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Computation of Sombor Indices of Certain Networks

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Abstract: *In Chemical science, the topological index computation can help determine chemical, biological, pharmacological, toxicological, and technically relevant information on molecules. This paper introduces the modified Sombor index, reduced modified Sombor index, first and second reduced (a, b)-KA indices of a molecular graph and compute exact formulas for certain chemical importance species, like silicate, chain silicate, oxide, and graphene networks.*

Mathematics Subject Classification: 05*C*05, 05*C*07, 05*C*90.

Keywords: *Sombor index, modified Sombor index, reduced (a, b)-KA indices, network.*

I. INTRODUCTION

Chemical graph theory has an important effect on the development of chemical sciences. The single number that can characterize some property of the molecular graph is called a topological index or a graph index of that graph. Several such graph indices [1] have been considered and have found various applications, especially in QSPR/QSAR studies see [2, 3].

Let G be a finite, simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex u is the number of vertices adjacent to u.

The Sombor index was introduced by one of the present authors in [4], defined as

$$SO(G)=\sum_{uv\in E(G)}\sqrt{d_G(u)^2+d_G(v)^2}.$$

We now define the modified Sombor index of a graph G as

$$^{m}SO(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_G(u)^2+d_G(v)^2}}.$$

In [5], the first (a, b)-KA index of a graph was introduced and defined as

$$KA^{1}_{a,b}(G)=\sum_{uv\in E(G)}\left[d_G(u)^a+d_G(v)^a\right]^b$$

Where a and b are suitably chosen real-number parameters.

The reduced Sombor index was defined as [4]

$$RSO(G)=\sum_{uv\in E(G)}\sqrt{\left(d_G(u)-1\right)^2+\left(d_G(v)-1\right)^2}.$$

We propose the reduced, modified Sombor index of a graph G, and it is defined as

$$^{m}RSO(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{\left(d_G(u)-1\right)^2+\left(d_G(v)-1\right)^2}}.$$

Furthermore, we put toward the first and second reduced (a, b)-KA indices of a graph G, defined as

$$RKA^{1}_{a,b}II(G)=\sum_{uv\in E(G)}\left[\left(d_G(u)-1\right)^a+\left(d_G(v)-1\right)^a\right]^b,$$

$$RKA^{2}_{a,b}(G)=\sum_{uv\in E(G)}\left[\left(d_G(u)-1\right)^a\left(d_G(v)-1\right)^a\right]^b.$$

Recently some other reduced indices were studied in [6, 7].

In this paper, we compute the Sombor index, modified Sombor index, reduced Sombor index, reduced, modified Sombor index, and KA-indices of certain networks such as silicate, chain silicate, oxide, and graphene networks.

II. Results for Silicate Networks

Silicate networks are obtained by fusing metal oxide or metal carbonates with sand. A silicate network is denoted by SL_n, where n is the number of hexagons between the center and boundary of SL_n. A silicate network of dimension 2 is shown in Figure 1.

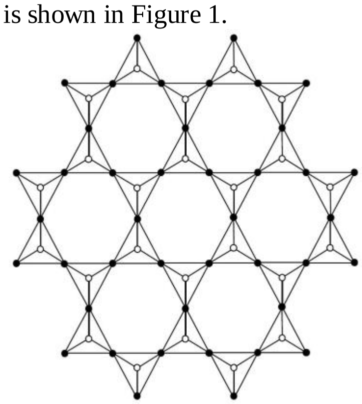

Figure 1. Silicate network of dimension two

Let G be the graph of SL_n. By calculation, we obtain that G has $15n^2+3n$vertices and $36n^2$edges. Also, by calculation, there are three types of edges in G based on the degree of end vertices of each edge, as in Table 1.

$d_G(u),d_G(v)\backslash$ $uv \in E(G)$	(3, 3)	(3,6)	(6, 6)
Number of edges	$6n$	$18n^2+6n$	$18n^2-12n$

Table 1.Edge partition of SL_n

In the following Theorem, we compute the first (a, b)-KA index of SL_n.

