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Hanoi 图的 K Banhatti 和 K 超 Banhatti 指数

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摘要：在理论化学领域存在各种拓扑指数，尤其是基于距离的拓扑指数和基于度的拓扑指数等. 而基于距离的拓扑指数取决于一对顶点之间的距离，基于度的拓扑指数则取决于顶点的程度. 指标是数字，描述相关化合物的拓扑. 在 QSAR/QSPR 研究中，拓扑指数例如 K Banhatti 指数和 K 超 Banhatti 指数用来表征化合物的物理化学性质. 因此，基于图结构的分析，计算了双轮图和 Hanoi 图的 K Banhatti 指数和 K 超Banhatti指数.

关键词：化学图论；Banhatti 指数；双轮图 DW_n；Hanoi 图 H_n
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K Banhatti and K Hyper Banhatti Indices of Hanoi Graph

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Abstract: In theoretical chemistry, there are various topological indices for example distance based topological indices and degree based topological indices etc. The distance based topological indices depends on the distances between pair of vertices and the degree based topological indices depends on the degrees of vertices. The indices are numerical numbers and describe the topology of concerned chemical compound. In QSAR/QSPR study, physiochemical properties and topological indices for example K Banhatti index and K Hyper Banhatti index are used to characterize the chemical compound. So based on the graph structure analysis, we computed the K Banhatti index and K Hyper Banhatti index of Double-wheel graph DW_n and Hanoi graph H_n.
Key words: chemistry graph theory; Banhatti indices; double-wheel graph DW_n; Hanoi graph H_n

0 Introduction

Chemical reaction network theory deals with an attempt to model the behavior of real world chemical systems. From the very beginning of its foundation, it is hot cake for research community; especially due to its importance in two important branches i. e. biochemistry and theoretical chemistry. It has also a signicant place in pure mathematics particularly due to its mathematical structures.

Cheminformatics is an upcoming and progressive area that deals with the relationships of qualitative structure activity (QSAR) and structure property (QSPR) and also predicts the biochemical activities and properties of nanomaterial. In these studies, for the prediction of bioactivity of the chemical compounds, some physcio-chemical properties and topological indices are used see [1—5].

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Mathematical chemistry is the branch of chemistry which discusses the chemical structures with the aid of mathematical tools. Molecular graph is a simple connected graph in chemical graph theory. This graph consists of atoms and chemical bonds and they are represented by vertices and edges respectively. The distance between two vertices u and v is represented as $d(u,v)$ and it is the shortest length between u and v in graph G. The degree of vertex is basically the number of vertices of G adjacent to a given vertex v and will be denoted by d_v. The topological index of a molecule can be used to quantify the molecular structure. To be simple, the topological index can be considered a function that assign each molecular structure to real number. Boiling point, heat of evaporation, heat of formation, chromate graphic retention times, surface tension, vapor pressure etc can be predicted by using topological indices. First and second Zagreb indices are degree based graph invariants have been studies extensively since 1970′s.

In this paper all molecular graphs are considered to be connected, finite, loop less and deprived of parallel edges. Let F be a graph with n vertices and m edges. The degree of a vertex is the number of vertices adjacent to q and is signified as $d(q)$. By these terminologies, certain topological indices are well-defined in the following way.

The first and second K Banhatti indices were introduced by Kulli in [6] as

$$B_1(G) = \sum_{ue}[d_G(u) + d_G(e)],$$

and

$$B_2(G) = \sum_{ue}[d_G(u)d_G(e)].$$

The following K hyper-Banahatti indices are defined in [7] as

$$HB_1(G) = \sum_{ue}[d_G(u) + d_G(e)]^2,$$

and

$$HB_2(G) = \sum_{ue}[d_G(u)d_G(e)]^2.$$

1 Main Results for Double-Wheel Graph

A double-wheel graph DW_n (see Figure 1) of size n can be composed of $2C_n + K_1, n \geqslant 3$, that is it contains two cycles of size n, where all the points of the two cycles are associated to a common center.

The degree based topological indices like K Banhatti index and K Hyper Banhatti index for Double-wheel graph are calculated in this section.

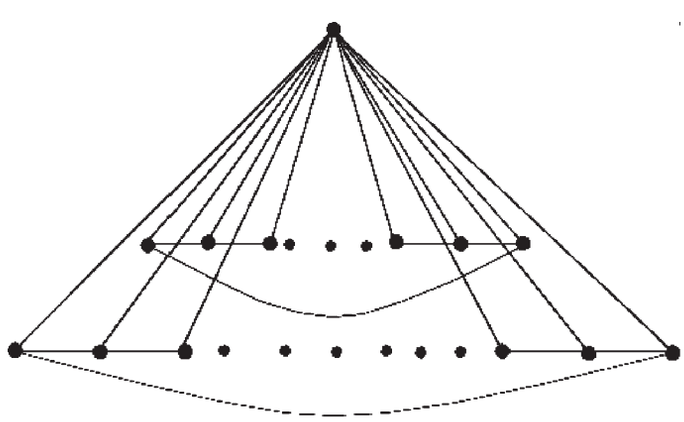

Figure 1 Double Wheel Graph DW_n

Theorem 1 For DW_n, we have

1. $B_1(DW_n) = 6n(2n+5)$;
2. $B_2(DW_n) = n(8n^2 + 8n - 45)$;

3. $HB_1(DW_n)=2n(20n^2+103)$;

4. $HB_2(DW_n)=2n(16n^4-16n^3+40n^2-36n+297)$.

