PACKING OF CERTAIN CARBON BASED NANOTUBES AND NANOTORUS

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Article History: Received: 03.04.2023 **Revised:** 11.05.2023 **Accepted:** 19.06.2023

Abstract

Packing in graphs is an influential steer, as it has numerous implementations in applied sciences. In computer science, it is one of the most studied and researched area, primarily due to its combinatorial aspects and algorithmic utilisations. Research outcomes and findings from packing theory have tremendous utilisations in code optimization, clustering, and component placing. P_3-packing concepts have quite a few promising applications in chemistry for illustrating chemical compounds or to problems of pattern recognition and image processing, few of which involve the use of hierarchical data structures of nanotubes. In this paper we give algorithms to find perfect H-packing of $\mathrm{TUC_4C_8}(S)$ nanostructure with H isomorphic to cyclooctane, butane, 3, 4-dimethyl hexane, cyclobutane and 2-methyl propane. We have also investigated that the V-Phenylenic nanostructure $\mathrm{VPH}[\mathrm{p},\mathrm{q}]$ admits a perfect H-packing with H isomorphic to cyclohexane, propane, 2, 3 - dimethyl butane, 2 - methyl pentane and 3 - methyl pentane. In addition we have also studied the F-packing of $\mathrm{VPH}[\mathrm{p},\mathrm{q}]$ where $\mathrm{F} \simeq \{\mathrm{C}_4, \mathrm{C}_8\}$.

Keywords: H-packing, F-packing, Perfect packing, $\mathrm{TUC_4C_8}(S)$ nanotube, V-Phenylenic VPH[p,q] nanotube;

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DOI: 10.31838/ecb/2023.12.s3.506

1. Introduction and Terminology

Nanotechnology studies the manipulation of matter on an atomic and molecular scale [16]. Many of these merchandises that are in use nowadays are products which have been progressively upgraded, in which some type of nanotechnology assisted process is used in the production center. There are numerous usages of this fast developing aspect in the areas of medical treatment and practices, chemistry, dynamism, farming, information and communication, heavy industry and consumer goods. The manufacturing of molecular goods needs to be processed out by robotic Machines, often called as nanorobots [11]

Nanorobotics is a fast developing area in the field of science and engineering which necessitates combined efforts between physicists, chemists, biologists, computer scientists, engineers and other specialists [6, 22, 27]. Today this technology is still progressing, mainly due to the tremendous contributions made by great scholars and researchers round the globe paying to this ever stimulating and rousing field. Nanorobotics emphasis on the plan, engineering, software design and control of the nanoscale robots. Controlling nanoscale robot is attained by appropriate scheduling, where scheduling is the method of determining how to obligate assets between a diversity of probable jobs and H-packing has significant applications in scheduling [4].

In this paper we have investigated the packing numbers of certain nanotubes such as $TUC_4C_8(S)$ nanotube and V-Phenylenic VPH[p,q] nanotube.

1. Definitions

1.1. Definition:

[7] An H - packing of a graph G is a set of vertex disjoint subgraphs of G, each of which is isomorphic to a fixed graph H. From the optimization point of view, maximum H – packing problem is to find the maximum number of vertex disjoint copies of H in G called the packing number denoted by λ (G, H). For our convenience λ(G, H) is sometimes represented as λ.

The vertices belonging to the subgraph H of an H-packing are said to be saturated by the H-packing and the other vertices are said to be unsaturated. A packing that saturates every vertex of G is said to be a perfect H - packing.

1.2. Definition**:**

[15] An F - packing is a natural generalization of H - packing concept. For a given family F of graphs, the problem is to identify a set of vertex-disjoint subgraphs of G, each isomorphic to a member of F. The F - packing problem is to find an F - packing in a graph G that covers the maximum number of vertices of G.

Throughout this paper a path on n vertices is denoted by $\mathbf{P_n}$, a cycle on n vertices is denoted by $\mathbf{C_n}$ and $\mathbf{K_{1,n}}$ to represent the star graph where star graph is a special type of graph in which n vertices have degree 1 and a single vertex has degree n.

2. $\mathbf{TUC_4C_8(S)}$ Carbon Nanotube

The carbon nanotube $TUC_4C_8(S)$ [23] is a trivalent arrangement obtained by interchanging squares C_4 and octagons C_8. In this section let q, an even number, signify the number of rows and p signify the number of squares induced by row i and row $i + 1$, i odd, $1 \leq i \leq q - 1$. The total number of vertices in $TUC_4C_8(S)$ is 4pq [26]. The nomenclature of the edges of the nanotube are; horizontal edges which are parallel to the plane and acute edges, which make an acute angle with the plane and obtuse edges, that make an obtuse angle with the plane as shown in Figure 1 [21].

