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# Saturation number of nanotubes

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**Abstract**

In the present paper we are interested in the saturation number of closed benzenoid chains and certain families of nanotubes. The saturation number of a graph is the cardinality of a smallest maximal matching in the graph. The problem of determining the saturation number is related to the edge dominating sets and efficient edge dominating sets in a graph. We establish the saturation number of some closed benzenoid chains and $C_4C_6$-tubes. Further, upper and lower bounds for the saturation number of armchair, zig-zag, $TUC_4C_8(S)$ and $TUC_4C_8(R)$ nanotubes are calculated.

*Keywords: Saturation number, maximal matching, edge domination number, efficient edge dominating set, closed benzenoid chain, armchair nanotube, zig-zag nanotube, tubulene, $TUC_4C_8(S)$ nanotube, $TUC_4C_8(R)$ nanotube.*

*Math. Subj. Class.: 92E10, 05C70, 05C69*

## 1 Introduction

The saturation number $s(G)$ of a graph $G$ is the cardinality of a smallest maximal matching in $G$. Maximal matchings serve as models of adsorption of dimers (those that occupy two adjacent atoms) to a molecule. It can occur that the double bonds in a molecule are not efficiently saturated by dimers, and therefore, their number is below the theoretical maximum. Hence, the saturation number provides an information on the worst possible

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case of adsorption. Besides in chemistry the saturation number has a list of interesting applications in engineering and networks.
A lot of work has been done on enumeration problems of different matchings in some chemical graphs, for example see [4, 5], but not much has been done on the smallest maximal matchings. Previous work on the saturation number includes research on benzenoid systems [8] and fullerenes [6, 1, 2]. Recent results on related concepts can be found in [3, 7].
The saturation number is closely related to the edge dominating sets. Actually, for any graph, the saturation number equals the edge domination number. The problem of determining the saturation number of a graph is NP-complete [13].
In this paper we show how to use an efficient edge dominating set in a graph to determine its saturation number. Also, the saturation number is established for certain closed benzenoid chains. Further, some bounds for the saturation number of different families of nanotubes are calculated.

## 2 Preliminaries

A *matching* $M$ in a graph G is a set of edges of G such that no two edges from $M$ share a vertex. A matching $M$ is a *maximum matching* if there is no matching in $G$ with greater cardinality. The cardinality of any maximum matching in G is denoted by $\nu(G)$ and called the *matching number* of $G$. If every vertex of $G$ is incident with an edge of $M$, the matching $M$ is called a *perfect matching* (in chemistry perfect matchings are known as *Kekulé structures*).
A matching $M$ in a graph $G$ is *maximal* if it cannot be extended to a larger matching in $G$. Obviously, every maximum matching is also maximal, but the opposite is generally not true. A matching $M$ is a *smallest maximal matching* if there is no maximal matching in $G$ with smaller cardinality. The cardinality of any smallest maximal matching in $G$ is the *saturation number* of $G$.
The following lemma is very useful for proving lower bounds for the saturation number. The proof can be found online, but for the sake of completeness we provide it.

**Lemma 2.1.** *Let $G$ be a graph and let $A$ and $B$ be maximal matchings in $G$. Then $|A| \geq \frac{|B|}{2}$ and $|B| \geq \frac{|A|}{2}$.*

*Proof.* First note that each edge in $B \setminus A$ can be adjacent to at most two edges in $A \setminus B$ since $A$ is a matching. Moreover, each edge in $A \setminus B$ is adjacent to an edge in $B \setminus A$ by maximality of $B$. Therefore,

$$|A \setminus B| \leq 2|B \setminus A|.$$

Hence, we obtain

$$|A| = |A \cap B| + |A \setminus B| \leq 2|B \cap A| + 2|B \setminus A| = 2|B|.$$

The other inequality can be proven analogously. □

An *independent set* is a set of vertices in a graph $G$, no two of which are adjacent. A *maximum independent set* is an independent set of largest possible cardinality for a given graph $G$. This cardinality is called the *independence number* of $G$, and denoted $\alpha(G)$. It is obvious that if $M$ is a maximal matching and $A$ is the set of endpoints of edges in

