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Chemical Applications on General Zagreb Indices of Composite Graphs

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ABSTRACT

A topological index is a quantity computed from the molecular graph, that finds application in chemistry, material science, computer science, and biological application-driven fields. Recently, the general Zagreb indices were studied, and methods for their calculation for composite graphs were established. In the present paper, we provide examples for chemical applications of these methods, computing the first and second general Zagreb indices of several composite molecular species, in particular of biphenyl, naphthalene, biphenylene, and bicoronylene.

In this paper, we compute the Nirmala index and its corresponding exponential of chloroquine, hydroxychloroquine and remdesivir. Also we determine the inverse Nirmal indices of chloroquine, hydroxychloroquine and remdesivir.

KEYWORDS: Topological index, General Zagreb indices, Composite graphs, Molecular graphs.

I. INTRODUCTIN

In this paper, we are concerned with the general first and second Zagreb indices, defined as

$$M_1^\alpha = M_1^\alpha(G) = \sum_{uv\in E(G)} [\delta(u)^\alpha + \delta(v)^\alpha]$$

and

$$M_2^\alpha = M_2^\alpha(G) = \sum_{uv\in E(G)} [\delta(u)\,\delta(v)]^\alpha$$

where α is some real-valued number. Special cases of M_1^α are several earlier investigated topological indices: the first Zagreb index ($\alpha = 1$, [8, 12]), forgotten index ($\alpha = 2$, [6]), and Y-index ($\alpha = 3$, [2]). Special cases of M_2^α are the second Zagreb index ($\alpha = 1$, [11]), second hyper-Zagreb index ($\alpha = 2$, [1]), Randić connectivity index ($\alpha = -1/2$, [15]), and the reciprocal Randić index ($\alpha = 1/2$, [9]).

In a recent paper [4], a method was elaborated for computing the general Zagreb indices of composite graphs. Here we apply this method to obtain results of chemical interest. Needless to say that by choosing a pertinent value of α, each expression for M_1^α or M_2^α of molecular graphs can be straightforwardly transformed into an expression for the above mentioned topological indices.

Throughout this paper, we consider a simple finite connected graph. The vertex and the edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The degree of the vertex u is the number of edges joined with this vertex denoted by $\delta(u)$. Graph theory is applied in various fields, such as computer science, biology, chemistry, and social sciences. In chemical graph theory, the atoms of molecules are represented by vertices, whereas chemical bonds by edges. Graph theory provides suitable tools for predicting properties of chemical species, such as melting, flash, boiling points, density, and thermodynamic properties [3, 10, 17].
In order to present the applicative potential of our theory [4], in what follows we outline the computation of the two general Zagreb indices of four chemical compounds: hexagonal cactus biphenyl [13], naphthalene [14], biphenylene [16], and dicoronylene [5].

Let G be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d(u)$ of a vertex u is the number of vertices adjacent to u. We refer [1], for other undefined notations and terminologies.

II. GENERAL ZAGREB INDICES OF Biphenyl

Biphenyl $(C_6H_5)_2$ is an aromatic compound consisting of two benzene rings connected by a single covalent bond.

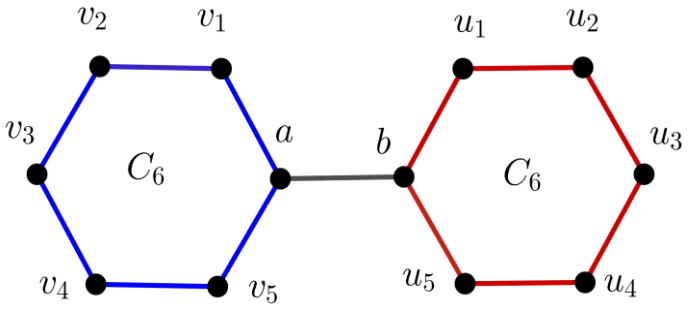

Figure 1. The molecular graph of biphenyl. By different colors is indicated how

Its composition from simpler structural features is done.

Theorem 1. The general Zagreb indices of biphenyl are

(1) $M_1^\alpha(G) = 10 \cdot 2^{\alpha+1} + 2 \cdot 3^{\alpha+1}$,

(2) $M_2^\alpha(G) = 8 \cdot 4^\alpha + 4 \cdot 6^\alpha + 9^\alpha$.

