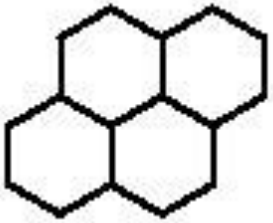
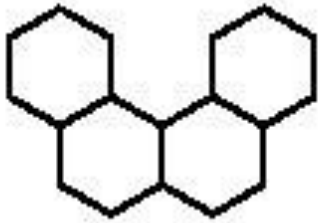
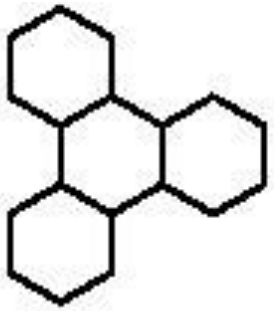
Benzenoid:Having the six-membered ring structure or aromatic properties of benzene.



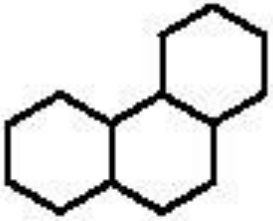
Pyrene



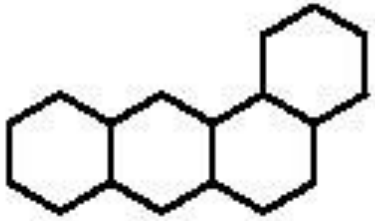
Benzo[c]phenanthrene



