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On Certain Topological Indices of Silicate, Honeycomb and Hexagonal Networks

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ABSTRACT

In the QSAR /QSPR study, physicochemical properties and topological indices such as Randić, Zagreb, and ABC index are used to predict bioactivity of the chemical compounds. Graph theory has found considerable use in Chemistry, particularly in modeling chemical structures. Topological indices are designed basically by transforming a molecular graph into a number. In this paper we calculate the Randić, Zagreb, and ABC index of Silicate, honeycomb and hexagonal networks.

Keywords: Silicate Network, honeycomb network, hexagonal network, Randić index, Zagreb index, ABC index.

1. INTRODUCTION

Cheminformatics is new subject which is a combination of chemistry, mathematics and information science. It studies Quantitative structure-activity (QSAR) and structure-property (QSPR) relationships that are used to predict the biological activities and properties of chemical compounds. In the QSAR /QSPR study, physicochemical properties and topological indices such as Szeged, Wiener, Randić index, Zagreb index, ABC index are used to predict bioactivity of the chemical compounds.

Graph theory has found considerable use in Chemistry, particularly in modeling chemical structures. Topological indices are designed basically by transforming a molecular graph into a number. The first use of a topological index was made in 1947 by the chemist Harold Wiener. Wiener introduced the notion of path number of a graph as the sum of distances between any two carbon atoms in the molecules, in terms of carbon-carbon bonds[1]. In graph theoretical language, the Wiener index is equal to the count of all shortest distances in a graph[2]. This molecular modeling is used to investigate the relationships between

structure, properties and activity of chemical compounds.

In this paper we calculate the Randić index, Zagreb index and ABC index of Honeycomb and Hexagonal Networks.

Definition 1: For a graph G = (V, E), the *general Randić index* $R_\alpha(G)$ of G is defined as the sum of $(d_u d_v)^\alpha$ over all edges $e = uv$ of G where d_u denotes the degree of $\in V$, i.e.,

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha$$

It is well known that $R_{-1/2}$ was introduced by Randić[3] in 1975 as one of the many graph-theoretical parameters derived from the graph underlying some molecule. Like other successful chemical indices, this index has been closely correlated with many chemical properties. The general Randić index was proposed by Bollobás and Erdös[4], and Amic *et al.*[5], independently, in 1998. Then it has been extensively studied by both mathematicians and theoretical chemists[6]. Many important mathematical properties have been established[7]. For a survey of results, we refer to the new book by Li and Gutman[8].

The graph invariant ZG_2, known under the name second Zagreb index, equal to the sum of the products of the degrees of pairs of adjacent vertices of the respective graph, was first considered in 1972. Since then, almost no result for ZG_2 was communicated in either the chemical or in mathematical literature.

Definition 2: The second Zagreb index is defined as $ZG_2(G) = \sum_{(u,v)\in E(G)}(d_u d_v)$ where d_u and d_v are the degrees of u and v.

One of the best known topological indices is the branching index introduced by Randić[3] in 1975. But, many physico-chemical properties depend on factor rather than branching. In order to take physico-chemical properties into account, at the same time to keep the soul of Randić index, Estrada et al. proposed a new index, the atom-bond connectivity (ABC) index[9,10].

Definition 3: The atom-bond connectivity (ABC) index is defined as $ABC(G) = \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$, where d_u denotes the degree of a vertex u in G.

2. SILICATE NETWORKS

The silicates are the largest, the most interesting and the most complicated class of minerals by far. The basic chemical unit of silicates is the (SiO_4) tetrahedron. A silicate sheet is a ring of tetrahedrons which are linked by shared oxygen nodes to other rings in a two dimensional plane that produces a sheet-like structure

Silicates are obtained by fusing metal oxides or metal carbonates with sand. Essentially all the silicates contain SiO_4 tetrahedra. In chemistry, the corner vertices of SiO_4 tetrahedran represent oxygen ions and the center vertex represents the silicon ion. In graph theory, we call the corner vertices as *oxygen nodes* and the center vertex as *silicon node*. See Figure 1.

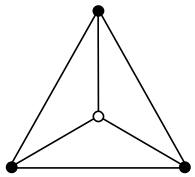

Figure 1: SiO_4 tetrahedra where the corner vertices represent oxygen ions and the center vertex the silicon ion

The minerals are obtained by successively fusing oxygen nodes of two tetrahedra of different silicates. The different types of silicate structure arise from the ways in which these tetrahedra are arranged: they may exist as separate unlinked entities, as linked finite arrays, as 1-dimensional chains, as 2-dimensional sheets or as 3-dimensional frameworks. Some of the structural units found in silicates are shown in Figures 2 and 3. They are termed orthosilicates, pyrosilicates, chain silicates, cyclic silicates and sheet silicates.

