Joshua Fenton* (jfenton@syr.edu), 805 Broad Street, Syracuse, NY 13210. Calculating Fries Deficit in Large Fullerenes.

A fullerene is a trivalent graph, representing a large carbon molecule, the faces of which are hexagons and 12 pentagons. A perfect matching of the edges in a fullerene is called a Kekulé structure. In this structure, a face which has 3 of its incident edges contained in the matching is called a benzene ring. The Fries number is the maximum number of benzene rings over all Kekulé structures. It is clear that for any vertex, at most 2 of the 3 incident faces could be benzene rings and so there is an upper bound on the Fries number of $\frac{2}{3}$ of the faces. Since the actual Fries number for any given fullerene may not reach this $\frac{2}{3}$ mark exactly, the difference between the true Fries number and $\frac{2}{3}$ of the faces is called the Fries deficit. I am developing tools to calculate the Fries deficit through the grouping of pentagons and measuring deficit generated in these groups. (Received September 25, 2018)