Toroidal azulenoids

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Abstract for **oral communication**

Azulene ($C_{10}H_8$) is a fully-conjugated bicyclic system that is iso-electronic with naphthalene. It consists of a five-ring and a seven-ring that share two carbon atoms and a bond. Within Huckel theory, aromatic behaviour might be expected on the grounds that, like naphthalene, it can be seen as a '*4n+2*' annulene with a bridging bond, and also that, should a pi-electron migrate towards the five membered ring then in principle two 'aromatic-sextets' could be formed. Consistent with this view is that it has a small dipole moment, and does indeed show some aromatic properties, under milder conditions. Some azulene derivatives can form stable salts with a strong acid. [1]

We don't yet know whether and how the electron mobility might manifest itself among azulenes embedded within a fullerene-style network, nor how many variations of such networks are theoretically possible. A fully resonant azulenoid is a network of carbon atoms such that there exists a partition of the atoms into azulenes. 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.

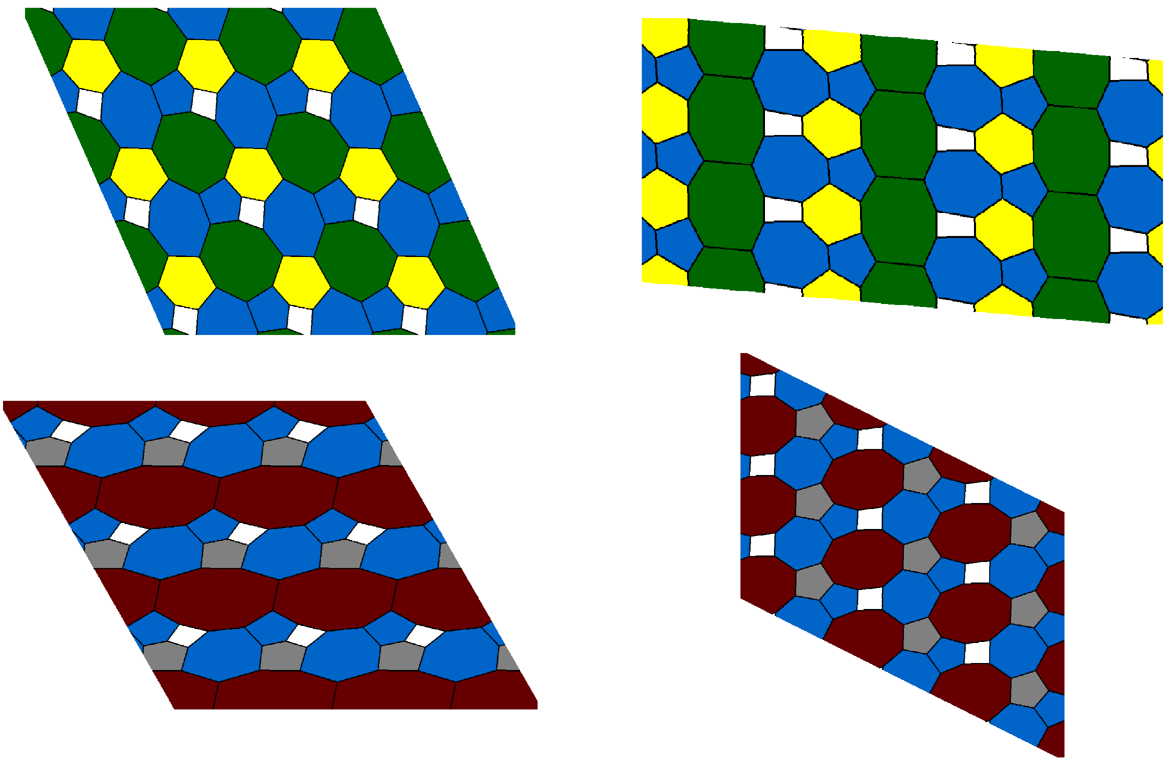
A tiling of the plane is a subdivision of the plane into faces (or tiles) in such a manner that everything is locally finite and the intersections of two different tiles are points or lines (respectively called the vertices and the edges of the tiling) or are empty. A tiling is said to be periodic when 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.

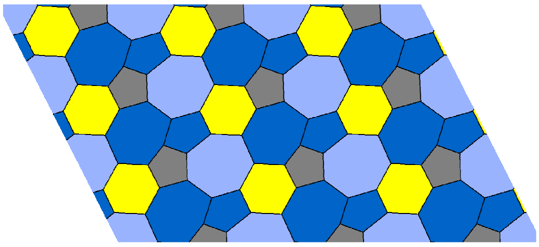
To enumerate and classify certain types of tilings we need a symbolic description for these tilings. Delaney symbols turned out to be a very efficient means for the purpose of enumerating two and three dimensional repetitive structures. [2]

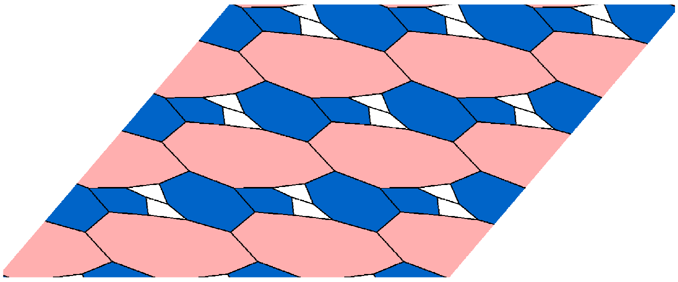
We decided that we would start by looking at all the fully-resonant azulenoids with only one orbit of azulenoids. This means that the complete network looks the same from each azulenes viewpoint. Our first task was to translate the restrictions on the azulenoids to restrictions on the Delaney symbols. 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.