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TOPOLOGICAL ASPECTS OF SILICATE NETWORK USING PSI_KPOLYNOMIAL

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ABSTRACT
Psi_K-polynomial is introduced as a graph polynomial to re-cover closed formulas of degree based topological indices by using some suitable operators. These topological indices have a predicting ability about the properties of organic molecules. Silicate network (phyllosilicates) belonging to an important group of minerals that includes talc, micas, serpentine, clay, and chlorite minerals. These minerals have much importance in the chemical industry. The aim of this paper is to explore the silicate network through M- polynomial and some degree-based topological indices. Results are also elaborate by plotting with graphs.

Keywords: Graph theory, Silicate network, Psi_K-polynomial, Topological indices.

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1. INTRODUCTION

Degree-based topological indices (TIs) are real numbers extract from the topology of the chemical species by using the chemical graph theory (CGT) tools. The widely studied topic in CGT is the computation of TIs for the chemical structure. These TIs have potential information about the structural characteristics of the organic compound [5, 8, 14]. Researchers have developed some algebraic functions, in which structural parameters such as the number of atoms or units and the number of bonds etc. used as input and in output relate with the characteristics of the molecules.

The first TI is the Wiener index introduced in 1947, which correlates with the boiling points of alkanes [20]. After that thousands of indices are designed up till now [19]. For the basics definitions see [12].

A degree dependent topological index for the graph G is defined as:

$$I(G) = \sum_{e=xy\in E_G} f(d_x, d_y). \qquad (1.1)$$

In the chemical graph, by counting the same end-degree edges, then the equation 1.1 rewrite as:

$$I(G) = \sum_{j\leq k} m_{jk} f(j,k). \qquad (1.2)$$

where $\{d_x, d_y\} = \{j,k\}$ and the total number of edges xy is denoted by mjk. Table 1 describes some important TIs.

Psi_K-polynomial is the representative of the structure of the chemical molecules. After applying some successive operations of derivatives and integrations on M-polynomial, we can find the TIs [1, 18,21-30]. E. Deutsch and S. Klavžar introduced this polynomial in 2015 [4]. Many researchers nowadays extensively used M-polynomial to obtain many TIs for molecular structures [3, 9, 10]. M-polynomial for the graph G is defined as:

$$M_G(u,v) = \sum_{\psi \le j \le k \le \Psi} m_{jk} u^j v^k.$$

Here $\psi = min\ \{d_x \mid x \in V_G\}$, $\Psi = max\ \{d_x \mid x \in V_G\}$. Closed form via Psi_K-polynomial of TIs mention in Table 1, is describe in Table 2.

Table 1: Some important topological indices

Topological Indices		Symbols		Formulas
reduced reciprocal randić index [7]	=	$RRR[G]$	=	$\sum_{xy\in E(G)} \sqrt{(d_x-1)(d_y-1)}$
firt arithmetic geometric index [16]	=	$AG_1[G]$	=	$\sum_{xy\in E(G)} \frac{d_x+d_y}{2\sqrt{d_x \cdot d_y}}$
SK index [17]	=	$SK[G]$	=	$\sum_{xy\in E(G)} \frac{d_x+d_y}{2}$
SK_1 index [17]	=	$SK_1[G]$	=	$\sum_{xy\in E(G)} \frac{d_x \cdot d_y}{2}$
SK_2 index [17]	=	$Sk_2[G]$	=	$\sum_{xy\in E(G)} (\frac{d_x+d_y}{2})^2$
first zagrab index in term of edge degree [13]	=	$EM_1[G]$	=	$\sum_{xy\in E(G)} (d_{xy})^2$
sum-connectivity index [6]	=	$SCI[G]$	=	$\sum_{xy\in E(G)} \frac{1}{\sqrt{d_x+d_y}}$
general sum-connectivity index [6]	=	$SCI_\lambda[G]$	=	$\sum_{xy\in E(G)} (d_x+d_y)^\lambda$
redefined third Zagreb index [15]	=	$ReZG_3[G]$	=	$\sum_{xy\in E(G)} \frac{d_x d_y}{d_x+d_y}$

