# Bipartite edge frustration of cactus chains

S. HAYAT[a,*], A. KHAN[b], F. YOUSAFZAI[b], M. IMRAN[a]
[a]*Department of Mathematics, School of Natural Sciences (SNS), National University of Sciences and Technology (NUST), Sector H-12, Islamabad, Pakistan*
[b]*School of Mathematical Sciences, University of Science and Technology of China (USTC), Hefei, Anhui, China*

A molecular graph is a graphical representation of a chemical structure which is constructed by using certain graph operation. Topological indices are global graph-theoretic parameters which are studied for molecular graphs and provide significant information related to physico-chemical properties of underlying chemical substances. Bipartite edge frustration is defined as the minimum number of edges whose deletion from the graph gives the bipartite spanning subgraph of given graph. Bipartite edge frustration is a topological index which is related to the chemical stability of various nanostructures such as Fullerenes. In this paper, the bipartite edge frustration of cactus chains are studied. We give an important conjecture generalizing this concept for whole family of cacti graphs at the end of the article.

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## 1. Introduction

Let $G=(V,E)$ be a simple graph, a graph without multiple edges and loops. A subgraph $H$ of $G$ is a graph whose set of vertices and set of edges are all subsets of $G$. A spanning subgraph is a subgraph that contains all the vertices of the original graph. The graph $G$ is called bipartite if the vertex set $V$ can be partitioned into two disjoint subsets $V_1$ and $V_2$ such that all edges of $G$ have one endpoint in $V_1$ and the other in $V_2$. Bipartite edge frustration of a graph $G$, denoted by $\phi(G)$, is the minimum number of edges that need to be deleted to obtain a bipartite spanning subgraph.

It is easy to see that $\phi(G)$ is a topological index and $G$ is bipartite if and only if $\phi(G)$ = 0. Thus $\phi(G)$ is a measure of bipartivity. It is a well-known fact that a graph $G$ is bipartite if and only if $G$ does not have odd cycles. Holme, Liljeros and Edling introduced the edge frustration as a measure in the context of complex network [15].

Fajtlowicz claimed that the chemical stability of fullerenes is related to the minimum number of vertices/edges that need to be deleted to make a fullerene graph bipartite [6, 7]. We mention here that before publishing the mentioned papers of Fajtlowicz, Schmalz et al. [19] observed that the isolated pentagon fullerenes (IPR fullerenes) have the best stability. Doslic [3], presented some computational results to confirm this relationship. So it is natural to ask about relationship between the degree of non-bipartivity and stability of chemical structures such as nanotubes, polyomino and cactus chains.

Throughout this paper all graphs considered are finite and simple. Our notations are standard and taken mainly from [8, 10]. We encourage the reader to consult papers by Doslic [3, 4, 5] for background material and more information on the problem.

We also encourage the reader to consult papers [2, 11, 12, 13, 14, 16, 17, 18] for some background material as well as basic computational methods on mathematical properties of nanomaterials and chemical networks.

## 2. Motivations, results and discussion

Topological indices play a vital role in the QSAR/QSPR studies, they predict certain physico-chemical properties of chemical compounds like nanotubes, nanocones, dendrimers, polyomino and cactus chains. Bipartite edge frustration is a topological index which correlate the chemical stability of Fullerenes and other chemical structures.

Ashrafi and co-authors [9] computed the bipartite edge frustration of various infinite families of carbon nanotubes. Doslic et al. [3, 4] studied the bipartite edge frustration of fullerenes. So its natural to ask for the bipartite edge frustration of polyomino and cactus chains which play an important role in polymer chemistry. In this paper, the bipartite edge frustration of various cactus chains is strong-minded.

### 2.1 Cactus chains

In this paper we consider a class of simple linear polymers called cactus chains. Cactus graphs were first known as Husimi trees; they appeared in the scientific literature some sixty years ago in papers by Husimi and Riddell concerned with cluster integrals in the theory of condensation in statistical mechanics [1].

A cactus graph is a connected graph in which no edge lies in more than one cycle. Consequently, each block of a cactus graph is either an edge or a cycle. If all blocks of a cactus $G$ are cycles of the same size $i$, the cactus is $i$-uniform. A triangular cactus is a graph whose blocks are triangles, i.e., a $3$-uniform cactus. A vertex shared by two or more triangles is called a cut-vertex. If each triangle of a triangular cactus G has at most two cut-vertices, and each cut-vertex is shared by exactly two triangles, we say that $G$ is a chain triangular cactus. By replacing triangles in this definitions by cycles of length $4$ we obtain cacti whose every block is $C_4$. We call such cacti square cacti. Note that the internal squares may differ in the way they connect to their neighbors. If their cut-vertices are adjacent, we say that such a square is an ortho-square; if the cut-vertices are not adjacent, we call the square a parasquare.

