SOME RESULTS ABOUT MODIFIED ZAGREB INDICES

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Abstract: Zagreb indices are the best known topological indices which reflect certain structural features of organic molecules. In this paper we point out that the modified Zagreb indices are worth studying and present some results about product graphs.

INTRODUCTION

Zagreb indices are the oldest and the best known topological indices [1, 2, 3, 4]. The *first Zagreb index* $M_1(G)$ and the *second Zagreb index* $M_2(G)$ are defined as follows [1, 2, 3, 4]: for a simple connected graph G, let $M_1(G) = \sum_{v\in V(G)} d(v)^2$, $M_2(G) = \sum_{uv\in E(G)} d(u)d(v)$, where d(u) and d(v) are the degrees of vertices u and v respectively.

However, some authors found we should amend Zagreb indices, because the contributing elements to the Zagreb indices give greater weights to the inner (interior) vertices and edges and smaller weights to outer (terminal) vertices and edges of a graph. This opposes intuitive reasoning that the outer atoms and bonds should have greater weights than inner vertices and bonds, because the outer vertices and bonds are associated with the larger part of the molecular surface and consequently are expected to make a greater contribution to physical, chemical and biological properties. One way to amend Zagreb indices is to input in the definitions of $M_1(G)$ and $M_2(G)$ inverse values of the vertex-degrees. We call these indices the *modified Zagreb indices* and denoted them by symbols ${}^mM_1$ and ${}^mM_2$ [5]. They are defined as follows [5]: for a simple connected graph G, let ${}^mM_1(G) = \sum_{v\in V(G)} \frac{1}{d(v)^2}$, ${}^mM_2(G) =$

$\sum_{uv\in E(G)} \frac{1}{d(u)d(v)}$.

PRELIMINARIES

For further details, see [8, 9].

Lemma 2.1[6]. The number of edges, m, in a k-regular graph is kn/2, where k is the regularity and n is the number of vertices of the graph.

Definition 2.2[8]. The *k-cube* is the graph whose vertices are the ordered k-tuples of 0's and 1's, two vertices being joined if and only if they differ in exactly one coordinate. The k-cube has 2^k vertices, $k2^{k-1}$ edges and is bipartite.

Definition 2.3[8] A k-regular graph of girth l with the least possible number of vertices is called a *(k, l)-cage.* If we denote by f(k,l) the number of vertices in a (k, l)-cage, we have f(2, l) = l and for $k \geq 3$, if n = 2r + 1, f(k, l) $\geq \frac{k(k-1)^r - 2}{k-2}$; if n = 2r, f(k, l) $\geq \frac{2(k-1)^r - 2}{k-2}$.

Definition 2.4[7]. The hexagonal system CC_2 shown in Figure 1 is referred to as the *coronene* (a name borrowed from chemistry). Circumscribing CC_2 by hexagons, we obtain the *circumcoronene* (see CC_3 in Figure 1). The structure of the further members CC_4, CC_5, ..., of the circumcoronene series is evident .

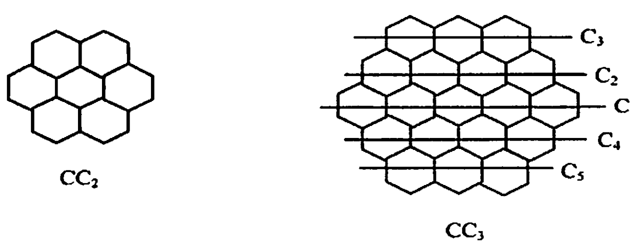

Figure 1. CC_k

Definition 2.5[10, 11]. The zeroth-order general Randic index $^0R_t(G) = \sum_{v\in V(G)} d(v)^t$ for general real number t, where d(v) is the degree of v. Randic index of graph G, denotes $\chi(G)$, is defined as follows: $\chi(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d(u)d(v)}}$.

Definition 2.6[8]. The product $G\times H$ of graphs G and H has the vertex set $V(G\times H) = V(G) \times V(H)$ and (a, x)(b, y) is an edge of $G\times H$ if a = b and xy $\in$ E(H) or ab $\in$ E(G) and x = y.

COMPARE MODIFIED ZAGREB INDICES WITH RANDIC INDEX

Theorem 3.1. Let G be a k-regular graph with n vertices, $n \geq 2$, we have

$$^{m}M_1(G) = \frac{n}{k^2},\quad ^{m}M_2(G) = \frac{n}{2k}.$$

Proof. By the definition of $^{m}M_1$ we have $^{m}M_1(G) = \frac{n}{k^2}$. By Lemma 2.1 and the definition of $^{m}M_2$ we have $^{m}M_2(G) = \frac{n}{2k}$. The theorem follows.

