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Saturation Number of Fullerene and Benzenoid Graphs

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Abstract

The saturation number of a graph G is the cardinality of any smallest maximal matching of G, and it is denoted by $S(G)$. Finding the saturation number of a graph is an NP-hard problem in general, but it is polynomial-time solvable for some special classes of graphs. For instance, it has been shown that the saturation number of a graph problem can be solved in linear time in trees. In this paper, we present a tight asymptotic bound on the saturation number of benzenoid parallelogram graph. Then we propose a mathematical model for determining the saturation number of a graph and analyze its efficacy on some fullerene and benzenoid graphs. Then by relaxation the mathematical model, we obtain a linear optimization model, that is a polynomial problem to find a lower bound for the saturation number of general graphs.

1 Introduction

Given a graph G, a matching M is a set of edges which are pairwise non-adjacent. If every vertex $v \in V$ is incident with an edge $e \in M$, we say that the matching M is perfect. A matching is said to be maximal if no other edge can be added to it while keeping the property of it being a matching. A matching M of G is maximum if $|M| \geq |N|$ for any other matching N in G. Vertices contained in edges of a matching are said to be saturated by this matching. A vertex which is not saturated by a matching is called exposed. The saturation number of a graph G is the cardinality of any smallest maximal matching of G, and it is denoted by $S(G)$.

Finding the saturation number of a graph is NP-hard in general. In [17], Yannakakis and Gavril show that the problem is NP-hard for several classes of graphs including bipartite (or

planar) graphs with maximum degree 3. In [10], Horton and Kilakos extended these results by showing the NP-hardness of the saturation number problem in planar bipartite graphs and planar cubic graphs.

On the other hand, polynomial time algorithms for the saturation number problem are designed for trees [13], for series-parallel graphs [14], for bipartite permutation graphs and cotrianglated graphs [16] and for clique-width bounded graphs [9].

The saturation number and its associated structure of a fullerene and benzenoid play a key role in molecular energy and stability [2].

In this paper, we propose a mathematical programming model for determining the saturation number of a graph. Then we obtain the saturation number of two class of chemically relevant graphs known as fullerene and benzenoid graphs by proposed model. In particular, we will give an explicit sharp bound on this quantity for some classes of benzenoid and related graphs.

This paper is organized as follows: First, we present a tight asymptotic bound on the saturation number of benzenoid parallelogram graph. Then we obtain the saturation number for three classes of benzenoid graphs by the mathematical model in section 3. Section 4 is devoted to obtaining the saturation number for some isomers of fullerenes by the mathematical model and finally, the conclusion part follows.

2 Saturation number of benzenoid graphs

A benzenoid system is a subset (with 1-connected interior) of a regular tiling of the plane by hexagonal tiles. To each benzenoid system, we can assign a graph, taking the vertices of hexagons as the vertices, and the sides of hexagons as the edges of the graph. The resulting simple, plane and bipartite graph is called a benzenoid graph [5].

All faces of a benzenoid graph except the unbounded one are hexagons. 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.

A benzenoid in a parallelogram-like shape called the benzenoid parallelogram and denoted by $P_{p,q}$, consists of $p \times q$ benzene rings, arranged in p rows, each row containing q benzene

rings, shifted by a half benzene ring to the right from the row immediately below. Clearly $P_{p,q}$ is the same as $P_{q,p}$, so $S(P_{p,q})$ is equal to $S(P_{q,p})$.

The saturation number of the benzenoid graph was studied by Došlić in [5], where the following bounds were established.

Theorem 1. [5] Let CB_h be a catacondensed benzenoid with h hexagons. Then

$$S(CB_h) \geq h + 2 .$$

Theorem 2. [5] Let B_h be a benzenoid chain on h hexagons. Then

$$h + 1 \leq S(B_h) \leq \left\lceil \frac{3h}{2} \right\rceil.$$

Theorem 3. [5] Let $P_{p,q}$ be a benzenoid parallelogram. Then

$$S(P_{p,q}) \leq \left\lceil \frac{2p+1}{3} \right\rceil q + p.$$

In what follows we construct maximal matching that provides an upper bound on the saturation number of benzenoid parallelograms for tightening the upper bound presented by Došlić in [5].

