradicts the maximality of G since

$$f(G') = f(G) + c_{13} - c_{22} + (c_{3i} - c_{2i}) + (c_{3j} - c_{2j}) \geq f(G) + V_1 > f(G).$$

- If u and v have a common neighbor w, then w has degree 3, else G has order $n = 3$. Also, the third neighbor x of w has degree at least two, else G has order $n = 4$.
  - If x has degree 2, then let y be its second neighbor and let $i \in \{1, 2, 3\}$ be the degree of y. We can obtain a chemical graph G' by replacing uv by vx. Then G' contradicts the maximality of G since

$$\begin{aligned} f(G') &= f(G) + c_{13} - c_{22} + (c_{3i} - c_{2i}) + (c_{33} - c_{23}) \\ &\geq f(G) + V_1 > f(G). \end{aligned}$$

  - If x has degree 3, then let y and z be the two other neighbors of x. We can obtain a chemical graph G' by replacing xy and xz by uy and vz. Then G' contradicts the maximality of G since

$$f(G') = f(G) + c_{13} - c_{22} + 2(c_{33} - c_{23}) \geq f(G) + V_1 > f(G). \quad \blacksquare$$

Lemma 2. *Let f be a degree-based topological index such that $V_1 > 0$ and $V_2 > 0$. A chemical graph G that maximizes f over all chemical graphs of the same order and size as G has no (1,2)-edge and no (2,2)-edge.*

Proof. We already know from Lemma 1 that G has no (2,2)-edge. Let uv be an edge in G with u of degree 1 and v of degree 2. Let w be the second neighbor of v. Note that w has degree 3, else G has order $n = 3$. Let x and y be the two other neighbors of w. At least one of them, say x has degree $i \geq 2$, else G has order $n = 5$. We can obtain a chemical graph G' by replacing uv and wx by uw and vx. Then G' contradicts the maximality of G since

$$f(G') = f(G) + c_{13} - c_{12} + (c_{2i} - c_{3i}) \geq f(G) + V_2 > f(G). \qquad \blacksquare$$

Lemma 3. *Let f be a degree-based topological index such that $V_3 > 0$. A chemical graph G that maximizes f over all chemical graphs of the same order and size as G has no (1,3)-edge.*

Proof. Let uv be an edge with u of degree 1 and v of degree 3, and let x and y be the two other neighbors of v. At least one of x and y, say y has degree at least two, else G has order $n = 4$. We can then obtain a chemical graph G' by replacing vy by uy. Let i be the degree of x and j the degree of y. Then G' contradicts the maximality of G since

$$f(G') = f(G) + c_{22} - c_{13} + (c_{2i} - c_{3i}) + (c_{2j} - c_{3j}) \geq f(G) + V_3 > f(G). \qquad \blacksquare$$

Lemma 4. *Let f be a degree-based topological index such that $V_4 > 0$. If a chemical graph G maximizes f over all chemical graphs of the same order and size as G then either $m = n - 1$ and G is P_n or $m \geq n$ and G has no (1,2)-edge.*

Proof. Let uv be an edge with u of degree 1 and v of degree 2. If G is not P_n, then there is a vertex w of degree 3 in G such that v and w are linked by a chain in which all internal vertices have degree 2 in G. Let x and y be the two neighbors of w that are not on the chain. We can obtain a chemical graph G' by replacing wx by ux. Let i be the degree of x and j the degree of y. Then G' contradicts the maximality of G since

$$f(G') = f(G) + 2c_{22} - c_{12} - c_{23} + (c_{2i} - c_{3i}) + (c_{2j} - c_{3j}) \geq f(G) + V_4 > f(G). \qquad \blacksquare$$

5 Characterization of extremal graphs

We first characterize the extremal graphs of 29 of the 33 degree-based topological indices of Table 1. The proofs involve the following values:

$$\begin{aligned} V_5 &= c_{13} - 4c_{23} + 3c_{33}, \\ V_6 &= c_{22} - 2c_{23} + c_{33}, \\ V_7 &= c_{12} - c_{13} - c_{23} + c_{33}, \\ V_8 &= -2c_{12} + 3c_{13} - 2c_{23} + c_{33}. \end{aligned}$$

5.1 Five graph families for 29 topological indices

We first show that the chemical graphs in F_1 maximize all degree-based topological indices such that V_1, V_2 and V_5 are strictly positive.

Theorem 5. *Let f be a degree-based topological index such that $V_1 > 0$, $V_2 > 0$ and $V_5 > 0$. A chemical graph G maximizes f over all chemical graphs of the same order and size as G if and only if $G \in F_1$.*

Proof. Let G be a chemical graph of order n, size m and with x_{ij} (i,j)-edges. Assume that it maximizes f over all chemical graphs of order n and size m. As shown in Lemma 2, $V_1 > 0$ and $V_2 > 0$ imply $x_{12} = x_{22} = 0$. Hence, $2n_2 = x_{23}$, which means that x_{23} is even.

If $x_{23} \leq 2$ then $n_2 = n \bmod 2$ (since the number $n_1 + n_3$ of odd degree vertices is even), which implies $x_{23} = 2(n \bmod 2)$. Equations (4) and (5) then give $x_{13} = \frac{3n-2m-(n \mod 2)}{2}$ and $x_{33} = \frac{4m-3n-3(n \mod 2)}{2}$, which means that G belongs to F_1.

If $x_{23} \geq 4$, then consider the vector $A = (0, 1, 0, -4, 3)$ associated with V_5 and let $(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33})$ be the $(A, \lfloor \frac{x_{23}}{4} \rfloor)$-transform of $(x_{12}, x_{13}, x_{22}, x_{23}, x_{33})$. We then have $x'_{12} = x'_{22} = 0$ and $x'_{23} \leq 2$. Since A is (n,m)-preserving, we conclude as above that $x'_{13} = \frac{3n-2m-(n \mod 2)}{2}$ and $x'_{33} = \frac{4m-3n-3(n \mod 2)}{2}$. Let G' be a graph in F_1 having exactly x'_{ij} (i,j)-edges. The maximality of G is contradicted by G' since

$$f(G') = f(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33}) = f(G) + V_5 \lfloor \tfrac{x_{23}}{4} \rfloor > f(G). \qquad \blacksquare$$

Theorem 6. *Let f be a degree-based topological index such that $V_3 > 0$, $V_4 > 0$ and $V_6 > 0$. A chemical graph G maximizes f over all chemical graphs of the same order and size as G if and only if $G \in F_2$.*

Proof. Let G be a chemical graph of order n, size m and with x_{ij} (i,j)-edges. Assume that it maximizes f over all chemical graphs of order n and size m. As shown by Lemmas 3 and 4, $V_3 > 0$ and $V_4 > 0$ imply $G = \mathsf{P}_n$ or $n_1 = 0$. Hence, if $m = n-1$, then $G = \mathsf{P}_n$ (since trees have vertices of degree 1), which means that $x_{12} = 2$, $x_{22} = m-2$ and $G \in F_2$. So assume $n \leq m < \frac{3n-3}{2}$, which implies that $n_1 = 0$ and x_{23} is even.

- If $m = n$, Equations (4) and (5) give $x_{23} = x_{33} = 0$, which implies $x_{22} = m$ and $G \in F_2$.
- If $m = n+1$, Equations (4) and (5) give $x_{23} + 2x_{33} = 6$, which implies $n_3 = 2$ and $x_{33} \leq 1$. Hence, there are only two possibilities:
  - $x_{22} = m-6$, $x_{23} = 6$,$x_{33} = 0$, or
  - $x_{22} = m-5$, $x_{23} = 4$,$x_{33} = 1$.