Figure 2: Different kinds of silicates

Simple orthosilicates contain discrete SiO_4 units. When two SiO_4 tetrahedra share an oxygen node, pyrosilicates are obtained. While tetrahedra are arranged linearly, chain silicates are obtained. See Figure 2.

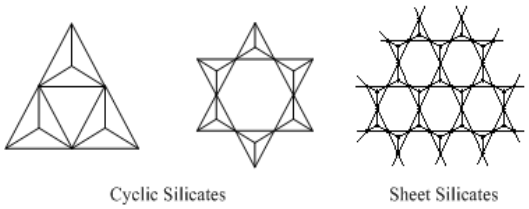

Figure 3: Cyclic and Sheet Silicates

A silicate network can be constructed in different ways. Here in this paper we describe the construction of a silicate network from a honeycomb network. Consider a honeycomb network $HC(n)$ of dimension$n$. Place silicon ions on all the vertices of $HC(n)$. Subdivide each edge of $HC(n)$ once. Place oxygen ions on the new vertices. Introduce $6n$ new pendant edges one each at the 2-degree silicon ions of $HC(n)$ and place oxygen ions at the pendent vertices. See Figure 4(a). With every silicon ion associate the three adjacent oxygen ions and form a tetrahedron as in Figure 4(b). The resulting network is a silicate network of dimension *n*, denoted $SL(n)$. The graph in Figure 4(b) is a silicate network of dimension two.

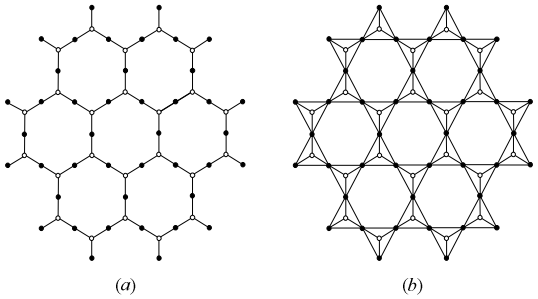

Figure 4: Silicate Network Construction

The number of nodes in $SL(n)$ is $15n^2 + 3n$. The number of edges of $SL(n)$ is $36n^2$. $SL(n)$ is a bi-regular graph. It has $6n^2 + 6n$ vertices of degree 3 and $9n^2 - 3n$ vertices of degree 6.

In a silicate network there are three types of edges based on the degree of the vertices of each edge. The following table gives the three types and gives the number of edges in each type.

(d_u, d_v) $where$ $u, v \in E(G)$	Total Number of edges
$(3,3)$	$6n$
$(3,6)$	$18n^2 + 6n$
$(6,6)$	$18n^2 - 12n$

From this table we have the following theorems.

Theorem 1: Let G be the silicate network $SL(n)$ of dimension n. Then the Randić index is

$R_{-1/2}(G) = (3 + 3\sqrt{2})n^2 + \sqrt{2}n$

Theorem 2: Let G be the silicate network $SL(n)$ of dimension n. Then the second Zagreb index is given by

$ZG_2(G) = 972n^2 - 270n$

Theorem 3: Let G be the silicate network $SL(n)$ of dimension n. Then the ABC index is given by

$ABC(G) = (\sqrt{10} + \sqrt{14})3n^2 + (4 + \sqrt{14} - 2\sqrt{10})n$

3. HEXAGONAL NETWORK

It is known that there exist three regular plane tessellations, composed of the same kind of regular polygons: triangular, square, and hexagonal. The triangular tessellation is used to define *Hexagonal network* and this is widely studied in[11].

A hexagonal network *HX(n)* of dimension n has $3n^2-3n+1$ vertices and $9n^2-15n+6$ edges, where n is the number of vertices on one side of the hexagon[11]. The diameter is $2n-2$. There are six vertices of degree three which we call as *corner vertices a, b, c, d, e, f*. See Figure 5. There is exactly one vertex *v* at distance $n-1$ from each of the corner vertices. This vertex is called the *centre* of *HX*(*n*) and is represented by *O*.

In a hexagonal network there are three types of vertices based on their degree. There are only 6 vertices with degree three. There are $6n-12$ vertices of degree 4. And there are $3n^2-9n+7$ vertices of degree six.

In a hexagonal network there are five types of edges based on the degree of the vertices of each edge. The following table gives the five types and gives the number of edges in each type.