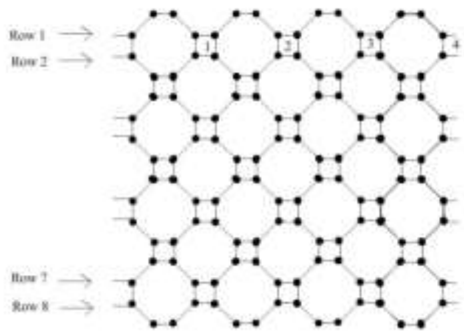

Figure 1: $TUC_4C_8(S)$

Packing patterns of $\mathbf{TUC_4C_8(S)}$

In this section we have shown that the carbon nanotube $TUC_4C_8(S)$ admits a perfect H -packing with H isomorphic to cyclooctane, butane and 3, 4-dimethyl hexane and have also studied the perfect $H-$packing of $TUC_4C_8(S)$ nanotorus with H isomorphic to cyclobutane and 2-methyl propane. The $H-$Packing of $TUC_4C_8(S)$ with these chemical graphs is complete when H is a graph on four or eight vertices, in the sense that, there exist no other connected graph H on four or eight vertices that perfectly packs $TUC_4C_8(S)$. If there exist a spannig subgraph $S \subseteq K_4$ or $S \subseteq K_8$ that perfectly packs $TUC_4C_8(S)$, then either S will be isomorphic to any one of the above mentioned chemical structures H or S will be a spanning subgraph of H.

2.1. Packing $TUC_4C_8(S)$ with Cyclooctane

A molecular graph $G = (V, E)$ is a simple graph having $|V|$ nodes and $|E|$ edges. The nodes $v_i \in V$ represent non-hydrogen atoms and the edges $(v_i, v_j) \in E$ represent bonds between the corresponding atoms. Specifically, hydrocarbons were formed only by carbon and hydrogen atoms and their molecular graphs characterize the carbon sketchwork of the molecule [24]. The graph H in figure 2a represents the well-known structure in chemistry, known as cyclooctane C_8H_{16}. In graph theoretical terms it represents a cycle on 8 vertices C_8.

2.1.1. Theorem The $TUC_4C_8(S)$ nanotube of dimension $p \times q$ admits a perfect packing with cyclooctane (C_8) for all values of p and q.

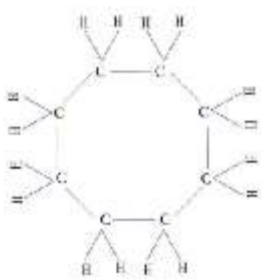

Figure a: Cyclooctane

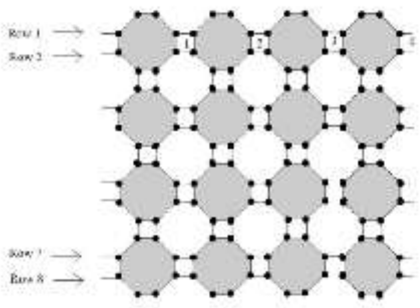

Figure b: Figure 2: -packing of

Proof. The total number of vertices is $TUC_4C_8(S)$ of dimension $p \times q$ is $4pq$, a multiple of four which supports a perfect $H-$ packing if the number of nodes in the H graph is four or multiples of four. The definition of $TUC_4C_8(S)$ imposes q to be an even number and hence the lower bound for the total number of vertices in $TUC_4C_8(S)$ is 8. Now select the octagons induced by row i and row $i+1$, i odd, $1 \leq i \leq q-1$ which divides the vertex set of $TUC_4C_8(S)$ into $(\frac{q}{2})$ times p copies of cyclooctane. Hence

$$\lambda(TUC_4C_8(S), C_8) = p(\frac{q}{2}).$$

2.2. Packing $TUC_4C_8(S)$ with Butane

Figure 3a shows C_4H_{10} butane structure, when on removal of hydrogen atoms it leaves a path P_4 in the place of butane.

2.2.1. Theorem The $TUC_4C_8(S)$ nanotube of dimension $p \times q$ admits a perfect packing with pq copies of butane (P_4) for all values of p and q.

The proof of the theorem follows from Theorem 3.1.1, where each cyclooctane is split into two copies of butane on the removal of either a pair of vertical edges or horizontal edges or acute edges or obtuse edges from each cyclooctane.

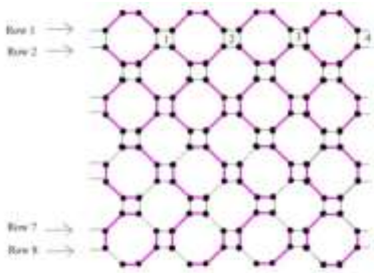

Figure b: $TUC_4C_8(S)$

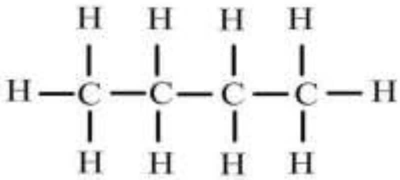

Figure a: Butane

Figure 3: P_4-packing of $TUC_4C_8(S)$

2.3. Packing $TUC_4C_8(S)$ with 3, 4 - dimethyl hexane

The graph H in figure 4a represents the familiar arrangement in chemistry, known as 3, 4 - dimethyl hexane. In graph theoretical terms it represents a caterpillar, a tree in where every vertex of the graph is on a central trunk or only one edge of the graph is away from the trunk, and on deletion of its endpoints we obtain a path graph.