$M$, then the set of vertices in $V(G) - A$ is an independent set of vertices in $G$. Therefore, $\alpha(G) \geq |V(G)| - 2s(G)$. Hence, we obtain another lower bound for the saturation number:

$$s(G) \geq \frac{|V(G)| - \alpha(G)}{2}.$$

Another graph invariant closely related to the saturation number is the edge domination number. An *edge dominating set* for a graph $G$ is a subset $D \subseteq E(G)$ such that every edge not in $D$ is incident to at least one edge in $D$. An *independent edge dominating set* is an edge dominating set in which no two elements are adjacent. An independent edge dominating set is in fact a maximal matching and a smallest independent edge dominating set is a smallest maximal matching, i.e. the cardinality of a smallest independent edge dominating set is the saturation number. The *edge domination number* of a graph $G$, $\gamma'(G)$, is the smallest cardinality taken over all edge dominating sets of $G$. If $M$ is a smallest maximal matching of $G$, then $M$ is also an edge dominating set, therefore $\gamma'(G) \leq s(G)$. For the contrary, if $D$ is a smallest edge dominating set with $k$ elements, we can construct a maximal matching of cardinality $k$ (for the details see [13]). Therefore, $s(G) \leq \gamma'(G)$. Hence, for every graph $G$ it holds

$$s(G) = \gamma'(G). \tag{2.1}$$

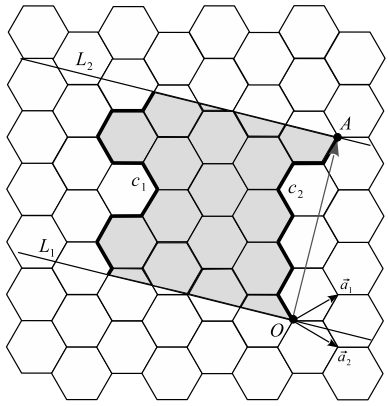


Figure 1: Illustration of a $(4, -3)$-type tubulene.

Since the paper focuses on nanotubes, we will formally define open-ended carbon nanotubes, also called *tubulenes* (see [11]). Choose any lattice point in the hexagonal lattice as the origin $O$. Let $\overrightarrow{a_1}$ and $\overrightarrow{a_2}$ be the two basic lattice vectors. Choose a vector $\overrightarrow{OA} = n\overrightarrow{a_1} + m\overrightarrow{a_2}$ such that $n$ and $m$ are two integers and $|n| + |m| > 1$, $nm \neq -1$. Draw two straight lines $L_1$ and $L_2$ passing through $O$ and $A$ perpendicular to $OA$, respectively. By rolling up the hexagonal strip between $L_1$ and $L_2$ and gluing $L_1$ and $L_2$ such that $A$ and $O$ superimpose, we can obtain a hexagonal tessellation $\mathcal{HT}$ of the cylinder. $L_1$ and $L_2$ indicate the direction of the axis of the cylinder. Using the terminology of graph theory, a *tubulene* $T$ is defined to be the finite graph induced by all the hexagons of $\mathcal{HT}$ that lie between $c_1$ and $c_2$, where $c_1$ and $c_2$ are two vertex-disjoint cycles of $\mathcal{HT}$ encircling the

axis of the cylinder. The vector $\overrightarrow{OA}$ is called the *chiral vector* of $T$ and the cycles $c_1$ and $c_2$ are the two open-ends of $T$.
For any tubulene $T$, if its chiral vector is $n\overrightarrow{a_1} + m\overrightarrow{a_2}$, $T$ will be called an $(n, m)$-type tubulene (see Figure 1). A tubulene $T$ is called *zig-zag* if $n = 0$ or $m = 0$ and *armchair* if $n = m$.

## 3 Graphs with an efficient edge dominating set

One other concept is also very useful in studying the saturation number. A matching $D$ of a graph $G$ is called an *efficient edge dominating set* if for each edge $e \in E(G) \setminus D$ there is exactly one edge $f$ in $D$ such that $e$ and $f$ are incident (this concept is equivalent to the efficient dominating set in the line graph of $G$, for the details see [10]). Using the following theorem we can exactly determine the saturation number for some graphs.

**Theorem 3.1.** *If a graph $G$ has an efficient edge dominating set $D$, then*

$$s(G) = |D|.$$

*Proof.* It follows from Equation 2.1 that $s(G) = \gamma'(G)$. Hence it is enough to show that $\gamma'(G) = |D|$ (see [9]).

