

## Domination in certain chemical graphs

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**Abstract** Domination theory is required for encryption of binary string into a DNA sequence. A dominating set of a graph  $G = (V, E)$  is a subset  $D$  of  $V$  such that every vertex not in  $D$  is adjacent to at least one vertex in  $D$ . The bondage number  $b(G)$  of a nonempty graph  $G$  is the minimum number of edges whose removal from  $G$  results in a graph with larger domination number than  $\gamma(G)$ . In this paper we determine the domination number and the bondage number for pyrene torus, Balaban 10-cage and hexabenzocoronene using  $H$ -packing. Further we compute the domination number of non-isomorphic graphs with same number of vertices namely  $H$ -phenylenic nanotube and  $H$ -naphthelene nanotube.

**Keywords** Pyrene torus ·  $H$ -packing · Perfect packing · Domination number · Bondage number · Balaban 10-cage ·  $H$ -phenylenic nanotube ·  $H$ -naphthelene nanotube · Hexabenzocoronene

**AMS Classification** 05C69

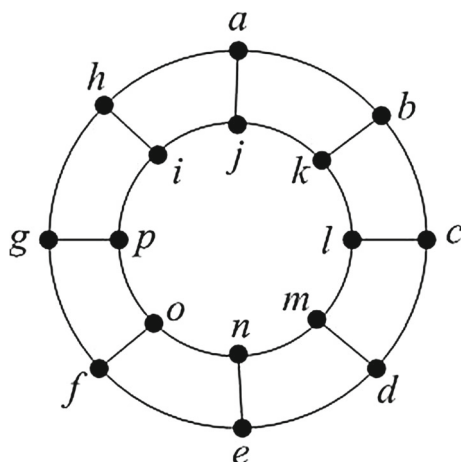
### 1 Introduction and preliminaries

Domination in graph theory is a natural model for many location problems in operations research. It has many other applications in dominating queens problem, school bus routing problem, computer communication network problems, social network theory, land surveying and kernels of games [9, 10]. Among them, the classical problems

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**Fig. 1**  $\gamma(P(8, 1)) = 4$  and  $b(G) = 2$

of covering chessboards by the minimum number of chess pieces are important in stimulating the study of domination, which commenced in the early 1970s.

Chemical structures are conveniently represented by graphs, where atoms correspond to vertices and chemical bonds correspond to edges. This representation inherits many useful information about chemical properties of molecules. It has been shown in QSAR and QSPR studies that many physical and chemical properties of molecules are well correlated with graph theoretical invariants that are termed topological indices or molecular descriptors. One of such graph theoretical invariants is domination number [16]. Domination theory is required for encryption of binary string into a DNA sequence. The methods like, basic method and insertion method encrypting any chemical formula using graph domination as the tool for encryption. Every chemical formula is converted into a binary string using graph domination and later encrypted using DNA steganography [22].

A set  $D$  of vertices in a graph  $G$  is said to be a *dominating set* if every vertex in  $V - D$  is adjacent to some vertex in  $D$ . The *domination number*  $\gamma(G)$  of a graph  $G$  is the minimum size of a dominating set of  $G$ . In Fig. 1, the dominating set of peterson graph is  $\{a, c, e, g, i, l, p\}$  but the minimum dominating set is  $\{a, e, l, p\}$  and can be  $\{b, f, m, i\}$ . In 1990, Fink et al. [7] introduced the bondage number as a parameter for measuring the vulnerability of an interconnection network under link failure. The *bondage number*  $b(G)$  of a nonempty graph  $G$  is the minimum number of edges whose removal from  $G$  results in a graph with larger domination number than  $\gamma(G)$ . If  $b(G)$  does not exist, for example empty graphs, we define  $b(G) = \infty$ . They also established the bondage number of cycles, paths, complete graphs and complete multipartite graphs and showed that  $b(T) \leq 2$  for any tree  $T$ . In [8], Hartnell et al. and Wang [21] gave an improved upper bound of the bondage number. The problem of determining bondage number for general graphs is NP-hard [15]. In Fig. 1, the bondage set is  $\{(a, j), (b, k), (b, c)\}$  but the minimum bondage set is  $\{(a, j), (b, k)\}$  and the bondage number is 2.

Molecules arranging themselves into predictable patterns on silicon chips could lead to microprocessors with much smaller circuit elements [19]. Mathematically,

assembling in predictable patterns is equivalent to *packing* in graphs. 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  $\lambda(G, H)$ . For our convenience  $\lambda(G, H)$  is sometimes represented as  $\lambda$ .

An *H*-packing in  $G$  is called *perfect* if it covers all vertices of  $G$ . If  $H$  is the complete graph  $K_2$ , the maximum *H*-packing problem becomes the familiar maximum matching problem. Structures realized by arrangements of regular hexagons in the plane are of interest in the chemistry of benzenoid hydrocarbons, where perfect matchings correspond to kekule structures and feature in the calculation of molecular energies associated with benzenoid hydrocarbon molecules. *H*-Packing, is of practical interest in the areas of scheduling, wireless sensor tracking, wiring-board design, code optimization and many others [19].