  Since $c_{22}-2c_{23}+c_{33}=V_6 > 0$, the second solution has a larger value, which implies $G \in F_2$.
- If $n+1 < m < \frac{3n-3}{2}$ and $x_{23} = 2$, then Equations (4) and (5) give $x_{22} = 3n-2m-1$ and $x_{33} = 3m-3n-1$, which implies $G \in F_2$. So assume $x_{23} \geq 4$, consider the vector $A = (0,0,1,-2,1)$ associated with V_6 and let $(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33})$ be the $(A, \frac{x_{23}-2}{2})$-transform of $(x_{12}, x_{13}, x_{22}, x_{23}, x_{33})$. Hence, $x'_{12} = x'_{13} = 0$ and $x'_{23} = 2$. Since A is (n,m)-preserving, we conclude as above that $x'_{22} = 3n-2m-1$ and $x'_{33} = 3m-3n-1$. Consider any chemical graph G' in F_2 having exactly x'_{ij} (i,j)-edges. The maximality of G is contradicted by G' since

$$f(G') = f(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33}) = f(G) + V_6(\tfrac{x_{23}-2}{2}) > f(G). \qquad \blacksquare$$

Corollary 7. *$F_1 \cup F_2$ is the set of extremal chemical graphs for the 13 degree-based topological indices ABSC, AG, AG-GA, Extended, GA, GouravaSC, Harmonic, Randić, Sombor, rSombor, SumConn, rSumConn and lnZagreb1.*

Proof. It is easy to check that

- V_1, V_2 and V_5 are strictly positive for ABSC, AG, AG-GA, Extended, rSumConn, Sombor, rSombor, lnZagreb1, $\overline{\text{GA}}$, $\overline{\text{GouravaSC}}$, $\overline{\text{Harmonic}}$, $\overline{\text{Randić}}$ and $\overline{\text{SumConn}}$, which implies that F_1 is the set of chemical graphs which maximize ABSC, AG, AG-GA, Extended, rSumConn, Sombor, rSombor, lnZagreb1 and minimize GA, GouravaSC, Harmonic, Randić and SumConn.
- V_3, V_4 and V_6 are strictly positive for $\overline{\text{ABSC}}$, $\overline{\text{AG}}$, $\overline{\text{AG-GA}}$, $\overline{\text{Extended}}$, $\overline{\text{Sombor}}$, $\overline{\text{rSombor}}$, $\overline{\text{rSumConn}}$, $\overline{\text{lnZagreb1}}$, GA, GouravaSC, Harmonic,Randić and SumConn, which implies that F_2 is the set of chemical graphs which minimize ABSC, AG, AG-GA, Extended, Sombor, rSombor, rSumConn, lnZagreb1 and maximize GA, GouravaSC, Harmonic, Randić and SumConn. ■

We now characterize the degree-based topological indices f for which the chemical graphs in F_3 and F_4 maximize f.

Theorem 8. *Let f be a degree-based topological index such that $V_1{>}0$, $V_6{>}0$, $V_7{>}0$ and $V_8{>}0$. A chemical graph G maximizes f over all graphs of the same order and size as G if and only if $G \in F_3$.*

Proof. Let G be a chemical graph of order n, size m and with x_{ij} (i, j)-edges. Assume that it maximizes f over all chemical graphs of order n and size m. As shown by Lemma 1, $V_1 > 0$ implies $x_{22} = 0$. Let W_{33} be the set of vertices of degree 2 in G with two neighbors of degree 3, and let W_{13} be the set of vertices of degree 2 in G with one neighbor of degree 1 and the other of degree 3. Since $n > 3$, we have $n_2 = |W_{33}| + |W_{13}|$.

- If $n_2 = 0$, then $x_{12} = x_{22} = x_{23} = 0$ and Equations (4) and (5) give $x_{13} = \frac{3n-2m}{2}$ and $x_{33} = \frac{4m-3n}{2}$, which implies that G belongs to F_3.
- If $n_2 = 1$, then let v be the vertex of degree 2 in G.
  - if $v \in W_{13}$ then $x_{12} = x_{23} = 1, x_{22} = 0$ and Equations (4) and (5) give $x_{13} = \frac{3n-2m-3}{2}$ and $x_{33} = \frac{4m-3n-1}{2}$;
  - if $v \in W_{33}$ then $x_{12} = x_{22} = 0, x_{23} = 2$ and Equations (4) and (5) give $x_{13} = \frac{3n-2m-1}{2}$ and $x_{33} = \frac{4m-3n-3}{2}$.

  Since $c_{12} - c_{13} - c_{23} + c_{33} = V_7 > 0$, the first case has a larger value $f(G)$, which implies that G belongs to F_3.

- If $n_2 > 1$, then the two neighbors of each vertex in W_{33} are adjacent. Indeed, if a vertex $v \in W_{33}$ has two non-adjacent neighbors u_1 and u_2, then consider any other vertex w of degree 2 and let u_3 be one of its neighbors: by replacing vu_1, vu_2, wu_3 by vw, vu_3 and u_1u_2, we get a chemical graph G' which contradicts the maximality of G since

$$f(G') = f(G) + c_{22} - 2c_{23} + c_{33} = f(G) + V_6 > f(G).$$

  Let us now show that $|W_{33}| \le 1$. Assume by contradiction that W_{33} contains at least two vertices v_1 and v_2. Since $n > 4$, there are two non-adjacent vertices u_1 and u_2 such that u_1 is adjacent to v_1 but not to v_2, while u_2 is adjacent to v_2 but not to v_1. Let w_1 be the second neighbor of v_1, and let G' be the chemical graph obtained from G by replacing v_1w_1 and v_2u_2 by v_1u_2 and v_2w_1. Then G' has $n_2 > 1$ vertices of degree 2 and one of them, namely v_1, has two non-adjacent neighbors u_1, u_2 of degree 3. We have shown above that this implies that G' does not maximize f while $f(G') = f(G)$, a contradiction.

  Hence, $|W_{33}| \le 1$, which implies $|W_{13}| \ge 1$. So let v be a vertex in W_{13}, let u be another vertex of degree 2, let w be the neighbor of v of degree 1, and let G' be the chemical graph obtained from G by replacing vw by uw:
  - if $u \in W_{13}$ then $f(G') = f(G) - 2c_{12} + 3c_{13} - 2c_{23} + c_{33} = f(G) + V_8 > f(G)$;
  - if $u \in W_{33}$ then $f(G') = f(G) - c_{12} + 2c_{13} - 3c_{23} + 2c_{33} = f(G) + V_7 + V_8 > f(G)$.

  In both cases, G' contradicts the maximality of G. ■

Theorem 9. *Let f be a degree-based topological index such that $V_3>0$, $V_4>0$ and $V_6<0$. A chemical graph G maximizes f over all graphs of the same order and size as G if and only if $G \in F_4$.*

Proof. Let G be a chemical graph of order n, size m and with x_{ij} (i, j)-edges. Assume that it maximizes f over all chemical graphs of order n and size m. As shown by Lemmas 3 and 4, $V_3 > 0$ and $V_4 > 0$ imply $G = \mathsf{P}_n$ or $n_1 = 0$. Hence, if $m = n - 1$, then $G = \mathsf{P}_n$, which means that $x_{12} = 2$,

$x_{22} = m - 2$ and $G \in F_4$. So assume $m > n - 1$, which implies $n_1 = 0$. Equations (4) and (5) give $x_{23} = 6n - 4m - 2x_{22}$ and $x_{33} = 5m - 6n + x_{22}$. Hence, $x_{22} \geq \max\{0, 6n - 5m\}$.

- If $x_{22} = 0$, then $x_{23} = 6n - 4m$, $x_{33} = 5m - 6n$ and $G \in F_4$.
- If $x_{22} = 6n - 5m > 0$, then $x_{23} = 6m - 6n$, $x_{33} = 0$ and $G \in F_4$.
- If $x_{22} > 0$ and $x_{22} \neq 6n - 5m$, then $x_{33} > 0$. Consider the vector $A = (0, 0, -1, 2, -1)$ associated with $-V_6$ and let $(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33})$ be the $(A, \min\{x_{22}, x_{22} - 6n + 5m\})$-transform of $(x_{12}, x_{13}, x_{22}, x_{23}, x_{33})$. Hence, $x'_{22} = \max\{0, 6n - 5m\}$ and $x'_{12} = x'_{13} = 0$. Since A is (n, m)-preserving we conclude as above that there is a chemical graph G' in F_4 having exactly x'_{ij} (i, j)-edges. Then G' contradicts the maximality of G since

$$f(G') = f(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33})$$
$$= f(G) - V_6 \min\{x_{22}, x_{22} - 6n + 5m\} > f(G). \qquad \blacksquare$$

Corollary 10. $F_3 \cup F_4$ *is the set of extremal chemical graphs for the 10 degree-based topological indices Gourava1, Gourava2, hGourava1, hGourava2, GouravaPC, InvSumDeg, rRandić, Zagreb2, hZagreb1, hZagreb2.*

Proof. It is easy to check that

- $V_1 > 0$, $V_6 > 0$, $V_7 > 0$ and $V_8 > 0$ for Gourava1, Gourava2, hGourava1, hGourava2, GouravaPC, InvSumDeg, rRandić, Zagreb2, hZagreb1, hZagreb2, which implies that F_3 is the set of chemical graphs which maximize these topological indices.
- $V_3 > 0, V_4 > 0$ and $V_6 < 0$ for $\overline{\text{Gourava1}}$, $\overline{\text{Gourava2}}$, $\overline{\text{hGourava1}}$, $\overline{\text{hGourava2}}$, $\overline{\text{GouravaPC}}$, $\overline{\text{InvSumDeg}}$, $\overline{\text{rRandić}}$, $\overline{\text{Zagreb2}}$, $\overline{\text{hZagreb1}}$, $\overline{\text{hZagreb2}}$, which implies that F_4 is the set of chemical graphs which minimize the 10 topological indices. $\blacksquare$

Note that $F_1 \cup F_3$ is the set of chemical graphs with x_{ij} (i, j)-edges such that

x_{12}	x_{13}	x_{22}	x_{23}	x_{33}	
0	$\frac{3n-2m}{2}$	0	0	$\frac{4m-3n}{2}$	if n if even
1	$\frac{3n-2m-3}{2}$	0	1	$\frac{4m-3n-1}{2}$	if n is odd
0	$\frac{3n-2m-1}{2}$	0	2	$\frac{4m-3n-3}{2}$	

Theorem 11. *Let f be a degree-based topological index such that $V_1{>}0$, $V_5{>}0$ and $V_7{=}0$. A chemical graph G maximizes f over all graphs of the same order and size as G if and only if $G \in F_1 \cup F_3$.*

Proof. Let G be a chemical graph of order n, size m and with x_{ij} (i,j)-edges. Assume that it maximizes f over all chemical graphs of order n and size m. Note that the two possibilities for the x_{ij} values when n is odd give the same value $f(G)$ since $c_{12} - c_{13} - c_{23} + c_{33} = V_7 = 0$. As shown by Lemma 1, $V_1 > 0$ implies $x_{22} = 0$. Moreover, $n > 3$ implies $x_{12} \leq x_{23}$, and x_{12} and x_{23} have the same parity.