Proof: From a graph-theoretical point of view, the molecular graph of biphenyl can be constructed by connecting two hexagons by means of a single edge (see Fig. 1). Bearing this in mind, we apply Propositions 3.1 and 3.2, and Corollary 3.1 of Ref. [4], noting that $d_G(a,b) = 1$. This results in

(1) $M_1^\alpha(G) = (n+m+1)2^{\alpha+1} + 3^{\alpha+1}$,

(2) $M_2^\alpha(G) = (n+m-4)4^\alpha + 4 \cdot 6^\alpha + 9^\alpha$.

Setting $n = m = 6$, yields the formulas in Theorem 1.

Table 1 gives the general Zagreb indices of biphenyl for $\alpha = 1,2,\ldots,9$.

Table 1. The general Zagreb indices of biphenyl.

α	M_1^α	M_2^α
1	58	65
2	134	353
3	322	2105
4	806	13793
5	2098	98345
6	5654	750833
7	15682	6033785
8	44486	50289473
9	128338	429828425

III. GENERAL ZAGREB INDICES OF NAPHTHALENE

Naphthalene, $C_{10}H_8$, is the simplest polycyclic aromatic hydrocarbon.

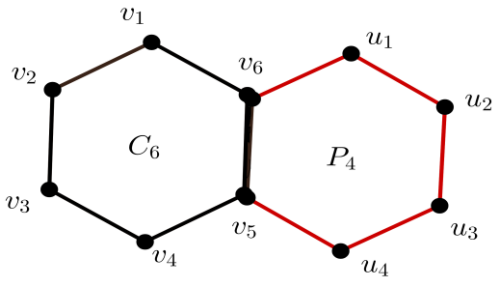

Figure 2. The molecular graph of naphthalene; for meaning of colors cf. Fig. 1.

Theorem 2. The general Zagreb indices of naphthalene are

(1) $M_1^\alpha(G) = 8 \cdot 2^{\alpha+1} + 2 \cdot 3^{\alpha+1}$,

(2) $M_2^\alpha(G) = 6 \cdot 4^\alpha + 4 \cdot 6^\alpha + 9^\alpha$.

Proof: The molecular graph of naphthalene can be constructed by attaching the endpoints of a 4-vertex path to adjacent vertices of a hexagon, see Fig. 2. Bearing this in mind, we can apply Propositions 2.2 and 4.1, and Corollary 4.1 of Ref. [4], recalling that $d_G(u_1,u_6) = d_G(u_4,u_5) = 1$. By this, we obtain

(1) $M_1^\alpha(G) = (n+m-4)2^{\alpha+1} + 2 \cdot 3^{\alpha+1}$,

(2) $M_2^\alpha(G) = (n+m-6)4^\alpha + 4 \cdot 6^\alpha + 9^\alpha$.

Setting $n = m = 6$, yields the formulas in Theorem 2.

Table 2 gives the general Zagreb indices of naphthalene $\alpha = 1,2,\ldots,9$.

Table 2. The general Zagreb indices of naphthalene.

α	M_1^α	M_2^α
1	50	57
2	118	321
3	290	1977
4	742	13281
5	1970	96297
6	5398	742641
7	15170	6001017
8	43462	50158401
9	126290	429304137

IV. GENERAL ZAGREB INDICES OF BIPHENYLENE

Biphenylene, $C_{12}H_8$, is the smallest aromatic compound that in addition to 6-membered rings, possesses an (antiaromatic) 4-membered ring.

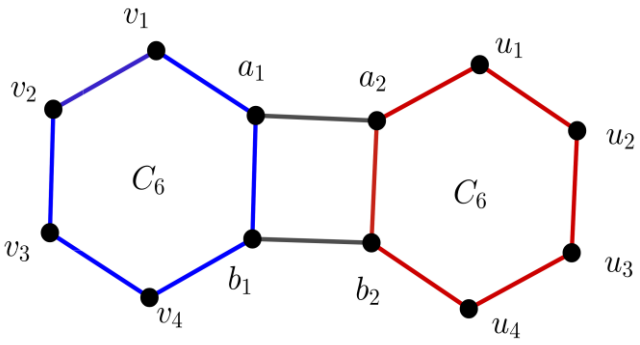

Figure 3. The molecular graph of biphenylene; for meaning of colors cf. Fig. 1.