Remark: Randic index has identical values for non-isomorphic regular graphs with different connectivities but with the same number of vertices [6], however, the modified Zagreb indices have different values. Hence, the modified Zagreb indices are worth studying.

By Theorem 3.1 we have

Theorem 3.2. Let G be the Petersen graph, we have $^{m}M_1(G) = \frac{10}{9}$, $^{m}M_2(G) = \frac{5}{3}$, where the Petersen graph is defined in [8].

By Definition 2.2 and Theorem 3.1 we have

Theorem 3.3. Let G be a k-cube, we have $^{m}M_1(G) = \frac{2^k}{k^2}$, $^{m}M_2(G) = \frac{2^{k-1}}{k}$.

By Definition 2.3 and Theorem 3.1 we have

Theorem 3.4. Let G be a (k, l)-cage.

(1). When k = 2, we have $^{m}M_1(G) = 0.25l$, $^{m}M_2(G) = 0.25l$.

(2). When $k \geq 3$ and $l = 2r + 1$, we have $^mM_1(G) \geq \frac{k(k-1)^r - 2}{k^2(k-2)}$, $^mM_2(G) \geq \frac{k(k-1)^r - 2}{2k(k-2)}$.

(3). When $k \geq 3$ and $l = 2r$, we have $^mM_1(G) \geq \frac{2(k-1)^r - 2}{k^2(k-2)}$, $^mM_2(G) \geq \frac{(k-1)^r - 1}{k(k-2)}$.

Theorem 3.5. Let CC_k be circumcoronene, we have

$$^mM_1(CC_k) = \frac{4k^2 + 5k}{6},\ ^mM_2(CC_k) = k^2 + \frac{1}{3}k + \frac{1}{6}.$$

Proof. Because there are $2k-1$ hexagons in C_1, see Figure 1, there are $4k-1$ vertices in the upper layer of C_1. Because there are $2k-2$ hexagons in C_2, there are $4k-3$ vertices in the upper layer of C_2. Similarly, there are $2k + 1$ vertices in the upper layer of C_k. Hence, the vertex number of CC_k is

$$2\times[(4k-1) + (4k-3) + \ldots + (2k+1)] = 6k^2.$$

Because there are k hexagons in C_k, there are $k + 2$ vertices with degrees 2 in the upper layer of C_k. Obviously, there are 2 vertices with degrees 2 in the upper layer of C_i, where $i = 1, 2, \ldots, k-1$. Hence, the total number of vertices of CC_k with degrees 2 is $[k + 2 + 2(k-1)] \times 2 = 6k$. By the definition of $^mM_1$ we have $^mM_1(CC_k) = (4k^2 + 5k)/6$.

Because $2m = \sum_{v\in V(CC_k)} d(v)$, where m is the edge number of CC_k, we have $m = 9k^2 - 3k$. In the upper layers of C_k, C_{2k-1} and the line of C_1, there are two edges whose vertices are with degrees 2. Hence, the total number of edges whose vertices are with degrees 2 is 6.

In the upper layer of C_1 there are two edges whose vertices are with degrees 2 and 3 respectively. In line C_2 there are two edges whose vertices are with degrees 2 and 3 respectively. In the upper layer of C_2 there are two edges whose vertices are with degrees 2 and 3 respectively. Similarly, in line C_k there are two edges whose vertices are with degrees 2 and 3 respectively. In the upper layer of C_k there are $2k-2$ edges whose vertices are with degrees 2 and 3 respectively. Hence, the total number of edges whose vertices are with degrees 2 and 3 is $[2 + 4(k-2) + 2 + (2k-2)]\times 2 = 12(k-1)$. By the definition of ${}^mM_2$ we have ${}^mM_2(CC_k) = 6/4 + 12(k-1)/6 + [9k^2-3k-6-12(k-1)]/9 = k^2 + k/3 + 1/6$. The theorem follows.

MAIN RESULTS ABOUT PRODUCT GRAPHS

Theorem 4.1. ${}^mM_1(P_m\times P_n) = \frac{1}{16}mn + \frac{7}{72}(m+n) + \frac{13}{36}$, where $m, n \geq 2$.

Proof. By Definition 2.6 we have $|V(G \times H)| = |V(G)||V(H)|$, $d_{G\times H}((u,v)) = d_G(u) + d_H(v)$. By the definition of ${}^mM_1(G)$ the theorem follows.