1. If $x_{12} = 0$ then, as shown in Theorem 5, $G \in F_1$, else there is a graph $G' \in F_1$ so that $f(G') > f(G)$.
2. If $x_{12} = 1$ then
   - if $x_{23} = 1$ then Equations (4) and (5) give $x_{13} = \frac{3n-2m-3}{2}$ and $x_{33} = \frac{4m-3n-1}{2}$, which implies that G belongs to F_3.
   - if $x_{23} \geq 3$, then consider the vector $A = (-1, 2, 0, -3, 2)$ associated with $V_5{-}V_7$ and let $(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33})$ be the $(A, 1)$-transform of $(x_{12}, x_{13}, x_{22}, x_{23}, x_{33})$. Note that $x'_{12} = x'_{22} = 0$ and A is (n,m)-preserving. Hence, we have shown in case 1. that there is a graph $G' \in F_1$ which contradicts the maximality of G since

$$
\begin{aligned}
f(G') &\geq f(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33}) \\
&= f(G) + V_5 - V_7 = f(G) + V_5 > f(G).
\end{aligned}
$$

3. If $x_{12} \geq 2$ then $x_{23} \geq x_{12} \geq 2$. Consider the vector $A = (-2, 3, 0, -2, 1)$ associated with $V_5 - 2V_7$ and let $(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33})$ be the $(A, \lfloor \frac{x_{12}}{2} \rfloor)$-transform of $(x_{12}, x_{13}, x_{22}, x_{23}, x_{33})$. Since $x'_{12} = x'_{22} = 0$ and A is (n,m)-preserving, we have shown in case 1. that there is a graph

$G' \in F_1$ which contradicts the maximality of G since

$$f(G') \geq f(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33}) = f(G) + \lfloor \frac{x_{12}}{2} \rfloor (V_5 - 2V_7)$$
$$= f(G) + \lfloor \frac{x_{12}}{2} \rfloor V_5 > f(G).$$ ■

Theorem 12. *Let f be a degree-based topological index such that $V_3>0$, $V_4>0$ and $V_6=0$. A chemical graph G maximizes f over all graphs of the same order and size as G if and only if $G \in F_5$.*

Proof. Let G be a chemical graph of order n, size m and with x_{ij} (i,j)-edges. Assume that it maximizes f over all chemical graphs of order n and size m. Note first that the two possibilities for the x_{ij} values when $m = n+1$ have the same value $f(G)$ since $c_{22} - 2c_{23} + c_{33} = V_6 = 0$. For the same reason, all solutions for $n+1 < m \leq \frac{3n-3}{2}$ have the same value.

As shown by Lemmas 3 and 4, $V_3 > 0$ and $V_4 > 0$ imply $G = \mathsf{P}_n$ or $n_1 = 0$. Hence, if $m = n-1$, then $G = \mathsf{P}_n$, which means that $x_{12} = 2$, $x_{22} = m-2$ and $G \in F_5$. So assume $n \leq m < \frac{3n-3}{2}$, which implies that $n_1 = 0$ and x_{23} is even.

- If $m = n$, Equations (4) and (5) give $x_{23} = x_{33} = 0$ and $x_{22} = m$, which implies $G \in F_5$.
- If $m = n+1$, Equations (4) and (5) give $x_{23} + 2x_{33} = 6$, which implies $n_3 = 2$ and $x_{33} \leq 1$. Hence, there are only two possibilities:
  - $x_{22} = m-6$, $x_{23} = 6$,$x_{33} = 0$, or
  - $x_{22} = m-5$, $x_{23} = 4$,$x_{33} = 1$,

  and both imply $G \in F_5$.
- If $n+1<m\leq\frac{3n-3}{2}$, then $x_{23} \geq 2$ and Equations (4) and (5) give $x_{22} = a$, $x_{23} = 6n-4m-2a$ and $x_{33} = 5m-6n+a$. Since $x_{33} \geq 0$ and $x_{23} \geq 2$, we have $\max\{0, 6n-5m\} \leq a \leq 3n-2m-1$, which implies $G \in F_5$. ■

Corollary 13. *$F_1 \cup F_3 \cup F_5$ is the set of extremal chemical graphs for the topological indices Forgotten, InvDeg, Zagreb1, lnZagreb2, lnZagreb3 and mZagreb.*

Proof. It is easy to check that

- $V_1{>}0$, $V_5{>}0$ and $V_7{=}0$ for Forgotten, InvDeg, Zagreb1, $\overline{\text{lnZagreb2}}$, lnZagreb3 and mZagreb which implies that $F_1 \cup F_3$ is the set of chemical graphs which maximize Forgotten, InvDeg, Zagreb1 and mZagreb and minimize lnZagreb2.
- $V_3{>}0, V_4{>}0$ and $V_6{=}0$ for $\overline{\text{Forgotten}}$, $\overline{\text{InvDeg}}$, $\overline{\text{Zagreb1}}$, lnZagreb2, $\overline{\text{lnZagreb3}}$ and $\overline{\text{mZagreb}}$, which implies that F_5 is the set of chemical graphs which minimize Forgotten, InvDeg, Zagreb1, mZagreb and maximize lnZagreb2. ■

5.2 Additional families of extremal chemical graphs

As proved in the previous section, the five families $F_1, \ldots, F_5$ are sufficient to characterize all extremal graphs of 29 topological indices. However, some degree-based topological indices have extremal chemical graphs that do not belong to any of the five families. We give here four examples. More precisely, we characterize the extremal chemical graphs of the topological indices ABC, Albertson, Sigma, and aZagreb. For this purpose, we define new families $F_6, \ldots, F_{11}$ of chemical graphs characterized by x_{ij} values. Here again, as explained in Section 3, it is easy to check that given x_{ij} values of one of the graph families, there is at least one chemical graph with x_{ij} (i,j)-edges. Examples of chemical graphs belonging to at least one of the families $F_6, \ldots, F_{11}$, but to none of the families $F_1, \ldots, F_5$ are given in figure 2.

Definition 11. *F_6 is the set of chemical graphs with the following numbers x_{ij} of (i,j)-edges:*

x_{12}	x_{13}	x_{22}	x_{23}	x_{33}
0	a	0	$6n-4m-4a$	$5m-6n+3a$

where a is any integer such that $\max\{0, \lceil\frac{6n-5m}{3}\rceil\} \leq a \leq \lfloor\frac{3n-2m}{2}\rfloor$.

Theorem 14. *Let f be a degree-based topological index such that $V_1{>}0$, $V_2{>}0$ and $V_5{=}0$. A chemical graph G maximizes f over all graphs of the same order and size as G if and only if $G \in F_6$.*

Proof. Let G be a chemical graph of order n, size m and with x_{ij} (i,j)-edges. Assume that it maximizes f over all chemical graphs of order n

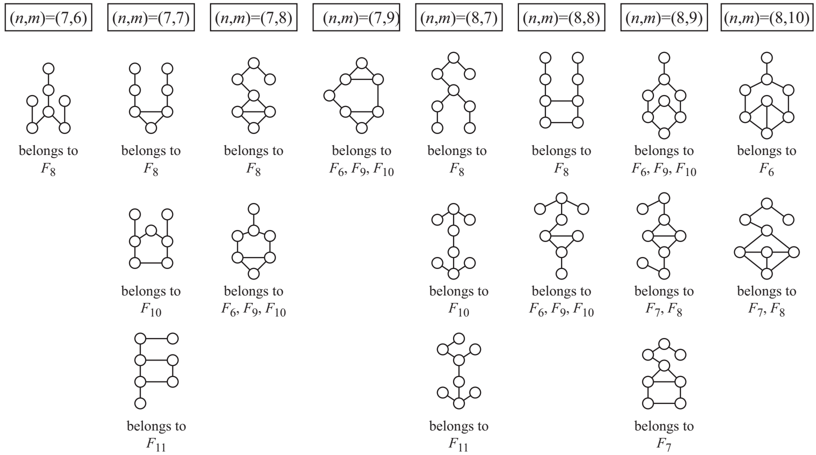

Figure 2. Examples of chemical graphs or order $n \in \{7, 8\}$ and size $m \leq n+2$ belonging to at least one of the families $F_6, \ldots, F_{11}$ but to none of the families $F_1, \ldots, F_5$.

