Face Independence Numbers of Fullerenes

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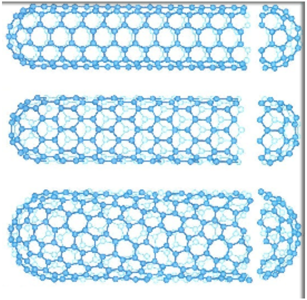
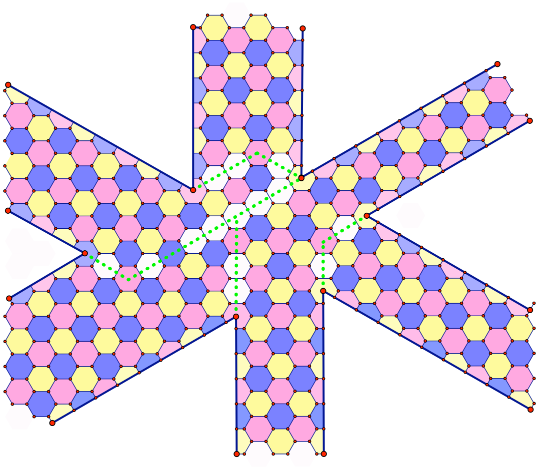
Nanotubes

Suppose we have a Fullerene with the pentagonal faces in two groups of 6.
Within each group, the pentagons are "close" to each other
This class of Fullerenes represents nanotubes

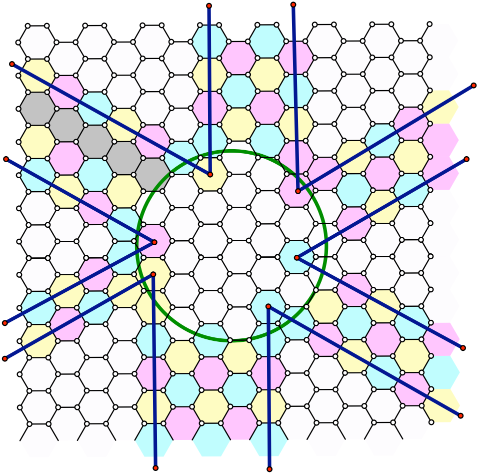


We would like to explore fullerenes of this type in which we are able to three color the hexagonal patch between the two groups of pentagons

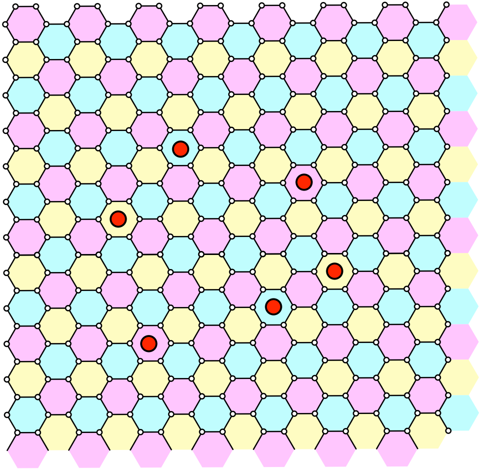
In the cap of this fullerene, the faces that cannot be 3-colored are only on the dotted segments between pentagons. The hexagonal faces outside of this group of pentagons can be 3-colored.



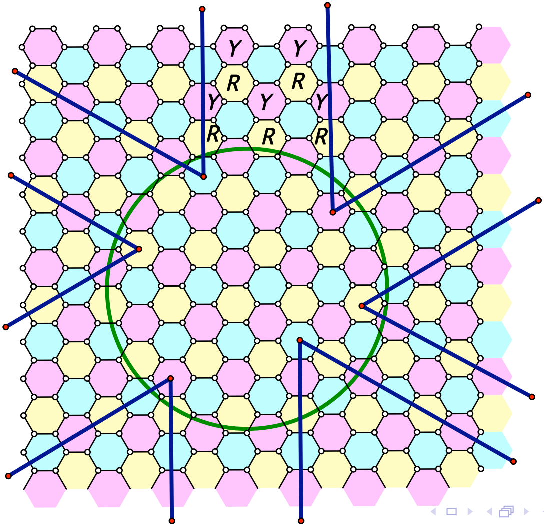
The hexagonal faces around this 6-set (outside the green circle) cannot be 3-colored. The gray line of faces cannot be colored and will extend until we reach the other cap of pentagonal faces.



Start with a 3-colored hexagonal tessellation of the plane. A cap of a nanotube-like Fullerene will contain 6 pentagonal faces.

