K₁ and K₂ Indices

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Abstract - In this paper, we introduce the K_1 and K_2 graphical indices of a graph. We compute these two indices for some standard graphs and certain important chemical structures such as nanostar dendrimers. Also we establish some bounds on these two indices.

Keywords - molecular structure, K_1 index, K_2 index, nanostar demdrimer.

Mathematics Subject Classification: 05C05, 05C09, 05C92.

I. INTRODUCTION

Let G be a 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 edges incident to u. We refer [1], for other undefined notations and terminologies.

A molecular graph is a graph such that its vertices correspond to the atoms and edges to the bonds. Chemical Graph Theory is a branch of mathematical chemistry, which has an important effect on the development of Chemical Sciences. Several graphical indices [2] have been considered in Theoretical Chemistry and have found some applications, see [3, 4, 5].

The Randic index [6] of a graph G was defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}.$$

Details of its Mathematical theory may be found in [7, 8].

This equation consists from 1 as numerator and geometric mean of end vertex degrees of an edge uv, $\sqrt{d_G(u)d_G(v)}$ as denominator.

Motivated by Randic index, we introduce the following graphical indices:

The K_1 index of a graph G is defined as

$$K_{1}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\left(d_{G}(u)^{2} + d_{G}(v)^{2}\right)/2}} = \sum_{uv \in E(G)} \frac{\sqrt{2}}{\sqrt{\left(d_{G}(u)^{2} + d_{G}(v)^{2}\right)}}.$$

This equation consists from 1 as numerator and quadratic mean of end vertex degrees of an edge uv, $\sqrt{\left(d_G(u)^2 + d_G(v)^2\right)/2}$ as denominator.

The K_2 index of a graph is defined as

$$K_{2}(G) = \sum_{uv \in E(G)} \frac{1}{\left(d_{G}(u)^{2} + d_{G}(v)^{2}\right) / \left(d_{G}(u) + d_{G}(v)\right)} = \sum_{uv \in E(G)} \frac{d_{G}(u) + d_{G}(v)}{d_{G}(u)^{2} + d_{G}(v)^{2}}.$$

This equation consists from 1 as numerator and contraharmonic mean of end vertex degrees of an edge uv, $\left(d_G(u)^2 + d_G(v)^2\right) / \left(d_G(u) + d_G(v)\right)$ as denominator.

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The harmonic index of a graph G is defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_G(u) + d_G(v)}$$

This index was studied by Favaron et al. [9] and Zhong [10].

Recently, some new graphical indices were studied, for example, in [11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24].

In this paper, we compute the K_1 and K_2 indices for some standard graphs and some nanostar dendrimers. Also we establish some properties of these indices. For dendrimers, see [25].

II. RESULTS FOR SOME STANDARD GRAPHS

A. K_1 index

Proposition 1. Let $K_{r,s}$ be a complete bipartite graph with $1 \le r \le s$, and $s \ge 2$ vertices. Then

$$K_1\left(K_{r,s}\right) = \frac{rs\sqrt{2}}{\sqrt{r^2 + s^2}}.$$

Proof: Let $K_{r,s}$ be a complete bipartite graph with r + s vertices and $rs \ edges$ such that $|V_1| = r$, $|V_2| = s$, $V(K_{r,s}) = V_1 \cup V_2$ for $1 \le r \le s$, and $s \ge 2$. Every vertex of V_1 is incident with s edges and every vertex of V_2 is incident with r edges.

$$K_1\left(K_{r,s}\right) = \frac{rs\sqrt{2}}{\sqrt{r^2 + s^2}}.$$

Corollary 1.1. Let $K_{r,r}$ be a complete bipartite graph with $r \ge 2$. Then

 $K_1(K_{r,r}) = r.$ Corollary 1.2. Let $K_{l,r-l}$ be a star with $r \ge 2$. Then

$$K_1(K_{1,r-1}) = \frac{(r-1)\sqrt{2}}{\sqrt{(r^2 - 2r + 2)}}$$

Proposition 2. If G is r-regular with n vertices and $r \ge 2$, then $K_1(G) = \frac{n}{2}$.