and size m. As shown in Lemma 2, $V_1 > 0$ and $V_2 > 0$ imply $x_{12} = x_{22} = 0$. Hence, it follows from Equations (4) and (5) that $x_{13} = a$, $x_{23} = 6n - 4m - 4a$ and $x_{33} = 5m - 6n + 3a$. Since $x_{23} \geq 0$ and $x_{33} \geq 0$, we have $\max\{0, \lceil \frac{6n-5m}{3} \rceil\} \leq a \leq \lfloor \frac{3n-2m}{2} \rfloor$. All possible solutions with the various values of a have the same value since $c_{13} - 4c_{23} + 3c_{33} = V_5 = 0$. ■

Definition 12. *F_7 is the set of chemical graphs with the following numbers x_{ij} of (i,j)-edges:*

	x_{12}	x_{13}	x_{22}	x_{23}	x_{33}	
	2	0	$m-2$	0	0	*if* $m = n-1$
	0	0	m	0	0	*if* $m = n$
	0	0	$m-5$	4	1	
	1	0	$m-7$	3	3	*if* $m = n+1$
$(n \geq 8)$	2	0	$m-9$	2	5	
	0	0	$3n-2m-1$	2	$3m-3n-1$	*if* $n+1 < m \leq \frac{3n-3}{2}$
	1	0	$3n-2m-3$	1	$3m-3n+1$	

Theorem 15. *Let f be a degree-based topological index such that $V_3 > 0$, $V_6 > 0$ and $V_5 + V_7 = 2V_6$. A chemical graph G maximizes f over all graphs of the same order and size as G if and only if $G \in F_7$.*

Proof. Let G be a chemical graph of order n, size m and with x_{ij} (i,j)-edges. Assume that it maximizes f over all chemical graphs of order n and size m. Note that the three possible cases for $m = n+1$ have the same value since $c_{12} - 2c_{22} - c_{23} + 2c_{33} = V_5 + V_7 - 2V_6 = 0$. For the same reason, the two possibilities for $n+1 < m < \frac{3n-3}{3}$ have the same value.

As shown by Lemma 3, $V_3 > 0$ implies $x_{13} = 0$. In what follows, for two integer a and b such that $(a,b) \neq (x_{12}, x_{23})$, we say that G is (a,b)-dominated if $a \leq x_{12}$, $b - a \leq x_{23} - x_{12}$, and there is a chemical graph of order n and size m which has a $(1,2)$-edges, b $(2,3)$-edges, and no $(1,3)$-edge. In such a case consider the (n,m)-preserving vector $A = (0,0,1,-2,1)$ associated with V_6 and let $(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33})$ be the $(A, \frac{x_{23}-x_{12}+a-b}{2})$-transform of $(x_{12}, x_{13}, x_{22}, x_{23}, x_{33})$. We thus have $x_{12} = x'_{12}$ and $x'_{23} = x_{12} + b - a$. Let $A' = (-1,0,3,-1,-1)$ be the (n,m)-preserving vector associated with $3V_6 - V_5 - V_7$ and let $(x''_{12}, x''_{13}, x''_{22}, x''_{23}, x''_{33})$ be the $(A', x_{12} - a)$-transform of $(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33})$. We now have $x''_{12} = a$ and $x''_{23} = b$. Let G' be a graph with x''_{ij} (i,j)-edges. Note that if $x_{12} = a$, then $x_{23} - x_{12} + a - b > 0$. Hence, G' contradicts the maximality of G since $3V_6 - V_5 - V_7 = V_6 > 0$ and

$$\begin{aligned} f(G') &= f(x''_{12}, x''_{13}, x''_{22}, x''_{23}, x''_{33}) = f(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33}) + (x_{12} - a)V_6 \\ &= f(G) + (\frac{x_{23} - x_{12} + a - b}{2})V_6 + (x_{12} - a)V_6 > f(G). \end{aligned}$$

Let us now analyze the possible values for m and use Equations (4) and (5) to derive x_{ij} values.

- If $m = n-1$, then assume $x_{23} > 0$. It follows that $3 \leq x_{12} \leq x_{23}$. Hence, $x_{12} = x_{23} = 3$, else G is $(3,3)$-dominated. We therefore have $x_{22} = m - 6$ and $x_{33} = 0$ and $f(\mathsf{P}_n) - f(G) = -c_{12} + 4c_{22} - 3c_{23} = 4V_6 - V_5 - V_7 = 2V_6 > 0$, which contradicts the maximality of G. Hence $x_{23} = 0$ which implies $G = \mathsf{P}_n \in F_7$.
- if $m = n$, then $x_{12} = x_{23} = 0$, else G is $(0,0)$-dominated. We therefore have $x_{22} = m$ and $x_{33} = 0$ which implies $G = \mathsf{C}_n \in F_7$.
- If $m = n+1$, then
  - if $x_{12} = 0$, then $x_{23} \geq 4$. Hence, $x_{23} = 4$ else G is $(0,4)$-dominated. We therefore have $x_{22} = m - 5$ and $x_{33} = 1$, mean-

ing that $G \in F_7$.

– if $x_{12} = 1$, then $x_{23} \geq 3$. Hence, $x_{23} = 3$ else G is $(1,3)$-dominated. We therefore have $x_{22} = m - 7$ and $x_{33} = 3$, meaning that $G \in F_7$.

– if $x_{12} = 2$, then $x_{23} \geq 2$. Hence, $x_{23} = 2$ else G is $(2,2)$-dominated. We therefore have $x_{22} = m - 9$ and $x_{33} = 5$, meaning that $G \in F_7$.

– if $x_{12} > 2$, then $x_{23} > 2$, which means that G is $(2,2)$-dominated, which contradicts the maximality of G.

- If $n + 1 < m \leq \frac{3n-3}{2}$ then
  – if $x_{12} = 0$, then $x_{23} \geq 2$. Hence, $x_{23} = 2$, else G is $(0,2)$-dominated. We therefore have $x_{22} = 3n - 2m - 1$ and $x_{33} = 3m - 3n - 1$, meaning that $G \in F_7$.
  – if $x_{12} = 1$, then $x_{23} \geq 1$. Hence, $x_{23} = 1$, else G is $(1,1)$-dominated. We therefore have $x_{22} = 3n - 2m - 3$ and $x_{33} = 3m - 3n + 1$, meaning that $G \in F_7$.
  – if $x_{12} \geq 2$, then $x_{23} \geq 2$. Hence, G is $(1,1)$-dominated, which contradicts the maximality of G. ■

Corollary 16. *$F_6 \cup F_7$ is the set of extremal chemical graphs for the topological index Sigma.*

Proof. It is easy to check that $V_1 > 0$, $V_2 > 0$ and $V_5 = 0$ for Sigma, while $V_3 > 0$, $V_6 > 0$ and $V_5 + V_7 = 2V_6$ for $\overline{\text{Sigma}}$, which means that F_6 is the set of chemical graphs which maximize Sigma, while F_7 is the set of chemical graphs which minimize Sigma. ■

Definition 13. *F_8 is the set of chemical graphs with the following numbers x_{ij} of (i,j)-edges:*

x_{12}	x_{13}	x_{22}	x_{23}	x_{33}	
2	0	$m-2$	0	0	*if $m+1=n \in \{7,8,9\}$*
3	0	$m-6$	3	0	
2	0	$m-7$	4	1	*if $m=n \in \{7,8\}$*
1	0	1	3	3	*if $n=7$ and $m=8$*
$\lfloor \frac{3n-2m}{3} \rfloor$	0	$m \bmod 3$	$\lfloor \frac{3n-2m}{3} \rfloor$	$\lfloor \frac{7m-6n}{3} \rfloor$	*otherwise*

Theorem 17. *Let f be a degree-based topological index such that $V_3{>}0$, $V_6{>}0$ and $V_5{+}V_7{=}4V_6$. A chemical graph G maximizes f over all graphs of the same order and size as G if and only if $G \in F_8$.*

Proof. Let G be a chemical graph of order n, size m and with x_{ij} (i,j)-edges. Assume that it maximizes f over all chemical graphs of order n and size m. As shown by Lemma 3, $V_3 > 0$ implies $x_{13} = 0$.

