

COMPUTING TWO ARITHMETIC-GEOMETRIC REVERSE INDICES OF CERTAIN NETWORKS

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ABSTRACT

In Chemical Science, the methods of topological index computation can help to find out the biological, chemical and medical information of drugs. In this paper, we propose the arithmetic-geometric reverse and multiplicative arithmetic-geometric reverse indices of a graph. Also we determine these reverse indices for silicate, chain silicate, hexagonal, oxide and honeycomb networks.

Keywords: arithmetic-geometric reverse index, multiplicative arithmetic-geometric reverse index, network.

Mathematics Subject Classification: 05C05, 05C07, 05C12.

1. INTRODUCTION

Chemical Graph Theory has an important effect on the development of Chemical Sciences. A topological index is a numerical parameter mathematically derived from the graph structure. Numerous topological indices have been considered in Theoretical Chemistry, especially in QSAR / QSPR study, see [1].

Let G be a finite, simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v . Let $\Delta(G)$ denote the maximum degree among the vertices of G . The reverse vertex degree of a vertex v in G is defined as $c_v = \Delta(G) - d_G(v) + 1$. The reverse edge connecting the reverse vertices u and v will be denoted by uv . For other undefined notations and terminology, readers are referred to [2].

Recently, Kulli [3] introduced the geometric-arithmetic reverse index of a graph G and it is defined as

$$GAC(G) = \sum_{uv \in E(G)} \frac{2\sqrt{c_u c_v}}{c_u + c_v}.$$

We now define the arithmetic - geometric reverse index of a graph as follows:

The arithmetic - geometric reverse index of a graph G is defined as

$$AGC(G) = \sum_{uv \in E(G)} \frac{c_u + c_v}{2\sqrt{c_u c_v}}. \quad (1)$$

In [4], Kulli introduced the multiplicative geometric-arithmetic reverse index of a graph G and it is defined as

$$GACII(G) = \prod_{uv \in E(G)} \frac{2\sqrt{c_u c_v}}{c_u + c_v}.$$

We now introduce the multiplicative arithmetic-geometric reverse index of a graph as follows:

The multiplicative arithmetic-geometric reverse index of a graph G is defined as

$$AGCII(G) = \prod_{uv \in E(G)} \frac{c_u + c_v}{2\sqrt{c_u c_v}}. \quad (2)$$

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For more information and recent results about reverse indices see [5, 6, 7]. Also some topological indices were studied, for example, in [8, 9].

Silicates are very important elements of Earth's crust. Sand and several minerals are constituted by silicates. The tetrahedron is a basic unit of silicates, in which the central vertex is silicon vertex and the corner vertices are oxygen vertices. For networks see [10]. In this paper, the arithmetic-geometric reverse index and the multiplicative arithmetic-geometric index of certain networks are computed.

2. RESULTS FOR SILICATE NETWORKS

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 . A 2-dimensional silicate network is presented in Figure 1.

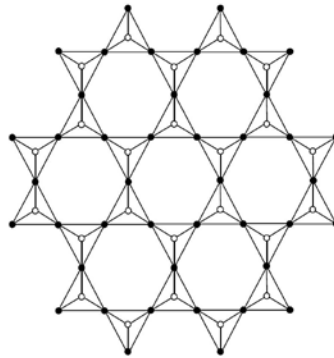


Figure-1: A 2-dimensional silicated network

Let G be the graph of a silicate network SL_n . From Figure 1, it is easy to see that the vertices of SL_n are either of degree 3 or 6. Therefore $\Delta(G) = 6$. Clearly we have $c_u = \Delta(G) - d_G(u) + 1 = 7 - d_G(u)$. The graph G has $15n^2 + 3n$ vertices and $36n^2$ edges. In G , by algebraic method, there are three types of edges based on the degree of end vertices of each edge as follows:

$$\begin{aligned} E_{33} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}, & |E_{33}| &= 6n. \\ E_{36} &= \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 6\}, & |E_{36}| &= 18n^2 + 6n. \\ E_{66} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 6\}, & |E_{66}| &= 18n^2 - 12n. \end{aligned}$$

Thus there are three types of reverse edges as given in Table 1.

