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Vertex-Cut Sets and Tenacity of Organic Compounds C_nH_{2n+2}

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Abstract Consider some vertices of a graph G are omitted, there are some criteria for measuring the vulnerability of the graph; *Tenacity* is one of them. In the definition of tenacity we use vertex cut S and some items, $\tau(G-S)$ and $\omega(G-S)$, such that $\tau(G-S)$ is the number of vertices in the largest component of $G-S$ and $\omega(G-S)$ is the number of components of $G-S$. In this paper we work on tenacity of organic compound C_nH_{2n+2}. The graph of this molecule is a tree. We try on tenacity of it by the definition of the tenacity.

Keywords Tenacity · Vertex cut · Organic compounds · Tree · C_nH_{2n+2} molecule

Mathematics Subject Classification (2010) 97k30

1 Introduction

Let G be a graph. Assume some vertices or some edges of G are removed. A question arises up, how much the graph G dangerous is. There are some criteria for measuring the vulnerability of G as connectivity, hardness, toughness, tenacity, etc. In [3], [7], [8], these criteria are compared and the results suggest that tenacity is a most suitable measure of stability or vulnerability in that

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for many graphs it is best able to distinguish between graphs that intuitively should have different levels of vulnerability. Some researchers are studied on tenacity of some graphs, for example, tenacity of complete graphs, tenacity of three classes of Harrary graphs, tenacity of corona product of graphs, etc [2,4,5,10–12]. In this paper we work on the tenacity of molecule C_nH_{2n+2} by the definition of tenacity. We explain some concepts of graphs and tenacity, some vertex cut-sets of graph of molecule C_nH_{2n+2}, main results and some examples in the sections, respectively.

2 Background

Definition 1 A graph $G = (V, E)$ consists of a nonempty set V of vertices and a set $E(G)$ of edges, with each edge of G is a set of two vertices of V (not necessarily distinct). We refer to $|V| = n$ as the order of the graph G, and to $|E| = m$ as the size of the graph G. If $m = 0$, the graph G is called empty. If $e_i = e_j$, these edges are called parallel. If $e = \{u, v\}$, then e is said to join u and v; the vertices u and v are called the ends of e. Two vertices u and v are incident to the edge e, also, u and v are adjacent. An edge with identical ends is called a loop. The degree $d_G(v)$ of a vertex v in G is the number of edges of G incident with v. A tree is a connected acyclic graph. If T is a tree and v is a vertex by degree 1, the vertex v is called a *leaf*. For every tree T, $m = n - 1$.

C_nH_{2n+2} molecule has n Carbon atoms and $2n + 2$ Hydrogen atoms, so the graph of C_nH_{2n+2} has $3n + 2$ vertices and $3n + 1$ edges, and it is tree. Every Carbon atom has degree 4 and every Hydrogen atom has degree 1.

Definition 2 A vertex v of G is a cut vertex if E can be partitioned into two nonempty subsets E_1 and E_2 such that $G[E_1]$ and $G[E_2]$ have just the vertex v in common. If G is loop less and nontrivial, then v is a cut vertex of G if and only if $\omega(G - v > \omega(G)$.
A vertex cut of G is a subset V' of V such that $G - V'$ is disconnected. A k-vertex cut is a vertex cut of k elements. A complete graph has no vertex cut; in fact, the only graphs which do not have vertex cuts are those that contain complete graphs as spanning sub-graphs.

See [1], for more information.

Definition 3 The tenacity of a graph G, $T(G)$, is

$$T(G) = min\{\frac{|S| + \tau(G - S)}{\omega(G - S)}\}, \qquad (1)$$

where the minimization is over all vertex cut-sets S, $\omega(G - S)$ is the number of components of $G - S$ and $\tau(G - S)$ is the number of vertices in the largest component of $G - S$ [2]. Edge-tenacity is defined similarly, except that S is an edge cut of G and $\tau(G - S)$ is the number of edges in the largest component of $G - S$. A Connected graph G is called T-tenacious, if for any subset S of vertices of G with $\omega(G-S) \geq 1$, we have $|S| + \tau(G-S) \geq T.\omega(G-S)$. If G is not a complete graph, then there is a largest number T, such that G is T-tenacious. Hence, the number T, is the tenacity of G. A connected graph G is called T-tenacious if $|S| + \tau(G-S) \geq T.\omega(G-S)$ holds for any subset S of vertices of G with $\omega(G-S) > 1$. If G is not complete, then there is a largest T such that G is T-tenacious; this T is the tenacity of G. On the other hand, a complete graph contains no vertex cut-set and so it is T-tenacious for every T. Accordingly, we define $T(K_p) = \infty$ for every p $(p \geq 1)$.A set $S \subset V(G)$ is said to be a T-set of G if $T(G) = \frac{|S|+\tau(G-S)}{\omega(G-S)}$ [2].

In this paper, the amount of $\frac{|S|+\tau(G-S)}{\omega(G-S)}$ is called the *" YIELD AMOUNT OF FRACTION (YAF) "*, made by the set S, and will be represented by symbol $YAF(S)$.

3 Vertex cut-sets of the Graph C_nH_{2n+2}

The aim of this paper is to investigate the tenacity of the graph of C_nH_{2n+2}. The tenacity of a graph is dependent on the vertex cut. So, first, we must obtain the vertex cut (for the graph of C_nH_{2n+2}). For carbon atom, we assign the index down, the graph of C_nH_{2n+2} appears in Figure 1.

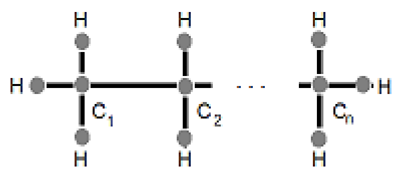

Fig. 1 Graph of C_nH_{2n+2}

Proposition 1 *Let T be a tree. $v \in V(T)$ is a cut vertex if and only if $d_T(v) > 1$.[1]*

Obviously, $v \in V(T)$ is a cut vertex if and only if v is a non-leaf. So in the graph of C_nH_{2n+2}, v is a cut vertex if and only if it is a Carbon atom in the graph of C_nH_{2n+2}. Therefore, each vertex cut-set must contain at least one Carbon atom.

