

Toroidal azulenoids

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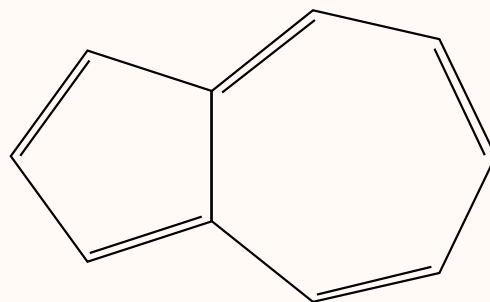
(Joint work with Gunnar Brinkmann, Olaf Delgado-Friedrichs and Edward Kirby)



Outline

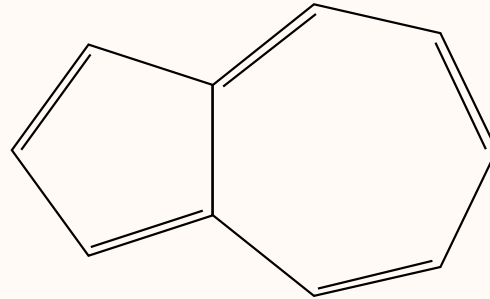
1. Motivation
2. Translation to tiles
3. Tools
4. Methods
5. Results

Azulenoids



Azulene

Azulenoids



An azulenoid is a carbon network (cubic) for which there exists a partition of the vertices into azulenes.

Question

How many variations of such networks are theoretically possible if there can only be one orbit of azulenes under the symmetry group?

Edward Kirby

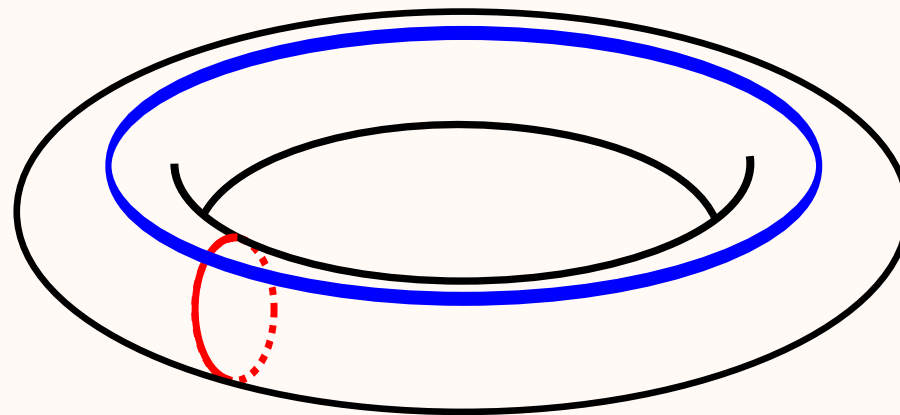
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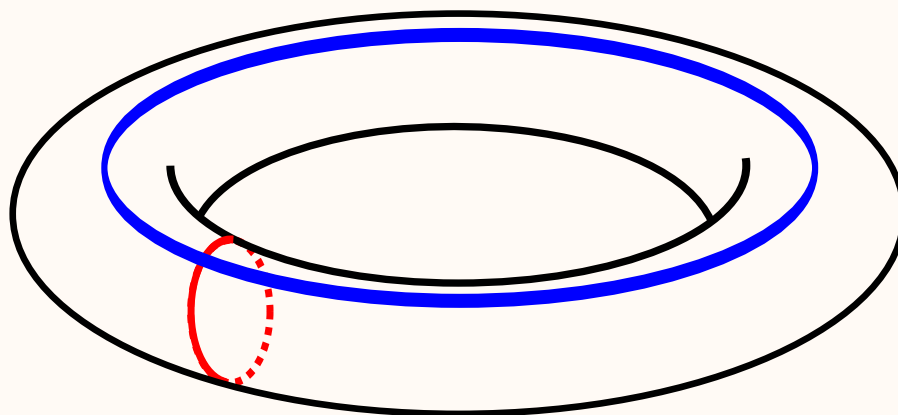
Edward Kirby

Toroidal, but also planar and cylindrical

Torus



Torus



Tiling

Tiling T = set of tiles t_1, t_2, \dots with $t_i \subset \mathbb{E}^2$, t_i homeomorph to $\overline{B}(0, 1)$ that satisfy the following conditions:

1. $\bigcup_{t \in T} t = \mathbb{E}^2$
2. $\forall t_i, t_j (i \neq j) \in T : t_i^\circ \cap t_j^\circ = \emptyset \wedge t_i \cap t_j \in \{\emptyset, \{\text{points}\}, \{\text{lines}\}\}$.
3. $\forall x \in \mathbb{E}^2 : x$ has a neighbourhood that only intersects a finite number of tiles.

Tiling

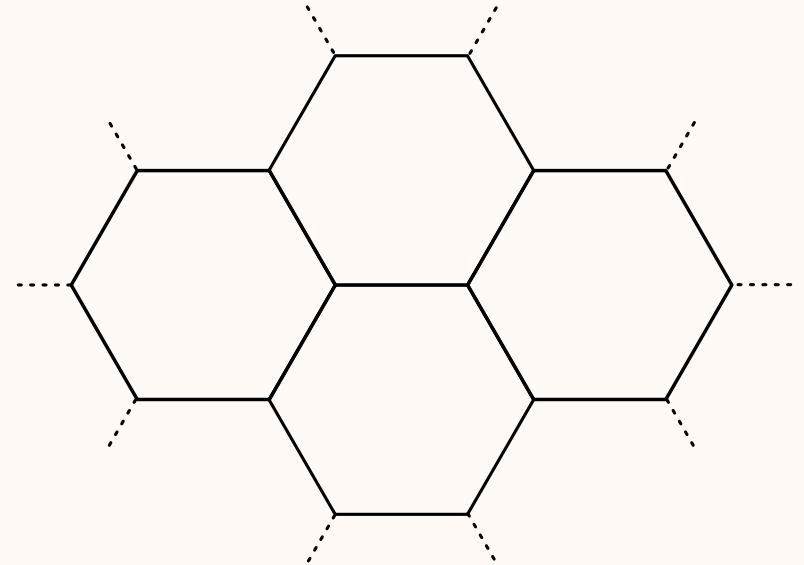
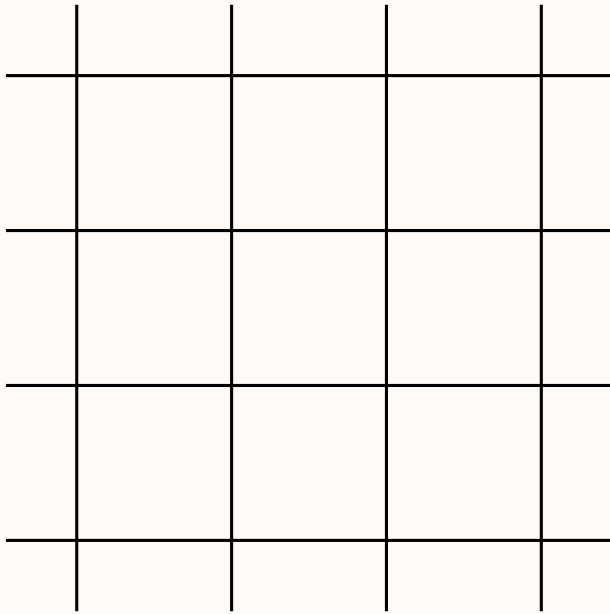
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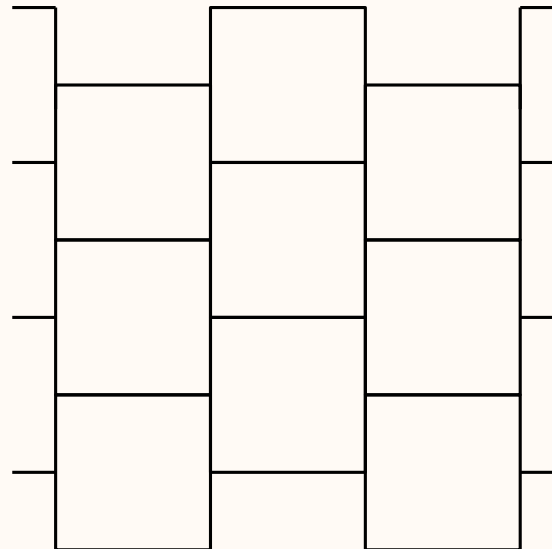
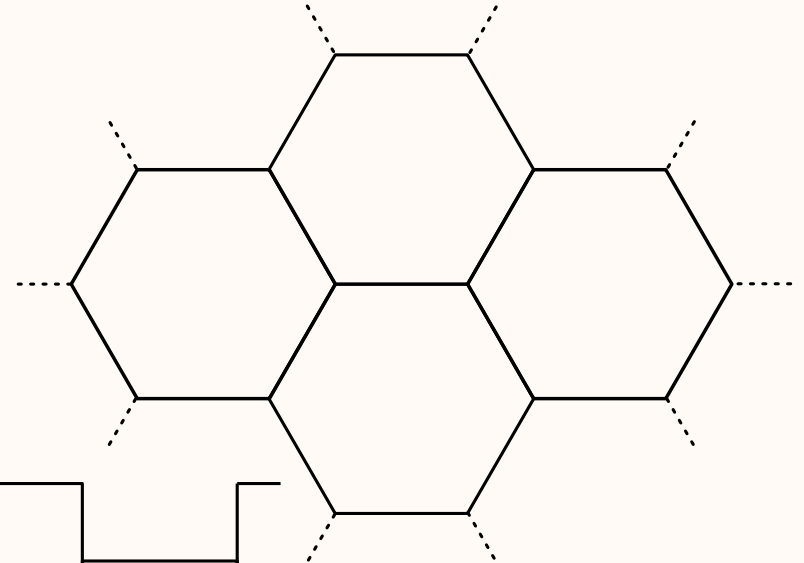
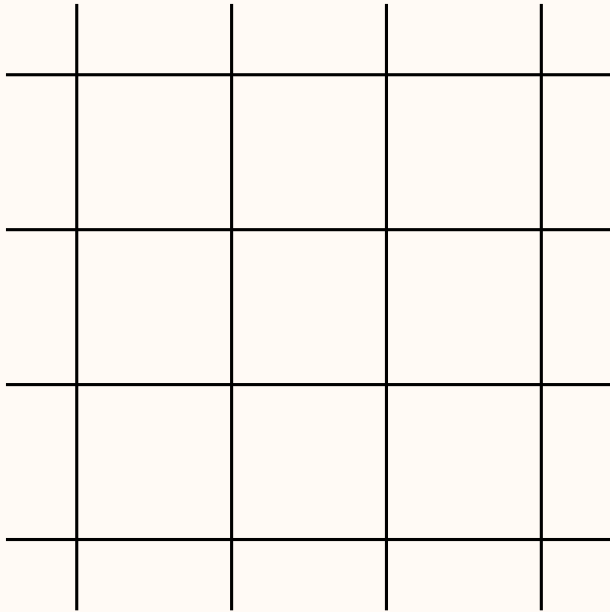
Periodic tiling \iff

symmetry group contains *two independent translations*

Example tiling



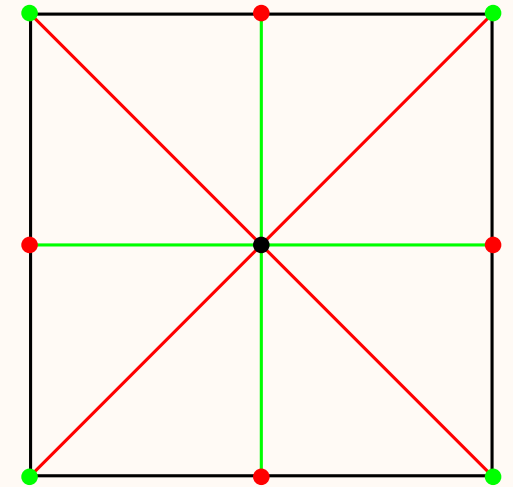
Example tiling



Barycentric subdivision

- For each face: one point
- For each edge: **one point**
- For each vertex: **one point**

⇒ subdivision consists of triangles



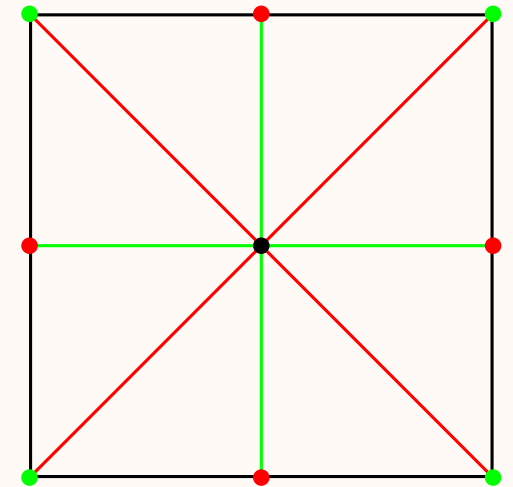
Chamber system

Define $\Sigma = \langle \sigma_0, \sigma_1, \sigma_2 \mid \sigma_i^2 = \mathbf{1} \rangle$

σ_0 : change the green point (vertex).

σ_1 : change the red point (edge).

σ_2 : change the black point (face).



