The First And Second Zagreb Indices Of Degree Splitting Of Molecular Graphs

S. Ragavi

Abstract: The first Zagreb index is the sum of the squares of the degree of the vertices and second Zagreb index is the sum of the product of degrees of pairs of adjacent vertices. My research is to find the first and second Zagreb index of degree splitting of molecular graphs like silicate networks, honey comb network.

Index Terms: Zagreb Index, Degree Splitting, Molecular Graphs.

INTRODUCTION:

The first and second Zagreb indices first appeared in a topological formula for the total π energy of conjugated molecules, were introduced by Gutman and Trinajstić in 1972. Since then these indices have been used as branching indices. The Zagreb indices are found to have applications in QSPR and QSAR studies. The First and Second Zagreb indices are defined in [5] as follows:

$$M_1(G) = \sum_{v \epsilon V(G)} d(v)^2$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

Let G = (V, E) be a graph with V = $S_1 \cup S_2 \cup \cdots, \cup S_t \cup T$ where each S_i is a set of vertices having at least two vertices and having the same degree and T = V − $\cup S_i$. The degree splitting graph of G is denoted by DS(G) is obtained from G by adding vertices $w_1, w_2, \cdots, w_t$ and joining w_i to each vertex of S_i ($1 \le i \le t$) [10].

The first and second Zagreb index of degree splitting of standard graphs and special graphs are studied in [11],[12]. My research is to find the first and second Zagreb index of degree splitting of molecular graphs like silicate networks, hexagonal network, honey comb network,

Theorem 1

For Triangular Benzenoid $T_n, n \ge 2$,

$$M_1(DS(T_n)) = n^4 + 2n^3 + 22n^2 + 57n + 8,$$

$$M_2(DS(T_n)) = 4n^4 + 8n^3 + 33n^2 + 116n + 1.$$

Proof:

The number of vertices in triangular oxide $|V(T_n)| = n^2 + 4n + 1$ and the number of edges $|E(T_n)| = \frac{3n(n+3)}{2}$.

The number of 3 and 4 degree vertices is 3n+3 and $n^2 + n - 2$ respectively.

Then there are 2 degree splitting vertices namely u_1 and u_2.

$$M_1(DS(T_n)) = \sum_{n^2+4n+1} d(v)^2$$

$$= \sum_{i=1}^{n^2+4n+1} d(v_i)^2 + d(u_1)^2 + d(u_2)^2$$

$$= \sum_{i=1}^{3n+3} 3^2 + \sum_{i=1}^{n^2+n-2} 4^2 + (3n+3)^2$$

$$+(n^2 + n - 2)^2$$

$$= 3^2(3n+3) + 4^2(n^2+n-2)$$

$$+(3n+3)^2 + (n^2+n-2)^2$$

$$= n^4 + 2n^3 + 22n^2 + 57n + 8$$

$$M_2(DS(T_n)) = \sum_{uv \in E} d(u)d(v)$$

$$= \sum_{i=1}^{6} 3(3) + \sum_{i=1}^{\frac{3n(n-1)}{2}} 3(4)$$

$$+ \sum_{i=1}^{6(n-1)} 4(4) + \sum_{i=1}^{3n+3} 3(3n+3)$$

$$+ \sum_{i=1}^{n^2+n-2} 4(n^2+n-2)$$

$$= 9(6) + 12\left(\frac{3n(n-1)}{2}\right) + 6(n-1)16$$

$$+3(3n+3)^2 + 4(n^2 + \mathrm{n} - 2)^2$$

$$= 54 + 18n(n-1) + 96(n-1)$$

$$+3(3n+3)^2 + 4(n^2 + \mathrm{n} - 2)^2$$

$$= 4n^4 + 8n^3 + 33n^2 + 116n + 1$$

Theorem 2

For Circumcoronene of Benzenoid H_k,

$$M_1(DS(H_k)) = 36k^4 - 72k^3 + 168k^2 + 54k - 96,$$

$$M_2(DS(H_k)) = 144k^4 - 288k^3 + 288k^2 - 96k + 6.$$

Proof:

The number of vertices in Circumcoronene $|V(H_k)| = 6k^2$ and the number of edges $|E(H_k)| = 9k^2 - 3k$.