Lemma 1 *Let $S_0 = \{C_1\}$ and S contains carbon atom C_1 only, then we have:*

$$YAF(S_0) \leq YAF(S). \quad (2)$$

Proof. Since $S_0 = \{C_1\}$, therefore

$$|S_0| = 1, \omega_0 = \omega(G - S_0) = 4, \tau_0 = \tau(G - S_0) = 3(n-1) + 1 = 3n - 2.$$

Let $S = S_0 \cup I \cup J$ such that the set I contains i hydrogen atoms connected to $C_1, (0 \leq i \leq 2)$ and the set J contains j hydrogen atoms unconnected to C_1, so

$$|S| = 1 + i + j, \omega = \omega(G - S) = \omega_0 - i, \tau = \tau(G - S) = \tau_0 - j, \tag{3}$$

therefore

$$\begin{aligned} YAF(S) = \tfrac{|S|+\tau}{\omega} &= \tfrac{|S_0|+i+j+\tau_0-j}{\omega_0-j} \\ &= \tfrac{|S_0|+i+\tau_0}{\omega_0-i} \\ &\geq \tfrac{|S_0|+\tau_0}{\omega_0} = YAF(S_0). \end{aligned}$$

□

The proof is similar for $S = \{C_n\}$.
Use τ and ω instead of $\tau(G - S)$ and $\omega(G - S)$, respectively, in the rest of this paper.

Lemma 2 *Let $S_0 = \{C_k\}$ ($2 \leq k \leq n-1$) and S contains atom carbon C_k only, then*

$$YAF(S_0) < YAF(S). \tag{4}$$

Proof. $S_0 = \{C_k\}$, so $|S_0| = 1$ and $\omega_0 = \omega(G - S_0) = 4$. Consider different cases for finding $\tau_0 = \tau(G - S_0)$, as follows:

1. If $k \leq \lceil \frac{n}{2} \rceil$, then the largest component of $G - S_0$ contains $n - k$ carbon atoms and $2(n-k) + 1$ hydrogen atoms. So there is $3(n-k) + 1$ vertices in the largest component of $G - S_0$.

2. If $k > \lceil \frac{n}{2} \rceil$, then the largest component of $G - S_0$ contains $k - 1$ carbon atoms and $2(k-1) + 1 = 2k - 1$ hydrogen atoms. so the largest component has $3(k-1) + 1 = 3k - 2$ vertices.
So

$$\tau(G - S_0) = \begin{cases} 3(n-k) + 1 \ , & k \leq \lceil \frac{n}{2} \rceil, \\ 3(k-1) + 1 \ , & k > \lceil \frac{n}{2} \rceil. \end{cases} \tag{5}$$

Accuracy, the function $\tau_0 = \tau(G - S_0)$ is continuous on $k = \lceil \frac{n}{2} \rceil$.
The graph of $C_nH_{2n+2} \backslash C_k$ has four components, two hydrogen atoms which are connected to C_k and two large components $C_{k-1}H_{2(k-1)+1}$ and $C_{n-k}H_{2(n-k)+1}$, name these components as A and B. Without reducing the generality consider $\nu(A) \geq \nu(B)$, so

$$\tau_0 = \tau(G - S_0) = \nu(A),$$

also $\nu(A) + \nu(B) + 3 = 3n + 2$.
Let $S = S_0 \cup I \cup J$ such that the set I has i hydrogen atoms connected to C_k,

$(0 \leq i \leq 2)$ and the set J has j hydrogen atoms unconnected to C_k. Also, let r members of J be in A and let s members of J be in B, $(r + s = j)$, so

$$|S| = |S_0| + i + j, \omega = \omega(G - S) = \omega_0 - i.$$

The set A transforms to A' after removing r hydrogen atoms from A and the set B transforms to B' after removing s hydrogen atoms from B, it means

$$\nu(A') = \nu(A) - r, \nu(B')\nu(B) - s.$$

Compare $\nu(A')$ and $\nu(B')$ for checking the tenacity of $G - S$

$$\begin{aligned} \nu(A') - \nu(B') &= \nu(A) - r - \nu(B) + s \\ &= 2\nu(A) - 3n - r + s + 1 \\ &\stackrel{\nu(A)=\tau_0}{=} 2\tau_0 - 3n - r + s + 1. \end{aligned}$$

If $2\tau_0 - 3n - r + s + 1 \geq 0$ then $\nu(A') \geq \nu(B')$ and so $\tau = \nu(A')$. Therefore,

$$\tau = \nu(A) - r = \tau_0 - r,$$

and

$$\begin{aligned} yaf(S) = \tfrac{|S|+\tau}{\omega} &= \tfrac{|S_0|+i+j+\tau_0-r}{\omega_0-i} \\ &= \tfrac{|S_0|+\tau_0+j+s}{\omega_0-i} \\ &\geq \tfrac{|S_0|+\tau_0}{\omega_0} = yaf(S_0). \end{aligned}$$

If $2\tau_0 - 3n - r + s + 1 < 0$ then $\nu(A') < \nu(B')$ and so $\tau = \nu(B')$. Therefore,

$$\begin{aligned} \tau = \nu(B) - s &= (3n + 2) - (\nu(A) + 3) - s \\ &= 3n - \nu(A) - 1 \\ &\stackrel{\nu(A)\tau_0}{=} 3n - \tau_0 - 1 - s. \end{aligned}$$

and

$$\begin{aligned} yaf(S) = \tfrac{|S|+\tau}{\omega} &= \tfrac{|S_0|+i+j+3n-\tau_0-1}{\omega_0-i} \\ &= \tfrac{|S_0|+3n+j-\tau_0-1-r}{\omega_0} \\ &\geq \tfrac{|S_0|+3n+j-\tau_0-1}{\omega_0} \\ &\geq \tfrac{|S_0|+\tau_0}{\omega_0} = yaf(S_0). \end{aligned}$$

The proof is complete. □

Lemma 3 *Suppose $S_0 = \{C_1, C_k\}$ and S contains two carbon atoms C_1 and C_k, then*

$$YAF(S_0) \leq YAF(S). \qquad (6)$$

Proof. Consider different cases
Case 1. Let $S_0 = \{C_1, C_2\}$, so

$$|S_0| = 2, \omega_0 = \omega(G - S_0) = 6, \tau_0 = \tau(G - S_0) = 3(n-2) + 1 = 3n - 5,$$

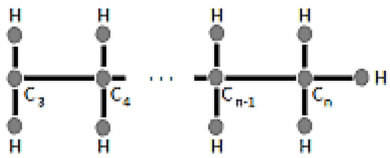

Fig. 2 The components of $G - S_0$

the largest component is in Figure 2.
Now suppose $S = S_0 \cup I \cup J$, that the set I contains i hydrogen atoms which are connected to C_1 or C_2 $(0 \leq i \leq 5)$, and the set J contains j hydrogen atoms which are unconnected to C_1 and C_2, so

$$|S| = |S_0| + i + j, \omega = \omega_0 - i, \tau = \tau_0 - j$$

and

$$\begin{aligned} YAF(S) = \tfrac{|S|+\tau}{\omega} &= \tfrac{|S_0|+i+j+\tau_0-j}{\omega_0-i} \\ &\geq \tfrac{|S_0|+i+\tau(G-S_0)}{\omega(G-S_0)} \\ &\geq \tfrac{|S_0|+\tau(G-S_0)}{\omega(G-S_0)} = YAF(S_0). \end{aligned}$$

