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Some Gourava Indices and Inverse Sum Indeg Index of Graphene andSilicate Networks

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Abstract: In chemical sciences, the topological indices are used in the analysis of drug molecular structure. These indices are helpful for chemical scientists to find out the chemical and biological characteristics of drugs. In this paper we compute first and second gourava indices, sum and product connectivity gourava indices, first and second hyper gourava indices and inverse sum indeg index of graphene and silicate networks are computed.

Keywords: First and second gourava indices, sum and product connectivity gourava indices, first and second hyper gourava indices, inverse sum indeg index, graphene, silicate networks.

1. Introduction

Topological index is the numerical value, which is used to characterize the physical and chemical nature of chemical molecules and they help us to predict certain physicochemical properties like boiling point, enthalpyof vaporization, stability, and so forth.[1]

Graphene is an atomic scale honeycomb lattice made of carbon atoms. It is the world's first 2D materialwhich was isolated from graphite in the year 2004 by Professor Andre Geim and Professor Kostya Novoselov. Graphene is 200 times stronger than steel, one million times thinner than a human hair, and world's most conductive material. So it has captured the attention of scientists, researchers, and industries worldwide. It is one of the most promising nanomaterials because of its unique combination of superb properties, which opens a way for its exploitation in a wide spectrum of applications ranging from electronics to optics, sensors, and biodevices. Also it is the most effective material for electromagnetic interference (EMI) shielding.[2]

Silicates are obtained by fusing metal oxide or metal carbonates with sand. A silicate network is symbolized by SL_n,where n is the number of hexagons between the center and boundary of SL_n.

Let G be a simple connected graph with vertex set V(G) and edge set E(G). Let $d_u(G)$ denotes the degree of the vertex u in G . $|V(G)|$ and $|E(G)|$ respectively denote the number of vertices and the number of edges in the graph G. [3]

Definition 1.1. The first and second Gourava indices were introduced by Kulli.[5] and are defined as,

$$GO_1(G) = \sum_{uv \in E} d_u + d_v + d_u.d_v \tag{1}$$

$$GO_2(G) = \sum_{uv \in E} (d_u + d_v).(d_u.d_v) \tag{2}$$

Definition 1.2. The sum connectivity gourava index[7] of a graph G is given by,

$$SGO(G) = \sum_{uv \in E} \frac{1}{\sqrt{d_u + d_v + d_u.d_v}} \tag{3}$$

Definition 1.3. The product connectivity gourava index[8] of a graph G is defined as,

$$PGO(G) = \sum_{uv \in E} \frac{1}{\sqrt{(d_u + d_v).(d_u.d_v)}} \tag{4}$$

Definition 1.4. The first and second hyper - gourava indices[6] are defined as,

$$HGO_1(G) = \sum_{uv \in E} [d_u + d_v + d_u.d_v]^2 \tag{5}$$

$$HGO_2(G) = \sum_{uv \in E} [(d_u + d_v).(d_u.d_v)]^2 \tag{6}$$

Definition 1.5. The Inverse sum indeg index[4] of a graph G is defined as,

$$ISI(G) = \sum_{uv \in E} \frac{d_u.d_v}{d_u + d_v} \tag{7}$$

2. Main Results

Two-dimensional structure of Graphene with n benzene rings in each of m rows is shown in figure 1. On the basis of degree of end vertices of each edge, there are three types of edges in the edge partition of Graphene.In the first type, the degree of both the end vertices u and v is 2, In the second type, the degree of the end vertices u and v as 2 and 3 respectively and in the third type, the degree of end vertices u and v as 3 and 3 respectively. Thus the edge partition of graphene is given in table(1).

A two-dimensional silicate network is shown in Figure 2. It is easy to see that the vertices of SL_n are either of degree three or six. Based on the degree of end vertices the edges of SL_n are divided into three types, first set of edges with degree of end vertices three, second set of edges with degree of end vertices three and six, and third set of edges with degree of end vertices six. The edge partition of SL_n is given in table(2).