$c_u, c_v \setminus uv \in E(G)$	(4, 4)	(4, 1)	(1, 1)
Number of edges	$6n$	$18n^2 + 6n$	$18n^2 - 12n$

Table-1: Reverse edge partition of SL_n

Theorem 1: The arithmetic-geometric reverse index of a silicate network SL_n is

$$AGC(SL_n) = \frac{81}{2}n^2 + \frac{3}{2}n.$$

Proof: Let G be the molecular graph of SL_n . By using equation (1) and Table 1, we deduce

$$\begin{aligned} AGC(SL_n) &= \sum_{uv \in E(G)} \frac{c_u + c_v}{2\sqrt{c_u c_v}} \\ &= \left(\frac{4+4}{2\sqrt{4 \times 4}} \right) 6n + \left(\frac{4+1}{2\sqrt{4 \times 1}} \right) (18n^2 + 6n) + \left(\frac{1+1}{2\sqrt{1 \times 1}} \right) (18n^2 - 12n) \\ &= \frac{81}{2}n^2 + \frac{3}{2}n. \end{aligned}$$

Theorem 2: The multiplicative arithmetic-geometric reverse index of a silicate network SL_n is

$$AGCH(SL_n) = \left(\frac{5}{4} \right)^{18n^2 + 6n}.$$

Proof: Let G be the molecular graph of SL_n . By using equation (2) and Table 1, we deduce

$$\begin{aligned}
 AGCH(SL_n) &= \prod_{uv \in E(G)} \frac{c_u + c_v}{2\sqrt{c_u c_v}} \\
 &= \left(\frac{4+4}{2\sqrt{4 \times 4}} \right)^{6n} + \left(\frac{4+1}{2\sqrt{4 \times 1}} \right)^{18n^2+6n} + \left(\frac{1+1}{2\sqrt{1 \times 1}} \right)^{18n^2-12n} \\
 &= \left(\frac{5}{4} \right)^{18n^2+6n}.
 \end{aligned}$$

3. RESULTS FOR CHAIN SILICATE NETWORKS

We now consider a family of chain silicate networks. This network is symbolized by CS_n and is obtained by arranging $n \geq 2$ tetrahedral linearly, see Figure 2.

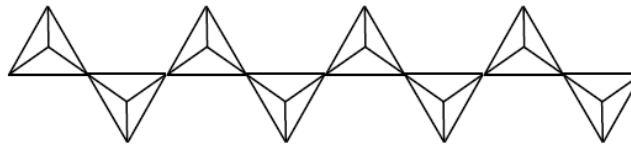


Figure-2: Chain silicate network

Let G be the graph of a chain silicate network CS_n with $3n+1$ vertices and $6n$ edges. From Figure 2, it is easy to see that the vertices of CS_n are either of degree 3 or 6. Therefore $\Delta(G) = 6$. Thus $c_u = \Delta(G) - d_G(u) + 1 = 7 - d_G(u)$. In G , by algebraic method, there are three types of edges based on the degree of end vertices of each edge as follows:

$$\begin{aligned}
 E_{33} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}, & |E_{33}| &= n + 4. \\
 E_{36} &= \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 6\}, & |E_{36}| &= 4n - 2. \\
 E_{66} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 6\}, & |E_{66}| &= n - 2.
 \end{aligned}$$

Thus there are three types of reverse edges as given in Table 2.

$c_u, c_v \setminus uv \in E(G)$	(4, 4)	(4, 1)	(1, 1)
Number of edges	$n + 4$	$4n - 2$	$n - 2$

Table-2: Reverse edge partition of CS_n

Theorem 3: The arithmetic-geometric reverse index of a chain silicate network CS_n is

$$AGC(CS_n) = 7n - \frac{1}{2}.$$

Proof: Let G be the molecular graph of CS_n . By using equation (1) and Table 2, we derive

$$\begin{aligned}
 AGC(CS_n) &= \sum_{uv \in E(G)} \frac{c_u + c_v}{2\sqrt{c_u c_v}} \\
 &= \left(\frac{4+4}{2\sqrt{4 \times 4}} \right)(n+4) + \left(\frac{4+1}{2\sqrt{4 \times 1}} \right)(4n-2) + \left(\frac{1+1}{2\sqrt{1 \times 1}} \right)(n-2) \\
 &= 7n - \frac{1}{2}.
 \end{aligned}$$

