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TOSHA INDEX FOR GRAPHS

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ABSTRACT. A topological index of a chemical structure (graph) is a number that correlates the chemical structure with chemical reactivity or physical properties. There are several topological indices have been defined on graphs using degrees of vertices/edges, for instance first and second Zagreb indices. In this paper, we introduce a new topological index for graphs called Tosha index using tension on edges. Further, we establish some inequalities and compute Tosha index for some standard graphs.

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1. INTRODUCTION

Mathematical chemistry deals with the molecular structures using mathematical methods. These methods solve many of the problems in chemistry. The theory of chemical graphs gives connectivity between chemistry and graph theory, and solves many of the difficult problems of mathematical chemistry using graph theory. A topological index of a chemical structure(graph) is a number that correlates the chemical structure with chemical reactivity or physical properties. Topological indices of large chemical structures such as metal organic frameworks can be extremely useful in both characterization of structures and computing their physicochemical properties that are otherwise difficult to compute for such large networks of importance in reticular chemistry. Topological indices numerically represent the structural characteristics of molecules that are obtained by the use of graph-theoretical concepts applied to these large networks of interest in reticular chemistry. Hence every topological index defined on graphs using degrees, distances, shortest paths etc., must reflect some chemical properties of molecules. Therefore there is a scope for defining new topological indices for graphs.

For standard terminology and notion in graphs, we refer the reader to the text-book of Harary [1]. The non-standard will be given in this paper as and when required.

Throughout this paper, $G = (V, E)$ denotes a graph (finite, undirected and simple) and $V = V(G)$ and $E = E(G)$ denote vertex set and edge set of G, respectively. Two non-distinct edges in a graph are adjacent if they

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are incident on a common vertex. We consider that an edge in a graph is not adjacent to itself. The degree of a vertex v in a graph G is the number of edges associated with it and is denoted by $d(v)$.

The distance between two vertices u and v in G, denoted by $d(u,v)$ is the number of edges in a shortest path (also called a graph geodesic) connecting them. We say that a graph geodesic P is passing through an edge e in G if e is an edge in P. The number of geodesics in G is denoted by f.

The notion of tension on edge in a graph has been studied recently by K. Bhargava, N.N. Dattatreya, and R. Rajendra in their paper [2]. Let G be a graph and e be an edge in G. The tension on e, denoted by $\tau_G(e)$ or simply $\tau(e)$, is defined as the number of geodesics in G passing through e. A graph G is said to be k-tension-regular if all its edges are of tension k. The total tension of G, denoted by $N_\tau(G)$, is defined as:

$$N_\tau(G) = \sum_{e \in E} \tau(e). \tag{1}$$

The first Zagreb index $M_1(G)$ of a simple graph G is defined (see [3, 4]) as

$$M_1(G) = \sum_{v \in V(G)} d(v)^2. \tag{2}$$

The Zagreb indices have been defined using degrees of vertices in a graph to explain some properties of chemical compounds at molecular level [3, 4]. It is exciting to study concepts involving values on edges like tosha-degree, tension etc., [see [2], [6], [7] and [8]]. The recent contribution towards the topological indices, the readers suggested to refer the papers [5, 9, 10]. Hence by the motivation of Zagreb indices, in this paper we introduce a new index on graphs called Tosha index of a graph using tensions of edges and we try to obtain some results.

2. Tosha index of a graph

Definition 2.1. *The Tosha index $\mathcal{T}(G)$ of a graph G is defined by*

$$\mathcal{T}(G) = \sum_{e \in E(G)} \tau(e)^2. \tag{3}$$

Example 2.1. *We compute the peripheral Harary index of the hydrogen-depleted molecular graph G of 1-Ethyl-2-methylcyclobutane C_7H_{14}. We label the vertices of G as shown in Figure 1.*

The tensions on the edges of G are as follows:

$$\begin{aligned} &\tau(ab) = 7, \quad \tau(ac) = 6, \quad \tau(bh) = 7, \quad \tau(bd) = 11, \\ &\tau(cd) = 8, \quad \tau(de) = 12, \quad \tau(ef) = 7. \end{aligned}$$

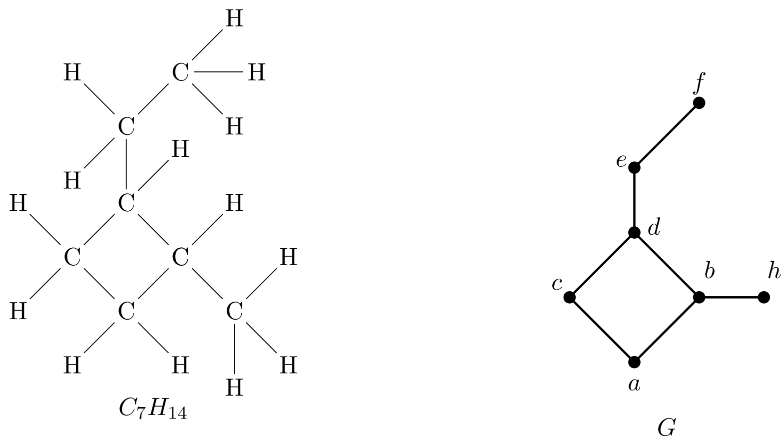

FIGURE 1. 1-Ethyl-2-methylcyclobutane C_7H_{14} and the corresponding hydrogen-depleted molecular graph G

