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Forgotten Topological Index and Revan Indices of Cayley Tree, Silicate Layer and Molybdenum Disulphide

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ABSTRACT

A topological index is a real number derived from a graph. In 2015, The forgotten topological index was introduced by Furtula and Gutman and in 2017, Kulli has introduced Revan indices. In this paper we compute the forgotten topological index, first, second and third Revan indices of Cayley tree, silicate layer and molybdenum disulfide nanostructure.

Keywords : Forgotten Topological Index, Revan Indices, Cayley Tree, Silicate Layer and Molybdenum Disulfide.

I. INTRODUCTION

In theoretical chemistry topological indices are used for studying the physical, biological properties of the chemical compounds and they are used to predict certain physicochemical properties like boiling point, stability, enthalpy of vaporization and so forth [2][3][4]. There are certain types of topological indices such as degree based topological indices, distance based topological indices and counting related topological indices etc. Consider a graph G which is a finite, simple and connected with vertex set V(G) and edge set E(G). The degree d_v of a vertex v is the number of vertices adjacent to v. For additional definitions and notations, the reader may refer to [1].

In 2015, Furtula and Gutman [5] introduced Forgotten topological index (or, F-index) which is stated as

$$F(G) = \sum_{v\in V(G)}(d_v)^3 = \sum_{uv\in E(G)}[(d_u)^2 + (d_v)^2] \qquad (1)$$

In 2017, Kulli [6] defined a novel degree concept in graph theory: The Revan vertex degree of a vertex v in G is defined as $r_G(v) = \Delta(G) + \delta(G) - d_v$. The first, second and third Revan indices were defined as

$$R_1(G) = \sum_{uv\in E(G)}[r_G(u) + r_G(v)] \qquad (2)$$

$$R_2(G) = \sum_{uv\in E(G)} r_G(u).r_G(v) \qquad (3)$$

$$R_3(G) = \sum_{uv\in E(G)}|r_G(u) - r_G(v)| \qquad (4)$$

To derive the topological index for a chemical compound first their topological representation called molecular graph must be derived. A molecular graph is a collection of points representing the atoms in the molecule and set of lines representing the covalent bonds. These points are named vertices and the lines are named edges in graph theory language. Once the molecular graph is defined the edge partition table of the graph (sometimes degree partition may also be required) should be computed. The edge partition is nothing, but the classification of the edges based on the degree of the vertices they connect. The edge partition table gives the number of edges corresponding to each type of edge. The index is then computed based on the formula defined for that particular index.

II. MATERIALS AND METHODS

The Cayley Tree Γ^k:

The Cayley tree Γ^k of order $k \geq 1$ is an infinite and symmetric regular tree, that is, a graph without cycles, from each vertex of which exactly k + 1 edges are issued. In this paper, we consider the Cayley tree $\Gamma_n^2 = (V, E, i)$ of order 2 and with n levels from the root x_0, where V is the set of vertices of Γ_n^2, E is the set of edges of Γ_n^2, and 'i' is the incidence function associating each edge $e \in E$ with its end vertices.

It is easy to compute the number of vertices reachable in step n or in level n starting from the root x_0, which is $|W_n| = 3.2^{(n-1)}$. The number of vertices of Γ_n^2 is $|V_n| = 1 + 3(2^n - 1)$, and the number of edges of Γ_n^2 is $|E_n| = 3(2^n - 1)$, as is shown in Figure 1 below.

Silicate Layer:

Silicates are obtained by fusing metal oxides or metal carbonates with sand. A silicate network in symbolized by SL_n where n is the number of hexagons between the centre and boundary of SL_n. A 2-dimensional silicate layer network is shown in Fig 2.

Molybdenum disulphide:

The MoS_2 (Molybdenum disulphide) is an inorganic compound with layered structure where a plane of Molybdenum atoms is sandwiched by planes of sulphide ions. As it has a low friction and robustness, it is used as a lubricant and it is also used as co-catalyst. Schematic representation of side view of a monolayer of is given in fig. 3. The layered structure makes it to be used as lubricant, capable of handling shear stress.

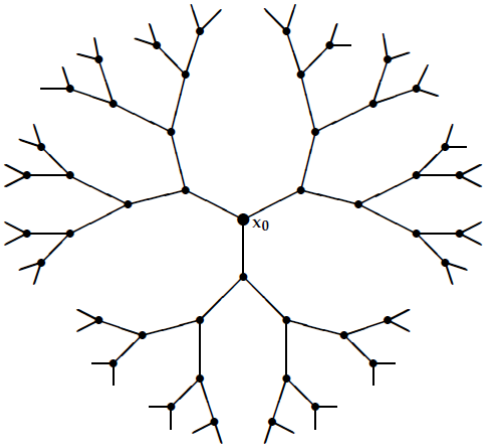

Fig 1: Cayley tree Γ_n^2 of order 2 with n levels, where $n \geq 1$.