Obviously, if $D$ is an efficient edge dominating set then $D$ is also an edge dominating set. Therefore, $\gamma'(G) \leq |D|$. Conversely, let $P$ be a smallest edge dominating set and let $e \in D$. It follows that either $e \in P$ or there is an edge $f \in P$ such that $e$ and $f$ are incident. Therefore, for an edge $e \in D$ there always exists $f_e \in P$ such that $e = f_e$ or $e$ and $f_e$ are incident. It is also clear that since $D$ is an efficient edge dominating set, for given edges $e$ and $e'$ in $D$, $e \neq e'$, it follows that $f_e \neq f_{e'}$. Hence, $|D| \leq |P| = \gamma'(G)$. The proof is complete. □

**Example 3.2.** One infinite family of graphs with an efficient edge dominating set are $C_4C_6$-tubes, which are constructed of cycles $C_4$ and $C_6$ - see Figure 2. Let $T(p, q)$ be a $C_4C_6$-tube with $p$ layers of hexagons and with $q$ hexagons in every layer. The set of double edges in Figure 2 is obviously an efficient edge dominating set of cardinality $pq = 15$. Therefore, by Theorem 3.1, the saturation number of $T(p, q)$ is $s(T(p, q)) = pq$.

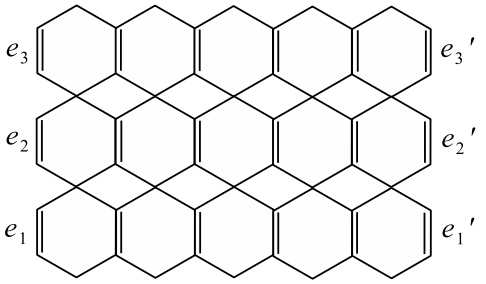


Figure 2: A $C_4C_6$-tube $T(3, 5)$. Edges $e_1$, $e_2$ and $e_3$ are joined with edges $e'_1$, $e'_2$ and $e'_3$, respectively.

For example, polyacenes and closed polyacenes are also such graphs (see Section 4). However, not many graphs posses an efficient edge dominating set.

## 4 Closed benzenoid chains

Recall that *benzenoid graphs* are 2-connected subgraphs of the hexagonal lattice such that every bounded face is a hexagon. The vertices lying on the border of the non-hexagonal face of a benzenoid graph are called *external*; other vertices, if any, are called *internal*. A benzenoid graph without internal vertices is called *catacondensed*. If no hexagon in a catacondensed benzenoid is adjacent to three other hexagons, we say that the benzenoid is a *chain*. In each benzenoid chain there are exactly two hexagons adjacent to one other hexagon; those two hexagons are called *terminal*, while any other hexagons are called *interior*. An interior hexagon is called *straight* if the two edges it shares with other hexagons are parallel, i.e., opposite to each other. If the shared edges are not parallel, the hexagon is called *kinky*. If all interior hexagons of a benzenoid chain are straight, we call the chain a *polyacene*.

Let $B$ be a benzenoid chain with terminal hexagons $h$ and $h'$. Let $e = uv$ and $e' = u'v'$ be edges of $h$ and $h'$, respectively, such that vertices $u, v, u', v'$ have degree 2 in $B$. Furthermore, suppose that there exist a path from $u$ to $u'$ in the perimeter of $B$, which does not contain neither $v$ nor $v'$. A graph obtained by identifying edges $e$ and $e'$ is called a *closed benzenoid chain*. For example see Figure 3.

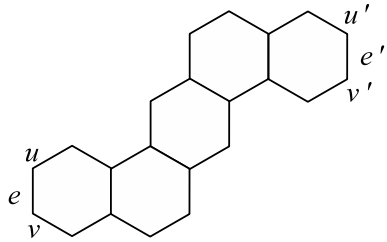


Figure 3: A closed benzenoid chain. Edges $e$ and $e'$ are joined together.

Similar as before, a hexagon of a closed benzenoid chain is called *straight* if the two edges it shares with other hexagons are opposite to each other. If the shared edges are not parallel, the hexagon is called *kinky*.

**Remark 4.1.** Note that not every closed benzenoid chain is a tubulene in the sense of the definition in the preliminaries. In fact, if we consider benzenoid chain embedded in the hexagonal lattice, it is not difficult to see that a closed benzenoid chain is a tubulene if and only if the distance from $u$ to $u'$ in the hexagonal lattice is an even number and the edge $e$ is parallel to $e'$.

In this section we compute the saturation number of some closed benzenoid chains. The following lemma claims that every closed benzenoid chain has a perfect matching.