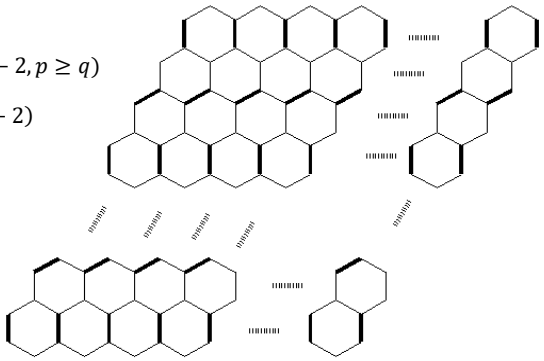
Theorem 4. Let $P_{p,q}$ be a benzenoid parallelogram and $k, k' \in \mathbb{N}$. Then

$$S(P_{p,q}) \leq \begin{cases} (2k-1)(q+1) & p = 3k-2, q = 3k'-2, p \geq q ; \\ (2k-1)(q+1) & p = 3k-2, q \neq 3k'-2 ; \\ 2k(q+1) & p = 3k-1, q \neq 3k'-2 ; \\ 2k(q+1)+q & p = 3k, q = 3k', p \geq q . \end{cases}$$

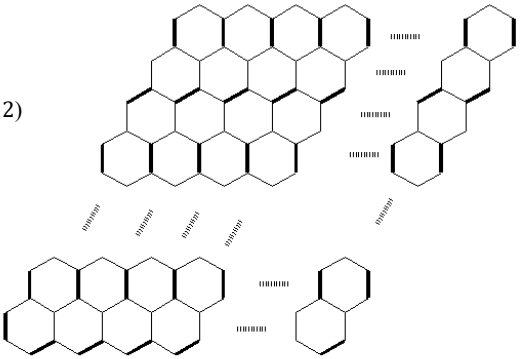
Proof.

If $(p = 3k-2, q = 3k'-2, p \geq q)$ or $(p = 3k-2, q \neq 3k'-2)$, since the matching M shown in bold in Figure 1.a is maximal, then $S(P_{p,q}) \leq (2k-1)(q+1)$. If $(p = 3k-1, q \neq 3k'-2)$, therefore $S(P_{p,q}) \leq 2k(q+1)$ (Figure 1.b). Similarly, if $(p = 3k , q = 3k')$, then $S(P_{p,q}) \leq 2k(q+1)+q$ (Figure 1.c).

a. $(p = 3k - 2, q = 3k' - 2, p \geq q)$
Or
$(p = 3k - 2, q \neq 3k' - 2)$



b. $(p = 3k - 1, q \neq 3k' - 2)$



c. $(p = 3k, q = 3k', p \geq q)$

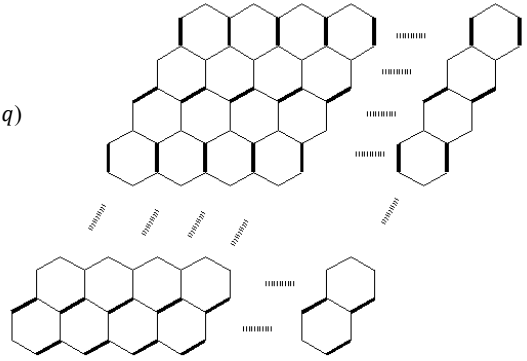


Figure 1. The upper bound on the saturation number and corresponding structure of $P_{p,q}$.

Conjecture 1. The upper bound presented in theorem 4, for $P_{p,q}$ with $(p = 3k-2, q = 3k'-2, p \geq q)$ or $(p = 3k-2, q \neq 3k'-2)$ that $k, k' \in \mathbb{N}$, is the saturation number of $P_{p,q}$, i.e.,

$$S(P_{p,q}) = (2k-1)(q+1).$$

Theorem 5. Our upper bound for the saturation of a benzenoid parallelogram in theorem 4 is sharper than the upper bound obtained by Došlić in [5].

Proof. Taking into account different values for p and q, proof is straightforward.