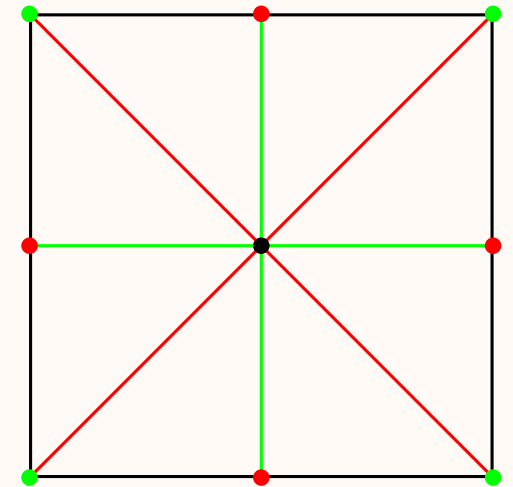
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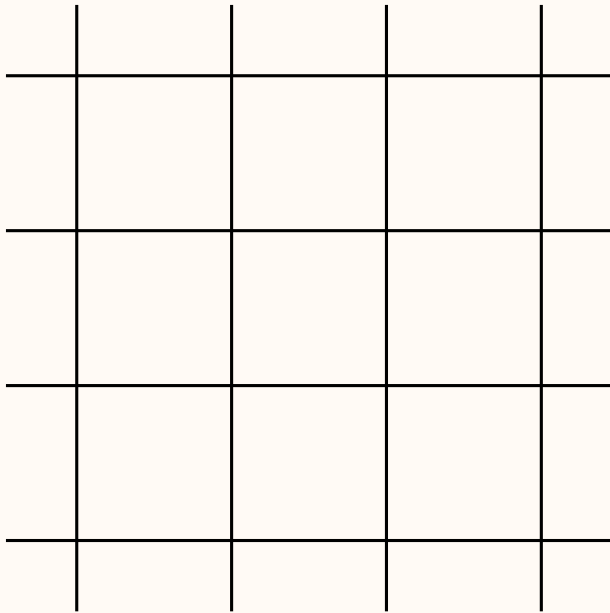


Chamber system \mathcal{C} of $T =$ barycentric subdivision together with Σ

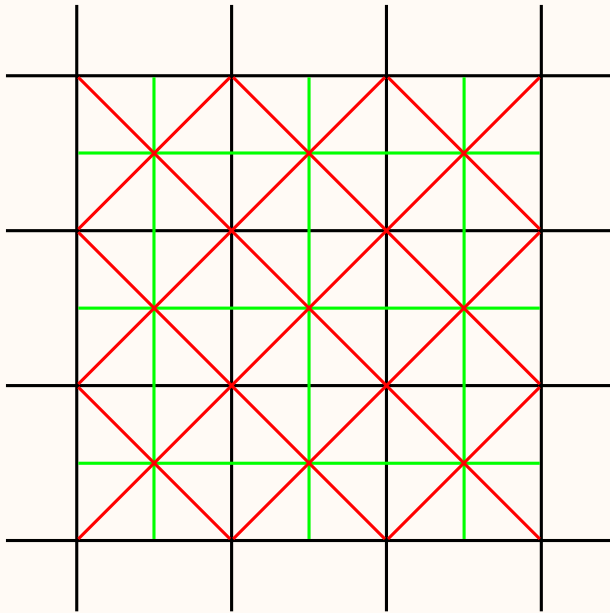
Delaney/Dress graph

The Delaney/Dress graph \mathcal{D} of a periodic tiling is the set of *orbits of the chambers* of the chamber system of the tiling under the symmetry group.

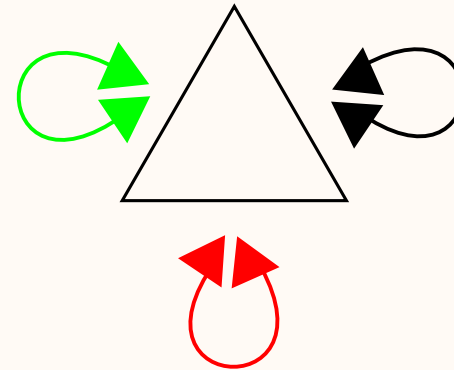
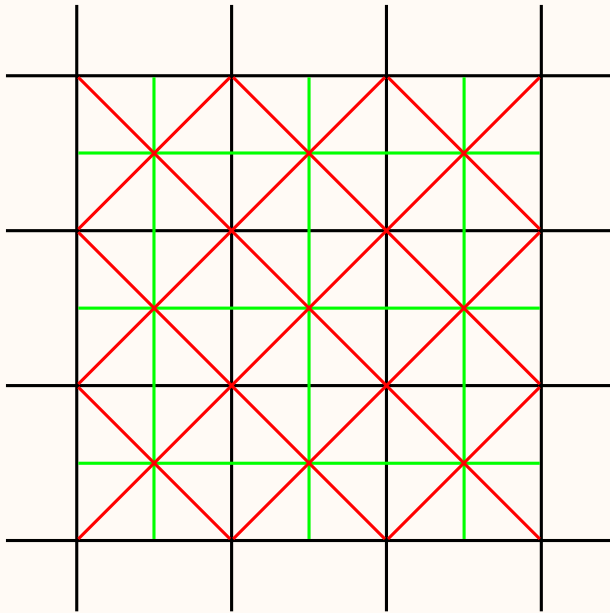
Example Delaney/Dress graph



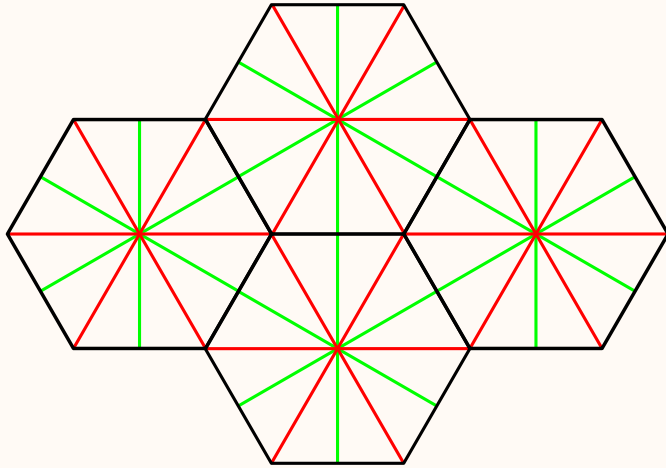
Example Delaney/Dress graph



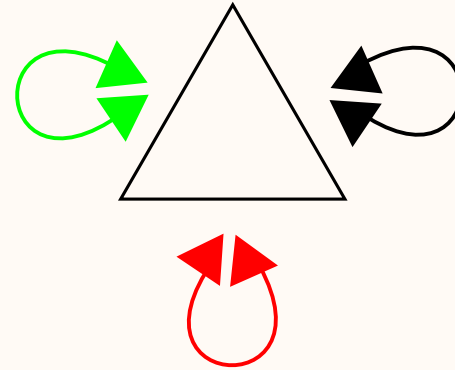
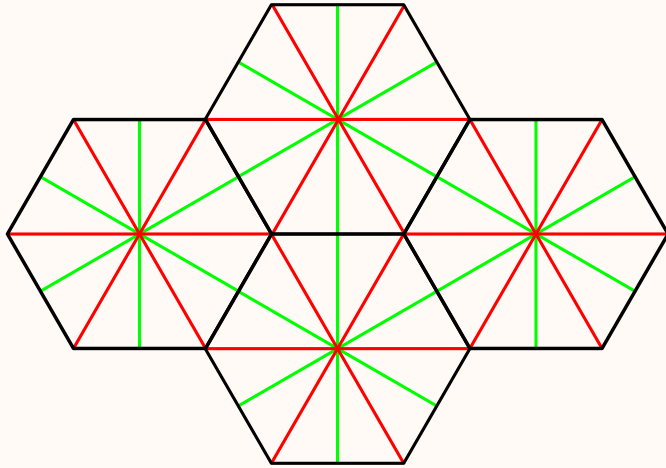
Example Delaney/Dress graph



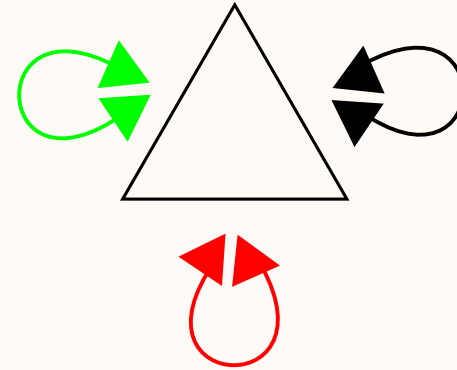
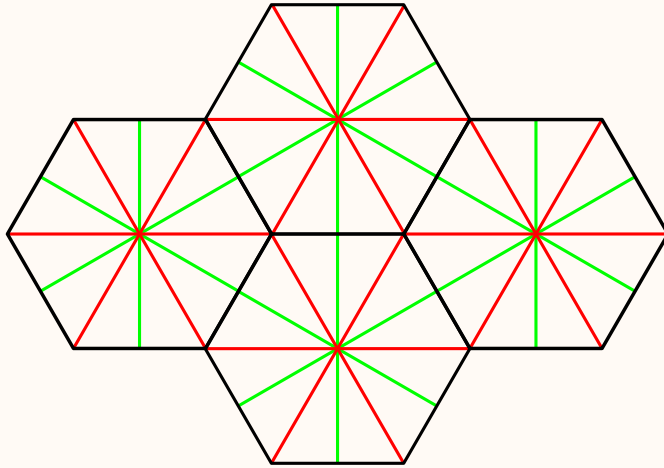
Example Delaney/Dress graph



Example Delaney/Dress graph



Example Delaney/Dress graph



⇒ Delaney/Dress graph is not sufficient to distinguish between tilings!

Delaney/Dress symbol

Define functions $r_{ij} : \mathcal{C} \rightarrow \mathbb{N}; c \mapsto r_{ij}(c)$ with $r_{ij}(c)$ the smallest number for which $c(\sigma_i \sigma_j)^{r_{ij}(c)} = c$.

Delaney/Dress symbol

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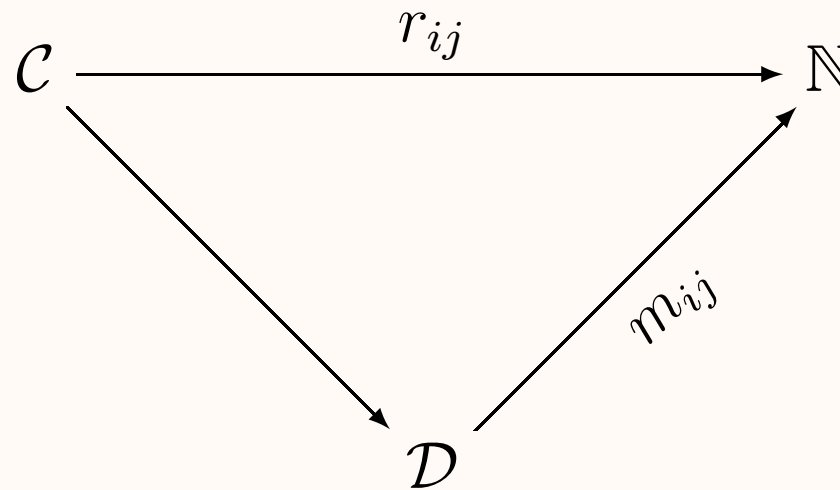
r_{02} is a constant function with value 2.

$r_{01}(c)$ is the size of the face of T that belongs to c .

$r_{12}(c)$ is the number of faces that meet in the vertex that belongs to c .

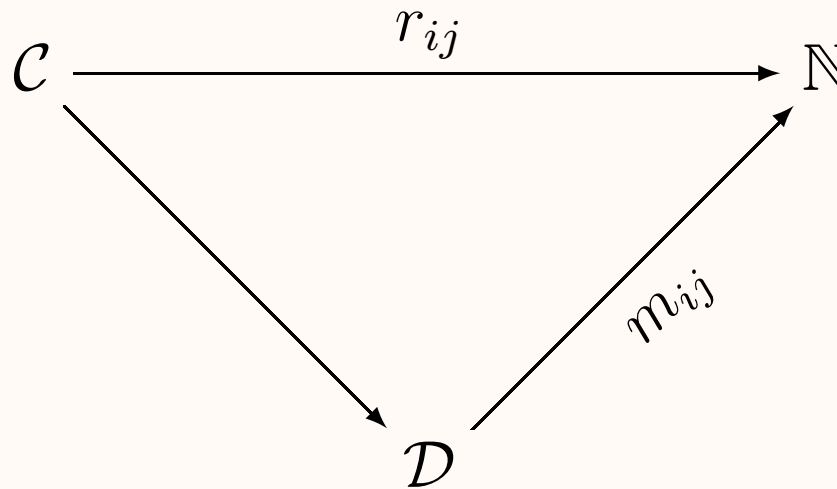
Delaney/Dress symbol

Define functions $m_{ij} : \mathcal{D} \rightarrow \mathbb{N}; d \mapsto m_{ij}(d)$ in such a manner that the following diagram is commutative:



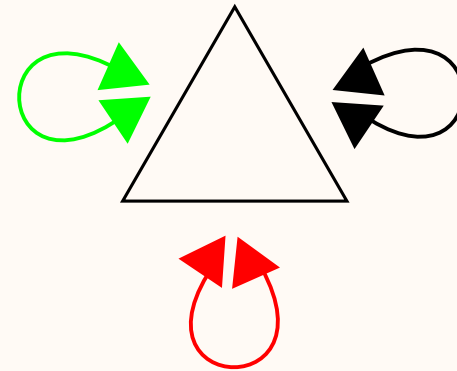
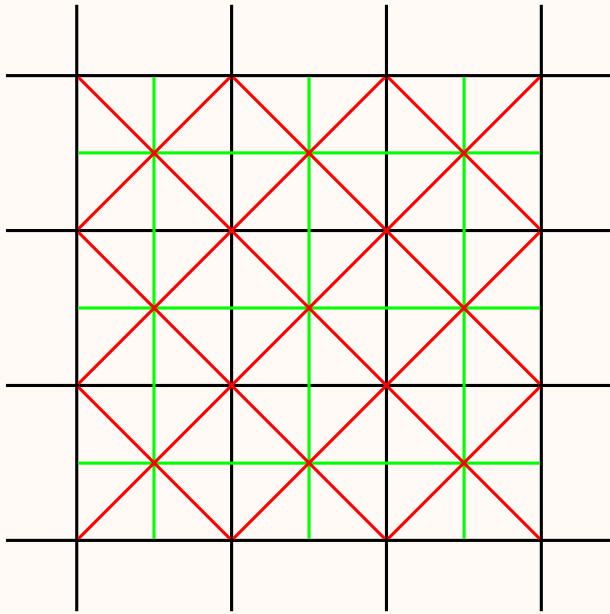
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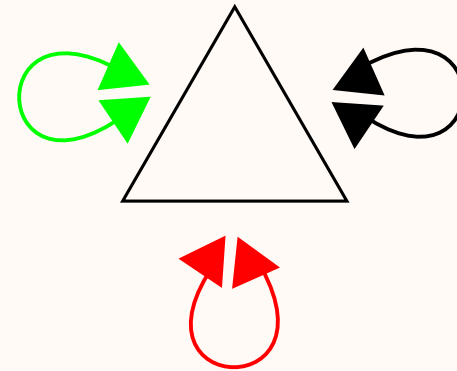
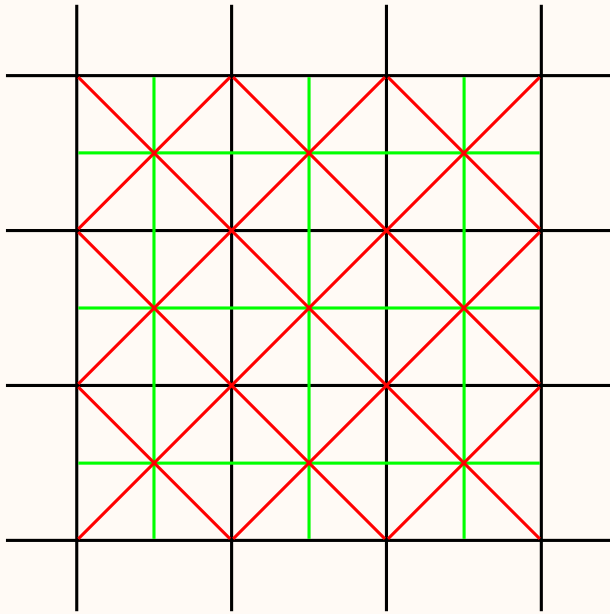