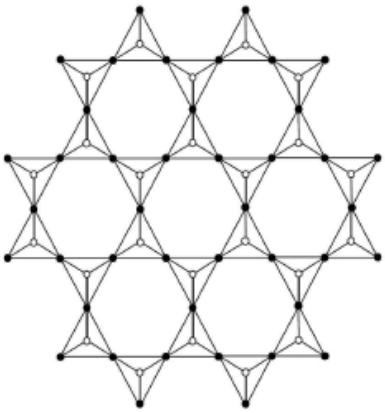

Fig 2: A two-dimensional silicate network.

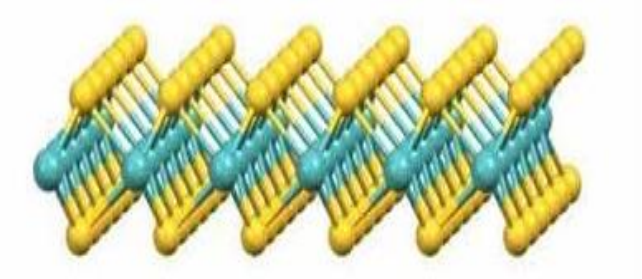

Fig 3: Schematic representation of side view of a monolayer of MoS_2

III. RESULTS AND DISCUSSION

Referring to Fig 1, there are two types of edges in Γ_n^2 on the basis of the degrees of the end vertices of each edge, as follows: the first type, for $e = uv \in E(\Gamma_n^2)$, is such that $d_u = 1$ and $d_v = 3$; the other type is, for $e = uv \in E(\Gamma_n^2)$, is such that $d_u = d_v = 3$. In the first type, there are 3.2^{n-1} edges, and in the other type, there are $3(2^{n-1} - 1)$ edges, as is shown in Table 1. The edge partition of Γ_n^2 on the basis of revan vertex degrees of end vertices is shown TABLE 2.

TABLE 1: Edge partition of Γ_n^2 on the basis of degrees of end vertices of each edge.

(d_u, d_v) where $uv \in E(\Gamma_n^2)$	Number of Edges
(1,3)	3.2^{n-1}
(3,3)	$3(2^{n-1}-1)$

TABLE 2: Edge partition of Γ_n^2 on the basis of revan vertex degrees of end vertices of each edge.

(d_u, d_v) where $uv \in E(\Gamma_n^2)$	$r_G(u)$	$r_G(u)$	Number of Edges
(1,3)	3	1	3.2^{n-1}
(3,3)	1	1	$3(2^{n-1}-1)$

TABLE 3: Edge partition of SL_n on the basis of degrees of end vertices of each edge.

(d_u, d_v) where $uv \in E(SL_n)$	Number of Edges
(3,3)	$6n$
(3,6)	$18n^2+6n$
(6,6)	$18n^2-12n$

TABLE 4: Edge partition of SL_n on the basis of revan vertex degrees of end vertices of each edge.

(d_u, d_v) where $uv \in E(SL_n)$	$r_G(u)$	$r_G(u)$	Number of Edges
(3,3)	6	6	$6n$
(3,6)	6	3	$18n^2+6n$
(6,6)	3	3	$18n^2-12n$

In SL_n, by algebraic method, there are three types of edges based on the degree of the vertices of each edge as follows: the first type, for $e = uv \in E(SL_n)$, is such that $d_u = d_v = 3$; the second type, for $e = uv \in E(SL_n)$, is such that $d_u = 3 \; and \; d_v = 6$; the third type, for $e = uv \in E(SL_n)$, is such that $d_u = d_v = 6$. In the first type, there are $6n$ edges, In the second type, there are $18n^2 + 6n$ edges and in the third type, there are $18n^2 - 12n$ edges as shown in TABLE 3. The Edge partition of SL_n on the basis of revan vertex degrees of end vertices is shown in TABLE 4.

There are three types of edges in MoS_2, one connecting vertex with degree two to another vertex with degree two, second type of edge connects vertex with degree two to vertex with degree four and the third type of vertex connects vertex with degree four to vertex with degree four. The number of edges for each type of edges for MoS_2 is given in the TABLE 5. The Edge partition of MoS_2 on the basis of revan vertex degrees of end vertices is shown in TABLE 6.

TABLE 5: Edge partition of MoS_2 on the basis of degrees of end vertices of each edge.

(d_u, d_v) where $uv \in E(MoS_2)$	Number of Edges
(2,2)	4
(2,4)	$4p + 4q - 8$
(4,4)	$4pq - 4p - 4q + 4$

TABLE 6: Edge partition of MoS_2 on the basis of revan vertex degrees of end vertices of each edge.

