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Research Article

Computation of Modified Möbius Indices of Some Oxide and Silicate Related Networks

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Abstract. Topological indices describes the topology of chemical graphs in terms of mathematical expressions to comprehend both physical and chemical features of the compounds involved. The scientific study of chemical graphs is a significant discipline in the applied mathematics to support the ideas evolved with respect to chemical graphs by means of different topological indices. The specific formulations of recently designated degree-based adapted Möbius indices have been determined in this piece through evaluating a number of oxide and silicate networks as well as their various variations.

Keywords. Topological index, Silicate networks, Oxide networks, Modified Möbius indices, Dominating, Rhombus, Regular triangulene

Mathematics Subject Classification (2020). 05C10, 05C90, 05C92

1. Introduction

Various types of silicate and oxide networks are examined in this paper. Cuvettes, eyeglasses, and prisms are all made of silicates. Numerous construction materials, such as concrete and bricks, are made from silicate, a natural resource. Salts with silicon (Si) and oxygen (O) anions are called silicates. A total of four atoms of oxygen, each situated in a regular tetrahedron's corner, surround and correspond to a single silicon atom, to form the fundamental structural unit of all silicate minerals. Silicates are diverse due to the wide range of possible silicon-to-oxygen ratios. However, silicon atoms tend to accumulate at the center of tetrahedrons of all silicates, whereas oxygen molecules are somewhat positioned at the margins. As the most prevalent group of minerals that form rocks, silicates are the most significant mineral class. The combination of different tetrahedron silicates allows us to create a variety of silicate structures. It is possible to create silicate networks from various silicate structures. When silicon atoms are removed from the center of tetrahedra, oxide networks can be created.

Besides, the networks of copper (I) oxide (Cu_2O) and copper (II) oxide (CuO) are being investigated. The oxide of copper (II) forms the inorganic chemical compound CuO. Copper (II) oxide is an innovative addition to consumption and commercial products along with medical equipment, even though it is an authorized form of copper in mineral and vitamin supplements. Chemical graphs serve to represent chemical compounds, with atoms acting as vertex $V(G)$ and bonds of chemicals acting as edges $E(G)$. A topological indices comprises a real numeric which symbolizes the graph under specific circumstances. This study considers $V(G)$ and $E(G)$ as the vertex set and edge set, duly, for any simple graph dot. The topology of a chemical graph structure is described. Both the QSPR and QSAR models use topological indices to describe various physical-chemical characteristics of chemical compounds. A wide range of graph invariants have been used to introduce and study topological indices (TI). In the present work, silicates and oxides are capable of being deployed to obtain the exact manifestations of modified Möbius indices (Gao *et al.* [5]) for governing silicate as well as oxide networks, regular triangulene silicate as well as oxide networks, rhombus silicate and oxide networks, copper(I) and copper (II) oxide networks regarding $m \times n$ layers. Just in case you forgot, here are the amended Möbius indices.

First Modified Möbius Index:

$$\widetilde{M}_1(G) = \sum_{uv \in E} [\mu(d_u) + \mu(d_v)].$$

d_u = vertex degree of 'u' and $\mu(d_u)$ = Möbius function value of d_u.

We refer, Aravinth and Ravi [2] for the basic definition.

Second Modified Möbius Index:

$$\widetilde{M}_2(G) = \sum_{uv \in E} (\mu(d_u) \cdot \mu(d_v)).$$

Third Modified Möbius Index:

$$\widetilde{M}_3(G) = \sum_{uv \in E} |\mu(d_u) - \mu(d_v)|.$$

2. Main Results

In this section, we shall derive certain exact expressions of above said TI's for regular triangulene silicate (RTSL(n)) and regular triangulene oxide (RTOX(n)) types, dominating silicate (DSL(n)) and dominating oxide (DOX(n)) types, rhombus silicate (RHSL(n)) and rhombus oxide (RHOX(n)) networks, copper (I) oxide ($Cu_2$2O) and copper (II) oxide (CuO) types. A honeycomb structure with one dimension (the quantity of hexagonal layers) could potentially be leveraged to build all three of the first kinds of networks described. The nomenclature for every network's edge split according to the degree of its edges' end vertices is as follows: $E_{p,q} = \{uv \in E(G) : d_u = p, d_v = q\}$ and $|E_{p,q}|$ = cardinality of $E_{p,q}$.

