

The enumeration of space fullerenes

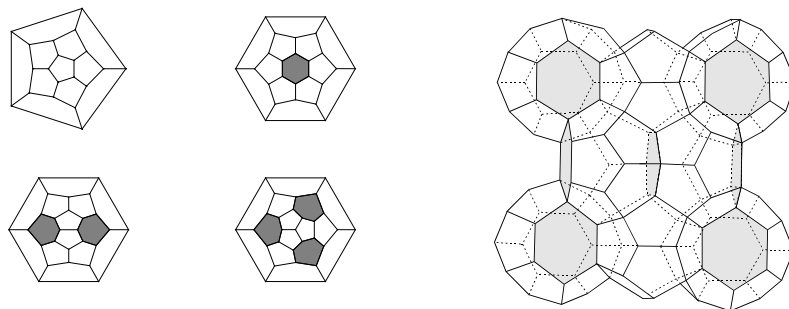
Mathieu DUTOUR

November 11, 2009

Abstract

A fullerene is a 3-valent plane graphs whose faces are pentagons and hexagons. A fullerene is said to be IHR if its hexagons are adjacent, i.e. are adjacent only to pentagons. A *space fullerene* is a 4-valent tiling of the space by IHR fullerenes. Space fullerenes are interesting in crystallography and in Discrete geometry.

See below the 4 IHR fullerene and a space fullerene:



We enumerate the space fullerenes with a small fundamental domain under their translation groups. The technique is decomposed into two steps:

- The use of Delaney symbols, i.e. flag systems, as the basic model for storing combinatorial informations and the use of the softwares **3dt** and **Systre** by Olaf Delgado for transforming combinatorial description into topological and metric ones.
- The design of programs for enumerating space-fullerenes, using all the tricks in the books of combinatorial enumeration in order to achieve the highest speed possible.