3 Mathematical programming formulation for finding the saturation number

In this section, we formally define the problem considered in this paper. Here we denote by $A_{n\times n}$ the adjacency matrix describing graph G. Let d_i degree of vertex i and for each edge (i,j), joining the vertices i and j, a binary variable x_{ij} is associated. Given a maximal matching as a set of edges, the x_{ij} in which participated take the value 1 and otherwise 0.

With respect to the above parameters and variables definition, the mathematical binary integer linear programming problem (BILP) for finding the saturation number of a graph would be as follows:

$$\text{Minimize} \sum_{(i,j)\in E} x_{ij} \tag{1}$$

Subject to

$$\sum_{(i,j)\in E} x_{ij} \leq 1 \qquad \forall i \in V \tag{2}$$

$$d_i \sum_{(i,j)\in E} x_{ij} + \sum_{(i,j)\in E,(k,j)\in E} x_{jk} \geq d_i \quad \forall i \in V \tag{3}$$

$$x_{ij} \in \{0,1\} \qquad \forall (i,j) \in E \tag{4}$$

Having in mind the definition of x_{ij}, constraints (2) ensures that no two edges of M have a vertex in common. Therefore, it is easy to see that edges of G satisfying the first group of constraints forms a matching of G. Constraints (3) guarantees that node i will not be covered by matching obtained by the constraints (2) if and only if each vertex adjacent to node i are covered by matching M. It is clear that constraints (2), (3) ensure that matching obtained by the constraints (2) is a maximal matching. The feasible solution space of the above

mathematical programming problem, determined by inequality constraints (2) and (3), is a set of all possible maximal matching of graph G.

The model proposed in this paper minimize the number of edges over all maximal matching of graph G. Considering the above stated, it is clear that the optimal value of the objective function is the saturation number of a graph.

Summarizing these results we have the following theorem.

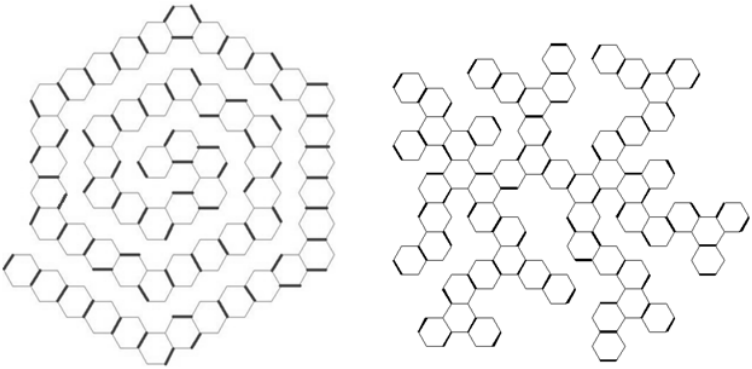
Theorem 6. There is a one-to-one correspondence between the saturation number as well as its associated maximal matching of graph G and the optimal objective value and optimal solution of the binary integer linear programming problem, respectively.

Since the degree of vertices in benzenoid graph is 2 or 3, to obtain the saturation number of benzenoid graph, the constraints (3) of the model presented becomes as follows:

$$3\sum_{(i,j)\in E} x_{ij} + \sum_{(i,j)\in E,(k,j)\in E} x_{jk} \geq 3 \qquad \forall i \in V \tag{5}$$

$$2\sum_{(i,j)\in E} x_{ij} + \sum_{(i,j)\in E,(k,j)\in E} x_{jk} \geq 2 \qquad \forall i \in V \tag{6}$$

We obtain the saturation number for three classes of benzenoid graphs by the mathematical model. For example, three structures of the benzenoid graph corresponding to its saturation number are illustrated in Figures 2 and 3.