**Lemma 4.2.** *Let $B$ be a closed benzenoid chain. Then $B$ has a perfect matching.*

*Proof.* Let $G$ be a benzenoid chain from which $B$ is obtained by identifying edges $e$ and $e'$. Since every internal hexagon in $G$ has exactly $4$ edges on the perimeter and both terminal hexagons have $5$ edges on the perimeter, there is always an even number of edges on the perimeter of $G$. Therefore, let $M$ be a perfect matching of the perimeter of $G$ such that $e \in M$. Obviously, $M$ is a perfect matching of $G$. Now we consider two cases:

1. If $e' \in M$, then after identifying $e$ and $e'$ into the new edge $f$, the set $(M \setminus \{e, e'\}) \cup \{f\}$ is a perfect matching of $B$.
2. If $e' \notin M$, then after identifying $e$ and $e'$, the set $M \setminus \{e\}$ is a perfect matching of $B$.

Hence, we have seen that $B$ has a perfect matching. □

In the next proposition we prove a lower bound for the saturation number of closed benzenoid chains.

**Proposition 4.3.** *Let $B$ be a closed benzenoid chain with $h$ hexagons. Then $s(B) \geq h$.*

*Proof.* Let $M$ be a perfect matching of $B$. Since there is $4h$ vertices in $B$ and every edge in $M$ covers exactly 2 vertices, perfect matching $M$ contains $2h$ edges. Therefore, by Lemma 2.1, any maximal matching contains at least half of the number of edges in $M$. Hence, $s(B) \geq \frac{2h}{2} = h$. □

A closed benzenoid chain $B$ is called a *closed polyacene* (or a *hexagonal belt*) if it does not contain kinky hexagons (see Figure 4).

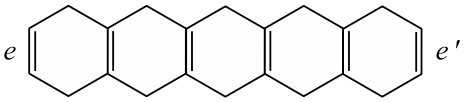


Figure 4: A maximal matching of a closed polyacene with 5 hexagons.

**Proposition 4.4.** *Let $B$ be a closed polyacene with $h$ hexagons. Then $s(B) = h$.*

*Proof.* Obviously, the set of vertical edges of $B$ (see the edges in matching $M$ from Figure 4) is an efficient edge dominating set and $|M| = h$. Therefore, by Theorem 3.1 it follows $s(B) = h$. □

The following theorem completely characterizes closed polyacenes among closed benzenoid chains according to saturation number.

**Theorem 4.5.** *Let $B$ be a closed benzenoid chain with $h$ hexagons. Then $s(B) = h$ if and only if $B$ is a closed polyacene.*

*Proof.* Let $B$ be a closed polyacene with $h$ hexagons. It follows from Proposition 4.4 that $s(B) = h$.

For the converse suppose that $B$ is a closed benzenoid chain with $h$ hexagons and $s(B) = h$. Let $M$ be a maximal matching with $h$ edges. Those edges cover exactly $2h$ vertices. Let $A$ be the set of vertices that are not covered by edges in $M$. Since $B$ has $4h$ vertices, there are $2h$ vertices in $A$. Since $M$ is a maximal matching, no two vertices in $A$ are adjacent. Let $A'$ be the set of edges that are incident to vertices in $A$. Since the degree of every vertex in $B$ is at least 2, it follows $|A'| \geq 4h$. But $A' \subseteq E(B) \setminus M$ and therefore, $|A'| \leq 5h - h = 4h$. Hence, every vertex in $A$ has degree 2 and every hexagon contains exactly two elements of $A$. Therefore, every hexagon of $B$ has 2 non-adjacent vertices of degree 2. It follows that $B$ is a closed polyacene. □

In the next theorem we compute the saturation number of closed benzenoid chains with exactly one kinky hexagon. However, such closed benzenoid chain is never a tubulene since the distance between $u$ and $u'$ is odd.

**Theorem 4.6.** *Let $B$ be a closed benzenoid chain with $h$ hexagons such that exactly one of them is a kinky hexagon. Then $s(B) = h + 1$.*

*Proof.* Let $M$ be the set of edges in $B$ that lie on exactly two hexagons. Moreover, let one other edge of the kinky hexagon be in $M$. Then it is easy to see that $M$ is a maximal matching and therefore, $s(B) \leq h + 1$.
Since $B$ is not a closed polyacene, $s(B) \geq h + 1$ and the proof is complete. □

**Proposition 4.7.** *Let $B$ be a closed benzenoid chain with exactly two kinky hexagons which are consecutive. Then $s(B) = h + 1$.*

*Proof.* Let $M$ be a maximal matching with $h+1$ edges from Figure 5. Hence, $s(B) \leq h+1$.