Where the operator used are defined as

$$D_u^{\frac{1}{2}} M_G(u,v) = \sqrt{u \frac{\partial}{\partial u} M_G(u,v)} \cdot \sqrt{M_G(u,v)},$$

$$D_u M_G(u,v) = u \frac{\partial}{\partial u} M_G(u,v),$$

$$D_v^{\frac{1}{2}} M_G(u,v) = \sqrt{v \frac{\partial}{\partial v} M_G(u,v)} \cdot \sqrt{M_G(u,v)},$$

$$D_v M_G(u,v) = v \frac{\partial}{\partial v} M_G(u,v),$$

$$S_u^{\frac{1}{2}} M_G(u,v) = \sqrt{\int_0^u \frac{M_G(t,v)}{t} dt} \cdot \sqrt{M_G(u,v)},$$

$$Q_{u(\alpha)} M_G(u,v) = u^\alpha M_G(u,v),$$

$$S_v^{\frac{1}{2}} M_G(u,v) = \sqrt{\int_0^v \frac{M_G(u,t)}{t} dt} \cdot \sqrt{M_G(u,v)},$$

$$JM_G(u,v) = M_G(u,u).$$

Table 2: Topological indices derive from $MG(u,v)$

$$
\begin{aligned}
RRR[G] &= D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} Q_{u(-1)} Q_{v(-1)} M_G(u,v)|_{u=v=1} \\
AG_1[G] &= \frac{1}{2} D_u J S_u^{\frac{1}{2}} S_v^{\frac{1}{2}} M_G(u,v)|_{u=1} \\
SK[G] &= \frac{1}{2}(D_u + D_v) M_G(u,v)|_{u=v=1} \\
SK_1[G] &= \frac{1}{2} D_u D_v M_G(u,v)|_{u=v=1} \\
Sk_2[G] &= \frac{1}{4} D_u^2 J M_G(u,v)|_{u=1} \\
EM_1[G] &= D_u^2 Q_{u(-2)} J M_G(u,v)|_{u=1} \\
SCI[G] &= S_u^{\frac{1}{2}} J M_G(u,v)|_{u=1} \\
SCI_\lambda[G] &= D_u^\lambda J M_G(u,v)|_{u=1} \\
ReZG_3[G] &= D_u D_v (D_u + D_v) M_G(u,v)|_{u=v=1}
\end{aligned}
$$

1. Chemical Graph of Silicate network

The 2D silicate network sheet has a general chemical formula $(Si_2O_5)_m^{2m-}$. Each $SiO4$ tetrahedron shares three of its oxygen atoms with others and so the two-dimensional sheets of silicate network are formed. The chemical graph of silicate network (SL_n) is shown in Figure 1, where n is the total number of hexagons present between center of the network to the boundary of SL_n. Table 3 shows the vertex partitions and Table 4 represents the edge partitions of SL_n. In this article we are concerned about topological indices, mention in Table 2, via M-polynomial of SL_n.