a. $S(B_{57}) = 70$ b. $S(CB_{56}) = 71$

Figure 2. The saturation number and corresponding structures of B_{57}, CB_{56}

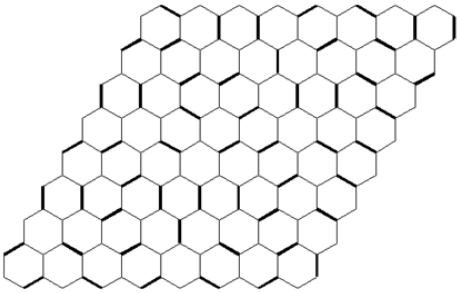


Figure 3. $S(P_{8,8}) = 53$

Although binary integer linear programming problem is an NP-hard problem in general, but by relaxation the mathematical model, we obtain a linear programming model as follows, that can also be solved in polynomial time and allows the computation of strong lower bounds for the saturation number problems.

$$\text{Minimize} \sum_{(i,j)\in E} x_{ij}$$

Subject to

$$\sum_{(i,j)\in E} x_{ij} \leq 1 \qquad \forall i \in V$$

$$d_i \sum_{(i,j)\in E} x_{ij} + \sum_{(i,j)\in E,(k,j)\in E} x_{jk} \geq d_i \qquad \forall i \in V$$

$$0 \leq x_{ij} \leq 1 \qquad \forall (i,j) \in E$$

4 Saturation number of a fullerene graph

A fullerene is a 3-regular plane graph consisting only of pentagonal and hexagonal faces. The vertices of the graph represent carbon atoms and edges represent chemical bonds between them. As a direct consequence of Euler's formula, every fullerene C_n has exactly 12 pentagons and $m = n/2 - 10$ hexagons [8]. It is well known that C_n exists for any even $n \geq 20$ except $n = 22$ [6]. For small n, a constructive enumeration of fullerene isomers with n vertices was given [7]. Fullerenes have wide application in various fields including electronic and optic engineering [7], medical science and biotechnology and have received a lot of recent chemists and mathematicians' attention [1, 11, 12,15].

The saturation number of fullerene graph was studied in [2, 3, 6, 8], where the following bounds were established.

Theorem 7. [8] Let G be a fullerene graph on p vertices. Then

$$\left\lceil \frac{p}{4} + 1 \right\rceil \leq S(G) \leq \frac{p}{2} - 2.$$

Theorem 8. [8] Let G be a d-regular graph. Then the size of any maximal matching in G is at most $\left(2 - \frac{1}{d}\right) S(G)$.

Theorem 9. [6] Let G be a fullerene graph on p vertices. Then

$$S(G) \geq \frac{3p}{10}$$

Theorem 10. [3] Let G be a fullerene graph on p vertices. Then

$$\frac{p}{3} - 2 \ \leq \ S(G) \leq \frac{p}{3} + O(\sqrt{p}).$$

Theorem 11. [4] Let G be a fullerene graph on p vertices. Then

$$s(G) \leq \frac{p}{2} - \frac{1}{4}(diam(G) - 2).$$

In particular,

$$s(G) \leq \frac{p}{2} - \frac{\sqrt{24p - 15} - 15}{24}.$$

Since the fullerene graph is a 3-regular graph, to obtain the saturation number of fullerene graph, the constraint (3) of the model presented in section3 becomes as follows:

$$3 \sum_{(i,j) \in E} x_{ij} + \sum_{(i,j) \in E, (k,j) \in E} x_{jk} \geq 3 \qquad \forall i \in V \tag{7}$$

We obtained the saturation number for all isomers of fullerenes $C_{20} - C_{80}$ and one isomer of each fullerene $C_{82} - C_{160}$, C_{180} and C_{192} from our model using CPLEX 12.6 under Matlab (R2013 a) on an Intel Pentium Core i2 CPU running at 2.2 GHz with 4 KB cache and 4 GB RAM under the Windows 7 operating system (64-bit). The results are reported in Table 1 and Table 2.