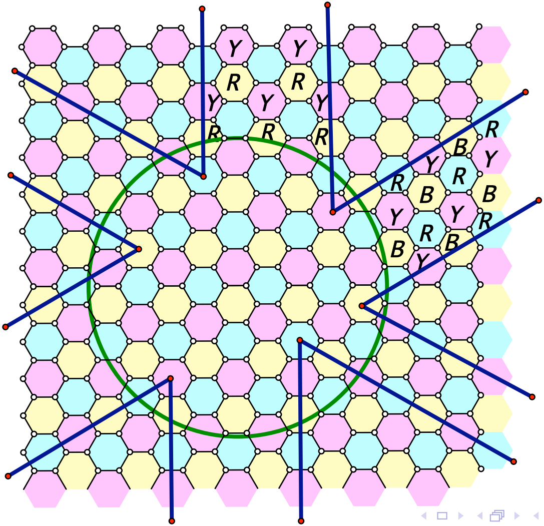


When we make a hexagonal face into a pentagonal face, we cut out a 60 degree angle and identify the two edges of the cut. As we go clockwise around the cut for the blue pentagonal face, we have interchanged the red and yellow faces, but fixed the blue faces.

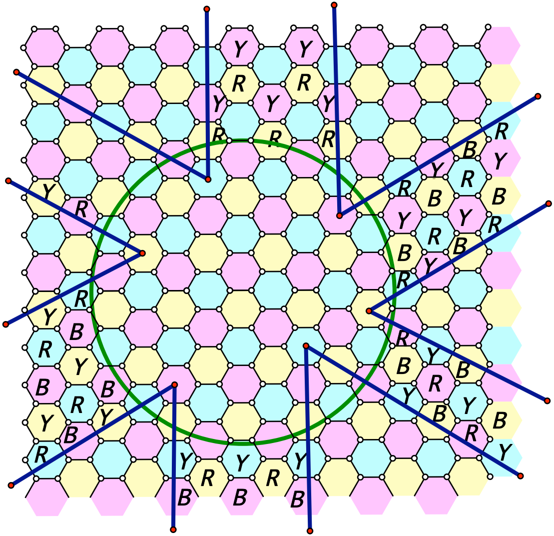


The next face in clockwise order is red.

The Blue face permuted the red and yellow faces while fixing the blue faces. A red face will permute the original yellow and blue faces while fixing the red. If we apply these two permutations in order, we have (by)(ry)= (rby)



All 6 pentagonal faces in clockwise order are blue, red, yellow, blue red, yellow. The permutations associated with these will be (br)(by)(ry)(br)(by)(ry). Composing these permutations, we get the identity.



Inserting a pentagonal face is equivalent to a permuting the color classes of the faces. This permutation fixes the color corresponding to the pentagonal face, and permutes the remaining two colors. The colors of the pentagonal faces are just elements of the permutation group S_3 acting on the set of color classes.

The faces outside a set of pentagons can be 3-colored exactly when the permutations compose to give the identity. When the composition of permutations is the identity, each color is mapped to itself, and so the 3-coloring matches up around the outside of the set of pentagons. Thus the colors of the pentagonal faces in the original 3-coloring of the hexagonal tessellation of the plane and the circular order of the cuts determines whether or not the coloring matches up around a set of pentagons.

Group Table

I	B	R	Y	A	A^{-1}
B	I	A	A^{-1}	R	Y
R	A^{-1}	I	A	Y	B
Y	A	A^{-1}	I	B	R
A	Y	B	R	A^{-1}	I
A^{-1}	R	Y	B	I	A

B= (ry)   R= (by)   Y = (br)   A=(byr) A^{-1}=(bry)

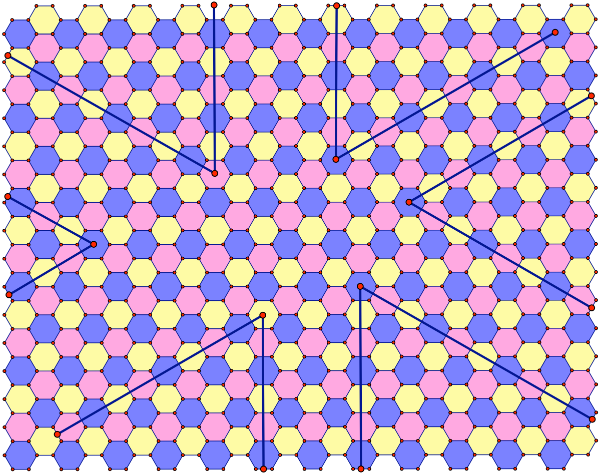
- The composition of any odd set of pentagons will give a permutation of two colors. The coloring cannot close around an odd set of pentagons, and exactly one color will be fixed outside the grouping.
- In an even cluster of pentagons, either the coloring works around the outside or all three colors are permuted.

