ZAGREB INDICES, HYPER ZAGREB INDICES AND REDEFINED ZAGREB INDICES OF CONICAL GRAPHS

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ABSTRACT. A topological index of graph G is a numerical parameter related to G which char- acterizes its topology and is preserved under isomorphism of graphs. Properties of the chemical compounds and topological indices are correlated. In this paper, we compute some topological indices such as Zagreb indices, Hyper Zagreb indices and Redefined Zagreb indices of conical graphs $G(m, n)$. Moreover we compute the correlation coefficients between them.

1. INTRODUCTION

A new subject which is combination of chemistry, information sciences and mathematics. Topological indices are real numbers related to a graph, that must be a structural invariant. Topological indices play an important role in mathematical chemistry, especially QSAR/QSPR investigations [2, 5, 7]. Throughout this paper, we consider a finite connected graph G that has no loops or multiple edges. The vertex and the edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The degree of the vertex a is the number of edges joined with this vertex denoted by $\delta(a)$. In practical applications, Zagreb Indices are among the best applications to recognize the physical properties, and chemical reactions. First Zagreb index $M_1(G)$, and Second Zagreb index $M_2(G)$ were

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firstly considered by I.Gutman and N.Trinajstic in 1972 [13]. They are defined as:

$$M_1(G) \;=\; \sum_{uv \in E(G)} \delta_G(u) + \delta_G(v), \quad M_2(G) = \sum_{uv \in E(G)} \delta_G(u)\,\delta_G(v).$$

These Indices were deduced within the study of the dependence of total pi-electron energy on molecular structures and are measures of branching of the molecular carbon-atom skeleton. Furtula and Gutman in 2015 introduced forgotten index (F-index) [9] which defined as:

$$F(G) = \sum_{uv \in E(G)} \big(\delta_G{}^2(u) + \delta_G{}^2(v)\big).$$

Furtula and Gutman raised that the predictive ability of forgotten index is almost similar to that of first Zagreb index and for the acentric factor and entropy, and both of them obtain correlation coefficients larger than 0.95. This fact implies the reason why forgotten index is useful for testing the chemical and pharmacological properties of drug molecular structures and reported that this index can reinforce the physicochemical exibility of Zagreb indices. [14,17]. In 2013, Ranjini et al re-defined the Zagreb indices [15], i.e., the redefined first, second and third Zagreb indices for a graph G defined as:

$$ReZG_1(G) = \sum_{uv \in E(G)} \frac{\delta(u) + \delta(v)}{\delta(u)\delta(v)}, \quad ReZG_2(G) = \sum_{uv \in E(G)} \frac{\delta(u)\delta(v)}{\delta(u) + \delta(v)},$$

$$ReZG_3(G) = \sum_{uv \in E(G)} (\delta_G(u)\,\delta_G(v))(\delta_G(u) + \delta_G(v)).$$

In 2013, Shirdel et al [10] introduced distance-based of Zagreb indices named Hyper- Zagreb index as:

$$HM(G) = \sum_{uv \in E(G)} (\delta_G(u) + \delta_G(v))^2.$$

In 2016, Gao et al [11] defined a new distance-based of Zagreb indices named second Hyper-Zagreb index as:

$$HM_2(G) = \sum_{uv \in E(G)} (\delta_G(u)\,\delta_G(v))^2.$$

In 2018, S. Ghobadi and M. Ghorbaninejad [16] introduced a new Zagreb index named Hyper F-index Forgotten topological index as:

$$HF(G) = \sum_{uv \in E(G)} [\delta_G{}^2(u) + \delta_G{}^2(v)]^2.$$

In 2020, Ayache et al [6] introduced the conical graph $G(m,n)$ with $|V(G)| = nm + 1$ vertices and $|E(G)| = 2nm$ edges, that consists of a center O and mn-cycles $C_n^1, C_n^2, ..., C_n^m$ interposed as it is illustrated in Figure 1. Here, we compute some topological indices, namely, first Zagreb index, second Zagreb index, forgotten index (F-index), Hyper Zagreb index, second Hyper Zagreb index, Hyper forgotten index (HF-index) and re-defined the Zagreb indices of conical graphs $G(m,n)$ that generalizes the classic wheel graph. Finally the correlation coefficients between these topological indices are computed. Any unexplained terminology is standard, typically as in [1,3,4,8,12].
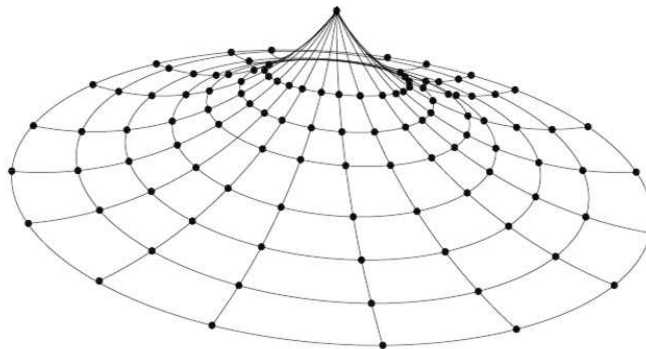