The number of 2 and 3 degree vertices is $6k$ and $6k(k-1)$ respectively.

Then there are 2 degree splitting vertices namely u_1 and u_2.

Also $|E_{33}| = 6, |E_{44}| = 9k^2 - 15k + 6, |E_{34}| = 12(k-1)$.

$$M_1(DS(H_k)) = \sum d(v)^2$$

$$= \sum_{i=1}^{6k^2} d(v_i)^2 + d(u_1)^2 + d(u_2)^2$$

$$= \sum_{i=1}^{6k} 3^2 + \sum_{i=1}^{6k(k-1)} 4^2 + (6k)^2$$

$$+(6k(k-1))^2$$

$$= 3^2(6k) + 4^2(6k^2 - 6k) + (6k)^2$$

$$+(6k^2 - 6k)^2$$

$$= 36k^4 - 72k^3 + 168k^2 + 54k - 96$$

$$M_2(DS(H_k)) = \sum_{uv \in E} d(u)d(v)$$

$$= \sum_{i=1}^{6} 3(3) + \sum_{i=1}^{12(k-1)} 3(4) + \sum_{i=1}^{9k^2-15k+6} 4(4)$$

$$+ \sum_{i=1}^{6k} 3(6k) + \sum_{i=1}^{6k^2-6k} 4(6k^2 - 6k)$$

$$= 9(6) + (12k - 12)(12) + (9k^2 - 15k + 6)16 + 3(6k)^2 + 4(6k^2 - 6k)^2$$

$$= 54 + 144k - 144 + 96k^2 - 240k + 96 + 108k^2 + 144k^4 + 144k^2 - 288k^3$$

$$= 144k^4 - 288k^3 + 288k^2 - 96k + 6$$

Theorem 3

For Rhombus Oxide Network $RHOX(n)$,

$M_1(DS(RHOX(n))) = 9n^4 - 12n^3 + 68n^2 + 4n$,

$M_2(DS(RHOX(n))) = 45n^4 - 60n^3 + 218n^2 - 80n + 26$.

Proof:

The number of vertices in triangular oxide $|V(RHOX(n))| = 3n^2 + 2n$ and the number of edges $|E(RHOX(n))| = 6n^2$.

The number of 2 and 3 degree vertices is 4n and $3n^2 - 2n$ respectively.

Then there are 2 degree splitting vertices namely u_1 and u_2.

$$M_1\left(DS\left(RHOX(n)\right)\right) = \sum d(v)^2$$

$$= \sum_{i=1}^{3n^2+2n} d(v_i)^2 + d(u_1)^2 + d(u_2)^2$$

$$= \sum_{i=1}^{4n} 3^2 + \sum_{i=1}^{3n^2-2n} 4^2 + (4n)^2$$

$$+ (3n^2 - 2n)^2$$

$$= 3^2(4n) + 4^2(3n^2 - 2n) + 16n^2 + 9n^4$$

$$+ 4n^2 - 12n^3$$

$$= 9n^4 - 12n^3 + 68n^2 + 4n$$

$$M_2\left(DS\left(RHOX(n)\right)\right) = \sum_{uv \in E} d(u)d(v)$$

$$= \sum_{i=1}^{4} 3(3) + \sum_{i=1}^{4(2n-1)} 3(5)$$

$$+ \sum_{i=1}^{6n^2-8n+2} 5(5) + \sum_{i=1}^{4n} 3(4n)$$

$$+ \sum_{i=1}^{3n^2-2n} 5(3n^2 - 2n)$$

$$= 9(4) + 15(8n - 4)$$

$$+25(6n^2 - 8n + 2) + 12n(4n)$$

$$+5(3n^2 - 2n)^2$$

$$= 45n^4 - 60n^3 + 218n^2 - 80n + 26$$

Theorem 4

For Silicate Network SL_n,

$M_1(DS(SL_n)) = 117n^4 + 18n^3 + 654n^2 - 51n$,

$M_2(DS(SL_n)) = 711n^4 - 90n^3 + 1658n^2 - 321n$.