Similarly, we have

Theorem 4.2. ${}^mM_1(K_m\times K_n) = \frac{mn}{(m+n-2)^2}$, where $m, n \geq 2$.

Theorem 4.3. ${}^mM_1(C_m\times C_n) = \frac{mn}{16}$, where $m, n \geq 3$.

Theorem 4.4. ${}^mM_1(K_{1,\,m-1}\times K_{1,\,n-1}) =$
$\frac{(m-1)(n-1)}{4} + \frac{1}{(m+n-2)^2} + \frac{n-1}{m^2} + \frac{m-1}{n^2}$, where $m, n \geq 2$.

Proof. By Definition 2.6, in $K_{1,\,m-1}\times K_{1,\,n-1}$ there are $(m-1)(n-1)$ vertices with degree 2, there is one vertex with degree $m+n-2$, there are $n-1$ vertices with degree m, there are $m-1$ vertices with degree n. By the definition of ${}^mM_1$ the theorem follows.

Theorem 4.5. ${}^mM_1(P_m\times C_n) = \frac{mn}{16} + \frac{7n}{72}$, where $m \geq 2$, $n \geq 3$.

Theorem 4.6. ${}^mM_1(P_m\times K_{1,\,n-1}) = \frac{n-1}{2} + \frac{2}{n^2} + \frac{(m-2)(n-1)}{9} +$
$\frac{m-2}{(n+1)^2}$, where $m, n \geq 2$.

Theorem 4.7. ${}^mM_1(C_m\times K_{1,\,n-1}) = \frac{m(n-1)}{9} + \frac{m}{(n+1)^2}$, where $m \geq 3$,

$n \geq 2$.

Theorem 4.8. ${}^{m}M_1(P_m \times K_n) = \frac{2}{n} + \frac{n(m-2)}{(n+1)^2}$, where $m, n \geq 2$.

Theorem 4.9. ${}^{m}M_1(C_m \times K_n) = \frac{mn}{(n+1)^2}$, where $m \geq 3, n \geq 2$.

Theorem 4.10. ${}^{m}M_1(K_m \times K_{1,n-1}) = \frac{n-1}{m} + \frac{m}{(m+n-2)^2}$, where m, $n \geq 2$.

Theorem 4.11. Let G and H be simple connected graphs, we have

$\frac{mn}{(m+n-2)^2} \leq {}^{m}M_1(G \times H) \leq \min\{\frac{1}{4}{}^{0}R_{-1}(G)\,{}^{0}R_{-1}(H)$, $\frac{(m-1)(n-1)}{4} + \frac{1}{(m+n-2)^2} + \frac{n-1}{m^2} + \frac{m-1}{n^2}\}$, where ${}^{0}R_{-1}(G)$ is defined in Definition 2.5, $m = |V(G)| \geq 2$, $n = |V(H)| \geq 2$.

Proof. By Definition 2.6 we have $d((u, v)) = d(u) + d(v)$. Since $d(u) + d(v) \geq 2(d(u)d(v))^{0.5}$, by the definition of ${}^{m}M_1$ we have

${}^{m}M_1(G \times H) = \sum_{(u,v)\in V(G\times H)} \frac{1}{d(u,v)^2} \leq \sum_{(u,v)\in V(G\times H)} \frac{1}{4d(u)d(v)} = \frac{1}{4}{}^{0}R_{-1}(G)$ ${}^{0}R_{-1}(H)$. Since $G \times H$ is a subgraph of $K_m \times K_n$, by Theorem 4.2 and the definition of ${}^{m}M_1$ we have ${}^{m}M_1(G \times H) \geq \frac{mn}{(m+n-2)^2}$.

Claim 1: When $m = 2$ we have ${}^{m}M_1(G \times H) \leq {}^{m}M_1(K_{1,1} \times K_{1,n-1})$.

In fact, since $m = 2$, we have $G = K_{1,1}$. When $H \neq K_{1,n-1}$, H has at most $n-2$ vertices with degrees 1 and at least 2 vertices with degrees at least 2. By the definition of ${}^{m}M_1$ we have ${}^{m}M_1(G \times H) \leq \frac{2(n-2)}{4} + \frac{4}{9}$. By Theorem 4.4 Claim 1 follows.

By symmetry we have

Claim 2: When $n = 2$ we have ${}^{m}M_1(G \times H) \leq {}^{m}M_1(K_{1,m-1} \times K_{1,1})$

Claim 3: When $m = 3$ we have ${}^{m}M_1(G \times H) \leq {}^{m}M_1(K_{1,2} \times K_{1,n-1})$.

We prove Claim 3 as follows:

Case 3.1. $G = K_{1,2}$, $H \neq K_{1,n-1}$.

