Automated Conjecturing VI: Domination Number of Benzenoids

L. Hutchinson, V. Kamat, C. E. Larson[1], S. Mehta, D. Muncy, N. Van Cleemput[2]

Department of Mathematics and Applied Mathematics
Virginia Commonwealth University
Richmond, VA 23284, USA
[2]*Department of Applied Mathematics, Computer Science and Statistics*
Ghent University
9000 Ghent, Belgium
[1]*Corresponding Author:* `clarson@vcu.edu`

Abstract

We demonstrate the use of a conjecturing program that can be a tool for researchers investigating bounds of invariants of chemical graphs by investigating upper bounds for the domination number of a benzenoid. The program is open-source, of general use, and can be used to generate conjectured bounds for *any* invariant of *any* class of chemical graphs.

1 Introduction

A *benzenoid* is a graph that represents the carbon structure of a benzenoid hydrocarbon molecule. Mathematically, it is the graph corresponding to any cycle in the infinite hexagonal lattice. (These graphs are variously called *benzenoid systems*, *polyhexs*, and *hexagonal systems*, among many others; see [1, 2, 3]). A *dominating set D* in a connected graph is a set of vertices such that all remaining vertices are each adjacent to at least one in D. The *domination number* of a graph is the cardinality of a minimum dominating set. The domination number of a general graph is a widely-studied NP-hard-to-compute graph invariant [4, 5].

Study of the domination number of a benzenoid is limited; formulas for specific classes of benzenoids may be found in [6, 7]. While minimum dominating sets and domination numbers in benzenoids have no apparent chemical relevance, chemically unmotivated graph invariants *can* have surprising chemical correlations: small order stable fullerenes, for instance, tend to minimize their graph theoretic independence number [8]—initially surprising—but an analogous fact was known to hold for benzenoids.

The results presented here all follow from conjectures of a computer program, CONJECTURING, developed by the third and sixth authors. The motivation of this research is to demonstrate the utility of this program in chemical graph theory. CONJECTURING can be used to generate conjectured bounds for *any* invariant of *any* class of chemical graphs; it is one more tool that mathematical chemists can use to help advance their research goals. This investigation of upper bounds of the domination number of a benzenoid is presented as a demonstration of what is possible.
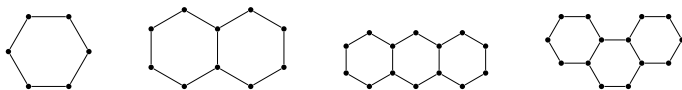

Table 1: Four small benzenoids: benzene, anthracene, naphthalene, phenanthrene

The program CONJECTURING produces invariant-relation conjectures and is based on a heuristic of Fajtlowicz [9]. This program and several experiments are described in [10]. The user of this program may input example objects of any type, choose invariants (numbers that can be computed from the objects, specified as functions) that may appear in the conjecture statements, choose a specific invariant that will appear on the left-hand side of the conjecture, and choose the form of the inequality: either upper bounds or lower bounds for the chosen invariant. The reported conjectures came from the domains of graph theory, matrix theory, number theory, and combinatorial game theory. CONJECTURING is open-source, and operates in Sage (a free and growing mathematical computing environment, similar to Maple, Matlab and Mathematica). The program, examples, and set-up instructions are available at: `http://nvcleemp.github.io/conjecturing/`

The program produces inequalities between algebraic relations of the input invariants (the expression generator is a descendant from Grinvin [11]). Here the objects are benzenoids. By the design of the program, each produced conjecture is "significant" with

respect to the previously produced conjectures—in the sense that each conjecture gives a better bound for one of the example benzenoids than any previously produced conjecture. This also implies that each newly produced conjecture is not implied by the previously produced conjectures. Furthermore, it means that the number of conjectures (of any particular form) cannot exceed the number of example benzenoids.

Figure 1: A sample run. Here is how a call to CONJECTURING looks to a user of the SageMathCloud interface. Some number of `invariants` and `objects` are defined and these are input as parameters to the `conjecture` function call.

CONJECTURING comprises an expression generator, code for evaluating expressions involving specified invariants and example objects, and uses Fajtlowicz's *Dalmatian* heuristic to conjecture relations between real number invariants of benzenoids. This Dalmatian heuristic comprises a truth-test and a significance test. The inequalities produced by the program are then checked if they are true for all examples that are provided to the program. This is the *truth test*. If a produced statement is false for an input benzenoid, the statement is rejected as a potential conjecture. Each statement is then tested for *significance* with respect to the input benzenoids and the database of previously produced conjectures. Informally, a statement is "significant" if it is not implied by the totality of previously made conjectures. By the design of the program, each produced conjecture is then "significant" with respect to the previously produced conjectures.

