On the Clar Number of Benzenoid Graphs

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This is joint work with István Estélyi, Riste Škrekovski, and Niko Tratnik.

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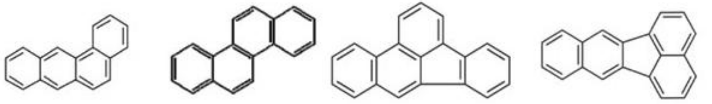
Benzenoids

PAHs (Polycyclic aromatic hydrocarbons):



Benzo[a]anthracen Chrysene Benzo[b]anthracen Benzo[k]anthracen

benzenoids . . . hexagonal rings only

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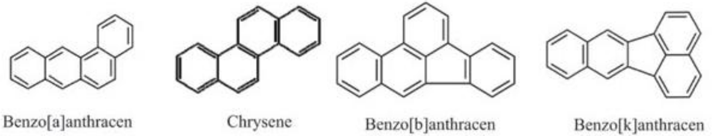
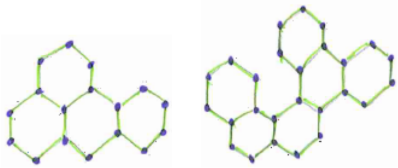


benzenoids . . . hexagonal rings only

Fusenes and benzenoid graphs

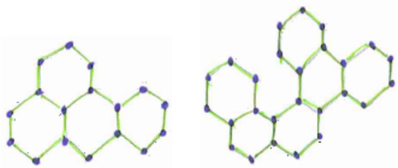


Definition used here:

A fusene is a 2-connected plane graph in which all inner faces are hexagons (and all hexagons are faces), such that two hexagons are either disjoint or have exactly one common edge, and no three hexagons share a common edge.

The above definition also includes graphs that cannot be embedded into the regular hexagonal grid.

Fusenes and benzenoid graphs



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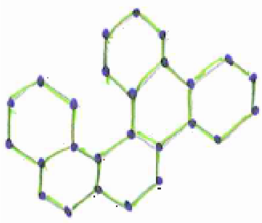
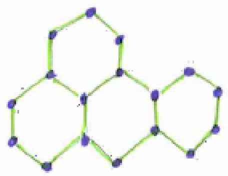
Benzenoid graphs
Catacondensed vs. pericondensed



Catacondensed



pericondensed

(Perfect) matchings

1. matching M in a graph G: $M \subseteq E(G)$ s.t. no two edges from M share a vertex
2. perfect matching: $2|M| = |V(G)|$
   (in chemistry perfect matchings are known as Kekulé structures)

Kekulé structures of the phenanthrene graph

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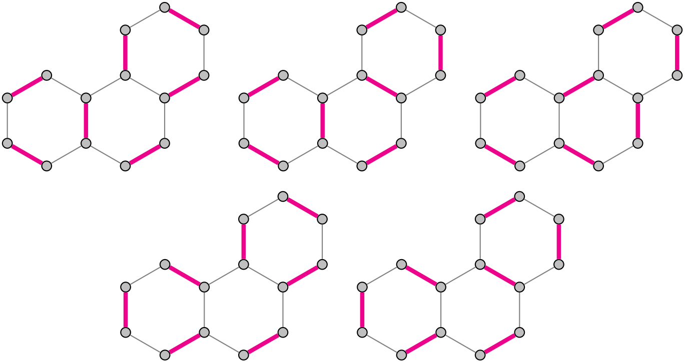

Kekulé structures of the phenanthrene graph

Perfect matchings and alternating hexagons

B ... benzenoid graph, $h \in B$ ... hexagon

1. h is an *M-alternating* hexagon: M contains exactly 3 edges of h (in such cases we often draw a circle in h)

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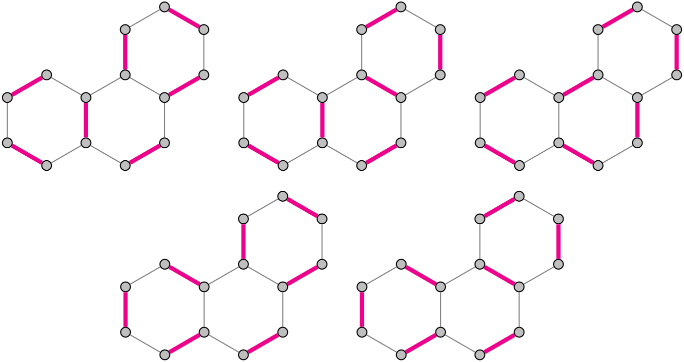

Kekulé structures of the phenanthrene graph

Clar set and Clar number

A Clar set C is a maximum set of independent M-alternating hexagons over all perfect matchings M of benzenoid B.

The Clar number of B, denoted by $\mathrm{Cl}(B)$, is the number of hexagons in a Clar set for B.

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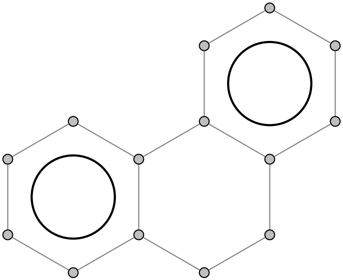
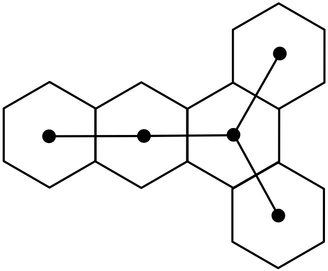


The dualist graph

The dualist graph of a benzenoid graph B consists of vertices corresponding to hexagons of B; two vertices are adjacent if and only if the corresponding hexagons have a common edge.