Delaney/Dress symbol of the tiling is $(\mathcal{D}; m_{01}, m_{12})$

Example Delaney/Dress symbol



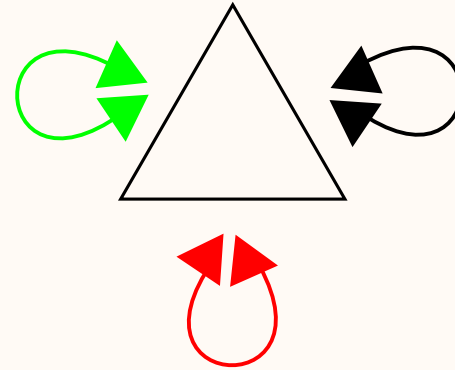
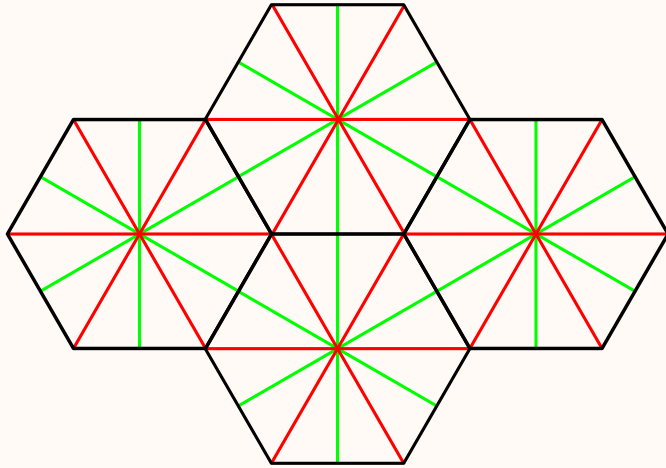
Example Delaney/Dress symbol



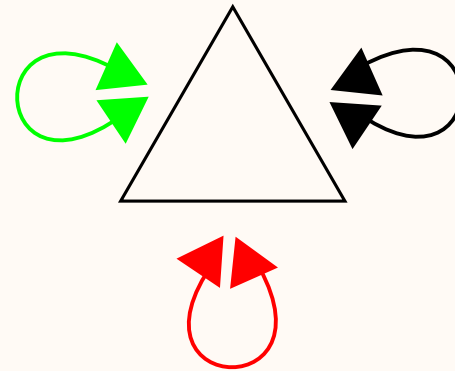
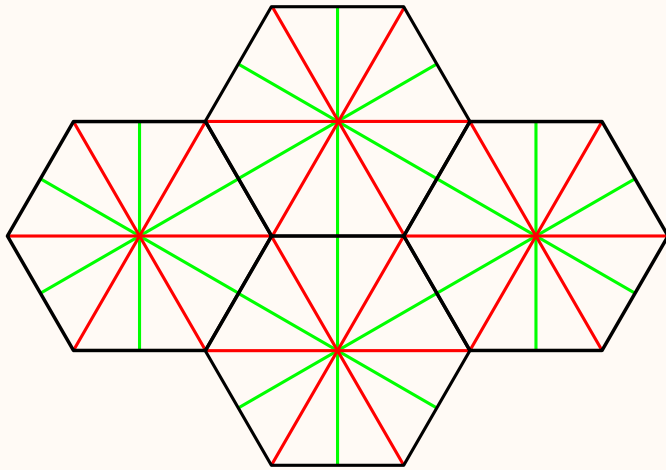
$$m_{01} = 4$$

$$m_{12} = 4$$

Example Delaney/Dress symbol



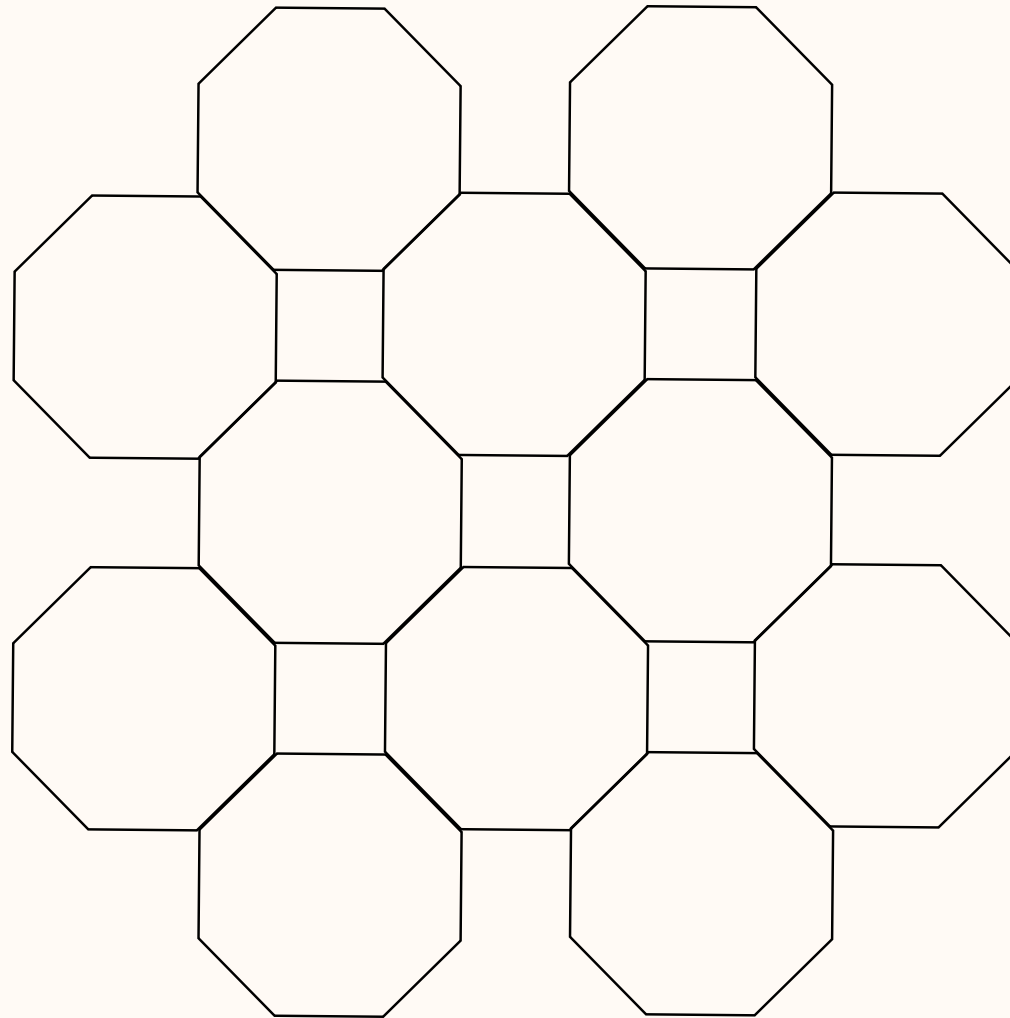
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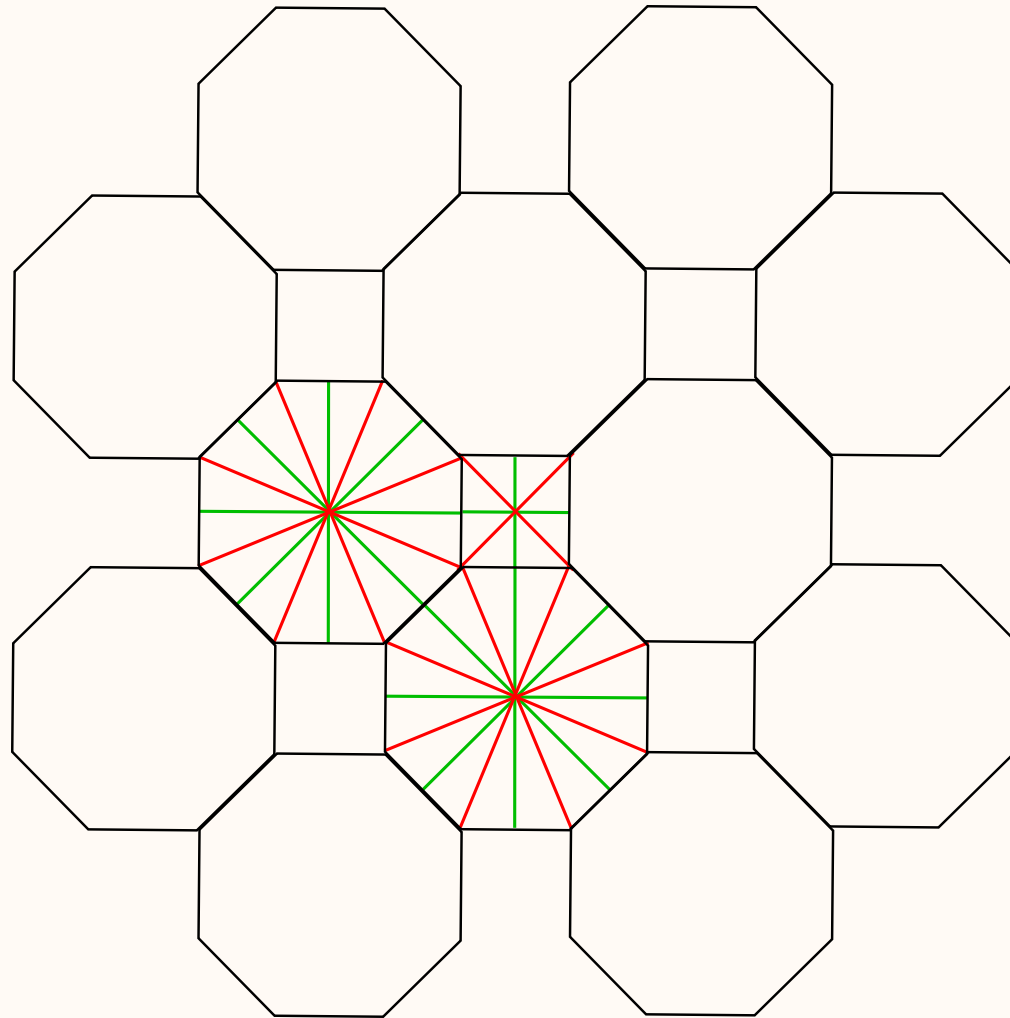
$$m_{01} = 6$$

$$m_{12} = 3$$

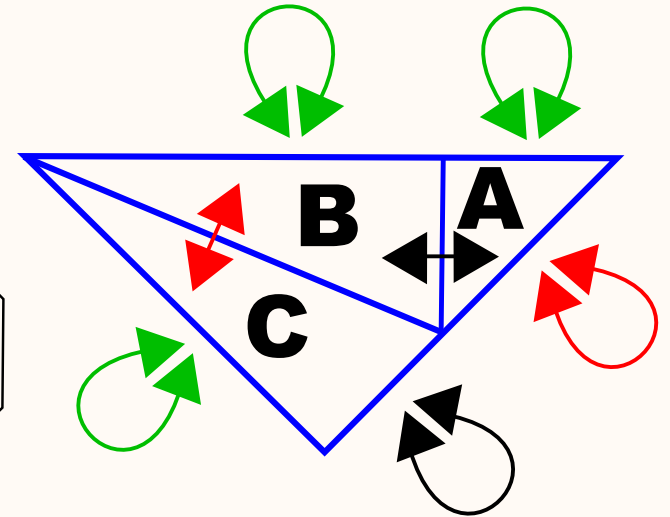
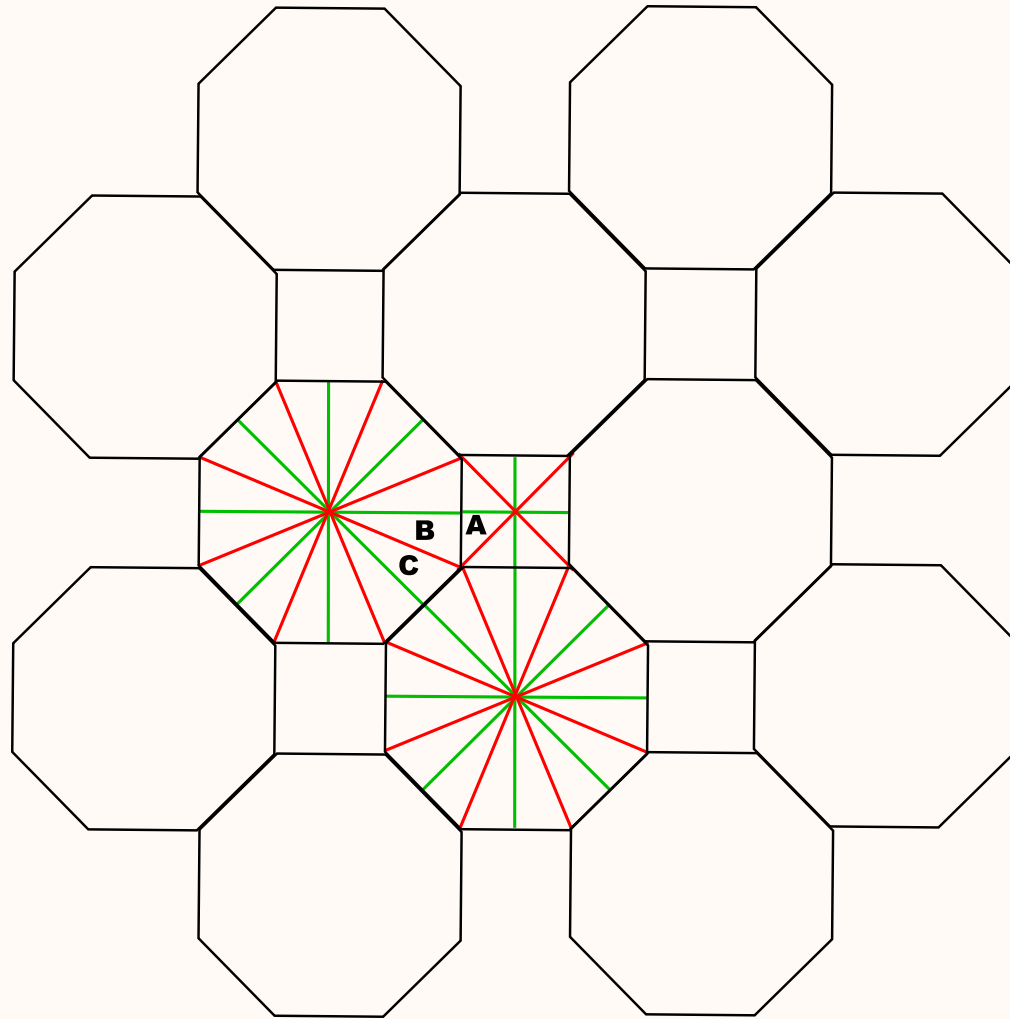
Example Delaney/Dress symbol