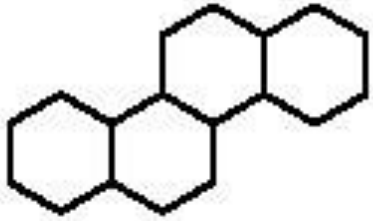
Triphenylene



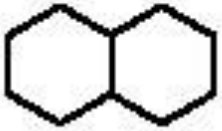
Phenanthrene



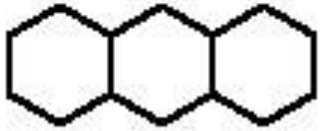
Benz[a]anthracene



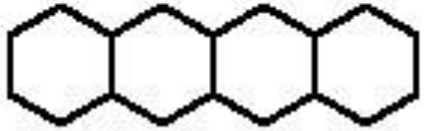
Chrysene



Naphthalene



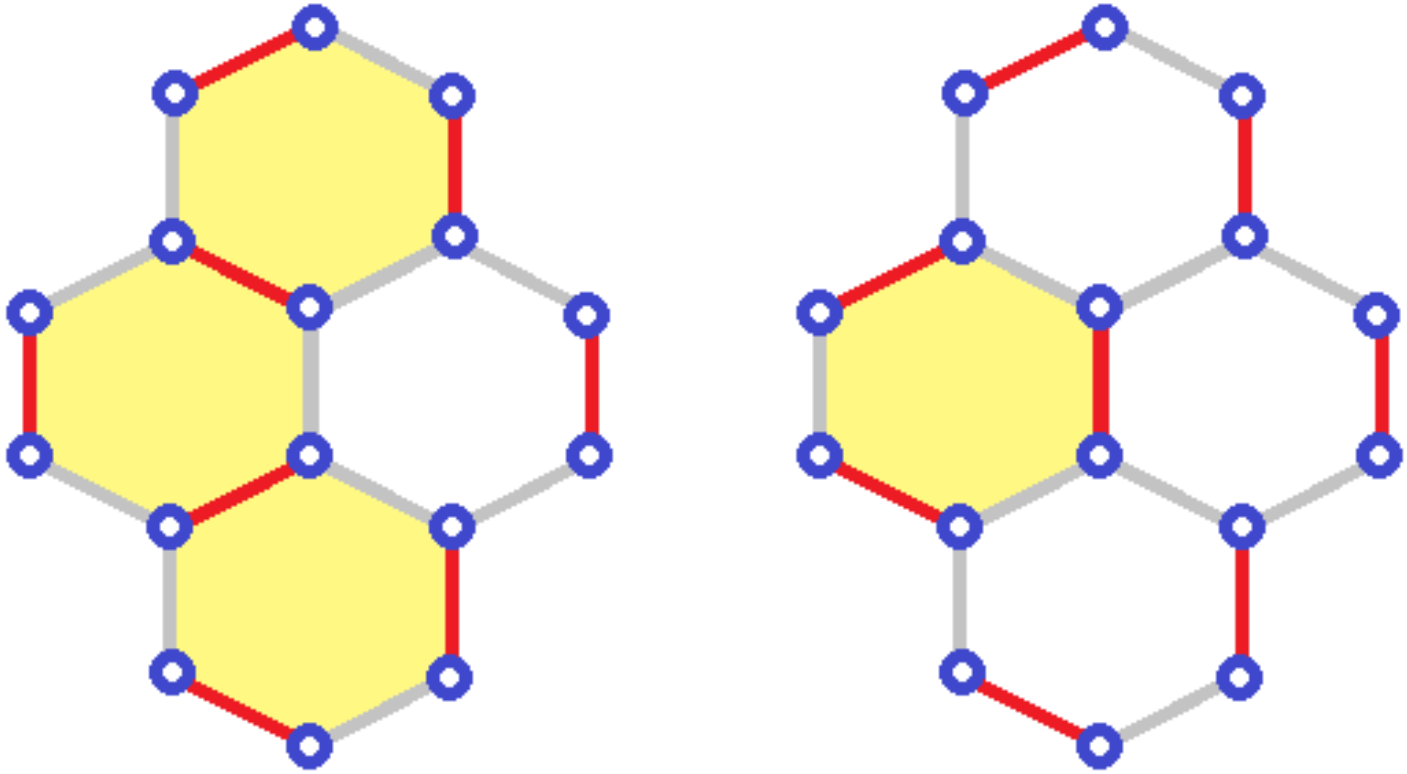
Anthracene