It is also possible to inform the program of existing "theory", or theoretical knowledge. The program is required to produce conjectures that are mathematically significant in a

precise sense: they will give better invariant value predictions for some objects than any known bounds will. This keeps the program both from repeating already-proved conjectures and from making conjectures that were implied by existing theory. See Fig. 2.

```
10  load("conjecturing.py")
11  load("objects_and_invariants.sage")
12
13  benzenoids = [napthalene, anthracene, phenanthrene, benz_5_face_ce, benzene, throwing_star, twi
    L14, twisted_strip3]
14
15  invariants = [domination_number, Graph.order, Graph.size, degree_2_vertices, degree_3_vertices,
    number_of_2_3_edges, internal_vertices, external_vertices, ratio_of_internal_to_external, numbe
    number_of_internal_3_3_edges, number_of_external_3_3_edges]
16
17  theory = [two_hexs, n_over_2_minus_1]
18
19  invariant = invariants.index(domination_number)
20
21  conjectures = conjecture(benzenoids, invariants, invariant, theory = theory)
22
23  for c in conjectures:
24      print c

    domination_number(x) <= degree_2_vertices(x) - hexagons(x)
    domination_number(x) <= maximum(number_of_3_3_edges(x), 1/2*degree_2_vertices(x))
    domination_number(x) <= number_of_3_3_edges(x) + 2
    domination_number(x) <= maximum(degree_3_vertices(x), sqrt(order(x)))

    antlers_show()
```

Figure 2: Here the `theory` variable is defined and contains two proved upper bounds for the domination number of a benzenoid: `two_hexs` and `n_over_2_minus_1`, representing Theorems 3.3 and 3.5 below. After telling the program about these known bounds, new conjectures must "improve" on these bounds—that is, a new conjecture must give a bound that is better for at least one input object than either of these bounds.

There are many useful programs available to chemical graph theorists. One that is included in Sage and that we made heavy use of in searching for counterexamples to conjectures is Brinkmann and Caporossi's benzenoid generator BENZENE [12]. A benzenoid embedding program derived from `CaGe` [13] is another useful package included in Sage.

2   Notation, Definitions, Basic Results

We use the following notation: a benzenoid B contains n vertices, m edges and h hexagons (hexagonal faces). The hexagons in B are denoted $H_1, \ldots, H_h$. For a face H_i, edge $e \in H_i$ is *shared* if it also belongs to another H_j, $j \neq i$; otherwise, the edge is *independent*. For a hexagon H in B, parallel (or antipodal) edges in H are *pairs*. If e is an edge in a hexagon H, the edge that forms a pair with e in hexagon H is denoted e'_H.

For a graph $G = (V, E)$, a set of vertices $S \subseteq V$ forms a *dominating set* if each vertex in the graph either belongs to S or is adjacent to some vertex in S. The *domination*

number $\gamma(G)$ of a graph G is the size of a smallest dominating set in G.

By definition benzenoids are *planar graphs*, that is, graphs which can be embedded in the plane. The *dual* of a planar graph G, denoted D_G, is constructed by having a vertex for every face in G and an edge between two vertices if and only if the two corresponding faces of G share an edge. We are interested in the *inner dual* of G, denoted I_G, which is the subgraph of D_G obtained by deleting the vertex representing the outer (unbounded) face of G. The vertices of the inner dual I_B of a benzenoid B benzenoid B are $\{v_1, \ldots, v_h\}$, where v_i is the vertex corresponding to hexagon H_i in B. A hexagon H_i is called a *leaf* if v_i has degree 1 in I_B.

A *catacondensed* benzenoid is a benzenoid whose inner dual is a *tree*, that is, a graph which is connected and acyclic. For a hexagon H in a catacondensed benzenoid B, at most three of its edges are shared. Call a hexagon H_i in B *branching* if either v_i has degree 3 in G_B or v_i has degree 2 and the two shared edges in H_i do not form a pair. We call the two types of branching hexagons 3-branching and 2-branching respectively. Let b and l denote the number of branching and leaf hexagons in B.

A catacondensed benzenoids whose inner dual is a *path* is a *snake*. A snake that has the additional property that there are *no* branching (2-branching, to be precise) hexagons is a *linear* benzenoid.