Proof: Let *G* is *r*-regular with *n* vertices and $r \ge 2$ and $\frac{nr}{2}$ edges. Then

$$K_1(G) = \frac{nr}{2} \frac{\sqrt{2}}{\sqrt{(r^2 + r^2)}} = \frac{n}{2}.$$

Corollary 1.1. Let C_n be a cycle with $n \ge 3$ vertices. Then $K_1(C_n) = \frac{n}{2}$.

Corollary 1.1. Let K_n be a complete graph with $n \ge 3$ vertices. Then

$$K_1(K_n)=\frac{n}{2}.$$

Proposition 3. If G is a path with $n \ge 3$ vertices, then $K_1(P_n) = \frac{n}{2} + \frac{2\sqrt{2}}{\sqrt{5}} - \frac{3}{2}$.

B. K₂ index

Proposition 4. Let $K_{r,s}$ be a complete bipartite graph with $1 \le r \le s$, and $s \ge 2$ vertices. Then

$$K_2(K_{r,s}) = \frac{rs(r+s)}{r^2 + s^2}.$$

Proof: Let $K_{r,s}$ be a complete bipartite graph with r + s vertices and $rs \ edges$ such that $|V_1| = r$, $|V_2| = s$, $V(K_{r,s}) = V_1 \cup V_2$ for $1 \le r \le s$, and $s \ge 2$. Every vertex of V_1 is incident with s edges and every vertex of V_2 is incident with r edges.

$$K_2(K_{r,s}) = \frac{rs(r+s)}{r^2 + s^2}.$$

Corollary 4.1. Let $K_{r,r}$ be a complete bipartite graph with $r \ge 2$. Then $K_2(K_{r,r}) = r$.

Corollary 4.2. Let $K_{l,r-l}$ be a star with $r \ge 2$. Then

$$QGK_2(K_{1,r-1}) = \frac{r(r-1)}{r^2 - 2r + 2}.$$

Proposition 5. If G is r-regular with n vertices and $r \ge 2$, then $K_2(G) = \frac{n}{2}$.

Proof: Let *G* is *r*-regular with *n* vertices and $r \ge 2$ and $\frac{nr}{2}$ edges. Then

$$K_2(G) = \frac{nr(r+r)}{2(r^2+r^2)} = \frac{n}{2}.$$

Corollary 5.1. Let C_n be a cycle with $n \ge 3$ vertices. Then $K_2(C_n) = \frac{n}{2}$.

Corollary 5.1. Let K_n be a complete graph with $n \ge 3$ vertices. Then

$$QGK_2(K_n)=\frac{n}{2}.$$

Proposition 6. If G is a path with $n \ge 3$ vertices, then $K_2(P_n) = \frac{n}{2} - \frac{3}{10}$.

III. BOUNDS ON K1 INDEX OF GRAPHS

Theorem 1. Let H(G) be the harmonic index of a graph G. Then

$$\frac{\sqrt{2}}{2}H(G) \le K_1(G) \le H(G).$$

Proof. Let $a \ge b \ge 1$ be real numbers. Then $(a-b)^2 \ge 0$.

 $a^2 + b^2 \ge 2ab$, this implies $2a^2 + 2b^2 \ge a^2 + b^2 + 2ab = (a+b)^2$

implying

$$\frac{2}{a+b} \ge \frac{\sqrt{2}}{\sqrt{a^2+b^2}}$$

For $a = d_G(u)$, $b = d_G(v)$, then the above inequality becomes

$$\frac{2}{d_{G}(u) + d_{G}(v)} \ge \frac{\sqrt{2}}{\sqrt{\left(d_{G}(u)^{2} + d_{G}(v)^{2}\right)}}$$

By definitions, we have

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_G(u) + d_G(v)} \ge \sum_{uv \in E(G)} \frac{\sqrt{2}}{\sqrt{(d_G(u)^2 + d_G(v)^2)}} = K_1(G).$$

Equality holds if and only if G is a regular graph.