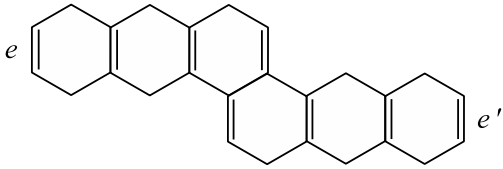


Figure 5: A closed benzenoid chain with two consecutive kinky hexagons and its maximal matching.

Since $B$ is not a closed polyacene, $s(B) \geq h + 1$ and the proof is complete. □

## 5 Zig-zag tubulenes

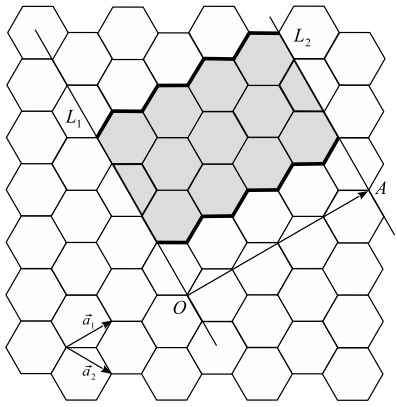


Figure 6: Zig-zag tubulene $ZT(3, 4)$.

Let $T$ be a zig-zag tubulene such that $c_1, c_2$ are the shortest possible cycles encircling the axis of the cylinder (see Figure 6). If $T$ has $n$ layers of hexagons, each containing

exactly $h$ hexagons, then we denote it by $ZT(n,h)$. Note that $ZT(n,h)$ is a $(0,h)$ or $(h,0)$-type tubulene. First we show an upper bound for the saturation number of $ZT(n,h)$, which is essentially of order $\frac{2nh}{3}$.

**Theorem 5.1.** *Let $ZT(n,h)$ be a zig-zag tubulene. Then*

$$s(ZT(n,h)) \leq \begin{cases} \frac{h(2n+3)}{3}, & 3 \mid n \\ \frac{h(2n+1)}{3}, & 3 \mid n-1 \\ \frac{h(2n+2)}{3}, & 3 \mid n-2. \end{cases}$$

*Proof.* Let $ZT(n,h)$ be drawn in a plane such that some edges are vertical and such that cycles $c_1$ and $c_2$ lie on the bottom and on the top. To show an upper bound, we construct a maximal matching of $ZT(n,h)$. This maximal matching is obtained by alternating two different layers of edges - vertical and non-vertical. We start with vertical edges in the first layer (at the bottom of a tubulene) and we need 2 layers of edges for every 3 layers of hexagons. Obviously we have exactly $h$ edges in every layer. Now consider three different cases.

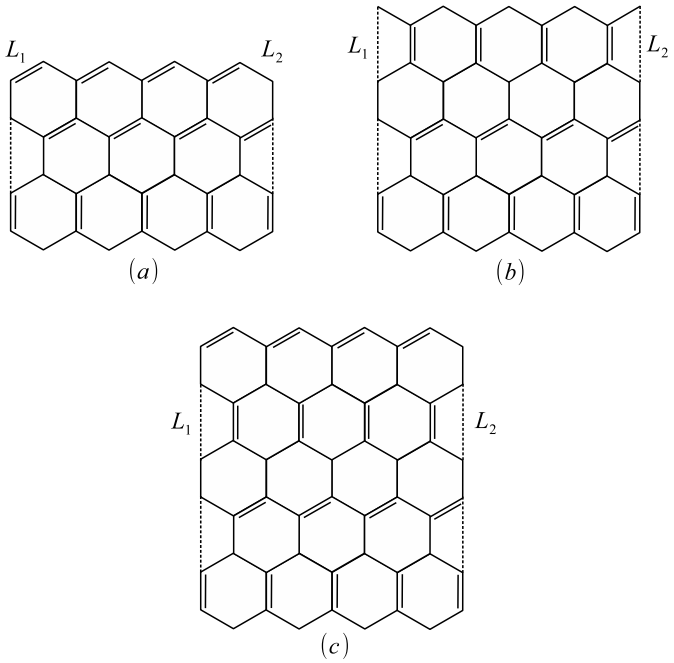


Figure 7: A maximal matching of zig-zag tubulenes. Lines $L_1$ and $L_2$ are joined together.

1. If $3 \mid n$: then we need $\frac{2n}{3}$ layers of edges and one additional layer at the top of a tubulene. Hence, we obtain $\frac{h(2n+3)}{3}$ edges in $M$. See Figure 7$(a)$.
2. If $3 \mid n-1$: in this case we need $\frac{2(n-1)}{3}$ layers of edges and we have to add one vertical layer. Hence, $|M| = \frac{h(2n+1)}{3}$. See Figure 7$(b)$.