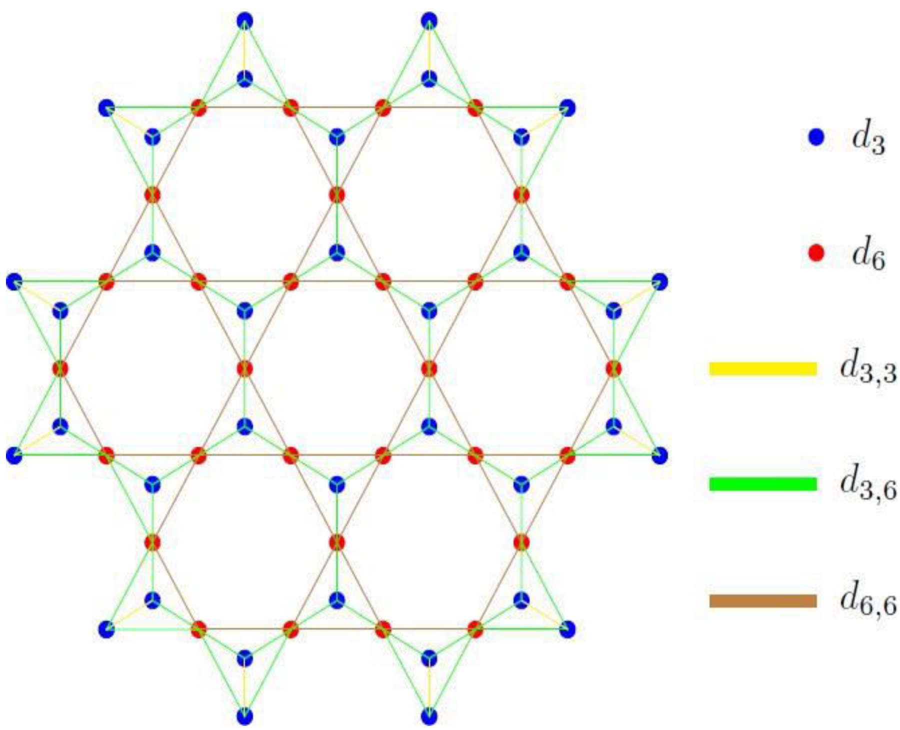

Figure 1. Chemical graph of silicate network (SL_2)

Table 3. Vertex partition of SL_n

d_x	Number of vertices
3	$6n(n+1)$
6	$3n(3n-1)$
Total vertices	$3n(5n+1)$

Table 4. Edge partition of SL_n.

(d_x, d_y)	Number of edges
$(3,3)$	$6n$
$(3,6)$	$6n(3n+1)$
$(6,6)$	$6n(3n-2)$
Total edges	$36n^2$

1. Psi_K-Polynomial and Topological Indices of Silicatenetwork

Theorem 3.1.. *If SL_n represent a silicate network then M-polynomial of SL_n is*

$MSL_n(u,v) = 6nu^3v^3 + 6n(3n+1)u^3v^6 + 6n(3n-2)u^6v^6$ *[2, 11].*

Theorem 3.2. *Let SL_n represent the silicate network and*

$MSL_n(u,v) = 6nu^3v^3 + 6n(3n+1)u^3v^6 + 6n(3n-2)u^6v^6$. *Then*

(1) $RRR[SL_n] = 18(5+\sqrt{10})n^2 - 6(8-\sqrt{10})n.$

(2) $AG_1[SL_n] = \frac{9}{2}(4+3\sqrt{2})n^2 - \frac{3}{2}(4-3\sqrt{2})n.$

(3) $SK[SL_n] = 189n^2 - 27n.$

(4) $SK_1[SL_n] = 486n^2 - 135n.$

(5) $SK_2[SL_n] = \frac{2025}{2}n^2 - \frac{513}{2}n.$

(6) $EM_1[SL_n] = 2682n^2 - 810n.$

(7) $SCI[SL_n] = 3(2+\sqrt{3})n^2 + (2+\sqrt{6}-2\sqrt{3})n.$

(8) $SCI_\lambda[SL_n] = 18(9^\lambda + 12^\lambda)n^2 + 6(6^\lambda + 9^\lambda - 2\cdot 12^\lambda)n.$

(9) $ReZG_3[SL_n] = 10692n^2 - 3888n.$$

Proof.