Proof Let $G=DW_n$. We have two partitions of the edge set $E(DW_n)$ as follows

$$E_{(3,3)}=\{uv\in E(G):d_G(u)=d_G(v)=3\},|E_{(3,3)}|=2n;$$

$$E_{(3,2n)}=\{uv\in E(G):d_G(u)=3,d_G(v)=2n\},|E_{(3,2n)}|=2n.$$

The edge degree partition is given in table 1.

Table 1　Edge Degree Partition of DW_n

$d_G(u),d_G(v):e=uv\in E(G)$	$(3,3)$	$(3,2n)$
$d_G(e)$	4	$2n-1$
Number of edges	$2n$	$2n$

1. First K Banhatti index.

$$\begin{aligned}B_1(G)&=\sum_{ue}[d_G(u)+d_G(e)]\\&=\sum_{e=uv\in E_{(3,3)}}[(d_G(u)+d_G(e))+(d_G(v)+d_G(e))]+\sum_{e=uv\in E_{(3,2n)}}[(d_G(u)+d_G(e))+(d_G(v)+d_G(e))]\\&=(2n)[(3+4)+(3+4)]+(2n)[(3+2n-1)+(2n+2n-1)]\\&=2n(14)+2n(6n+1)\\&=6n(2n+5).\end{aligned}$$

2. Second K Banhatti index.

$$\begin{aligned}B_2(G)&=\sum_{ue}[d_G(u)d_G(e)]\\&=\sum_{e=uv\in E_{(3,3)}}[(d_G(u)d_G(e))+(d_G(v)d_G(e))]+\sum_{e=uv\in E_{(3,2n)}}[(d_G(u)d_G(e))+(d_G(v)d_G(e))]\\&=(2n)[(3)(4)+(3)(4)]+(2n)[(3)(2n-1)+(2n)(2n-1)]\\&=2n(24)+2n(4n^2+4n-3)\\&=n(8n^2+8n-45).\end{aligned}$$

3. First Hyper K Banhatti index.

$$\begin{aligned}HB_1(G)&=\sum_{ue}[d_G(u)+d_G(e)]^2\\&=\sum_{e=uv\in E_{(3,3)}}[(d_G(u)+d_G(e))^2+(d_G(v)+d_G(e))^2]+\sum_{e=uv\in E_{(3,2n)}}[(d_G(u)+d_G(e))^2+(d_G(v)\\&\quad+d_G(e))^2]\\&=(2n)[(3+4)^2+(3+4)^2]+(2n)[(3+2n-1)^2+(2n+2n-1)^2]\\&=2n(98)+2n(20n^2+5)\\&=2n(20n^2+103).\end{aligned}$$

4. Second Hyper K Banhatti index.

$$\begin{aligned}HB_2(G)&=\sum_{ue}[d_G(u)d_G(e)]^2\\&=\sum_{e=uv\in E_{(3,3)}}[(d_G(u)d_G(e))^2+(d_G(v)d_G(e))^2]+\sum_{e=uv\in E_{(3,2n)}}[(d_G(u)d_G(e))^2+(d_G(v)d_G(e))^2]\\&=(2n)[((3)(4))^2+((3)(4))^2]+(2n)[((3)(2n-1))^2+((2n)(2n-1))^2]\\&=2n(288)+2n(16n^4-16n^3+40n^2-36n+9)\\&=2n(16n^4-16n^3+40n^2-36n+297).\end{aligned}$$

2　Main Results for Hanoi Graph

The Hanoi graph H_n (see Figure 2) can be created by taking the vertices to be the odd binomial coefficients of pascal′s triangle calculated on the integers from 0 to 2^n-1 and drawing a line when coefficients are together

diagonally or horizontally. The graph H_n has 3^n vertices and $(3^{n+1}-15)/2$ edges. Every Hanoi graph has a unique Hamiltonian cycle.

The degree based topological indices like K Banhatti index and K Hyper Banhatti index for Hanoi graph H_n are computed in this section.