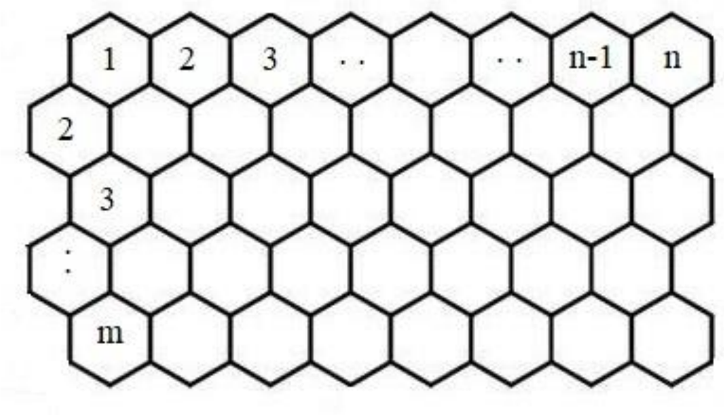

Figure 1: Schematic representation of side view of a monolayer of Graphene

(d_u, d_v) for $uv \in E(G)$	Number of edges
(2, 2)	$m + 4$
(2, 3)	$2m + 4n - 4$
(3, 3)	$3mn - 2n - m - 1$

Table 1: Edge partition of Graphene

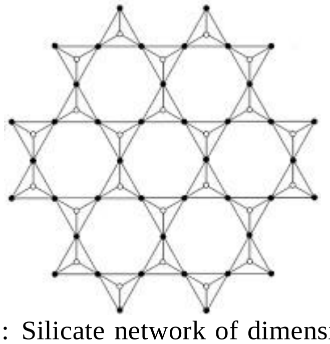

Figure 2: Silicate network of dimension two

Theorem 2.1. The first and second gourava indices, sum and product connectivity gourava indices of graphene(G)are given by

(i) $GO_1(G) = 45mn + 15m + 14n - 27$
(ii) $GO_2(G) = 162mn + 22m + 12n - 110$
(iii) $SGO(G) = 0.7746mn + 0.6984m + 0.6896n - 0.05$
(iv) $PGO(G) = 0.4082mn + 0.4791m + 0.4581n - 0.1336$

Proof. (i) from (1) , $GO_1(G) = \sum_{uv \in E} d_u + d_v + d_u.d_v$

using table(1) we get

$$GO_1(G) = (m + 4)(2 + 2 + 2.2) + (2m + 4n - 4)(2 + 3 + 2.3) + (3mn - 2n - m - 1)(3 + 3 + 3.3)$$

$\therefore GO_1(G) = 45mn + 15m + 14n - 27.$

(ii) from (2), $GO_2(G) = \sum_{uv \in E} (d_u + d_v).(d_u.d_v)$

using table(1) we get

$$GO_2(G) = (m + 4)(2 + 2)(2.2) + (2m + 4n - 4)(2 + 3)(2.3) + (3mn - 2n - m - 1)(3 + 3)(3.3)$$

$\therefore GO_2(G) = 162mn + 22m + 12n - 110.$

(iii) from (3), $SGO(G) = \sum_{uv \in E} \frac{1}{\sqrt{d_u + d_v + d_u.d_v}}$

(d_u, d_v) for $uv \in E(G)$	Number of edges
(3, 3)	$6n$
(3, 6)	$18n^2 + 6n$
(6, 6)	$18n^2 - 12n$

Table 2: Edge partition of SLn

using table(1) we get

$$SGO(G) = (m+4)\frac{1}{\sqrt{2+2+2.2}} + (2m+4n-4)\frac{1}{\sqrt{2+3+2.3}} + (3mn-2n-m-1)\frac{1}{\sqrt{3+3+3.3}}$$