Case 2. Let $S_0 = \{C_1, C_n\}$.

$$|S_0| = 2, \omega_0 = 7, \tau_0 = 3(n-2).$$

Now suppose $S = S_0 \cup I \cup J$ that I contains i hydrogen atoms only which are connected to C_1 or C_n and J contains j hydrogen atoms only which are unconnected to C_1 and C_n, so

$$|S| = |S_0| + i + j, \omega = \omega_0 - i, \tau = \tau_0 - j$$

and

$$\begin{aligned} YAF(S) = \tfrac{|S|+\tau}{\omega} &= \tfrac{|S_0|+i+j+\tau_0-j}{\omega_0-i} \\ &= \tfrac{|S_0|+i+\tau_0}{\omega_0-i} \end{aligned}$$

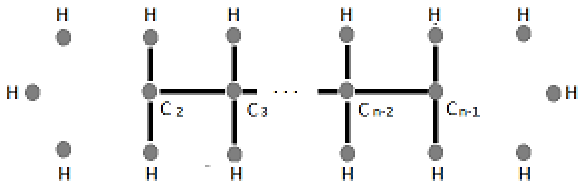

Fig. 3 The components of $G - S_0$

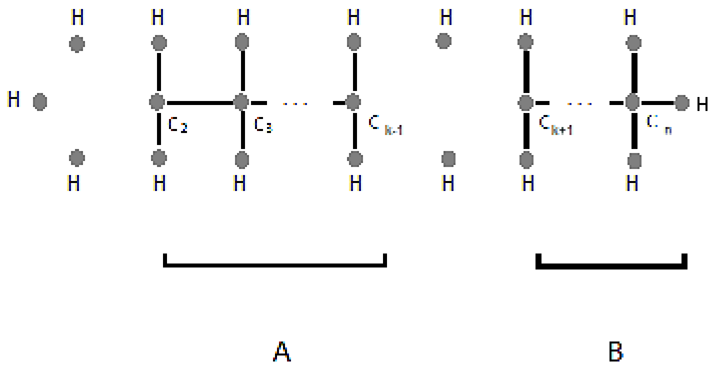

Fig. 4 The components of $G - S_0$

$$\geq \frac{|S_0|+\tau_0}{\omega_0} = YAF(S_0)$$

Case 3. Let $S_0 = \{C_1, C_k\}$ that $3 \leq k \leq n-1$.
Name the large components of $G - S_0$ by A and B as before, so

$$\nu(A) = 3(k-2), \nu(B) = 3(n-k)+1, \nu(B) - \nu(A) = 3n - 6k + 7,$$

So if $k \leq \frac{n}{2} + \frac{7}{6}$, then $\nu(B) \geq \nu(A)$ and $\tau_0 = \nu(B)$, and if $k > \frac{n}{2} + \frac{7}{6}$, then $\nu(A) > \nu(B)$ and $\tau_0 = \nu(A)$. Therefore

$$|S| = 2, \omega_0 = 7, \tau_0 = \begin{cases} 3(n-k)+1 & , k \leq \frac{n}{2} + \frac{7}{6}, \\ 3(k-2) & , k > \frac{n}{2} + \frac{7}{6}. \end{cases}$$

Suppose $S = S_0 \cup I \cup J$ that the set I contains i hydrogen atoms which are connected to C_1 or C_k, and the set J contains j hydrogen atoms which are unconnected to C_1 and C_k, so

$$|S| = |S_0| + i + j, \omega = \omega_0 - i.$$

Without reducing the generality, suppose $\nu(A) > \nu(B)$, therefore $\tau_0 = \nu(A)$. Let r members of J be in A and s members of J be in B, $(r + s = i)$, so A transforms to A' and B transforms to B' after removing S from C_nH_{2n+2}. Also,

$$\nu(A') = \nu(A) - r, \nu(B') = \nu(B) - s,$$

and

$$\begin{aligned} \nu(A') - \nu(B') &= \nu(A) - (3n - \nu(A) - 5) - r + s \\ &= 2\nu(A) - 3n + 5 - r + s \\ &\overset{\tau_0=\nu(A)}{=} 2\tau_0 - 3n + 5 - r + s. \end{aligned}$$

So if $2\tau_0 - 3n + 5 - r + s \geq 0$, then

$$\tau = \nu(A') = \nu(A) - r = \tau_0 - r,$$

and

$$\begin{aligned} YAF(S) = \tfrac{|S|+\tau}{\omega} &= \tfrac{|S_0|+i+j+\tau_0-r}{\omega_0-i} \\ &= \tfrac{|S_0|+\tau_0+(i+j-r)}{\omega_0-i} \\ &\geq \tfrac{|S_0|+\tau_0}{\omega_0} = YAF(S_0) \end{aligned}$$

And if $2\tau_0 - 3n + 5 - r + s < 0$, then

$$\tau = \nu(B') = \nu(B) - s = 3n - \nu(A) - 5 - 3 \overset{\nu(A)=\tau_0}{=} 3n - \tau_0 - 5 - s,$$

also

$$\begin{aligned} \nu(A') - \nu(B') < 0 \quad &\Rightarrow \quad 2\tau_0 - 3n + 5 + s - r < 0 \\ &\Rightarrow -2\tau_0 + 3n - 5 - s + r > 0 \\ &\Rightarrow -2\tau_0 + 3n - 5 - s > -r \\ &\Rightarrow -2\tau_0 + 3n - 5 + j - s > j - r > 0 \\ &\Rightarrow i + (j - s) + 3n - 2\tau_0 - 5 > 0, \end{aligned}$$

therefore

$$\begin{aligned} YAF(S) = \tfrac{|S|+\tau}{\omega} &= \tfrac{|S_0|+i+j+3n-\tau_0-5-s}{\omega_0-i} \\ &\geq \tfrac{|S_0|+\tau_0+(i+(j-s)+3n-2\tau_0-5)}{\omega_0-i} \\ &\geq \tfrac{|S_0|+\tau_0}{\omega_0} = YAF(S_0). \end{aligned}$$

The proof is complete. □

Lemma 4 *Let* $S_0 = \{C_k, C_{k+1}\}$ *that* $k \neq 1, k \neq n-1$*, and* S *contains two carbon atoms* C_k *and* C_{k+1}*, then*

$$YAF(S_0) \leq YAF(S). \tag{7}$$

Proof. Since $S_0 = \{C_k, C_{k+1}\}$, then $|S_0| = 2$ and $\omega_0 = 6$.