3. If $3 \mid n-2$: in this case we have $\frac{2(n-2)}{3}$ layers of edges and we have to add 2 additional layers (one vertical and one non-vertical) to obtain a maximal matching. Hence, $|M| = \frac{h(2n+2)}{3}$. See Figure 7$(c)$.

It is obvious that in such a way we always obtain a maximal matching. Therefore, the proof is complete. □

In the next lemma we prove a lower bound.

**Lemma 5.2.** *Let $ZT(n,h)$ be a zig-zag tubulene. Then*

$$s(ZT(n,h)) \geq \frac{(n+1)h}{2}.$$

*Proof.* Obviously $ZT(n,h)$ has a perfect matching with $(n+1)h$ edges. Therefore, by Lemma 2.1, any maximal matching contains at least $\frac{(n+1)h}{2}$ edges. □

Theorem 5.1 and Lemma 5.2 together imply the following corollary.

**Corollary 5.3.** *Let $ZT(n,h)$ be a zig-zag tubulene. Then*

$$\frac{(n+1)h}{2} \leq s(ZT(n,h)) \leq \begin{cases} \frac{h(2n+3)}{3}, & 3 \mid n \\ \frac{h(2n+1)}{3}, & 3 \mid n-1 \\ \frac{h(2n+2)}{3}, & 3 \mid n-2. \end{cases}$$

## 6 Armchair tubulenes

Let $T$ be an armchair tubulene such that $c_1$ and $c_2$ are the shortest possible cycles encircling the axis of the cylinder and such that there is the same number of hexagons in every column of hexagons (see Figure 8). If $T$ has $n$ vertical layers of hexagons, each containing exactly $p$ hexagons, then we denote it by $AT(n,p)$. Obviously, $n$ must be an even number. Note that $AT(n,p)$ is a $(\frac{n}{2}, \frac{n}{2})$-type tubulene. In the following theorem we prove an upper bound for the saturation number of $AT(n,p)$.

**Theorem 6.1.** *Let $AT(n,p)$ be an armchair tubulene. Then*

$$s(AT(n,p)) \leq \begin{cases} \frac{2n(p+1)}{3}, & 3 \mid n \\ \frac{(2n+1)(p+1)}{3}, & 3 \mid n-1 \\ \frac{2(n+2)(p+1)}{3}, & 3 \mid n-2. \end{cases}$$

*Proof.* Let $AT(n,p)$ be drawn in a plane such that some edges are horizontal and such that cycles $c_1$ and $c_2$ lie on the bottom and on the top. To show an upper bound, we construct a maximal matching of $AT(n,p)$. This maximal matching is obtained by alternating two different columns of edges - horizontal and non-horizontal. We start with horizontal edges in the first column (at the left side of a tubulene) and we need 2 columns of edges for every 3 columns of hexagons. Obviously we have exactly $p+1$ edges in every column. Now consider three different cases.

1. If $3 \mid n$: then we need $\frac{2n}{3}$ columns of edges to obtain a maximal matching. Hence, we obtain $\frac{2n(p+1)}{3}$ edges in $M$. See Figure 8.

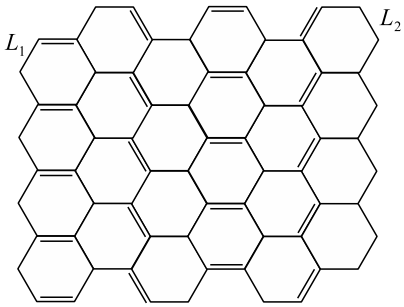


Figure 8: A maximal matching of armchair tubulene $AT(6,4)$. Curves $L_1$ and $L_2$ are joined together.

2. If $3 \mid n-1$: in this case we need $\frac{2(n-1)}{3}$ columns of edges and we have to add one horizontal column. Hence, $|M| = \frac{(2n+1)(p+1)}{3}$.
3. If $3 \mid n-2$: in this case we have $\frac{2(n-2)}{3}$ columns of edges and we have to add 2 additional horizontal layers of edges to obtain a maximal matching. Hence, $|M| = \frac{2(n+2)(p+1)}{3}$. See Figure 9.