2.1 DSL(n) and DOX(n) Type of Networks

We refer, Simonraj and George [7] for the basic diagrams and construction of DSL(n) and DOX(n) type of networks. We have the cardinalities of edge sets for such types of networks as follows:

$$|E(\mathrm{DSL}(n))| = 108n^2 - 108n + 36,$$
$$|E(\mathrm{DOX}(n))| = 54n^2 - 54n + 18.$$

We may note that

$$|E(\mathrm{DSL}(n))| = 2|E(\mathrm{DOX}(n))|.$$

Edge partition of DSL(n) is given as follows:

$$|E_{2,3}| = 12n - 6,$$
$$|E_{2,6}| = 24n - 12,$$
$$|E_{3,6}| = 54n^2 - 66n + 24,$$
$$|E_{6,6}| = 54n^2 - 78n + 30.$$

Edge partition of DOX(n) is given as follows:

$$|E_{2,4}| = 24n - 12,$$
$$|E_{4,4}| = 54n^2 - 78n + 30.$$

2.2 RTSL(n) and RTOX(n) Type of Networks

We refer [3] for the basic diagrams and construction of RTSL(n) and RTOX(n) types. We have the cardinalities of edge sets for such types as follows:

$$|E(\mathrm{RTSL}(n))| = 6n^2 + 12n,$$
$$|E(\mathrm{RTOX}(n))| = 3n^2 + 6n.$$

We note that

$$|E(\mathrm{RTSL}(n))| = 2|E(\mathrm{RTOX}(n))|.$$

Edge partition of RTSL(n) is given as follows:

$$|E_{3,3}| = 3n + 4,$$
$$|E_{3,6}| = 3n^2 + 9n - 2,$$
$$|E_{6,6}| = 3n^2 - 2.$$

Edge partition of RTOX(n) is given as follows:

$$|E_{2,2}| = 2,$$

$|E_{2,4}| = 6n,$

$|E_{4,4}| = 3n^2 - 2.$

2.3 RHSL(n) and RHOX(n) Networks

We have the cardinalities of edge sets as follows:

$|E(\text{RHSL}(n))| = 12n^2,$

$|E(\text{RHOX}(n))| = 6n^2.$

We note that

$|E(\text{RHSL}(n))| = 2|E(\text{RHOX}(n))|.$

Edge partition of RHSL(n) is given as follows:

$|E_{3,3}| = 4n + 2,$

$|E_{3,6}| = 6n^2 + 4n - 4,$

$|E_{6,6}| = 6n^2 - 8n + 2.$

Edge partition of RHOX(n) is given as follows:

$|E_{2,2}| = 2,$

$|E_{2,4}| = 8n - 4,$

$|E_{4,4}| = 6n^2 - 8n + 2.$

2.4 Copper (I) and Copper (II) Oxide Networks

One may refer [4, 6] for the basic diagrams and construction of these types of oxide networks. Also, $|E(\text{Cu}_2\text{O})| = 8mn$ ($m \times n$-layers) and $|E(\text{CuO})| = 12mn$.

Edge partitions of (Cu_2O) is as follows:

$|E_{1,2}| = 4n + 4m - 4,$

$|E_{2,2}| = 4mn - 4n - 4m + 4,$

$|E_{2,4}| = 4mn.$

Edge partitions of (CuO) is as follows:

$|E_{1,2}| = 2,$

$|E_{1,4}| = 2n - 2,$

$|E_{2,2}| = 2n + 2,$

$|E_{2,3}| = 4mn + 8m - 6,$

$|E_{3,4}| = 8mn - 8m - 4n + 4.$

Let us derive the exact expressions for modified Möbius indices of the considered various networks.