If $m + 1 = n \in \{7, 8, 9\}$, then there are only two possibilities: either $x_{12} = 2$ and $x_{22} = m - 2$, or $x_{12} = 3$, $x_{23} = 3$ and $x_{22} = m - 6$. Since $c_{12} - 4c_{22} + 3c_{23} = V_5 + V_7 - 4V_6 = 0$, we deduce that both cases correspond to an optimal graph G that belongs to F_8. We now assume $m \geq n$ or $m + 1 = n \geq 10$.

If $n_3 = 0$, then $G = \mathsf{P}_n$ and $m + 1 = n \geq 10$ or $G = \mathsf{C}_n$ and $n = m$.

- If $m + 1 = n \geq 10$, then the graph G' with $x_{12} = x_{23} = 4, x_{33} = 1$ and $x_{22} = m - 9$ has value $f(G') = f(G) + 2c_{12} - 7c_{22} + 4c_{23} + c_{33} = f(G) + 2V_5 + 2V_7 - 7V_6 = f(G) + V_6 > 0$, which contradicts the maximality of G.
- If $n = m$, then the graph G' with $x_{12} = 2, x_{23} = 4$, $x_{33} = 1$ and $x_{22} = m - 7$ has value $f(G') = f(G) + 2c_{12} - 7c_{22} + 4c_{23} + c_{33} = f(G) + 2V_5 + 2V_7 - 7V_6 = f(G) + V_6 > 0$, which contradicts the maximality of G.

If $n_3 > 0$, then consider the following 4 cases:

- If $m = n = 7$, then there are only two possibilities: either $x_{12} = 2$, $x_{23} = 4$ and $x_{33} = 1$, or $x_{12} = 1$, $x_{23} = 3$ and $x_{22} = 3$. Since $c_{12} + c_{23} + c_{33} - 3c_{22} = V_5 + V_7 - 3V_6 = V_6 > 0$, we deduce that the first solution is the best, which means that $G \in F_8$.
- If $m = n = 8$, then there are only three possibilities: either $x_{12} = 2$, $x_{22} = 1$, $x_{23} = 4$ and $x_{33} = 1$, or $x_{12} = 1$, $x_{23} = 3$ and $x_{22} = 4$, or $x_{12} = 2$ and $x_{23} = 6$. As in the previous case, the first solution is better than the second. Also, since $c_{22} - 2c_{23} + c_{33} = V_6 > 0$, we deduce that the first solution is better than the third one, which implies $G \in F_8$.
- If $n = 7$ and $m = 8$, there are four possibilities:
  - $x_{22} = 2$ and $x_{23} = 6$;
  - $x_{22} = 3$, $x_{23} = 4$ and $x_{33} = 1$;

- $x_{12} = 1$, $x_{23} = 5$ and $x_{33} = 2$;
- $x_{12} = x_{22} = 1$, $x_{23} = x_{33} = 3$.

The fourth is better than the first since $c_{12} - c_{22} - 3c_{23} + 3c_{33} = V_5 + V_7 - V_6 = 3V_6 > 0$. It is better than the second since $c_{12} - 2c_{22} - c_{23} + 2c_{33} = V_5 + V_7 - 2V_6 = 2V_6 > 0$. It is better than the third since $c_{22} - 2c_{23} + c_{33} = V_6 > 0$. Hence, $G \in F_8$.

- For the remaining case where $n \in \{7, 8, 9\}$ and $m \geq 9$, or $n \geq 10$, consider the two (n, m)-preserving vectors $A = (0, 0, 1, -2, 1)$ and $A' = (1, 0, -3, 1, 1)$ associated with V_6 and $V_5 + V_7 - 3V_6$, respectively. Let $(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33})$ be the $(A, \frac{x_{23}-x_{12}}{2})$-transform of $(x_{12}, x_{13}, x_{22}, x_{23}, x_{33})$. Note that $x'_{12} = x'_{23}$ and $x'_{13} = 0$. Let $(x''_{12}, x''_{13}, x''_{22}, x''_{23}, x''_{33})$ be the $(A', \lfloor\frac{x'_{22}}{3}\rfloor)$-transform of $(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33})$. Note that $x''_{13} = 0$, $x''_{12} = x''_{23}$ and $x''_{22} \leq 2$. Equations (4) and (5) then give $x''_{22} = m \bmod 3$, $x''_{12} = x''_{23} = \lfloor\frac{3n-2m}{3}\rfloor$, and $x''_{33} = \lfloor\frac{7m-6n}{3}\rfloor$. Consider any graph G' in F_8 with x''_{ij} (i, j)-edges. We then have

$$\begin{aligned} f(G') &= f(G) + \frac{x_{23} - x_{12}}{2}V_6 + \lfloor\frac{x'_{22}}{3}\rfloor(V_5 + V_7 - 3V_6) \\ &= f(G) + (\frac{x_{23} - x_{12}}{2} + \lfloor\frac{x'_{22}}{3}\rfloor)V_6. \end{aligned}$$

If $x_{23} - x_{12} > 0$, or $x_{23} - x_{12} = 0$ and $x_{22} = x'_{22} > 2$,then $f(G') > f(G)$, which contradicts the maximality of G. Hence, we can choose G' equal to G, which implies $G \in F_8$. ■

Definition 14. *F_9 is the set of chemical graphs with the following numbers x_{ij} of (i, j)-edges:*

x_{12}	x_{13}	x_{22}	x_{23}	x_{33}	
0	$\frac{6n-5m+(2m \bmod 3)}{3}$	0	$\frac{8m-6n-4(2m \bmod 3)}{3}$	$2m \bmod 3$	*if* $n - 1 \leq m \leq \frac{6n+2}{5}$
0	0	0	$6n - 4m$	$5m - 6n$	*if* $\frac{6n+3}{5} \leq m \leq \frac{3n-3}{2}$

Theorem 18. *Let f be a degree-based topological index such that $V_1 > 0$, $V_2 > 0$ and $V_5 < 0$. A chemical graph G maximizes f over all graphs of the same order and size as G if and only if $G \in F_9$.*

Proof. Let G be a chemical graph of order n, size m and with x_{ij} (i,j)-edges. Assume that it maximizes f over all chemical graphs of order n and size m. As shown by Lemma 2, $V_1 > 0$ and $V_2 > 0$ imply $x_{12} = x_{22} = 0$.

- If $x_{33} \leq 2$, Equations (4) and (5) give $x_{33} = (2m \bmod 3)$, $x_{13} = \frac{6n-5m+(2m \bmod 3)}{3}$ and $x_{23} = \frac{8m-6n-4(2m \bmod 3)}{3}$. Since $x_{13} \geq 0$, we have $6n - 5m \geq -2$, which implies $G \in F_9$.
- If $x_{33} \geq 3$ then
  - if $x_{13} = 0$, Equations (4) and (5) give $x_{23} = 6n - 4m$ and $x_{33} = 5m - 6n$. Since $x_{33} \geq 3$, we have $m \geq \frac{6n+3}{5}$, which implies $G \in F_9$.
  - if $x_{13}>0$, consider the (n,m)-preserving vector $A=(0,1,0,-4,3)$ associated with V_5, let $a = \min\{x_{13}, \lfloor\frac{x_{33}}{3}\rfloor\}$, and let $(x'_{12}, x'_{13}, x'_{22}, x'_{23}, x'_{33})$ be the $(A,-a)$-transform of $(x_{12}, x_{13}, x_{22}, x_{23}, x_{33})$. Then either $x'_{33} \leq 2$, or $x'_{33} \geq 3$ and $x_{13} = 0$. In both cases, we have seen that there is a graph $G' \in F_9$ with x'_{ij} (i,j)-edges. We therefore have $f(G') = f(G) - aV_5 > f(G)$, which contradicts the maximality of G. ■

Corollary 19. *$F_8 \cup F_9$ is the set of extremal chemical graphs for the topological index ABC.*

Proof. It is easy to check that $V_3 > 0$, $V_6 > 0$ and $V_5 + V_7 = 4V_6$ for $\overline{\text{ABC}}$, while $V_1 > 0$, $V_2 > 0$ and $V_5 < 0$ for ABC, which means that F_8 is the set of chemical graphs which minimize ABC, while F_9 is the set of chemical graphs which maximize ABC. ■

Theorem 20. *A chemical graph G maximizes the f=aZagreb topological index over all graphs of the same order and size as G if and only if $G \in F_8$, except in two cases where the x_{ij} values of G are as follows: if n=7 and m=8 then x_{12}=x_{13}=x_{23}=1, $x_{22} = 0$ and x_{33}=5; if n=8 and m=8 then x_{12}=x_{23}=2, x_{13}=1, $x_{22} = 0$ and x_{33}=3.*

Proof. The aZagreb topological index is defined by $c_{ij}=(\frac{ij}{i+j-2})^3$ (see Table 1). Let G be a chemical graph of order n, size m and with x_{ij} (i,j)-edges. Assume that it maximizes f over all chemical graphs of order n and size m.