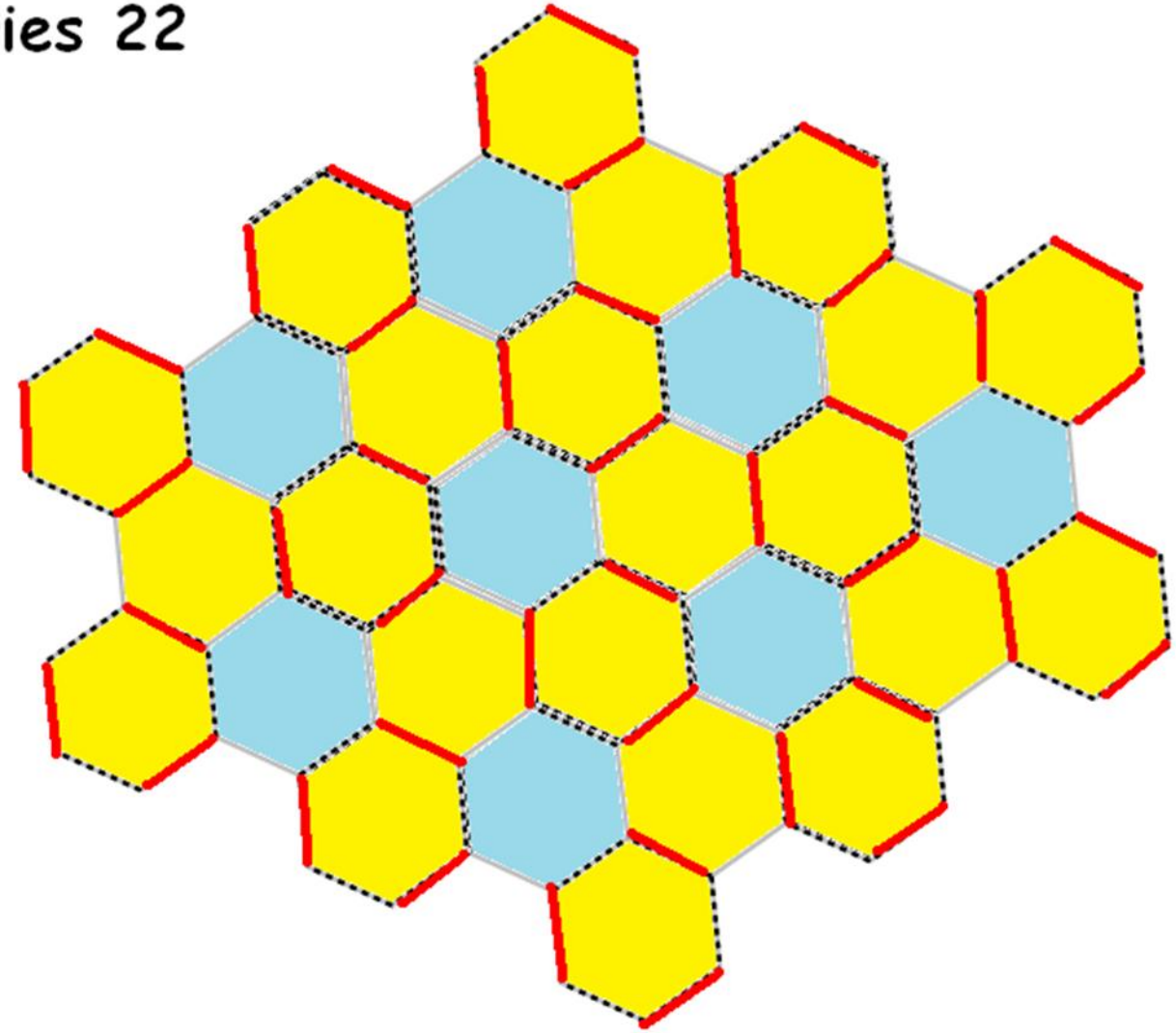
Tetracene

http://www.astrochem.org/sci/Cosmic_Complexity_PAHs.php

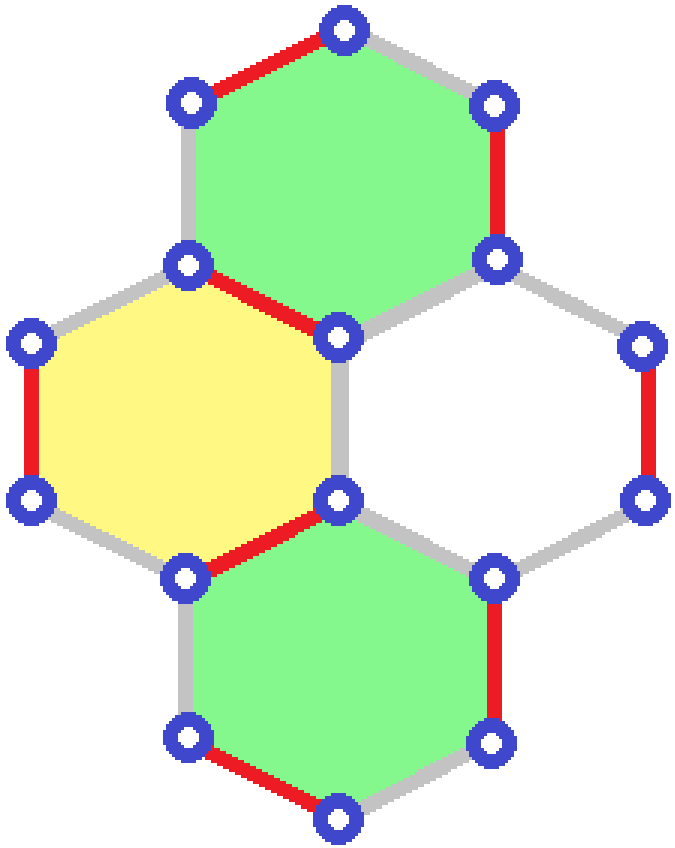
Matching: collection of disjoint edges.
Benzenoid hexagon: hexagon with 3 matching edges.
Fries number: maximum over all perfect matchings of the number of benzenoid hexagons.