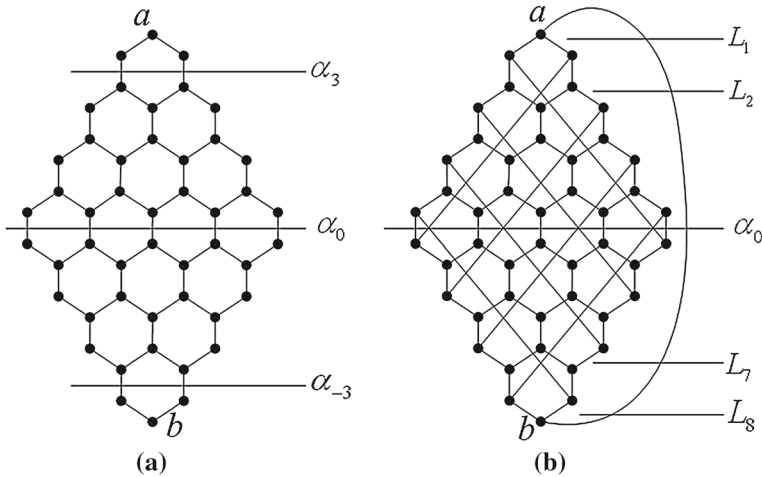
An *F*-packing is a natural generalization of *H*-packing concept. For a given family  $F$  of graphs, the problem is to identify a set of vertex-disjoint subgraphs of  $G$ , each isomorphic to a member of  $F$ . The *F*-packing problem is to find an *F*-packing in a graph  $G$  that covers the maximum number of vertices of  $G$ . When  $H$  is a connected graph with at least three vertices, Kirkpatrick and Hell proved that the maximum *H*-packing problem is *NP*-complete [11]. Packing lines in a hypercube has been studied in [6]. Identification of Bay Regions, enumeration of perfect matchings, Computer Generation of King and Color Polynomials of Graphs and Lattices, dimer statistics on graphs are highlighted by Balasubramanian et al. [3,4,13,20]. Clar's aromatic sextets and the associated sextet polynomials in the context of chemical graph theory are highlighted by Hosoya [12]. Algorithms are available for dense packing of trees of different sizes [23] and packing almost stars into the complete graph [5].

The rest of the paper is organized as follows. In Sect. 2, we compute bondage number of pyrene network. In Sect. 3, we discuss packing of certain chemical structures. In Sect. 4, we determine the domination number of non-isomorphic chemical graphs. Finally, concluding remarks and future work are given in Sect. 5.

## 2 Bondage number of pyrene network

The series of hypothetical benzenoid torus networks are derived by properly joining all the distant pairs of peripheral carbon atoms of 2-dimensional polycyclic aromatic hydrocarbons, namely coronene, pyrene and hexabenzocoronene [14]. This has vast applications in the field of chemistry.

Pyrene is an alternante polycyclic aromatic hydrocarbon (PAH) and consists of four fused benzene rings, resulting in a large flat aromatic system. It is a colorless or pale yellow solid which forms during incomplete combustion of organic materials and therefore can be isolated from coal tar together with a broad range of related compounds. In the last four decades, a number of research works have been reported on both the theoretical and experimental investigation of pyrene concerning its electronic structure, UV-vis absorption and fluorescence emission spectrum. Indeed, this polycyclic aromatic hydrocarbon exhibits a set of many interesting electrochemical and



**Fig. 2** **a** Pyrene network  $PY(4)$ , **b** pyrene torus network  $PT(4)$

photophysical attributes, which have results in its utilization in a variety of scientific areas. Like most PAHs, pyrene is used to make dyes, plastics and pesticides.

In order to study packing in pyrene networks, it is necessary to investigate its topological properties. Hence we introduce the axes for the pyrene network as follows: Let the centre line perpendicular to the vertical edge direction of hexagon of  $PY(n)$  and  $PT(n)$  be denoted by  $\alpha_0$  as shown in Fig. 2a. The lines which are parallel and in the anticlockwise direction of  $\alpha_0$  are denoted by  $\alpha_i$ ,  $1 \leq i \leq (n-1)$  and those in the clockwise direction of  $\alpha_0$  are denoted by  $\alpha_{-i}$ ,  $1 \leq i \leq (n-1)$ . Let the outer cycle of  $PY(n)$  be denoted by  $C_n^0$ . Let the topmost and bottommost vertices in  $PY(n)$  and  $PT(n)$  be denoted by  $a$  and  $b$ .

As given in [17] any zigzag line not containing vertical edges is called a *zigzag horizontal line*. The zigzag horizontal lines of  $PT(n)$  are denoted by  $L_j$ ,  $1 \leq j \leq 2n$ . See Fig. 2b. The number of vertices and edges of  $PT(n)$  are  $2n^2 + 4n$  and  $3n^2 + 6n$  respectively.

**Definition 2.1** The subgraph induced by  $L_j$  and  $L_{j+1}$  in  $PT(n)$  is called a 'zigzag horizontal channel' and is denoted by  $ZZC(j)$  for  $j = 1, 3, 5, \dots, 2n-1$ .

**Theorem 2.2** [19] Let  $G$  be a graph and  $H$  be a subgraph of  $G$ . Then  $\lambda(G, H) \leq \lfloor \frac{|V(G)|}{|V(H)|} \rfloor$ .

**Definition 2.3** [19] Given a vertex  $x$  in a hexagon, the unique vertex  $y$  at distance 3 from it is called the diagonally opposite vertex of  $x$ .

By definition of dominating set the proof of the following result is obvious.

**Lemma 2.4** Let  $S$  be a dominating set with the property that if every vertex  $a \in V(G)$  is dominated by exactly one vertex of  $S$ , then  $S$  is a minimum dominating set.

