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Saturation Number of Benzenoid Graphs

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Abstract

The saturation number of a graph is the cardinality of any smallest maximal matching in the graph. We present explicit results and tight asymptotic bounds on the saturation number of several classes of benzenoid graphs.

1 Introduction

Matching theory is a branch of graph theory concerned with study of structural and enumerative aspects of matchings, collections of edges of a graph that do not share a vertex. Its development has been strongly influenced and stimulated by chemical applications, in particular by the study of topological models of molecules representing conjugated compounds. A whole monograph [3] is devoted to the enumerative results on perfect matchings in just one class of chemically interesting graphs, the benzenoid graphs. Additional motivation came with discovery of fullerenes, again mostly concerning enumeration of perfect matchings [4, 5, 7, 10], but including also some structural results [2, 6]. This manuscript comes back to the roots, trying to elucidate some facts about structure of

large matchings in benzenoids. For a general background on matching theory and terminology we refer the reader to the classical monograph by Lovász and Plummer [8]; for graph theory terms not defined here we also recommend [9].

A **matching** M in a graph G is a collection of edges of G such that no two edges from M share a vertex. The cardinality of M is called the **size** of the matching. It is intuitively clear that matchings of small size are not interesting – each edge is a matching of size one, and the empty set is a matching of size 0. Hence, we will be interested in matchings that are, in a sense, "large", in fact, as large as possible.

A matching M is a **maximum matching** if there is no matching in G with greater size. The cardinality of any maximum matching in G is denoted by $\nu(G)$ and called the **matching number** of G. Since each vertex can be incident to at most one edge of a matching, it follows that no graph on n vertices can have matching number greater than $\lfloor n/2 \rfloor$. If each vertex of G is incident with an edge of M, the matching M is called **perfect**. Perfect matchings are obviously also maximum matchings. The study of perfect matchings, also known as **Kekulé structures** has a long history in both mathematical and chemical literature.

There is, however, another way to quantify the idea of "large" matchings. A matching M 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. Maximal matchings serve as models of adsorption of dimers to a substrate or a molecule; when that process is random, it is clear that the substrate can get "clogged" by a number of dimers way below the theoretical maximum. The cardinality of any smallest maximal matching in G is the **saturation number** of G. Hence, the saturation number provides an information on the worst possible case of clogging; it is a measure of how inefficient process of adsorption can be. The saturation number of a graph G we denote by $s(G)$. It is easy to see that the saturation number of a graph G is at least one half of the matching number of G, i.e., $s(G) \geq \nu(G)/2$.

Maximal matchings are much less researched that their maximum counterparts. That goes both for their structural and their enumerative aspects. The aim of this paper is to investigate the behavior of the saturation number of a class of chemically relevant graphs known as benzenoid graphs. In particular, we will give explicit formulas and/or sharp bounds on this quantity for several classes of benzenoid and related graphs.

2 Benzenoid chains

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**.

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; those two hexagons are called **terminal**, while any other hexagons are called **interior**. The number of hexagons in a benzenoid chain is called its **length**.

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**. (Note that the shared edges cannot be adjacent, since this would result in an internal vertex. Hence the above definitions cover all possible cases.)

If all $h-2$ interior hexagons of a benzenoid chain with h hexagons are straight, we call the chain a **polyacene** and denote it by A_h. If all interior hexagons are kinky, the chain is called a **polyphenacene** and denoted by Z_h. Since the number of perfect matchings in Z_h is equal to the $(h+2)$-nd Fibonacci number F_{h+2}, polyphenacenes are also known as **fibonacenes** [3].

In the rest of this section B_h denotes a generic benzenoid chain of length h.

Proposition 1

Let B_h be a benzenoid chain with h hexagons. Then $s(B_h) \geq h+1$.

Proof

The chain B_h has $4h+2$ vertices. Since B_h has a perfect matching, its matching number is equal to $2h+1$. Hence, $s(G) \geq (2h+1)/2$, and since it must be an integer, $s(G) \geq h+1$.

■

Proposition 2

$$s(B_h) + 1 \leq s(B_{h+1}) \leq s(B_h) + 2.$$

Proof

Let us suppose $s(B_{h+1}) \leq s(B_h)$ and let M be a maximal matching in B_{h+1} of cardinality $s(B_{h+1})$. Let us label the hexagons of B_{h+1} by $H_1, H_2, \ldots, H_{h+1}$. Then H_{h+1} must contain at least one edge of M such that neither of its end-vertices is shared with H_h. Let us denote that edge by $e = uv$. Now $M - e$ must be a maximal matching in $B_{h+1} \backslash e = B_{h+1} \backslash \{u, v\}$. If all edges of $M - e$ are also edges of B_h, we have a maximal matching in B_h of cardinality smaller than $s(B_h)$, a contradiction. Hence there must be an edge e' of $M - e$ with one end-vertex (say u') in B_h and another one (say v') in $B_{h+1} \backslash B_h$. Delete e'. If the rest is a maximal matching in B_h, we have a contradiction. If deleting of e' resulted in creating a pair of adjacent unsaturated vertices $\{u', w'\}$ in B_h by unsaturating u', extend $M - e - e'$ with $u'w'$. This is a maximal matching in B_h of cardinality smaller than $s(B_h)$, again a contradiction. Hence $s(B_{h+1}) > s(B_h)$, i.e., at least $s(B_{h+1}) \geq s(B_h) + 1$.