Observe that every vertex in a benzenoid B has degree two or three. For a benzenoid B, and $i, j \in \{2, 3\}$, let d_i be the number of vertices having degree i, let an (i, j)-edge be an edge adjacent to two vertices with degrees i and j respectively, and let e_{ij} be the number of (i, j)-edges. Similarly, let ex_{ij} denote the number of (i, j)-edges on the outer face of B; these are *exterior* edges. All other edges are *interior* edges. Vertices on the outer face are exterior vertices; the number of these is n_e. The number of interior vertices is n_i. The *perimeter* is the number of edges on the bounding face; which is also n_e.

The following useful relations between benzenoid invariants are recorded in Cyvin and Gutman's standard and extremely useful reference [1].

Theorem 2.1. *For any benzenoid,*

1. $n = 4h + 2 - n_i$

2. $m = 5h + 1 - n_i$

3. $m = n + h - 1$

4. $n_e = 4h + 2 - 2n_i$

5. $d_2 = 2h + 4 - n_i$

6. $d_3 = 2h - 2$

7. *internal vertices of degree two* $= 0$

8. *external vertices of degree two* $= 2h + 4 - n_i$

9. *internal vertices of degree three* $= n_i$

10. *external vertices of degree three* $= 2h - 2 - n_i$

11. *internal edges* $= h - 1 + n_i$

12. *internal (3, 3)-edges* $= h - 1 + n_i$

3   Results

Some of the following results have been recorded in the Master's thesis of the fifth author [14].

Many of our proofs use the notion of hexagon *removal*. We say that a hexagon H is removed from a benzenoid B when all vertices and edges that belong to H but to no other hexagon in B are removed from B—and denote the resulting graph by $B - H$. A hexagon H in a benzenoid B is *removable* if H has at least one external edge and the graph obtained by removing H is a benzenoid.

We will frequently make use of the following result.

Lemma 3.1. *Every benzenoid on $h \geq 2$ hexagons contains a removable hexagon having at least two vertices of degree* 2*. Every non-trivial benzenoid has at least two removable hexagons.*

Proof. The first claim follows directly from Corollary 2 of [15]. Many further sophisticated results than we require may be found in [16] (for instance, Lemma 6.3.25). But what we need is much more basic. It can easily be verified for all small benzenoids, so assume that

B is a benzenoid with at least 7 hexagons. Let H be an external hexagon that is not removable. Let B_1 and B_2 be components of $B - H$. B_1 and B_2 cannot share any edges, and are smaller benzenoids which must each have a removable hexagon not sharing an edge with H. These must be removable in B. ∎

Note that for smaller benzenoids the two removable hexagons may be adjacent, as they are in naphthalene.

All theorems here were conjectured by a conjecturing program. The iteration of conjectures led to the creation of counterexamples—new knowledge—that was added to the program as well as new invariants. This both imitates how human mathematical research works, but is sped up and systematized by the use of a computer assistant.

We first prove some general upper bounds for all benzenoids, before proceeding to prove stronger results for catacondensed benzenoids.

We begin with an observation.

Observation 3.2. Let B be a benzenoid, and let H be a removable hexagon of B containing $t \in \{2, 3, 4\}$ vertices of degree 2. If $t \in \{2, 3\}$, then we have $\gamma(B) \leq \gamma(B - H) + 1$. Otherwise we have that $\gamma(B) \leq \gamma(B - H) + 2$.

This observation easily follows from seeing that if t is two or three, those vertices can be dominated by a single vertex, and if t is four, those can be dominated by two vertices.

The following upper bound, in terms of the number of hexagons h, is also not difficult to see.

Theorem 3.3. *A benzenoid with h hexagons has $\gamma \leq 2h$.*

Proof. It is easy to note that for any hexagon H, picking a pair of antipodal vertices dominates all vertices of that hexagon. For each $1 \leq i \leq h$, let $P_i = \{a_i, b_i\}$ be any arbitrarily chosen pair of antipodal vertices from hexagon H_i Let $D = \cup_{i \in [h]} P_i$. Clearly, D is a dominating set for benzenoid B. As $|D| \leq 2h$, the bound follows. ∎

We will now prove a useful lemma on the structure of minimal dominating sets in certain benzenoids. The lemma will be used in the proof of the following theorem, and then extensively to prove results on catacondensed benzenoids.