Consider the three (n,m)-preserving vectors A_1, A_2, A_3 associated with the three following strictly positive values W_1, W_2, W_3:

- $A_1{=}(1,-1,0,-1,1)$ is associated with $W_1{=}c_{12}{-}c_{13}{-}c_{23}{+}c_{33}{\approx}8.01$;
- $A_2{=}(1,-1,-1,1,0)$ is associated with $W_2{=}c_{12}{-}c_{13}{-}c_{22}{+}c_{23}{\approx}4.62$;
- $A_3{=}(2,-3,0,2,-1)$ is associated with $W_3{=}2c_{12}{-}3c_{13}{+}2c_{23} - c_{33}{\approx}10.48$.

Let

- $(x^1_{12},x^1_{13},x^1_{22},x^1_{23},x^1_{33})$ be the $(A_1, \max\left\{0, \min\{x_{13}, \frac{x_{23}-x_{12}}{2}\}\right\})$-transform of $(x_{12},\, x_{13},\, x_{22},\, x_{23},\, x_{33})$;
- $(x^2_{12}, x^2_{13}, x^2_{22}, x^2_{23}, x^2_{33})$ be the $(A_2, \min\{x^1_{13}, x^1_{22}\})$-transform of $(x^1_{12},\, x^1_{13},\, x^1_{22},\, x^1_{23},\, x^1_{33})$;
- $(x^3_{12}, x^3_{13}, x^3_{22}, x^3_{23}, x^3_{33})$ be the $(A_3, \lfloor\frac{x^2_{13}}{3}\rfloor)$-transform of $(x^2_{12},\, x^2_{13},\, x^2_{22},\, x^2_{23},\, x^2_{33})$.

Note that if $x^2_{13} > 0$, then $x^2_{22} = 0$ and $x^2_{12} = x^2_{23}$, which implies $x^2_{33} > 0$, else G has order $n \leq 6$. We then have $x^3_{13} \leq 2$ and if $x^3_{13} = 0$, then $x^3_{12} = x^3_{23}$ and $x^3_{22} = 0$. There are therefore only 3 possible cases for which we can derive the x^3_{ij} values using Equations (4) and (5):

(1) if $x^3_{13} = 0$, then $G \in F_8$. Indeed the proof of Theorem 17 uses the fact that $V_3 > 0$ only to show that $x_{13} = 0$, and it is easy to check that $V_6 > 0$ and $V_5 + V_7 = 4V_6$ for the aZagreb topological index. Therefore,
   - if $x_{13} = 0$, then all x_{ij} values are equal to the x^3_{ij} values and as in Theorem 17, we conclude that $G \in F_8$;
   - if $x_{13} > 0$, then as in Theorem 17, we know that there exists a graph $G' \in F_8$ of order n and size m which contradicts the maximality of G since

$$\begin{aligned}
f(G') \geq& f(x^3_{12}, x^3_{13}, x^3_{22}, x^3_{23}, x^3_{33})\\
&= f(G) + \max\left\{0, \min\{x_{13}, \frac{x_{23}-x_{12}}{2}\}\right\} W_1\\
&\quad + \min\{x^1_{13}, x^1_{22}\} W_2 + \lfloor\frac{x^2_{13}}{3}\rfloor W_3\\
&> f(G).
\end{aligned}$$

(2) if $x^3_{13} = 1$, $x^3_{12} = x^3_{23}$ and x^3_{22}=0, then Equations (4) and (5) give $x^3_{12} = x^3_{23} = \frac{3n-2m-2}{3}$ and $x^3_{33} = \frac{7m-6n+1}{3}$, which implies $m \bmod 3 = 2$.

(3) if $x^3_{13} = 2$, $x^3_{12} = x^3_{23}$ and x^3_{22}=0, then Equations (4) and (5) give $x^3_{12} = x^3_{23} = \frac{3n-2m-4}{3}$ and $x^3_{33} = \frac{7m-6n+2}{3}$, which implies $m \bmod 3 = 1$.

Let us analyze the situation according to the value of $m \bmod 3$:

- if $m \bmod 3 = 0$ then $G \in F_8$ (since we are in Case (1));
- if $m \bmod 3 = 1$, then
  - if $m \geq 10$ or $m+1 = n = 8$, then Case (1) is better than Case (3) since $c_{12} - 2c_{13} + c_{22} + c_{23} - c_{33} \approx 5.85 > 0$. Hence, $G \in F_8$.
  - if $m = n = 7$, then Case (1) is better than Case (3) since $c_{12} - 2c_{13} + 3c_{23} - 2c_{33} \approx 2.46 > 0$. Hence $G \in F_8$.
- if $m \bmod 3 = 2$,
  - if $m \geq 11$ or $m+1 = n = 9$ then Case (1) is better than Case (2) since $-c_{13} + 2c_{22} - c_{33} \approx 1.23 > 0$. Hence $G \in F_8$.
  - if $m = 8$ and $n \in \{7, 8\}$ then Case (2) is better than Case (1) since $c_{13} - c_{22} - 2c_{23} + 2c_{33} \approx 2.15 > 0$. Moreover, the x_{ij} values of G are equal to the x^3_{ij} values else the graph G' with x^3_{ij} (i,j)-edges is such that $f(G') > f(G)$. Hence, $x_{12} = x_{13} = x_{23} = 1$ and $x_{33} = 5$ if $n = 7$ and $x_{12} = x_{23} = 2$, $x_{13} = 1$ and $x_{33} = 3$ if $n = 8$. ■

Definition 15. *F_{10} is the set of chemical graphs with the following numbers x_{ij} of (i,j)-edges:*

x_{12}	x_{13}	x_{22}	x_{23}	x_{33}	
0	$\frac{6n-5m}{3}$	0	$\frac{8m-6n}{3}$	0	*if* $n-1 \leq m \leq \frac{6n-2}{5}$ *and* m *mod* 3=0
0	$\frac{6n-5m-1}{3}$	1	$\frac{8m-6n-2}{3}$	0	*if* $n-1 \leq m \leq \frac{6n-2}{5}$ *and* m *mod* 3=1
0	$\frac{6n-5m+1}{3}$	0	$\frac{8m-6n-4}{3}$	1	*if* $n-1 \leq m \leq \frac{6n-2}{5}$ *and* m *mod* 3=2
0	0	1	$m-1$	0	*if* $m = \frac{6n-1}{5}$
0	0	0	$6n-4m$	$5m-6n$	*if* $\frac{6n}{5} \leq m \leq \frac{3n-3}{2}$

Theorem 21. *A chemical graph G minimizes the f=aZagreb topological index over all graphs of the same order and size as G if and only if $G \in F_{10}$.*

Proof. As in the previous theorem, we have $c_{ij}=(\frac{ij}{i+j-2})^3$. Let G be a chemical graph of order n, size m and with x_{ij} (i,j)-edges. Assume that it minimizes f over all chemical graphs of order n and size m. Note that $G \neq \mathsf{P}_n$ since for $n = m-1$, the chemical graph G' with $x'_{12} = 1$, $x'_{13} = 2$, $x'_{23} = 1$ and $x'_{22} = m-4$ would have value $f(G') = f(G) - c_{12} + 2c_{13} - 2c_{22} + c_{23} \approx f(G) - 9.25$. Hence, $x_{12} \leq x_{23}$.

Consider the five (n,m)-preserving vectors A_1, A_2, A_3, A_4, A_5 associated with the five following strictly negative values W_1, W_2, W_3, W_4, W_5:

- $A_1{=}(-1,1,1,-1,0)$ is associated with $W_1{=}-c_{12}{+}c_{13}{+}c_{22}{-}c_{23}{\approx}-4.62$;
- $A_2{=}(0,1,-2,0,1)$ is associated with $W_2 = c_{13} - 2c_{22} + c_{33} \approx -1.23$;
- $A_3{=}(0,-1,0,4,-3)$ is associated with $W_3{=}-c_{13}{+}4c_{23}{-}3c_{33}{\approx}-5.54$;
- $A_4{=}(0,0,-1,2,-1)$ is associated with $W_4{=}-c_{22}{+}2c_{23}{-}c_{33}{\approx}-3.39$;
- $A_5{=}(0,-1,1,2,-2)$ is associated with $W_5{=}-c_{13}{+}c_{22}{+}2c_{23}{-}2c_{33}{\approx}-2.15$.