Hence $s(B_h)$ is a strictly increasing function of h. To establish the upper bound on the growth rate of $s(B_h)$, note that adding a hexagon to B_h means adding a path with 4 internal vertices with the end-vertices adjacent in B_h. Such a path can be always trivially saturated with 2 edges. ■

Proposition 3

$s(B_h) = h + 1$ if and only if $B_h = A_h$.

Proof

All vertical edges of A_h make a maximal matching; hence, $s(A_h) \leq h + 1$. Together with Proposition 1 this yields $s(A_h) = h + 1$.

An alternative proof can be obtained by assuming that $s(A_h) \leq h$. Then a maximal matching M of length $s(A_h)$ leaves at least $2h+2$ unsaturated vertices. By the pigeonhole principle, at least one hexagon H must contain three unsaturated vertices. Since M is maximal, no two of them can be adjacent. But then the remaining vertices must be saturated by three edges whose other ends are not in H. That would imply that H is a branching hexagon, contrary to the fact that A_h is a chain.

Let us prove the converse. Let $s(B_h) = h + 1$. There are $4h + 2$ vertices in B_h, and $2h + 2$ are saturated by a maximal matching M of cardinality $h + 1$. Then the remaining $2h$ vertices must be incident by $4h$ edges not in M. Since there are no vertices of degree one, each unsaturated vertex must be incident with exactly two edges not in M. Further, no hexagon can contain three unsaturated vertices. Hence each hexagon contains two

unsaturated vertices of degree 2 which are not adjacent. That is possible only in A_h. ■

Proposition 3 gives the explicit formula for A_h. Now we start exploring what happens when B_h contains kinky hexagons. The simplest case is when there is exactly one kinky hexagon. Let $B_{h,1}$ denote a chain of length $h = k + m$ in which hexagon H_k is kinky and all other hexagons are straight. An example is shown in Fig. 1.

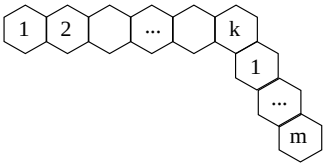

Figure 1: A chain with one kinky hexagon.

Proposition 4

$$s(B_{h,1}) = h + 2.$$

Proof

Chain $B_{h,1}$ has $k+m$ hexagons. The matching M that contains all $k+m-1$ shared edges, one edge in each terminal hexagon parallel with the shared edge, and one edge connecting the two vertices of degree 2 in the kinky hexagon is obviously maximal. Hence, $s(B_{h,1}) \leq k + m + 2$. On the other hand, by Proposition 3, $s(B_{h,1})$ must exceed $s(A_h) = k + m + 1$, i.e., $s(B_{h,1}) \geq k + m + 2 = h + 2$. ■

Hence one kinky hexagon means one more edge in the smallest maximal matching. This conclusion can be extended to the case of several kinky hexagons, as long as they are far enough. It turns out that far enough means not adjacent. The following result can be proved in a straightforward way using induction.

Proposition 5

Let $B_{h,k}$ be a benzenoid chain of length h with k kinky hexagons such that no two kinky hexagons are adjacent. Then $s(B_{h,k}) = h + k + 1$. ■

The following result shows that the above claim may remain valid even in case of adjacent kinky hexagons, as long as there are not too many of them.

Proposition 6

Let $S_{k,m}$ be a benzenoid chain shown in Fig. 2. Then $s(S_{k,m}) = k + m + 2$.

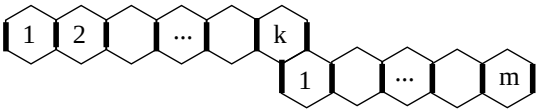

Figure 2: A chain with adjacent kinky hexagons.

Proof

Matching M shown by bold lines in Fig. 2 is obviously maximal, hence $s(S_{k,m}) \leq k+m+2$. On the other hand, by Proposition 3, we have $s(S_{k,m}) > k+m+1$, and the claim follows. ■

What happens when more than two kinky hexagons follow each other? A bit of experimenting shows that in some situation it still suffices to add just one new edge. It turns out, however, that every three consecutive kinky hexagons demand at least four new edges.

Proposition 7

Let Z_h be a fibonacene of length h. Then $s(Z_h) = \lfloor \frac{4h}{3} \rfloor + 1$.