FIGURE 1. $G_{19}(7)$

2. THE ZAGREB INDICES OF CONICAL GRAPHS

In this section we will find the first zagreb index, second zagreb index and F-index of conical graph $G(m,n)$, first we begin with

Theorem 2.1. *Let $G(m,n)$ be a conical graph with*

$$|V(G)| = nm + 1, \qquad |E(G)| = 2nm,$$

Then,

$$M_1(G) = n(n + 16m - 7),$$

$$M_2(G) = n(4n + 32m - 27),$$

$$F(G) = n(n^2 + 64m - 37).$$

Proof. The vertex set of $G(m, n)$ can be written as:

$$V(G) = \{u_0, u_1^1, u_2^1, ..., u_n^1, u_1^2, u_2^2, ..., u_n^2, ..., u_1^m, u_2^m, ..., u_n^m\}$$

$$\begin{cases} n & : u = u_0 = O \\ 3 & : u = u_i^m \\ 4 & : \text{otherwise}, \end{cases}$$

and the edge set of $G(m, n)$ can be written as:

$$E(G) = \bigcup_{k=0}^{3} E_k : \quad \bigcap E_k = \phi,$$

where

$$E_0 = \{u_0 u_1^1, u_0 u_2^1, ..., u_0 u_n^1\} \Rightarrow |E_0| = n,$$

$$E_1 = \{u_1^{m-1} u_1^m, u_2^{m-1} u_2^m, ..., u_n^{m-1} u_n^m\} \Rightarrow |E_1| = n,$$

$$E_2 = \{u_1^m u_2^m, u_2^m u_3^m, ..., u_{n-1}^m u_n^m, u_n^m u_1^m\} \Rightarrow |E_2| = n,$$

and $E_3 = E_+ \cup E_*$ such that $\forall j = 1, 2, ..., m - 1$.

$$E_+ = \{u_1^j u_2^j, u_2^j u_3^j, ..., u_{n-1}^j u_n^j, u_n^j u_1^j\} \Rightarrow |E_+| = n(m - 1),$$

$$E_* = \{u_1^{j-1} u_1^m, u_2^{j-1} u_2^m, ..., u_n^{j-1} u_n^m\} \Rightarrow |E_*| = n(m - 2),$$

Thus, $|E_3| = |E_+| + |E_*| = n(m - 1) + n(m - 2) = n(2m - 3)$.
For $i = 1, 2, ..., n$, we have, $E(G) = \bigcup_{k=0}^{3} E_k$, and

- If $uv \in E_0$, then $\delta u = \delta u_0 = n, \delta v = \delta u_i^1 = 4$.
- If $uv \in E_1$, then $\delta u = \delta u_i^{m-1} = 4, \delta v = \delta u_i^m = 3$.
- If $uv \in E_2$, then $\delta u = \delta v = \delta u_i^m = 3$.
- If $uv \in E_3$, then $\delta u = \delta v = 4$.

By Table 1 and definitions of first, second and forgotten indices we give:

$M_1(G)$

$$
\begin{aligned}
&= \sum_{uv \in E_0} (n+4) + \sum_{uv \in E_1} (7) + \sum_{uv \in E_2} (6) + \sum_{uv \in E_3} (8) \\
&= (n+4) \sum_{uv \in E_0} (1) + 7 \sum_{uv \in E_1} (1) + 6 \sum_{uv \in E_2} (1) + 8 \sum_{uv \in E_3} (1) \\
&= (n+4)(n) + 7(n) + 6(n) + 8n(2m-3) \\
&= n(n+4+7+6+16m-24) = n(n+16m-7).
\end{aligned}
$$

