Toroidal azulenoids

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A carbon network is an azulenoid if there exists a partition of the atoms into azulenes (a five ring and a seven ring that share an edge). Azulenoids might have interesting chemical properties. [1] The question we will discuss is what the possible forms of toroidal azulenoids are, i.e. azulenoids that form a torus.

When we cut open a torus along two topologically different fundamental cycles we get a rectangle in which the opposite sides coincide to each other. These can then be used for an infinite periodic tiling of the plane. Therefore the problem of finding torus tessellations is equivalent to finding periodic tilings of the plane.

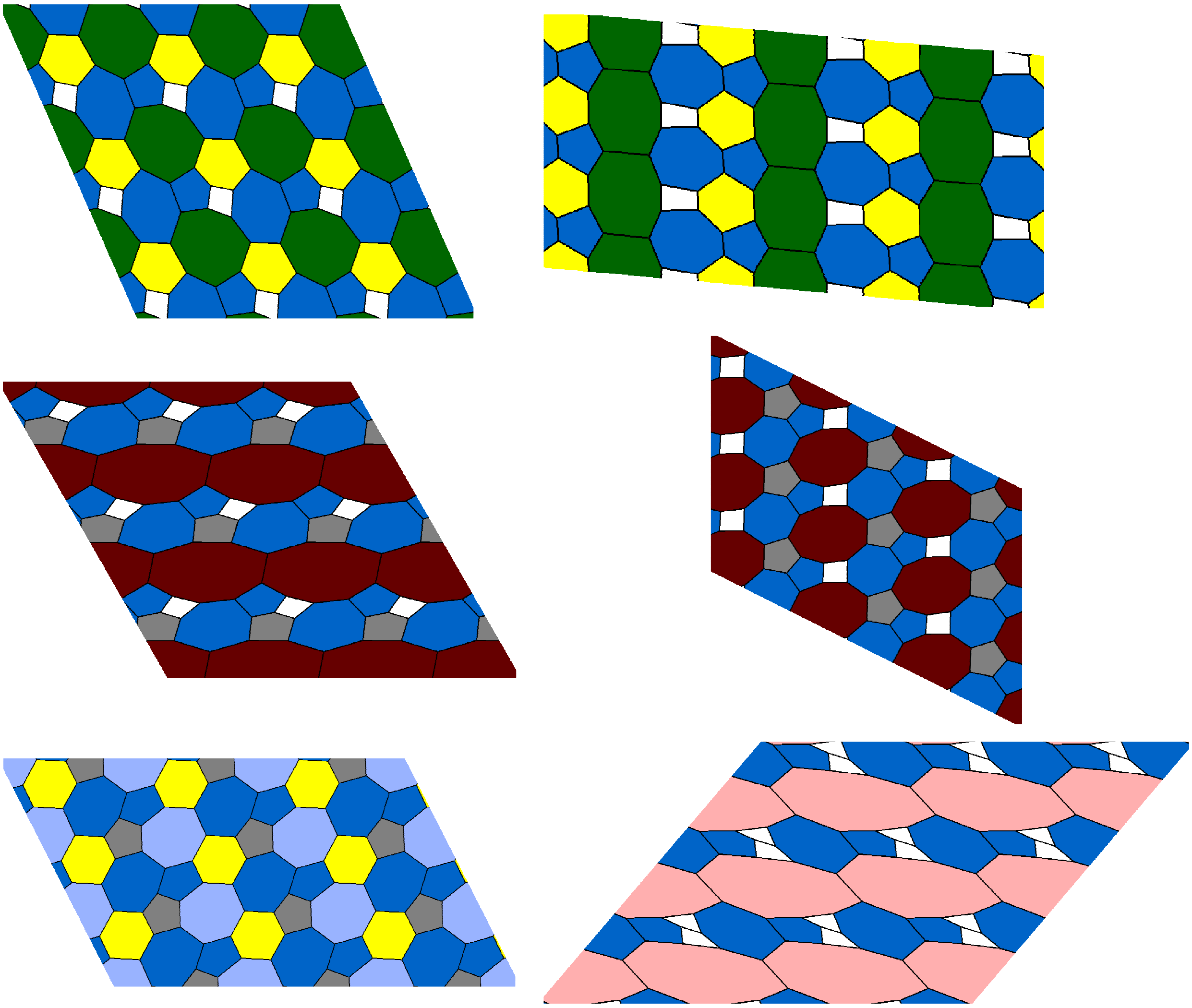
A tiling of the plane is a subdivision of the plane into faces (or tiles) in such a manner that everything is locally finite and the intersections of two different tiles are points or lines (respectively called the vertices and the edges of the tiling) or are empty. A tiling is said to be periodic when the symmetry group contains two independent translations. Intuitively this means that we only need a finite set of tiles and can then repeatedly shift this in several directions to reproduce the entire tiling.

To enumerate and classify certain types of tilings we need a symbolic description for these tilings. Delaney symbols turned out to be a very efficient means for the purpose of enumerating two and three dimensional repetitive structures. [2]

Our first task was to translate the restrictions on the azulenoids to restrictions on the Delaney symbols. Since azulene has only 8 external bonds we can start by generating tilings containing octagons and then paste in the azulenes. Therefore we started looking for tilings of the plane containing at least one orbit of octagons with the property that it is a partition of the vertices of the tiling, and where each vertex has degree 3.

We found 383 of these tilings leading to 1274 azulenoids. These numbers were confirmed by two independent approaches to the problem. A first interesting subset we can isolate is the azulenoids where there is one orbit of azulenes under the subgroup of translations. Intuitively this means that all the azulenes are pointing in the same directions. There are six of these azulenoids and they are shown in the illustration below.

Ongoing work is to search these tilings chemically interesting and realistic structures.



References

[1] Douglas Lloyd (**1984**) Non-Benzenoid Conjugated Carbon Compounds. *Studies in Organic Chemistry Vol. 16*, Elsevier, Chapter 8, p350. ISBN 0-444-42346-X.

[2] O. Delgado-Friedrichs, A.W.M. Dress, D.H. Huson, J. Klinowski and A.L. Mackay (**1999**) Systematic enumeration of crystalline nets. *Nature*, **400**, 644-647.