2.3.1. Theorem The $TUC_4C_8(S)$ nanotube of dimension $p \times q$ admits a perfect packing with 3, 4 - dimethyl hexane for all values of p and q.

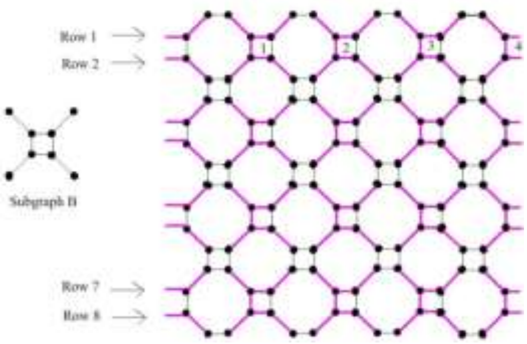

Figure b: $TUC_4C_8(S)$

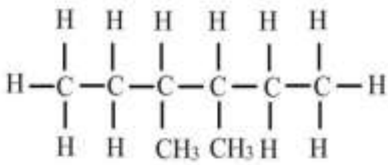

Figure a: 3, 4 - dimethyl hexane

Figure 4: H-packing of $TUC_4C_8(S)$

Proof. In $TUC_4C_8(S)$ of dimension $p \times q$ select all the squares induced by vertices in row i and row $i+1$, i odd, $1 \leq i \leq q-1$ which yields p times $(\frac{q}{2})$ copies of C_4. To the selected squares, adjoin the four edges that are incident with its corner vertices resulting in the graph B as shown in figure 4b. From the graph B if any one of the edges of the square is removed it results in the chemical structure 3, 4 – dimethyl hexane thus vertex decomposing the nanotube $TUC_4C_8(S)$ into $p(\frac{q}{2})$ copies of the graph H. In the tube formation of $TUC_4C_8(S)$ the last square gets sequentially arranged next to the first square and hence disclosing a perfect $H-$packing of $TUC_4C_8(S)$.

3. $\mathbf{TUC_4C_8(S)}$ Nanotorus

The $TUC_4C_8(S)$ nanotorus can be assimilated by amalgamating pairs of nodes of degree two of the $TUC_4C_8(S)$ nanotube. In order to accomplish vertex symmetry, the finest selection for enfolding around is the pairs of nodes that are mirror symmetric with respect to the horizontal line, travrsing through the center of the $TUC_4C_8(S)$ nanotube. Figure 5 shows how to wraparound $TUC_4C_8(S)$ nanotube of dimension $p \times q$ to obtain a $TUC_4C_8(S)$ nanotorus of dimension $p \times q$.

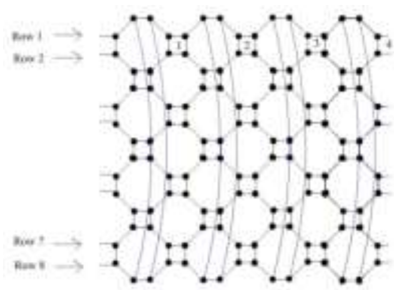

Figure 5: $TUC_4C_8(S)$ nanotorus

3.1. Packing $TUC_4C_8(S)$ nanotorus with Cyclobutane

Figure 6a shows C_4H_8 cyclobutane structure, when on removal of hydrogen atoms it leaves a cycle C_4 in the place of cyclobutane.

3.1.1. Theorem: The $TUC_4C_8(S)$ nanotorus of dimension $p \times q$ admits a perfect packing with cyclobutane for all values of p and q.

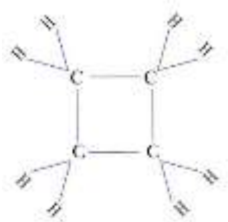

Figure a: Cyclobutane

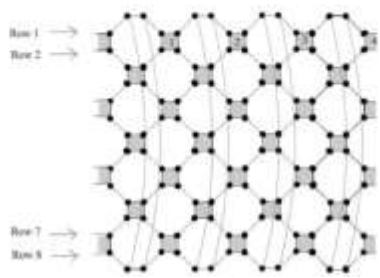

Figure b: $TUC_4C_8(S)$ nanotorus

Figure 6: C_4-packing of $TUC_4C_8(S)$ nanotorus

Proof. In $TUC_4C_8(S)$ nanotorus of dimension $p \times q$ select all the squares induced by vertices in row i and row $i+1$, i odd, $1 \leq i \leq q-1$ which yields p times $(\frac{q}{2})$ copies of C_4 . Now select all the squares induced by vertices in row i and row $i+1$, i even, $2 \leq i \leq q-2$ which yields p times $\{(\frac{q}{2})-1\}$ copies of C_4. The torus formation of $TUC_4C_8(S)$ yields another row of p squares induced by the vertices of row 1 and row q. Thus we see that the $TUC_4C_8(S)$ nanotorus is vertex degenerated into $\{p(\frac{q}{2})+p((\frac{q}{2})-1)+p\}$ copies of cyclobutane which on simplification gives pq copies of C_4 saturating all the vertices of $TUC_4C_8(S)$.

