Exploring connections between chemistry, computer science, and graph theory

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The goal of this talk is to illustrate interconnections between chemistry and interesting theoretical and algorithmic questions in graph theory.

We will consider several classes of molecules that can be represented by planar graphs that have maximum degree three. A *fullerene* is an all carbon molecule that corresponds to a 3-regular planar graph with face sizes five or six. *Fusenes* are hydrocarbon molecules that correspond to simple planar 2-connected graphs embedded in the plane such that all internal faces are hexagons, all vertices not on the external face have degree 3 and vertices on the external face have degree 2 or 3. *Benzenoids* have similar structure but can contain holes.

Various graph theory concepts are of chemical relevance. A subset S of the vertices of a graph forms an *independent set* if the vertices of S are pairwise non-adjacent. Independent sets model addition possibilities for reactions with bulky addends. Given a perfect matching of a graph, a *benzenoid hexagon* is a hexagon which contains three matching edges. One simple chemical model for stability of benzenoid molecules uses the *Fries number* (the maximum number of benzenoid hexagons over all the perfect matchings of the molecular graph). Another model uses the *Clar number* (the maximum number of independent benzenoid hexagons over all perfect matchings). A *conjugated circuit* of a graph G is a cycle C such that $G - C$ has a perfect matching. Several simplified models for currents are based on enumerating contributions from conjugated circuits.

This talk will summarize the work we have done so far on independent sets, the Clar and Fries numbers, and currents in molecules. The work discussed has been done in collaboration with Patrick Fowler, a chemist from the University of Sheffield, and several students at the University of Victoria: William H. Bird, Matthew J. Imrie, and Sean Daugherty (currently at Metron Inc.).