Resonance graphs of kinky benzenoid systems are daisy cubes

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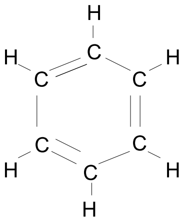
Outline

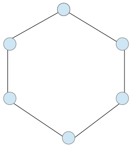
Benzenoid systems

Benzenoid systems are 2-connected planar graphs such that every interior face is a hexagon.

Molecule of benzene

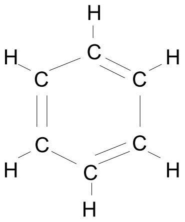


benzene

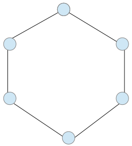


benzenoid system

Molecule of benzene

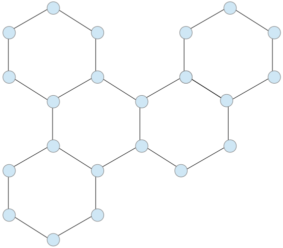


benzene

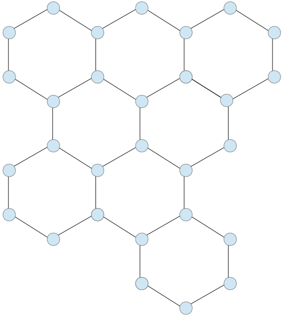


benzenoid system

Cata- and pericondensed benzenoid systems



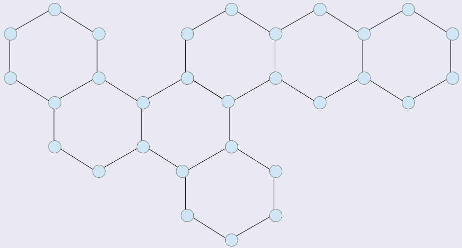
catacondensed b.s.



pericondensed b.s.

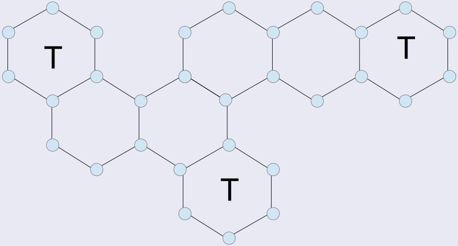
Catacondensed benzenoid systems

Types of hexagons



Catacondensed benzenoid systems

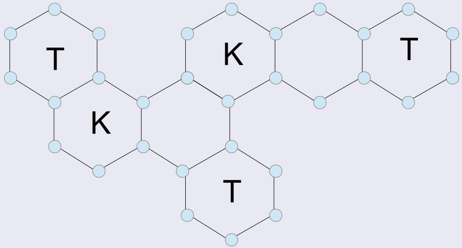
Types of hexagons



T ... terminal hexagon

Catacondensed benzenoid systems

Types of hexagons

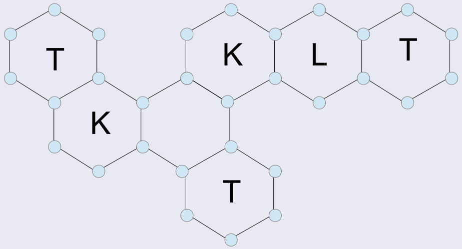


T ... terminal hexagon

K ... a kink (or an angularly connected hexagon)

Catacondensed benzenoid systems

Types of hexagons



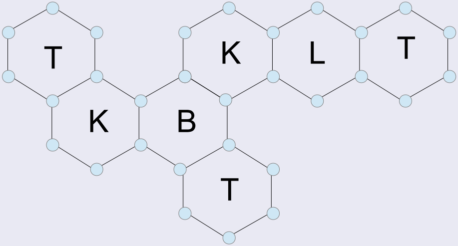
T ... terminal hexagon

K ... a kink

L ... linear hexagon

Catacondensed benzenoid systems

Types of hexagons



T ... terminal hexagon

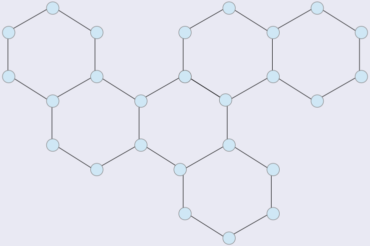
K ... a kink

L ... linear hexagon

B ... branched hexagon

Kinky benzenoid systems

No L



Perfect matchings

- a **1-factor** of a benzenoid system B is a spanning subgraph of B such that every vertex has degree one