Theorem 1. The first (a, b)-KA index of a silicate network SL_n is

$$KA_{a,b}^1(SL_n)=\left(2\times 3^a\right)^b 6n+\left(3^a+6^a\right)^b\left(18n^2+6n\right)$$

Proof: By definition and by using Table 1, we deduce

$$KA_{a,b}^1(SL_n)=\sum_{uv\in E(G)}\left[d_G(u)^a+d_G(v)^a\right]^b$$
$$=\left(3^a+3^a\right)^b 6n+\left(3^a+6^a\right)^b\left(18n^2+6n\right)$$
$$+\left(6^a+6^a\right)^b\left(18n^2-12n\right)$$
$$=\left(2\times 3^a\right)^b 6n+\left(3^a+6^a\right)^b\left(18n^2+6n\right)$$
$$+\left(2\times 6^a\right)^b\left(18n^2-12n\right).$$

From Theorem 1, we obtain the following results.

Corollary 1.1. The Sombor index of SL_n is

$$SO(SL_n)=\left(\sqrt{5}-2\sqrt{2}\right)54n^2+\left(\sqrt{5}-3\sqrt{2}\right)18n.$$

Corollary 1.2. The modified Sombor index of SL_n is

$${}^mSO(SL_n)=\left(\frac{6}{\sqrt{5}}+\frac{3}{\sqrt{2}}\right)n^2\times\left(\frac{2}{\sqrt{5}}\right)n.$$

In the following Theorem, we compute the general reduced first (a, b)-KA index of SL_n.

Theorem 2. The first reduced (a, b)-KA index of SL_n is

$$RKA_{a,b}^1(SL_n)=\left(2\times 2^a\right)^b 6n+\left(2^a+5^a\right)^b\left(18n^2+6n\right)$$
$$+\left(2\times 5^a\right)^b\left(18n^2-12n\right).$$

Proof: By definition and Table 1, we deduce

$$RAK_{a,b}^1(SL_n)=\sum_{uv\in E(G)}\left[\left(d_G(u)-1\right)^a+\left(d_G(v)-1\right)^a\right]^b.$$
$$=\left[(3-1)^a+(3-1)^a\right]^b 6n$$
$$+\left[(3-1)^a+(6-1)^a\right]^b\left(18n^2+6n\right)$$
$$+\left[(6-1)^a+(6-1)^a\right]^b\left(18n^2-12n\right).$$
$$=\left(2\times 2^a\right)^b 6n+\left(2^a+5^a\right)^b\left(18n^2+6n\right)$$
$$+\left(2\times 5^a\right)^b\left(18n^2-12n\right).$$

Using Theorem 2, we establish the following results.

Corollary 2.1. The reduced Sombor index of SL_n is

$$SO(SL_n)=\left(\sqrt{29}+5\sqrt{2}\right)18n^2+\left(\sqrt{29}-8\sqrt{2}\right)6n.$$

Corollary 2.2. The reduced, modified Sombor index of SL_n is

$${}^mRSO(SL_n)=\left(\frac{1}{\sqrt{29}}+\frac{1}{5\sqrt{2}}\right)18n^2$$
$$+\left(\frac{2}{\sqrt{29}}+\frac{1}{\sqrt{2}}-\frac{4}{5\sqrt{2}}\right)3n.$$

III. Results for Chain Silicate Networks

In this section, we consider a family of chain silicate networks. This network is denoted by CS_n and is obtained by arranging n tetrahedral linearly, see Figure 2.

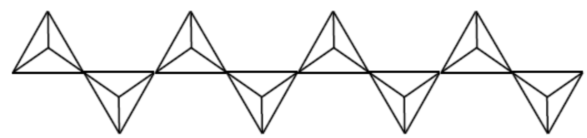

Figure 2.Chain silicate network

Let G be the graph of CS_n with $3n+1$ vertices and $6n$ edges. By calculation, there are three types of edges in CS_n, $(n \geq 2)$based on the degree of end vertices of each edge as given in Table 2.

