Maximum Nullity for Benzenoids

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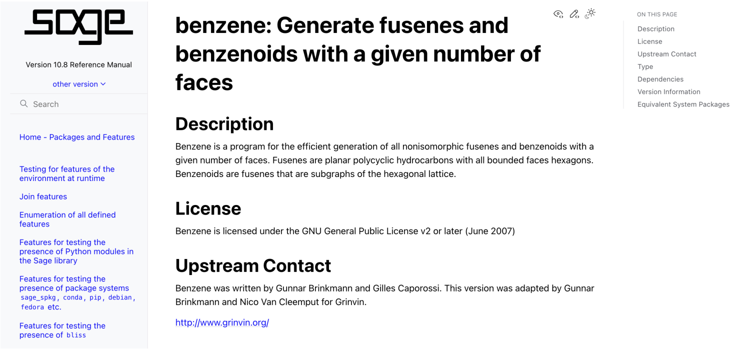
Computers in Scientific Discovery

1. `Sage` (or `SageMath`)

2. `benzene` (Brinkmann & Caporossi, 2007) for fast, complete generation of benzenoids

3. `Conjecturing` (L. & Van Cleemput, 2016)

Ghent Combinatorial Structure Generation



Version 10.8 Reference Manual

other version

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Testing for features of the environment at runtime

Join features

Enumeration of all defined features

Features for testing the presence of Python modules in the Sage library

Features for testing the presence of package systems `sage_spkg`, `conda`, `pip`, `debian`, `fedora` etc.

Features for testing the presence of `bliss`

benzene: Generate fusenes and benzenoids with a given number of faces

Description

Benzene is a program for the efficient generation of all nonisomorphic fusenes and benzenoids with a given number of faces. Fusenes are planar polycyclic hydrocarbons with all bounded faces hexagons. Benzenoids are fusenes that are subgraphs of the hexagonal lattice.

License

Benzene is licensed under the GNU General Public License v2 or later (June 2007)

Upstream Contact

Benzene was written by Gunnar Brinkmann and Gilles Caporossi. This version was adapted by Gunnar Brinkmann and Nico Van Cleemput for Grinvin.

http://www.grinvin.org/

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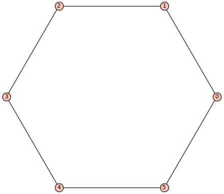
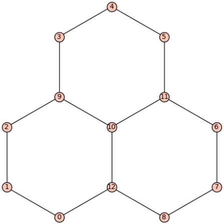
Ghent Combinatorial Structure Generation

Patrick's Question

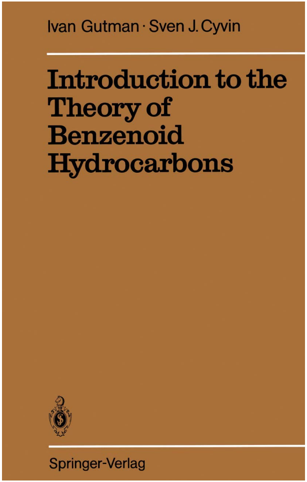
Which benzenoids with h hexagonal faces have maximum nullity η?





Benzene has $\eta = 0$, Phenalene has $\eta = 1$.

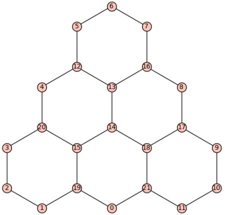
Gutman & Cyvin, 1989

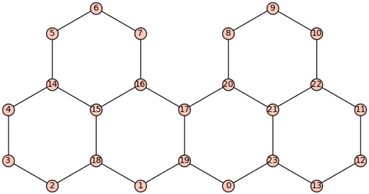


Facts about Benzenoids

1. Bounded region of the hexagonal lattice.
2. Bipartite.
3. Pairing theorem implies that if λ is an eigenvalue then $-\lambda$ is an eigenvalue.
4. Any with odd order have a 0 eigenvalue ($\eta > 0$).
5. Kőnig-Egerváry Theorem implies independence number α plus the matching number μ equals the order n ($\alpha + \mu = n$).

Even-order Benzenoids can have $\eta > 0$

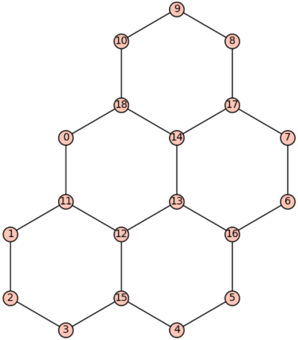




Triangulene with odd order and $\eta = 1$,

Two fused phenalenes with even order and $\eta = 2$.