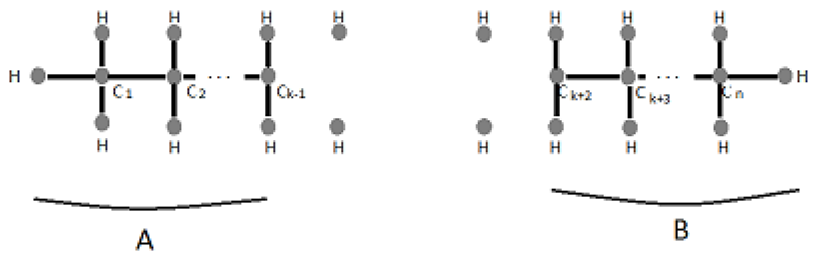

Fig. 5 The components of $G - S_0$

The graph $G - S_0$ has four isolated components and two large components, name the large components by A and B, so

$$\nu(A) = 3(k-1) + 1, \nu(B) = 3(n - (k+1)) + 1.$$

Therefore, if $n - 2k \geq 0$ then $\nu(B) \geq \nu(A)$ and

$$\tau_0 = \tau(G - S) = \nu(B) = 3(n - (k+1)) + 1$$

and if $n - 2k \leq 0$, then $\nu(A) \geq \nu(B)$ and

$$\tau_0 = \tau(G - S_0) = \nu(A) = 3(k-1) + 1.$$

Without reducing the generality consider $\nu(A) \geq \nu(B)$.
Suppose $S = S_0 \cup I \cup J$ that the set I contains i hydrogen atoms which are connected to C_k or C_{k+1}, and the set J contains j hydrogen atoms which are unconnected to C_k and C_{k+1}, so

$$|S| = |S_0| + i + j, \omega = \omega_0 - i.$$

Let r members of J be in A and s members of J be in B $(r + s = j)$, so the set A transforms to A' and the set B transforms to B' after omitting the set J, thus

$$\nu(B') = \nu(B) - s, \nu(B') = \nu(B) - s.$$

Therefor if $\nu(A') \geq \nu(B')$ then

$$\tau = \nu(A') = \nu(A) - r \overset{\nu(A)=\tau_0}{=} \tau_0 - r,$$

and

$$\begin{aligned} YAF(S) = \tfrac{|S|+\tau}{\omega} &= \tfrac{|S_0|+i+j+\tau_0-r}{\omega_0-i} \\ &\geq \tfrac{|S_0|+\tau_0}{\omega_0} = YAF(S_0), \end{aligned}$$

and if $\nu(A') < \nu(B')$ then

$$\tau = \nu(B') = \nu(B) - s = 3n - 4 - \nu(A) - s \overset{\nu(A)=\tau_0}{=} 3n - \tau_0 - 4 - s,$$

also $i + j - s + 3n - 4 > 0$, so

$$\begin{aligned} YAF(S) = \tfrac{|S|+\tau}{\omega} &= \tfrac{|S_0|+i+j+3n-4-\tau_0-s}{\omega_0-i} \\ &= \tfrac{|S_0|+\tau_0+(i+j-s+3n-4)}{\omega_0-i} \\ &\geq \tfrac{|S_0|+\tau_0}{\omega_0} = YAF(S_0). \end{aligned}$$ □

Lemma 5 *Let $S_0 = \{C_1, C_2, \cdots, C_k\}$ that $k < n$, and S contains k carbon atoms $C_1, C_2, \cdots, C_k$, then*

$$YAF(S_0) \leq YAF(S). \tag{8}$$

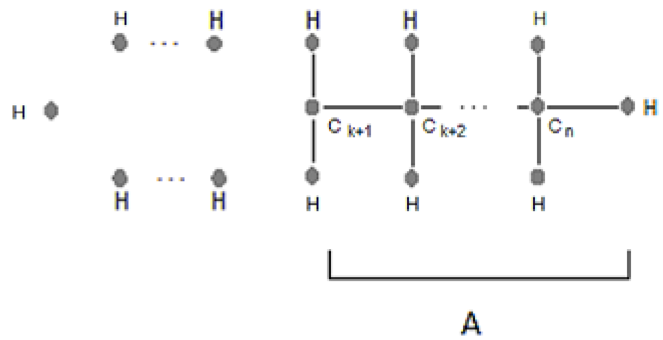

Fig. 6 The components of $G - S_0$

Proof. Obviously, $G - S_0$ has $2k + 2$ components, so

$$|S_0| = k, \omega_0 = 2k + 2, \tau_0 = 3(n - k) + 1.$$

Consider $S = S_0 \cup I \cup J$ where I contains i hydrogen atoms which are connected to C_1 or C_2 or $\cdots$ or C_k ($0 \le i \le 2k$), and J contains j hydrogen atoms which are unconnected to C_1 and C_2 and $\cdots$ and C_k, then

$$|S| = |S_0| + i + j, \omega = \omega_0 - i, \tau = \tau_0 - j$$

and

$$\begin{aligned} YAF(S) = \tfrac{|S|+\tau}{\omega} = & \tfrac{|S_0|+i+j+\tau_0-j}{\omega_0-i} \\ & = \tfrac{|S_0|+\tau_0+i}{\omega_0-i} \\ & \ge \tfrac{|S_0|+\tau_0}{\omega_0} = YAF(S_0). \end{aligned}$$ □

Lemma 6 *Let* $S_0 = \{C_k, C_{k+1}, \cdots, C_{k'}\}$ *($k > 1$, $k' < n$), and* S *contains carbon atoms* $C_k, C_{k+1}, \cdots, C_{k'}$*, then*

$$YAF(S_0) \le YAF(S) \tag{9}$$

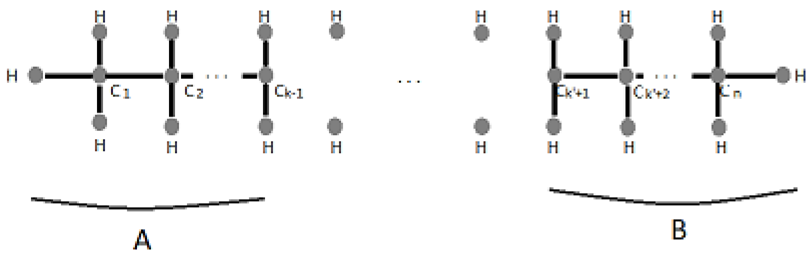

Fig. 7 components of $G - S_0$

Proof. Obviously, $G - S_0$ has $2k' - 2k + 4$ components, see Figure 7. We have

$$|S_0| = k' - k + 1, \omega(G - S_0) = 2k' - 2k + 4$$

and

$$\nu(A) - \nu(B) = (3(k-1)+1) - (3(n-k')+1) = 3(k+k'-n-1).$$

So, $\nu(A) - \nu(B) \ge 0$ if and only if $n + 1 \le k + k'$; therefore

$$\tau(G - S_0) = \begin{cases} 3(k-1)+1 & , k+k' \ge n+1, \\ 3(n-k')+1 & , k+k' < n+1. \end{cases}$$