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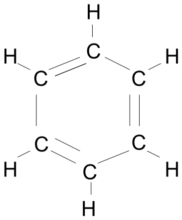
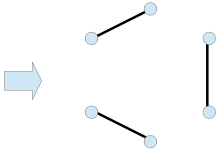
- a **1-factor** of a benzenoid system B is a spanning subgraph of B such that every vertex has degree one
- edges of 1-factor form an independent set of edges $\mathcal{M}(B)$ called **perfect matchings** (chemicaly known as **Kekulé structures**)

Kekulé structure vs 1-factor (perfect matching)

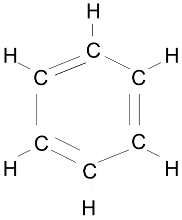


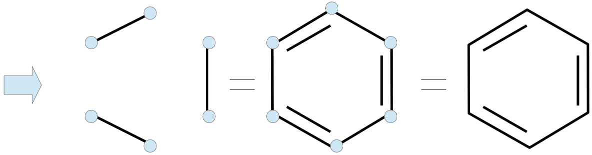
Kekule structure



1-factor

Kekulé structure VS 1-factor (perfect matching)

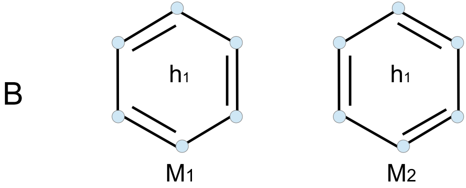




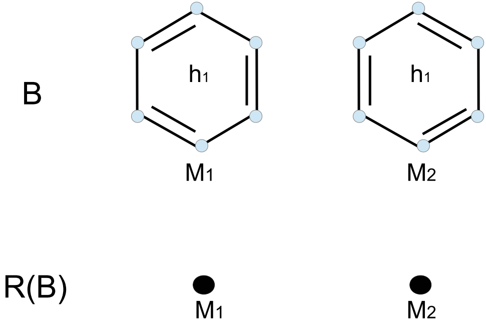
Kekule structure

1-factor

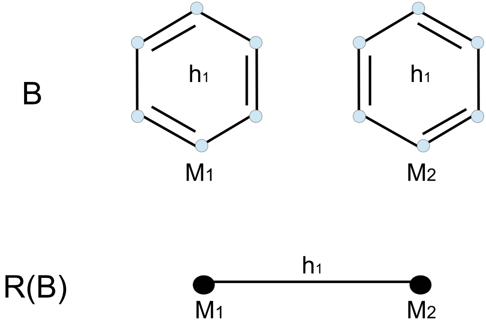
Resonance graph of benzene



Resonance graph of benzene



Resonance graph of benzene



Definition of the resonance graph $R(B)$

vertices of $R(B)$ ... perfect matchings of B

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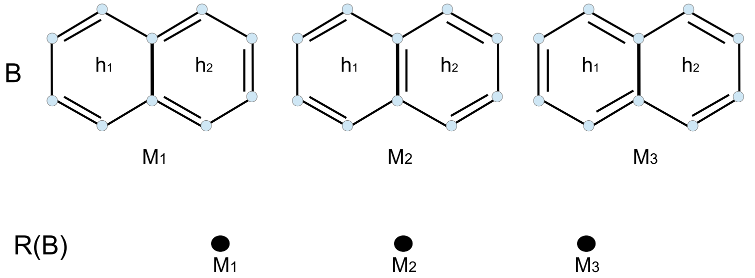
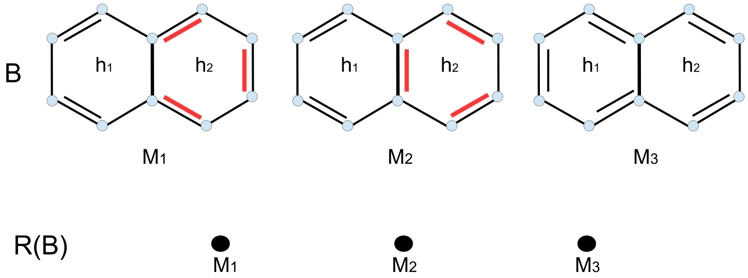
M_1M_2 is an edge in $R(B)$ ... $M_1 \oplus M_2$ is a hexagon of B