The Tosha index of G is,

$$\begin{aligned}\mathcal{T}(G) &= \tau(ab)^2+\tau(ac)^2+\tau(bh)^2+\tau(bd)^2+\tau(cd)^2+\tau(de)^2+\tau(ef)^2\\ &= 7^2+6^2+7^2+11^2+8^2+12^2+7^2\\ &= 512.\end{aligned}$$

Proposition 2.2. *For any graph G, we have the following inequalities:*

$$N_\tau(G) \le \mathcal{T}(G) \le |E|f^2 \tag{4}$$

and

$$N_\tau(G) \le \mathcal{T}(G) \le N_\tau(G)^2. \tag{5}$$

Proof. Since $\tau(e) \le \tau(e)^2$, $\forall e \in E(G)$, from the equations (1) and (3), from the (3), we have

$$N_\tau(G) \le \mathcal{T}(G). \tag{6}$$

Since $\tau(e) \le f$, $\forall e \in E(G)$, we have

$$\mathcal{T}(G) \le |E|f^2 \tag{7}$$

Combining (6) and (7), we get (4).

From (1), we have

$$N_\tau(G)^2 = \left[\sum_{e\in E}\tau(e)\right]^2 = \sum_{e\in E}\tau(e)^2 + \sum_{e,e'\in E}\tau(e)\tau(e')$$

which implies

$$,\sum_{e\in E}\tau(e)^2 = N_\tau(G)^2 - \sum_{e,e'\in E}\tau(e)\tau(e').$$

Therefore

$$\mathcal{T}(G) = \sum_{e \in E} \tau(e)^2 \leq N_\tau(G)^2. \tag{8}$$

Combining (6) and (8), we get (5). □

Proposition 2.3. *If G is k-tension regular, then*

$$\mathcal{T}(G) = k^2|E| \tag{9}$$

Proof. If G is k-tension regular, then $\tau(e) = k$, $\forall e \in E(G)$ and so from (3), we have

$$\mathcal{T}(G) = \sum_{e \in E(G)} k^2 = k^2|E|.$$

□

Corollary 2.4. *(i) For the complete graph K_n on n vertices, $\mathcal{T}(K_n) = \binom{n}{2}$.*

(ii) For the complete bipartite graph $K_{m,n}$, $\mathcal{T}(K_{m,n}) = mn(m+n-1)^2$.

(iii) For the cycle C_n on n vertices,

$$\mathcal{T}(C_n) = \begin{cases} \dfrac{n(n-1)^2(n+1)^2}{64}, & \text{if } n \text{ is odd;} \\ \dfrac{n^3(n+2)^2}{64}, & \text{if } n \text{ is even.} \end{cases}$$

Proof. (i) In the complete graph K_n, for any edge e, we have $\tau(e) = 1$. Therefore K_n is 1-tension regular graph. Hence by Proposition 2.3, we have

$$\mathcal{T}(K_n) = 1^2|E(K_n)| = \binom{n}{2}.$$

(ii) In the complete bipartite graph $K_{m,n}$, for any edge e, we have $\tau(e) = m+n-1$. Therefore $K_{m,n}$ is $(m+n-1)$-tension regular graph. Hence by Proposition 2.3, we have

$$\mathcal{T}(K_{m,n}) = (m+n-1)^2|E(K_{m,n})| = (m+n-1)^2 mn.$$

(iii) Let e be any edge in the cycle graph C_n on n vertices. Then

$$\tau(e) = \begin{cases} \dfrac{(n-1)(n+1)}{8}, & \text{if } n \text{ is odd} \\ \dfrac{n(n+2)}{8}, & \text{if } n \text{ is even.} \end{cases}$$

Therefore C_n is

$$\begin{cases} \dfrac{(n-1)(n+1)}{8}\text{-tension regular}, & \text{if } n \text{ is odd;} \\ \dfrac{n(n+2)}{8}\text{-tension regular}, & \text{if } n \text{ is even.} \end{cases}$$

Hence by Proposition 2.3, we have

$$\mathcal{T}(C_n) = \begin{cases} \left[\dfrac{(n-1)(n+1)}{8}\right]^2 |E(C_n)|, & \text{if } n \text{ is odd;} \\ \left[\dfrac{n(n+2)}{8}\right]^2 |E(C_n)|, & \text{if } n \text{ is even.} \end{cases}$$

$$= \begin{cases} \dfrac{n(n-1)^2(n+1)^2}{64}, & \text{if } n \text{ is odd;} \\ \dfrac{n^3(n+2)^2}{64}, & \text{if } n \text{ is even.} \end{cases}$$