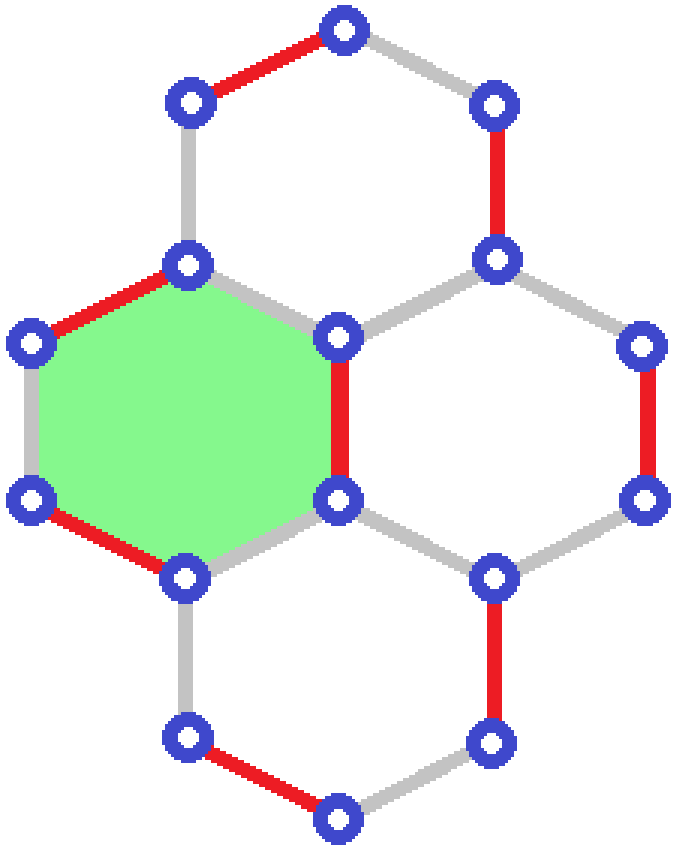


Fries 22

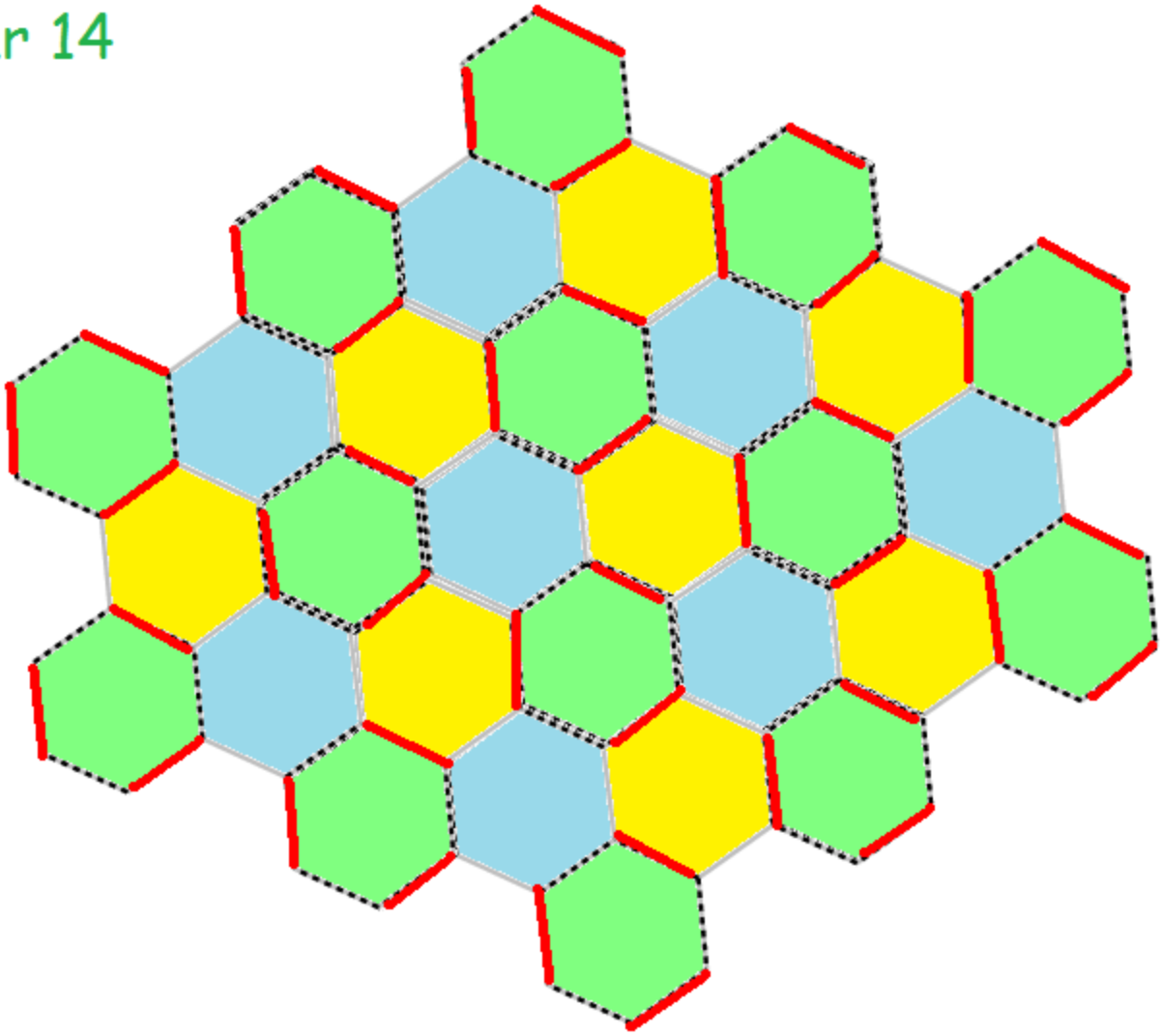


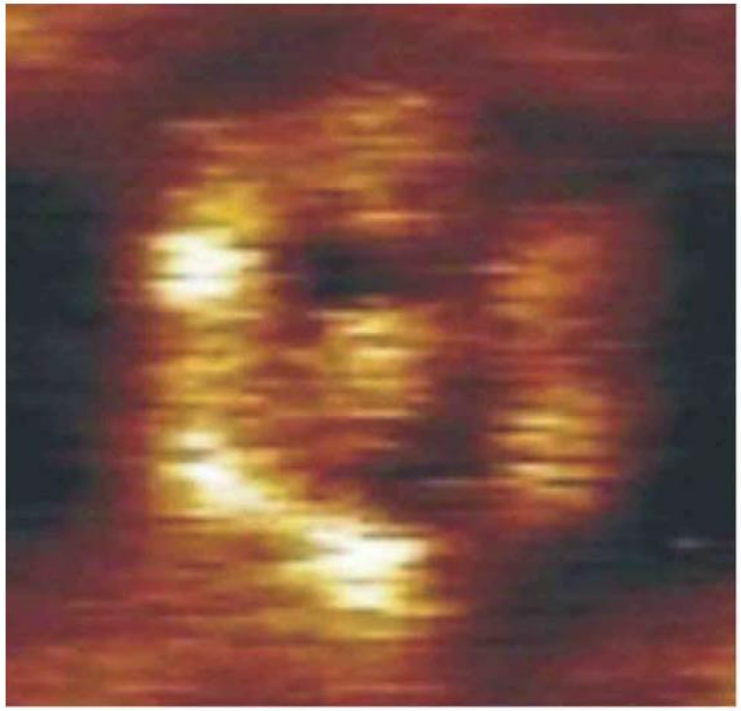
Clar number: maximum over all perfect matchings of the number of independent benzenoid hexagons.

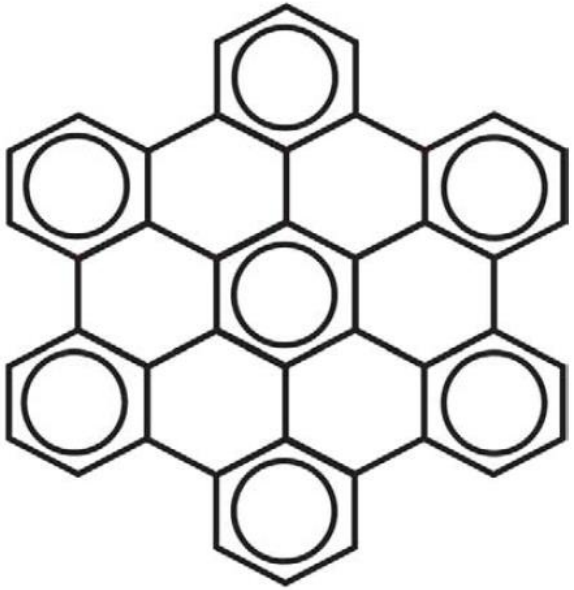