If $S = S_0 \cup I \cup J$ that I contains i hydrogen atoms H which are connected to C_k or C_{k+1} or $\cdots$ or $C_{k'}$, and J contains j hydrogen atoms H' which are unconnected to C_k and C_{k+1} and $\cdots$ and $C_{k'}$, then

$$|S| = k' - k + 1 + i + j = |S_0| + i + j, \omega(G - S) = \omega(G - S_0) - i.$$

Without reducing the generality suppose $\nu(A) \geq \nu(B)$. Let r members of J be in A and s members of J be in B, $(r + s = j)$, therefore the set A transforms to A' and the set B transforms to B' after removing the set J. So,

$$\nu(A') = \nu(A) - r, \nu(B') = \nu(B) - s.$$

On the other hand

$$\nu(A) + \nu(B) + 3|S_0| = \nu = 3n + 2,$$

so

$$\nu(B) = \nu - 3|S_0| - \nu(A) = \nu - 3|S_0| - \tau_0$$

and

$$\nu(A') - \nu(B') = 2\tau_0 + 3|S_0| - \nu - r + s.$$

If $\nu(A') \geq \nu(B')$, then

$$\tau(G - S) = \tau(G - S_0) - r = \nu(A'),$$

thus

$$\begin{aligned} YAF(S) &= \tfrac{|S|+\tau(G-S)}{\omega(G-S)} = \tfrac{|S_0|+i+j+\tau(G-S_0)-r}{\omega(G-S_0)-i} \\ &= \tfrac{|S_0|+\tau(G-S_0)+i+s}{\omega(G-S_0)-i} \\ &\geq \tfrac{|S_0|+\tau(G-S_0)}{\omega(G-S_0)} = YAF(S_0), \end{aligned}$$

and if $\nu(A') < \nu(B')$, then

$$\tau(G - S) = \nu(B') = \nu(B) - s = \nu - 3|S_0| - \tau_0 - s$$

and because

$$\begin{aligned} \nu(A') - \nu(B') < 0 \quad &\Leftrightarrow \quad 2\tau_0 + 3|S_0| - \nu - r + s < 0 \\ &\Leftrightarrow \quad \tau_0 < \nu - 3|S_)| + r - s - \tau_0 \\ &\qquad < \nu - 3|S_0| + r - \tau_0 \\ &\qquad < \nu - 3|S_0| + r - \tau_0 - i, \end{aligned}$$

we have

$$\begin{aligned} YAF(S) = \tfrac{|S|+\tau(G-S)}{\omega(G-S)} &= \tfrac{|S_0|+\tau_0+(i+j+\nu-3|S_0|-2\tau_0-s)}{\omega(G-S_0)-i} \\ &= \tfrac{|S_0|+\nu-3|S_0|+r-\tau_0+i}{\omega(G-S_0)-i} \\ &\geq \tfrac{|S_0|+\tau(G-S_0)}{\omega(G-S_0)} = YAF(S_0). \end{aligned}$$

□

Lemma 7 *let n be odd, $S_0 = \{C_1, C_3, \cdots, C_{2t+1}, \cdots, C_n\}$, and S contains carbon atoms $C_1, C_3, \cdots, C_n$, then*

$$YAF(S_0) \leq YAF(S). \tag{10}$$

Proof. $S_0 = \{C_1, C_3, \cdots, C_{2t+1}, \cdots, C_n\}$ so

$$|S_0| = \frac{n+1}{2}, \omega_0 = 2(\frac{n+1}{2}) + 2 + \frac{n-1}{2} = \frac{3n-5}{2}, \tau_0 = 3.$$

Suppose $S = S_0 \cup I \cup I$, where I contains i hydrogen atoms only which are connected to C_1 or C_3 or $\cdots$ or C_{2t+1} or $\cdots$ or C_n, and J contains j hydrogen atoms only which are unconnected to C_1 and C_3 and $\cdots$ and C_{2t+1} and $\cdots$ and C_n, so

$$|S| = \frac{n+1}{2} + i + j = |S_0| + i + j, \omega = \omega_0 - i,$$

also

$$\tau(G-S) = \begin{cases} 1 & , j = n-1, \\ 2 & , j = n-2, \\ 2 \ or \ 3 & , j < n-2, \end{cases}$$

thus

$$j + \tau = \begin{cases} j+1 = n-1+1 = n & , j = n-1, \\ j+2 = n-2+2 = n & , j = n-2, \\ j+2 \ or \ j+3 & , j < n-2. \end{cases}$$

Therefore $j + \tau \geq 3$, and

$$\begin{aligned} YAF(S) = \tfrac{|S|+\tau}{\omega} &= \tfrac{|S_0|+i+j+\tau}{\omega_0 - i} \\ &\geq \tfrac{|S_0|+i+3}{\omega_0 - i} \\ &= \tfrac{|S_0|+i+\tau_0}{\omega_0 - i} \\ &\geq \tfrac{|S_0|+\tau_0}{\omega_0} = YAF(S_0). \end{aligned}$$

The proof is complete. □

Lemma 8 *Let n be odd, $S_0 = \{C_2, C_4, \cdots, C_{2t}, \cdots, C_{n-1}\}$, and S contains carbon atoms $C_2, C_4, \cdots, C_{2t}, \cdots, C_{n-1}$, then we have*

$$YAF(S_0) \leq YAF(S). \tag{11}$$

Proof. We can see

$$|S_0| = \frac{n-1}{2}, \tau_0 = 4, \omega_0 = 2(\frac{n-1}{2}) + \frac{n+1}{2} = \frac{3n-1}{2}.$$

Suppose $S = S_0 \cup I \cup J$, taht I contains i hydrogen atoms which are connected to C_2 or C_4 or $\cdots$ or C_{2t} or $\cdots$ or C_{n-1}, and J contains j hydrogen atoms only which are unconnected to C_2 and C_4 and $\cdots$ and C_{2t} and $\cdots$ and C_{n-1}, then

$$|S| = |S_0| + i + j, \omega(G - S) = \omega(G - S_0) - i.$$

Obviously, $j + \tau \geq 4 = \tau_0$, and therefore

$$\begin{aligned} YAF(S) = \tfrac{|S|+\tau(G-S)}{\omega(G-S)} &= \tfrac{|S_0|+i+j+\tau(G-S)}{\omega(G-S_0)-i} \\ &\geq \tfrac{|S_0|+i+4}{\omega(G-S_0)-i} \\ &= \tfrac{|S_0|+\tau(G-S_0)+i}{\omega(G-S_0)-i} \\ &\geq \tfrac{|S_0|+\tau(G-S_0)}{\omega(G-S_0)} = YAF(S_0). \end{aligned}$$ □