(d_u, d_v) $where$ $u, v \in E(G)$	Total Number of edges
$(3,4)$	12
$(3,6)$	6
$(4,4)$	$6(n-3)$
$(4,6)$	$12(n-2)$
$(6,6)$	$9n^2-33n+30$

From this table we have the following theorems.

Theorem 4: Let G be the hexagonal network $HX(n)$ of dimension n. Then the Randić index is

$R_{-1/2} = \frac{3}{2}n^2 + (\sqrt{6}-4)n + \sqrt{2} + 2\sqrt{3}(1-\sqrt{2}) + \frac{1}{2}$

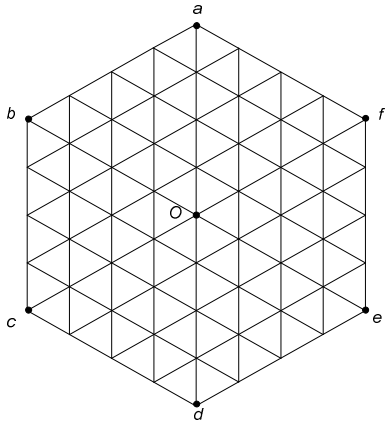

Figure 5: HX(5)

In the appendix, we also give the MATLAB coding to calculate the general Randić Index of $HX(n)$.

Theorem 5: Let G be the hexagonal network $HX(n)$ of dimension n. Then the second Zagreb index is given by

$$ZG_2 = 12(24n^2 - 56n + 29)$$

Theorem 6: Let G be the hexagonal network $HX(n)$ of dimension n. Then the ABC index is given by

$$ABC(G) = \frac{\sqrt{15}}{2}n^2 + \left(\frac{3\sqrt{6} + 8\sqrt{3} - 11\sqrt{10}}{2}\right)n + 22\sqrt{5} + 2\sqrt{42} - 27\sqrt{2} - 54$$

4. HONEYCOMB NETWORKS

Built recursively using the hexagon tessellation[12], honeycomb networks are widely used in computer graphics[12], cellular phone base stations[13], image processing, and in chemistry as the representation of benzenoid hydrocarbons. Honeycomb network $HC(n)$ is obtained from $HC(n-1)$ by adding a layer of hexagons around the boundary of $HC(n-1)$. The parameter n of $HC(n)$ is determined as the number of hexagons between the centre and boundary of $HC(n)$. See Figure 6. The number of vertices and edges of $HC(n)$ are $6n^2$ and $9n^2 - 3n$ respectively. The diameter is $4n - 1$[12].

All the carbon nanotubes are formed by folding a honeycomb sheet of infinite length in different ways. Or it is can be also considered as a graphite sheet when n is sufficiently large. Honeycomb network $HC(n)$ is a bounded dual of hexagonal network $HX(n+1)$.

In honeycomb network, there are $6n$ vertices of degree two and the remaining vertices are of degree 3.

In a honeycomb network there are three types of edges based on the degree of the vertices of each edge. The following table gives the three types and gives the number of edges in each type.

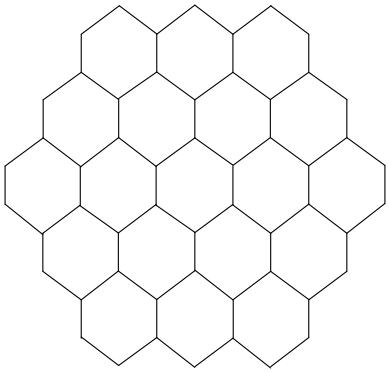

Figure 6: Honeycomb network of dimension 3

(d_u, d_v) $where$ $u, v \in E(G)$	Total Number of edges
$(2,2)$	6
$(2,3)$	$12(n-1)$
$(3,3)$	$(9n^2 - 15n + 6)$

From this table we have the following theorems.

Theorem 7: Let G be the honeycomb network $HC(n)$ of dimension n. Then the Randić index is

$$R_{-1/2} = 3n^2 + (2\sqrt{6} - 5)n + 5 - 2\sqrt{6}$$

Theorem 8: Let G be the honeycomb network $HC(n)$ of dimension n. Then the second Zagreb index is given by

$$ZG_2 = 3(27n^2 - 21n + 2)$$

Theorem 9: Let G be the honeycomb network $HC(n)$ of dimension n. Then the ABC index is given by

$$ABC(G) = 6n^2 + (6\sqrt{2} - 10)n + \frac{8 + 5\sqrt{2}}{2}$$

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