We have

$$\frac{1}{\sqrt{a^2 + b^2}} = \frac{1}{\sqrt{(a+b)^2 - 2ab}} \ge \frac{1}{\sqrt{(a+b)^2}} = \frac{1}{(a+b)}$$

Implying

$$\frac{\sqrt{2}}{\sqrt{a^2+b^2}} \ge \frac{\sqrt{2}}{2} \frac{2}{(a+b)}$$

For $a = d_G(u)$, $b = d_G(v)$, by using the above inequality and definitions, we have

$$K_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{2}}{\sqrt{\left(d_G(u)^2 + d_G(v)^2\right)}} \ge \frac{\sqrt{2}}{2} \sum_{uv \in E(G)} \frac{2}{d_G(u) + d_G(v)} = \frac{\sqrt{2}}{2} H(G).$$

Theorem 2. Let R(G) be the Randic index of a graph G. Then

$$K_1(G) \leq R(G).$$

Proof. Let $a \ge b \ge 1$ be real numbers. Then $(a-b)^2 \ge 0$.

We get
$$a^2 + b^2 \ge 2ab$$
. This implies $\frac{\sqrt{2}}{\sqrt{a^2 + b^2}} \le \frac{1}{\sqrt{ab}}$.

For $a = d_G(u)$, $b = d_G(v)$, by using the above inequality and definitions, we have

$$K_{1}(G) = \sum_{uv \in E(G)} \frac{\sqrt{2}}{\sqrt{\left(d_{G}(u)^{2} + d_{G}(v)^{2}\right)}} \leq \sum_{uv \in E(G)} \frac{1}{\sqrt{d_{G}(u)d_{G}(v)}} = R(G).$$

Equality holds if and only if G is a regular graph

In literature, there exist many upper bounds on the Randic index. Thus one can establish many upper bounds on the K_1 index by using Theorem 2. For example, It is a well-known fact that if G is a graph without isolated vertices then

$$R(G) \leq \frac{n}{2}.$$

Corollary 2.1. Let G be a graph with n vertices and minimum degree at least 1. Then

 $K_1(G) \leq \frac{n}{2}.$

with equality if and only if G is a regular graph

IV. BOUNDS ON K2 INDEX OF GRAPHS

Theorem 3. Let G be a connected graph G with m edges and minimum degree δ . Then

$$K_2(G) \leq \frac{m}{\delta}.$$

Proof. For any edge uv in E (G), we can easily see that

$$\frac{d_G(u) + d_G(v)}{d_G(u)^2 + d_G(v)^2} \le \frac{1}{\delta}.$$

with equality if and only if $d_G(u) = d_G(v) = \delta$. That is, equality holds if and only if G is regular.

By using the above inequality and definitions, we have

$$K_{2}(G) = \sum_{uv \in E(G)} \frac{d_{G}(u) + d_{G}(v)}{d_{G}(u)^{2} + d_{G}(v)^{2}} \le \sum_{uv \in E(G)} \frac{1}{\delta} = \frac{m}{\delta}$$

Theorem 4. Let G be a connected graph. Then

$$K_2(G) > \frac{1}{2}H(G).$$

Proof. Let $a \ge b \ge 1$ be real numbers. Then $(a+b)^2 = a^2 + b^2 + 2ab > a^2 + b^2$.

implying
$$\frac{a+b}{a^2+b^2} > \frac{2}{2(a+b)}$$
.

For $a = d_G(u)$, $b = d_G(v)$, by using the above inequality and definitions, we have

$$K_{2}(G) = \sum_{uv \in E(G)} \frac{d_{G}(u) + d_{G}(v)}{d_{G}(u)^{2} + d_{G}(v)^{2}} > \sum_{uv \in E(G)} \frac{2}{d_{G}(u) + d_{G}(v)} = \frac{1}{2}H(G).$$

Theorem 5. Let G be a connected graph with m edges. Then

$$K_2(G) \leq \frac{m}{2}.$$

Proof. Let $a \ge b \ge 2$ be real numbers. Then $(a+b)^2 = a^2 + b^2 + 2ab > a^2 + b^2$.

Implying
$$\frac{a+b}{a^2+b^2} \le \frac{1}{2}$$
.

