A graph-theoretical solution to a chemical problem: dominating sets and polyhedral carbon-nitrogen cages

Patrick Fowler (University of Sheffield, UK)

A problem arising in the context of a chemical synthesis programme is to find cubic polyhedral molecular frameworks in which all the atoms (vertices) are either nitrogen (N) or singly hydrogenated carbon (C), the N forming an independent dominating set and the C a perfect matching of the remaining vertices. The polyhedra have $10q$ vertices, of which $4q$ are N and $6q$ are C. A complete solution is presented for those polyhedra that are *aza-fullerenes*, i.e. based on the chemically interesting fullerene polyhedra (cubic polyhedra with 12 pentagonal faces and all other faces hexagonal). Unique solutions exist for fullerenes with 20, 40 and 50 vertices; for 60-vertex fullerenes, there is a family of eight solutions related by transformations of the underlying polyhedra. It is straightforward to prove that no fullerene solution with more than 60 vertices exists.

This is joint work with Peter Portius, Joseph Clarke, Tom Black, Rory M Campbell (University of Sheffield) and Wendy Myrvold (University of Victoria).

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