Claudia Justus

(Universität Bielefeld, visiting Syracuse University)

Applications of Graph Theory in Fullerene Chemistry

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Fullerenes are chemical molecules consisting of carbon atoms that can be arranged on the surface of a sphere, where each atom is directly bonded to three neighbors so that all the faces formed by the bondings are either pentagons or hexagons. In terms of graph theory, we have a trivalent plane graph with faces of size 5 or 6. The Euler formula yields that the number of pentagons in a fullerene always has to be 12.

Especially interesting in both math and chemistry are local transformations between fullerenes, where a subgraph (a so-called *patch*) is replaced by a different patch that fits into the same boundary. In some cases, those patches may have a different number of faces so that the fullerene grows through this operation (see Figure 1). It was already shown that hexagonal patches without pentagons that have the same boundary always contain the same number of faces and therefore can never be growth patches; on the other hand, we know growth patches with two or more pentagons. The only open question was whether there exist growth patches with exactly one pentagon, which is important for large fullerenes because otherwise they cannot grow through local transformations. I will give a sketch of the proof that the number of faces of such a patch with hexagons and exactly one pentagon is uniquely determined by its boundary, which means that growth patches with one pentagon cannot exist.

Click here to view the Endo-Kroto growth patches.

I dealt with the question whether the number of faces of such a *disordered* patch is determined by its boundary also in a more general context with arbitrary vertex degrees and face sizes. In order to completely solve this question, a different, more topological approach can be used which I also would like to present briefly.

In the last part of my talk I would like to give an idea of my current work that deals with the *expander constant* of a fullerene, which is a measure for the connectivity of a graph.