$M_2(G)$

$$
\begin{aligned}
&= \sum_{uv \in E_0} (4n) + \sum_{uv \in E_1} (12) + \sum_{uv \in E_2} (9) + \sum_{uv \in E_3} (16) \\
&= (4n) \sum_{uv \in E_0} (1) + 12 \sum_{uv \in E_1} (1) + 9 \sum_{uv \in E_2} (1) + 16 \sum_{uv \in E_3} (1) \\
&= (4n)(n) + 12(n) + 9(n) + 16n(2m-3) \\
&= n(4n+32m-27).
\end{aligned}
$$

$F(G)$

$$
\begin{aligned}
&= \sum_{uv \in E_0} (n^2+16) + \sum_{uv \in E_1} (25) + \sum_{uv \in E_2} (18) + \sum_{uv \in E_3} (32) \\
&= (n^2+16) \sum_{uv \in E_0} (1) + 25 \sum_{uv \in E_1} (1) + 18 \sum_{uv \in E_2} (1) + 32 \sum_{uv \in E_3} (1) \\
&= (n^2+16)(n) + 25(n) + 18(n) + 32n(2m-3) \\
&= n(n^2+64m-37).
\end{aligned}
$$

TABLE 1. Relationship between Zagreb indices and it's degrees of conical graphs.

No.	$uv \in E(G)$	$uv \in E_0$	$uv \in E_1$	$uv \in E_2$	$uv \in E_3$
1.	$\delta(u)+\delta(v)$	$n+4$	7	6	8
2.	$\delta(u)\delta(v)$	$4n$	12	9	16
3.	$\delta^2(u)+\delta^2(v)$	n^2+16	25	18	32

□

Example 1. *Suppose that G with m=4 levels and n=5 vertices, then, by theorem 2.1 we have*

$$M_1(G) = 310, \quad M_2(G) = 605, \quad F(G) = 1220.$$

3. THE HYPER ZAGREB INDICES OF CONICAL GRAPHS

In this section we will find the first Hyper Zagreb index, second Hyper Zagreb index and HF-index of $G(m,n)$.

Firstly, by using Theorem 2.1 we give the relationship between Hyper Zagreb indices and it's degrees of conical graph $G(m,n)$ in the Table 2.

TABLE 2. Relationship between Hyper Zagreb indices and it's degrees of conical graphs.

No.	$uv \in E(G)$	$uv \in E_0$	$uv \in E_1$	$uv \in E_2$	$uv \in E_3$
1.	$(\delta(u) + \delta(v))^2$	$(n+4)^2$	49	36	64
2.	$\delta^2(u)\delta^2(v)$	$16n^2$	144	81	256
3.	$(\delta^2(u) + \delta^2(v))^2$	$(n^2 + 16)^2$	625	324	1024

TABLE 3. Relationship between Redefined Zagreb indices and it's degrees of conical graphs.

No.	$uv \in E(G)$	$uv \in E_0$	$uv \in E_1$	$uv \in E_2$	$uv \in E_3$
1.	$\dfrac{\delta(u) + \delta(v)}{\delta(u)\delta(v)}$	$\dfrac{n+4}{4n}$	$\dfrac{7}{12}$	$\dfrac{2}{3}$	$\dfrac{1}{2}$
2.	$\dfrac{\delta(u)\delta(v)}{\delta(u) + \delta(v)}$	$\dfrac{4n}{n+4}$	$\dfrac{12}{7}$	$\dfrac{3}{2}$	2
3.	$\delta(u)\delta(v)(\delta(u) + \delta(v))$	$4n(n+4)$	84	54	128

Theorem 3.1. *Let $G(m,n)$ be a conical graph with*

$$|V(G)| = nm + 1, \quad |E(G)| = 2nm.$$

Then,

$$HM_1(G) = n(n^2 + 8n + 128m - 91),$$
$$HM_2(G) = n(16n^2 + 512m - 543),$$
$$HF(G) = n(n^4 + 32n^2 + 2048m - 1867).$$

Proof. By using Table 2 and definitions of Hyper Zagreb index we have,

$HM_1(G)$

$$
\begin{aligned}
&= \sum_{uv \in E_0} (n+4)^2 + \sum_{uv \in E_1} (49) + \sum_{uv \in E_2} (36) + \sum_{uv \in E_3} (64) \\
&= (n+4)^2 \sum_{uv \in E_0} (1) + 49 \sum_{uv \in E_1} (1) + 36 \sum_{uv \in E_2} (1) + 64 \sum_{uv \in E_3} (1) \\
&= (n+4)^2(n) + 49(n) + 36(n) + 64n(2m-3) \\
&= (n^2 + 8n + 16)(n) + 49(n) + 36(n) + 64n(2m-3) \\
&= n(n^2 + 8n + 128m - 91).
\end{aligned}
$$