Theorem 2.1. *Let G be the dominating silicate network* DSL(n), *then its modified Möbius indices are:*

(i) $\widetilde{M}_1(\mathrm{DSL}(n)) = 108n^2 - 180n + 72$,

(ii) $\widetilde{M}_2(\mathrm{DSL}(n)) = 12 - 24n$,

(iii) $\widetilde{M}_3(\mathrm{DSL}(n)) = 108n^2 - 84n + 24$.

Proof. Let $G \cong \mathrm{DSL}(n)$. Based on Möbius function, we have $\mu(2) = \mu(3) = -1$, $\mu(6) = 1$.

(i)
$$\begin{aligned}\widetilde{M}_1(\mathrm{DSL}(n)) &= |E_{2,3}|[\mu(2)+\mu(3)]+|E_{2,6}|[\mu(2)+\mu(6)]+|E_{3,6}|[\mu(3)+\mu(6)]+|E_{6,6}|[\mu(6)+\mu(6)]\\ &= (12n-6)[-1-1]+(24n-12)[-1+1]+(54n^2-66n+24)[-1+1]\\ &\quad +(54n^2-78n+30)[1+1]\\ &= (12n-6)(-2)+(54n^2-78n+30)(2)\\ &= (2)[54n^2-78n+30-12n+6]\\ &= 108n^2-180n+72.\end{aligned}$$

(ii)
$$\begin{aligned}\widetilde{M}_2(\mathrm{DSL}(n)) &= |E_{2,3}|[\mu(2)\cdot\mu(3)]+|E_{2,6}|[\mu(2)\cdot\mu(6)]+|E_{3,6}|[\mu(3)\cdot\mu(6)]+|E_{6,6}|[\mu(6)\cdot\mu(6)]\\ &= (12n-6)[-1\times -1]+(24n-12)[-1\times 1]+(54n^2-66n+24)[-1\times 1]\\ &\quad +(54n^2-78n+30)[1\times 1]\\ &= (12n-6)+(12-24n)+(66n-54n^2-2)+54n^2-78n+30\\ &= 12n-24n+66n-78n-6+12-24+30\\ &= 12-24n.\end{aligned}$$

(iii)
$$\begin{aligned}\widetilde{M}_3(\mathrm{DSL}(n)) &= |E_{2,3}||\mu(2)-\mu(3)|+|E_{2,6}||\mu(2)-\mu(6)|+|E_{3,6}||\mu(3)-\mu(6)|+|E_{6,6}||\mu(6)-\mu(6)|\\ &= (12n-6)|-1-(-1)|+(24n-12)|-1-1|\\ &\quad +(54n^2-66n+24)|-1-1|+(54n^2-78n+30)|-1-(-1)|\\ &= (12n-6)(0)+(24n-12)(2)+(54n^2-66n+24)(2)+(54n^2-78n+30)(0)\\ &= (2)[24n-12+54n^2-66n+24]\\ &= 108n^2-84n+24.\end{aligned}$$

□

Theorem 2.2. *Let G be the dominating oxide network* $\mathrm{DOX}(n)$*, then its modified Möbius indices are:*

(i) $\widetilde{M}_1(\mathrm{DOX}(n)) = 12 - 24n$,

(ii) $\widetilde{M}_2(\mathrm{DOX}(n)) = 0$,

(iii) $\widetilde{M}_3(\mathrm{DOX}(n)) = 24n - 12$.

Proof. Let $G \cong \mathrm{DOX}(n)$. Based on Möbius function, we have $\mu(2) = -1$, $\mu(4) = 0$.

(i)
$$\begin{aligned}\widetilde{M}_1(\mathrm{DOX}(n)) &= |E_{2,4}|[\mu(2)+\mu(4)]+|E_{4,4}|[\mu(4)+\mu(4)]\\ &= (24n-12)[-1+0]+(54n^2-78n+30](0)\\ &= 12-24n.\end{aligned}$$

(ii)
$$\begin{aligned}\widetilde{M}_2(\mathrm{DOX}(n)) &= (24n-12)(-1\times 0)+(54n^2-78n+30)(0)\\ &= 0.\end{aligned}$$

(iii) $$\begin{aligned}\widetilde{M}_3(\mathrm{DOX}(n)) &= (24n-12)|-1-0| + (54n^2-78n+30)|0-0| \\ &= 24n-12. \end{aligned}$$ □

Theorem 2.3. *Let G be the regular triangulene silicate network* RTSL(n)*, then its modified Möbius indices are:*

(i) $\widetilde{M}_1(\mathrm{RTSL}(n)) = 6n^2-6n-12$,

(ii) $\widetilde{M}_2(\mathrm{RTSL}(n)) = 4-6n$,

(iii) $\widetilde{M}_3(\mathrm{RTSL}(n)) = 6n^2+18n-4$.