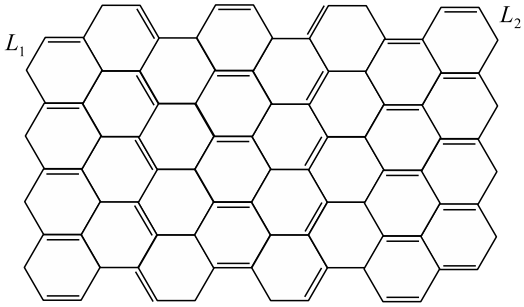


Figure 9: A maximal matching of armchair tubulene $AT(8,4)$. Curves $L_1$ and $L_2$ are joined together.

It is obvious that in such a way we always obtain a maximal matching. Therefore, the proof is complete. □

In the next lemma we prove a lower bound.

**Lemma 6.2.** *Let $AT(n,p)$ be an armchair tubulene. Then*

$$s(AT(n,p)) \geq \frac{n(p+1)}{2}.$$

*Proof.* Obviously $AT(n,p)$ has a perfect matching with $n(p+1)$ edges (we can put all horizontal edges in a perfect matching). Therefore, by Lemma 2.1, any maximal matching contains at least $\frac{n(p+1)}{2}$ edges. □

Theorem 6.1 and Lemma 6.2 together imply the following corollary.

**Corollary 6.3.** *Let $AT(n,h)$ be an armchair tubulene. Then*

$$\frac{n(p+1)}{2} \leq s(AT(n,p)) \leq \begin{cases} \frac{2n(p+1)}{3}, & 3 \mid n \\ \frac{(2n+1)(p+1)}{3}, & 3 \mid n-1 \\ \frac{2(n+2)(p+1)}{3}, & 3 \mid n-2. \end{cases}$$

## 7 $TUC_4C_8(S)$ nanotubes

A $C_4C_8$ net is a trivalent pattern made by alternating squares $C_4$ and octagons $C_8$. Identifying some edges in such a lattice we obtain a $TUC_4C_8(S)$ nanotube (see Figure 10). Such nanotubes could appear by successive low energy Stone-Wales edge flipping [12] in polyhex nanotubes. In this section we prove an upper and a lower bound for the saturation number of $TUC_4C_8(S)$ nanotubes. We denote nanotube with $q$ layers and $p$ squares (or octagons) in every layer with $TS(p,q)$.

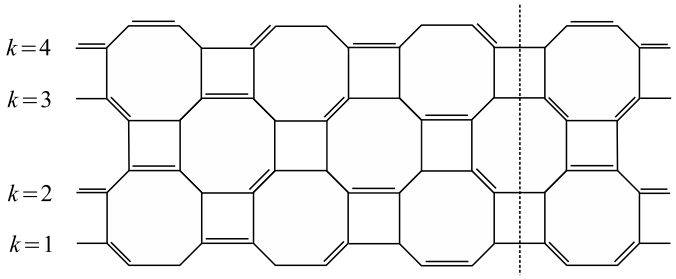


Figure 10: $TS(4,4)$ with a maximal matching.

**Theorem 7.1.** *Let $TS(p,q)$ be a $TUC_4C_8(S)$ nanotube. Then*

$$s(TS(p,q)) \leq \begin{cases} \frac{4pq}{3}, & 3 \mid p \\ \frac{(4p+2)q}{3}, & 3 \mid p-1 \\ \frac{(4p+1)q}{3}, & 3 \mid p-2. \end{cases}$$

*Proof.* To prove the theorem we construct a maximal matching for nanotube $TS(p,q)$. In every layer we put every third edge in the matching $M$. In layer with $k=1$ we put the first edge in $M$ and in layer with $k=2$ we start with the second edge (see Figure 10). Next, in the third layer, we repeat the first layer.

Now consider the following cases:

1. If $3 \mid p$, then we have $\frac{4pq}{3}$ edges in $M$.
2. If $3 \mid p-1$: in this case we have $\frac{4(p-1)q}{3}$ edges and we have to add 2 additional edges in every layer to obtain a maximal matching. Hence, $|M| = \frac{4(p-1)q}{3} + 2q = \frac{(4p+2)q}{3}$.
3. If $3 \mid p-2$: in this case we have $\frac{4(p-2)q}{3}$ edges and we have to add 3 additional edges in every layer to obtain a maximal matching. Hence, $|M| = \frac{4(p-2)q}{3} + 3q = \frac{(4p+1)q}{3}$.

□

In the next proposition we prove a lower bound.