3.2. Packing $TUC_4C_8(S)$ nanotorus with 2 – methyl propane

Figure 7a shows C_4H_{10} , 2 – methyl propane or isobutane structure, when on removal of hydrogen atoms it leaves a claw $K_{1,3}$ in the place of 2 – methyl propane.

3.2.1. Theorem The $TUC_4C_8(S)$ nanotorus of dimension $p \times q$ admits a perfect packing with 2 – methyl propane for all values of p and q.

Proof. In $TUC_4C_8(S)$ nanotorus of dimension $p \times q$ select the obtuse edges in all the i rows, $1 \leq i \leq q$ which yields pq copies of P_2. Each of these obtuse edges are incident with two nodes, the above one called as the upper node and the below one called as the lower node say α_{ij}, $1 \leq i \leq q$ and $1 \leq j \leq p$. Adjoin the lower node α_{ij} with the vertical and horizontal edges that are incident with it consequently forming a claw with α_{ij} as the internal node and the vertical, horizontal and obtuse edges as the spikes of the claw. The α_{ij} nodes of the obtuse edges selected in the q^{th} row will be of degree two, but on torus formation, yields degree three together with the edges adjoining the vertices of row 1 and henceforth admitting a perfect packing of $TUC_4C_8(S)$ nanotorus with 2 – methyl propane for all values of p and q.

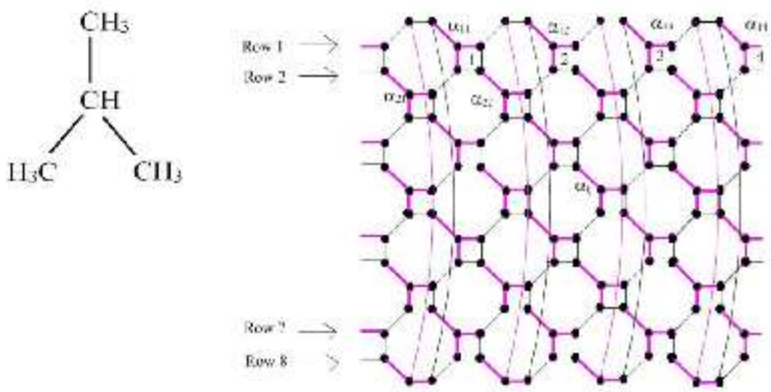

Figure a: 2 – methyl propane Figure b:

Figure 7: Packing $TUC_4C_8(S)$ nanotorus with 2 – methyl propane

4. V-Phenylenic VPH[p, q] Nanotube

V-Phenylenic nanotubes VPH[p, q] are molecular graphs that are covered by C_6, C_4 and C_8. In this section, perfect packings and packing numbers of V -phenylenic VPH[p, q] nanotube are investigated. In the V -phenylenic VPH[p, q] nanotube, p represents the number of hexagons in each column and q represents the number of hexagons in each row and the total number of vertices in V-Phenylenic VPH[p, q] nanotube is 6pq [3]. See figure 8.

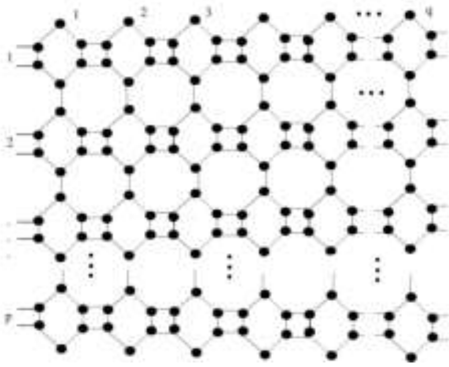

Figure 8: V-Phenylenic VPH[p, q] nanotube

Packing patterns of V-Phenylenic VPH[p, q] Nanotube

In this section we have shown that the V-Phenylenic nanotubes VPH[p, q] admits a perfect H-packing with H isomorphic to cyclohexane, propane, 2, 3 - dimethyl butane and 2 - methyl pentane and have also studied the perfect H − packing of VPH[p, q] nanotorus with H isomorphic to 3 - methyl pentane. The H − Packing of VPH[p, q] with these chemical graphs is complete when H is a graph on three or six vertices, in the sense that, there exist no other connected graph H on three or six vertices that perfectly packs VPH[p, q]. If there exist a spannig subgraph $S \subseteq K_3$ or $S \subseteq K_6$ that perfectly packs VPH[p, q], then either S will be isomorphic to any one of the above mentioned chemical structures H or S will be a spanning subgraph of H. Furthermore we have also investigated the F-packing of VPH[p, q] where $F \simeq \{C_4, C_8\}$.

4.1. Packing $VPH[p,q]$ nanotube with Cyclohexane

The graph H in figure 9a represents the common carbon skeleton in chemistry, known as cyclohexane C_6H_{12}. In graph theoretical terms it represents a cycle on 6 vertices C_6.

4.1.1. Theorem The V-Phenylenic $VPH[p,q]$ nanotube admits a perfect packing with pq copies of cyclohexane for all values of p and q.