Note: the dualist graph of B is a tree if and only if B is catacondensed. Moreover, it is a subcubic tree.
If the dualist is a path then the catacondensed benzenoid is called unbranched, otherwise branched.

Catacondensed benzenoids with large Clar number

Theorem

Let B be a catacondensed benzenoid graph with h hexagons. Then

$$\mathrm{Cl}(B) \leq \left\lfloor \frac{2h+1}{3} \right\rfloor .$$

Independent set and vertex cover

An independent set is a set of vertices in a graph G, no two of which are adjacent.
The independence number of G, denoted by $\alpha(G)$, is the size of the maximum independent set.

A vertex cover of a graph is a set of vertices such that each edge of the graph is incident to at least one vertex of the set.
The vertex covering number of G, denoted by $\tau(G)$, is the size of any smallest vertex cover of G.

A results about trees

Lemma

Let T be a subcubic tree on $n \geq 1$ vertices with independence number $\alpha(T)$. Then

$$\alpha(T) \leq \left\lceil \frac{2n+1}{3} \right\rceil.$$

Idea of proof: use the Gallai identity.

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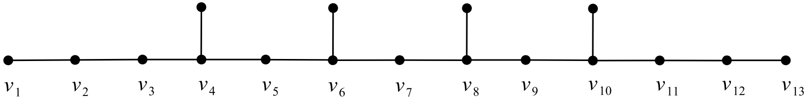
More about trees

Definition

Let $k \geq 2$ be an integer. The tree T_k is composed of the path on vertices $v_1, \ldots, v_{2k+1}$ with $k-2$ additional leaves which are attached to the vertices $v_4, v_6, \ldots, v_{2k-2}$.



T_6

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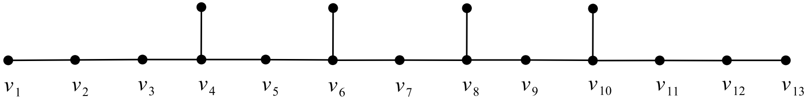

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More about trees (cont'd)

Theorem

Let T be a subcubic tree on $n \geq 3$ vertices with independence number

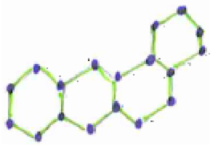
$$\left\lceil \frac{2n+1}{3} \right\rceil.$$

Then exactly one of the following statements holds:

(i) *T has a vertex that is adjacent to (at least) two leaves.*

(ii) *T is isomorphic to T_k for some $k \geq 2$.*

A hexagon h of a catacondensed benzenoid graph B adjacent to exactly two other hexagons possesses two vertices of degree 2. If these two vertices are adjacent, then h is angularly connected. If these two vertices are not adjacent, then h is linearly connected.

tetraphene: 

Lemma

Let B be a catacondensed benzenoid graph with n hexagons such that $T(B) \simeq T_k$ for some $k \geq 2$. Then $\mathrm{Cl}(B) = \left[\frac{2n+1}{3}\right]$ if and only if the two hexagons corresponding to vertices v_2 and v_{2k} are both angular.

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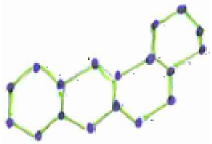
tetraphene: 

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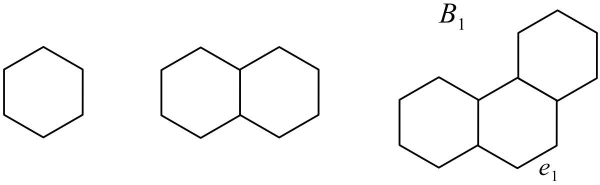
Family $\mathcal{B}$ of catacondensed benzenoid graphs:

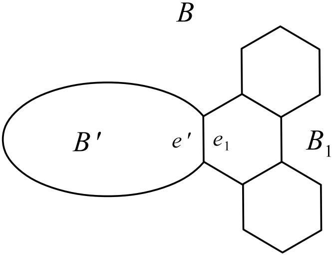
(*i*) The following benzenoid graphs belongs to $\mathcal{B}$:



(*ii*) A catacondensed benzenoid graph B, s.t. $T(B) \simeq T_k$ for some $k \geq 2$ and s.t. the two hexagons corresponding to vertices v_2 and v_{2k} are both angular, belongs to $\mathcal{B}$.

Family $\mathcal{B}$ of catacondensed benzenoid graphs:

(iii) Let $B' \in \mathcal{B}$ and let e' be any edge of B' with both endvertices of degree 2. Let B_1 be the phenanthrene graph (see above) and let e_1 be the edge of the angular hexagon with both endvertices of degree 2.

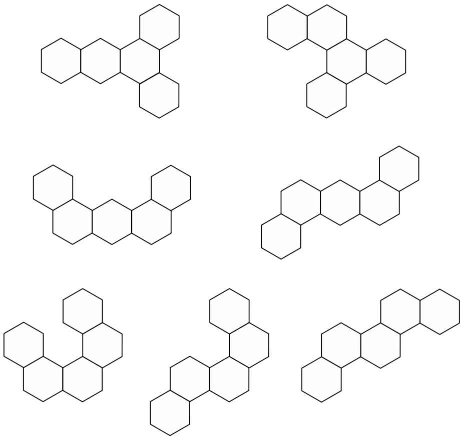


Benzenoid that is obtained from B' and B_1 by identifying edges e' and e_1 belongs to $\mathcal{B}$.

Catacondensed benzenoids with large Clar number

Characterisation (cont^{3}d)

Examples:



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Theorem

Let B be a catacondensed benzenoid graph with h hexagons. Then

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and equality holds if and only if B belongs to $\mathcal{B}$.


Thats all Folks!