Lemma 3.4. *Let H be a leaf hexagon in a benzenoid B, and let e be its shared edge. Then B has a minimum dominating set S that contains a vertex from e'_H.*

Proof. Let H be a leaf hexagon in a benzenoid B. Let $\{v_1, \ldots, v_6\}$ be the vertices of the hexagon, and let $\{v_1v_2, v_2v_3, v_3v_4, v_4v_5, v_5v_6, v_6v_1\}$ (with $v_iv_j = \{v, v_j\}$) be the set of edges in H. Without loss of generality, let v_1v_2 be the shared edge of H, and let $e'_H = v_4v_5$. We will construct a minimum dominating set that contains either v_4 or v_5. Let S be a mininum dominating set that contains neither. This implies that $\{v_3, v_6\} \in S$. So the set $S' = S \setminus \{v_3, v_6\} \cup \{v_1, v_4\}$ is a minimum dominating set containing v_4. ∎

Theorem 3.5. *For any benzenoid, $\gamma \leq \frac{n}{2} - 1$.*

After the program conjectured this and we found a proof, we then added the result to the "theory" of the program. We omit the proof as the program then made the following conjecture which implies and supersedes it. Benzenoids are connected bipartite graphs. In chemistry this concept for benzenoids is often referred to as alternant, and the different partite sets are referred to as starred/non-starred sites. Since either of the partite sets is a dominating set, then the cardinality of the smaller of these must also be a dominating set. Let sp be the cardinality of a the smaller partite set. It follows immediately that $\gamma \leq sp$ for benzenoids. And in fact this can give a great improvement over the $\frac{n}{2}$ bound: the difference between the smaller and larger partite sets can be arbitrarily large. In [1] Cyvin and Gutman showed that the difference between the cardinalities of these sets in a benzenoid is the same as the difference between the number of *peaks* and the number of *valleys*. In the triangular-shaped benzenoids (*triangulenes*) the number of peaks is exactly one, while the number of valleys grows with the number of "layers" of the triangulene (see Fig. 3).

In fact the program made a slightly better conjecture.

Theorem 3.6. *For any benzenoid, $\gamma \leq sp - 1$.*

Proof. Let B be a benzenoid. We denote by $\mathcal{B}_s(B)$, respectively $\mathcal{B}_l(B)$, the smaller, respectively larger, bipartite set of B. If the two sets have the same size, we choose $\mathcal{B}_s(B)$ and $\mathcal{B}_l(B)$ arbitrarily, but distinct.

The claim can easily be checked for benzenoids with one or two hexagons. Let B' be a benzenoid with at least three hexagons. We assume the claim is true for benzenoids
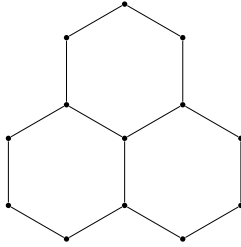
Figure 3: A triangulene with two layers, one peak and two valleys.

with fewer hexagons than B'. Let H be a removable hexagon in B', and let $B = B - H$. Below we several times use Observation 3.2 to get the relation between $\gamma(B')$ and $\gamma(B)$.

First, suppose that H has two degree-2 vertices. Since H has only two degree-2 vertices, they must be adjacent. As the vertices are adjacent, each one belongs to a separate bipartite set. Notice that $|\mathcal{B}_s(B)| = |\mathcal{B}_s(B')| - 1$ and $|\mathcal{B}_l(B)| = |\mathcal{B}_l(B')| - 1$. By assumption, $\gamma(B) \leq |\mathcal{B}_s(B)| - 1$. It must be that

$$\gamma(B') \leq \gamma(B) + 1 \leq (|\mathcal{B}_s(B)| - 1) + 1 = |\mathcal{B}_s(B)| = |\mathcal{B}_s(B')| - 1.$$

Now suppose the case that H has four degree-2 vertices. This case is very similar to the first one. It must be that removing H removes two vertices from each bipartite set. Then $|\mathcal{B}_s(B)| = |\mathcal{B}_s(B')| - 2$ and $|\mathcal{B}_l(B)| = |\mathcal{B}_l(B')| - 2$. By assumption $\gamma(B) \leq |\mathcal{B}_s(B)| - 1$. Observe that

$$\gamma(B') \leq \gamma(B) + 2 \leq (|\mathcal{B}_s(B)| - 1) + 2 = |\mathcal{B}_s(B')| - 1.$$

Consider the final case where H has three degree-2 vertices. In the first subcase, only one of the three vertices that we remove from B' are in $\mathcal{B}_s(B')$. Then $|\mathcal{B}_s(B)| = |\mathcal{B}_s(B')| - 1$ (even if the larger partition becomes the smaller one after this removal) and

$$\gamma(B') \leq \gamma(B) + 1 \leq (|\mathcal{B}_s(B)| - 1) + 1 = |\mathcal{B}_s(B')| - 1.$$

