
JENNIFER EDMOND, Syracuse University
Chain Configurations of 4-Clusters in Fullerenes

Fullerenes can be considered to be either a molecule of pure carbon or the trivalent plane graph with all pentagonal or hexagonal faces that models the molecule. Pairs of pentagonal faces can be connected by sequences of edges and faces in the hexagonal tessellation that we call chains. These chains are used to compute the Clar number, a parameter of much interest to chemists as it appears to indicate information about the stability of the molecule. Clusters in a fullerene are formed when a number of pentagons are isolated from the others. Pairing the four pentagons in a 4-cluster requires chains in complex configurations. The chains often wrap around one another each simultaneously affecting the other. We discuss how the configurations of 4-clusters enter into the computation of the Clar number.