Proof. Let $G \cong \mathrm{RTSL}(n)$. Based on Möbius function, we have $\mu(3)=-1$, $\mu(6)=1$.

(i) $$\begin{aligned}\widetilde{M}_1(\mathrm{RTSL}(n)) &= |E_{3,3}|[\mu(3)+\mu(3)] + |E_{3,6}|[\mu(3)+\mu(6)] + |E_{6,6}|[\mu(6)+\mu(6)] \\ &= [3n+4](-1-1) + (3n^2+9n-2)(-1+1) + [3n^2-2](1+1) \\ &= (3n+4)(2) + (3n^2-2)(2) \\ &= (2)[3n^2-2-3n-4] \\ &= (2)[3n^2-3n-6] \\ &= 6n^2-6n-12. \end{aligned}$$

(ii) $$\begin{aligned}\widetilde{M}_2(\mathrm{RTSL}(n)) &= (3n+4)[-1\times -1] + (3n^2+9n-2)[-1\times 1] + (3n^2-2)[1\times 1] \\ &= 3n+4-3n^2-9n+2+3n^2-2 \\ &= 4-6n. \end{aligned}$$

(iii) $$\begin{aligned}\widetilde{M}_3(\mathrm{RTSL}(n)) &= (3n+4)|-1-1) + (3n^2+9n-2)|-1-1| + (3n^2-2)|1-1| \\ &= 2(3n^2+9n-2) \\ &= 6n^2+18n-4. \end{aligned}$$ □

Theorem 2.4. *Let G be the regular triangulene oxide network* RTOX(n)*, then its modified Möbius indices are:*

(i) $\widetilde{M}_1(\mathrm{RTOX}(n)) = -4-6n$,

(ii) $\widetilde{M}_2(\mathrm{RTOX}(n)) = 2$,

(iii) $\widetilde{M}_3(\mathrm{RTOX}(n)) = 6n$.

Proof. Let $G \cong \mathrm{RTOX}(n)$. Based on Möbius function, we have $\mu(2)=-1$, $\mu(4)=0$.

(i) $$\begin{aligned}\widetilde{M}_1(\mathrm{RTOX}(n)) &= |E_{2,2}|[\mu(2)+\mu(2)] + |E_{2,4}|[\mu(2)+\mu(4)] + |E_{4,4}|[\mu(4)+\mu(4)] \\ &= (2)[-1-1] + (6n)[-1+0] + (3n^2-2)(0+0) \\ &= -4-6n. \end{aligned}$$

(ii) $$\begin{aligned}\widetilde{M}_2(\mathrm{RTOX}(n)) &= |E_{2,2}|[\mu(2)\cdot\mu(2)] + |E_{2,4}|[\mu(2)\cdot\mu(4)] + |E_{4,4}|[\mu(4)\cdot\mu(4)] \\ &= (2)[-1\times -1] + (6n)[-1\times 0 + (3n^2-2)[0\times 0] \\ &= 2. \end{aligned}$$

(iii) $$\widetilde{M}_3(\mathrm{RTOX}(n)) = |E_{2,2}||\mu(2)-\mu(2)| + |E_{2,4}||\mu(2)-\mu(4)| + |E_{4,4}||\mu(4)-\mu(4)|$$

$$
\begin{aligned}
&= (6n)|-1-0| \\
&= 6n. \qquad \square
\end{aligned}
$$

Theorem 2.5. *Let G be the rhombus silicate network* RHSL(n)*, then its modified Möbius indices are:*

(i) $\widetilde{M}_1(\mathrm{RHSL}(n)) = 12n^2 - 24n$,

(ii) $\widetilde{M}_2(\mathrm{RHSL}(n)) = 8 - 8n$,

(iii) $\widetilde{M}_3(\mathrm{RHSL}(n)) = 12n^2 + 8n - 8$.