**Theorem 2.5** *In a graph  $G$ , if there exists a perfect  $H$ -packing when  $H \cong K_{1,\Delta(G)}$ , then  $\gamma(G) = \lambda$ , where  $\Delta(G)$  and  $\lambda$  are the maximum degree and the packing number of  $G$  respectively.*

*Proof* It is clear that  $\gamma(K_{1,\Delta(G)}) = 1$ . In a perfect  $H$ -packing when  $H \cong K_{1,\Delta(G)}$ , all the vertices are dominated by exactly one vertex. Hence, it is obvious that the packing number and the domination number of  $G$  are same. In other words  $\gamma(G) = \lambda$ .  $\square$

**Theorem 2.6** *Let  $G$  be a pyrene network of dimension  $n$ . Then*

$$\gamma(G) = \begin{cases} (\frac{2n^2+4n}{4}) + 1, & \text{if } n \text{ is even} \\ \lceil \frac{2n^2+4n}{4} \rceil, & \text{if } n \text{ is odd} \end{cases}$$

*Proof* Start at a vertex  $a$  as shown in Fig. 3b and call it saturated.

Case (i) ( $n$  is odd)

Saturate a sequence of diagonally opposite vertices of hexagons beginning with vertex  $a$  and proceed till vertex  $b$  is reached.

Case (ii) ( $n$  is even)

The  $\alpha_0$ -line divides  $PY(n)$  into two subgraphs  $H_1$  and  $H_2$  which are mirror images of each other along  $\alpha_0$ . See Fig. 3a. Saturate the vertices as in Case (i) till  $\alpha_{-1}$ -line is reached. Next saturate a vertex  $b$  in  $H_2$  which is the mirror image of  $a$ . Saturate a sequence of diagonally opposite vertices of hexagons beginning with vertex  $b$ . Proceed till  $\alpha_{-1}$ -line is reached.

By Lemma 2.4, since all the vertices on graph are dominated exactly once, the saturated vertices form a minimum dominating set. Therefore,  $\gamma(G) = (\frac{2n^2+4n}{4}) + 1$ , if  $n$  is even and  $\gamma(G) = \lceil \frac{2n^2+4n}{4} \rceil$ , if  $n$  is odd.  $\square$

**Theorem 2.7** *If  $G$  is a pyrene network, then  $b(G) = 1$ .*

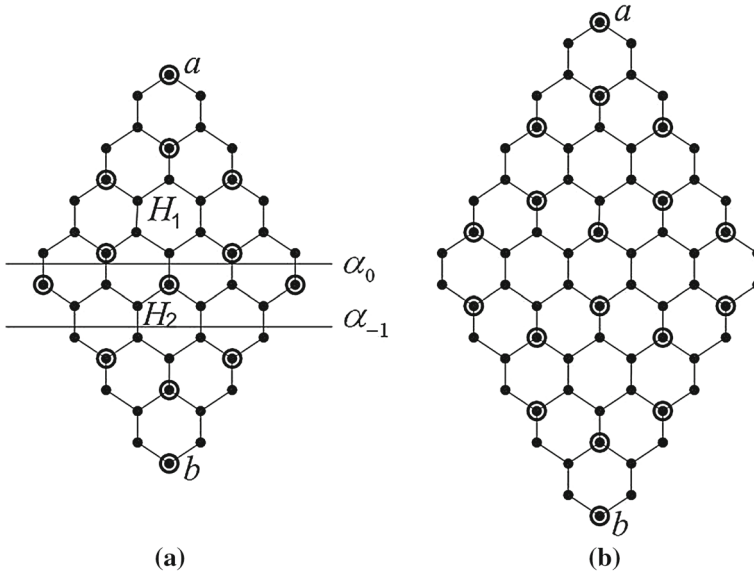
*Proof* Clearly all the saturated vertices form a minimum dominating set of  $G$  by Theorem 2.6. Removal of an edge which is adjacent to saturated vertices, increases the domination number to  $(\frac{2n^2+4n}{4}) + 2$  if  $n$  is even and  $\lceil \frac{2n^2+4n}{4} \rceil + 1$  if  $n$  is odd.  $\square$

### 3 Packing of certain chemical structures

In this section, we compute packing of certain chemical structures, such as, pyrene torus, hexabenzocoronene sheet, hexabenzocoronene torus and Balaban 10-cage network.

#### 3.1 Packing of pyrene torus $PT(n)$ with $K_{1,3}$

**Theorem 3.1** *If  $G$  is a pyrene torus and  $H \cong K_{1,3}$ , then  $\lambda = \lfloor \frac{2n^2+4n}{4} \rfloor$ , where  $\lambda$  is the packing number of  $G$ .*



**Fig. 3** **a** Pyrene network  $PY(4)$ , **b** pyrene network  $PY(5)$

*Proof* Start at a vertex  $a$  as shown in Fig. 4b and call it saturated.