(d_u, d_v) where $uv \in E(MoS_2)$	$r_G(u)$	$r_G(u)$	Number of Edges
(2,2)	4	4	4
(2,4)	4	2	$4p + 4q - 8$
(4,4)	2	2	$4pq - 4p - 4q + 4$

Theorem 1: The Forgotten topological index of Cayley tree, Silicate layer network and molybdenum disulphide are: i. $F(\Gamma_n^2) = 21.2^{n+1} - 54$.

ii. $F(SL_n) = 2106n^2 - 486n$

iii. $F(MoS_2) = 128pq - 48(p + q)$

Proof:

i. Using (1) and TABLE 1, we get

$F(\Gamma_n^2) = 3.2^{n-1}(1^2 + 3^2) + 3(2^{n-1} - 1)(3^2 + 3^2)$ $F(\Gamma_n^2) = 21.2^{n+1} - 54$

ii. Using (1) and TABLE 3, we get

$$F(SL_n) = 6n(3^2 + 3^2) + (18n^2 + 6n)(3^2 + 6^2) + (18n^2 - 12n)(6^2 + 6^2)$$

$F(SL_n) = 2106n^2 - 486n$

iii. Using (1) and TABLE 5, we get

$$F(MoS_2) = 4(2^2 + 2^2) + (4p + 4q - 8)(2^2 + 4^2) + (4pq - 4p - 4q + 4)(4^2 + 4^2)$$

$F(MoS_2) = 128pq - 48(p + q)$

Theorem 2: The first, second and third revan indices of Cayley tree Γ_n^2 are:

i. $R_1(\Gamma_n^2) = 9.2^n - 6$

ii. $R_2(\Gamma_n^2) = 21.2^n - 3$

iii. $R_3(\Gamma_n^2) = 3.2^n$.

Proof:

i. Using (2) and TABLE 2 we get

$R_1(\Gamma_n^2) = 3.2^{n-1}(3 + 1) + 3(2^{n-1} - 1)(1 + 1)$

$R_1(\Gamma_n^2) = 9.2^n - 6$.

ii. Using (3) and TABLE 2 we get

$R_2(\Gamma_n^2) = 3.2^{n-1}(3.1) + 3(2^{n-1} - 1)(1.1)$

$R_2(\Gamma_n^2) = 21.2^{n-1} - 3.$

iii. Using (4) and TABLE 2 we get

$R_3(\Gamma_n^2) = 3.2^{n-1}|3 - 1| + 3(2^{n-1} - 1)|1 - 1|$

$R_3(\Gamma_n^2) = 3.2^{n+1}.$

Theorem 3: The first, second and third revan indices of Silicate layer network SL_n are:

i. $R_1(SL_n) = 270n^2 + 54n$

ii. $R_2(SL_n) = 486n^2 + 216n$

iii. $R_3(SL_n) = 54n^2 + 18n.$

Proof:

i. Using (2) and TABLE 4 we get

$R_1(SL_n) = 6n(6 + 6) + (18n^2 + 6n)(6 + 3) + (18n^2 - 12n)(3 + 3)$

$R_1(SL_n) = 270n^2 + 54n$.

ii. Using (3) and TABLE 4 we get

$R_2(SL_n) = 6n(6.6) + (18n^2 + 6n)(6.3) + (18n^2 - 12n)(3.3)$

$R_2(SL_n) = 486n^2 + 216n.$

iii. Using (4) and TABLE 4 we get

$R_3(SL_n) = 6n|6 - 6| + (18n^2 + 6n)|6 - 3| + (18n^2 - 12n)|3 - 3|$

$R_3(SL_n) = 54n^2 + 18n.$

Theorem 4: The first, second and third revan indices of Molybdenum disulphide MoS_2 are:

i. $R_1(MoS_2) = 16pq + 8p + 8q$

ii. $R_2(MoS_2) = 16pq + 16p + 16q + 16$

iii. $R_3(MoS_2) = 8p + 8q - 16.$

Proof:

i. Using (2) and TABLE 4 we get

$R_1(MoS_2) = 4(4 + 4) + (4p + 4q - 8)(4 + 2) + (4pq - 4p - 4q + 4)(2 + 2)$

$R_1(MoS_2) = 16pq + 8p + 8q$.

ii. Using (3) and TABLE 4 we get

$R_2(MoS_2) = 4(4.4) + (4p + 4q - 8)(4.2) + (4pq - 4p - 4q + 4)(2.2)$

$R_2(MoS_2) = 16pq + 16p + 16q + 16.$

iii. Using (4) and TABLE 4 we get

$R_3(MoS_2) = 4|4 - 4| + (4p + 4q - 8)|4 - 2| + (4pq - 4p - 4q + 4)|2 - 2|$

$$R_3(MoS_2) = 8p + 8q - 16.$$

IV. CONCLUSION

In this paper, certain degree-based topological indices, namely, the Forgotten topological index, first, second and third Revan indices are studied. We have determined and computed these indices for Cayley tree, Silicate layer network and molybdenum disulphide nano material. These results are novel and significant contributions in graph theory and network science, and they provide a good basis to understand the topology of these graphs and networks.

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