Clar 14



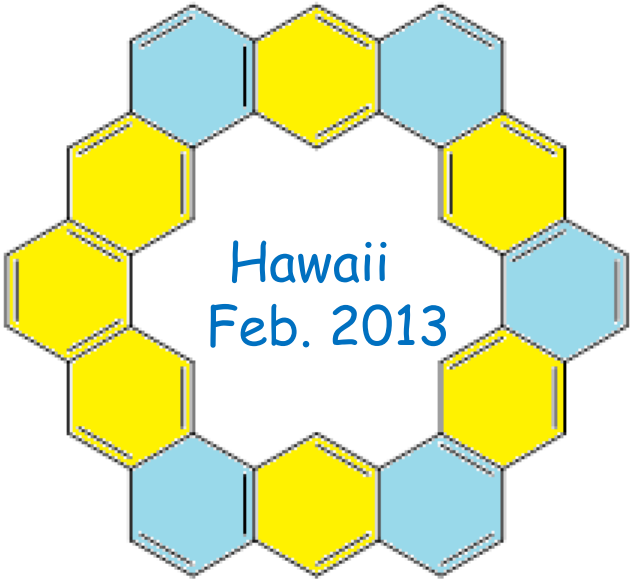




STM current-image of hexabenzocoronene

from
I Gutman, Ž Tomović, K Müllen, J P Rabe,
Chemical Physics Letters 397 (2004) 412–416

Counterexamples to a proposed algorithm for finding the Fries number of a benzenoid