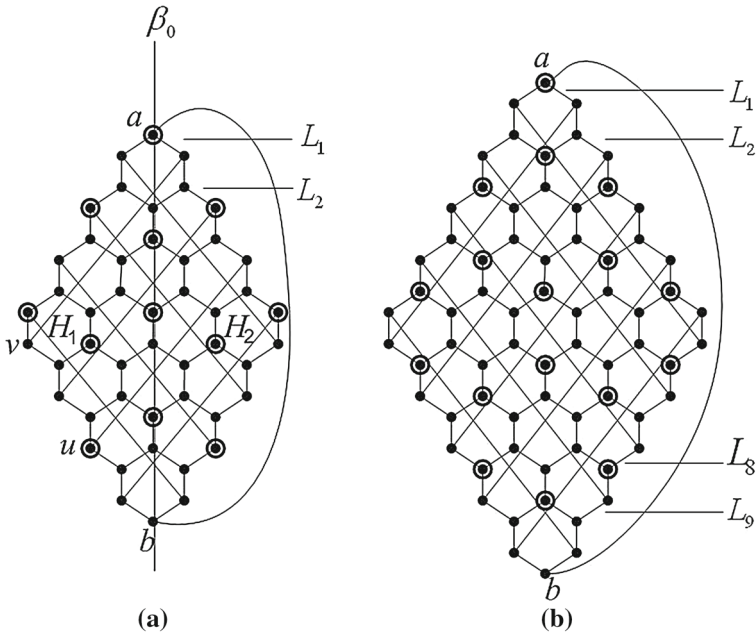
Case (i) ( $n$  is odd)

Saturate a sequence of diagonally opposite vertices of hexagons beginning with vertex  $a$  till a diagonally opposite vertex of  $b$  is reached.

Case (ii) ( $n$  is even)

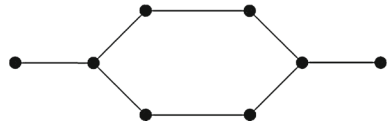
Saturate the vertices as in Theorem 2.6 of the subgraph  $H \cong PY(n-2)$  obtained by deleting the boundary vertices and the diagonally opposite vertices of  $a$  and  $b$  in  $PY(n)$ . Draw the vertical line  $\beta_0$  through the vertices  $a$  and  $b$  as shown in Fig. 4a. The  $\beta_0$  line divides  $PT(n)$  into two subgraphs  $H_1$  and  $H_2$  which are mirror images of each other along  $\beta_0$ . Let the boundary line of  $H_1$  and  $H_2$  be  $C_1$  and  $C_2$  respectively. Label  $C_1$  as follows: Begin with vertex  $u$  at distance 3 from  $b$  as in Fig. 4a and call it saturated. Traversing in the anticlockwise sense, choose the next vertex  $v$  at distance 4 from the saturated vertex and saturate it provided the vertex at distance 4 from  $u$  has no neighbour in zigzag horizontal line  $L_1$ . If not, saturate the next vertex on  $C_n^0$  adjacent to  $b$ . Proceed till  $\beta_0$  is reached. Now we saturate the vertex  $a$  and the vertices in  $C_2$  which are mirror images of saturated vertices on  $C_1$ .

The subgraph induced by  $N[a]$  when  $a$  is a saturated vertex is isomorphic to  $K_{1,3}$ . Now  $N[a] \cap N[u] = \emptyset$  for all pairs of saturated vertices. The wraparound edge incident with  $a$  together with the two vertices on  $C_n^0$  adjacent to  $a$ , induce  $K_{1,3}$ . For  $n$  even, the subgraph  $H \cong PY(n-2)$  contains  $\frac{(n-1)^2+1}{2}$  number of saturated vertices and  $C_n^0$  contains  $2n-1$  number of saturated vertices. The closed neighbourhoods of these saturated vertices together cover  $4 \times [\frac{(n-1)^2+1}{2} + (2n-1)] = 2n^2 + 4n$  vertices. Therefore, the  $H$ -packing is perfect and  $\lambda = \frac{2n^2+4n}{4}$ .



**Fig. 4** **a** Pyrene torus  $PT(4)$ , **b** pyrene torus  $PT(5)$

**Fig. 5** 1,4-dimethyl cyclohexane



For  $n$  odd,  $ZZC(k)$  contains  $k + 1$  number of saturated vertices,  $k = 1, 3, 5, \dots, n$  and  $2n + 1 - k$  number of saturated vertices,  $k = n + 2, n + 4, \dots, 2n - 3$ . The last zigzag horizontal channel contains a saturated vertex. The closed neighbourhoods of these saturated vertices together cover  $4 \times [2 + 4 + 6 + \dots + (n + 1) + (n - 1) + (n - 3) + \dots + 6 + 4] + 4 = [2n^2 + 4n] - 2$  vertices.

Therefore,  $\lambda \geq \lfloor \frac{2n^2+4n}{4} \rfloor$ . By Theorem 2.2,  $\lambda \leq \lfloor \frac{2n^2+4n}{4} \rfloor$ . Hence,  $\lambda = \lfloor \frac{2n^2+4n}{4} \rfloor$ .  $\square$

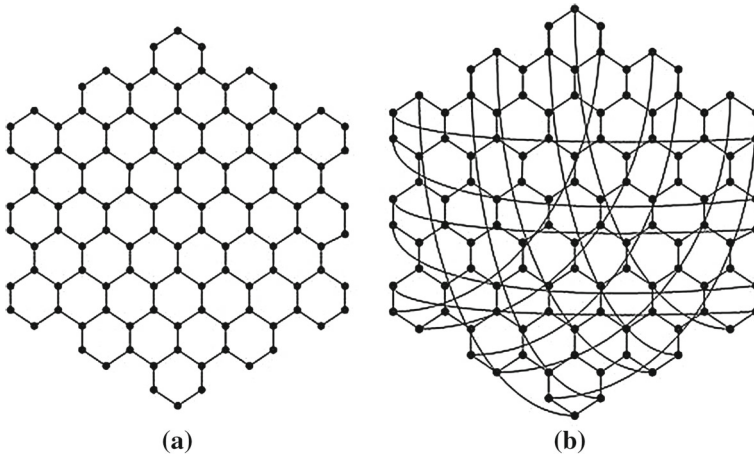
The graph in Fig 5 is known as 1,4-dimethyl cyclohexane in chemistry.