Proof. Let $G \cong$ RHSL(n). Based on Möbius function, we have $\mu(3) = -1$, $\mu(6) = 1$.

(i)
$$
\begin{aligned}
\widetilde{M}_1(\mathrm{RHSL}(n)) &= |E_{3,3}|[\mu(3)+\mu(3)] + |E_{3,6}|[\mu(3)+\mu(6)] + |E_{6,6}|[\mu(6)+\mu(6)] \\
&= (4n+2)(-1-1) + (6n^2+4n-4)(-1+1) + (6n^2-8n+2)(1+1) \\
&= (4n+2)(-2) + (6n^2+4n-4)(0) + (6n^2-8n+2)(2) \\
&= (2)[-4n-2+6n^2-8n+2] \\
&= (2)[6n^2-12n] \\
&= 12n^2-24n.
\end{aligned}
$$

(ii)
$$
\begin{aligned}
\widetilde{M}_2(\mathrm{RHSL}(n)) &= (4n+2)(-1\times -1) + (6n^2+4n-4)(-1\times 1) + (6n^2-8n+2)(1\times 1) \\
&= 4n+2-6n^2-4n+4+6n^2-8n+2 \\
&= 8-8n.
\end{aligned}
$$

(iii)
$$
\begin{aligned}
\widetilde{M}_3(\mathrm{RHSL}(n)) &= (4n+2)|-1-1| + (6n^2+4n-4)|-1-1| + (6n^2-8n+2)|1-1| \\
&= (6n^2+4n-4)(2) \\
&= 12n^2+8n-8. \qquad \square
\end{aligned}
$$

Theorem 2.6. *Let G be the rhombus oxide network* RHOX(n)*, then its modified Möbius indices are:*

(i) $\widetilde{M}_1(\mathrm{RHOX}(n)) = -8n$.

(ii) $\widetilde{M}_2(\mathrm{RHOX}(n)) = 2$.

(iii) $\widetilde{M}_3(\mathrm{RHOX}(n)) = 8n - 4$.

Proof. Let $G \cong$ RHOX(n). Based on Möbius function, we have $\mu(2) = -1$, $\mu(4) = 0$.

(i)
$$
\begin{aligned}
\widetilde{M}_1(\mathrm{RHOX}(n)) &= |E_{2,2}|[\mu(2)+\mu(2)] + |E_{2,4}|[\mu(2)+\mu(4)] + |E_{4,4}|[\mu(4)+\mu(4)] \\
&= (2)[-1-1] + (8n-4)(-1+0) + (6n^2-8n+2)(0+0) \\
&= -4-8n+4 \\
&= -8n.
\end{aligned}
$$

(ii)
$$
\begin{aligned}
\widetilde{M}_2(\mathrm{RHOX}(n)) &= (2)(-1\times -1) + (8n-4)(-1\times 0) + (6n^2-8n+2)(0) \\
&= 2.
\end{aligned}
$$

(iii)
$$
\widetilde{M}_3(\mathrm{RHOX}(n)) = (2)|-1-(-1)| + (8n-4)|-1-0| + (6n^2-8n+2)|0-0|
$$

$$= (2)(0) + (8n-4)(1) + 0$$
$$= 8n - 4. \qquad \square$$

Theorem 2.7. *Let G be the copper (I) oxide-network (Cu_2O), then its modified Möbius indices are*

(i) $\widetilde{M}_1$(copper (I) oxide-network) $= 8n + 8m - 12mn - 8$,

(ii) $\widetilde{M}_2$(copper (I) oxide-network) $= -8n - 8m + 4mn + 8$,

(iii) $\widetilde{M}_3$(copper (I) oxide-network) $= 8n + 8m + 4mn - 8$.

Proof. Let $G \cong$ copper (I) oxide-network. Based on Möbius function, we have $\mu(1) = 1$, $\mu(2) = -1$, $\mu(4) = 0$.