$d_G(u),d_G(v)\backslash$ $uv \in E(G)$	(3, 3)	(3,6)	(6, 6)
Number of edges	$n+4$	$4n-2$	$n-2$

Table 2. Edge partition of CS_n

Theorem 3. The first (a, b)-KA index of CS_n is

$$KA_{a,b}^1(CS_n)=\left(2\times 3^a\right)^b(n+4)+\left(3^a+6^a\right)^b(4n-2)$$
$$+\left(2\times 6^a\right)^b(n-2).$$

Proof: Bydefinition and using Table 2, we derive

$$KA_{a,b}(CS_n)=\sum_{uv\in E(G)}\left[d_G(u)^a+d_G(v)^a\right]^b.$$
$$=\left(3^a+3^a\right)^b(n+4)+\left(3^a+6^a\right)^b(4n-2)$$
$$+\left(6^a+6^a\right)^b(n-2)+\left(2\times 6^a\right)^b(n-2).$$
$$=\left(2\times 3^a\right)^b(n+4)+\left(3^a+6^a\right)^b(4n-2)$$
$$+\left(2\times 6^a\right)^b(n-2).$$

By using Theorem 3, we establish the following results.

Corollary 3.1. The Sombor index of CS_n is

$$SO(CS_n)=\left(4\sqrt{5}+3\sqrt{2}\right)3n-6\sqrt{5}.$$

Corollary 3.2. The modified Sombor index of CS_n is

$${}^mSO(CS_n)=\left(\frac{1}{3\sqrt{2}}+\frac{4}{3\sqrt{5}}+\frac{1}{6\sqrt{2}}\right)n+\frac{1}{\sqrt{2}}-\frac{2}{3\sqrt{5}}.$$

Theorem 4. The first reduced (*a*, *b*)-*KA* index of CS_n is

$$RKA^1_{a,b}(CS_n) = (2\times 2^a)^b (n+4) + (2^a+5^a)^b (4n-2) + (2\times 5^a)^b (n-2).$$

Proof: By using the definition and Table 2, we obtain

$$RKA^1_{a,b}(CS_n) = \sum_{uv\in E(G)} \left[(d_G(u)-1)^a + (d_G(v)-1)^a\right]^b.$$

$$= \left[(3-1)^a + (3-1)^a\right]^b (n+4) + \left[(3-1)^a + (6-1)^a\right]^b (4n-2) + (2\times 5^a)^b (n-2).$$

$$= (2\times 2^a)^b (n+4) + (2^a+5^a)^b (4n-2) + (2\times 5^a)^b (n-2).$$

From Theorem 4, we get the following results.

Corollary 4.1. The reduced Sombor index of CS_n is

$$RSO(CS_n) = (7\sqrt{2} - 4\sqrt{29})n - 2\sqrt{2} - 2\sqrt{29}.$$

Corollary 4.2. The reduced, modified Sombor index of CS_n is

$$^m RSO(CS_n) = \left(\frac{1}{2\sqrt{2}} + \frac{4}{\sqrt{29}} + \frac{1}{5\sqrt{2}}\right)n + \frac{8}{5\sqrt{2}} - \frac{2}{\sqrt{29}}.$$

IV. Results for Oxide Networks

Oxide networks are of vital importance in the study of silicate networks. An oxide network of dimension *n* is denoted by OX_n. An oxide network of dimension five is presented in Figure 3.

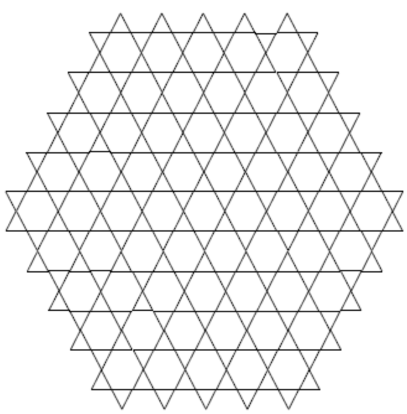

Figure 3. Oxide network of dimension five

Let *G* be the graph of OX_n. Then*G* has $9n^2+3n$ vertices and $18n^2$ edges. By calculation, there are two types of edges in OX_n based on the degree of end vertices of each edge, as given in Table 3.

$d_G(u),d_G(v) \backslash uv \in E(G)$	(2, 4)	(4, 4)
Number of edges	$12n$	$18n^2 - 12n$

Table 3. Edge partition of OX_n

Theorem 5. The first (*a*, *b*)-*KA* index of OX_n is

$$KA^1_{a,b}(OX_n) = (2^a+4^a)^b 12n + (2\times 4^a)^b (18n^2 - 12n).$$

Proof: By using the definition and Table 3, we deduce

$$KA^1_{a,b}(OX_n) = \sum_{uv\in E(G)} \left[d_G(u)^a + d_G(v)^a\right]^b.$$

$$= (2^a+4^a)^b 12n + (4^a+4^a)^b (18n^2-12n)$$

$$= (2^a+4^a)^b 12n + (2\times 4^a)^b (18n^2-12n).$$

From Theorem 5, we get the following results.