Theorem 4: The multiplicative arithmetic-geometric reverse index of a chain silicate network CS_n is

$$AGCH(CS_n) = \left(\frac{5}{4} \right)^{4n-2}.$$

Proof: Let G be the molecular graph of CS_n . By using equation (2) and Table 2, we derive

$$\begin{aligned}
 AGCH(CS_n) &= \prod_{uv \in E(G)} \frac{c_u + c_v}{2\sqrt{c_u c_v}} = \left(\frac{4+4}{2\sqrt{4 \times 4}} \right)^{n+4} \times \left(\frac{4+1}{2\sqrt{4 \times 1}} \right)^{4n-2} \times \left(\frac{1+1}{2\sqrt{1 \times 1}} \right)^{n-2} \\
 &= \left(\frac{5}{4} \right)^{4n-2}.
 \end{aligned}$$

4. RESULTS FOR HEXAGONAL NETWORKS

It is known that there exist three regular plane tilings with composition of some kind of regular polygons such as triangular, hexagonal and square. Triangular tiling is used in the construction of hexagonal networks. This network is symbolized by HX_n , where n is the number of vertices in each side of hexagon. A hexagonal network of dimension six is shown in Figure 3.

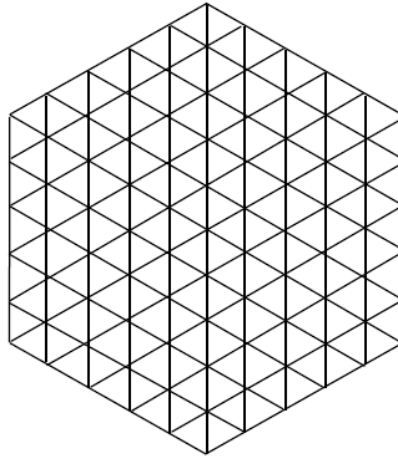


Figure-3: Hexagonal network of dimension six

Let G be the graph of a hexagonal network HX_n . The graph G has $3n^2-3n+1$ vertices and $9n^2-15n+6$ edges. From Figure 3, it is easy to see that the vertices of HX_n are either of degree 3, 4 or 6. Therefore $\Delta(G)=6$ and $\delta(G) = 3$. Thus $c_u = \Delta(G) - d_G(u) + 1 = 7 - d_G(u)$. In G , by algebraic method, there are five types of edges based on the degree of end vertices of each edge as follows:

$$\begin{aligned} E_{34} &= \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 4\}, & |E_{34}| &= 12. \\ E_{36} &= \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 6\}, & |E_{36}| &= 6. \\ E_{44} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 4\}, & |E_{44}| &= 6n - 18. \\ E_{46} &= \{uv \in E(G) \mid d_G(u) = 4, d_G(v) = 6\}, & |E_{46}| &= 12n - 24. \\ E_{66} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 6\}, & |E_{66}| &= 9n^2 - 33n + 30. \end{aligned}$$

Thus there are five types of reverse edges as given in Table 3.

$c_u, c_v \setminus uv \in E(G)$	(4, 3)	(4, 1)	(3, 3)	(3, 1)	(1, 1)
Number of edges	12	6	$6n - 18$	$12n - 24$	$9n^2 - 33n + 30$

Table-3: Reverse edge partition of HX_n

Theorem 5: The arithmetic-geometric reverse index of a hexagonal network HX_n is

$$AGC(HX_n) = 9n^2 + \left(\frac{24}{\sqrt{3}} - 27 \right) n + \frac{39}{2} - \frac{27}{\sqrt{3}}.$$

Proof: Let G be the molecular graph of HX_n . By using equation (1) and Table 3, we obtain

$$\begin{aligned} AGC(HX_n) &= \sum_{uv \in E(G)} \frac{c_u + c_v}{2\sqrt{c_u c_v}} \\ &= \left(\frac{4+3}{2\sqrt{4 \times 3}} \right) 12 + \left(\frac{4+1}{2\sqrt{4 \times 1}} \right) 6 + \left(\frac{3+3}{2\sqrt{3 \times 3}} \right) (6n - 18) + \left(\frac{3+1}{2\sqrt{3 \times 1}} \right) (12n - 24) \\ &\quad + \left(\frac{1+1}{2\sqrt{1 \times 1}} \right) (9n^2 - 33n + 30) \\ &= 9n^2 + \left(\frac{24}{\sqrt{3}} - 27 \right) n + \frac{39}{2} - \frac{27}{\sqrt{3}}. \end{aligned}$$