Proof

According to Proposition 3, there is no maximal matching of cardinality 4 in Z_3. Hence any three consecutive kinky hexagons in a chain contribute at least 4 to its saturation number. On the other hand, it is easy to see that two consecutive kinky hexagons can always be added to B_h at a price of one edge each. That shows that three consecutive kinky hexagons do not require more that 4 new edges. The exact formula now follows by fitting the general form to the saturation numbers of short fibonacenes. ■

It follows that the saturation number of a benzenoid chain cannot exceed four thirds of its length by more than one.

3 Catacondensed benzenoids

Any catacondensed benzenoid CB_h that is not a chain must have at least one branching hexagon. Let us consider a case when there is exactly one branching hexagon H. Then the three branches of lengths h_i, $i = 1, 2, 3$, are rooted at three independent edges of H. Here we have $h = h_1 + h_2 + h_3 + 1$, i.e., the branching hexagon is not counted in the length of a branch. If we delete all vertices and incident edges of the branch of length h_3, the remaining benzenoid is a chain of length $h_1 + h_2 + 1$, and H is its kinky hexagon.

Hence, any maximal matching in it must contain at least $h_1 + h_2 + 3$ edges. No matter how we extend it to branch 3, we cannot do it by less than h_3 edges. Hence, any maximal matching in CB_h must contain at least $h_1 + h_2 + h_3 + 3 = h + 2$ edges.

Proposition 8

Let CB_h be a catacondensed benzenoid with h hexagons. Then $s(CB_h) \geq h + 2$. ■

Unlike the case of chains, the minimum value can be achieved by more than one graph, as can be seen from Fig. 3. In fact, it could be shown with some care that any catacondensed benzenoid on h hexagons whose saturation number is equal to $h+2$ could be obtained by appending polyacenic branches of appropriate lengths to one of the graphs from Fig. 3.

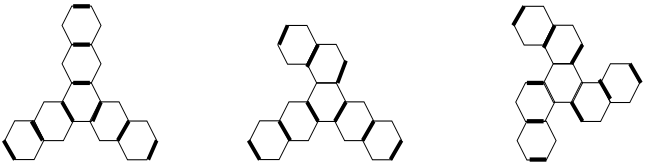

Figure 3: Catacondensed graphs on h hexagons with the saturation number equal to $h+2$.

4 Pericondensed benzenoids

Pericondensed benzenoids have internal vertices, and their number brings an additional structural parameter that must be accommodated. That makes it difficult to formulate and prove elegant results valid for all such graphs. Instead, we will concentrate on some special cases that can be illustrative for the whole class.

We start with benzenoid parallelograms. Take a configuration of $p \times q$ congruent regular hexagons arranged in p rows, each row of q hexagons, shifted for half a hexagon to the right from the row immediately below. An example is shown in Fig. 4. The arrangement is such that two hexagons either share a whole edge or are completely disjoint. To each such configuration we assign a graph by taking the vertices of hexagons as vertices of the graph, and the edges of hexagons as its edges. The resulting planar and bipartite graph is called a **benzenoid parallelogram** and denoted by $P_{p,q}$. It has pq hexagonal faces, $2(pq+p+q)$ vertices and $3pq+2p+2q-1$ edges. For $p = q$ we obtain a **benzenoid rhombus** P_p.

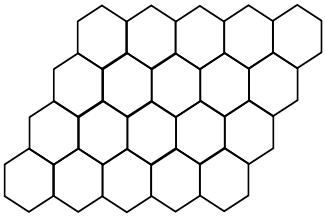

Figure 4: Benzenoid parallelogram $P_{4,5}$.

In what follows we construct maximal matchings that provide upper bounds on the saturation number of benzenoid parallelograms. The upper bounds will be asymptotically tight. With sufficient care they could be turned into exact expressions; however, we prefer to keep the exposition smooth.

Proposition 9

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

Proof

Let us start by considering $P_{1,q}$. Since it is nothing else than A_q, (Fig. 5 a)), we obtain $s(P_{1,q}) = q + 1$. By adding one row of q hexagons, we obtain $P_{2,q}$. Since the matching M

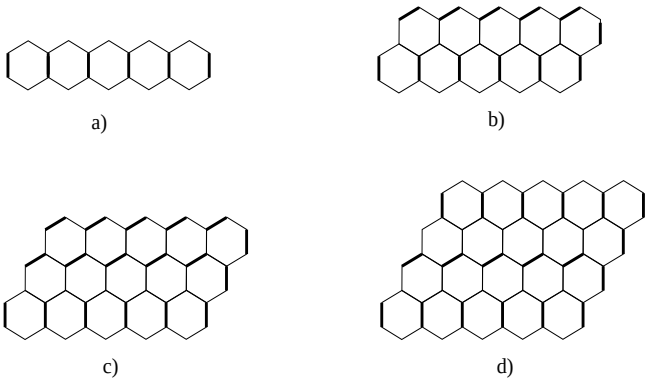

Figure 5: Adding rows of hexagons to $P_{p,q}$.