Corollary 5.1. The Sombor index of OX_n is

$$SO(OX_n) = 72\sqrt{2}n^2 + (\sqrt{5} - 2\sqrt{2})24n.$$

Corollary 5.2. The modified Sombor index of OX_n is

$$^m SO(OX_n) = \frac{9}{2\sqrt{2}} n^2 + \left(\frac{6}{\sqrt{5}} - \frac{3}{\sqrt{2}}\right)n.$$

Theorem 6. The first reduced (*a*, *b*)-*KA* index of OX_n is

$$RKA^1_{a,b}(OX_n) = (1+3^a)^b 12n + (2\times 3^a)^b (18n^2-12n).$$

Proof: By using the definition and Table 3, we have

$$RKA^1_{a,b}(OX_n) = \sum_{uv\in E(G)} \left[(d_G(u)-1)^a + (d_G(v)-1)^a\right]^b.$$

$$= \left[(2-1)^a + (4-1)^a\right]^b 12n + \left[(4-1)^a + (4-1)^a\right]^{bb} (18n^2-12n).$$

$$= (1+2^a)^b 12n + (2\times 3^a)^b (18n^2-12n).$$

Using Theorem 6, we obtain the following results.

Corollary 6.1. The reduced Sombor index of OX_n is

$$RSO(OX_n) = 54\sqrt{2}n^2 + (\sqrt{10} - 3\sqrt{2})n.$$

Corollary 6.2. The reduced, modified Sombor index of OX_n is

$$^m RSO(OX_n) = \left(\frac{1}{\sqrt{2}}\right)6n^2 \times \left(\frac{1}{\sqrt{10}} - \frac{1}{3\sqrt{2}}\right)12n.$$

V. Results for Graphene Networks

Graphene is a material consisting of carbon, in which carbon atoms are arranged in a single layer, forming a two-dimensional hexagonal (honeycomb) lattice. If one considers graphene as an infinitely large network, its graph representation is an infinite 3-regular graph, Figure 4.

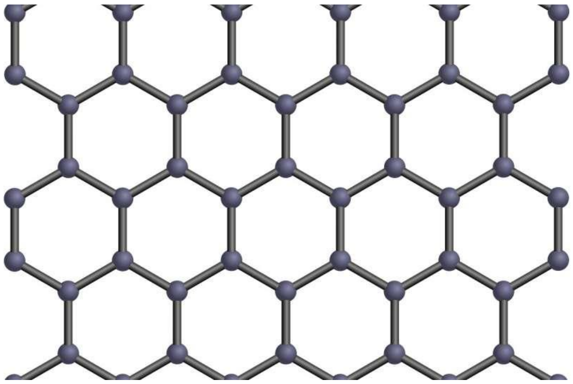

Figure 4. The graphene network considered as an infinite 3-regular graph *GR*

If G is any regular graph of degree r, with n vertices, then it has $m=\frac{1}{2}nr$ edges, and its Sombor index is

$$SO(G)=\frac{1}{2}\mathrm{nr}\left(\sqrt{r^2+r^2}\right)=\frac{\sqrt{2}}{2}\mathrm{nr}^2 .$$

This implies that the Sombor index of the graphene graph (GR), expressed per carbon atom, is

$$\frac{1}{n}SO(GR)=\frac{9\sqrt{2}}{2}.$$

In the same way, one can find expressions for the other above listed topological indices. For instance,

$$\frac{1}{n}KA^1_{a,b}(GR)=2^{b-1}3^{ab+1}$$

$$\frac{1}{n}RKA^1_{a,b}(GR)=3\cdot 2^{2ab-1}.$$

In reality, graphene consists of a finite number of carbon atoms. Thus, it has a boundary, and its graph representation is a finite graph $GR_{n,h}$, such as the one depicted in Figure 5.