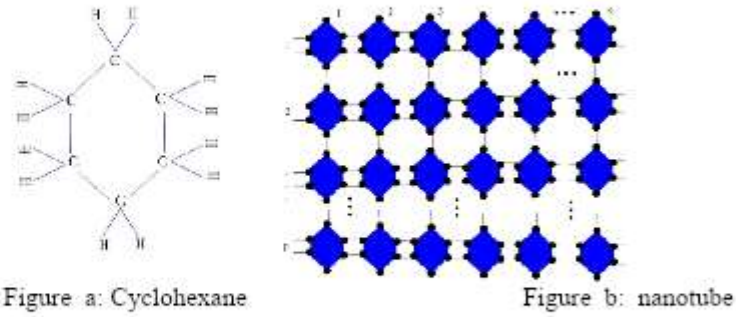

Figure 9: C_6 packing of VPH[p, q] nanotube

Proof. Though the chemical graph structure of V-Phenylenic nanotube is covered by C_6, C_4 and C_8, the nanotube does not admit a perfect H − packing when $H \simeq C_4$ or $H \simeq C_8$ except for $H \simeq C6$. The graph of VPH[p, q] consist of p number of cyclohexanes in each column and q number of cyclohexanes in each row which totally contributes pq copies of cyclohexane saturating the $6pq$ vertices of the $VPH[p,q]$ nanotube as shown in figure 9b. Hence $\lambda(VPH[p,q], C_6) = pq$.

4.2. Packing $VPH[p,q]$ nanotube with Propane

The graph H in figure 10a signifies the common carbon sketch in chemistry, known as propane C_3H_8 . In graph theoretical terms it represents a path on 3 vertices P_3.

4.2.1. Theorem The V-Phenylenic $VPH[p,q]$ nanotube admits a perfect packing with 2pq copies of propane for all values of p and q.

The proof of this theorem follows from theorem 5.1.1, where each cyclohexane is split into two copies of propane on the removal of either a pair of vertical edges or acute edges or obtuse edges from each cyclohexane as shown in figure 10b. Hence $\lambda(VPH[p,q], P_3) = 2pq$.

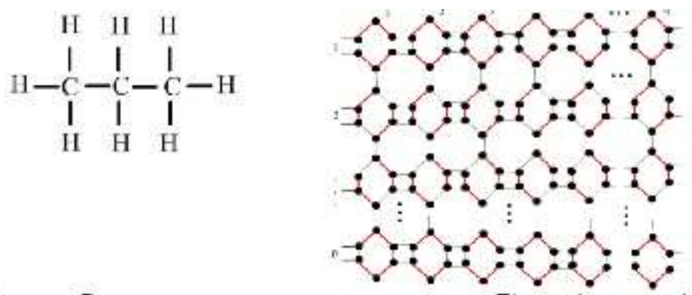

Figure a: Propane Figure b: nanotube

Figure 10: P_3 packing of $VPH[p,q]$ nanotube

4.3. Packing $VPH[p,q]$ nanotube with 2, 3 – dimethyl butane

The graph H in figure 11a signifies the common carbon skeleton in chemistry, known as 2, 3 – dimethyl butane. In graph theoretical terms it represents a double star, a graph obtained by joining the center of two stars $K_{1,2}$.

4.3.1. Theorem The V-Phenylenic $VPH[p,q]$ nanotube admits a perfect packing with pq copies of 2, 3 – dimethyl butane for all values of p and q.

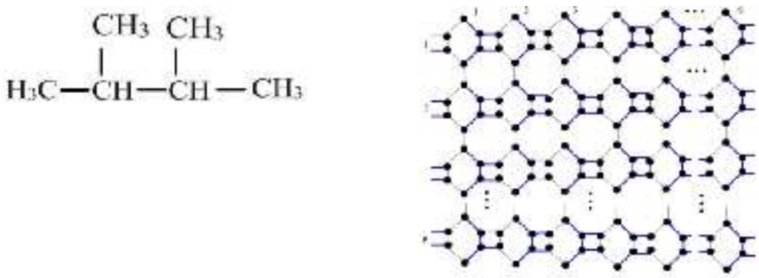

Figure a: 2, 3 – dimethyl butane Figure b: nanotube

Figure 11: Packing $VPH[p,q]$ nanotube with 2, 3 – dimethyl butane

Proof. In the V-Phenylenic $VPH[p,q]$ nanotube select all the q squares in the p rows contributing pq copies of C_4. In each of these squares there are two vertical edges, call them as the left edge and right edge say. Now remove the right edge of all the selected squares resulting in pq copies of path P_4. In each of these paths P_4, there are two internal vertices which are incident with an acute edge and an obtuse edge from the cycle C_6. To the path P_4 adjoin these two edges from the cycle C_6 which ensues pq copies of 2, 3 – dimethyl butane saturating all the $6pq$ vertices of the V-Phenylenic $VPH[p,q]$ nanotube as shown in figure 11b.