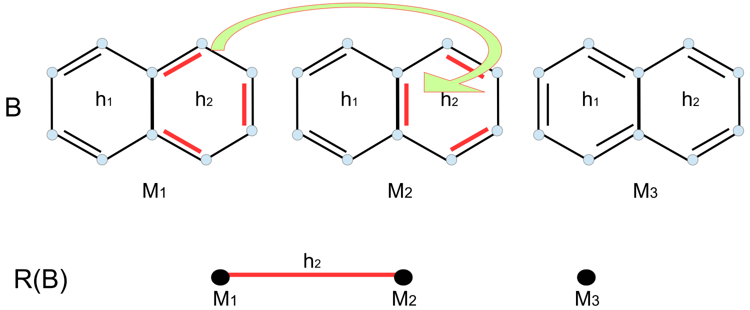
Resonance graph of naphtalene



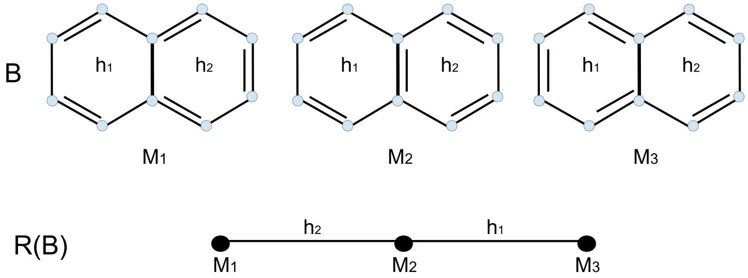
Resonance graph of naphtalene



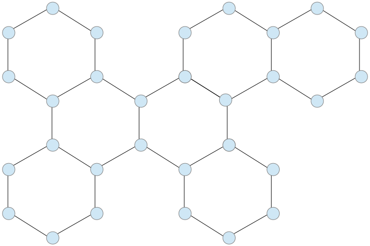
Resonance graph of naphtalene



Resonance graph of naphtalene



The binary coding procedure [Klavžar et al. (2001)]



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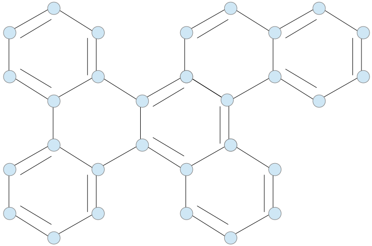
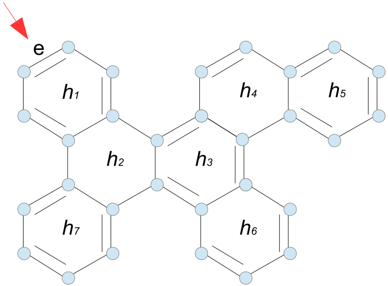
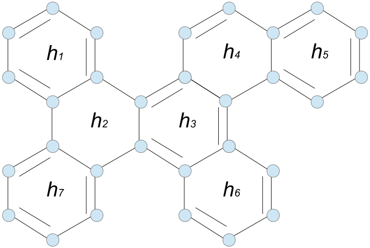


The binary coding procedure



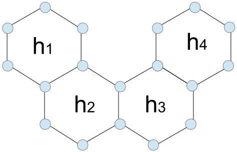
The binary coding procedure



$\ell(M) = 1010101$

Figure: The binary label of perfect matching M.

An example - fibonaccene



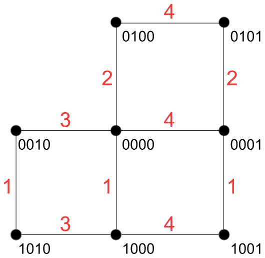
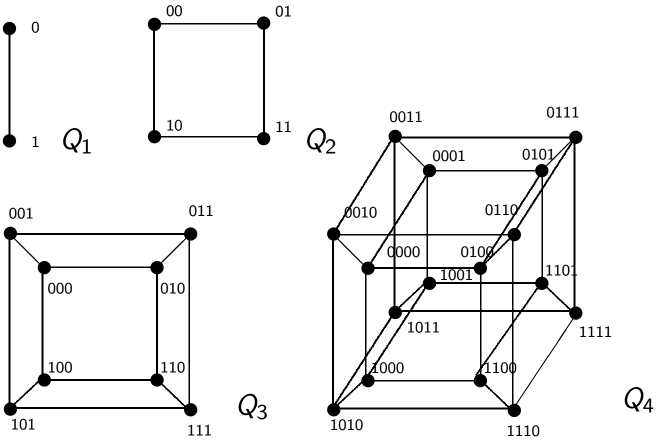


Figure: The resonance graph is isomorphic to the Fibonacci cube Γ_4.