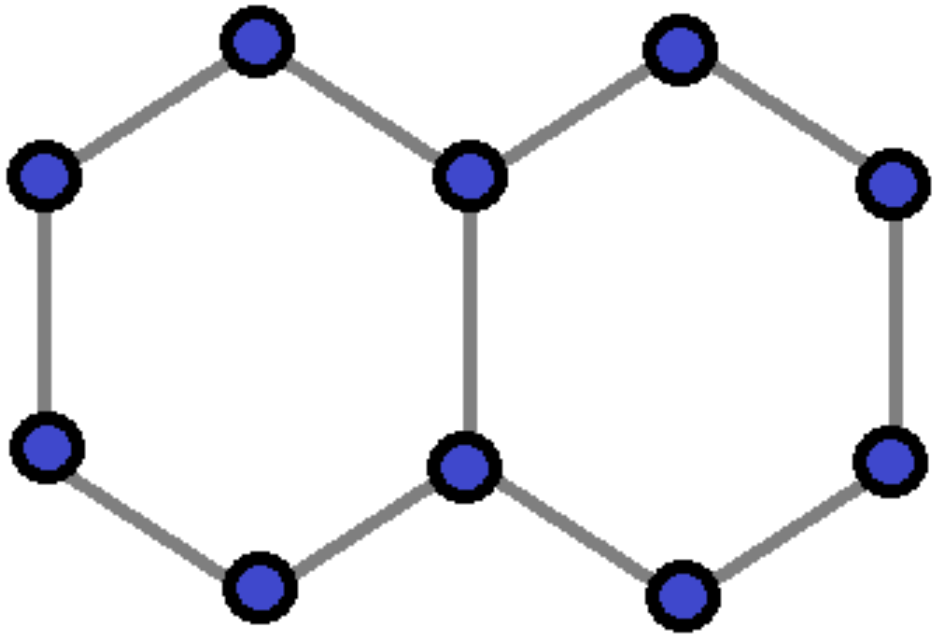
Wendy Myrvold, Patrick W. Fowler

and William H. Bird

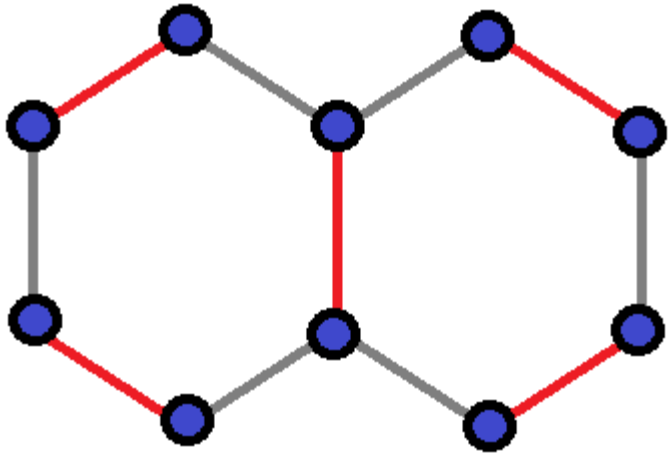
Published in: Journal of Mathematical Chemistry, Oct. 2012, Volume 50, Issue 9, pp. 2408-2426.

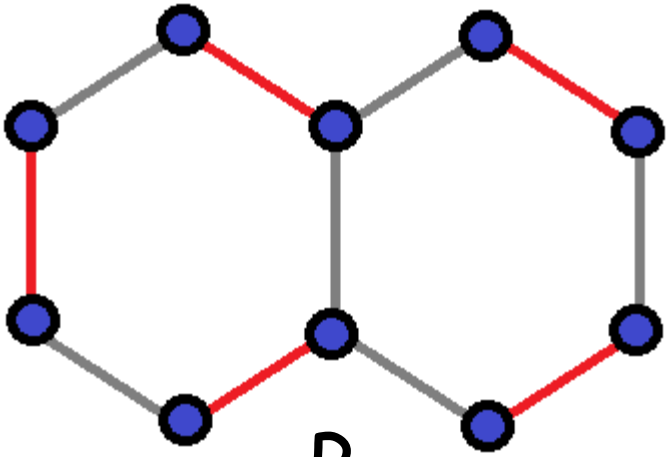
How many perfect matchings does this graph have?

What are the perfect matchings?