Lemma 9 *Let n be even, $S_0 = \{C_1, C_3, \cdots, C_{2t+1}, \cdots, C_{n-1}\}$ and S contains carbon atoms $C_1, C_3, \cdots, C_{2t+1}, \cdots, C_{n-1}$, then*

$$YAF(S_0) \leq YAF(S). \tag{12}$$

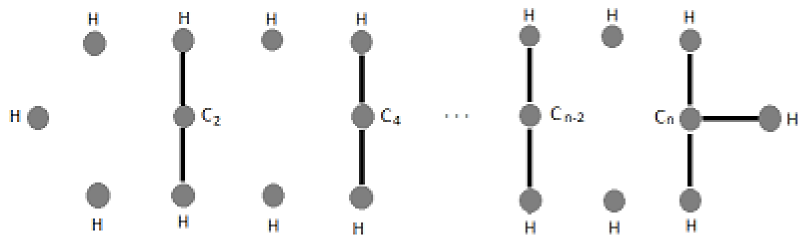

Fig. 8 components of $G - S_0$

Proof. The graph of $G - S_0$ is shown in Figure 8, so

$$|S_0| = \frac{n}{2}, \omega_0 = \frac{3}{2n+1}, \tau_0 = 4.$$

Suppose $S = S_0 \cup I \cup J$, that I contains i hydrogen atoms only which are connected to C_1 or C_3 or $\cdots$ or C_{2t+1} or $\cdots$ or C_{n-1}, and J contains j hydrogen atoms only which are unconnected to C_1 and C_3 and $\cdots$ and C_{2t+1} and $\cdots$ and C_{n-1}. Therefore

$$|S| = |S_0| + i + j, \omega = \omega_0 - i,$$

obviously, $j + \tau \geq 4 = \tau_0$, so

$$YAF(S) = \frac{|S|+\tau(G-S)}{\omega(G-S)} = \frac{|S_0|+i+j+\tau(G-S)}{\omega(G-S_0)-i} \geq \frac{|S_0|+i+4}{\omega_0-i} = \frac{|S_0|+\tau_0+i}{\omega} \geq \frac{|S_0|+\tau_0}{\omega_0} = YAF(S_0).$$ □

Lemma 10 *Let $S_0 = \{C_1, C_2, \cdots, C_n\}$ then for every cut set S that contains all Carbon atoms, we have*

$$YAF(S_0) \leq YAF(S). \tag{13}$$

Proof. $S_0 = \{C_1, C_2, \cdots, C_n\}$, so

$$|S_0| = n, \omega_0 = 2n+2, \tau_0 = 1.$$

Let $S = S_0 \cup I$ that I contains i hydrogen atoms then

$$|S| = | + i, \omega = \omega_0 - i, \tau = \tau_0,$$

therefore
$YAF(S) = \frac{|S|+\tau}{\omega} = \frac{|S_0|+i+\tau_0}{\omega_0-i} \geq \frac{|S_0|+\tau_0}{\omega_0} = YAF(S_0)$,
and the proof is complete. □

4 Tenacity of C_nH_{2n+2}

The tenacity of a graph G is

$$T(G) = min\frac{|S| + \tau(G-S)}{\omega(G-S)},$$

that minimization is over all vertex cut-sets S, $\tau(G-S)$ is the number of vertices in the largest component of $G-S$ and $\omega(G-S)$ is the number of components of $G-S$. Every vertex cut of C_nH_{2n+2} must have a Carbon atom at least, the number of it's vertex cut-sets is $2^n - 1$ and it is a big number, so checking all vertex cut-sets is a hard work, therefore we use the vertex cut-sets and lemmas of the previous section. We compare these cut sets by the cut set $S = \{C_1, C_2, \cdots, C_n\}$.

Theorem 1 *Suppose $S_0 = \{C_k\}$ and $S = \{C_1, C_2, \cdots, C_n\}$, then*

$$YAF(S) \leq YAF(S_0). \tag{14}$$

Proof. Since $S_0 = \{C_k\}$, therefore $\omega(G - S_0) = 4$ and

$$\tau(G - S_0) = \begin{cases} 3(n-k)+1 & ,k \leq \lceil \frac{n}{2} \rceil, \\ 3(k-1)+1 & ,k > \lceil \frac{n}{2} \rceil, \end{cases}$$

and since $S = \{C_1, C_2, \cdots, C_n\}$, therefore

$$\omega(G - S) = 2n + 2, \tau(G - S) = 1.$$

We consider two cases

1. If $k \leq \lceil \frac{n}{2} \rceil$, then

$$YAF(S_0) = \frac{|S_0| + \tau(G-S_0)}{\omega(G-S_0)} = \frac{1+3(n-k)+1}{4} = \frac{3(n-k)+2}{4}.$$

We know that $3(n - k) \geq 0$, therefore $3(n - k) + 2 \geq 2$, thus $\frac{3n-3k+2}{4} \geq \frac{1}{2}$. So $YAF(S_0) \geq \frac{1}{2}$, and since $YAF(S) = \frac{1}{2}$, we have $YAF(S_0) \geq YAF(S)$.

2. If $k > \lceil \frac{n}{2} \rceil$, then

$$YAF(S_0) = \frac{|S_0| + \tau(G-S_0)}{\omega(G-S_0)} = \frac{1+3(k-1)+1}{4} = \frac{3k-1}{4}.$$

We know $3k \geq 3$ thus $3k - 1 \geq 2, so \frac{3k-1}{4} \geq \frac{1}{2}$. From above relations, we obtain that $YAF(S_0) \geq YAF(S)$. □

Theorem 2 *Suppose* $S_0 = \{C_i, C_j\}$ *and* $S = \{C_1, C_2, \cdots, C_n\}$*, then*

$$YAF(S_0) \geq YAF(S). \tag{15}$$

Proof. For proof, we consider different cases of the following

1. Suppose $S_0 = \{C_1, C_k\}$ $(k \neq 2)$ (or $S_0 = \{C_1, C_n\}$), then

$$\omega(G - S_0) = 7, \tau(G - S_0) = \begin{cases} 3(n-k)+1 & ,6k \leq 3n+7, \\ 3(k-2) & ,6k > 3n+7, \end{cases}$$

If $6k \leq 3n+7$, then $6n-6k > 1$; therefore $\frac{2+3(n-k)+1}{7} > \frac{1}{2}$, which implies that $YAF(S_0) \geq YAF(S)$. And if $6k > 3n + 7$, then $\frac{2+3(k-2)}{7} > \frac{1}{2}$, which implies that $YAF(S) < YAF(S_0)$.