Computer Search for more Examples



$n = 18,\ h = 5,\ \eta = 1.$

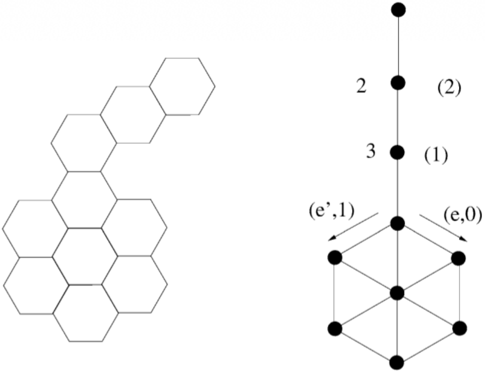
Computer Search for more Examples

G. Brinkmann et al. / Journal of Algorithms 45 (2002) 155–166 165

Table 1

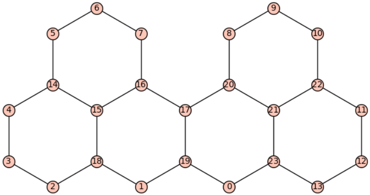
Hexagons	Fusenes	Benzenoids	Inner duals	Inner duals with trivial group
1	1	1	1	1
2	1	1	1	0
3	3	3	2	0
4	7	7	4	0
5	22	22	8	0
6	82	81	21	5
7	339	331	53	22
8	1 505	1 435	151	90
9	7 036	6 505	458	342
10	33 836	30 086	1 477	1 247
11	166 246	141 229	4 918	4 491
12	829 987	669 584	16 956	16 095
13	4 197 273	3 198 256	59 494	57 906
14	21 456 444	15 367 577	212 364	209 170
15	110 716 585	74 207 910	766 753	760 830
16	576 027 737	359 863 778	2 796 876	2 784 913
17	3 018 986 040	1 751 594 643	10 284 793	10 262 649
18	15 927 330 105	8 553 649 747	38 096 072	38 051 063
19	84 530 870 455	41 892 642 772	141 998 218	141 914 613
20	451 069 339 063	205 714 411 986	532 301 941	532 131 882
21	2 418 927 725 532	1 012 565 172 403	2 005 638 293	2 005 320 952
22	13 030 938 290 472	4 994 807 695 197	7 592 441 954	7 591 794 561
23	70 492 771 581 350	24 687 124 900 540	28 865 031 086	28 863 820 538
24	382 816 374 644 336	122 238 208 783 203	110 174 528 925	110 172 051 829
25	2 086 362 209 298 079		422 064 799 013	422 060 152 511
26	11 408 580 755 666 756		1 622 379 252 093	1 622 369 728 951

Inner Duals



A Conjecture

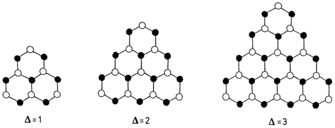
Patrick's idea: edge fusions of phenalenes and triangulenes might maximize nullity for a given number of hexagons.



What can we prove?

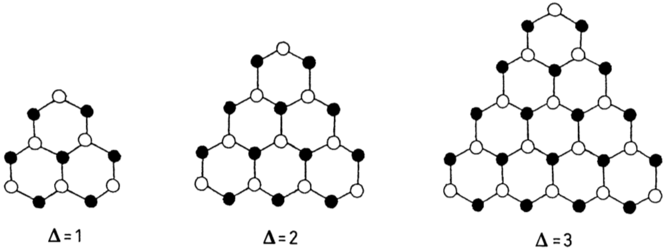
A Formula for Nullity

Fajtlowicz, John and Sachs (2005) proved that $\eta = \alpha - \mu$, where α is the independence number and μ is the matching number.



The black vertices are a maximum independent set.

Color Excess



Let the partite sets be B and W (assume $|B| \geq |W|$). The color excess is $\Delta = |B| - |W|$.

Color Excess

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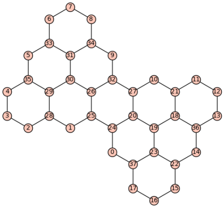
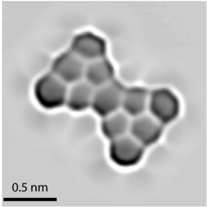
If $|B| > |W|$ there can't be a perfect matching. The Kőnig-Egerváry Theorem implies $\alpha > \mu$ and $\alpha - \mu > 0$.