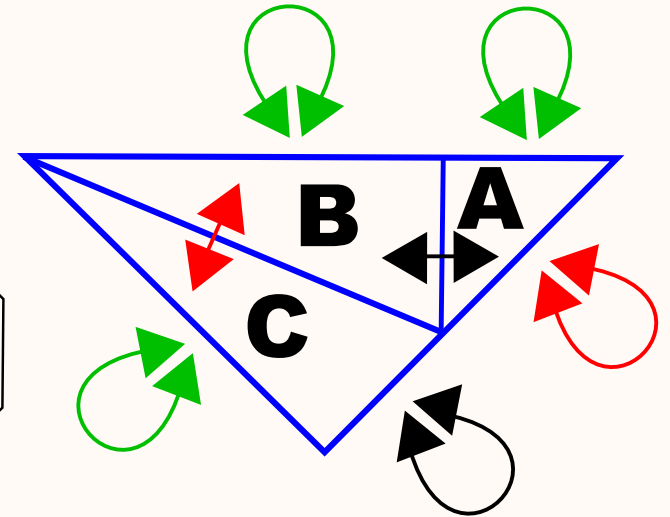
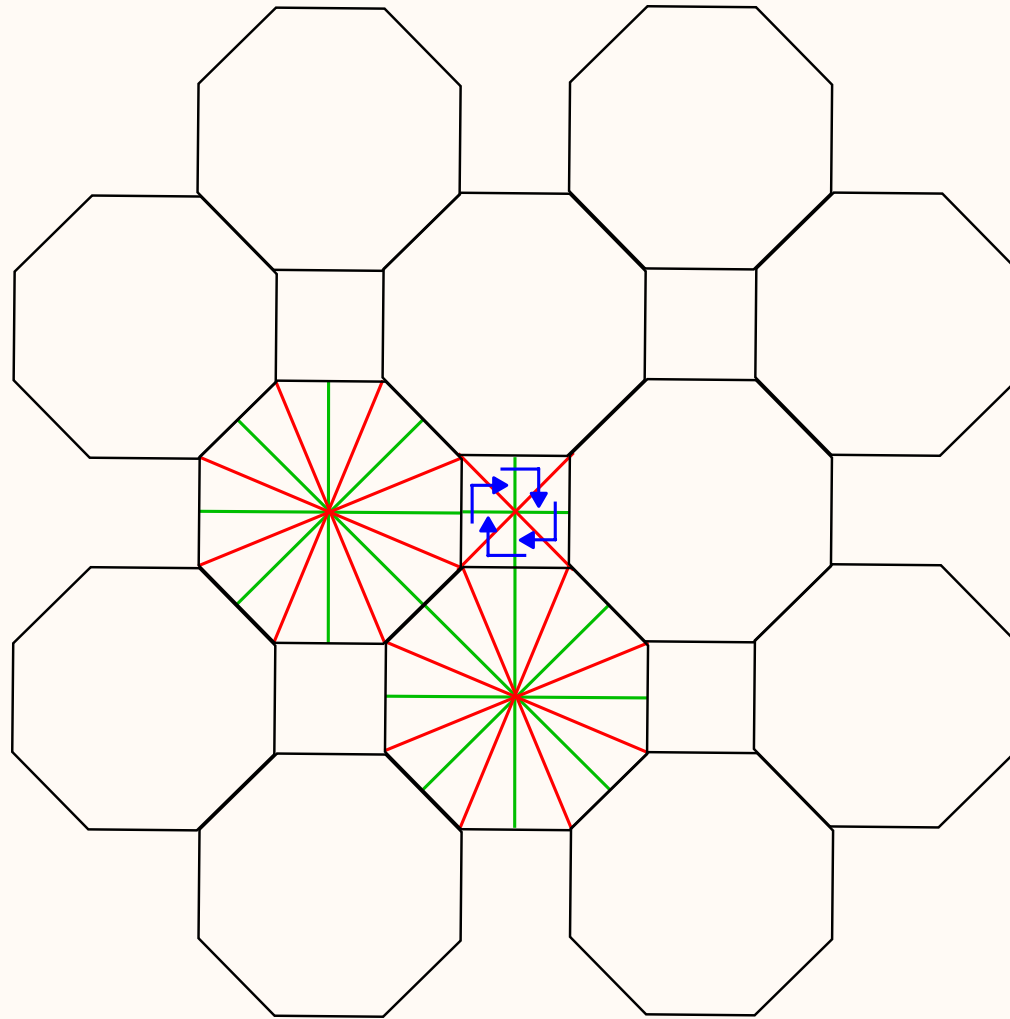
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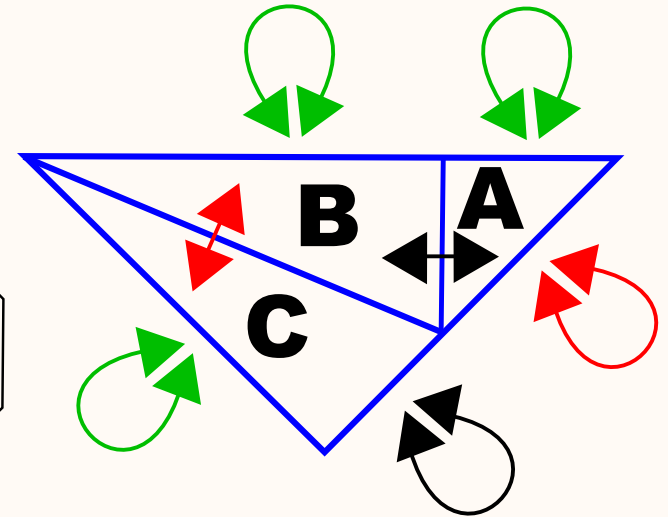
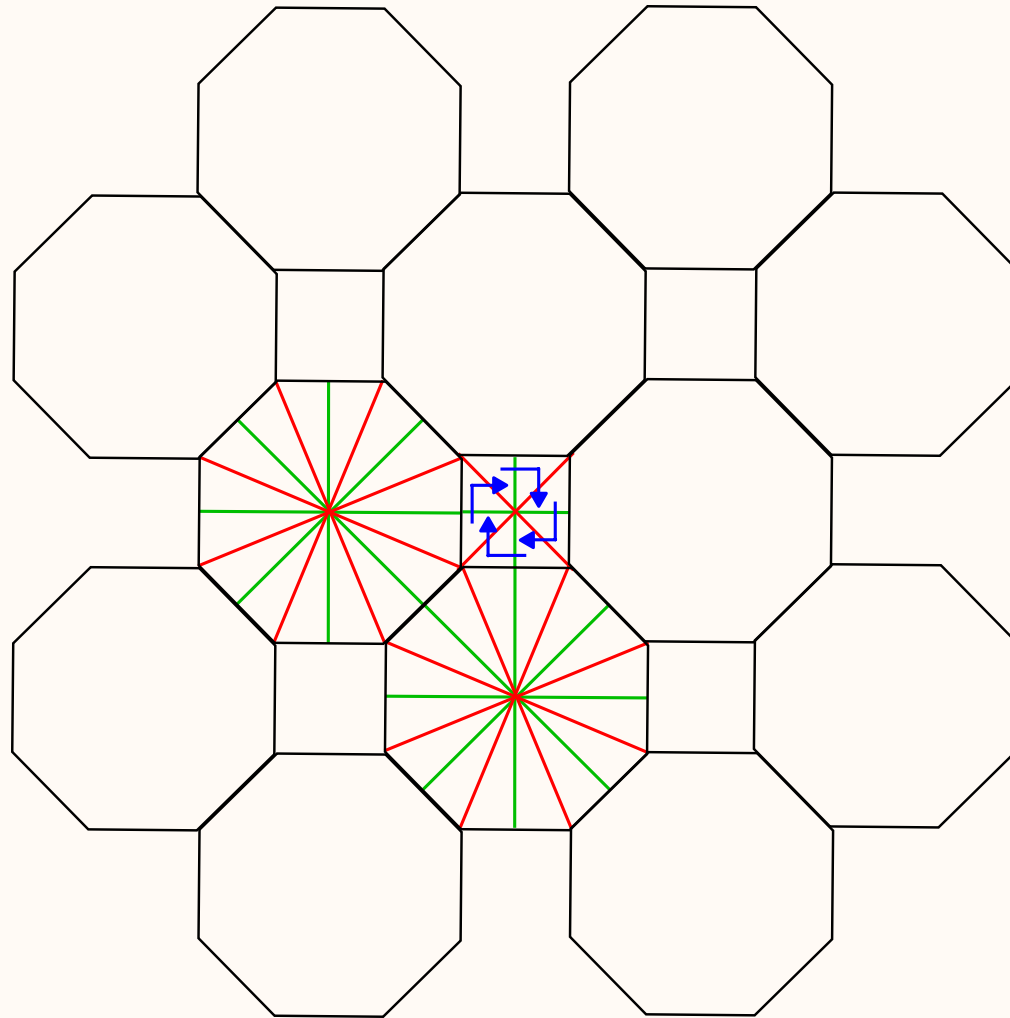
Example Delaney/Dress symbol



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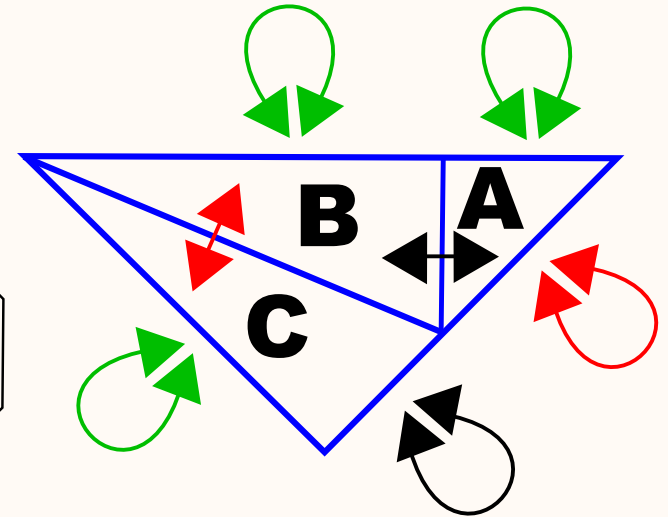
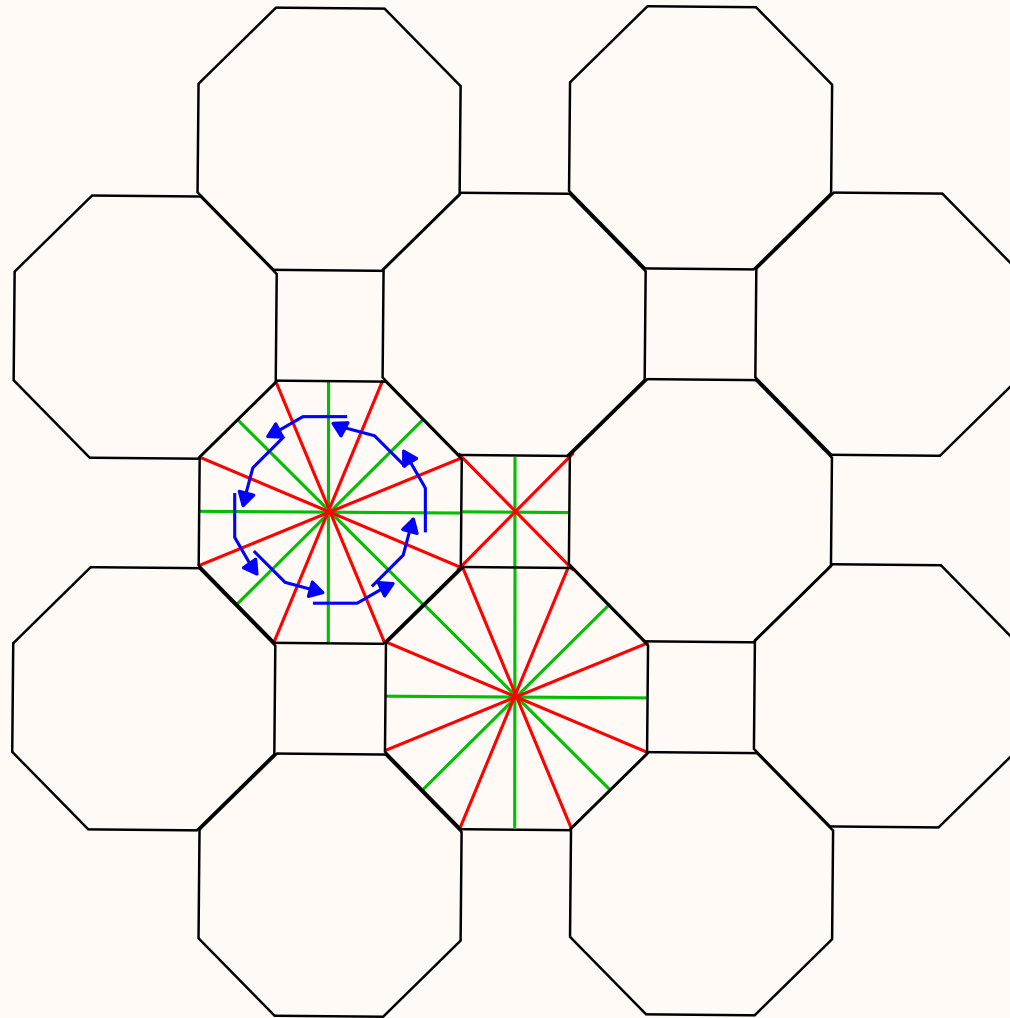