For $a = d_G(u)$, $b = d_G(v)$, by using the above inequality and definitions, we have

$$K_{2}(G) = \sum_{uv \in E(G)} \frac{d_{G}(u) + d_{G}(v)}{d_{G}(u)^{2} + d_{G}(v)^{2}} \le \sum_{uv \in E(G)} \frac{1}{2} = \frac{m}{2}.$$

V. RESULTS FOR POLY ETHYLENE AMIDE AMINE DENDRIMER PETAA

We consider the family of poly ethylene amide amine dendrimers. This family of dendrimers is denoted by *PETAA*. The molecular graph of *PETAA* is presented in Figure 1.



Fig 1. The molecular graph of PETAA

Let *G* be the molecular graph of *PETAA*. By calculation, we find that *G* has $44 \times 2^n - 18$ vertices and $44 \times 2^n - 19$ edges. In *PETAA*, there are three types of edges based on degrees of end vertices of each edge as given in Table 1.

Table 1. Edge partition of PETAA

$d_G(u), d_G(v) \setminus uv \in E(G)$	(1, 2)	(1, 3)	(2, 2)	(2, 3)
Number of edges	4×2^n	$4 \times 2^n - 2$	$16 \times 2^{n} - 8$	$20 \times 2^n - 9$

In the following theorem, we determine the K_1 and K_2 indices of *PETAA*. **Theorem 6.** Let *PETAA* be the family of poly ethylene amide amine dendrimers. Then

(i)
$$K_1(PETAA) = \left(\frac{4\sqrt{2}}{\sqrt{5}} + \frac{4}{\sqrt{5}} + 8 + \frac{20\sqrt{2}}{\sqrt{13}}\right)2^n - \frac{2}{\sqrt{5}} - 4 - \frac{9\sqrt{2}}{\sqrt{13}}.$$

(ii)
$$K_2(PETAA) = \frac{256 \times 2^n}{13} - \frac{537}{65}$$
.

Proof: By using definitions and Table 1, we obtain

(i)
$$K_{1}(PETAA) = \sum_{uv \in E(G)} \frac{\sqrt{2}}{\sqrt{\left(d_{G}(u)^{2} + d_{G}(v)^{2}\right)}}$$
$$= \frac{4 \times 2^{n} \sqrt{2}}{\sqrt{\left(1^{2} + 2^{2}\right)}} + \frac{\left(4 \times 2^{n} - 2\right) \sqrt{2}}{\sqrt{\left(1^{2} + 3^{2}\right)}} + \frac{\left(16 \times 2^{n} - 8\right) \sqrt{2}}{\sqrt{\left(2^{2} + 2^{2}\right)}} + \frac{\left(20 \times 2^{n} - 9\right) \sqrt{2}}{\sqrt{\left(2^{2} + 3^{2}\right)}}$$

After simplification, we obtain the desired result.

(ii)
$$K_{2}(PETAA) = \sum_{uv \in E(G)} \frac{d_{G}(u) + d_{G}(v)}{d_{G}(u)^{2} + d_{G}(v)^{2}}$$
$$= \frac{4 \times 2^{n} (1+2)}{1^{2} + 2^{2}} + \frac{(4 \times 2^{n} - 2)(1+3)}{1^{2} + 3^{2}} + \frac{(16 \times 2^{n} - 8)(2+2)}{2^{2} + 2^{2}} + \frac{(20 \times 2^{n} - 9)(2+3)}{2^{2} + 3^{2}}$$
giving the desired result

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VI. RESULTS FOR PROPYL ETHER IMINE DENDRIMER PETIM

We consider the family of propyl ether imine dendrimers. This family of dendrimers is denoted by *PETIM*. The molecular graph of *PETIM* is depicted in Figure 2.



Fig 2. The molecular graph of PETIM

Let *G* be the molecular graph of *PETIM*. By calculation, we find that *G* has $24 \times 2^n - 23$ vertices and $24 \times 2^n - 24$ edges. In *PETIM*, there are three types of edges based on degrees of end vertices of each edge as given in Table 2.