$$Q_{v(-1)}M_{SL}(u,v) = 6nu^3v^2 + 6n(3n+1)u^3v^5 + 6n(3n-2)u^6v^5,$$
$$Q_{u(-1)}Q_{v(-1)}M_{SL}(u,v) = 6nu^2v^2 + 6n(3n+1)u^2v^5 + 6n(3n-2)u^5v^5,$$
$$D_v^{\frac{1}{2}}Q_{u(-1)}Q_{v(-1)}M_{SL}(u,v) = 6\sqrt{2}nu^2v^2 + 6\sqrt{5}n(3n+1)u^2v^5 + 6\sqrt{5}n(3n-2)u^5v^5,$$
$$D_u^{\frac{1}{2}}D_v^{\frac{1}{2}}Q_{u(-1)}Q_{v(-1)}M_{SL}(u,v) = 12nu^2v^2 + 6\sqrt{10}n(3n+1)u^2v^5 + 30n(3n-2)u^5v^5,$$
$$S_v^{\frac{1}{2}}M_{SL}(u,v) = 2\sqrt{3}nu^3v^3 + \sqrt{6}n(3n+1)u^3v^6 + \sqrt{6}n(3n-2)u^6v^6,$$
$$S_u^{\frac{1}{2}}S_v^{\frac{1}{2}}M_{SL}(u,v) = 2nu^3v^3 + \sqrt{2}n(3n+1)u^3v^6 + n(3n-2)u^6v^6,$$
$$JS_u^{\frac{1}{2}}S_v^{\frac{1}{2}}M_{SL}(u,v) = 2nu^6 + \sqrt{2}n(3n+1)u^9 + n(3n-2)u^{12},$$
$$D_uJS_u^{\frac{1}{2}}S_v^{\frac{1}{2}}M_{SL}(u,v) = 12nu^6 + 9\sqrt{2}n(3n+1)u^9 + 12n(3n-2)u^{12},$$
$$\frac{1}{2}D_uJS_u^{\frac{1}{2}}S_v^{\frac{1}{2}}M_{SL}(u,v) = 6nu^6 + \frac{9\sqrt{2}}{2}n(3n+1)u^9 + 6n(3n-2)u^{12},$$
$$D_uM_{SL}(u,v) = 18nu^3v^3 + 18n(3n+1)u^3v^6 + 36n(3n-2)u^6v^6,$$
$$D_vM_{SL}(u,v) = 18nu^3v^3 + 36n(3n+1)u^3v^6 + 36n(3n-2)u^6v^6,$$
$$(D_u + D_v)M_{SL}(u,v) = 36nu^3v^3 + 54n(3n+1)u^3v^6 + 72n(3n-2)u^6v^6,$$
$$\frac{1}{2}(D_u + D_v)M_{SL}(u,v) = 18nu^3v^3 + 27n(3n+1)u^3v^6 + 36n(3n-2)u^6v^6,$$
$$D_uD_vM_{SL}(u,v) = 54nu^3v^3 + 108n(3n+1)u^3v^6 + 216n(3n-2)u^6v^6,$$
$$\frac{1}{2}(D_uD_v)M_{SL}(u,v) = 27nu^3v^3 + 54n(3n+1)u^3v^6 + 108n(3n-2)u^6v^6,$$
$$JM_{SL}(u,v) = 6nu^6 + 6n(3n+1)u^9 + 6n(3n-2)u^{12},$$
$$D_u^2JM_{SL}(u,v) = 216nu^6 + 486n(3n+1)u^9 + 864n(3n-2)u^{12},$$
$$\frac{1}{4}D_t^2JM_{SL}(u,v) = 54nu^6 + \frac{243}{2}n(3n+1)u^9 + 216n(3n-2)u^{12},$$
$$Q_{u(-2)}JM_{SL}(u,v) = 6nu^4 + 6n(3n+1)u^7 + 6n(3n-2)u^{10},$$
$$D_u^2Q_{u(-2)}JM_{SL}(u,v) = 96nu^4 + 294n(3n+1)u^7 + 600n(3n-2)u^{10},$$
$$S_u^{\frac{1}{2}}JM_{SL}(u,v) = \sqrt{6}nu^6 + 2n(3n+1)u^9 + \sqrt{3}n(3n-2)u^{12},$$
$$D_u^\lambda JM_{SL}(u,v) = 6\cdot 6^\lambda nu^6 + 6\cdot 9^\lambda n(3n+1)u^9 + 6\cdot 12^\lambda n(3n-2)u^{12},$$
$$D_v(D_u + D_v)M_{SL}(u,v) = 108nu^3v^3 + 162n(3n+1)u^3v^6 + 432n(3n-2)u^6v^6,$$
$$D_uD_v(D_u + D_v)M_{SL}(u,v) = 324nu^3v^3 + 972n(3n+1)u^3v^6 + 2592n(3n-2)u^6v^6.$$