In the same way, by replacing the $C_4$ by $C_5, C_6, \ldots, C_k$ for some positive integer $k$ we get 2-parametric class of cactus chains. We denote it $HT_n^k$ after their original name i.e. Husimi trees, where $k$ is the length of the cycle we replace and $n$ is the dimension of the chain. In this paper, we study the bipartite edge frustration of three families of cactus chains named as triangular, square and pentagonal cactus chains. We formulate a conjecture for the general $k$ in $HT_n^k$ as well. Now we compute bipartite edge frustration of triangular cactus chains.

### 2.2 Bipartite edge frustration of chain triangular cactus

We call the number of triangles in $G$, the length of the chain. An example of a chain triangular cactus is shown in Fig. 1. Obviously, all chain triangular cacti of the same length are isomorphic. Hence, we denote the chain triangular cactus of length $n$ by $T_n$ which is isomorphic to $HT_n^k$ with $k = 3$.

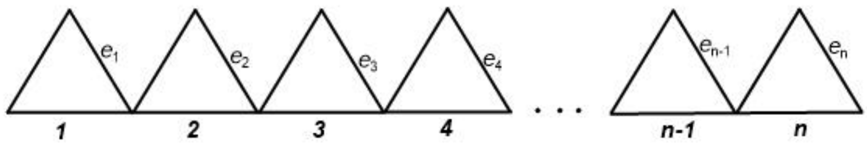


*Fig. 1. Triangular chain cactus $HT_n^k$ with $k = 3$.*

Now we compute bipartite edge frustration index of triangular cactus graph.

**Theorem 2.2:** Let $T_n$ be the triangular cactus graph, then

$$\phi(T_n) = n$$

***Proof.*** Consider $T_n$ be the triangular chain cactus. There exist no 2-coloring of $T_n$ which turns out that $\phi(T_n) > 0$. To prove that it is exactly $n$, we need to prove both of the inequalities i.e. $\phi(T_n) \geq n$ and $\phi(T_n) \leq n$. Since for $n > 1$, there is a cut vertex between two triangles which means we only need to delete one edge in every cycle to make it a spanning tree which is surely a bipartite. In Fig 1, $e_i$, $i = 1,2,3,\ldots,n$ are the edges which are needed to be deleted to make it spanning tree. This implies that $\phi(T_n) \leq n$.

On the other hand, it can easily be seen that there is no less number of edges which makes its edges deleted subgraph a bipartite spanning subgraph. This turns out that $\phi(T_n) \geq n$. And the proof is complete.

### 2.3 Bipartite edge frustration of chain square cacti

By replacing triangles in the definitions of triangular cactus, by cycles of length $4$ we obtain cacti whose every block is $C_4$. We call such cacti, square cacti. An example of a square cactus chain is shown in Fig. 2.

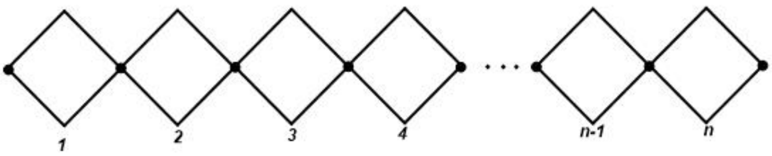


*Fig. 2. An $n$-dimensional para-chain square cactus.*

We see that the internal squares may differ in the way they connect to their neighbors. If their cut-vertices are adjacent, we say that such a square is an ortho-square; if the cut-vertices are not adjacent, we call the square a para-square.

We denote the para-chain square cactus graph of length $n$ as $Q_n$, and ortho-chain square cactus graph of length $n$ as $O_n$. An $n$-dimensional ortho-chain square cactus graph is depicted in Fig. 3.