4.4. Packing $VPH[p,q]$ nanotube with 2 – methyl pentane

The graph H in figure 12a represents the common carbon skeleton in chemistry, known as 2 – methyl pentane. In graph theoretical terms it represents a star $K_{1,3}$ where one of its edges is replaced by a path P_4.

4.4.1. Theorem The V-Phenylenic $VPH[p,q]$ nanotube admits a perfect packing with pq copies of 2 – methyl pentane for all values of p and q.

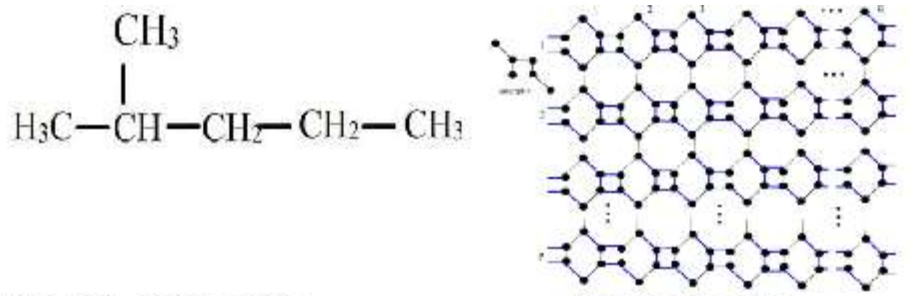

Figure a: 2 – methyl pentane Figure b: nanotube

Figure 12: Packing $VPH[p,q]$ nanotube with 2 – methyl pentane

Proof. In the V-Phenylenic $VPH[p,q]$ nanotube select all the q squares in the p rows contributing pq copies of C_4 . We now select any two alternating edges incident with the corner vertices of each of these squares resulting in the graph S as shown in figure 12b. From the graph S if any one of the edges of the square is removed, results in the chemical structure 2 – methyl pentane, thus vertex decomposing the nanotube $VPH[p,q]$ into pq copies of the graph H.

5. V-Phenylenic $VPHY[p,q]$ Nanotorus

The torus structure of the V- Phenylenic $VPH[p,q]$ nanotube is denoted as $VPHY[p,q]$ obtained by joining the two degree nodes of the first row with the two degree nodes in the last row as shown in figure 13.

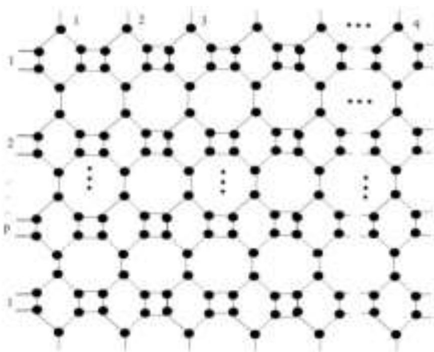

Figure 13: V-Phenylenic $VPHY[p,q]$ nanotorus

5.1. Packing $VPHY[p,q]$ nanotorus with 3 – methyl pentane

The graph H in figure 14a represents the common carbon sketch in chemistry, known as 3 – methyl pentane. In graph theoretical terms it represents a star $K_{1,3}$ where two of its edges are replaced by path P_3.

5.1.1. Theorem The V-Phenylenic VPHY[p,q] nanotorus admits a perfect packing with 3 – methyl pentane for all values of p and q.

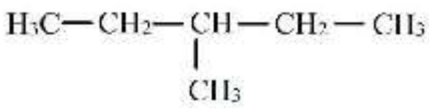

Figure a: 3 – methyl pentane

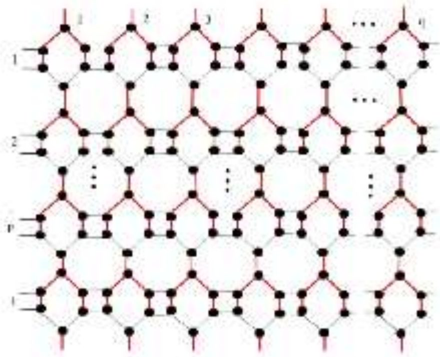

Figure b: nanotorus

Figure 14: Packing $VPHY[p,q]$ nanotorus with 3 – methyl pentane

Proof. Select the vertical edges of the nanotorus which links the hexagons between the p rows. Together with the vertical edges adjoin the pair of acute and obtuse edges that are incident with the lower node of each of these vertical edges. This results in the formation of pq copies of claw $K_{1,3}$. Now affix the pair of parallel vertical edges present in the formation of every hexagon to the acute and obtuse edges of the claw $K_{1,3}$ transforming it into pq copies of 3 – methyl hexane. The pq copies of 3 – methyl hexane deduced while packing the nanotorus, saturates all the $6pq$ vertices of the graph as the total number of vertices in the H graph is 6 assuring a perfect packing of the V-Phenylenic $VPHY[p,q]$ nanotorus. Refer figure 14b.

5.2. Packing $VPHY[p,q]$ nanotorus with $\{C_4, C_8\}$

5.2.1. Theorem The nanotorus V-Phenylenic $VPHY[p,q]$, $p > 2,\ q > 2$ admits a perfect F - packing when $q \equiv 0\ (mod\ 2)$ and a maximum F – packing when $q \equiv 1\ (mod\ 2)$ where $F \simeq \{C_4, C_8\}$.