Theorem 6: The multiplicative arithmetic-geometric reverse index of a hexagonal network HX_n is

$$AGCII(HX_n) = \left(\frac{7}{4\sqrt{3}}\right)^{12} \times \left(\frac{5}{4}\right)^6 \times \left(\frac{2}{\sqrt{3}}\right)^{12n-24}.$$

Proof: Let G be the molecular graph of HX_n . By using equation (2) and Table 3, we obtain

$$\begin{aligned} AGCII(HX_n) &= \prod_{uv \in E(G)} \frac{c_u + c_v}{2\sqrt{c_u c_v}} \\ &= \left(\frac{4+3}{2\sqrt{4 \times 3}}\right)^{12} \times \left(\frac{4+1}{2\sqrt{4 \times 1}}\right)^6 \times \left(\frac{3+3}{2\sqrt{3 \times 3}}\right)^{6n-18} \\ &\quad \times \left(\frac{3+1}{2\sqrt{3 \times 1}}\right)^{12n-24} \times \left(\frac{1+1}{2\sqrt{1 \times 1}}\right)^{9n^2-33n+30} \\ &= \left(\frac{7}{4\sqrt{3}}\right)^{12} \times \left(\frac{5}{4}\right)^6 \times \left(\frac{2}{\sqrt{3}}\right)^{12n-24}. \end{aligned}$$

5. RESULTS FOR OXIDE NETWORKS

The oxide networks are of vital importance in the study of silicate networks. An oxide network of dimension n is denoted by OX_n . A 5-dimensional oxide network is shown in Figure 4.

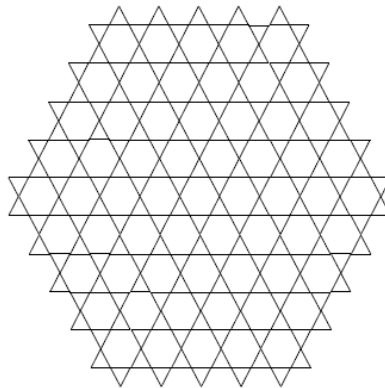


Figure-4: Oxide network of dimension 5

Let G be the graph of an oxide network OX_n . From Figure 4, it is easy to see that the vertices of OX_n are either of degree 2 or 4. Therefore $\Delta(G)=4$. Thus $c_u = \Delta(G) - d_G(u) + 1 = 5 - d_G(u)$. By calculation, we obtain that G has $9n^2+3n$ vertices and $18n^2$ edges. In G , by algebraic method, there are two types of edges based on the degree of end vertices of each edge as follows:

$$\begin{aligned} E_{24} &= \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 4\}, & |E_{24}| &= 12n. \\ E_{44} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 4\}, & |E_{44}| &= 18n^2 - 12n. \end{aligned}$$

Thus there are two types of reverse edges as given in Table 4.

$c_u, c_v \setminus uv \in E(G)$	(3, 1)	(1, 1)
Number of edges	$12n$	$18n^2 - 12n$

Table-4: Reverse edge partition of OX_n

Theorem 7: The arithmetic-geometric reverse index of an oxide network OX_n is

$$AGC(OX_n) = 18n^2 + \left(\frac{24}{\sqrt{3}} - 12\right)n.$$

Proof: Let G be the molecular graph of OX_n . By using equation (1) and Table 4, we deduce

$$\begin{aligned} AGC(OX_n) &= \sum_{uv \in E(G)} \frac{c_u + c_v}{2\sqrt{c_u c_v}} = \left(\frac{3+1}{2\sqrt{3 \times 1}}\right)12n + \left(\frac{1+1}{2\sqrt{1 \times 1}}\right)(18n^2 - 12n) \\ &= 18n^2 + \left(\frac{24}{\sqrt{3}} - 12\right)n. \end{aligned}$$