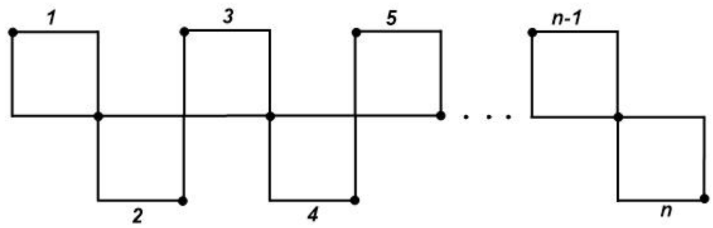


*Fig. 3. An ortho-chain square cactus of dimension $n$.*

**Theorem 2.3:** Let $Q_n$ and $O_n$ be the para and ortho chain square cacti respectively, then

$$\phi(Q_n) = \phi(O_n) = 0$$

***Proof.*** A graph $G$ is bipartite if and only if $\phi(G) = 0$. So, to prove them having zero bipartite edge frustration it suffices to prove them bipartite. Fig. 2 shows a 2-coloring of $Q_n$, in which bold vertices can be put in one partite set and rest of them can be put in other partition. Which clearly shows that $Q_n$ is bipartite.

In the similar manner, we can prove ortho-chain square cactus bipartite. Fig. 3 shows a bipartition of $O_n$ having bold vertices in one partition and remaining in other partition. Hence $O_n$ is bipartite.

### 2.4 Bipartite edge frustration of chain pentagonal cactus

By replacing pentagons in the definition of triangular chain cactus, we get chain pentagonal cactus having each block as $C_5$. Of course, all chain pentagonal cacti of same dimension are isomorphic. For sake of convenience, we denote it as $P_n$ which is equivalent to the $HT_n^5$. Fig. 4 shows a chain pentagonal cactus.

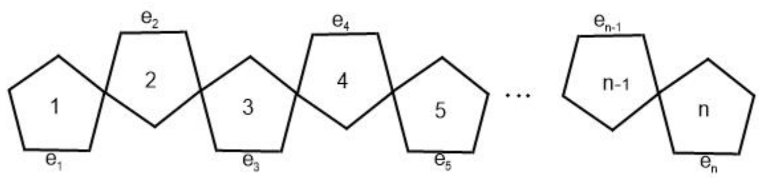


*Fig. 4. An n-dimensional chain pentagonal cactus.*

We compute bipartite edge frustration of chain pentagonal cactus in the following result.

**Theorem 2.4:** Let $P_n$ be the chain pentagonal square cactus, then

$$\phi(P_n) = n$$

***Proof.*** We prove $\phi(P_n) = n$, we need to prove these two inequalities, $\phi(P_n) \le n$, and $\phi(P_n) \ge n$. There does not exist any 2-coloring of $P_n$, which turns us out $\phi(P_n) > 0$. The presence of cut-vertex shared by any two pentagons ensures us that deletion of one edge from each 5-gon turns out a spanning tree of $P_n$ for $n > 1$. In Fig. 4, $e_i$, $i = 1,2,3,...,n$ are the edges which are needed to be deleted to make it spanning tree. Hence $\phi(P_n) \le n$.

It can easily be seen that there is no less number of edges present in $P_n$ whose deletion gives a spanning tree. Hence $\phi(P_n) \ge n$, which completes the proof.

### 2.5 Conjecture on $HT_n^k$

By replacing a cycle of any length i.e. $k$ where $k$ is positive integer, we get general cactus chain i.e. $HT_n^k$. If we study some parameter for triangular, square and pentagonal cactus chains, then it is natural to ask the study of this parameter for general cactus graph. After doing lot of calculation and their verification, we come across this result for $HT_n^k$. Since we do not find some rigorous graph-theoretic mathematical arguments to prove this result. So we leave it to the readers for future research work by formulating it as a conjecture.

**Conjecture:** The bipartite edge frustration of $HT_n^k$ is as follows:

$$\phi(HT_n^k) = \begin{cases} 0, & k \cong 0 \bmod (2) \\ n, & k \cong 1 \bmod (2) \end{cases}$$

## 3. Conclusion and general remarks

Topological indices are the numerical descriptors, which provide us very valuable information in theoretical chemistry and nanotechnology. Bipartite edge frustration is an important topological index which is closely related to the chemical stability of chemical compounds. This index has been extensively studied for nanotubes and Fullerenes, In this paper, we extend this concept to the cactus chains which are important structures in chemistry due to their chemical significance. We have found results for three classes of cactus chains and formulate a conjecture to make this concept generalized for whole family of cactus chain graphs.

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*Corresponding author: sakander1566@gmail.com