similarly the second Hyper Zagreb index and HF-index are equals

$$
HM_2(G) = n(16n^2 + 512m - 543),
$$

$$
HF(G) = n(n^4 + 32n^2 + 2048m - 1867).
$$

$\square$

Example 2. *Suppose that G with m=3 levels and n=4 vertices, then, by theorem 3.1 we have*

$$
HM_1(G) = 1364, \quad HM_2(G) = 4996, \quad HF(G) = 20180.
$$

4. THE REDEFINED ZAGREB INDICES OF CONICAL GRAPHS

In this section we will find the first, second and third Redefined Zagreb Indices of conical graphs $G(m,n)$. By using similar method via the proof of Theorem 2.1 and Theorem 3.1 given in the following Theorem:

Theorem 4.1. *If $G(m,n)$ is a conical graph with*

$$
|V(G)| = nm + 1, \qquad |E(G)| = 2nm,
$$

Then,

$$
ReZG_1(G) = [1 + mn],
$$

$$
ReZG_2(G) = \frac{n}{14(n+4)} (56nm + 17n + 224m - 156),
$$

$$
ReZG_3(G) = n(4n^2 + 16n + 256m - 246).
$$

TABLE 4. The Zagreb Indices, Hyper Zagreb indices and Redefined Zagreb indices of conical graphs $G(m, n)$.

$m =$	3	4	5	6	7	8	9	10
M_1	180	244	308	372	436	500	564	628
M_2	340	468	596	724	852	980	1108	1236
F	684	940	1196	1452	1708	1964	2220	2476
HM	136	1876	2388	2900	3412	3924	4436	4948
HM_2	4996	7044	9092	11140	13188	15236	17284	19332
HF	20144	28336	36528	44720	52912	61104	69296	77488
$ReZG_1$	13	17	21	25	29	33	37	41
$ReZG_2$	44.86	60.86	76.86	92.86	108.86	124.86	140.86	156.86
$ReZG_3$	2600	3624	4648	5672	6696	7720	8744	9768

TABLE 5. The correlation coefficient of conical graphs $G(m, n)$, between the Zagreb Indices, Hyper Zagreb indices and Redefined Zagreb indices.

Correl.	M_1	M_2	F	HM	HM_2	HF	$ReZG_1$	$ReZG_2$	$ReZG_3$
M_1	1	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
M_2	1.000	1	1.000	1.000	1.000	1.000	1.000	1.000	1.000
F	1.000	1.000	1	1.000	1.000	1.000	1.000	1.000	1.000
HM	1.000	1.000	1.000	1	1.000	1.000	1.000	1.000	1.000
HM_2	1.000	1.000	1.000	1.000	1	1.000	1.000	1.000	1.000
HF	1.000	1.000	1.000	1.000	1.000	1	1.000	1.000	1.000
$ReZG_1$	1.000	1.000	1.000	1.000	1.000	1.000	1	1.000	1.000
$ReZG_2$	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1	1.000
$ReZG_3$	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1

Example 3. *Suppose that G with 3 levels and 3 vertices, then, by Theorem 4.1 we have*

$$ReZG_1(G) = 10, \quad ReZG_2(G) = \frac{3213}{98} = 32.79, \quad ReZG_3(G)(G) = 1818.$$

5. CORRELATION COEFFICIENT OF SOME SPECIAL CONICAL GRAPHS

In this section we calculate the Coefficient Correlation for Zagreb Indices, Hyper Zagreb indices and Redefined Zagreb indices of conical graphs $G(m, n)$. with m level where $m = 3, 4, ..., 10$, and $n = 4$ vertices, we have $|V(G)| = nm + 1 = 4m + 1$, $|E(G)| = 2nm = 8m$, where, $m = 3, 4, ..., 10$

Then, the Zagreb Indices, Hyper Zagreb indices and Redefined Zagreb indices of conical graphs $G(m, n)$ given in the Table 4. The correlation coefficient of conical graphs $G(m, n)$ are found in Table 5.

In Table 5. We select those physicochemical properties of some spacial cases of conical graphs for which give perfect correlations, i.e., we can say that, some spacial cases of conical graphs are possible tools for QSPR researches.

6. CONCLUSION

Several articles are concerned the calculations of topological indices for different types of graphs. Some of them have found applications, but others were devoted to the mathematical side in order to throw more light on the relationship between these various concepts. In this paper, we have evaluated a useful tool for building new graphs with some topological indices that may open a wide window for other researches in the future.

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