Let

- $(x^1_{12}, x^1_{13}, x^1_{22}, x^1_{23}, x^1_{33})$ be the (A_1, x_{12})-transform of $(x_{12}, x_{13}, x_{22}, x_{23}, x_{33})$;
- $(x^2_{12}, x^2_{13}, x^2_{22}, x^2_{23}, x^2_{33})$ be the $(A_2, \lfloor\frac{x^1_{22}}{2}\rfloor)$-transform of $(x^1_{12}, x^1_{13}, x^1_{22}, x^1_{23}, x^1_{33})$;
- $(x^3_{12}, x^3_{13}, x^3_{22}, x^3_{23}, x^3_{33})$ be the $(A_3, \min\{\lfloor\frac{x^2_{33}}{3}\rfloor, x^2_{13}\})$-transform of $(x^2_{12}, x^2_{13}, x^2_{22}, x^2_{23}, x^2_{33})$;
- $(x^4_{12}, x^4_{13}, x^4_{22}, x^4_{23}, x^4_{33})$ be the $(A_4, \min\{x^3_{22}, x^3_{33}\})$-transform of $(x^3_{12}, x^3_{13}, x^3_{22}, x^3_{23}, x^3_{33})$;
- $(x^5_{12}, x^5_{13}, x^5_{22}, x^5_{23}, x^5_{33})$ be the $(A_5, \min\{x^4_{13}, \lfloor\frac{x^4_{33}}{2}\rfloor\})$-transform of $(x^4_{12}, x^4_{13}, x^4_{22}, x^4_{23}, x^4_{33})$.

We then have $x^5_{12} = 0, x^5_{22} \leq 1$, $x^5_{13} = 0$ or $x^5_{33} \leq 1$, and $x^4_{22} + x^4_{33} \leq 1$. There are therefore only 5 possible cases for which we can derive the x^5_{ij} values using Equations (4) and (5):

- if $x^5_{22} = x^5_{33} = 0$ and $x^5_{13} \geq 1$, then $x^5_{13} = \frac{6n-5m}{3}$ and $x^5_{23} = \frac{8m-6n}{3}$, which implies $6n - 5m \geq 3$ and $m \bmod 3 = 0$;
- if $x^5_{22} = 1, x^5_{33} = 0$ and $x^5_{13} \geq 1$, then $x^5_{13} = \frac{6n-5m-1}{3}$ and $x^5_{23} = \frac{8m-6n-2}{3}$, which implies $6n - 5m \geq 4$ and $m \bmod 3 = 1$;

- if $x^5_{22} = 0, x^5_{33} = 1$ and $x^5_{13} \geq 1$, then $x^5_{13} = \frac{6n-5m+1}{3}$ and $x^5_{23} = \frac{8m-6n-4}{3}$, which implies $6n - 5m \geq 2$ and $m \bmod 3 = 2$;
- if $x^5_{22} = x^5_{13} = 0$ and $x^5_{33} \geq 0$, then $x^5_{33} = 5m-6n$ and $x^5_{23} = 6n-4m$, which implies $6n - 5m \leq 0$;
- if $x^5_{22} = 1$ and $x^5_{13} = x^5_{33} = 0$, then $x^5_{33} = 5m - 6n + 1$ and $x^5_{23} = 6n - 4m - 2$, which implies $6n - 5m = 1$.

Hence all possible x^5_{ij} values correspond to those in F_{10}. So, let G' be a graph with x^5_{ij} (i, j)-edges. We have

$$\begin{aligned} f(G') =& f(G) + x_{12}W_1 + \lfloor \frac{x^1_{22}}{2} \rfloor W_2 + \min\{\lfloor \frac{x^2_{33}}{3} \rfloor, x^2_{13}\}W_3 \\ &+ \min\{x^3_{22}, x^3_{33}\}W_4 + \min\{x^4_{13}, \lfloor \frac{x^4_{33}}{2} \rfloor\}W_5. \end{aligned}$$

If G does not belong to F_{10} then at least one of the five values x_{12}, $\lfloor \frac{x^1_{22}}{2} \rfloor$, $\min\{\lfloor \frac{x^2_{33}}{3} \rfloor, x^2_{13}\}$, $\min\{x^3_{22}, x^3_{33}\}$ and $\min\{x^4_{13}, \lfloor \frac{x^4_{33}}{2} \rfloor\}$ is strictly positive, which implies $f(G') < f(G)$, a contradiction. ∎

Definition 16. *Family F_{11} is obtained from F_{10} by adding the following possible values:*

x_{12}	x_{13}	x_{22}	x_{23}	x_{33}	
1	$\frac{6n-5m-4}{3}$	0	$\frac{8m-6n+1}{3}$	0	*if* $n-1 \leq m \leq \frac{6n-2}{5}$ *and* m *mod* $3 = 1$
0	$\frac{6n-5m+2}{3}$	0	$\frac{8m-6n-8}{3}$	2	
0	1	0	$m-3$	2	*if* $m = \frac{6n-1}{5}$

Theorem 22. *A chemical graph G maximizes the f=Albertson topological index over all graphs of the same order and size as G if and only if $G \in F_{11}$.*

Proof. The Albertson topological index is defined by $c_{ij} = |i-j|$ (see Table 1). Let G be a chemical graph of order n, size m and with x_{ij} (i, j)-edges. Assume that it maximizes f over all chemical graphs of order n and size m. Note that the two possible cases for $m = \frac{6n-1}{5}$ have the same value since $c_{13} - c_{22} - 2c_{23} + 2c_{33} = 0$. Also, the case in F_{10} for $m \leq \frac{6n-2}{5}$ and $m \bmod 3 = 1$ has the same value as the two new possibilities in F_{11} since $c_{12} - c_{13} - c_{22} + c_{23} = c_{13} - c_{22} - 2c_{23} + 2c_{33} = 0$. Moreover, $G \neq \mathsf{P}_n$ since for $n = m-1$, the chemical graph G' with $x'_{12} = 1$, $x'_{13} = 2$, $x'_{23} = 1$ and $x'_{22} = m-4$ would have value $f(G') = f(G) - c_{12} + 2c_{13} - 2c_{22} + c_{23} = f(G) + 4$. Hence, $x_{12} \leq x_{23}$.

Consider the five following (n,m)-preserving vectors A_1, A_2, A_3, A_4, A_5, A_6:

- $A_1 = (-2,3,0,-2,1)$ is associated with $-2c_{12} + 3c_{13} - 2c_{23} + c_{33} = 2$;
- $A_2{=}(-1,2,-1,-1,1)$ is associated with $-c_{12}{+}2c_{13}{-}c_{22}{-}c_{23}{+}c_{33}{=}2$;
- $A_3 = (0,1,-2,0,1)$ is associated with $c_{13} - 2c_{22} + c_{33} = 2$;
- $A_4 = (0,0,-1,2,-1)$ is associated with $-c_{22} + 2c_{23} - c_{33} = 2$;
- $A_5 = (-1,1,0,1,-1)$ is associated with $-c_{12} + c_{13} + c_{23} - c_{33} = 2$;
- $A_6 = (0,-1,0,4,-3)$ is associated with $-c_{13} + 4c_{23} - 3c_{33} = 2$.

Let

- $(x^1_{12}, x^1_{13}, x^1_{22}, x^1_{23}, x^1_{33})$ be the $(A_1, \lfloor \frac{x_{12}}{2} \rfloor)$-transform of $(x_{12}, x_{13}, x_{22}, x_{23}, x_{33})$;
- $(x^2_{12}, x^2_{13}, x^2_{22}, x^2_{23}, x^2_{33})$ be the $(A_2, \min\{x^1_{12}, x^1_{22}\})$-transform of $(x^1_{12}, x^1_{13}, x^1_{22}, x^1_{23}, x^1_{33})$;
- $(x^3_{12}, x^3_{13}, x^3_{22}, x^3_{23}, x^3_{33})$ be the $(A_3, \lfloor \frac{x^2_{22}}{2} \rfloor)$-transform of $(x^2_{12}, x^2_{13}, x^2_{22}, x^2_{23}, x^2_{33})$;
- $(x^4_{12}, x^4_{13}, x^4_{22}, x^4_{23}, x^4_{33})$ be the $(A_4, \min\{x^3_{22}, x^3_{33}\})$-transform of $(x^3_{12}, x^3_{13}, x^3_{22}, x^3_{23}, x^3_{33})$;
- $(x^5_{12}, x^5_{13}, x^5_{22}, x^5_{23}, x^5_{33})$ be the $(A_5, \min\{x^4_{12}, x^4_{33}\})$-transform of $(x^4_{12}, x^4_{13}, x^4_{22}, x^4_{23}, x^4_{33})$;
- $(x^6_{12}, x^6_{13}, x^6_{22}, x^6_{23}, x^6_{33})$ be the $(A_6, \min\{x^5_{13}, \lfloor \frac{x^5_{33}}{3} \rfloor\})$-transform of $(x^5_{12}, x^5_{13}, x^5_{22}, x^5_{23}, x^5_{33})$.