Proof:

The number of vertices in silicate network $|V(SL_n)| = 15n^2 + 3n$ and the number of edges $|E(SL_n)| = 36n^2$.

The number of 3 and 6 degree vertices is $6n^2 + 6n$ and $9n^2 - 3n$ respectively.

Then there are 2 degree splitting vertices namely u_1 and u_2.

$$M_1(DS(SL_n)) = \sum d(v)^2$$

$$= \sum_{i=1}^{15n^2+3n} d(v_i)^2 + d(u_1)^2 + d(u_2)^2$$

$$= \sum_{i=1}^{6n^2+6n} 4^2 + \sum_{i=1}^{9n^2-3n} 7^2 + (6n^2+6n)^2$$
$$+ (9n^2-3n)^2$$
$$= 4^2(6n^2+6n) + 7^2(9n^2-3n) + (6n^2+6n)^2$$
$$+ (9n^2-3n)^2$$
$$= 117n^4 + 18n^3 + 654n^2 - 51n$$

$$M_2(\,DS(SL_n)) = \sum_{uv\in E} d(u)d(v)$$
$$= \sum_{i=1}^{6n} 4(4) + \sum_{i=1}^{18n^2+6n} 4(7) + \sum_{i=1}^{18n^2-12n} 7(7)$$
$$+ \sum_{i=1}^{6n^2+6n} 3(6n^2+6n) + \sum_{i=1}^{9n^2-3n} 5(9n^2-3n)$$

$$= 16(6n) + 28(18n^2+6n)$$
$$+ 49(18n^2-12n) + 5(9n^2-3n)^2$$
$$+5(9n^2-3\mathrm{n})^2$$
$$= 711n^4 - 90n^3 + 1658n^2 - 321n$$

Theorem 5

For Triangular Silicate Network TSL_n,

$$M_1(\,DS(TSL_n)) = \frac{5n^4 - 6n^3 + 475n^2 - 266n + 338}{4}.$$

$$M_2(\,DS(TSL_n)) = \frac{29n^4 - 78n^3 + 2191n^2 - 3258n + 1576}{4}.$$

Proof:

The number of vertices in silicate network $|V(TSL_n)| = \frac{3n^2+3n+2}{2}$ and the number of edges $|E(TSL_n)| = \frac{3n^2+3n}{2}$.

The number of 3, 7 and 12 degree vertices is $n^2+3, 3n-3$ and $\frac{n^2-3n+2}{2}$ respectively.

Then there are 3 degree splitting vertices namely u_1, u_2 and u_3.

$$M_1(\,DS(TSL_n)) = \sum_{i=1}^{\frac{3n^2+3n+2}{2}} d(v_i)^2 + d(u_1)^2 + d(u_2)^2$$
$$+d(u_3)^2$$
$$= \sum_{i=1}^{n^2+3} 4^2 + \sum_{i=1}^{3n-3} 8^2 + \sum_{i=1}^{\frac{n^2-3n+2}{2}} 13^2$$
$$+(n^2+3)^2 + (3n-3)^2$$
$$+\left(\frac{n^2-3n+2}{2}\right)^2$$
$$= 4^2(n^2+3) + 8^2(3n-3)$$
$$+13^2\left(\frac{n^2-3n+2}{2}\right) + (n^2+3)^2$$
$$+(3n-3)^2 + \left(\frac{n^2-3n+2}{2}\right)^2$$
$$= \frac{5n^4 - 6n^3 + 475n^2 - 266n + 338}{4}$$