Example Delaney/Dress symbol



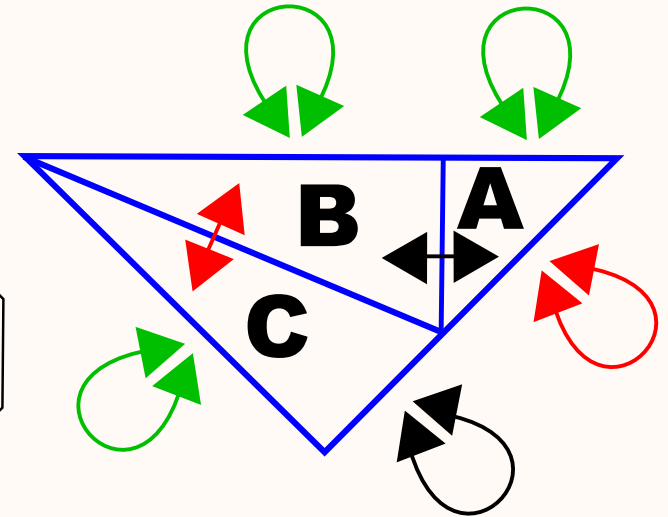
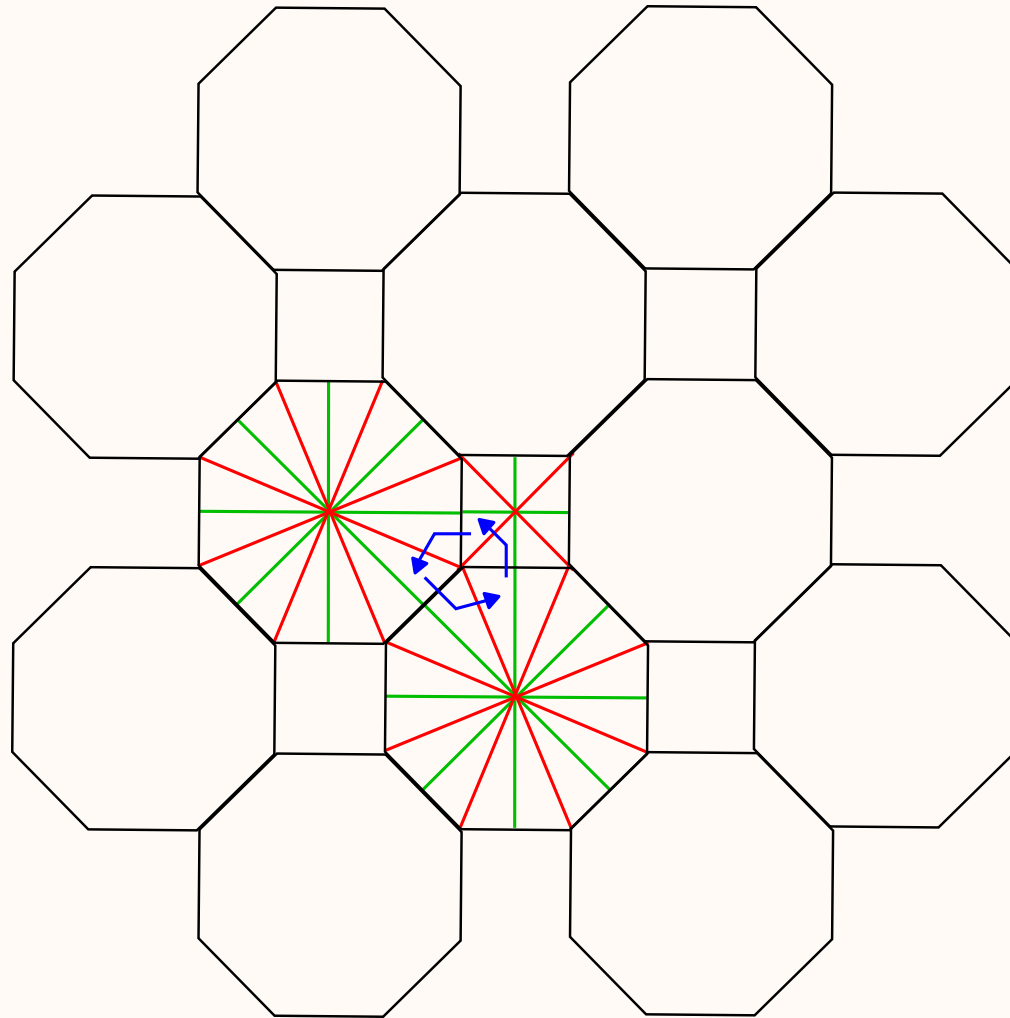
	m_{01}	m_{12}
A	4	
B		
C		

Example Delaney/Dress symbol



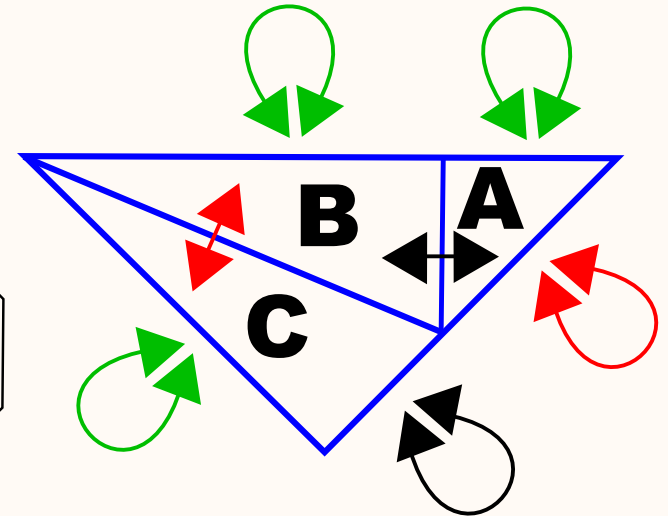
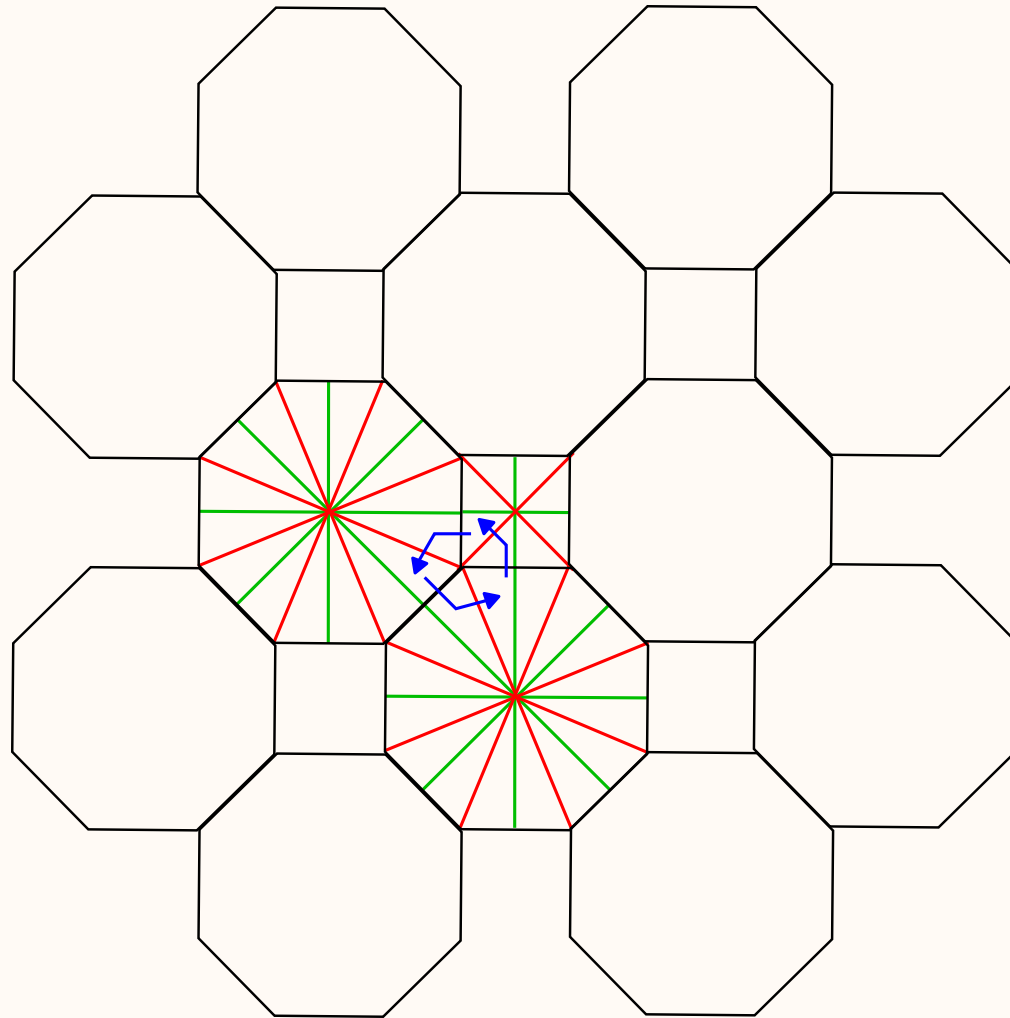
	m_{01}	m_{12}
A	4	
B	8	
C	8	

Example Delaney/Dress symbol



	m_{01}	m_{12}
A	4	
B	8	
C	8	

Example Delaney/Dress symbol



	m_{01}	m_{12}
A	4	3
B	8	3
C	8	3

Delaney/Dress symbol

$(\mathcal{D}; m_{01}, m_{12})$ is the Delaney/Dress symbol of a periodic tiling iff

1. \mathcal{D} is finite
2. Σ works transitively on \mathcal{D}
3. m_{01} is constant on $\langle \sigma_0, \sigma_1 \rangle$ orbits and
 $\forall d \in \mathcal{D} : d(\sigma_0 \sigma_1)^{m_{01}(d)} = d$
4. m_{12} is constant on $\langle \sigma_1, \sigma_2 \rangle$ orbits and
 $\forall d \in \mathcal{D} : d(\sigma_1 \sigma_2)^{m_{12}(d)} = d$
5. $\forall d \in \mathcal{D} : d(\sigma_0 \sigma_2)^2 = d$

Delaney/Dress symbol

$$K(\mathcal{D}) = \sum_{d \in \mathcal{D}} \left(\frac{1}{m_{01}(d)} + \frac{1}{m_{12}(d)} - \frac{1}{2} \right)$$

1. $K(\mathcal{D}) < 0$
2. $K(\mathcal{D}) = 0$
3. $K(\mathcal{D}) > 0$

Delaney/Dress symbol

$$K(\mathcal{D}) = \sum_{d \in \mathcal{D}} \left(\frac{1}{m_{01}(d)} + \frac{1}{m_{12}(d)} - \frac{1}{2} \right)$$

1. $K(\mathcal{D}) < 0 \rightarrow$ hyperbolic plane
2. $K(\mathcal{D}) = 0$
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Delaney/Dress symbol

$$K(\mathcal{D}) = \sum_{d \in \mathcal{D}} \left(\frac{1}{m_{01}(d)} + \frac{1}{m_{12}(d)} - \frac{1}{2} \right)$$

1. $K(\mathcal{D}) < 0 \rightarrow$ hyperbolic plane
2. $K(\mathcal{D}) = 0 \rightarrow$ euclidean plane
3. $K(\mathcal{D}) > 0$

Delaney/Dress symbol

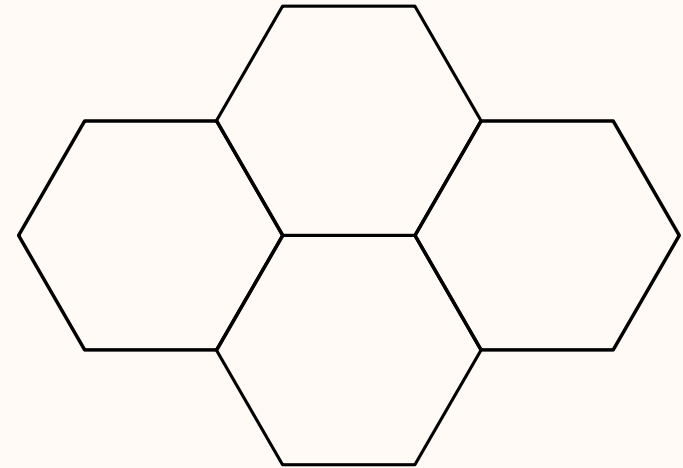
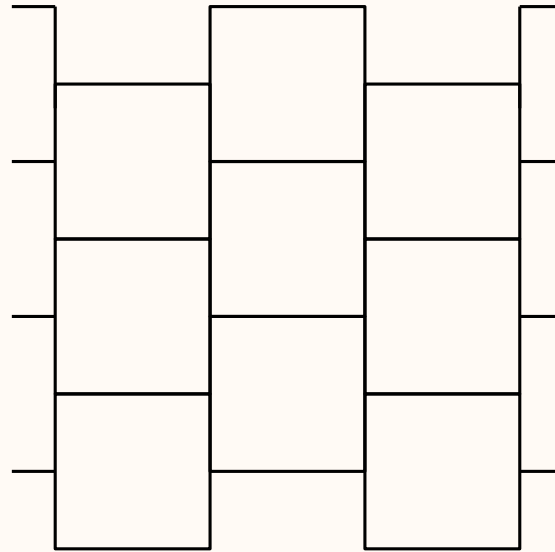
$$K(\mathcal{D}) = \sum_{d \in \mathcal{D}} \left(\frac{1}{m_{01}(d)} + \frac{1}{m_{12}(d)} - \frac{1}{2} \right)$$

1. $K(\mathcal{D}) < 0 \rightarrow$ hyperbolic plane
2. $K(\mathcal{D}) = 0 \rightarrow$ euclidean plane
3. $K(\mathcal{D}) > 0 \rightarrow$ sphere iff $\frac{4}{K(\mathcal{D})} \in \mathbb{N}$