Table 2. Edge partition of PETIM

$d_G(u), d_G(v) \setminus uv \in E(G)$	(1, 2)	(2, 2)	(2, 3)
Number of edges	2×2^n	$16 \times 2^{n} - 18$	$6 \times 2^n - 6$

In the following theorem, we compute the K_1 and K_2 indices of *PETIM*. **Theorem 7.** Let *PETIM* be the family of porpyl ether imine dendrimers. Then

(i)
$$K_1(PETIM) = \left(\frac{2\sqrt{2}}{\sqrt{5}} + 8 + \frac{6\sqrt{2}}{\sqrt{13}}\right)2^n - 9 - \frac{6\sqrt{2}}{\sqrt{13}}.$$

(ii)
$$K_2(PETIM) = \frac{748 \times 2^n}{65} - \frac{147}{13}.$$

Proof: By using definitions and Table 2, we obtain

(i)
$$K_{1}(PETIM) = \sum_{uv \in E(G)} \frac{\sqrt{2}}{\sqrt{\left(d_{G}(u)^{2} + d_{G}(v)^{2}\right)}}$$
$$= \frac{2 \times 2^{n} \sqrt{2}}{\sqrt{\left(1^{2} + 2^{2}\right)}} + \frac{\left(16 \times 2^{n} - 18\right)\sqrt{2}}{\sqrt{\left(2^{2} + 2^{2}\right)}} + \frac{\left(6 \times 2^{n} - 6\right)\sqrt{2}}{\sqrt{\left(2^{2} + 3^{2}\right)}}$$

giving the desired result

(ii)
$$K_2(PETIM) = \sum_{uv \in E(G)} \frac{d_G(u) + d_G(v)}{d_G(u)^2 + d_G(v)^2}$$

= $\frac{2 \times 2^n (1+2)}{1^2 + 2^2} + \frac{(16 \times 2^n - 18)(2+2)}{2^2 + 2^2} + \frac{(6 \times 2^n - 6)(2+3)}{2^2 + 3^2}.$

After simplification, we obtain the desired result.

VII. RESULTS FOR ZINC PROPHYRIN DENDRIMER DPZ_N We consider the family of zinc prophyrin dendrimers. This family of dendrimers is denoted by DPZ_n , where *n* is the steps of growth in this type of dendrimers. The molecular graph of DPZ_n is shown in Figure 3.



Fig 3. The molecular graph of DPZ_n

Let G be the molecular graph of DPZ_n . By calculation, we obtain that G has $56 \times 2^n - 7$ vertices $64 \times 2^n - 4$ edges. In DPZ_n , there are four types of edges based on degrees of end vertices of each edge as given in Table 3.

Table 3. Edge partition of *DPZ_n*

$d_G(u), d_G(v) \setminus uv \in E(G)$	(2, 2)	(2, 3)	(3, 3)	(3, 4)
Number of edges	$16 \times 2^{n} - 4$	$40 \times 2^{n} - 16$	$8 \times 2^{n} + 12$	4

In the following theorem, we determine the K_1 and K_2 indices of DPZ_n . **Theorem 8.** Let DPZ_n be the family of zinc prophyrin dendrimers. Then

(i)
$$K_1(DPZ_n) = \left(\frac{32}{3} + \frac{10\sqrt{2}}{\sqrt{13}}\right)2^n + 2 - \frac{16\sqrt{2}}{\sqrt{13}} + \frac{4\sqrt{2}}{5}$$

(ii)
$$K_2(DPZ_n) = \frac{566 \times 2^n}{39} - \frac{986}{325}.$$

Proof: From definitions and by using Table 3, we deduce

(i)
$$K_{1}(DPZ_{n}) = \sum_{uv \in E(G)} \frac{\sqrt{2}}{\sqrt{\left(d_{G}(u)^{2} + d_{G}(v)^{2}\right)}} = \frac{\left(16 \times 2^{n} - 4\right)\sqrt{2}}{\sqrt{\left(2^{2} + 2^{2}\right)}} + \frac{\left(40 \times 2^{n} - 16\right)\sqrt{2}}{\sqrt{\left(2^{2} + 3^{2}\right)}} + \frac{\left(8 \times 2^{n} + 12\right)\sqrt{2}}{\sqrt{\left(3^{2} + 3^{2}\right)}} + \frac{4\sqrt{2}}{\sqrt{\left(3^{2} + 4^{2}\right)}}$$
This gives the desired result of the simplification

This gives the desired result after simplification.