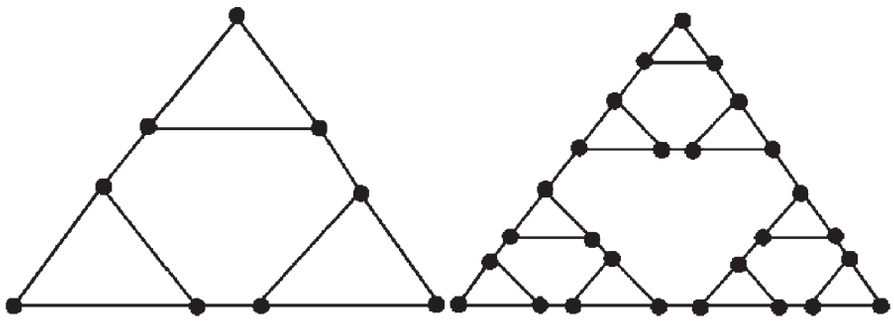

Figure 2 Hanoi Graph H_n

Theorem 2 For H_n, we have

1. $B_1(H_n)=3(7\times 3^n-13)$;
2. $B_2(H_n)=9(4\times 3^n-10)$;
3. $HB_1(H_n)=3(49\times 3^n-123)$;
4. $HB_2(H_n)=2(216\times 3^n-729)$.

Proof Let $G=H_n$, where $n\geqslant 3$. We have two partitions of the edge set $E(H_n)$ as follows

$$E_{(2,3)}=\{uv\in E(G):d_G(u)=2,d_G(v)=3\},|E_{(3,3)}|=6;$$

$$E_{(3,3)}=\{uv\in E(G):d_G(u)=d_G(v)=3\},|E_{(3,3)}|=\frac{3^{n+1}-15}{2}.$$

The edge degree partition is given in table 2.

Table 2 Edge Degree Partition of H_n

$d_G(u),d_G(v):e=uv\in E(G)$	(2,3)	(3,3)
$d_G(e)$	3	4
Number of edges	6	$(3^{n+1}-15)/2$

1. First K Banhatti index.

$$\begin{aligned}B_1(G)&=\sum_{ue}[d_G(u)+d_G(e)]\\&=\sum_{e=uv\in E_{(2,3)}}[(d_G(u)+d_G(e))+(d_G(v)+d_G(e))]+\sum_{e=uv\in E_{(3,3)}}[(d_G(u)+d_G(e))+(d_G(v)+d_G(e))]\\&=(6)[(2+3)+(3+3)]+\frac{3^{n+1}-15}{2}[(3+4)+(4+4)]\\&=6(11)+\frac{3^{n+1}-15}{2}(14)\\&=3(7\times 3^n-13).\end{aligned}$$

2. Second K Banhatti index.

$$\begin{aligned}B_2(G)&=\sum_{ue}[d_G(u)d_G(e)]\\&=\sum_{e=uv\in E_{(2,3)}}[(d_G(u)d_G(e))+(d_G(v)d_G(e))]+\sum_{e=uv\in E_{(3,3)}}[(d_G(u)d_G(e))+(d_G(v)d_G(e))]\\&=(6)[(2)(3)+(3)(3)]+\frac{3^{n+1}-15}{2}[(3)(4)+(4)(4)]\end{aligned}$$

$$=6(15)+\frac{3^{n+1}-15}{2}(24)$$

$$=9(4\times 3^{n}-10).$$

3. First Hyper K Banhatti index.

$$HB_1(G)=\sum_{ue}[d_G(u)+d_G(e)]^2$$

$$=\sum_{e=uv\in E_{(2,3)}}[(d_G(u)+d_G(e))^2+(d_G(v)+d_G(e))^2]+\sum_{e=uv\in E_{(3,3)}}[(d_G(u)+d_G(e))^2+(d_G(v)+d_G(e))^2]$$

$$=(6)[(2+3)^2+(3+3)^2]+\frac{3^{n+1}-15}{2}[(3+4)^2+(4+4)^2]$$

$$=6(61)+\frac{3^{n+1}-15}{2}(98)$$

$$=3(49\times 3^{n}-123).$$

4. Second Hyper K Banhatti index.

$$HB_2(G)=\sum_{ue}[d_G(u)d_G(e)]^2$$

$$=\sum_{e=uv\in E_{(2,3)}}[(d_G(u)d_G(e))^2+(d_G(v)d_G(e))^2]+\sum_{e=uv\in E_{(3,3)}}[(d_G(u)d_G(e))^2+(d_G(v)d_G(e))^2]$$

$$=(6)[((2)(3))^2+((3)(3))^2]+\frac{3^{n+1}-15}{2}[((3)(4))^2+((4)(4))^2]$$

$$=6(117)+\frac{3^{n+1}-15}{2}(288)$$

$$=2(216\times 3^{n}-729).$$

3 Conclusion

Topological indices are important, because with the help of topological indices, one can predict properties of chemical compounds. In this paper, we have computed Banhatti indices, hyper Banhatti indices and multiplicative versions of Banhatti indices for some important classes of graphs. Our results can pay a vital role in new drugs formation.

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