Falsifying some conjectures in organic chemistry on the structure of perfect matchings in subgraphs of the honeycomb lattice

Robert D. Barish

Division of Medical Data Informatics, Human Genome Center, Institute of Medical Science, University of Tokyo, 4-6-1 Shirokanedai, Minato-ku, Tokyo 108-8639, Japan
rbarish@ims.u-tokyo.ac.jp
tshibuya@hgc.jp

This is joint work with Tetsuo Shibuya.

Abstract

In mathematical chemistry, we abstract the *carbon skeleton* of a molecular structure as an undirected graph, where vertices represent carbon atoms, edges represent single carbon-carbon bonds, and we ignore the presence of other atom types (e.g., hydrogen). Here, a *polyhex* is a connected carbon skeleton that is isomorphic to an induced subgraph of the honeycomb lattice with minimum degree 2. If a polyhex has at most one face (respectively, more than one face) of length ≥ 7, corresponding to the outer boundary (respectively, outer boundary or a hole), then we may refer to it as a *benzenoid* (respectively, a *coronoid*). Letting G be a polyhex, we refer to a perfect matching for G as a *Kekulé structure*, and for a particular Kekulé structure $\mathcal{M}$, we refer to any 6-sided face in G with 3 edges in $\mathcal{M}$ as a *resonant benzene face*. We can now define the *Fries number* $F(G)$ [4] for G as the maximum number of resonant benzene faces that can be realized by any Kekulé structure. Additionally, we can define the *Clar number* $C(G)$ [2] for G as the maximum number of mutually vertex-disjoint resonant benzene faces that can be realized by any Kekulé structure. Finally, we can define the *Fries set* $\mathcal{F}$ (respectively, *Clar set* $\mathcal{C}$) for G as the set of all Kekulé structures inducing $F(G)$ resonant benzene faces (respectively, $C(G)$ mutually vertex-disjoint resonant benzene faces).

In this talk, we will elaborate on coronoid counterexamples we have discovered for the well-known *Clar–Fries conjecture* [1,3,5,6,7] for polyhexes (or bipartite planar carbon skeletons more generally [1]) that at least one Clar set is a subset of a Fries set. It was previously only known that the Clar–Fries conjecture was false for fullerenes [6,7] (i.e., necessarily non-bipartite 3-regular planar graphs with pentagonal and hexagonal faces), and true for special classes of fullerenes [6,7] and benzenoids [5].

References

1. E. Bérczi-Kovács and A. Frank. A network flow approach to a common generalization of Clar and Fries numbers. *Discrete Math.*, 347(11):114145:1–114145:14, 2024. doi:10.1016/j.disc.2024.114145.
2. E. Clar. *The aromatic sextet.* Wiley, London, 1972.
3. J. Fenton, J. E. Graver, and E. J. Hartung. The Clar-Fries mystery. *Art Discrete Appl. Math.*, 9(1):1–10, 2026. doi:10.26493/2590-9770.1519.4b6.
4. K. Fries. Über bicyclische verbindungen und ihren vergleich mit dem naphtalin. III. Mitteilung. *Justus Liebigs Annalen der Chemie*, 454(1):121–324, 1927. doi:10.1002/jlac.19274540108.
5. J. E. Graver, E. J. Hartung, and A. Y. Souid. Clar and Fries numbers for benzenoids. *J. Math. Chem.*, 51:1981–1989, 2013. doi:10.1007/s10910-013-0193-0.
6. E. J. Hartung. *The Clar structure of fullerenes.* PhD thesis, Syracuse University, Syracuse, New York, 2012.
7. E. J. Hartung. Clar chains and a counterexample. *J. Math. Chem.*, 52(3):990–1006, 2014. doi:10.1007/s10910-014-0305-5.

This work was supported by JSPS Kakenhi grant 25K21149.
The material in this extended abstract is currently under review for publication elsewhere.