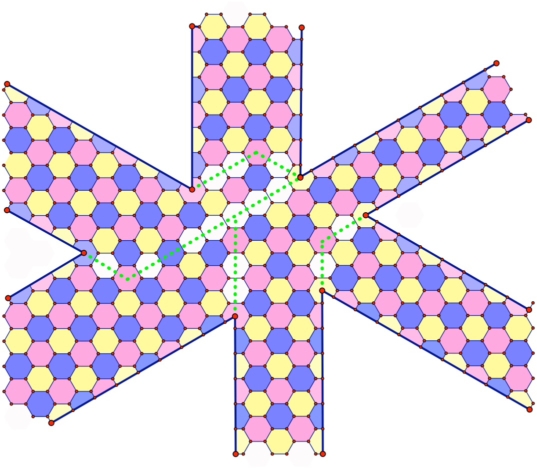
The previous example was a 6-set: The coloring works around these 6 pentagons, but there are no smaller clusters around which the coloring works. Groups of 6 pentagons around which the coloring works can break up into a set of 4 and a set of 2, or into 3 2-sets.

In clockwise order, the pentagonal faces are RBBBYB. The permutations are (ry)(br)(ry)(ry)(ry)(by)=(ry)(br)(ry)(by)

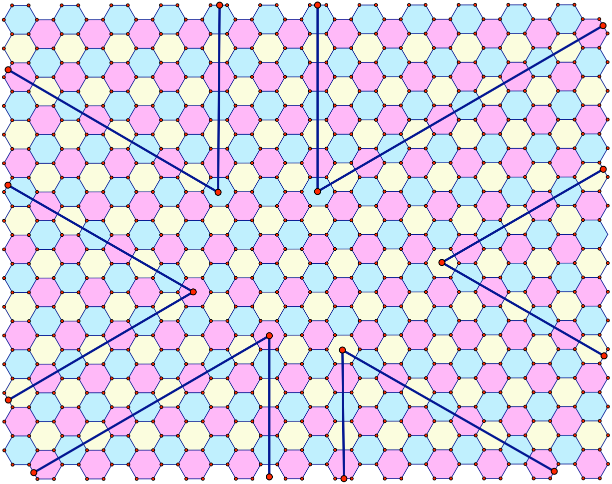
$$b \to y \to r \to b \qquad y \to b \to r \to y \qquad r \to y \to r$$

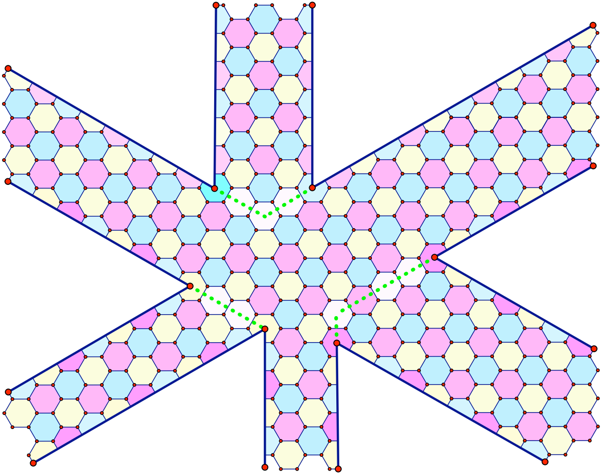
Two permutations compose to give the identity, as do the remaining 4.





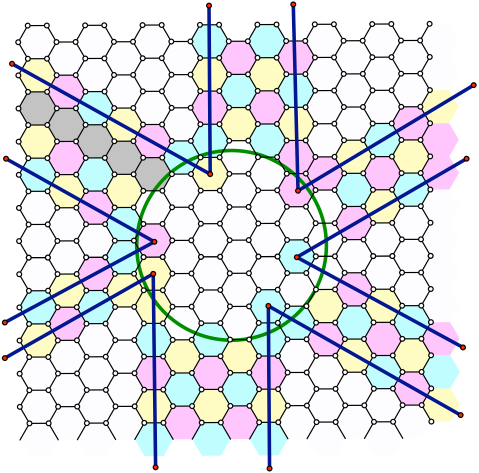
The pentagonal faces on the cap of this fullerene are BBYYRR.
The permutations are (by)(by)(br)(br)(ry)(ry)
These 6 pentagons will break up into 3 pairs around which the coloring works.





The 3-coloring does not match up around the outside of these 6 pentagons. All 3 colors are permuted in the final composition. YRBBYR
(by)(br)(ry)(ry)(by)(br)=(by)(br)(by)(br)

$$b \to r \to b \to y \qquad r \to b \to y \to b \qquad y \to b \to r$$



We want to determine the maximal face independent set within a 6-set where the coloring works. Connecting the pentagonal faces with different segments can change the face independence number and the Kekule Structure.