In the second subcase, two of the three vertices we remove from B' are in $\mathcal{B}_s(B')$. Note that we are also in this situation if both partitions of B' have the same size. Notice that $|\mathcal{B}_s(B)| = |\mathcal{B}_s(B')| - 2$ and

$$\gamma(B') \leq \gamma(B) + 1 \leq (|\mathcal{B}_s(B)| - 1) + 1 = |\mathcal{B}_s(B')| - 2 \leq |\mathcal{B}_s(B')| - 1.$$

It follows by induction that $\gamma(B) \leq |\mathcal{B}_s(B)| - 1 = sp - 1$. ∎

Theorem 3.7. *For any benzenoid,* $\gamma \leq e_{33} + 2$.

Proof. Let B be a benzenoid. We proceed by induction on the number of hexagons h. The statement is trivial for $h = 1$ (where $e_{33} = 0$ and $\gamma = 2$) and $h = 2$ (where $e_{33} = 1$ and $\gamma = 3$), so suppose B has at least 2 hexagons. Using Lemma 3.1, we know that B contains a removable hexagon, say H, containing $2 \leq t \leq 4$ degree-2 vertices. If $t \in \{2, 3\}$, then the induction proceeds easily as Observation 3.2 gives us that $\gamma(B) \leq \gamma(B - H) + 1$, and by removing H we destroy at least two (3,3)-edges, so $e_{33}(B - H) \leq e_{33}(B) - 2$. Combining everything and using the induction hypothesis, we get

$$\gamma(B) \leq \gamma(B - H) + 1 \leq (e_{33}(B - H) + 2) + 1 \leq e_{33}(B) + 1.$$

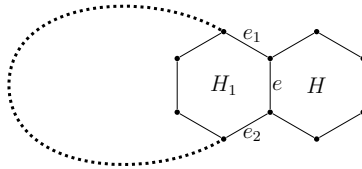So now we assume that $t = 4$, and we use the naming conventions as shown in Figure 4.

Figure 4: A removable hexagon H with 4 vertices of degree 2.

Suppose first that either e_1 or e_2 is a (3,3)-edge. In this instance, we have $e_{33}(B - H) \leq e_{33}(B) - 2$ as e and at least one of e_1 and e_2 are no longer (3,3)-edges in $B - H$. Combining this with Observation 3.2 and the induction hypothesis, we get

$$\gamma(B) \leq \gamma(B - H) + 2 \leq (e_{33}(B - H) + 2) + 2 \leq e_{33}(B) + 2.$$

Finally we assume that neither e_1 nor e_2 is a (3,3)-edge. This implies that H_1 is a leaf hexagon in $B - H$, and so Lemma 3.4 gives us that $\gamma(B) \leq \gamma(B - H) + 1$.

The edge e is no longer a (3,3)-edge in $B - H$, so $e_{33}(B - H) = e_{33}(B) - 1$. Combining this with the induction hypothesis, we get

$$\gamma(B) \leq \gamma(B - H) + 1 \leq (e_{33}(B - H) + 2) + 1 \leq (e_{33}(B) + 1) + 1 \leq e_{33}(B) + 2.$$

∎

We now prove several upper bounds for the domination number of catacondensed benzenoids. First we state and prove some observations and a technical lemma that we use in the proof of the theorems.

Observation 3.8. Every tree T is either a path or contains a vertex of degree at least 3.

Lemma 3.9. *For a tree T on n vertices, there exists a leaf such that its neighbor either has degree two, or is adjacent to another leaf.*

Proof. Consider a tree T and suppose P is a maximum length path in this tree. Let u and v be the endpoints of this path. Consider v, which is clearly a leaf as the path is maximal. Let x be its neighbor which also lies on P. If x does not have degree 2, then it is adjacent to another vertex, say w, which is not in P. Clearly w must be a leaf, otherwise we can extend the path between u and w to obtain one longer than P, which contradicts the maximality of P. ∎

Finally, we make some observations on the number of vertices and edges in catacondensed benzenoids in terms of the number of hexagons. These follow immediately from Theorem 1, together with the observation that catacondensed benzenoids have no internal vertices and $n_i = 0$.

Observation 3.10. A catacondensed benzenoid with n vertices, m edges and h hexagons has $n = 4h + 2$ and $m = 5h + 1$.