(ii)
$$K_{2}(DPZ_{n}) = \sum_{uv \in E(G)} \frac{d_{G}(u) + d_{G}(v)}{d_{G}(u)^{2} + d_{G}(v)^{2}}$$
$$= \frac{(16 \times 2^{n} - 4)(2 + 2)}{2^{2} + 2^{2}} + \frac{(40 \times 2^{n} - 16)(2 + 3)}{2^{2} + 3^{2}} + \frac{(8 \times 2^{n} + 12)(3 + 3)}{3^{2} + 3^{2}} + \frac{4(3 + 4)}{3^{2} + 4^{2}}$$

After simplification, we obtain the desired result.

VIII. RESULTS FOR PORPHYRIN DENDRIMER $D_N P_N$

We consider the family of porphyrin dendrimers. This family of dendrimers is denoted by $D_n P_n$. The molecular graph of $D_n P_n$ is shown in Figure 4.



Fig 4. The molecular graph of $D_n P_n$

Let *G* be the molecular graph of $D_n P_n$. By calculation, we find that *G* has 96n - 10 vertices and 105n - 11 edges. In $D_n P_n$, there are six types of edges based on degrees of end vertices of each edge as given in Table 4.

Table 4. Edge partition of $D_n P_n$

$d_G(u), d_G(v) \setminus uv \in E(G)$	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(3, 3)	(3, 4)
Number of edges	2n	24 <i>n</i>	10n - 5	48n - 6	13 <i>n</i>	8 <i>n</i>

In the following theorem, we compute the K_1 and K_2 indices of $D_n P_n$. **Theorem 9.** Let $D_n P_n$ be the family of porphyrin dendrimers. Then

(i)
$$K_1(D_nP_n) = \left(\frac{2}{\sqrt{5}} + \frac{24\sqrt{2}}{\sqrt{17}} + 5 + \frac{48\sqrt{2}}{\sqrt{13}} + \frac{13}{3} + \frac{8\sqrt{2}}{5}\right)n - \frac{5}{2} - \frac{6\sqrt{2}}{\sqrt{13}}.$$

(ii)
$$K_2(D_nP_n) = \left(\frac{4}{5} + \frac{120}{17} + 5 + \frac{240}{13} + \frac{15}{3} + \frac{36}{25}\right)n - \frac{123}{26}.$$

Proof: From definitions and by using Table 4, we deduce

(i)
$$K_1(D_n P_n) = \sum_{uv \in E(G)} \frac{\sqrt{2}}{\sqrt{(d_G(u)^2 + d_G(v)^2)}}$$

 $= \frac{2n\sqrt{2}}{\sqrt{(1^2 + 3^2)}} + \frac{24n\sqrt{2}}{\sqrt{(1^2 + 4^2)}} + \frac{(10n - 5)\sqrt{2}}{\sqrt{(2^2 + 2^2)}} + \frac{(48n - 6)\sqrt{2}}{\sqrt{(2^2 + 3^2)}} + \frac{13n\sqrt{2}}{\sqrt{(3^2 + 3^2)}} + \frac{8n\sqrt{2}}{\sqrt{(3^2 + 4^2)}}$

After simplification, we get the desired result.

(ii)
$$K_2(D_nP_n) = \sum_{uv \in E(G)} \frac{d_G(u) + d_G(v)}{d_G(u)^2 + d_G(v)^2}$$

= $\frac{2n(1+3)}{1^2 + 3^2} + \frac{24n(1+4)}{1^2 + 4^2} + \frac{(10n-5)(2+2)}{2^2 + 2^2} + \frac{(48n-6)(2+3)}{2^2 + 3^2} + \frac{13n(3+3)}{3^2 + 3^2} + \frac{8n(3+4)}{3^2 + 4^2}$

giving the desired result

IX. CONCLUSION

In this paper, we have introduced two novel graphical indices which are K_1 and K_2 indices and computed exact values of some standard graphs. Furthermore we have determined these two indices for certain nanostar dendrimers. Also we have obtained some properties of these indices.

- Many questions are suggested by this research, among them are the following:
- 1. Characterize the K_1 and K_2 indices in terms of other degree based topological indices.
- 2. Obtain the extremal values and extremal graphs of K_1 and K_2 indices.
- 3. Compute these two indices for other chemical nanostructures.

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