fullerene	Number of isomers	Max	Min	Average time (sec.)
C_{20}	1	6	6	0.030
C_{24}	1	8	8	0.031
C_{26}	1	9	9	0.031
C_{28}	2	9	9	0.048
C_{30}	3	10	10	0.031
C_{32}	6	11	10	0.047
C_{34}	6	11	11	0.068
C_{36}	15	12	11	0.046
C_{38}	17	13	12	0.136
C_{40}	40	13	12	0.098
C_{42}	45	14	13	0.106
C_{44}	89	15	14	0.158
C_{46}	116	15	14	0.126
C_{48}	199	16	15	0.176
C_{50}	271	17	15	0.166
C_{52}	437	17	16	0.150
C_{54}	580	18	17	0.181
C_{56}	924	18	18	0.173
C_{58}	1205	19	18	0.178
C_{60}	1812	20	18	0.177
C_{62}	2385	21	19	0.171
C_{64}	3465	21	20	0.174
C_{66}	4478	22	21	0.181
C_{68}	6332	23	21	0.181
C_{70}	8149	23	22	0.184
C_{72}	11190	24	22	0.190
C_{74}	14246	25	23	0.194
C_{76}	19151	25	24	0.200
C_{78}	24109	26	25	0.212
C_{80}	31924	27	25	0.197

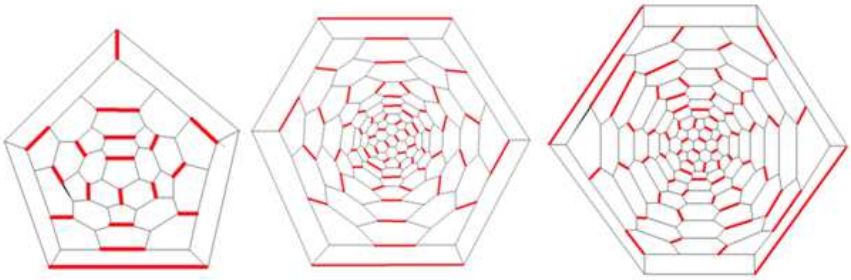
Table 1. The saturation number for fullerene isomers $C_{24} - C_{80}$.

In Table 1, column 'Min' is the minimum saturation number over all isomers of fullerene graph. Similarly, column 'Max' represents the maximum saturation number over all isomers of fullerene graph. Column 'average time' is average CPU time for computing the saturation number over all isomers of fullerene graph. Since there are too many isomers for each fullerene $C_n, n \geq 82$, we obtained the saturation number for one isomer of each fullerene $C_{82} - C_{160}$ and C_{180}, C_{192}. The results are illustrated in Table 2.

fullerene	Saturation number	CPU time
C_{82}	27	0.235
C_{84}	28	0.469
C_{86}	29	0.985
C_{88}	29	0.344
C_{90}	30	0.875
C_{92}	30	0.500
C_{94}	31	0.843
C_{96}	32	2.078
C_{98}	33	5.093
C_{100}	33	0.954
C_{102}	34	5.984
C_{104}	34	1.141
C_{106}	35	2.187
C_{108}	36	6.375
C_{110}	37	5.891
C_{112}	37	3.719
C_{114}	38	7.985
C_{116}	38	5.985
C_{118}	39	9.938
C_{120}	40	9.906
C_{122}	41	57.328
C_{124}	41	14.265
C_{126}	42	42.891
C_{128}	42	11.156
C_{130}	43	11.063
C_{132}	44	54.328
C_{134}	45	126.141
C_{136}	45	33.516
C_{138}	46	118.094
C_{140}	47	226.266
C_{142}	47	113.735
C_{144}	48	131.266
C_{146}	49	134.546
C_{148}	49	121.344
C_{150}	50	214.25
C_{152}	50	56.672
C_{154}	51	273.110
C_{156}	52	280.120
C_{158}	52	296.656
C_{160}	53	185.735
C_{180}	58	201.240
C_{192}	62	258.010

Table 2. The saturation number for some fullerene isomers $C_{82} - C_{160}$ and C_{180}, C_{192}

The saturation number and their corresponding structure for some isomers of fullerenes computed by solving our model are illustrated in Figure 4.



a. $S(C_{60}) = 18$ b. $S(C_{180}) = 58$ c. $S(C_{192}) = 62$

Figure 4. The saturation number and corresponding structures of C_{60}, C_{180} and C_{192}.

5 Conclusion

In this paper, we presented a tight asymptotic bound on the saturation number of benzenoid parallelogram graph and proposed a mathematical programming model for determining the saturation number of a graph. The results show that our mathematical model is able to find the saturation number of relatively large size instances of fullerene and benzenoid graphs.

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