$$M_2(\,DS(TSL_n)) = \sum_{uv\in E} d(u)d(v)$$
$$= \sum_{i=1}^{3} 4(4) + \sum_{i=1}^{9n-3} 4(8)$$
$$+ \sum_{i=1}^{3n-3} 8(8) + \sum_{i=1}^{3n^2-9n+6} 4(13)$$
$$+ \sum_{i=1}^{6n-12} 8(13) + \sum_{i=1}^{3\left(\frac{n^2-5n+6}{2}\right)} 13(13)$$
$$+ \sum_{i=1}^{n^2+3} 4(n^2+3) + \sum_{i=1}^{3n-3} 8(3n-3)$$
$$+ \sum_{i=1}^{\frac{n^2-3n+2}{2}} 13\left(\frac{n^2-3n+2}{2}\right)$$

$$= 16(3) + 32(9n-3) + 64(3n-3)$$
$$+52(3n^2-9n+6) + 104(6\mathrm{n}-12)$$
$$+169\left(\frac{3n^2-15n+18}{2}\right) + 4(n^2+3)^2$$
$$+8(3n+3)^2 + 13\left(\frac{n^2-3n+2}{2}\right)^2$$
$$= \frac{29n^4 - 78n^3 + 2191n^2 - 3258n + 1576}{4}$$

Theorem 6

For Chain Silicate Network $CS_n, n \geq 2$,

$M_1(\,DS(CS_n)) = 5n^2 + 87n - 12$, $M_2(\,DS(CS_n)) = 23n^2 - 179n - 67$.

Proof:

The number of vertices in hexagonal network$|V(CS_n)| = 3n + 1$ and the number of edges $|E(CS_n)| = 6n$.

The number of 3 and 6 degree vertices is$2n + 2$ and $n - 1$ respectively.

Then there are 2 degree splitting vertices namely $u_1$and u_2.

$$M_1(\,DS(CS_n)) = \sum d(v)^2$$
$$= \sum_{i=1}^{3n+1} d(v_i)^2 + d(u_1)^2 + d(u_2)^2$$
$$= \sum_{i=1}^{2n+2} 4^2 + \sum_{i=1}^{n-1} 7^2 + (2n+2)^2 + (n-1)^2$$
$$= 16(2n+2) + 49(n-1) + 4n^2 + 8\text{n} + 4$$
$$+ n^2 - 2\text{n} + 1$$
$$= 5n^2 + 87n - 12$$

$$M_2(\,DS(CS_n)) = \sum_{uv\in E} d(u)d(v)$$
$$= \sum_{i=1}^{n+4} 4(4) + \sum_{i=1}^{4n-2} 7(4) + \sum_{i=1}^{n-2} 7(7)$$
$$+ \sum_{i=1}^{2n+2} 4(2n+2)$$
$$+ \sum_{i=1}^{n-1} 7(n-1)$$
$$= 16(n+4) + 28(4n-2) + 49(n-2)$$
$$+ 4(2n+2)^2 + 7(\text{n}-1)^2$$
$$= 23n^2 - 179n - 67$$

Theorem 7

For Triangular oxide network, $M_1(\,DS(TOX_n)) = \frac{n^4-6n^3+147n^2-78n+80}{4}$,

$$M_2(\,DS(TOX_n)) = \frac{7n^4 - 42n^3 + 565n^2 - 774n + 460}{4}.$$

Proof:

The number of vertices in triangular oxide $|V(TOX_n)| = \frac{(n+1)(n+2)}{2}$ and the number of edges $|E(TOX_n)| = \frac{3(n+1)}{2}$.

The number of 3, 5 and 7 degree vertices is 3, 3(n-1) and $\frac{(n-1)(n-2)}{2}$ respectively.

Then there are 3 degree splitting vertices namely $u_1, u_2$and u_3.