Proof. The chemical structure of V-Phenylenic $VPHY[p,q]$ nanotorus is an arrangement of C_6 , C_4 and C_8 in a predefined manner. The parameter p represents the number of hexagons in each column and q represents the number of hexagons in each row. The total count of the hexagons agrees with the total number of squares in the nanotorus. In $VPHY[p,q]$ there are p rows of octagons with q copies in each row where each octagon shares four vertices, two each with the octagons on its left and right. This induces a constraint that on selecting an octagon, the preceding and the succeeding octagons in that row cannot be selected. Mark the columns in the $VPHY[p,q]$ nanotorus as shown in figure 15.

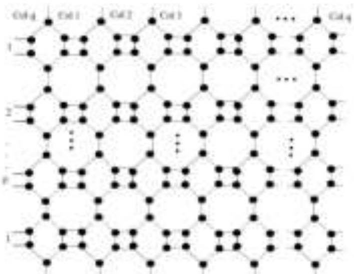

Figure 15: $VPHY[p,q]$ nanotorus

Case 1: $q \equiv 0\ \ (mod\ \ 2)$

For q even, select the p copies of C_8 in all the even columns C_j , $2 \leq j \leq q$ which yields $p(\frac{q}{2})$ copies of C_8 saturating $4pq$ vertices of the V-Phenylenic $VPHY[p,q]$

nanotorus. Now select all the p squares in the odd columns C_j, $1 \leq j \leq q-1$ which produces another $p(\frac{q}{2})$ copies of C_4 saturating the remaining $2pq$ vertices of the V-Phenylenic $VPHY[p,q]$ nanotorus. Hence the $VPHY[p,q]$ nanotorus admits a perfect $F-packing$ when $q \equiv 0 \pmod 2$ with $F \simeq \{C_4, C_8\}$.

Case 2: $q \equiv 1 \pmod 2$

For q odd, select the p copies of C_8 in all the even columns C_j, $2 \leq j \leq q-1$ which yields $p(\frac{q-1}{2})$ copies of C_8 saturating $4p(q-1)$ vertices of the V-Phenylenic $VPHY[p,q]$ nanotorus. Now select all the p squares in the odd columns C_j, $1 \leq j \leq q$ which produces $p(\frac{q+1}{2})$ copies of C_4 saturating another set of $2p(q+1)$ vertices of the nanotorus. The current selection of C_8 and C_4 saturates 6pq-2p vertices of the nanotorus leaving 2p vertices unsaturated. Since the selection of two adjacent octagons are incompatible, these 2p vertices that lie in the intersecting nodes of the p octagons between the first and the last odd columns are unsaturated. Hence the VPHY[p, q] nanotorus admits a maximum $F-packing$ when $q \equiv 1 \pmod 2$ with $F \simeq \{C_4, C_8\}$.

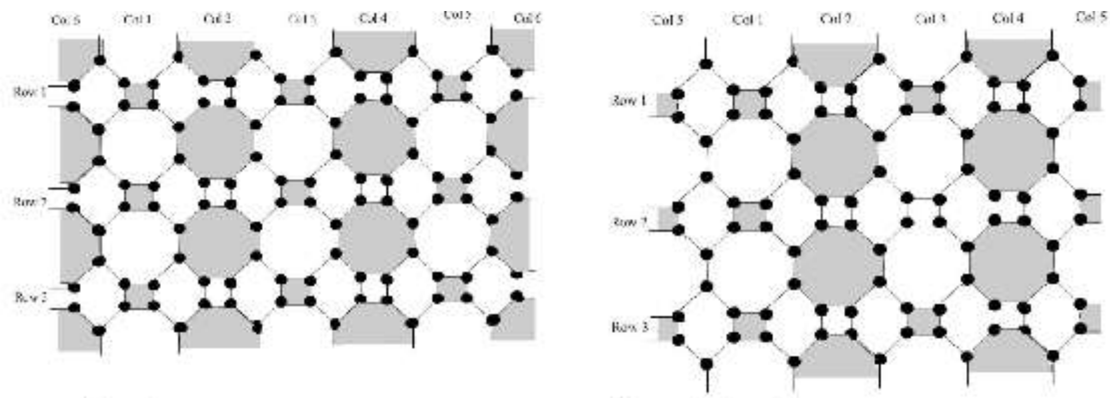

Figure a: Case 1: Figure b: Case 2:

Figure 16: F-Packing of VPHY[p, q] nanotorus

2. Conclusion

In this paper we have investigated the various chemical structures implanted in the carbon nanotubes $TUC_4C_8(S)$ and V − PhenylenicVPH[p, q] by studying the perfect H -packing of $TUC_4C_8(S)$ nanostructure with H isomorphic to cyclooctane, butane, 3, 4-dimethyl hexane, cyclobutane and 2-methyl propane. We have also studied that the V-Phenylenic nanostructure VPH[p, q] admits a perfect H -packing with H isomorphic to cyclohexane, propane, 2, 3 - dimethyl butane, 2 - methyl pentane and 3 - methyl pentane. In addition we have also studied the F -packing of VPH[p, q] where $F \simeq \{C_4, C_8\}$.