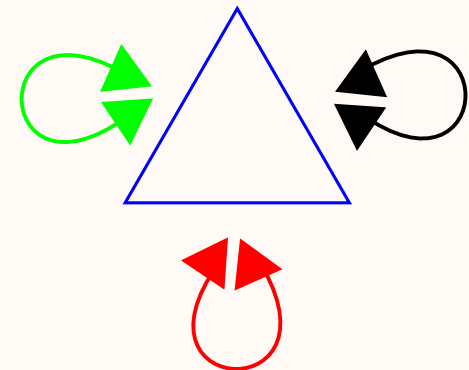
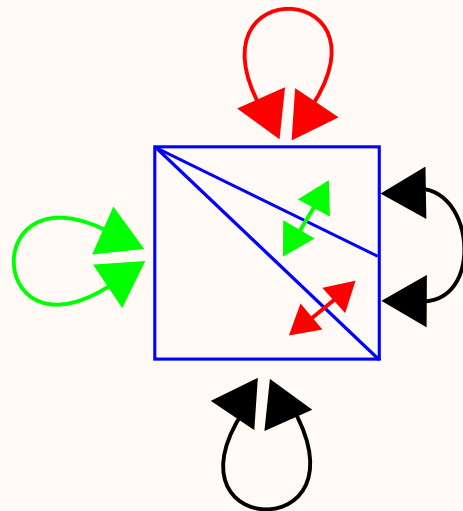
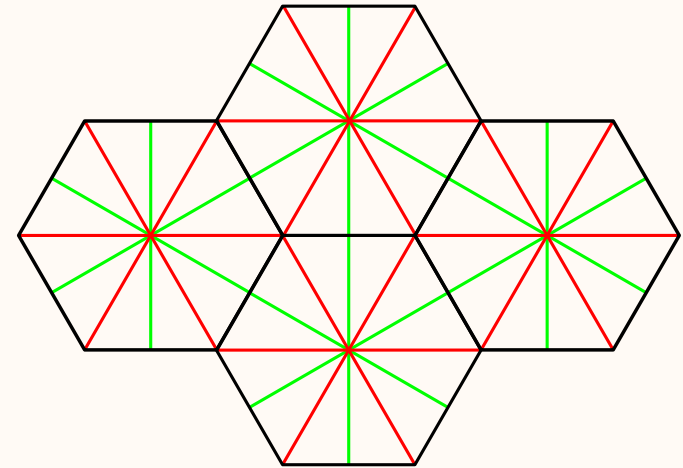
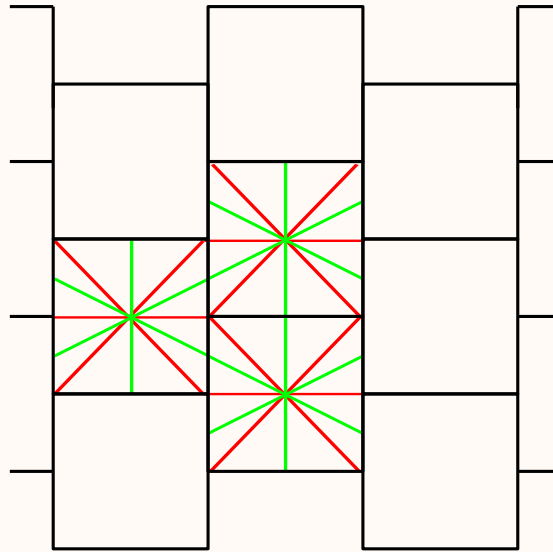
Representation

	σ_0	σ_1	σ_2	m_{01}	m_{12}
1	$\sigma_0(1)$	$\sigma_1(1)$	$\sigma_2(1)$	$m_{01}(1)$	$m_{12}(1)$
2	$\sigma_0(2)$	$\sigma_1(2)$	$\sigma_2(2)$	$m_{01}(2)$	$m_{12}(2)$
3	$\sigma_0(3)$	$\sigma_1(3)$	$\sigma_2(3)$	$m_{01}(3)$	$m_{12}(3)$
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots
N	$\sigma_0(N)$	$\sigma_1(N)$	$\sigma_2(N)$	$m_{01}(N)$	$m_{12}(N)$

Minimal symbol



Minimal symbol



Minimal symbol

add symmetry



Minimal symbol

add symmetry \Rightarrow map orbits onto each other

Minimal symbol

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- Choose two orbits c and d

Minimal symbol

add symmetry \Rightarrow map orbits onto each other

- Choose two orbits c and d
- Is $m_{ij}(c) = m_{ij}(d)$?

Minimal symbol

add symmetry \Rightarrow map orbits onto each other

- Choose two orbits c and d
- Is $m_{ij}(c) = m_{ij}(d)$?
- index priority depth-first traversal from c and d

$\sigma_i(c)$ maps onto $\sigma_i(d)$

Minimal symbol

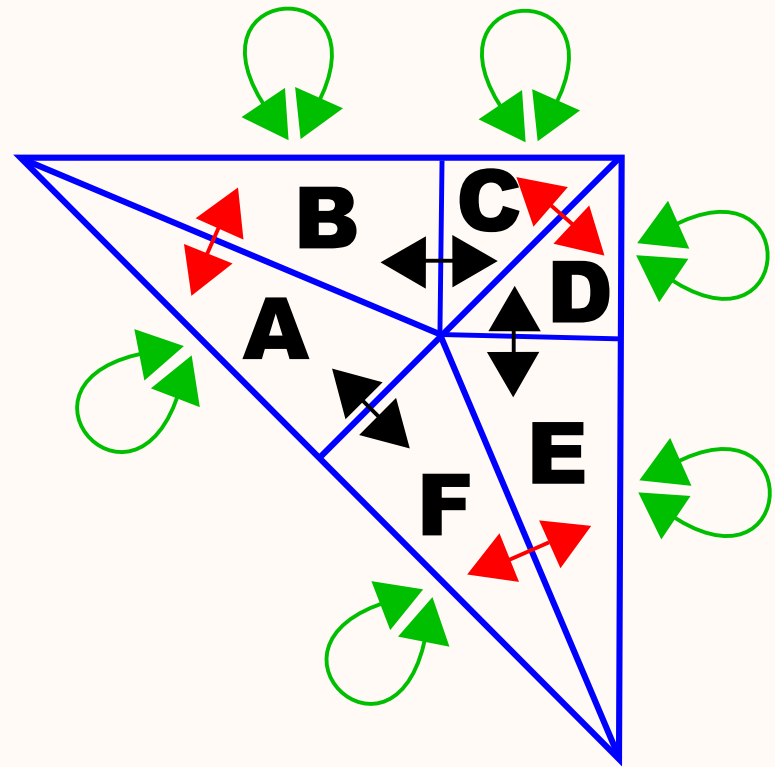
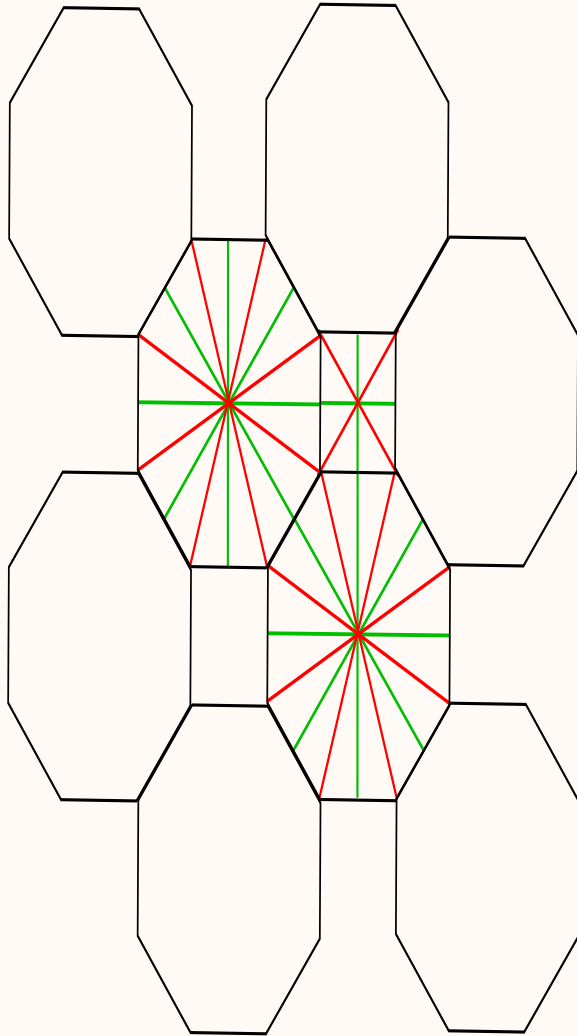
add symmetry \Rightarrow map orbits onto each other

- Choose two orbits c and d
- Is $m_{ij}(c) = m_{ij}(d)$?
- index priority depth-first traversal from c and d

$\sigma_i(c)$ maps onto $\sigma_i(d)$

$m_{ij}(\cdot) = m_{ij}(\cdot)$?

Example minimal symbol



Example minimal symbol

	σ_0	σ_1	σ_2	m_{01}	m_{12}	
A	A	B	F	8	3	A
B	B	A	C	8	3	B
C	C	D	B	4	3	C
D	D	C	E	4	3	D
E	E	F	D	8	3	E
F	F	E	A	8	3	F

C

D

Example minimal symbol

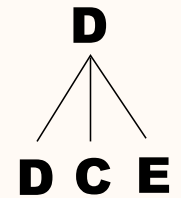
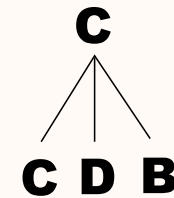
	σ_0	σ_1	σ_2	m_{01}	m_{12}	
A	A	B	F	8	3	A
B	B	A	C	8	3	B
C	C	D	B	4	3	a
D	D	C	E	4	3	a
E	E	F	D	8	3	E
F	F	E	A	8	3	F

C

D

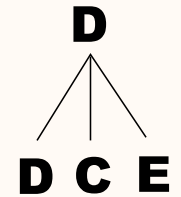
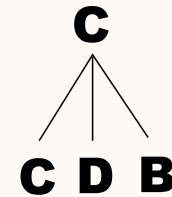
Example minimal symbol

	σ_0	σ_1	σ_2	m_{01}	m_{12}	
A	A	B	F	8	3	A
B	B	A	C	8	3	B
C	C	D	B	4	3	a
D	D	C	E	4	3	a
E	E	F	D	8	3	E
F	F	E	A	8	3	F



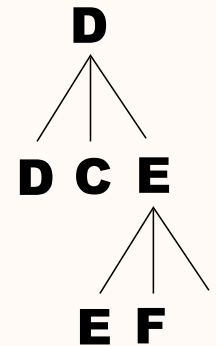
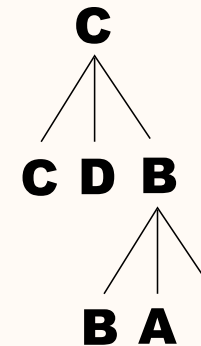
Example minimal symbol

	σ_0	σ_1	σ_2	m_{01}	m_{12}	
A	A	B	F	8	3	A
B	B	A	C	8	3	b
C	C	D	B	4	3	a
D	D	C	E	4	3	a
E	E	F	D	8	3	b
F	F	E	A	8	3	F



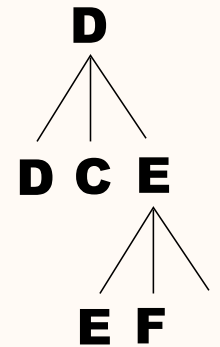
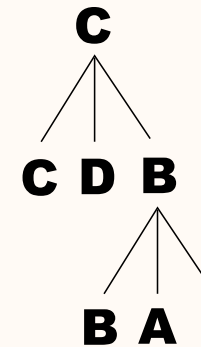
Example minimal symbol

	σ_0	σ_1	σ_2	m_{01}	m_{12}	
A	A	B	F	8	3	A
B	B	A	C	8	3	b
C	C	D	B	4	3	a
D	D	C	E	4	3	a
E	E	F	D	8	3	b
F	F	E	A	8	3	F



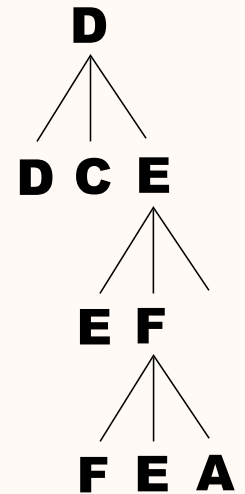
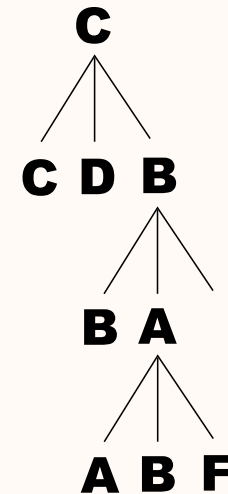
Example minimal symbol

	σ_0	σ_1	σ_2	m_{01}	m_{12}	
A	A	B	F	8	3	c
B	B	A	C	8	3	b
C	C	D	B	4	3	a
D	D	C	E	4	3	a
E	E	F	D	8	3	b
F	F	E	A	8	3	c



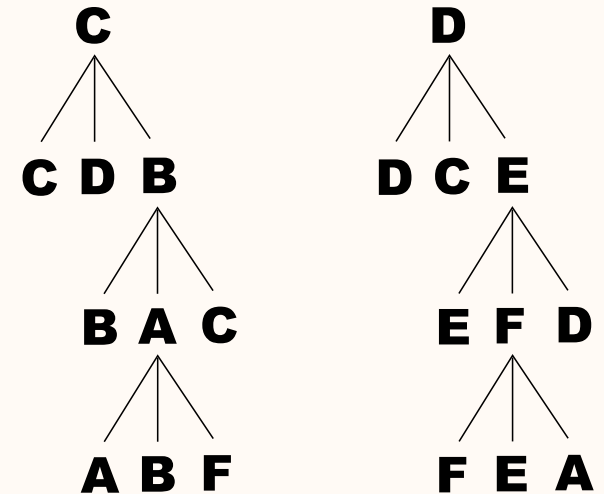
Example minimal symbol

	σ_0	σ_1	σ_2	m_{01}	m_{12}	
A	A	B	F	8	3	c
B	B	A	C	8	3	b
C	C	D	B	4	3	a
D	D	C	E	4	3	a
E	E	F	D	8	3	b
F	F	E	A	8	3	c