**Corollary 3.2** *If  $H$  is isomorphic to 1,4-dimethyl cyclohexane, then there exists a perfect  $H$ -packing of  $PT(n)$  when  $n$  is even.*

*Proof* It is clear that the vertex set of each selected  $H$  obtained from Theorem 3.1 can be partitioned into two disjoint sets each inducing a subgraph isomorphic to  $K_{1,3}$ .  $\square$

**Theorem 3.3** *If  $G$  is a Pyrene torus, then  $\gamma(G) = \lceil \frac{2n^2+4n}{4} \rceil$ .*

*Proof* Clearly a pyrene torus  $PT(n)$  has a perfect  $H$ -packing when  $n$  is even and an  $H$ -packing of  $PT(n)$  with at most two unsaturated vertices, if  $n$  is odd by Theorem 3.1. Therefore,  $\gamma(G) = \lceil \frac{2n^2+4n}{4} \rceil$  by Theorem 2.5.  $\square$



**Fig. 6** **a** Hexabenzocoronene  $HBC(3)$ , **b** hexabenzocoronene torus  $HBCT(3)$

**Theorem 3.4** *If  $G$  is a pyrene torus network, then  $b(G) = 1$ .*

*Proof* Clearly a pyrene torus  $PT(n)$  has a perfect  $H$ -packing when  $n$  is even and an  $H$ -packing of  $PT(n)$  with at most two unsaturated vertices, if  $n$  is odd by Theorem 3.1. Removal of an edge which is adjacent to saturated vertices, increases the domination number to  $\lceil \frac{2n^2+4n}{4} \rceil + 1$  if  $n$  is even. Removal of an edge which is adjacent to  $a$  and  $b$  except the wraparound edge  $e = (a, b)$ , increases the domination number to  $\lceil \frac{2n^2+4n}{4} \rceil + 1$  if  $n$  is odd. Hence,  $b(G) = 1$ .  $\square$

### 3.2 Packing of hexabenzocoronene $HBC(n)$ with $\{K_{1,3}, K_{1,2}\}$

Hexabenzocoronene ( $HBC$ ) or hexa-peri-benzocoronene existing in yellow crystalline state is noted for its extreme stability. See Fig. 6a. It does not dissolve into concentrated sulfuric acid, and its melting point could not be determined because the melting point tube melted long before the hydrocarbon [14].

Hexabenzocoronene  $HBC(n)$  is obtained by adding a layer of six hexagons to the honeycomb network  $HC(2(n-1))$  as shown in Fig. 6a. We call the vertices of degree 2 of these six hexagons as top vertices. The number of vertices and edges of  $HBC(n)$  are  $6(n^2 + 2n + 4)$  and  $3(3n^2 + 5n + 10)$  respectively.

One of the most widely studied packing is claw-packing [5]. A claw is another name for the complete bipartite graph  $K_{1,3}$ .

**Procedure PACKING** ( $HBC(n), \{K_{1,3}, K_{1,2}\}$ )

**Input:** A hexabenzocoronene network  $G$  of dimension  $n$  and  $F = \{K_{1,3}, K_{1,2}\}$ .

**Algorithm:**

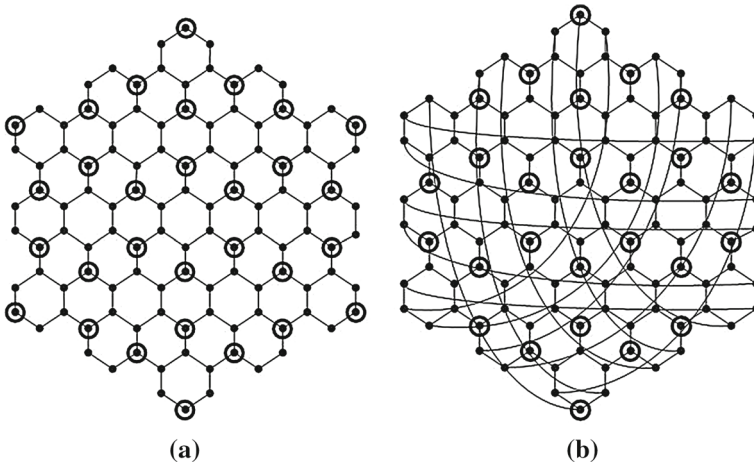
(i) Invoke Procedure PACKING ( $HC(2(n-1)), K_{1,3}$ ) [19]

(ii) Select  $K_{1,2}$  induced by the top vertices and two of its adjacent vertices.

End PACKING

**Output:** An  $F$ -packing of  $HBC(n)$  with  $\lfloor \frac{6(n^2+2n+4)}{4} \rfloor - 4$  copies of  $K_{1,3}$  and six copies of  $K_{1,2}$





**Fig. 7** a Hexabenzocoronene  $HBC(3)$ , b hexabenzocoronene torus  $HBCT(3)$

*Proof of Correctness:* The copies of  $K_{1,3}$  and  $K_{1,2}$  selected by the procedure are disjoint and cover  $4 \times (\lfloor \frac{6(n^2+2n+4)}{4} \rfloor - 4) + 6 \times 3 = 6(n^2 + 2n + 4)$  vertices.

