Spectral clustering of combinatorial fullerene isomers based on their facet graph structure

Artur Bille

(*Ulm University*)

After Curl, Kroto and Smalley were awarded 1996 the Nobel Prize in chemistry, fullerenes have been subject of much research. One part of that research is the prediction of a fullerene's stability using topological descriptors. It was mainly done by considering the distribution of the twelve pentagonal facets on its surface, calculations mostly were performed on all isomers of C_{40}, C_{60} and C_{80}. We suggest a novel method for the classification of combinatorial fullerene isomers using spectral graph theory. The classification presupposes an invariant scheme for the facets based on the Schlegel diagram. The main idea is to find clusters of isomers by analyzing their graph structure of hexagonal facets only. We also show that our classification scheme can serve as a formal stability criterion, which became evident from a comparison of our results with recent quantum chemical calculations.

We apply our method to classify all isomers of C_{60} and give an example of two different cospectral isomers of C_{44}. The only input for our algorithms is the vector of positions of pentagons in the facet spiral.