□

Proposition 2.5. *If T is a tree with m edges $e_1, e_2, ..., e_m$, then*

$$\mathcal{T}(T) = \sum_{i=1}^{m} |V(C_{i1})|^2 |V(C_{i2})|^2,$$

where C_{i1} and C_{i2} are the components of $T - e_i$, $1 \le i \le m$. Further, for a path P_n with n vertices,

$$\mathcal{T}(P_n) = \frac{1}{30} n(n^4 - 1).$$

Proof. For the edge e_i in T, let C_{i1} and C_{i2} be the components of $T - e_i$. Then

$$\tau(e_i) = |V(C_{i1})||V(C_{i2})|, \ 1 \le i \le m.$$

Hence from (3), we have $\mathcal{T}(T) = \sum_{i=1}^{m} |V(C_{i1})|^2 |V(C_{i2})|^2$.

A path P_n with n vertices, has $n - 1$ edges $e_1, e_2, ..., e_{n-1}$ (shown in the following figure).

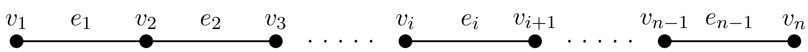

Figure 2. The path P_n on n vertices.

Clearly, $|V(C_{i1})| = i$ and $|V(C_{i2})| = n - i$ in $T - e_i$. Hence

$$\mathcal{T}(P_n) = \sum_{i=1}^{n-1} |V(C_{i1})|^2 |V(C_{i2})|^2 = \sum_{i=1}^{n-1} i^2 (n-i)^2 = \frac{1}{30} n(n^4 - 1).$$

□

Proposition 2.6. *Let W_n denote the wheel graph on $n \ge 5$ vertices. Then*

$$\mathcal{T}(W_n) = (n-1)(n^2 - 6n + 18).$$

Proof. For the wheel graph W_n with $n \ge 5$, there are $(n-1)$ radial edges and $(n-1)$ peripheral edges. If e_p is a peripheral edge in W_n, then $\tau(e_p) = 3$

and if e_r is a radial edge in W_n, then $\tau(e_r) = n - 3$. Hence from (3), we have

$$\begin{aligned}\mathcal{T}(W_n) &= \sum_{\text{peripheral edges}} \tau(e_p)^2 + \sum_{\text{radial edges}} \tau(e_p)^2 \\ &= (n-1)\cdot 3^2 + (n-1)\cdot(n-3)^2 \\ &= (n-1)(n^2 - 6n + 18).\end{aligned}$$

□

Proposition 2.7. *Let F_n denote the friendship graph on $2n+1$ vertices. Then*

$$\mathcal{T}(F_n) = 8n^3 + 8n^2 + 3n.$$

Proof. In F_n, there are $3n$ edges, out of them $2n$ radial edges and n peripheral edges. If e_p is a peripheral edge in F_n, then $\tau(e) = 1$ and if e_r is a radial edge in F_n, then $\tau(e_r) = 2n+1$. Hence from (3), we have

$$\begin{aligned}\mathcal{T}(F_n) &= \sum_{\text{peripheral edges}} \tau(e_p)^2 + \sum_{\text{radial edges}} \tau(e_p)^2 \\ &= n\cdot 1^2 + 2n\cdot(2n+1)^2 \\ &= 8n^3 + 8n^2 + 3n.\end{aligned}$$

□

Proposition 2.8. *If G is a subgraph of a tree T, then $\mathcal{T}(G) \leq \mathcal{T}(T)$.*

Proof. Let G be a subgraph of a tree T. Since, in a tree, between any two vertices there is one and only one path, $\tau_G(e) \leq \tau_T(e)$ for any edge e in G. Therefore, from (3),

$$\mathcal{T}(G) = \sum_{e\in E(G)} \tau_G(e)^2 \leq \sum_{e\in E(G)} \tau_T(e)^2 \leq \sum_{e\in E(T)} \tau_T(e)^2 = \mathcal{T}(T).$$

□

Remark 2.9. If G is a subgraph of a graph G', then the inequality $\mathcal{T}(G) \leq \mathcal{T}(G')$ need not be true, if G' is not a tree. For example, consider the complete graph K_n which contains a path P_n. From the Corollary 2.4 (i) and Proposition 2.5, we have $\mathcal{T}(K_n) = \binom{n}{2} = \frac{1}{2}n(n-1)$ and $\mathcal{T}(P_n) = \frac{1}{30}n(n^4-1)$. Clearly for $n \geq 3$, $\mathcal{T}(P_n) = \frac{1}{30}n(n^4-1) > \frac{1}{2}n(n-1) = \mathcal{T}(K_n)$.

Conclusion

All graphs considered in this manuscript are simple. We have introduced a new topological index of a graph called Tosha index using tension on edges. Further, we established some inequalities and compute Tosha index for some standard graphs. The fact that modelling a molecule by a graph gives us many required information on the physico-chemical properties of the molecule at the end of some mathematical calculations made on the graph has been used in the last seven decades. In future, we would like to develop the theory of Tosha index, by finding methods of computation and its relations with chemical properties of molecules.

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