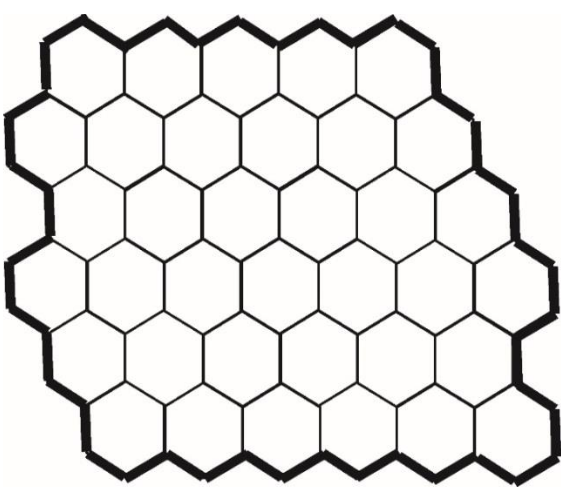

Figure 5. The graph representation of a graphene fragment $GR_{n,h}$ whose boundary is indicated by a heavy line. By n and h are denoted the number of vertices (i.e., carbon atoms) and hexagons, respectively; in this example, $n=96$, $h=36$. In reality, graphene fragments possess many carbon atoms, of order 10^9 or greater.

To arrive at formulas for Sombor and KA-indices of graphene fragments, we first have to determine some basic structural parameters of the graph $GR_{n,h}$.

The vertices of $GR_{n,h}$ can be divided into internal (lying inside the boundary) and external (lying on the boundary). Let their numbers be denoted by n_{int} and n_{ext} so that $n_{int}+n_{ext}=n$. In the theory of hexagonal systems, it is well known [8] that $n=4h+2-n_{\mathrm{int}}$, from which it directly follows

$$n_{\mathrm{int}}=4h+2-n \qquad \text{and}$$

$$n_{ext}=2n-4h-2 .$$

The number of edges of $GR_{n,h}$ is $m=n+h-1$. There are three types of edges, those connecting two vertices of degree 3, those connecting two vertices of degree 2, and those connecting a vertex of degree 3 with a vertex of degree 2. Their numbers will be denoted by m_{33}, m_{22}, and m_{32}, respectively. All internal vertices are of degree 3, whereas degree 2 vertices exist only on the boundary.

Because we are dealing with very large values of the parameter n, and because the shape of the boundary of graphene fragments is expected to be convex, it is reasonable to assume that the boundary of $GR_{n,h}$ contains no or a negligibly small number of features such as bays, coves, and fjords [8] and that the number of (2,2)-type edges is negligibly small. It is well known [8], and easy to prove, that $m_{33}=2h-2$. Therefore, in addition $m_{22}\approx 0$, we have

$$m_{32}\approx m-m_{33}=n+h-1-(2\mathrm{h}-2)=n-h+1 .$$

Knowing the above relations, it is possible to calculate expressions for various topological indices of the graphene fragment $GR_{n,h}$. For instance, in the case of the Sombor index, we have

$$\begin{aligned}SO(GR_{n,h}) &= \sqrt{3^2+3^2}\,m_{33}\\ &+\sqrt{3^2+2^2}\,m_{32}+\sqrt{2^2+2^2}\,m_{22}\\ &\approx 3\sqrt{2}(2h-2)+\sqrt{13}(n-h+1)\\ &=\sqrt{13}n+(6\sqrt{2}-\sqrt{13})h+\sqrt{13}-6\sqrt{2}\\ &=3.606\,n+4.880(h-1).\end{aligned}$$

In the same manner, one finds expressions for the other above listed topological indices. For instance,

$$^{m}SO\left(GR_{n,h}\right)\approx\frac{1}{\sqrt{13}}n+\left(\frac{\sqrt{2}}{3}-\frac{1}{\sqrt{13}}\right)(h-1)$$

$$RSO\left(GR_{n,h}\right) \approx \sqrt{5}\,\mathrm{n} + (4\sqrt{2} - \sqrt{5})(h-1)$$

$$^{m}RSO\left(GR_{n,h}\right) \approx \frac{1}{\sqrt{5}}n + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{5}}\right)(h-1)$$

$$KA_{a,b}^{1}\left(GR_{n,h}\right) \approx (3^{a} + 2^{a})^{b} n + \left[2^{b+1} \cdot 3^{ab} - (3^{a} + 2^{a})^{b}\right](h-1)$$

$$RKA_{a,b}^{1}\left(GR_{n,h}\right) = 2^{ab} n + \left(2^{2ab+1} - 2^{ab}\right)(h-1).$$

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