Theorem 3. The general Zagreb indices of biphenylene are

(1) $M_1^{\alpha}(G) = (8)2^{\alpha+1} + 4 \cdot 3^{\alpha+1}$,

(2) $M_2^{\alpha}(G) = (6)4^{\alpha} + 4 \cdot 6^{\alpha} + 4 \cdot 9^{\alpha}$.

Proof: From a graph-theoretical point of view, the molecular graph of biphenylene is constructed by joining adjacent vertices of two hexagons by means of two edges (see Fig. 3). This makes it possible to apply Proposition 5.1 and 5.2, and Corollary 5.1 of Ref. [4], for $r = s = 6, n = 2$, and $d_G(a_1, b_1) = d_G(a_2, b_2) = 1$. We then get

(1) $M_1^{\alpha}(G) = (r + s + n - 3n)2^{\alpha+1} + 2n3^{\alpha+1}$,

(2) $\mathrm{M}_2^{\alpha}(\mathrm{G}) = (\mathrm{r+s-2n-2})4^{\alpha} + 4.6^{\alpha} + (3n-2)9^{\alpha}$.

In our case, $r = s = 6$ and $n = 2$ (see Fig. 3), by which we obtain the formulas in Theorem 3.

Table 3 gives the general Zagreb indices of biphenylene for $\alpha = 1,2, \ldots, 9$.

Table 3. The general Zagreb indices of biphenylene.

α	M_1^{α}	M_2^{α}
1	68	84
2	172	564
3	452	4164
4	1228	32964
5	3428	273444
6	9772	2336964
7	28292	20349924
8	82828	179298564
9	244388	1591565604

V. GENERAL ZAGREB INDICES OF DICORONYLENE

We conclude this study with the following result, that represents a more complex variant of the previous theorem. Dicoronylene, $C_{48}H_{20}$, is one of the largest known polycyclic aromatic hydrocarbons [7, 18].

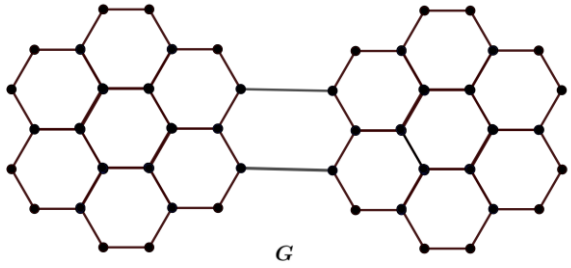

Figure 4. The molecular graph of dicoronylene.

Theorem 4. The general Zagreb indices of dicoronylene are

(1) $M_1^{\alpha}(G) = 28 \cdot 3^{\alpha+1} + 20 \cdot 2^{\alpha+1}$,

(2) $M_2^{\alpha}(G) = 8 \cdot 4^{\alpha} + 24 \cdot 6^{\alpha} + 30 \cdot 9^{\alpha}$.

Proof: Similar as in the case of biphenylene, the molecular graph of dicoronylene is constructed by joining a pair of vertices of two coronene units by means of two edges (see Fig. 4). These two edges connect pairs of degree-two vertices of the coronene units that are at smallest distance to each other. Bearing this in mind, we can apply Propositions 5.1 and 5.2 of [4]. In order to do this, we first need to determine the properties of the coronene graph H, depicted in Fig. 5.

The coronene graph has 6 edges connecting vertices of degree 2, 12 edges connecting vertices of degree 2 and 3, and 12 edges connecting vertices of degree 3. Taking this into account, we directly obtain

$$\mathrm{M}_1^{\alpha}(H) = 6.(2^{\alpha} + 2^{\alpha}) + 12.(2^{\alpha} + 3^{\alpha}) + 12.(3^{\alpha} + 3^{\alpha})$$

$$= 24 \cdot 2^{\alpha} + 36 \cdot 3^{\alpha}$$

and

$$M_2^{\alpha}(H) = 6 \cdot (2^{\alpha} \cdot 2^{\alpha}) + 12 \cdot (2^{\alpha} \cdot 3^{\alpha}) + 12 \cdot (3^{\alpha} \cdot 3^{\alpha})$$