$\therefore SGO(G) = 0.7746mn + 0.6984m + 0.6896n - 0.05.$

(iv) from (4), $PGO(G) = \sum_{uv \in E} \frac{1}{\sqrt{(d_u + d_v).(d_u.d_v)}}$

using table(1) we get

$$PGO(G) = (m+4)\frac{1}{\sqrt{(2+2)(2.2)}} + (2m+4n-4)\frac{1}{\sqrt{(2+3)(2.3)}} + (3mn-2n-m-1)\frac{1}{\sqrt{(3+3)(3.3)}}$$

$\therefore PGO(G) = 0.4082mn + 0.4791m + 0.4581n - 0.1336.$

□

Theorem 2.2. The first and second hyper gourava indices and inverse sum indeg index of graphene(G) aregiven by

(i) HGO1(G) = 675mn + 81m + 34n − 453
(ii) HGO2(G) = 6588mn − 140m − 792n − 4772
(iii) ISI(G) = $\frac{1}{10}$[45mn + 19m + 18n − 23]

Proof. (i) from (5) , $HGO_1(G) = \sum_{uv \in E} [d_u + d_v + d_u.d_v]^2$
using table(1) we get

$HGO_1(G) = (m + 4)(2 + 2 + 2.2)^2 + (2m + 4n - 4)(2 + 3 + 2.3)^2 + (3mn - 2n - m - 1)(3 + 3 + 3.3)^2$

$\therefore HGO_1(G) = 675mn + 81m + 34n - 453.$

(ii) from (6), $HGO_2(G) = \sum_{uv \in E} [(d_u + d_v).(d_u.d_v)]^2$

using table(1) we get

$HGO_2(G) = (m + 4)((2 + 2)(2.2))^2 + (2m + 4n - 4)((2 + 3)(2.3))^2 + (3mn - 2n - m - 1)((3 + 3)(3.3))^2$

$\therefore HGO_2(G) = 6588mn - 140m - 792n - 4772.$

(iii) from (7), $ISI(G) = \sum_{uv \in E} \frac{d_u.d_v}{d_u + d_v}$

using table(1) we get

$$ISI(G) = (m + 4)\left(\frac{2.2}{2+2}\right) + (2m + 4n - 4)\left(\frac{2.3}{2+3}\right) + (3mn - 2n - m - 1)\left(\frac{3.3}{3+3}\right)$$
$$\therefore ISI(G) = \frac{1}{10}[45mn + 19m + 18n - 23].$$

Theorem 2.3. The first and second gourava indices, sum and product connectivity gourava indices of silicatenetwork(SL_n) are given by

(i) $GO_1(SL_n) = 1350n^2 - 324n$
(ii) $GO_2(SL_n) = 9972n^2 - 3888n$
(iii) $SGO(SL_n) = 6.0621n^2 + 0.9718n$
(iv) $PGO(SL_n) = 2.2802n^2 - 0.7105n$

Proof. (i) from (1) , $GO_1(G) = \sum_{uv \in E} d_u + d_v + d_u.d_v$
using table(2) we get

$GO_1(SL_n) = (6n)(3 + 3 + 3.3) + (18n^2 + 6n)(3 + 6 + 3.6) + (18n^2 - 12n)(6 + 6 + 6.6)$

$\therefore GO_1(SL_n) = 1350n^2 - 324n.$

(ii) from (2), $GO_2(G) = \sum_{uv \in E} (d_u + d_v).(d_u.d_v)$

using table(2) we get

$GO_2(SL_n) = (6n)(3 + 3)(3.3) + (18n^2 + 6n)(3 + 6)(3.6) + (18n^2 - 12n)(6 + 6)(6.6)$

$\therefore\ GO_2(SL_n) = 9972n^2 - 3888n.$

(iii) from (3), $SGO(G) = \sum_{uv \in E} \frac{1}{\sqrt{d_u + d_v + d_u.d_v}}$

using table(2) we get

$$SGO(SL_n) = (6n)\frac{1}{\sqrt{3+3+3.3}} + (18n^2 + 6n)\frac{1}{\sqrt{3+6+3.6}} + (18n^2 - 12n)\frac{1}{\sqrt{6+6+6.6}}$$