2. Suppose $S_0 = \{C_k, C_{k+1}\}$ (or $S_0 = \{C_1, C_2\}$), then

$$\omega(G - S_0) = 6, \tau(G - S_0) = \begin{cases} 3(n-(k+1))+1 & ,2k \leq n, \\ 3(k-1)+1 & ,2k > n. \end{cases}$$

If $2k \leq n$, then

$$\begin{aligned} k \leq \tfrac{n}{2} \quad &\Rightarrow \quad k+1 \leq \tfrac{n}{2} + 1 < n \\ &\Rightarrow \quad n - k \geq 1 \end{aligned}$$

$$\begin{aligned}
&\Leftrightarrow \tfrac{n-k}{2} \geq \tfrac{1}{2}\\
&\Leftrightarrow \tfrac{n-(k+1)+1}{2} \geq \tfrac{1}{2}\\
&\Leftrightarrow \tfrac{3n-3(k+1)+3}{6} \geq \tfrac{1}{2}\\
&\Leftrightarrow \tfrac{2+3n-3(k+1)+1}{6} \geq \tfrac{1}{2}\\
&\Leftrightarrow \tfrac{|S_0|+\tau(G-S_0)}{\omega(G-S_0)} \geq \tfrac{|S|+\tau(G-S)}{\omega(G-S)} \quad \Leftrightarrow \quad YAF(S_0) \geq YAF(S).
\end{aligned}$$

And if $2k > n$, then

$$\begin{aligned}
k > \tfrac{n}{2} \quad &\Rightarrow \quad k > 1\\
&\Rightarrow \tfrac{k}{2} \geq \tfrac{1}{2}\\
&\Leftrightarrow \tfrac{3(k-1)+3}{6} \geq \tfrac{1}{2}\\
&\Leftrightarrow \tfrac{2+3(k-1)+1}{6} \geq \tfrac{1}{2}\\
&\Leftrightarrow \tfrac{|S_0|+\tau(G-S_0)}{\omega(G-S_0)} \geq \tfrac{|S|+\tau(G-S)}{\omega(G-S)} \quad \Leftrightarrow \quad YAF(S_0) \geq YAF(S).
\end{aligned}$$

Thus for all cases we get that $YAF(S_0) \geq YAF(S)$. □

Theorem 3 *Suppose* $S_0 = \{C_k, C_{k+1}, \cdots, C_{k'}\}$ *(that* $k \neq 1$, $k' \neq n$*) and* $S = \{C_1, C_2, \cdots, C_n\}$*, then*

$$YAF(S_0) \geq YAF(S). \tag{16}$$

Proof. we have

$$|S_0| = k' - k + 1, \omega(G - S_0) = 2(k' - k + 1) + 2,$$

$$\tau(G - S_0) = \begin{cases} 3(k-1)+1 & , k + k' \geq n + 1, \\ 3(n-k')+1 & , k + k' < n + 1. \end{cases}$$

If $k + k' \geq n + 1$, then

$$\begin{aligned}
k \geq 1 \ , \ k' \geq k+2 \quad &\Rightarrow \quad k' - k + 2 > 0\\
&\Rightarrow \tfrac{3(k-1)}{k'-k+2} > 0\\
&\Rightarrow \tfrac{k'-k+2+3(k-1)}{k'-k+2} > 1\\
&\Rightarrow \tfrac{k'-k+1+3(k-1)+1}{2(k'-k+1)+2} > \tfrac{1}{2}.
\end{aligned}$$

And if $k + k' < n + 1$, then

$$\frac{3(n-k')}{k'-k+2} > 0 \quad (\ because(k' \leq n-1 \Rightarrow n - k' > 0), k' - k + 2 > 0)$$

$$\Leftrightarrow \tfrac{k'-k+1+3(n-k')+1}{k'-k+2} > 1$$

$$\Leftrightarrow \tfrac{k'-k+1+3(n-k')+1}{2(k'-k+1)+2} > \tfrac{1}{2}.$$

Thus we get that $YAF(S_0) > YAF(S)$. □

Lemma 11 *Suppose n is odd, $S_1 = \{C_1, C_3, \cdots, C_{2t+1}, \cdots, C_n\}$, and $S_2 = \{C_2, C_4, \cdots, C_{2t}, \cdots, C_{n-1}\}$, then*

$$YAF(S_1) \geq YAF(S_2). \tag{17}$$

Proof. We have

$$|S_1| = \frac{n+1}{2}, \omega(G-S_1) = \frac{3n-5}{2}, \tau(G-S_1) = 3$$
$$|S_2| = \frac{n-1}{2}, \omega(G-S_2) = \frac{3n-1}{2}, \tau(G-S_2) = 4.$$

Therefore

$$\begin{aligned} 3n-1 \geq 3n-5 \quad &\Leftrightarrow \quad \tfrac{n+7}{3n-5} \geq \tfrac{n+7}{3n-1} \\ &\Leftrightarrow \quad \tfrac{\frac{n+1}{2}+3}{\frac{3n-5}{2}} \geq \tfrac{\frac{n-1}{2}+4}{\frac{3n-1}{2}} \\ &\Leftrightarrow \quad \tfrac{|S_1|+\tau(G-S_1)}{\omega(G-S_1)} \geq \tfrac{|S_2|+\tau(G-S_2)}{\omega(G-S_2)} \\ &\Leftrightarrow \quad YAF(S_1) \geq YAF(S_2). \end{aligned}$$

□

The above results will be useful in the rest of the paper. We find upper bound of tenacity of C_nH_{2n+2} by using them in the following theorems.

5 Main results

In this section, we find upper bound for the cases n odd and n even.

Theorem 4 *If n is odd, then*

$$T(C_nH_{2n+2}) \leq \begin{cases} \frac{1}{2} & , n \leq 15 \\ \frac{n+7}{3n-1} & , n > 15 \end{cases}. \tag{18}$$

Proof. We consider two cases as follows

1. If $n \leq 15$, then

$$\begin{aligned} 2n+14 \geq 3n-1 \quad &\Leftrightarrow \quad \tfrac{n+7}{3n-1} \geq \tfrac{1}{2} \\ &\Leftrightarrow \quad \tfrac{\frac{n-1}{2}+4}{\frac{3n-1}{2}} \geq \tfrac{1}{2} \quad \Leftrightarrow \quad YAF(S_2) \geq YAF(S) = \tfrac{1}{2}, \end{aligned}$$

therefore

$$T(C_nH_{2n+2}) \leq \frac{1}{2}.$$

2. If $n > 15$, then

$$T(C_nH_{2n+2}) \leq YAF(S_2) = \frac{n+7}{3n-1}.$$

□

Theorem 5 *If n is even, then*

$$T(C_nH_{2n+2}) \leq \begin{cases} \frac{1}{2} & , n \leq 15 \\ \frac{n+8}{3n+1} & , n > 15 \end{cases}. \tag{19}$$