Theorem 3.11. *For any catacondensed benzenoid, $\gamma \leq \frac{n}{3}$.*

Proof. The statement can easily be verified for catacondensed benzenoids with $h \leq 3$. Let B be a benzenoid with $h > 3$. Following Observation 3.8 there are two cases to consider.

If the inner dual I_B is a path $v_1 - v_2 - \ldots - v_h$, we let B_3 be the subgraph of B formed by the hexagon H_1, H_2, H_3 corresponding to vertices v_1, v_2, v_3. Let e_3 be the unique shared edge of H_3 that also belongs to H_4. Let B' be the benzenoid obtained from B by deleting every vertex in B_3 except the two endpoints of e_3. It follows from the induction hypothesis that $\gamma(B') \leq \frac{n-12}{3}$ and $\gamma(B_3) \leq 4$. We find that $\gamma(B) \leq \gamma(B') + \gamma(B_3) \leq \frac{n-12}{3} + 4 = \frac{n}{3}$.

If the inner dual I_B is not a path, and thus contains a 3-branching vertex v, let H be the corresponding hexagon. Let e and f be any two shared edges in H; and note that they cannot contain a common vertex. Let e_1, e_2, e_3 be the three independent edges in H,

and f_1, f_2, f_3 be the three shared edges. Let G be the graph obtained by removing edges e_1, e_2, e_3 from B. G is a disjoint union of three benzenoids, say B_1, B_2, B_3 (containing edges f_1, f_2, f_3 respectively), each of which necessarily contains fewer hexagons than B. Moreover, $\gamma(B) \leq \sum_{i=1}^{3} \gamma(B_i)$. Let $|B_i| = n_i$. The induction hypothesis implies that $\gamma(B_i) \leq \frac{n_i}{3}$. This implies that $\gamma(B) \leq \sum_{i=1}^{3} \frac{n_i}{3} = \frac{n}{3}$. ∎

Theorem 3.12. *For any catacondensed benzenoid, $\gamma \leq \frac{m}{2} - h$.*

Proof. First, using Observation 3.10, we have that $m/2 - h = (3h+1)/2$. Also, for $h \geq 1$, it is easy to verify that $(4h + 2)/3 \leq (3h + 1)/2$. Thus, using Theorem 3.11, we get $\gamma \leq m/2 - h$. ∎

4   Conjectures & Open Problems

As conjectures are the lifeblood of mathematics, we conclude with a selection of some of the conjectures that we worked on and tested but could not solve. We hope they are of interest to the reader.

We proved above that for catacondensed benzenoids, $\gamma \leq m/2 - h$. In fact, this conjecture appears regularly in the general (non-catacondensed) case. Despite our best efforts, publicizing it, and even offering a \$10 prize for its resolution, it has not been resolved. We can prove it for certain well-structured benzenoids. It is true for linear chains, triangulenes, and the family of graphs derived from coronene by successively adding an extra ring of hexagons (these include circumcoronene and circum-circumcoronene). But our ideas do not apply to less structured cases, and exhaustive computer search of relatively small examples did not produce a counterexample.

These conjectures below are presented in the form they were output by the CONJECTURING program—except `domination_number` was replaced with the symbol γ in order to fit the conjectures on single lines.

This first list of conjectures should be interpreted as applying to catacondensed benzenoids. The invariants here include numbers of coves, bays, fissures, and fjords—topological features of the benzenoid boundary which happened to be easy to code, and will be familiar to all readers of [1].

1. $\gamma(x)$ <= `number_of_2_3_edges(x)` + 2

2. `γ(x) <= size(x)/coves(x)`

3. `γ(x) <= maximum(degree_3_vertices(x), sqrt(order(x)))`

4. `γ(x) <= maximum(degree_3_vertices(x), hexagons(x)+1)`

5. `γ(x) <= bays(x) + 1/2*degree_2_vertices(x)`

6. `γ(x) <= maximum(hexagons(x), number_of_3_3_edges(x))+1`

 The remaining conjectures should be interpreted for *all* benzenoids.

1. `γ(x) <= hexagons(x)+number_of_external_3_3_edges(x)+1`

2. `γ(x) <= 1/2*number_of_2_2_edges(x)+`
           `number_of_internal_3_3_edges(x)-1`

3. `γ(x) <= -number_of_external_3_3_edges(x) + 1/2*size(x)`

4. `γ(x) <= 1/2*degree_2_vertices(x) +`
           `2*number_of_2_3_edges(x)`

5. `γ(x) <= maximum(hexagons(x), number_of_2_3_edges(x))+1`

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