$\therefore\ SGO(SL_n) = 6.0621n^2 + 0.9718n.$

(iv) from (4), $PGO(G) = \sum_{uv \in E} \frac{1}{\sqrt{(d_u + d_v).(d_u.d_v)}}$

using table(2) we get

$$PGO(SL_n) = (6n)\frac{1}{\sqrt{(3+3)(3.3)}} + (18n^2 + 6n)\frac{1}{\sqrt{(3+6)(3.6)}} + (18n^2 - 12n)\frac{1}{\sqrt{(6+6)(6.6)}}$$

$\therefore\ PGO(SL_n) = 2.2802n^2 - 0.7105n.$

Theorem 2.4. The first and second hyper gourava indices and inverse sum indeg index of silicate network (SL_n)are given by

(i) $HGO_1(SL_n) = 54594n^2 - 21924n$
(ii) $HGO_2(SL_n) = 3831624n^2 - 2064528n$
(iii) $ISI(SL_n) = 90n^2 - 15n$

Proof. (i) from (5) , $HGO_1(G) = \sum_{uv \in E} [d_u + d_v + d_u.d_v]^2$

using table(2) we get

$HGO_1(SL_n) = (6n)(3 + 3 + 3.3)^2 + (18n^2 + 6n)(3 + 6 + 3.6)^2 + (18n^2 - 12n)(6 + 6 + 6.6)^2$

$\therefore\ HGO_1(SL_n) = 54594n^2 - 21924n.$

(ii) from (6), $HGO_2(G) = \sum_{uv \in E} [(d_u + d_v).(d_u.d_v)]^2$

using table(2) we get

$HGO_2(SL_n) = (6n)((3 + 3)(3.3))^2 + (18n^2 + 6n)((3 + 6)(3.6))^2 + (18n^2 - 12n)((6 + 6)(6.6))^2$

$\therefore\ HGO_2(SL_n) = 3831624n^2 - 2064528n.$

(iii) from (7), $ISI(G) = \sum_{uv \in E} \frac{d_u.d_v}{d_u + d_v}$

using table(2) we get

$$ISI(SL_n) = (6n)\left(\frac{3.3}{3+3}\right) + (18n^2 + 6n)\left(\frac{3.6}{3+6}\right) + (18n^2 - 12n)\left(\frac{6.6}{6+6}\right)$$

$\therefore ISI(SL_n) = 90n^2 - 15n.$

3. Conclusion

The problem of finding the general formula for first and second gourava indices, sum and product connectivity gourava indices, first and second hyper gourava indices and inverse sum indeg index of graphene and silicate networks is solved here analytically without using computers.

References

[1] I.Gutman and N.Trinajstic, Graph theory and molecular orbitals, Total π-electron energy of alternant hydrocarbons,Chem. Phys. Lett., 17(1972), 535-538.

[2] Geim, A. K.; Novoselov, K. S. (26 February 2007). ”The rise of graphene”. Nature Materials. 6 (3): 183–191.

[3] F. HARARY, “Graph Theory”, Addison-Wesley, 1969.

[4] Pattabiraman, K. (2018). Inverse sum indeg index of graphs. AKCE Int. J. Graphs Comb.15(2):155–167.

[5] V. R. Kulli, The Gourava indices and coindices of graphs, Annals of Pure and Applied Mathematics, 14(1),21- 26 (2017).

[6] V.R. Kulli, On hyper-Gourava indices and coindices, International Journal of Mathematical Archive, 8(12) (2017) 116-120.

[7] V.R.Kulli, On the sum connectivity Gourava index, International Journal of Mathematical Archive, 8(7) (2017) 211-217.

[8] V. R. Kulli, The product connectivity Gourava index, Journal of Computer and Mathematical Sciences, 8(6) (2017) 235-242.