$$= 6 \cdot 4^{\alpha} + 12 \cdot 6^{\alpha} + 12 \cdot 9^{\alpha}.$$

Now, by Propositions 5.1 and 5.2 of [4]

$$\mathrm{M}_1^{\alpha}(G) = 2M_1^{\alpha}(H) + 2(3^{\alpha+1} - 2^{\alpha+1}) + 2(3^{\alpha+1} - 2^{\alpha+1}) + 2(1-1)2^{\alpha+1}$$

and we arrive at formula (1) of Theorem 4.

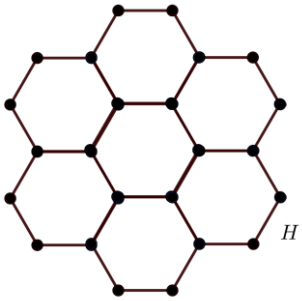

Figure 5. The molecular graph of coronene, H.

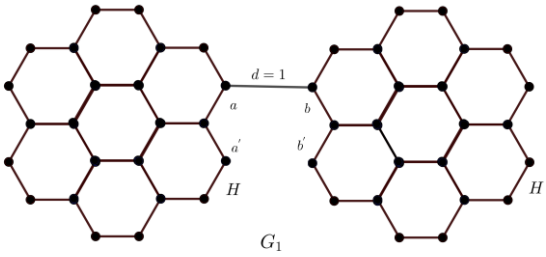

Figure 6. The dicoronylene graph with one of its connecting edges deleted.

In order to calculate the second general Zagreb index, we will proceed by two steps:

Step 1: Let G_1 be the graph depicted in Fig. 6. We have

$$M_2^{\alpha}(G_1) = 2R^{\alpha}(H) + 2A_H^{\alpha}(a)\Delta_H^{\alpha}(a) + 3^{\alpha}\,3^{\alpha}$$
$$= 2\left(6.4^{\alpha} + 12.6^{\alpha} + 12.9^{\alpha}\right)$$
$$+2\left(3^{\alpha} + 2^{\alpha}\right)\left(3^{\alpha} - 2^{\alpha}\right) + 3^{\alpha}3^{\alpha}$$
$$= 10 \cdot 4^{\alpha} + 24 \cdot 6^{\alpha} + 27 \cdot 9^{\alpha}.$$

Step 2: The dicoronylene graph G is results by joining a', b' in G_1 by an edge. Recall that $d(a', b') > 1, m = 2$. Then

$$M_2^{\alpha}(G) = 2R^{\alpha}(G_1) + 2A_{G_1}^{\alpha}(a)\Delta_{G_1}^{\alpha}(a) + 3^{\alpha}\,3^{\alpha}$$
$$= 10.4^{\alpha} + 24.6^{\alpha} + 27.9^{\alpha}$$
$$+2\left(3^{\alpha} + 2^{\alpha}\right)\left(3^{\alpha} - 2^{\alpha}\right) + 3^{\alpha}3^{\alpha}$$
$$= 8 \cdot 4^{\alpha} + 24 \cdot 6^{\alpha} + 30 \cdot 9^{\alpha}$$

which completes the proof of Theorem 4.

Table 4 gives the general Zagreb indices of the dicoronylene for $\alpha = 1,2,\ldots,9$.

Table 4: The general Zagreb indices of the dicoronylene.

α	M_1^{α}	M_2^{α}
1	332	446
2	916	3422
3	2588	27566
4	7444	229982
5	21692	1966286
6	63796	17095742
7	188828	150338606
8	561364	1332236702
9	1673852	11866576526

VI. CONCLUSION

Calculating the topological descriptors of chemical compounds enables researchers in chemistry and pharmacology to discuss and predict some of molecular properties using mathematical methods without necessarily referring to quantum mechanics. It was noted that most of the chemical graphs were the result of some operations such as gluing two graphs at one or more vertices or joining them by one or several paths. For this reason, we have focused our study on these kinds of operations. In this paper we show how our general results [4] can be applied to chemically relevant molecular species.

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