So, Δ is related to nullity η ($\Delta > 0$ implies $\eta > 0$).





(Fasel, Empa, 2019). But some benzenoids have $\Delta = 0$ and $\eta = \alpha - \mu > 0$.

Color Excess

Brunvoll, Cyvin, and Gutman (1988) proved that $\Delta \leq \lfloor \frac{h}{3} \rfloor$, where h is the number of hexagons.

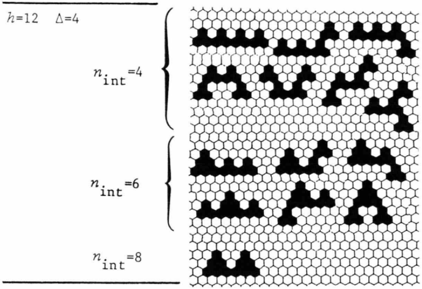


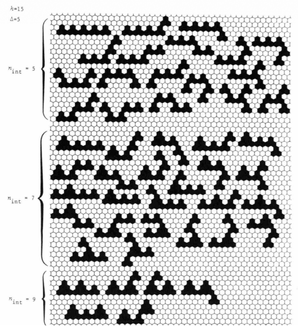
Fig. 8. Benzenoid systems with $\Delta = \Delta_{\max}$ for $h = 12$, classified according to their numbers of internal vertices (n_{int}).

They define the class of TP benzenoids.

And prove for these graphs $\Delta = \lfloor \frac{h}{3} \rfloor$.

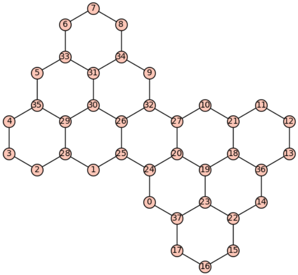
Color Excess

Brunvoll, Cyvin, and Gutman proved that $\Delta \leq \lfloor \frac{h}{3} \rfloor$, where h is the number of hexagons.



Patrick's intuition was that these should be the nullity-maximizing benzenoids. Computational experiments confirmed this.

Color Excess vs. Nullity



But $\Delta \neq \eta$ in general: this example has $\Delta = 0$, and $\eta = 2$.

So what can be said?

Color Excess vs. Nullity

For any bipartite graph with bipartition (B, W) ($|B| \geq |W|$), we have

$$\alpha \geq |B| \geq |W| \geq \mu.$$

So,

$$\eta = \alpha - \mu \geq |B| - |W| = \Delta.$$

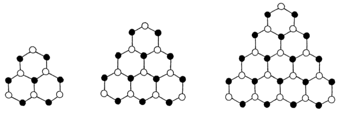
Color Excess vs. Nullity

If we can prove,

$$\Delta \leq \eta = \alpha - \mu \leq \lfloor \frac{h}{3} \rfloor.$$

for any benzenoid, then we'd have the class of TP graphs are in fact nullity-maximizing.

Nullity of TP Benzenoids

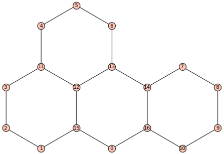


1. The triangulenes T_k (including phenalene and triangulene) have unique maximum independent sets and can be fused to maintain this property (Pepper, 2008).

2. Let TP_3 and TP_6 be TP benzenoids with 3 or 6 hexagons. These have unique maximum independent sets and $\alpha - \mu = \frac{h}{3}$.

3. Let TP_{3k} be the TP benzenoids which are 2-2 edge fusions of TP_{3r} and TP_{3s} $(3r + 3s = 3k)$. These have unique maximum independent sets and $\alpha - \mu = \frac{h}{3}$.

Nullity of TP-1 Benzenoids



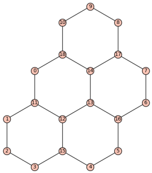
1. A TP-1 benzenoid G is a benzenoid formed by the 2-2 edge fusion of benzene H to a TP benzenoid $G - H$ (in the inner dual this will be a pendant vertex).

2. These have unique independent sets.

3. $\eta = \alpha - \mu$ remains unchanged.

4. $\alpha(G) - \mu(G) = \alpha(G - H) - \mu(G - H) = \frac{h(G-H)}{3} = \lfloor \frac{h(G)}{3} \rfloor$.

Nullity of TP-2 Benzenoids



1. A TP-2 benzenoid G is a benzenoid formed by the 2-2 edge fusion of benzene H to a TP-1 benzenoid $G - H$ (with 4 new degree-2 vertices) or a fusion of benzene into a bay region (with 2 new degree-2 vertices).