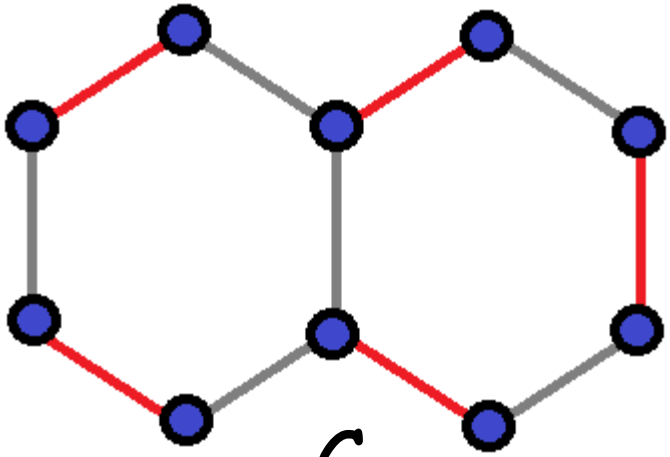


A



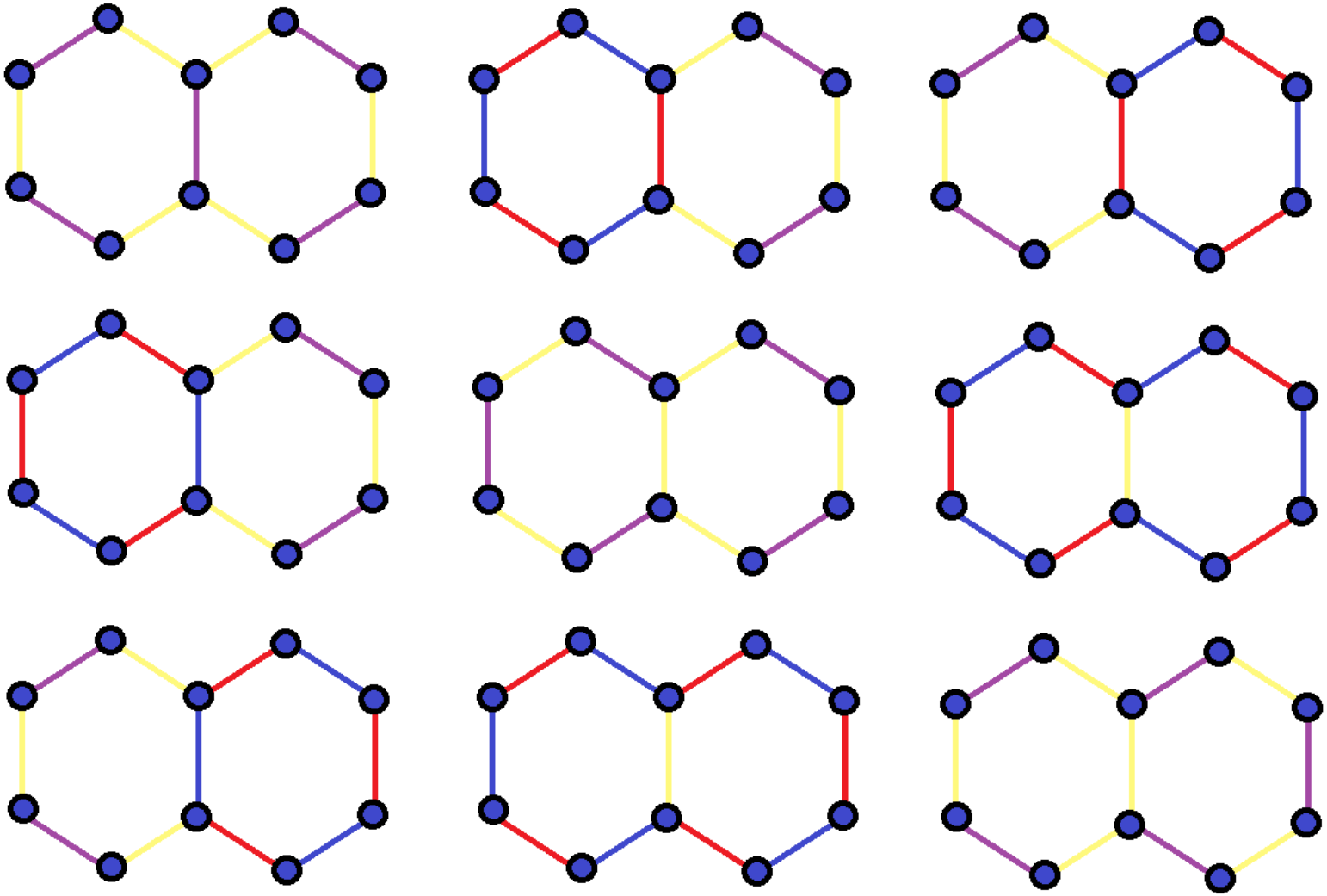


B

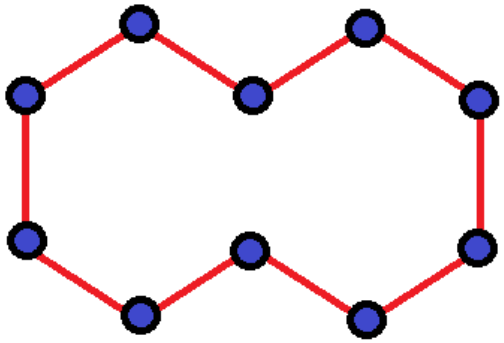


C

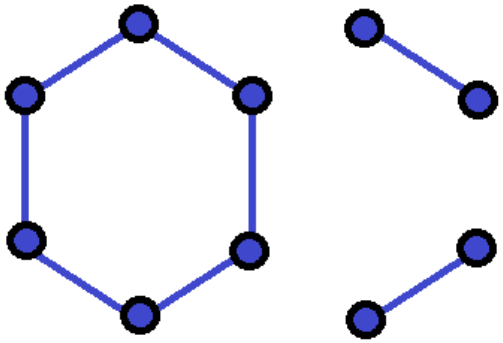
Randic current model: Consider ordered pairs of perfect matchings.



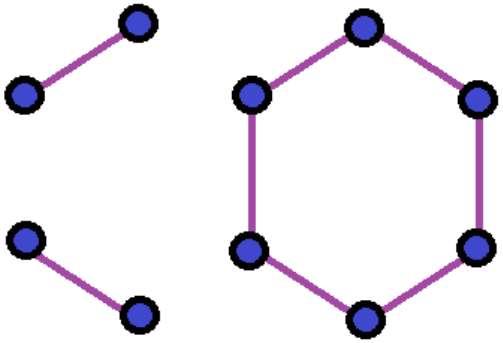
Conjugated Circuits:



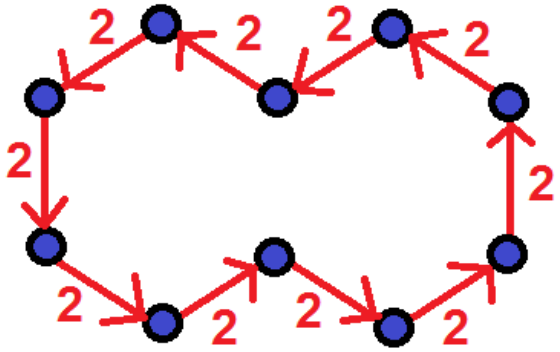
Occurs 2 times
(BC, CB).

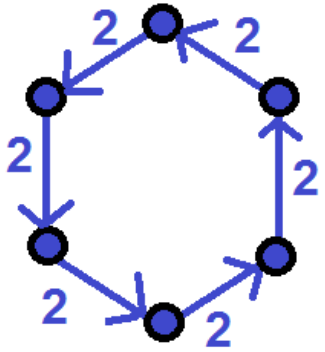