Hypercubes Q_1, Q_2, Q_3, Q_4



Daisy cubes

Let $\leq$ be a partial order on $\{0,1\}^n$ defined with

$$u_1 \ldots u_n \leq v_1 \ldots v_n \ \text{ if } u_i \leq v_i, \forall\, i \in [n]\,.$$

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For example:

$$000 \leq 010 \leq 011 \leq 111$$

Daisy cubes

[Klavžar, Mollard (2018)]

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$$u_1 \ldots u_n \leq v_1 \ldots v_n \text{ if } u_i \leq v_i, \forall\, i \in [n]\,.$$

For $X \subseteq \{0,1\}^n$ we define the graph $Q_n(X)$ as the subgraph of Q_n with $Q_n(X) = \langle\{u \in \{0,1\}^n; u \leq x \text{ for some } x \in X\}\rangle$ and say that $Q_n(X)$ is a *daisy cube* (generated by X).

The vertex sets of daisy cubes are also known as hereditary or downwards closed sets.

$Q_n(X) = \langle \{u \in \{0,1\}^n ; u \le x \text{ for some } x \in X\} \rangle$

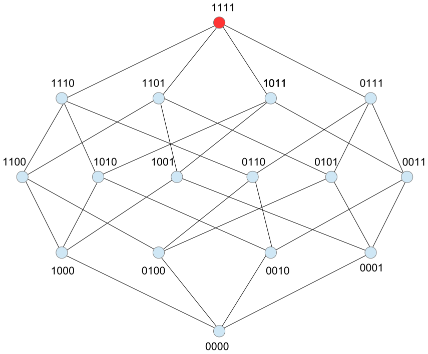

Figure: $X = \{1^n\} \Rightarrow Q_n(X) = Q_n$

$Q_n(X) = \langle \{u \in \{0,1\}^n ; u \leq x \text{ for some } x \in X\} \rangle$

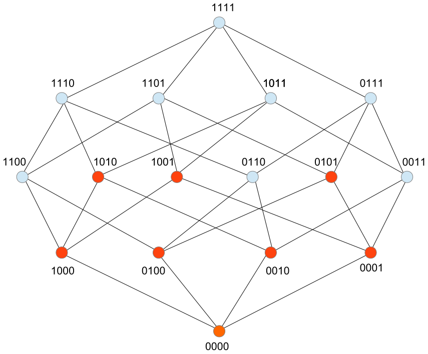

Figure: $X = \{u_1 \ldots u_n ; u_i \cdot u_{i+1} = 0, i \in [n-1]\}$

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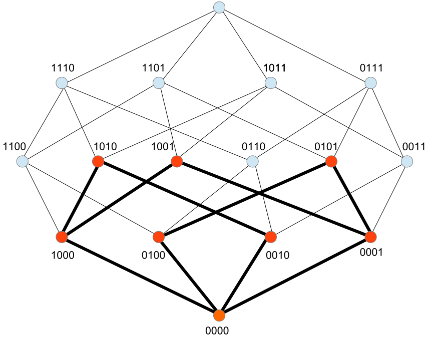

Figure: $X = \{u_1 \ldots u_n; u_i \cdot u_{i+1} = 0, i \in [n-1]\} \Rightarrow Q_n(X) = \Gamma_n$ (a Fibonacci cube)

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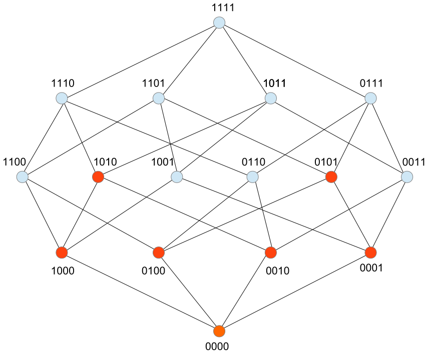

Figure: $X = \{u_1 \ldots u_n; u_i \cdot u_{i+1} = 0, i \in [n-1], u_1 \cdot u_n = 0\}$

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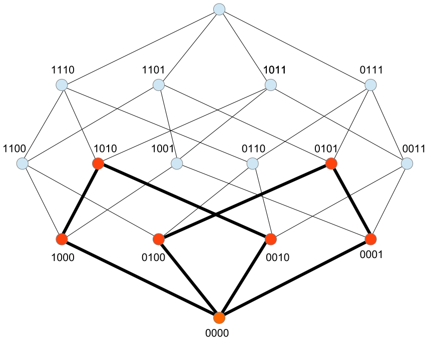

Figure:
$X = \{u_1 \ldots u_n;\, u_i \cdot u_{i+1} = 0, i \in [n-1], u_1 \cdot u_n = 0\} \Rightarrow Q_n(X) = \Lambda_n$ (a Lucas cube)