**Theorem 3.5** *If  $G$  is a hexabenzocoronene of dimension  $n$ , then  $\gamma(G) = \lceil \frac{6(n^2+2n+4)}{4} \rceil + 1$ .*

*Proof* The Procedure PACKING ( $HBC(n), \{K_{1,3}, K_{1,2}\}$ ) gives a  $F$ -packing of  $HBC(n)$  with  $\lfloor \frac{6(n^2+2n+4)}{4} \rfloor - 4$  copies of  $K_{1,3}$  and six copies of  $K_{1,2}$ . Saturate the vertex of degree 3 in each  $K_{1,3}$  and the vertex of degree 2 in each  $K_{1,2}$ . See Fig. 7a. The saturated vertices of  $HBC(n)$  form a minimum dominating set of  $G$ . Therefore,  $\gamma(G) = \lceil \frac{6(n+1)^2+18}{4} \rceil + 1 = \lceil \frac{6(n^2+2n+4)}{4} \rceil + 1$ .  $\square$

### 3.3 Packing of hexabenzocoronene torus $HBCT(n)$ with $K_{1,3}$

Hexabenzocoronene torus ( $HBCT$ ) is a hypothetical torus-shaped network derived by properly connecting the nine pairs of peripheral carbon atoms of the hexabenzocoronene skeleton; See Fig. 6b. The interesting mathematical properties of the supersymmetry of  $HBCT$  are (a)  $C_6$  Rotational symmetry (b)  $C_7$  Rotational symmetry (c) Hamiltonian cycle and Heawood graph. This network is vertex-transitive as well as edge-transitive. In other words both the topcities of vertex and edge of  $HBCT$  are unity [14].

**Procedure PACKING** ( $HBCT(n), K_{1,3}$ )

**Input:** A hexabenzocoronene torus network  $G$  of dimension  $n$  and  $H \cong K_{1,3}$ .

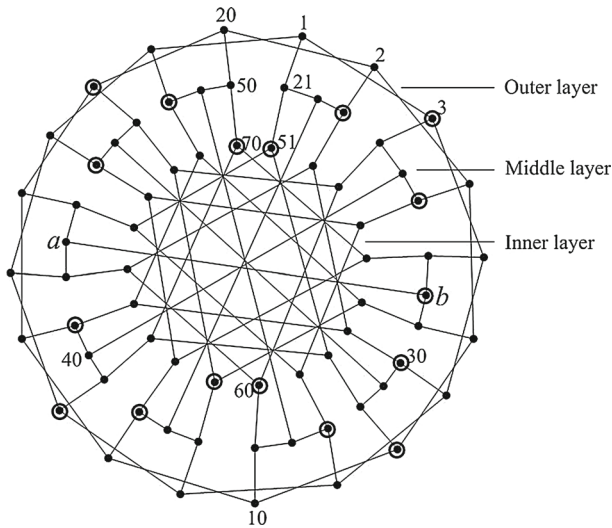
**Algorithm:**

(i) Invoke Procedure PACKING ( $HC(2(n - 1)), K_{1,3}$ ) [19]

(ii) Select  $K_{1,2}$  induced by the top vertices and two of its adjacent vertices.

End PACKING

**Output:** An  $H$ -packing of  $HBCT(n)$  with at most 10 unsaturated vertices.



**Fig. 8** Balaban 10-cage

*Proof of Correctness:* The copies of  $K_{1,3}$  selected by the procedure are disjoint and cover  $4 \times (\lfloor \frac{6(n^2+2n+4)}{4} \rfloor - 2) = 6(n^2 + 2n + 4) - 10$  vertices.

**Theorem 3.6** *If  $G$  is a hexabenzocoronene torus of dimension  $n$ , then  $\lceil \frac{6(n^2+2n+4)}{4} \rceil \leq \gamma(G) \leq \lceil \frac{6(n^2+2n+4)}{4} \rceil + 1$ .*

*Proof* The  $K_{1,3}$  selected in the algorithm Procedure PACKING ( $HBCT(n), K_{1,3}$ ) do not cover 10 vertices. Hence,  $\lceil \frac{6(n^2+2n+4)}{4} \rceil \leq \gamma(G) \leq \lceil \frac{6(n^2+2n+4)}{4} \rceil + 1$ .  $\square$

### 3.4 Packing of Balaban 10-cage graph with $K_{1,3}$

In the mathematical field of graph theory, the Balaban 10-cage or Balaban (3–10)-cage is a 3-regular graph and a bipartite graph with 70 vertices and 105 edges named after A. T. Balaban Published in 1972 [2]. It was the first (3–10)-cage discovered but is not unique. Cages and related graphs have found their applications in chemistry, e.g. in modelling chemical reactions and degenerate rearrangements [18]. The vertices of Balaban 10-cage graph are labelled as shown in Fig. 8.

**Procedure PACKING** (Balaban 10-cage,  $K_{1,3}$ )

**Input:** A Balaban 10-cage and  $H \cong K_{1,3}$ .

**Algorithm:**

- (i) Select the vertices 3,8,13,18 from the outer layer of Balaban 10-cage.
- (ii) Select the vertices 23,26,28,30,33,38,41,45,48 from the middle layer.
- (iii) Select the vertices 51,60,61,70 from the inner layer.