2. These have unique independent sets.

3. $\eta = \alpha - \mu$ remains unchanged.

4. $\alpha(G) - \mu(G) = \alpha(G - H) - \mu(G - H) = \lfloor \frac{h(G-H)}{3} \rfloor = \lfloor \frac{h(G)}{3} \rfloor$.

Proof of the Nullity Bound

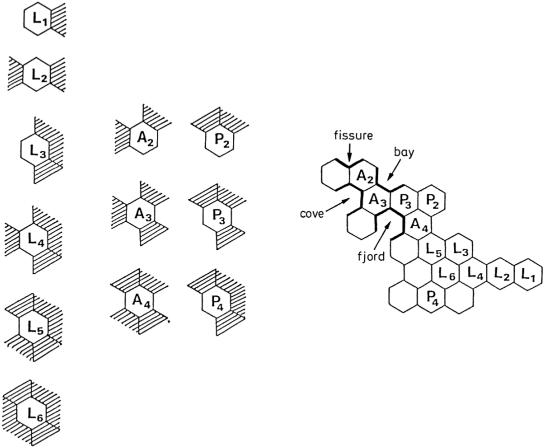


Fig. 3.2. The twelve possible modes of hexagons in benzenoid systems and the notation proposed for them. Definition of some structural features of the perimeter

Proof of the Nullity Bound

1. Assume $\alpha - \mu \leq \frac{h}{3}$ for benzenoids with fewer than h hexagons, and let G be a benzenoid with h hexagons.

2. If G is a 2-2 edge fusion (has a cut edge in its inner dual) with sub-benzenoids B_1 and B_2,

$$\alpha(B_1) - \mu(B_1) \leq \frac{h(B_1)}{3} \text{ and}$$

$$\alpha(B_2) - \mu(B_2) \leq \frac{h(B_2)}{3} \text{ implies}$$

$$\alpha(G) - \mu(G) \leq \frac{h(G)}{3}.$$

Proof of the Nullity Bound

3. If G has only degree-2 and degree-4 vertices in its inner dual then G is in the triangulene family and $\alpha(G) - \mu(G) \leq \frac{h(G)}{3}$.

4. If G has a degree-3 vertex in its inner dual then there is a hexagon H with 2 unique degree-2 vertices. By assumption,

$$\alpha(G - H) - \mu(G - H) \leq \frac{h(G - H)}{3}.$$

   As H adds no more than a single vertex to any maximum independent set and adds a single edge to every maximum matching, we have

$$\alpha(G) - \mu(G) \leq \alpha(G - H) - \mu(G - H) \leq \frac{h(G - H)}{3} \leq \frac{h(G)}{3}.$$

Characterization of Benzenoids with Maximum Nullity

Conjecture: A benzenoid G has maximum nullity among benzenoids with h hexagons if and only if G is TP, TP-1, or TP-2.

Proved: If G is TP, TP-1, or TP-2 then nullity is maximized (and equals $\lfloor \frac{h}{3} \rfloor$).

Characterization of Benzenoids with Maximum Nullity

1. Small benzenoids with $\alpha - \mu = \frac{h}{3}$ are TP.
2. Assume this is true for benzenoids with fewer than h hexagons.
3. Let G be a benzenoid with h hexagons, and $\alpha(G) - \mu(G) = \frac{h(G)}{3}$.
4. The inner dual cannot have a pendant vertex.
5. G cannot have a degree-3 vertex in the inner dual.
6. (Case: no cut edges in the inner dual). Then G has only degree-2 and degree-4 vertices in the inner dual and is in the triangulene class. So its in phenalene or triangulene.
7. (Case: there is a cut edge in the inner dual). G is two benzenoids B_1 and B_2 fused at a 2-2 edge. It can be shown that it must be that $\alpha(B_1) - \mu(B_1) = \frac{h(B_1)}{3}$ and $\alpha(B_2) - \mu(B_2) = \frac{h(B_2)}{3}$ with a *proper* fusion.
8. The inductive hypothesis implies B_1 and B_2 are TP and then G is TP.

Characterization of Benzenoids with Maximum Nullity

Theorem: A benzenoid G has maximum nullity among benzenoids with $h = 3k$ hexagons if and only if G is TP,

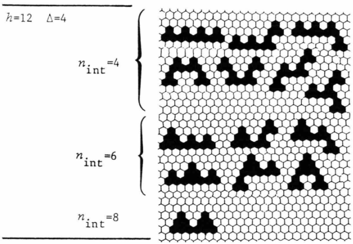


Fig. 8. Benzenoid systems with $\Delta = \Delta_{max}$ for $h = 12$, classified according to their numbers of internal vertices (n_{int}).