(1) $RRR[SL_n] = D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} Q_{u(-1)} Q_{v(-1)} M_{SL}(u,v)|_{u=v=1}$,

$RRR[SL_n] = 18(5+\sqrt{10})n^2 - 6(8-\sqrt{10})\,n.$

(2) $AG_1[SL_n] = \frac{1}{2} D_u J S_u^{\frac{1}{2}} S_v^{\frac{1}{2}} M_{SL}(u,v)|_{u=1}$,

$AG_1[SL_n] = \frac{9}{2}(4+3\sqrt{2})n^2 - \frac{3}{2}(4-3\sqrt{2})n.$

(3) $SK[SL_n] = \frac{1}{2}(D_u + D_v) M_{SL}(u,v)|_{u=v=1}$,

$SK[SL_n] = 189n^2 - 27n.$

(4) $SK_1[SL_n] = \frac{1}{2} D_u D_v M_{SL}(u,v)|_{u=v=1}$,

$SK_1[SL_n] = 486n^2 - 135n.$

(5) $Sk_2[SL_n] = \frac{1}{4} D_u^2 J M_{SL}(u,v)|_{u=1}$,

$SK_2[SL_n] = \frac{2025}{2}n^2 - \frac{513}{2}n.$

(6) $EM_1[SL_n] = D_u^2 Q_{u(-2)} J M_{SL}(u,v)|_{u=1}$,

$EM_1[SL_n] = 2682n^2 - 810n.$

(7) $SCI[SL_n] = S_u^{\frac{1}{2}} J M_{SL}(u,v)|_{u=1}$,

$SCI[SL_n] = 3(2+\sqrt{3})n^2 + (2+\sqrt{6}-2\sqrt{3})n.$

(8) $SCI_\lambda[SL_n] = D_u^\lambda J M_{SL}(u,v)|_{u=1}$,

$SCI_\lambda[SL_n] = 18(9^\lambda + 12^\lambda)n^2 + 6(6^\lambda + 9^\lambda - 2\cdot 12^\lambda)n.$

(9) $ReZG_3[SL_n] = D_u D_v (D_u + D_v) M_{SL}(u,v)|_{u=v=1}$,

$ReZG_3[SL_n] = 10692n^2 - 3888n.$

The plotting of topological indices of SL_n shown inFigure 2.■

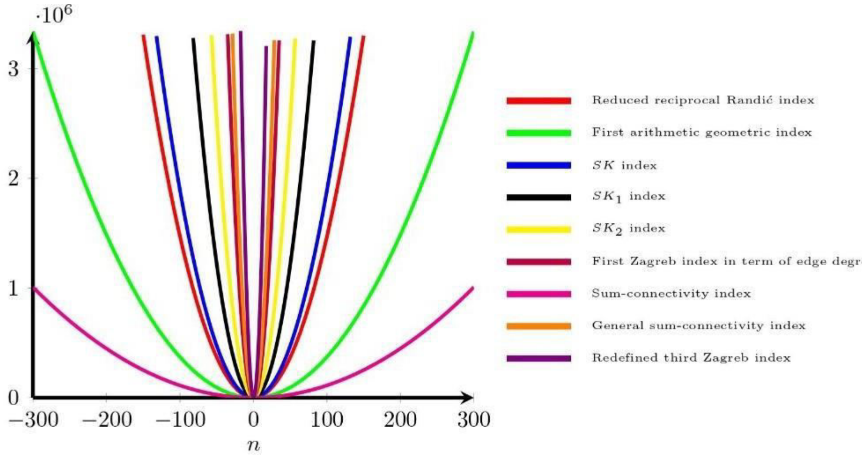

Figure 2. Plot of topological indices of silicate network (SL_n).

2. CONCLUSIONS

We computed the M-polynomial of and important classes of minerals known as silicate network and then used the M-polynomial to recover some degree based topological indices mention in Table 2. These results have many applications in structural chemistry and can be used to detect some chemical and physical properties of the silicate network. Visualization forms of results are also given.

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