Example minimal symbol

	σ_0	σ_1	σ_2	m_{01}	m_{12}	
A	A	B	F	8	3	c
B	B	A	C	8	3	b
C	C	D	B	4	3	a
D	D	C	E	4	3	a
E	E	F	D	8	3	b
F	F	E	A	8	3	c



Example minimal symbol

	σ_0	σ_1	σ_2	m_{01}	m_{12}
a	a	a	b	4	3
b	b	c	a	8	3
c	c	a	b	8	3

Translation

Restrictions azulenoïd:

- 1 orbit of azulenes
- every atom part of exactly one azulene in that orbit

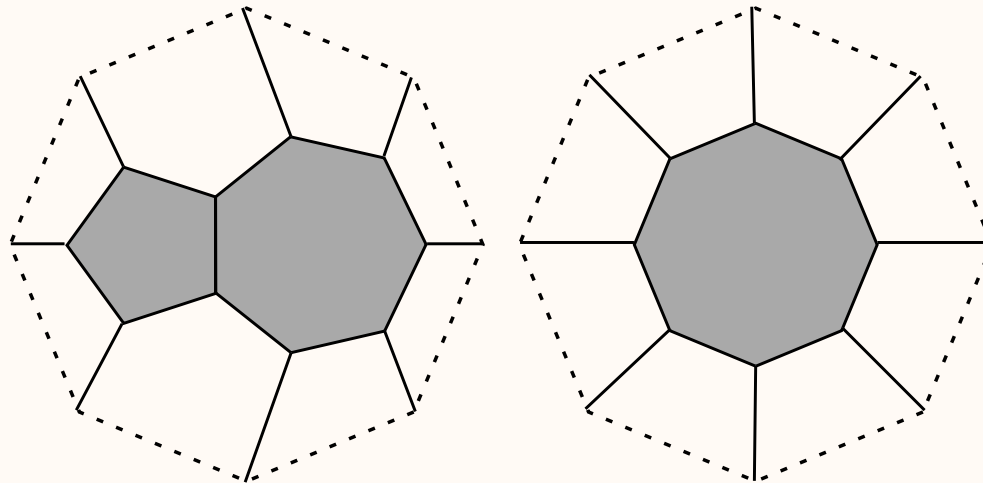
Translation

Restrictions azulenoid:

- 1 orbit of azulenes
- every atom part of exactly one azulene in that orbit

Restrictions Delaney/Dress symbol:

- $\exists \sigma_0 \sigma_1$ orbit O :
$$\left\{ \begin{array}{l} r_{01}(O) = 8 \\ \forall \sigma_1 \sigma_2 \text{ orbit } V : O \cap V \neq \emptyset \\ \forall d \in O : \sigma_2(d) \notin O \end{array} \right.$$



Translation

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Restrictions Delaney/Dress symbol:

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- $\forall \sigma_1 \sigma_2$ orbit V : $r_{12}(V) = 3$

Translation

Restrictions azulenoïd:

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Restrictions Delaney/Dress symbol:

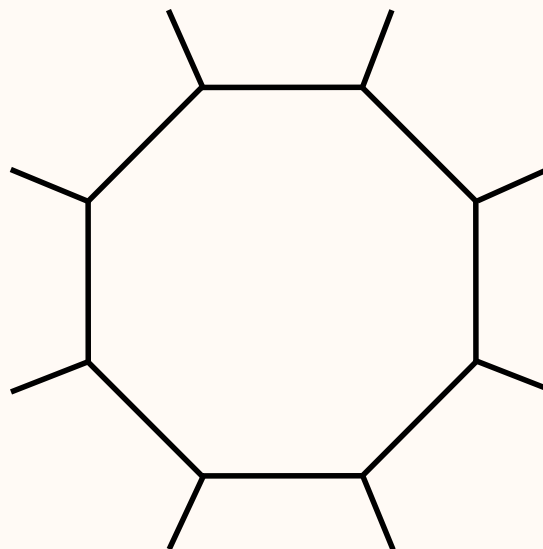
- $\exists \sigma_0 \sigma_1$ orbit O :
$$\left\{ \begin{array}{l} r_{01}(O) = 8 \\ \forall \sigma_1 \sigma_2 \text{ orbit } V : O \cap V \neq \emptyset \\ \forall d \in O : \sigma_2(d) \notin O \end{array} \right.$$

- $\forall \sigma_1 \sigma_2$ orbit V : $r_{12}(V) = 3$

- $$\sum_{d \in \mathcal{D}} \left(\frac{1}{m_{01}(d)} + \frac{1}{m_{12}(d)} - \frac{1}{2} \right) = 0$$

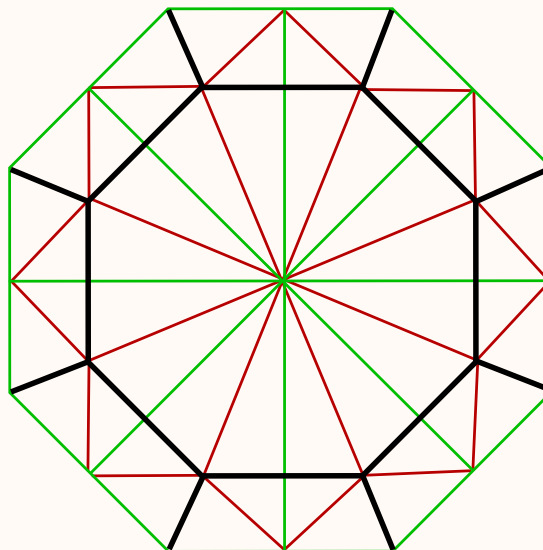
Method

- Octagon and the different vertex orbits



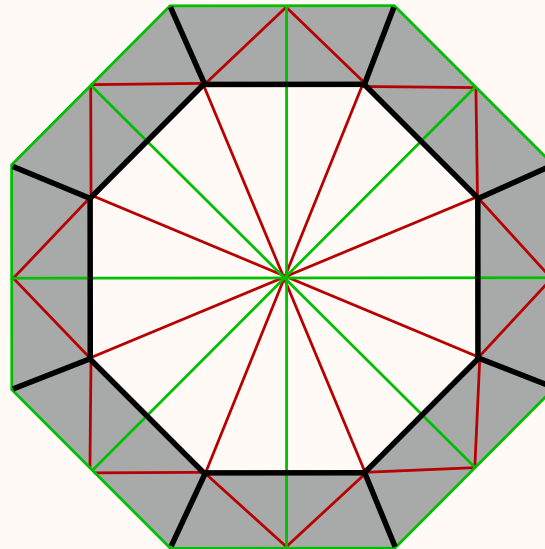
Method

- Octagon and the different vertex orbits



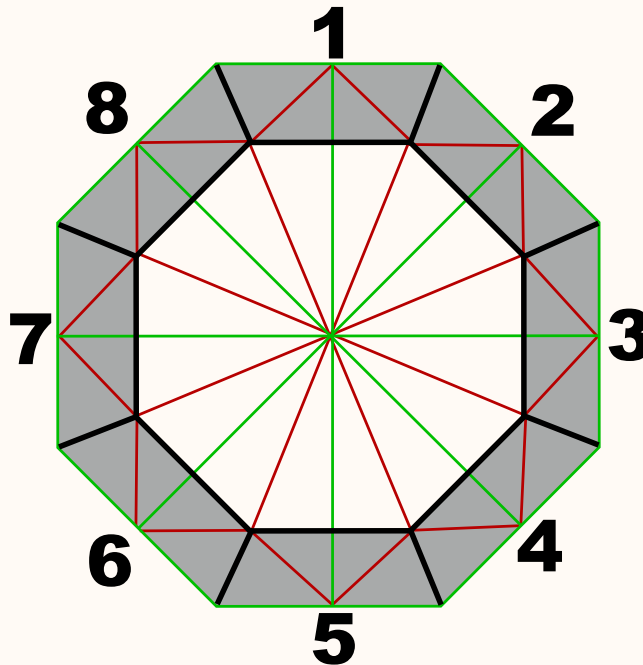
Method

- Octagon and the different vertex orbits
- Calculate and assign remaining m_{01} values



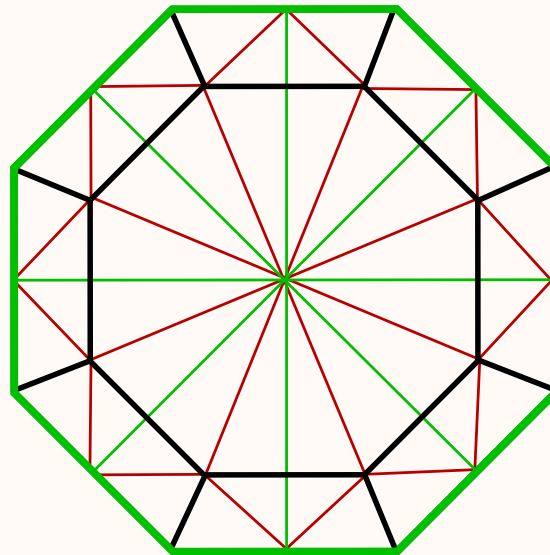
Method

- Octagon and the different vertex orbits
- Calculate and assign remaining m_{01} values



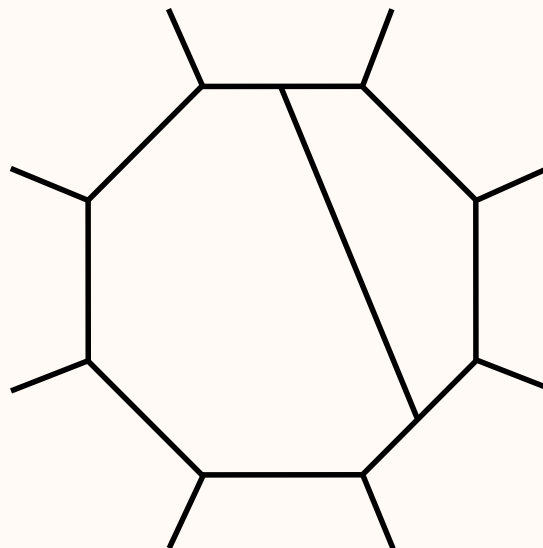
Method

- Octagon and the different vertex orbits
- Calculate and assign remaining m_{01} values
- Assign remaining σ_0 's



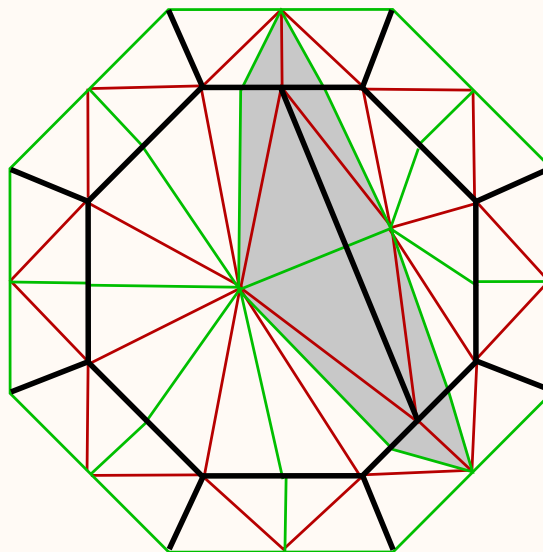
Method

- Octagon and the different vertex orbits
- Calculate and assign remaining m_{01} values
- Assign remaining σ_0 's
- Replace octagon with azulene



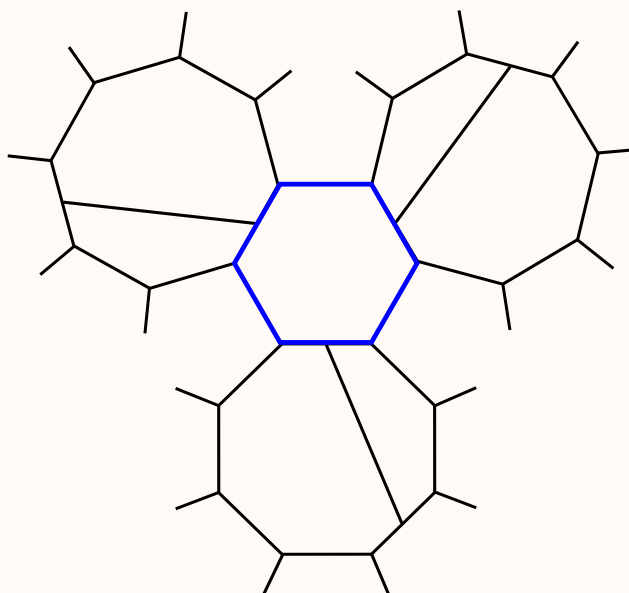
Method

- Octagon and the different vertex orbits
- Calculate and assign remaining m_{01} values
- Assign remaining σ_0 's
- Replace octagon with azulene



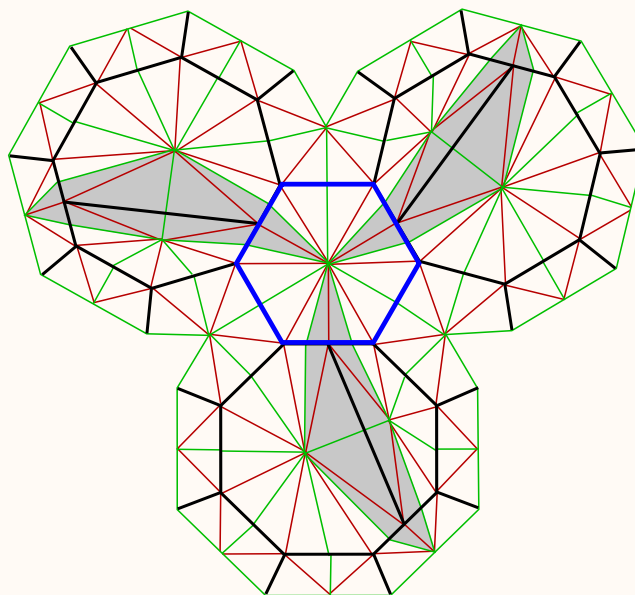
Method

- Octagon and the different vertex orbits
- Calculate and assign remaining m_{01} values
- Assign remaining σ_0 's
- Replace octagon with azulene