Conjectures

```
:  load("benzenoids.sage")

   max_nullity_graphs = [phenalene,phenalene_plus1,max_nullity5A,max_nullity5B,max_nullity5C,max_nullity6A,max_nu

   benzenoids = [naphthalene, anthracene, phenanthrene, phenalene, flying_saucer, benz_5_face_ce, benzene, throwi
   twisted_strip2, sunflower, bug_eye, snowflake, heptacene, antlers, L12, L13, L14, twisted_strip3, throwing_cha
   snake_25, snake_29, circulene_7, excess_4, circulene_9, circulene_8, circulene_15, circulene_16, circulene_17,
   big_throwing_star, dancer, dancer_CE, dancer_CE_two, dancer_CE_three, dancer_CE_four, twisted_strip4, pentahex
   throwing_star_CE, octahexagons, throwing_star_8, jaggedy, bone]

   objects = max_nullity_graphs + [benzene] + benzenoids

   #invariants = [nullity, independence_number, matching_number, Graph.order, Graph.size]
   invariants = [nullity,matching_number, Graph.order, Graph.size, degree_2_vertices, degree_3_vertices, hexagons
   number_of_3_3_edges, number_of_2_3_edges, internal_vertices, external_vertices, ratio_of_internal_to_external,
   number_of_internal_3_3_edges, number_of_external_3_3_edges, smaller_bipartite_set, larger_bipartite_set, match
   Graph.diameter, fissures, bays, coves, fjords, faces_with_1_external_edge, faces_with_2_external_edges, faces_
   faces_with_4_external_edges, faces_with_5_external_edges, faces_with_0_external_edges, branching_number]

   invariant = invariants.index(nullity)

   conjs = conjecture(objects, invariants, invariant, upperBound = False)

   for conj in conjs:
       print(conj)

:  benzenoid embedder loaded
   conjecturing loaded!!
   nullity(x) >= color_excess(x)
```

Conjectures

```
load("benzenoids.sage")

max_nullity_graphs = [phenalene,phenalene_plus1,max_nullity5A,max_nullity5B,max_nullity5C,max_nullity6A,max_nul

benzenoids = [clars_goblet,naphthalene, anthracene, phenanthrene, phenalene, flying_saucer, benz_5_face_ce, ben
twisted_strip, twisted_strip2, sunflower, bug_eye, snowflake, heptacene, antlers, L12, L13, L14, twisted_strip3
tree_13_bays, snake_25, snake_29, circulene_7, excess_4, circulene_9, circulene_8, circulene_15, circulene_16,
big_throwing_star, dancer, dancer_CE, dancer_CE_two, dancer_CE_three, dancer_CE_four, twisted_strip4, pentahexa
throwing_star_CE, octahexagons, throwing_star_8, jaggedy, bone]

objects = max_nullity_graphs + [benzene] + benzenoids

#invariants = [nullity, independence_number, matching_number, Graph.order, Graph.size]
invariants = [nullity,matching_number, Graph.order, Graph.size, degree_2_vertices, degree_3_vertices, hexagons,
number_of_3_3_edges, number_of_2_3_edges, internal_vertices, external_vertices, ratio_of_internal_to_external,
number_of_internal_3_3_edges, number_of_external_3_3_edges, smaller_bipartite_set, larger_bipartite_set, matchi
Graph.diameter, fissures, bays, coves, fjords, faces_with_1_external_edge, faces_with_2_external_edges, faces_w
faces_with_4_external_edges, faces_with_5_external_edges, faces_with_0_external_edges, branching_number]

invariant = invariants.index(nullity)

conjs = conjecture(objects, invariants, invariant, upperBound = True)

for conj in conjs:
    print(conj)
```

```
benzenoid embedder loaded
conjecturing loaded!!
nullity(x) <= internal_vertices(x)
nullity(x) <= maximum(color_excess(x), tan(degree_3_vertices(x)))
nullity(x) <= degree_3_vertices(x)
nullity(x) <= color_excess(x) + number_of_external_3_3_edges(x)
nullity(x) <= maximum(color_excess(x), tan(number_of_2_3_edges(x)))
```

Thank You!

Automated Conjecturing in Sage:
http://nvcleemp.github.io/conjecturing/

clarson@vcu.edu