$$M_1(\,DS(TOX_n)) = \sum_{i=1}^{\frac{(n+1)(n+2)}{2}} d(v_i)^2 + d(u_1)^2 + d(u_2)^2 + d(u_3)^2$$
$$= \sum_{i=1}^{3} 3^2 + \sum_{i=1}^{3(n-1)} 5^2 + \sum_{i=1}^{\frac{(n-1)(n-2)}{2}} 7^2 + 3^2$$
$$+(3(n-1))^2 + \left(\frac{(n-1)(n-2)}{2}\right)^2$$
$$= 3^2(3) + 5^2(3n-3)$$
$$+7^2\left(\frac{(n-1)(n-2)}{2}\right) + 9 + (3n-3)^2$$
$$+ \left(\frac{(n-1)(n-2)}{2}\right)^2$$
$$= 9(3) + 25(3n-3)$$
$$+49\left(\frac{(n-1)(n-2)}{2}\right) + 9 + 9n^2$$
$$+9 - 18\text{n} + \left(\frac{n^2-3n+2}{2}\right)^2$$
$$= \frac{n^4 - 6n^3 + 147n^2 - 78n + 80}{4}$$

$$M_2(\,DS(TOX_n)) = \sum_{uv\in E} d(u)d(v)$$
$$= \sum_{i=1}^{6} 3(5) + \sum_{i=1}^{3(n-1)} 5(5)$$
$$+ \sum_{i=1}^{6(n-2)} 5(7) + \sum_{i=1}^{\frac{3(n-3)(n-2)}{2}} 7(7)$$
$$+ \sum_{i=1}^{3} 3(3) + \sum_{i=1}^{3n-3} 5(3n-3)$$
$$+ \sum_{i=1}^{\frac{(n-1)(n-2)}{2}} 7\left(\frac{(n-1)(n-2)}{2}\right)$$
$$= 15(6) + 25(3n-3) + 35(6n-12)$$
$$+49\frac{3(n-3)(n-2)}{2}$$

$$+9(3)+5(3n-3)^2+7\left(\frac{(n-1)(n-2)}{2}\right)^2$$
$$=\frac{7n^4-42n^3+565n^2-774n+460}{4}.$$

Theorem 8

For Hexagonal Network HX_n,

$M_1(DS(HX_n)) = 9n^4-54n^3+306n^2-561n+368,$

$M_2(DS(HX_n)) = 63n^4-378n^3+1482n^2-2649n+1795.$

Proof:

The number of vertices in hexagonal network$|V(HX_n)| = 3n^2-3n+1$ and the number of edges $|E(HX_n)| = 9n^2-15n+6.$

The number of 3, 4 and 6 degree vertices is6, $6n-12$ and $3n^2-9n+7$ respectively.

Then there are 3 degree splitting vertices namely u_1,$u_2$and u_3.

$$M_1\big(DS(HX_n)\big) = \sum_{i=1}^{3n^2-3n+1} d(v_i)^2+d(u_1)^2+d(u_2)^2+d(u_3)^2$$
$$=\sum_{i=1}^{6}4^2+\sum_{i=1}^{6n-12}5^2+\sum_{i=1}^{3n^2-9n+7}7^2+6^2$$
$$+(6n-12)^2+(3n^2-9n+7)^2$$

$$=4^2(6)+5^2(6n-12)+7^2(3n^2-9n+7)+(6n-12)^2+(3n^2-9n+7)^2$$

$$=9n^4-54n^3+306n^2-561n+368$$

$$M_2\big(DS(HX_n)\big)=\sum_{uv\in E} d(u)d(v)$$
$$=\sum_{i=1}^{12}4(5)+\sum_{i=1}^{6}4(7)+\sum_{i=1}^{6n-18}5(5)$$
$$+\sum_{i=1}^{9n^2-33n+30}7(7)+\sum_{i=1}^{6}4(6)+\sum_{i=1}^{12n-24}5(7)$$
$$+\sum_{i=1}^{6n-12}5(6n-12)$$
$$+\sum_{i=1}^{3n^2-9n+7}7(3n^2-9n+7)$$
$$=20(12)+28(6)+25(6n-18)$$
$$+35(12n-24)^2+4(6)^2$$
$$+5(6n-12)^2+49(9n^2-33n+30)$$
$$+7(3n^2-9n+7)^2$$
$$=63n^4-378n^3+1482n^2-2649n$$
$$+1795$$

Theorem 9

For Honey Comb Network HC_n,

$M_1(DS(HC_n)) = 36n^4-72n^3+168n^2-42n,$

$M_2(DS(HC_n)) = 144n^4-288n^3+576n^2-96n+6.$

Proof:

The number of vertices in hexagonal network$|V(HC_n)| = 6n^2$ and the number of edges $|E(HC_n)| = 9n^2-3n.$

The number of 2 and 3 degree vertices is$6n$ and $6n^2-6n$ respectively.