$Q_n(X) = \langle \{u \in \{0,1\}^n ; u \leq x \text{ for some } x \in X\} \rangle$

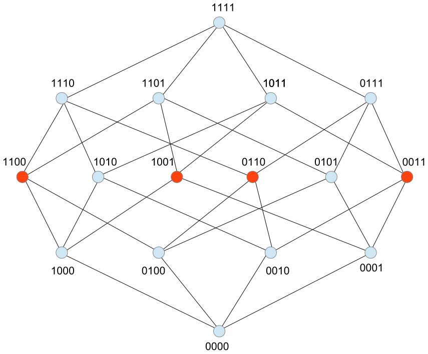

Figure: $X = \{110^{n-2}, 01100^{n-3}, \ldots, 0^{n-2}11, 10^{n-2}1\}$

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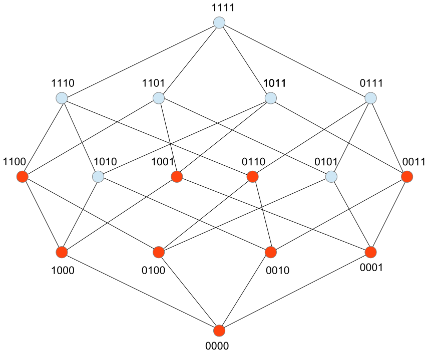

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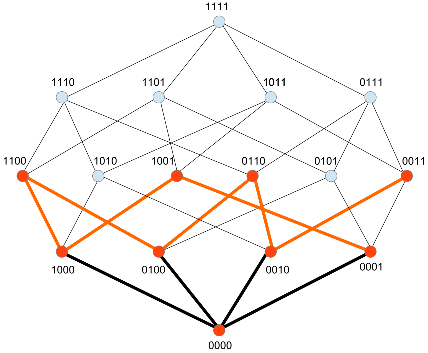
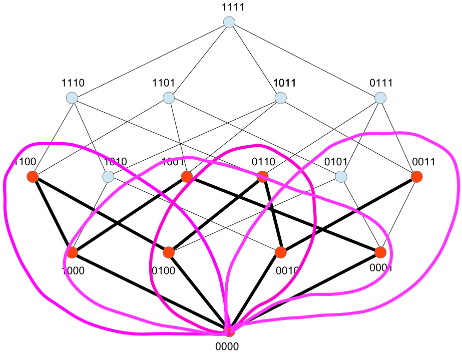


Figure: $X = \{110^{n-2}, 01100^{n-3}, \ldots, 0^{n-2}11, 10^{n-2}1\} \Rightarrow Q_n(X) = \mathrm{BW}_n$ (a bipartite wheel)

A daisy cube

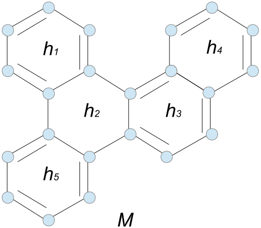

1111
1110
1101
1011
0111
1100
1010
1001
0110
0101
0011
1000
0100
0010
0001
0000

The main result

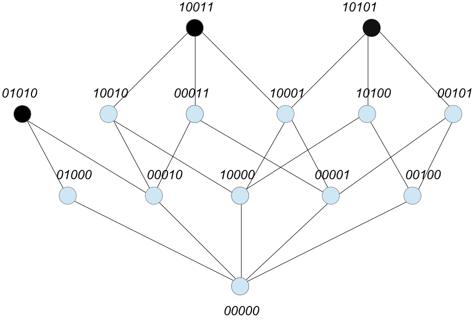
[P. Ž. P. (2018)]

The resonance graph of a kinky benzenoid system is a daisy cube.

An example


h_1
h_2
h_3
h_4
h_5

M


10011
10101
01010
10010
00011
10001
10100
00101
01000
00010
10000
00001
00100
00000

Problem-linear hexagons

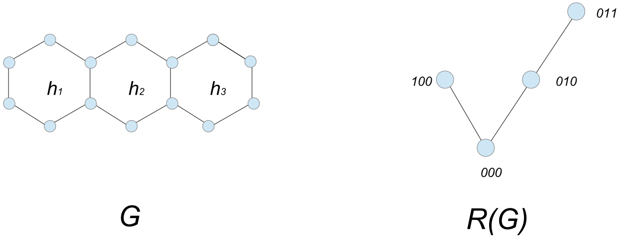


Figure: The resonance graph is not a daisy cube.

Thanks for your attention!