End PACKING

**Output:** An  $H$ -packing of Balaban 10-cage with at most two unsaturated vertices.

*Proof of Correctness:* The subgraph induced by the selected vertices is isomorphic to  $K_{1,3}$ . The copies of  $K_{1,3}$  selected by the procedure are disjoint and cover  $4 \times (4 + 9 + 4) - 2 = 70 - 2$  vertices. Therefore, the packing number  $\lambda = \lfloor \frac{70}{4} \rfloor = 17$ .

**Theorem 3.7** *If  $G$  is a Balaban 10-cage graph, then  $\gamma(G) = \lceil \frac{70}{4} \rceil = 18$ .*

*Proof* The Procedure PACKING (Balaban 10-cage,  $K_{1,3}$ ) gives a  $H$ -packing with at most two non adjacent unsaturated vertices. Since a vertex  $a = 43$  dominates the two non adjacent unsaturated vertices, the saturated vertices and the vertex  $a$  form a minimum dominating set of  $G$ . Therefore,  $\gamma(G) = \lceil \frac{70}{4} \rceil = 18$ .  $\square$

**Theorem 3.8** *If  $G$  is a Balaban 10-cage graph, then  $b(G) = 1$ .*

*Proof* Clearly a Balaban 10-cage graph has a  $H$ -packing with at most 2 unsaturated vertices by the Procedure PACKING (Balaban 10-cage,  $K_{1,3}$ ). Removal of an edge which is adjacent to  $a = 43$  and  $b = 28$  except an edge  $e = (a, b)$ , increases the domination number to 19. Hence,  $b(G) = 1$ .  $\square$

#### 4 Domination number of non-isomorphic chemical structures

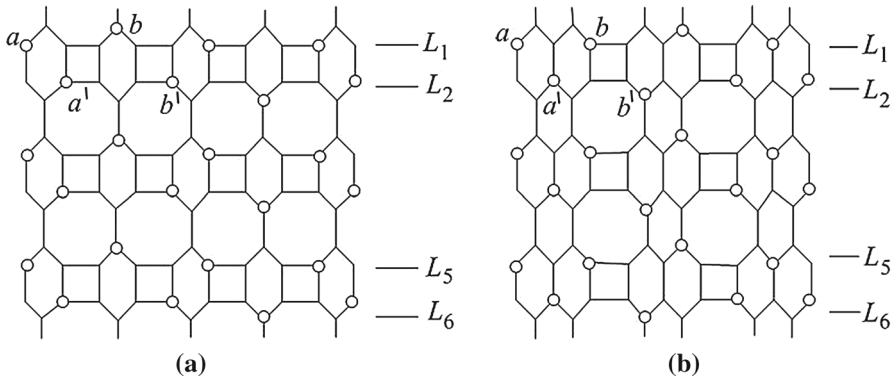
A nanotube is a tube-like structure having a diameter close to 1 nanometer. Carbon nanotubes are molecular cylinders that are rapidly extending our ability to fabricate nanoscale devices by providing molecular probes, pipes, wires, bearings and springs. They are the strongest and stiffest materials known and thus have many potential applications in various technologies.

A carbon nanotube is like a cylinder rolled up from a single sheet of graphite, whose atoms are arranged in hexagons. This type of structure can be used in many applications to improve the stability, efficiency and reliability of computing. Nanotechnology creates many new materials and devices with a wide range of applications in medicine, electronics, and computers. In this section we exhibit a domination number of two non-isomorphic graphs with same number of vertices namely  $H$ -Phenylenic nanotube and  $H$ -Naphthelenic nanotube.

$H$ -Phenylenic nanotubes  $HPH[p, q]$  are molecular graphs that are covered by  $C_6$ ,  $C_4$  and  $C_8$  [1]. In the  $H$ -Phenylenic  $HPH[p, q]$  nanotube,  $p$  represents the number of hexagons(rows) in each column and  $q$  represents the number of hexagons(columns) in each row. The number of vertices in  $H$ -Phenylenic  $HPH[p, q]$  nanotube is  $6pq$ . See Fig. 9a.  $H$ -Naphthalenic Nanotubes are obtained by the sequence  $C_6, C_6, C_4, C_6$  and  $C_6 \dots C_6, C_6, C_4, C_6, C_6$  and the repeat unit  $C_6, C_6, C_4$  [24]. See Fig. 9b.

**Theorem 4.1** *Let  $G$  be a  $HC_6C_4C_8(p, q)$  nanotube and  $q$ -odd. Then  $\gamma(G) = p(3q + 1)/2$ .*

*Proof* For each level  $i$  where  $i$  is odd, start at a vertex  $a$  as shown in Fig. 9a and call it saturated. Traversing through the level  $i(L_i)$  vertices choose the next vertex  $b$  at distance 4 from  $a$  and saturate it. For each level  $i$  where  $i$  is even, start at a vertex  $a'$  as shown in Fig. 9a and call it saturated. Traversing through the level  $i(L_i)$  vertices choose the next vertex  $b'$  at distance 4 from  $a'$  and saturate it. Continue the



**Fig. 9** *a* *H*-Phenylene nanotube, *b* *H*-Naphthalenic nanotube

process till all the levels are traversed. By Lemma 2.4, since all the vertices on graph  $G$  are dominated exactly once, the saturated vertices form a minimum dominating set. Therefore,  $\gamma(G) = p(3q + 1)/2$ .  $\square$

In the view of Theorem 4.1, we have the following result.