Since $H \neq K_{1,n-1}$, H has at most $n-2$ vertices with degrees 1 and at least 2 vertices with degrees at least 2. By the definition of ${}^{m}M_1$

we have ${}^{m}M_1(K_{1,2}\times H) \le \frac{2(n-2)}{4}+\frac{n-2}{9}+\frac{2}{16}+\frac{4}{9}$. By Theorem 4.4 we have ${}^{m}M_1(K_{1,2}\times K_{1,n-1}) = \frac{2(n-1)}{4}+\frac{1}{(n+1)^2}+\frac{n-1}{9}+\frac{2}{n^2}$. Claim 3 follows.

Case 3.2. $G = C_3$, $H = K_{1,n-1}$.

By Theorem 4.7 and Theorem 4.4, Claim 3 follows.

Case 3.3. $G = C_3$, $H \neq K_{1,n-1}$.

Similar to Case 3.1 we have ${}^{m}M_1(C_3\times H) \le \frac{3(n-2)}{9}+\frac{6}{16}$. Claim 3 follows.

By symmetry we have

Claim 4: When $n = 3$ we have ${}^{m}M_1(G\times H) \le {}^{m}M_1(K_{1,m-1}\times K_{1,2})$.

Claim 5: When $m \ge 4$, $n \ge 4$ we have ${}^{m}M_1(K_{1,m-1}\times H) \le {}^{m}M_1(K_{1,m-1}\times K_{1,n-1})$.

In fact, when $H \neq K_{1,n-1}$, H has at most $n-2$ vertices with degrees 1 and at least 2 vertices with degrees at least 2. By the definition of ${}^{m}M_1$ we have ${}^{m}M_1(K_{1,m-1}\times H) \le \frac{(m-1)(n-2)}{4}+\frac{2(m-1)}{9}+\frac{n-2}{m^2}+\frac{2}{(m+1)^2}$. When $m \ge 4$ we have $\frac{2(m-1)}{9}+\frac{1}{(m+1)^2} < \frac{m-1}{4}$. By Theorem 4.4 Claim 5 follows.

Similarly, we have

Claim 6: When $m \ge 4$, $n \ge 4$ we have ${}^{m}M_1(G\times K_{1,n-1}) \le {}^{m}M_1(K_{1,m-1}\times K_{1,n-1})$.

Claim 7: When $m \ge 4$, $n \ge 4$, $G \neq K_{1,m-1}$, $H \neq K_{1,n-1}$, we have ${}^{m}M_1(G\times H) \le {}^{m}M_1(K_{1,m-1}\times K_{1,n-1})$.

In fact, when $G \neq K_{1,m-1}$, G has at most $m-2$ vertices with degrees 1 and at least 2 vertices with degrees at least 2. Similarly, when $H \neq K_{1,n-1}$, H has at most $n-2$ vertices with degrees 1 and at least 2 vertices with degrees at least 2. By the definition of ${}^{m}M_1$ we have ${}^{m}M_1(G\times H) \le \frac{(m-2)(n-2)}{4}+\frac{2(m-2)}{9}+\frac{2(n-2)}{9}+\frac{4}{16}$. By

Claim 5 we have ${}^{m}M_1(K_{1,m-1}\times H) \le \frac{(m-1)(n-2)}{4} + \frac{2(m-1)}{9} + \frac{n-2}{m^2} + \frac{2}{(m+1)^2}$. When $n \ge 4$ we have $\frac{2(n-2)}{9} + \frac{1}{4} < \frac{n-2}{4} + \frac{2}{9}$. Hence, we have $\frac{(m-2)(n-2)}{4} + \frac{2(m-2)}{9} + \frac{2(n-2)}{9} + \frac{4}{16} \le \frac{(m-1)(n-2)}{4} + \frac{2(m-1)}{9} + \frac{n-2}{m^2} + \frac{2}{(m+1)^2}$. By Claim 5 Claim 7 follows.

From these Claims above we have

Claim 8: When $m \ge 2$, $n \ge 2$, we have ${}^{m}M_1(G\times H) \le {}^{m}M_1(K_{1,m-1}\times K_{1,n-1})$. The theorem follows.

Similarly, we have

Theorem 4.12. ${}^{m}M_2(P_m\times P_n) = \frac{1}{8}mn + \frac{11}{144}(m+n) + \frac{1}{12}$, where $m, n \ge 3$.

Theorem 4.13. ${}^{m}M_2(K_m\times K_n) = \frac{mn}{2(m+n-2)}$, where $m, n \ge 2$.