shown in bold in Fig. 5 b) is maximal, we have $s(P_{2,q}) \leq 2(q+1)$. Similarly, $s(P_{3,q}) \leq 3(q+1)$ (Fig 5 c)). However, the pattern breaks when we add the fourth row of q hexagons: Fig. 5 d) shows that it is possible to construct a maximal matching in $P_{4,q}$ at the expense on only one new edge. By continuing this process, it is clear that any addition of 3 rows

of hexagons requires roughly $2(q+1)+1$ additional edges. The expression of Proposition 9 now follows by fine-tuning the parameters p and q. ■

More interesting than the exact formulas is the asymptotic behavior of the saturation number. We can see that the saturation number of $P_{p,q}$ is of the order $\frac{2pq}{3}$, i.e., $s(P_{p,q}) \sim \frac{2}{3}h$, where h is the number of hexagons. Hence, for large enough pericondensed benzenoids the saturation number can be smaller than the number of hexagons. Further, for large p and q the fraction of external vertices tends to zero, and almost all vertices are shared by three hexagons. Hence, we see that there are maximal matchings covering no more than two thirds of the vertices. That makes our bounds asymptotically tight. Namely, that leaves on average 2 unsaturated vertices per hexagon, and a recent result by Andova *et al.* on nanotubes shows that we cannot do better than that (Proposition 3.1 of [2]).

We can similarly alternate between radial and non-radial edges in successive layers of hexagons to construct maximal matchings of size roughly $h/3$ in hexagonal patches such as shown in Fig. 6. Another way to obtain the result would be to split H_m to three rhombi

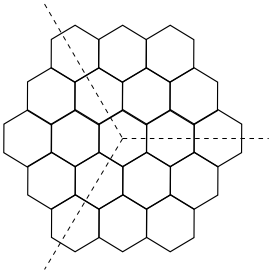

Figure 6: Hexagonal benzenoid H_3.

$P_{m-1,m-1}$ as indicated by dashed lines in Fig. 6 and to construct maximal matchings of size $\sim \frac{2}{3}m^2$ in each of them. Their union augmented by a matching of size at most linear in m will be a maximal matching in H_m of a size $\sim h/3$.

5 Concluding remarks

We have presented several results concerning the saturation number of various classes of benzenoid graphs. In particular, we have solved the problem for benzenoid chains and we have given asymptotically tight bounds for large pericondensed graphs, indicating thusly the behavior of the saturation number of graphene sheets. However, many questions still

remain open. For example, it would be interesting to investigate how the number of branching hexagons influences the saturation number of a catacondensed benzenoid. Further, there are other polymer-like graphs such as spiro-graphs and polyphenylenes whose saturation number is completely unexplored. Also, very little is known abut saturation numbers of polytopal graphs such as fullerenes; some recent progress is reported in [2], along with a conjecture that is worth exploring. A promising starting point could be a study of hexagonal nanocones with a single non-hexagonal defect at the apex [1]. Finally, it would be interesting to explore the saturation number of finite portions of various plane lattices and its asymptotic behavior.

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References

[1] Y. Alizadeh, M. Azari, T. Došlić, Computing the eccentricity–related invariants of single-defect carbon nanocones, *J. Comput. Theor. Nanosci.* **10** (2013) 1297–1300.

[2] V. Andova, F. Kardoš, R. Škrekovski, Sandwiching saturation number of fullerene graphs, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 501–518.

[3] S. J. Cyvin, I. Gutman, *Kekulé Structures in Benzenoid Hydrocarbons*, Springer, Berlin, 1988.

[4] T. Došlić, On lower bounds of number of perfect matchings in fullerene graphs,*J. Math. Chem.* **24** (1998) 359–364.

[5] T. Došlić, Fullerene graphs with exponentially many perfect matchings, *J. Math. Chem.* **41** (2007) 183–192.

[6] T. Došlić, Saturation number of fullerene graphs, *J. Math. Chem.* **43** (2008) 647–657.

[7] F. Kardoš, D. Král', J. Miškuf, J. S. Sereni, Fullerene graphs have exponentially many perfect matchings, *J. Math. Chem.* **46** (2009) 443–447.

[8] L. Lovász, M. D. Plummer, *Matching Theory*, North–Holland, Amsterdam, 1986.

[9] D. B. West, *Introduction to Graph Theory*, Prentice Hall, Upper Saddle River, 1996.

[10] H. Zhang, F. Zhang, New lower bounds on the number of perfect matchings of fullerene graphs, *J. Math. Chem.* **30** (2001) 343–347.