**Lemma 7.2.** *Let $TS(p,q)$ be a $TUC_4C_8(S)$ nanotube. Then $s(TS(p,q)) \geq pq$.*

*Proof.* First notice that $TS(p,q)$ always has a perfect matching. For example, we can take every second edge in every layer. Since the number of vertices in $TS(p,q)$ is $4pq$, a perfect matching of $TS(p,q)$ contains $2pq$ edges, since every edge covers two vertices. Now it follows from Lemma 2.1 that every maximal matching contains at least $pq$ edges. Hence, $s(TS(p,q)) \geq pq$. □

Theorem 7.1 and Lemma 7.2 together imply the next corollary.

**Corollary 7.3.** *Let $TS(p,q)$ be a $TUC_4C_8$ nanotube. Then*

$$pq \leq s(TS(p,q)) \leq \begin{cases} \frac{4pq}{3}, & 3 \mid p \\ \frac{(4p+2)q}{3}, & 3 \mid p-1 \\ \frac{(4p+1)q}{3}, & 3 \mid p-2. \end{cases}$$

## 8 $TUC_4C_8(R)$ nanotubes

Again we begin with a $C_4C_8$ net, but this time squares are not in the horizontal position. Identifying some edges in such a lattice we obtain a $TUC_4C_8(R)$ nanotube (see Figure 11). In this section we prove an upper and a lower bound for the saturation number of $TUC_4C_8(R)$ nanotubes. We denote a nanotube with $p$ octagons in every layer and $q$ octagons in every column with $TR(p,q)$.

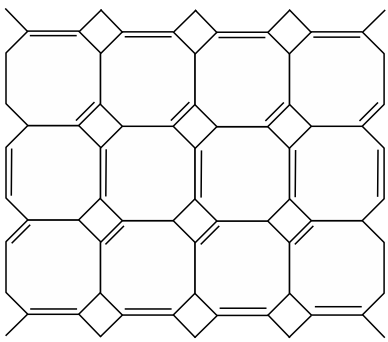

Figure 11: $TR(4,3)$ with a maximal matching. Left and right side are joined.

**Theorem 8.1.** *Let $TR(p,q)$ be a $TUC_4C_8(R)$ nanotube. Then*

$$s(TR(p,q)) \leq \begin{cases} \frac{4qp}{3} + p, & 3 \mid q \\ \frac{4(q-1)p}{3} + 3p, & 3 \mid q-1 \\ \frac{4(q-2)p}{3} + 4p, & 3 \mid q-2. \end{cases}$$

*Proof.* We construct a maximal matching $M$ for nanotube $TR(p,q)$. For every 3 rows of octagons we put $4$ layers of edges in the matching $M$. Of course, every layer contains exactly $p$ edges. See Figure 11.

Now consider the following cases:

1. If $3 \mid q$: in this case we have $\frac{4qp}{3}$ edges in $M$ and we need one additional layer of horizontal edges at the top - see Figure 11.
2. If $3 \mid q-1$: in this case we have $\frac{4(q-1)p}{3}$ edges and we have to add 3 additional layers of edges to obtain a maximal matching. Hence, $|M| = \frac{4(q-1)p}{3} + 3p$.
3. If $3 \mid q-2$: in this case we have $\frac{4(q-2)p}{3}$ edges and we have to add $4$ additional layers of edges to obtain a maximal matching. Hence, $|M| = \frac{4(q-2)p}{3} + 4p$.

□

In the next lemma we prove a lower bound.

**Lemma 8.2.** *Let $TR(p,q)$ be a $TUC_4C_8(R)$ nanotube. Then $s(TR(p,q)) \geq p(q+1)$.*

*Proof.* First notice that $TR(p,q)$ always has a perfect matching. Since the number of vertices in $TR(p,q)$ is $4p(q+1)$, a perfect matching of $TR(p,q)$ contains $2p(q+1)$ edges, since every edge covers two vertices. Now it follows from Lemma 2.1 that every maximal matching contains at least $p(q+1)$ edges. Hence, $s(TR(p,q)) \geq p(q+1)$. □

Theorem 8.1 and Lemma 8.2 together imply the next corollary.

**Corollary 8.3.** *Let $TR(p,q)$ be a $TUC_4C_8(R)$ nanotube. Then*

$$p(q+1) \leq s(TR(p,q)) \leq \begin{cases} \frac{4qp}{3} + p, & 3 \mid q \\ \frac{4(q-1)p}{3} + 3p, & 3 \mid q-1 \\ \frac{4(q-2)p}{3} + 4p, & 3 \mid q-2. \end{cases}$$

## Concluding remarks

In the paper we have established some bounds for the saturation number of certain families of nanotubes. However, the exact values are unknown. There are still many open problems regarding the saturation number of molecular graphs, for example coronenes, coronoids, polyomino chains, etc.

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