(i)
$$\begin{aligned}\widetilde{M}_1(G) &= |E_{1,2}|[\mu(1)+\mu(2)] + |E_{2,2}|[\mu(2)+\mu(2)] + |E_{2,4}|[\mu(2)+\mu(4)]\\ &= (4n+4m-4)[1-1] + (4mn-4n-4m+4)[-1-1] + (4mn)[-1+0]\\ &= (4mn-4n-4m+4)(-2) + (4mn)(-1)\\ &= 8n+8m-8mn-8-4mn\\ &= 8n+8m-12mn-8.\end{aligned}$$

(ii)
$$\begin{aligned}\widetilde{M}_2(G) &= (4n+4m-4)(1\times -1) + (4mn-4n-4m+4)(-1\times -1) + (4mn)(-1\times 0)\\ &= -4n-4m+4+4mn-4n-4m+4\\ &= 4mn-8n-8m+8.\end{aligned}$$

(iii)
$$\begin{aligned}\widetilde{M}_3(G) &= (4n+4m-4)|1-(-1)| + (4mn-4n-4m+4)|-1-(-1)| + (4mn)|-1-0|\\ &= (4n+4m-4)(2) + 4mn\\ &= 8n+8m-8+4mn. \qquad \square\end{aligned}$$

Theorem 2.8. *Let $G \cong$* copper (II) oxide-network*, then then its modified Möbius indices are*

(i) $\widetilde{M}_1$(copper (II) oxide-network) $= 2n - 8m - 16mn + 2$,

(ii) $\widetilde{M}_2$(copper (II) oxide-network) $= 4mn + 2n + 8m - 6$,

(iii) $\widetilde{M}_3$(copper (II) oxide-network) $= 8mn - 2n - 8m + 6$.

Proof. Let $G \cong$copper (II) oxide-network. Based on Möbius function, we have $\mu(1) = 1$, $\mu(2) = -1$, $\mu(3) = -1$, $\mu(4) = 0$.

(i)
$$\begin{aligned}\widetilde{M}_1(G) &= |E_{1,2}|[\mu(1)+\mu(2)] + |E_{1,4}|[\mu(1)+\mu(4)] + |E_{2,2}|[\mu(2)+\mu(2)]\\ &\quad + |E_{2,3}|[\mu(2)+\mu(3)] + |E_{3,4}|[\mu(3)+\mu(4)]\\ &= (2)[1-1] + (2n-2)[1+0] + (2n+2)[-1-1]\\ &\quad + (4mn+8m-6)[-1-1] + (8mn-8m-4n+4)[-1+0]\\ &= 0 + 2n - 2 + (2n+2)(-2) + (4mn+8m-6)(-2) + (8mn-8m-4n+4)(-1)\\ &= 2n-2-4n-4-8mn-16m+12-8mn+8m+4n-4\\ &= -16mn+2n-8m+2.\end{aligned}$$

(ii) $$\begin{aligned}\widetilde{M}_2(G) &= (2)(1\times -1)+(2n-2)(1\times 0)+(2n+2)(-1\times -1)\\ &\quad +(4mn+8m-6)(-1\times -1)+(8mn-8m-4n+4)(-1\times 0)\\ &= -2+2n+2+4mn+8m-6+0\\ &= 2n+4mn+8m-6.\end{aligned}$$

(iii) $$\begin{aligned}\widetilde{M}_3(G) &= (2)|1-(-1)|+(2n-2)|1-0|+(2n+2)|-1-(-1)|\\ &\quad +(4mn+8m-6)|-1+1|+(8mn-8m-4n+4)|-1-0|\\ &= 2(2)+2n-2+8mn-8m-4n+4\\ &= 4+2n-2+8mn-8m-4n+4\\ &= 8mn-2n-8m+6\end{aligned}$$ □

3. Conclusion

We computed the modified Möbius indices on some silicate networks, oxide networks and copper oxide networks with respect to their different forms like dominating, regular triangulene and rhombus. We will derive the results related some more graph structures like silicon carbide graphs, hex derived networks and some nano tubes in future work.

Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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