Theorem 4.14. ${}^{m}M_2(C_m\times C_n) = \frac{mn}{8}$, where $m, n \ge 3$.

Theorem 4.15. ${}^{m}M_2(K_{1,m-1}\times K_{1,n-1}) = \frac{(m-1)(n-1)(m+n)}{2mn} + \frac{m^2+n^2-m-n}{mn(m+n-2)}$, where $m, n \ge 2$.

Theorem 4.16. ${}^{m}M_2(P_m\times C_n) = \frac{mn}{8} + \frac{11n}{144}$, where $m, n \ge 3$.

Theorem 4.17. ${}^{m}M_2(P_m\times K_{1,n-1}) = \frac{n-1}{n} + \frac{(m-2)(n-1)}{3(n+1)} + \frac{n-1}{3} + \frac{(m-3)(n-1)}{9} + \frac{2}{n(n+1)} + \frac{m-3}{(n+1)^2}$, where $m \ge 3$, $n \ge 2$.

Theorem 4.18. ${}^{m}M_2(C_m\times K_{1,n-1}) = \frac{m(n+4)(n-1)}{9(n+1)} + \frac{m}{(n+1)^2}$, where $m \ge 3$, $n \ge 2$.

Theorem 4.19. ${}^{m}M_2(P_m\times K_n) = \frac{n-1}{n} + \frac{mn^2-2n^2+mn+4}{2(n+1)^2}$, where $m \ge 3$, $n \ge 2$.

Theorem 4.20. ${}^{m}M_2(C_m \times K_n) = \frac{mn}{2(n+1)}$, where $m \geq 3$, $n \geq 2$.

Theorem 4.21. ${}^{m}M_2(K_m \times K_{1,n-1}) = \frac{n-1}{m+n-2} + \frac{(m-1)(n-1)}{2m}$

$+\frac{m(m-1)}{2(m+n-2)^2}$, where $m, n \geq 2$.

Theorem 4.22. Let G and H be simple connected graphs, we have ${}^{m}M_2(G\times H) \leq \frac{1}{4}({}^{0}R_{-1}(G)\chi(H) + {}^{0}R_{-1}(H)\chi(G))$, and ${}^{m}M_2(G\times H) = \frac{1}{4}({}^{0}R_{-1}(G)\chi(H) + {}^{0}R_{-1}(H)\chi(G))$ if and only if both G and H are k-regular graphs, where ${}^{0}R_{-1}(G)$ and $\chi(G)$ are defined in Definition 2.5, $m = |V(G)| \geq 2$, $n = |V(H)| \geq 2$.

Proof. ${}^{m}M_2(G\times H) = \sum_{(x,u)(y,v)\in E(G\times H)} d_{G\times H}(x,u)d_{G\times H}(y,v) = \sum_{x\in V(G)}\sum_{uv\in E(H)} \frac{1}{(d(x)+d(u))(d(x)+d(v))} + \sum_{u\in V(H)}\sum_{xy\in E(G)} \frac{1}{(d(x)+d(u))(d(u)+d(y))}$. Since $d(u) + d(x) \geq 2\sqrt{d(u)d(x)}$,

we have ${}^{m}M_2(G\times H) \leq \sum_{x\in V(G)}\sum_{uv\in E(H)} \frac{1}{4d(x)\sqrt{d(u)d(v)}} + \sum_{u\in V(H)}\sum_{xy\in E(G)} \frac{1}{4d(u)\sqrt{d(x)d(y)}} = \frac{1}{4}{}^{0}R_{-1}(G) \sum_{uv\in E(H)} \frac{1}{\sqrt{d(u)d(v)}} + \frac{1}{4}{}^{0}R_{-1}(H) \sum_{xy\in E(G)} \frac{1}{\sqrt{d(x)d(y)}} = \frac{1}{4}({}^{0}R_{-1}(G)\chi(H) + {}^{0}R_{-1}(H)\chi(G))$. Since $d(u) + d(x) = 2\sqrt{d(u)d(x)}$ if and only if $d(u) = d(x)$, we know that ${}^{m}M_2(G\times H) = \frac{1}{4}({}^{0}R_{-1}(G)\chi(H) + {}^{0}R_{-1}(H)\chi(G))$ if and only if both G and H are k-regular graphs. The theorem follows.

Acknowledgements: The project supported by the Natural Science Foundation of Department of Education of Zhejiang Province of China (No. 20070441); The project supported by the Invention

Group of Zhejiang Normal University; National Nature Science Foundation of China (No. 10971198), Zhejiang Provincial Natural Science Foundation of China (No. Y6090699).

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