Then there are 2 degree splitting vertices namely $u_1$and u_2.

$$M_1\big(DS(HC_n)\big)=\sum_{i=1}^{6n^2} d(v_i)^2+d(u_1)^2+d(u_2)^2$$
$$=\sum_{i=1}^{6n}3^2+\sum_{i=1}^{6n^2-6n}4^2+(6n)^2+(6n^2-6n)^2$$
$$=9(6n)+16(6n^2-6n)+36n^2+36n^4$$
$$-72n^3+36n^2$$
$$=36n^4-72n^3+168n^2-42n$$

$$M_2\big(DS(HC_n)\big)=\sum_{uv\in E} d(u)d(v)$$
$$=\sum_{i=1}^{6}3(3)+\sum_{i=1}^{12n-12}3(4)$$
$$+\sum_{i=1}^{9n^2-15n+6}4(4)+\sum_{i=1}^{6n}3(6n)$$
$$+\sum_{i=1}^{6n^2-6n}4(6n^2-6n)$$
$$=9(6)+12(12n-12)$$
$$+16(9n^2-15n+6)+3(6n)^2$$
$$+4(6n^2-6n)^2$$
$$=144n^4-288n^3+576n^2-96n+6$$

ACKNOWLDEGEMENT
This work is supported by Institutional Fund, Mannar Thirumalai Naicker College, Madurai

REFERENCES

[1]. J. Braun, A. Kerber, M. Meringer, C. Rucker **Similarity of molecular descriptors: the equivalence of Zagreb indices and walk counts,** MATCH Commun. Math. Comput. Chem., 54 (2005), pp. 163-176.

[2]. K.C. Das and I. Gutman, **Some properties of the second Zagreb index**, MATCH Commun. Math. Comput. Chem 52 (2004), no. 1, 103–112.

[3]. Gao . W., Farahani, M. R., Shi, L., 2016a. **Forgotten topological index of some drug structures**,Acta Med. Medit.

[4]. Gao. W, Muhammad Kamran Siddiqui, Muhammad Imran, Mohamad Kamran Jamil, Mohammad Reza Farahani, **Forgotten topological index of chemical structure in drugs**, Saudi Pharmaceutical Journal, 2016.

[5]. I. Gutman, O. Polansky, **Mathematical Concepts in Organic Chemistry**, Springer-Verlag, Berlin, 1986.

[6]. V.R.Kulli, **On the sum connectivity reverse index of oxide and honeycomb networks**, Journal of computer and Mathematical Sciences,8(9)(2017) 408-413.

[7]. V.R.Kulli, **Some topological indices of certain nanotubes**, Journal of Computer and Mathematical Sciences, 2018.

[8]. V.R.Kulli, **Ravan indices and their polynomials of certain rhombus networks**, International Journal of Current Research in Life Sciences, 7(5), May 2018 2110-2116.

[9]. F. Harary, **Graph Theory**, Addison-Wesley, Reading, Mass, (1969).

[10]. R. Ponraj and S. Soma Sundaram, **On the Degree Splitting of a Graphs**, NATL. ACAD. SCI. LETT., Vol-27, No.7 & 8, pp. 275 – 278, 2004.

[11]. S.Ragavi, **The First and Second Zagreb Indices of Degree Splitting of Graphs**, IJMTT, Volume-65 Issue-2 (2019),pp.31-36.

[12]. S.Ragavi, The First and Second Zagreb indices of some special types of graphs, Indian Journal of Applied Research, Volume 9, Issue 4, March 2019.

[13]. E. Sampathkumar and H.B.Walikar, **On the splitting of a graph**, The Karnataka University Journal Science Vol.XXV& XXVI (Combined) 1980-1981. Pp 13-16.