Theorem 8: The multiplicative arithmetic-geometric reverse index of an oxide network OX_n is

$$AGCII(OX_n) = \left(\frac{2}{\sqrt{3}} \right)^{12n}.$$

Proof: Let G be the molecular graph of OX_n . By using equation (2) and Table 4, we deduce

$$\begin{aligned} AGCII(OX_n) &= \prod_{uv \in E(G)} \frac{c_u + c_v}{2\sqrt{c_u c_v}} = \left(\frac{3+1}{2\sqrt{3 \times 1}} \right)^{12n} + \left(\frac{1+1}{2\sqrt{1 \times 1}} \right)^{18n^2-12n} \\ &= \left(\frac{2}{\sqrt{3}} \right)^{12n}. \end{aligned}$$

6. RESULTS FOR HONEYCOMB NETWORKS

Honeycomb networks are useful in Computer Graphics and Chemistry. A honeycomb network of dimension n is denoted by HC_n , where n is the number of hexagons between central and boundary hexagon. A 4-dimensional honeycomb network is shown in Figure 5.

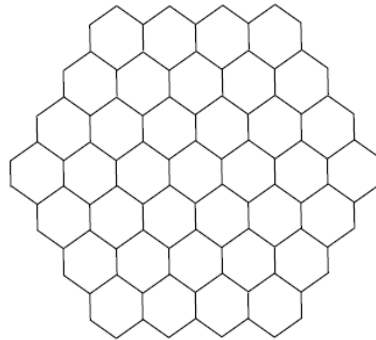


Figure-5: A 4-dimensional honeycomb network

Let G be the graph of a honeycomb network HC_n . From Figure 5, it is easy to see that the vertices of HC_n are either of degree 2 or 3. Thus $\Delta(G) = 3$. Therefore $c_u = \Delta(G) - d_G(u) + 1 = 4 - d_G(u)$. By calculation, we obtain that G has $6n^2$ vertices and $9n^2 - 3n$ edges. In G , by algebraic method, there are three types of edges based on the degree of end vertices of each edge as follows:

$$\begin{aligned} E_{22} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}, & |E_{22}| &= 6. \\ E_{23} &= \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}, & |E_{23}| &= 12n - 12. \\ E_{33} &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}, & |E_{33}| &= 9n^2 - 15n + 6. \end{aligned}$$

Thus there are three types of reverse edges as given in Table 5.

$c_u, c_v \setminus uv \in E(G)$	(2, 2)	(2, 1)	(1, 1)
Number of edges	6	$12n - 12$	$9n^2 - 15n + 6$

Table-5: Reverse edge partition of HC_n

Theorem 9: The arithmetic-geometric reverse index of a honeycomb network HC_n is

$$AGC(HC_n) = 9n^2 + \left(\frac{18}{\sqrt{2}} - 15 \right) n + 12 - \frac{18}{\sqrt{2}}.$$

Proof: Let G be the molecular graph of HC_n . By using equation (1) and Table 5, we deduce

$$\begin{aligned} AGC(HC_n) &= \sum_{uv \in E(G)} \frac{c_u + c_v}{2\sqrt{c_u c_v}} \\ &= \left(\frac{2+2}{2\sqrt{2 \times 2}} \right) 6 + \left(\frac{2+1}{2\sqrt{2 \times 1}} \right) (12n - 12) + \left(\frac{1+1}{2\sqrt{1 \times 1}} \right) (9n^2 - 15n + 6) \\ &= 9n^2 + \left(\frac{18}{\sqrt{2}} - 15 \right) n + 12 - \frac{18}{\sqrt{2}}. \end{aligned}$$

Theorem 10: The multiplicative arithmetic-geometric reverse index of a honeycomb network HC_n is

$$AGCII(HC_n) = \left(\frac{3}{2\sqrt{2}} \right)^{12n-12}.$$

Proof: Let G be the molecular graph of HC_n . By using equation (2) and Table 5, we obtain

$$\begin{aligned} AGCII(HC_n) &= \prod_{uv \in E(G)} \frac{c_u + c_v}{2\sqrt{c_u c_v}} = \left(\frac{2+2}{2\sqrt{2 \times 2}} \right)^6 + \left(\frac{2+1}{2\sqrt{2 \times 1}} \right)^{12n-12} + \left(\frac{1+1}{2\sqrt{1 \times 1}} \right)^{(9n^2-15n+6)} \\ &= \left(\frac{3}{2\sqrt{2}} \right)^{12n-12}. \end{aligned}$$

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