3. References

Al Mutairi A, Ali B, Manuel P, Packing in carbon nanotubes. J. Comb. Math. Comb. Comput. 92, 195–206 (2015)

Antony Xavier, Santiagu Theresal, Maria Jesu Raja S, Induced H‑packing k‑partition number for certain nanotubes and chemical graphs, Journal of Mathematical Chemistry, April (2020)

Bahrami A and Yazdani J, 2009, Vertex pi index of V- phenylenic nanotubes and nanotori, Digest Journal of Nanomaterials and Biostructures 4, 205.

Bar-Yehuda R, Halldorsson M, Naor J, Shachnai H and Shapira I, 2002, Scheduling split intervals, Proc.

Thirteenth Annu.ACM–SIAM Symp. On Discrete Algorithms, 732–741.

Bejar R, Krishnamachari B, Gomes C and Selman B, 2001, Distributed constraint satisfaction in a wireless sensor tracking system, Workshop on Distributed Constraint Reasoning, Internat. Joint Conf. on Artificial Intelligence.

Celasun S, 2013, Reviews in Theoretical Science 1, 319.

Czygrinow A and Hanckowiak M, 2007, Distibuted approximations for packing in unit-disk graphs, Distributed Computing, Proceedings of 21st International Symposium, Disc, Lemesos, Cyprus, September 24-26.

Dobson E, 1997, Packing almost stars into the complete graph, J. of Graph Theory, 10, 169-172.

Felzenbaum A, 1993, Packing lines in a hypercube, Discrete Mathematics 117, 107-112.

Galli G, Donadio D, 2010, Thermoelectric materials: silicon stops heat in its tracks. Nat. Nanotechnol., 5, 701–702.

Hamdi M and Ferreira A, 2011, Design, Modeling and Characterization of Bio-Nanorobotic Systems, Springer.

Hardesty L, 2010, Self-assembling computer chips, (MIT News Office, Cambridge, MA, 2010). Posted on 16 March 2010

Hell P and Kirkpatrick D, 1978, On the complexity of a generalized matching problem , Proceedings of Tenth ACM Symposium On Theory of Computing, pp. 309–318.

Hornyak T, 2010. MIT building self-assembling computer chips, CNET News, March 16, 6:28 PM PDT.

Indra Rajasingh, Albert Muthumalai, Bharati R and Shanthi A S, Packing in honeycomb networks, 2012, J. of Mathematical Chemistry, 50, no. 5, 1200-1209.

Indra Rajasingh, Paul Manuel and A. S. Shanthi, Excessive Index of Certain Nanotubes, Journal of Computational and Theoretical Nanoscience, Vol. 11, 1–6, (2014).

Jude Annie Cynthia V, Sindiya Therese, Packing of Certain Nanotubes and Nanosheet, International Journal of Mathematics and Computer Science, no. 4, 1135–1141, 15(2020).

Jude Annie Cynthia V and Sindiya Therese S, Packing of Certain Mesh Derived Architectures, International Journal of Pure and Applied Mathematics, Volume 120 No. 8, 99-107, 2018.

Jude Annie Cynthia V and Sindiya Therese S, Path Packing of Certain Class of Cyclic Split Graphs, International Journal of Pure and Applied Mathematics, Volume 120 No. 7, 117-124, 2018.

Muthumalai A, Rajasingh I and Shanthi A S, 2011, Packing of Hexagonal Networks, J. of Combinatorial Mathematics and Combinatorial Computation, 79, 121-127.

Manuel P, Rajasingh I, Rajan B, and Rajan R S, 2013 Total-Szeged Index of C4-Nanotubes, C4-Nanotori and Dendrimer Nanostars, J. Comput. Theoret. Nanosci. 10, 1515.

Manuel P, Rajasingh I, and Arockiaraj M, 2013, J. Comput. Theoret.Nanosci. 10, 405.

Manuel P, Rajasingh I, Rajan B, and Rajan R S, 2013, J. Comput. Theoret. Nanosci. 10, 1515.

Supriya Saha and Dilipkumar Pal, 2017, Mathematical Chemistry – An Emerging Field of Drug Discovery, Scholar's Press, ISBN: 978-3-330-65214-9.

Siddiqui H M A, Imran M, Computation of metric dimension and partition dimension of nanotubes, J. Comput. Theor. Nanosci. 12, 199–203 (2015)

Thalaya Al-Fozan, Paul Manuel, Indra Rajasingh, and Sundara Rajan R, 2014, Computing Szeged Index of Certain Nanosheets Using Partition Technique, MATCH Commun.

Math. Comput. Chem 72.1, 339-353.
Art and Future Challenges, Invited Chapter in Tissue Engineering and Artificial Organs The Biomedical Engineering Handbook, edited by M. L. Yarmush, CRC Press, Chap. 19.
Yap H P, 1988, Packing of graphs – A Survey, Discrete Mathematics, 72, 395-404.