We then have $x^6_{12} + x^6_{22} \leq 1$, $\min\{x^6_{12}, x^6_{33}\}{=}0$, $\min\{x^6_{22}, x^6_{33}\}{=}0$, and $x^6_{13} = 0$ or $x^6_{33} \leq 2$. Hence, there are 6 possible cases for which we can derive the x^6_{ij} values using Equations (4) and (5):

- if $x^6_{12} = 0$, $x^6_{22} = 1$ and $x^6_{33} = 0$, then $x^6_{13} = \frac{6n-5m-1}{3}$ and $x^6_{23} = \frac{8m-6n-2}{3}$, which implies $6n - 5m \geq 1$ and $m \bmod 3 = 1$;
- if $x^6_{12} = 1, x^6_{22} = 0$ and $x^6_{33} = 0$, then $x^6_{13} = \frac{6n-5m-4}{3}$ and $x^6_{23} = \frac{8m-6n+1}{3}$, which implies $6n - 5m \geq 4$ and $m \bmod 3 = 1$;
- if $x^6_{12} = x^6_{22} = x^6_{13} = 0$ then $x^6_{23} = 6n - 4m$ and $x^6_{33} = 5m - 6n$, which implies $6n - 5m \leq 0$;

- if $x_{12}^6 = x_{22}^6 = x_{33}^6 = 0$ and $x_{13}^6 \geq 1$, then $x_{13}^6 = \frac{6n-5m}{3}$ and $x_{23}^6 = \frac{8m-6n}{3}$, which implies $6n-5m \geq 3$ and $m \bmod 3 = 0$;
- if $x_{12}^6 = x_{22}^6 = 0$, $x_{33}^6 = 1$ and $x_{13}^6 \geq 1$, then $x_{13}^6 = \frac{6n-5m+1}{3}$ and $x_{23}^6 = \frac{8m-6n-4}{3}$, which implies $6n-5m \geq 2$ and $m \bmod 3 = 2$;
- if $x_{12}^6 = x_{22}^6 = 0$, $x_{33}^6 = 2$ and $x_{13}^6 \geq 1$, then $x_{13}^6 = \frac{6n-5m+2}{3}$ and $x_{23}^6 = \frac{8m-6n-8}{3}$, which implies $6n-5m \geq 1$ and $m \bmod 3 = 1$.

Hence all possible x_{ij}^6 values correspond to those in F_{11}. So, let G' be a graph with x_{ij}^6 (i,j)-edges. We have

$$\begin{aligned} f(G') =& f(G) + 2\left(\lfloor \frac{x_{12}}{2} \rfloor + \min\{x_{12}^1, x_{22}^1\}\right) \\ &+ 2\left(\lfloor \frac{x_{22}^2}{2} \rfloor + \min\{x_{22}^3, x_{33}^3\} + \min\{x_{12}^4, x_{33}^4\} + \min\{x_{13}^5, \lfloor \frac{x_{33}^5}{3} \rfloor\}\right) \end{aligned}$$

If G does not belong to F_{11} then at least one of the six values $\lfloor \frac{x_{12}}{2} \rfloor$, $\min\{x_{12}^1, x_{22}^1\}$, $\lfloor \frac{x_{22}^2}{2} \rfloor$, $\min\{x_{22}^3, x_{33}^3\}$, $\min\{x_{12}^4, x_{33}^4\}$, $\min\{x_{13}^5, \lfloor \frac{x_{33}^5}{3} \rfloor\}$ is strictly positive, which implies $f(G') > f(G)$, a contradiction. ■

Definition 17. *F_{12} is the set of chemical graphs with the following numbers x_{ij} of (i,j)-edges:*

	x_{12}	x_{13}	x_{22}	x_{23}	x_{33}	
	2	0	$m-2$	0	0	*if* $m = n-1$
	0	0	m	0	0	*if* $m = n$
$(n \geq 8)$	2	0	$m-9$	2	5	
	1	1	$m-8$	1	5	
	1	0	$m-7$	3	3	*if* $m = n+1$
	0	1	$m-6$	2	3	
	0	0	$m-5$	4	1	
	0	0	$3n-2m-1$	2	$3m-3n-1$	*if* $n+1 < m \leq \frac{3n-3}{2}$
	1	0	$3n-2m-3$	1	$3m-3n+1$	

Theorem 23. *A chemical graph G minimizes the f=Albertson topological index over all graphs of the same order and size as G if and only if $G \in F_{12}$.*

Proof. As in the previous theorem, we have $c_{ij} = |i-j|$. Let G be a chemical graph of order n, size m and with x_{ij} (i,j)-edges. Assume that it minimizes f over all chemical graphs of order n and size m. If $m = n-1$, then $G = \mathsf{P}_n$ since $f(\mathsf{P}_n) = 2$ while $f(G) \geq 6$ if $n_3 > 0$. Also, if $m = n$, then $G = \mathsf{C}_n$ since $f(\mathsf{C}_n) = 0$ while $f(G) > 0$ if $n_1 + n_3 > 0$ and $m < \frac{3n}{2}$. Hence, in these cases, we have $G \in F_{12}$.

Assume now $m \geq n+1$. We thus have $x_{12} \leq x_{23}$ and $f(G)$ is an even number at least equal to 2 (since $m < \frac{3n}{2}$). To reach value 2, there are only three possibilities:

- if $x_{13} = 1$ and $x_{12} = x_{23} = 0$, then $x_{22} = 0$ and Equations (4) and (5) give $x_{22} = 3n - 2m - 2$ and $x_{33} = 3m - 3n + 1$ which implies $m = \frac{3n-2}{2}$, a contradiction.
- if $x_{12} = x_{23} = 1$ and $x_{13} = 0$, then Equations (4) and (5) give $x_{22} = 3n - 2m - 3$ and $x_{33} = 3m - 3n + 1$, which implies $m > n+1$ (else $x_{33} = 4$ and $n_3 = 3$ imply $x_{33} = 4 > 3 = \frac{n_3((n_3-1)}{2}))$ and $G \in F_{12}$.
- if $x_{12} = 0$, $x_{23} = 2$ and $x_{13} = 0$, then Equations (4) and (5) give $x_{22} = 3n - 2m - 1$ and $x_{33} = 3m - 3n - 1$, which implies $m > n+1$ (else $x_{33} = 1$ and $n_3 = 1$ imply $x_{33} = 1 > 0 = \frac{n_3((n_3-1)}{2}))$ and $G \in F_{12}$.

Hence, if $m > n+1$ then $G \in F_{12}$. The remaining case is $m = n+1$ for which $f(G) \geq 4$. There are only six possibilities to reach the minimum value 4:

- if $x_{12} = x_{23} = 2$ and $x_{13} = 0$, then $x_{22} = m - 9$ and $x_{33} = 5$.
- if $x_{12} = x_{23} = 1$ and $x_{13} = 1$, then $x_{22} = m - 8$ and $x_{33} = 5$.
- if $x_{12} = 1$, $x_{23} = 3$ and $x_{13} = 0$, then $x_{22} = m - 7$ and $x_{33} = 3$.
- if $x_{12} = 0$, $x_{23} = 2$ and $x_{13} = 1$, then $x_{22} = m - 6$ and $x_{33} = 3$.
- if $x_{12} = 0$, $x_{23} = 4$ and $x_{13} = 0$, then $x_{22} = m - 5$ and $x_{33} = 1$.
- if $x_{12} = x_{23} = 0$ and $x_{13} = 2$, then $x_{22} = 0$ and $x_{33} = m - 2$, which implies $n = 6$.

Since G is of order $n \geq 7$, we have $G \in F_{12}$. ■

6 Conclusion

Many topological indices have been proposed to study the chemical properties of molecules, and many papers focus on extremal graphs for these indices, each paper dealing with a particular index. We have shown that many of these topological indices have the same extremal properties in the sense that the chemical graphs that maximize or minimize the values of these indices are often the same. Thus, for example, for 29 of these indices, one might expect 58 classes of extremal chemical graphs, while 5 families are sufficient to describe them all. Also, for another example, chemical graphs of even order n for which $x_{13} = \frac{3n-2m}{2}$, $x_{33} = \frac{4m-3n}{2}$ and $x_{12} = x_{22} = x_{23} = 0$ are extremal for 29 topological indices (since these graphs belong to $F_1 \cap F_3$).

Most of the characterizations we have given for extremal graphs are based on a set of 8 values $V_1, \ldots, V_8$. If new topological indices are proposed, it is therefore easy to check whether they have the same extremal properties of the indices studied in this paper. Note that some degree-based topological indices that we have not analyzed in this paper do not have any of the stated properties that allow us to characterize their extremal chemical graphs. For example, the reduced reciprocal Randić index (rrRandić) mentioned in [27] and defined by $c_{ij} = \sqrt{(i-1)(j-1)}$ is such that V_1, V_2, V_3 and V_4 are strictly negative. An analysis similar to those performed in Section 5 easily shows that the set of extremal chemical graphs of order $n \geq 10$ for the aZagreb index is strictly contained in that for rrRandić.

As Ivan Gutman pointed out [24], “today we have far too many topological indices, and there seems to lack a firm criterion to stop or slow down their proliferation”. We believe we have provided a tool to quickly test whether a new topological index has the same extremal properties as many existing indices.

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