**Theorem 4.2** *Let  $G$  be a  $H$ -Naphthalenic nanotube. Then  $G$  has a minimum dominating set.*

It is easy to see that the *H*-Phenylene nanotube and *H*-Naphthalenic nanotube are non-isomorphic graphs with 90 vertices. But the domination number of each graphs is same.

**Theorem 4.3** *Let  $G$  be a  $H$ -Phenylene nanotube or  $H$ -Naphthalenic nanotube. Then  $b(G) = 1$ .*

*Proof* Clearly all the saturated vertices form a minimum dominating set of  $G$  by Theorem 4.1. Removal of an edge which is adjacent to saturated vertices, increases the domination number. Therefore,  $b(G) = 1$ .  $\square$

## 5 Concluding remarks

In this paper, we determine the domination number and bondage number of pyrene torus, hexabenzocoronene, Balaban 10-cage, *H*-Phenylene nanotube and *H*-Naphthalenic nanotube. The problem of finding the domination number, the total domination number and the total bondage number of Rectangular twisted torus and various chemical graphs are under investigation.

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## References

1. A. Bahrami, J. Yazdani, PI Index of  $H$ -phenylenic nanotubes and nanotori. *Dig. J. Nanomater. Biostruct.* **3**(4), 265–276 (2008)
2. A.T. Balaban, A trivalent graph of girth ten. *J. Combin. Theory Ser.* **12**, 1–5 (1972)
3. K. Balasubramanian, R. Ramaraj, Computer-generation of king and color polynomials of graphs and lattices and their applications to statistical mechanics. *J. Comput. Chem.* **6**(5), 447–454 (1985)
4. K. Balasubramanian, J.J. Kaufman, W.S. Koski, A.T. Balaban, Graph theoretical characterization and computer-generation of certain carcinogenic benzenoid hydrocarbons and identification of bay regions. *J. Comput. Chem.* **1**(2), 149–157 (1980)
5. E. Dobson, Packing almost stars into the complete graph. *J. Graph Theory* **10**, 169–172 (1997)
6. A. Felzenbaum, Packing lines in a hypercube. *Discret. Math.* **117**, 107–112 (1993)
7. J.F. Fink, M.S. Jacobson, L.F. Kinch, J. Roberts, The bondage number of a graph. *Discret. Math.* **86**, 47–57 (1990)
8. B.L. Hartnell, D.F. RaU, Bounds on the bondage number of a graph. *Discret. Math.* **128**, 173–177 (1994)
9. T.W. Haynes, S.T. Hedetniemi, P.J. Slater (eds.), *Fundamentals of Domination in Graphs* (Marcel Dekker Inc, New York, 1998)
10. T.W. Haynes, S.T. Hedetniemi, P.J. Slater (eds.), *Domination in Graphs: Advanced Topics* (Marcel Dekker, New York, 1998)
11. P. Hell, D. Kirkpatrick, On the complexity of a generalized matching problem, in *Proceedings of Tenth ACM Symposium On Theory of Computing* (1978), pp. 309–318
12. H. Hosoya, Clar's aromatic sextet and sextet polynomial. *Adv. Theory Benzenoid Hydrocarb. Top. Curr. Chem.* **153**, 255–272 (1990)
13. H. Hosoya, K. Balasubramanian, Exact dimer statistics and characteristic polynomials of cacti lattices. *Theor. Chim. Acta* **76**(5), 315–329 (1989)
14. H. Hosoya, Y. Tsukano, K. Nakada, S. Iwata, U. Nagashima, Supersymmetry of Hexabenzocoronene Torus. *CCACAA* **77**(1–2), 89–95 (2004)
15. F.-T. Hu, J.-M. Xu, On the complexity of the bondage and reinforcement problems. *J. Complexity* **28**(2), 192–201 (2012)
16. S. Majstorovic, T. Doslic, A. Klobucar,  $K$ -Domination on hexagonal cactus chains. *Kragujev. J. Math.* **36**(2), 335–347 (2012)
17. P. Manuel, M. Guizani, Broadcasting algorithms of carbon nanotubes, UNESCO-HP, Kuwait University
18. T. Pisanski, M. Boben, D. Marusic, A. Orbanic, A. Graovac, The 10-cages and derived configuration. *Discret. Math.* **275**(1–3), 265–276 (2004)
19. I. Rajasingh, A. Muthumalai, R. Bharathi, A.S. Shanthi, Packing in honeycomb networks. *J. Math. Chem.* **50**, 1200–1209 (2012)
20. R. Ramaraj, K. Balasubramanian, Computer-generation of matching polynomials of chemical graphs and lattices. *J. Comput. Chem.* **6**(2), 122–141 (1985)
21. Y.L. Wang, Note on the bondage number of a graph. *Discret. Math.* **159**, 291–294 (1994)
22. M. Yamuna, K. Karthika, Chemical formula: encryption using graph domination and molecular biology. *ChemTech* **5**(6), 2747–2756 (2013)
23. H.P. Yap, Packing of graphs—a survey. *Discret. Math.* **72**, 395–404 (1988)
24. J. Yazdani, A. Bahrami, Topological descriptors of  $H$ -naphthalenic nanotubes. *Dig. J. Nanomater. Biostruct.* **4**(1), 209–212 (2009)