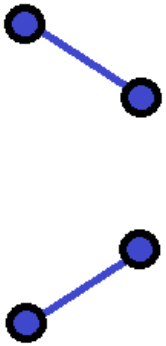
Occurs 2 times.
(AB, BA)

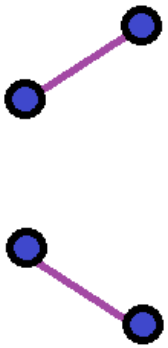


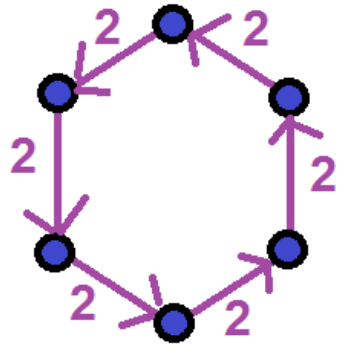
Occurs 2 times.
(AC, CA)

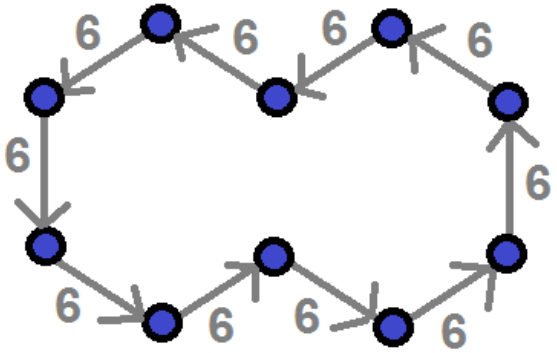












Milan Randic

Current flow: counterclockwise in 4n+2 cycles and clockwise in 4n cycles.

Sum the currents for each pair of matchings to get current estimate.