Proof. Let $S_=\{C_1, C_3, \cdots, C_{n-1}\}$. We consider two cases as follows

1. If $n \leq 15$, then

$$\begin{aligned} n \leq 15 \quad &\Leftrightarrow \quad 2n+16 \geq 3n+1 \\ &\Leftrightarrow \quad \tfrac{n+8}{3n+1} \geq \tfrac{1}{2} \\ &\Leftrightarrow \quad \tfrac{\frac{n}{2}+4}{\frac{3n+1}{2}} \geq \tfrac{1}{2} \quad \Leftrightarrow \quad YAF(S_3) \geq YAF(S) = \tfrac{1}{2}, \end{aligned}$$

therefore

$$T(C_nH_{2n+2}) \leq \frac{1}{2}.$$

2. If $n > 15$, then

$$T(C_nH_{2n+2}) \leq YAF(S_3) = \frac{n+8n}{3n+1}.$$

□

6 Examples

For all the cases that $n \geq 3$, we obtained an upper bound for the tenacity. In the end, for $n = 1$ and $n = 2$, we will calculate the tenacity for methane and ethane.

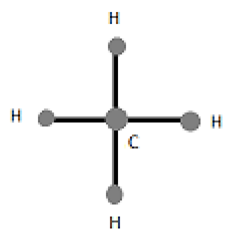

Fig. 9 Graph of methane

Example 1 Let $n = 1$, obtain tenacity of methane.
Solved. Graph of methane is in Figure 9. Also the vertex cutsets are as follows $S_0 = \{C\}$, $S_1 = S_0 \cup H_1$, where H_1 contains only one H and $S_2 = S_0 \cup H_2$, where H_2 contains only two H, then for any $i = 1, 2$, we have $|S_i| = |S_0| + i$, $\omega(G - S_i) = \omega(G - S_0) - i$, $\tau(G - S_i) = \tau(G - S_0)$; therefore

$$T(G) = min\{\frac{|S_i|+\tau(G-S_i)}{\omega(G-S_i)}|i = 0, 1, 2\}$$

$$= min\{\frac{|S_0|+i+\tau(G-S_0)}{\omega(G-S_0)-i}|i = 0, 1, 2\}$$

$$= min\{\frac{1+i+1}{4-i}|i = 0, 1, 2\}$$

$$= min\{\frac{2+i}{4-i}|i = 0, 1, 2\}$$

$$= min\{\frac{1}{2}, \frac{3}{3}, \frac{4}{2}\}$$

$$= min\{\frac{1}{2}, 1, 2\} = \frac{1}{2}.$$

The set $S = \{C\}$ is the $\frac{1}{2}$-tenasious.

Example 2 Let $n = 2$, obtain tenacity of ethanol.
Solved. The cut sets of above graph are
$S_i = \{C_1, C_2\} \cup A$, where A contains only i hydrogen atoms, $0 \le i \le 4$ and $S^k_{i,j} = \{C_k\} \cup B \cup C$, where B contains only i hydrogen atoms which are connected to C_k and C contains only j hydrogen atoms which are unconnected to C_k, $0 \le k \le 1$, $0 \le i \le 2$, $0 \le j \le 3$. So, we have

$|S_i| = 2 + i, (0 \le i \le 4)$
$|S^k_{i,j}| = 1 + i + j, (0 \le k \le 1, 0 \le i \le 3, 0 \le j \le 3)$
$|S^k_{0,0}| = 1, \omega(G - S^k_{0,0}) = 4, \tau(G - S^k_{0,0}) = 4$
$\omega(G - S^k_{i,j}) = \omega(G - S^k_{0,0}) - i = 4 - i, \tau(G - S^k_{i,j}) = \tau(G - S^k_{0,0}) - j = 4 - j$
$|S_0| = 2, \omega(G - S_0) = 6, \tau(G - S_0) = 1$
$\omega(G - S_i) = \omega(G - S_0) - i = 6 - i, \tau(G - S_i) = \tau(G - S_0) = 1.$

Now we consider two cases as follows

1. When $S = S^k_{i,j}$, so
$min\{\frac{|S^k_{i,j}|+\tau(G-S^k_{i,j})}{\omega(G-S^k_{i,j})}|0 \le i \le 2, 0 \le j \le 3\}$
$= min\{\frac{1+i+j+4-j}{4-i}|0 \le i \le 2, 0 \le j \le 3\}$
$= min\{\frac{5+i}{4-i}|0 \le i \le 2\}$
$= min\{\frac{5}{4}, 2, \frac{7}{2}, 8\} = \frac{5}{4}.$

2. When $S = S_i$, so
$min\{\frac{|S_i|+\tau(G-S_i)}{\omega(G-S_i)}|0 \le i \le 4\}$
$= min\{\frac{2+i+1}{6-i}|0 \le i \le 4\}$

$= min\{\frac{3+i}{6-i}|0 \le i \le 4\}$
$= min\{\frac{1}{2}, \frac{4}{5}, \frac{5}{4}, 2, \frac{7}{2}\} = \frac{1}{2}$.

Thus

$$T(C_2H_6) = min\{\frac{1}{2}, \frac{5}{4}\} = \frac{1}{2}.$$

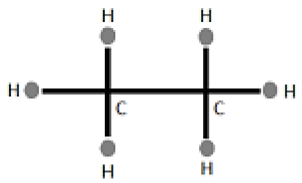

Fig. 10 Graph of ethan

The set $\{C_1, C_2\}$ is the $\frac{1}{2}$-tenasious.

7 conclusions and one open problem

In this paper we study vertex cut-sets and the tenacity of the graph of C_nH_{2n+2}. Our results show that the study of tenacity and vertex cut-sets are important. By using two examples 1 and 2, we see that the tenacity is exactly $\frac{1}{2}$ which obtained on $\{C_1\}$ for methane and on $\{C_1, C_2\}$ for ethanol. Also, in the last two theorems, we found the smallest upper bound on the $\{C_1, C_2, \cdots, C_n\}$. Therefore, an estimate it could be that the smallest upper bound of tenacity will obtained on vertex cut which has most carbon atom (for $n \ge 15$). These observations provide evidence for the fact that the study of the following conjecture ought to be challenging.

Conjecture: May be the tenacity of the graph of C_nH_{2n+2} is

$$T(C_nH_{2n+2}) = \begin{cases} min\{\frac{1}{2}, \frac{n+8}{3n+1}\} \text{ , } n \text{ is even,} \\ min\{\frac{1}{2}, \frac{n+7}{3n-1}\} \text{ , } n \text{ is odd.} \end{cases} \tag{20}$$

Obviously that if 20 is reached, then

$$\frac{1}{3} < T(C_nH_{2n+2}) \le \frac{1}{2}.$$

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