Method

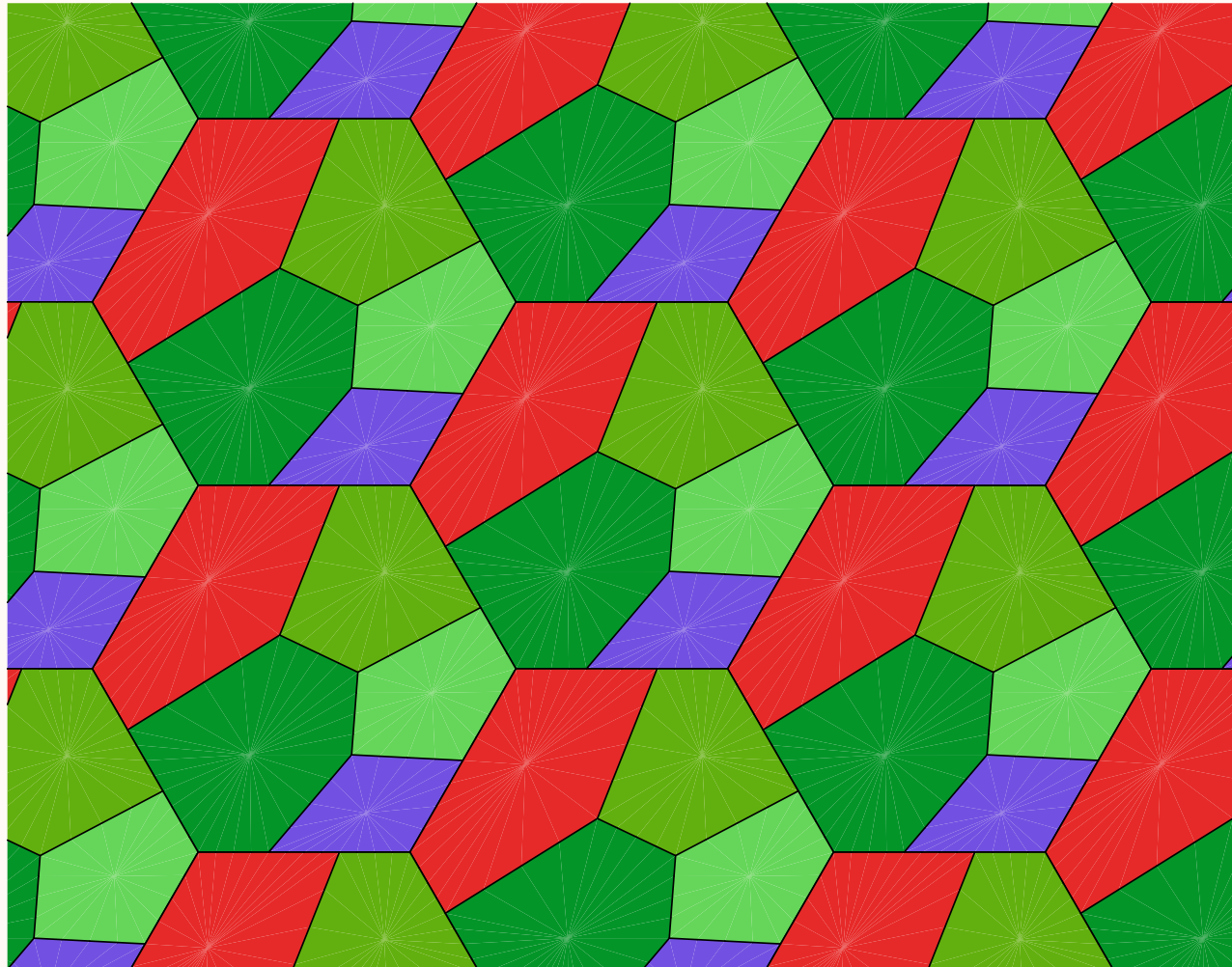
- Octagon and the different vertex orbits
- Calculate and assign remaining m_{01} values
- Assign remaining σ_0 's
- Replace octagon with azulene



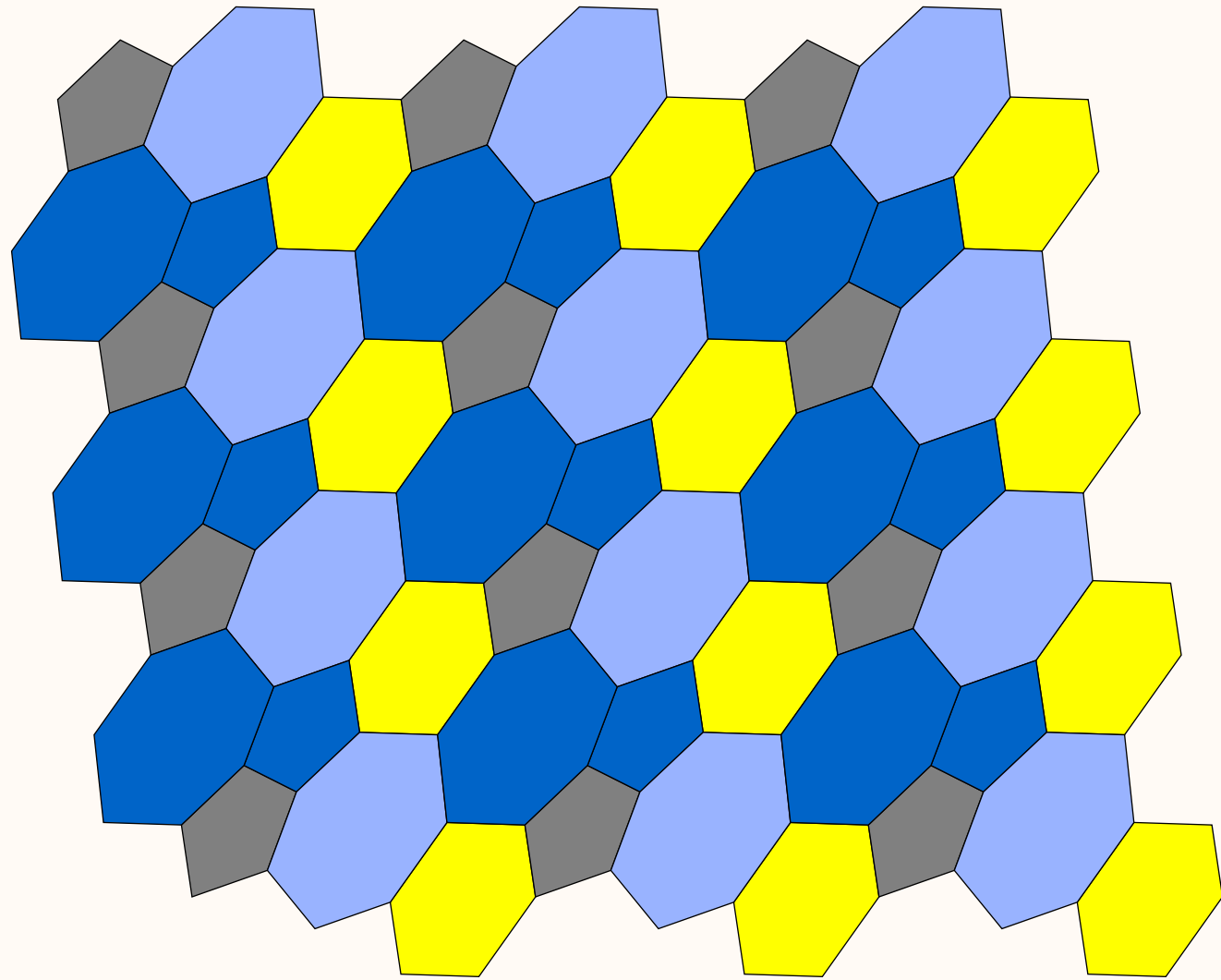
Visualisation



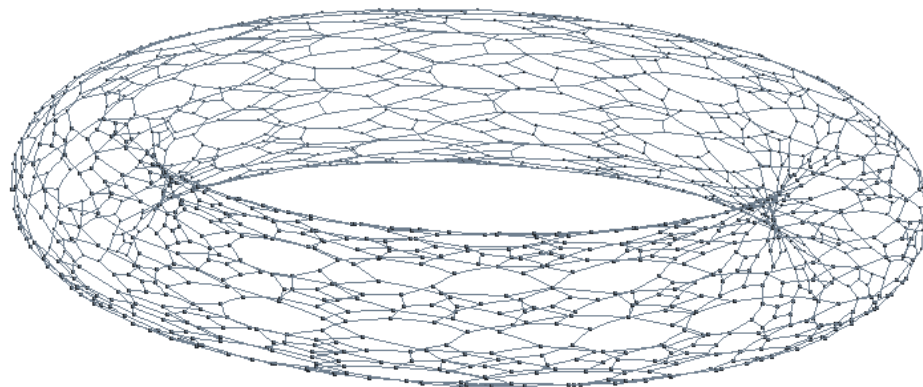
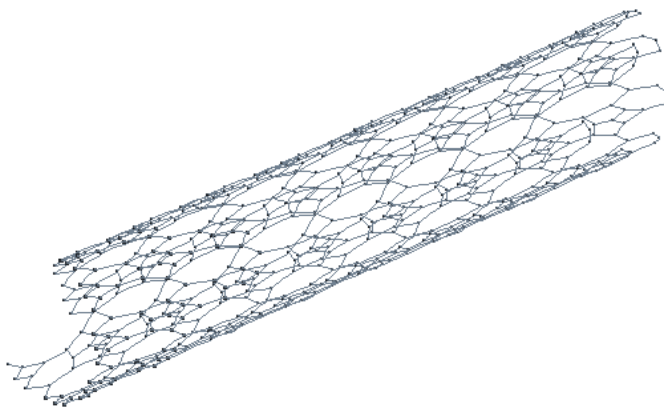
Visualisation



Visualisation



Visualisation



Results

	m_{01} values								# strings	# symbols
1	4	4	4	4	4	6	24	24	21	6
2	4	4	4	4	4	8	12	24	42	42
3	4	4	4	4	4	8	16	16	21	48
4	4	4	4	4	4	10	10	20	21	0
5	4	4	4	4	4	12	12	12	7	44
6	4	4	4	4	6	6	8	24	105	0
7	4	4	4	4	6	6	12	12	54	2
8	4	4	4	4	6	8	8	12	105	12
9	4	4	4	4	8	8	8	8	10	160
10	4	4	4	6	6	6	6	12	35	6
11	4	4	4	6	6	6	8	8	70	38
12	4	4	6	6	6	6	6	6	4	25

Results

383 symbols of tilings containing octagons

Results

383 symbols of tilings containing octagons



1274 minimal unmarked azulenoids

1324 minimal marked azulenoids

Marked vs. Unmarked

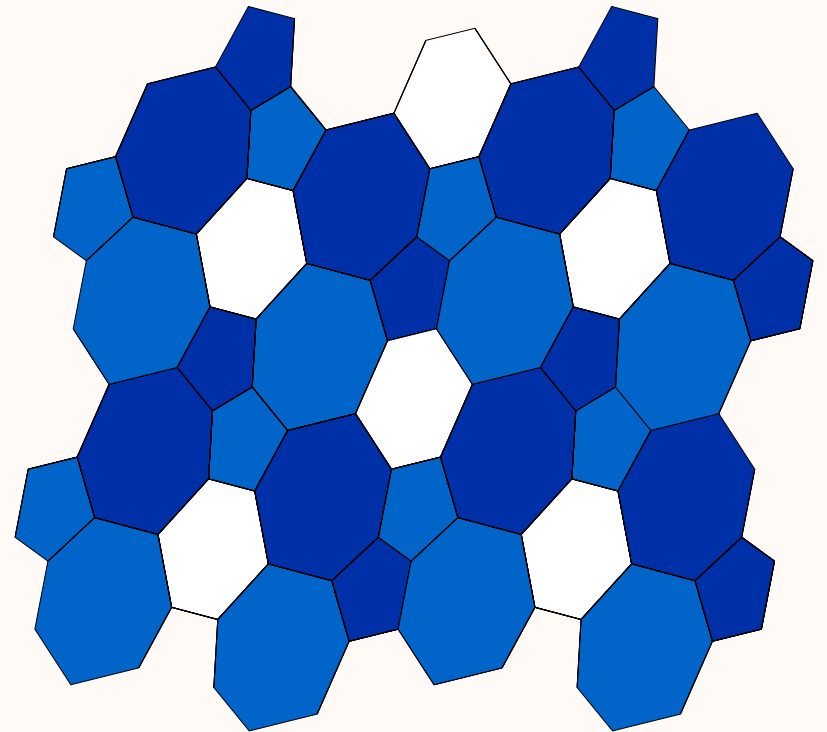
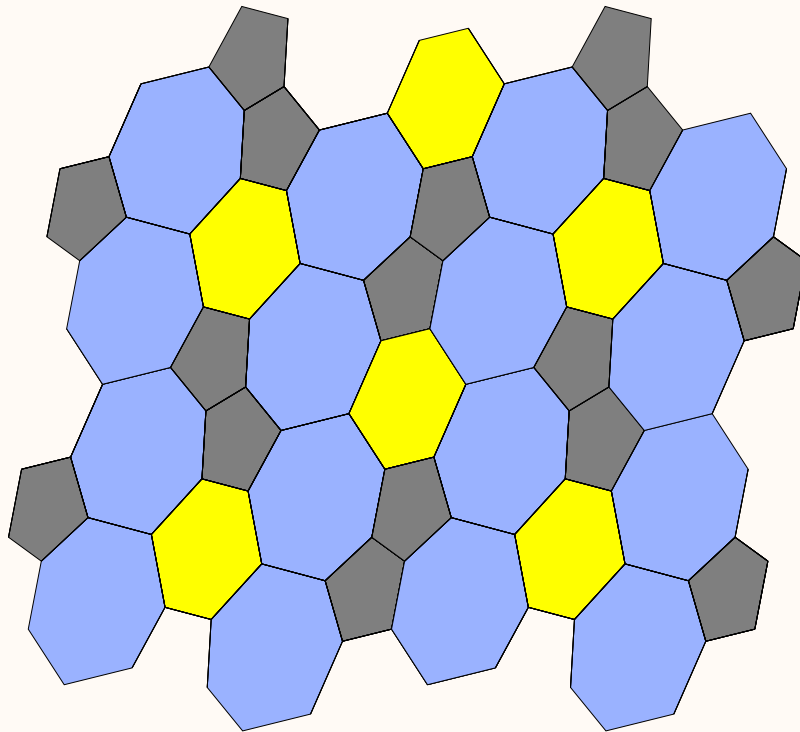
structures that have an azulenoïd set

vs.

structures with their azulenoïd set

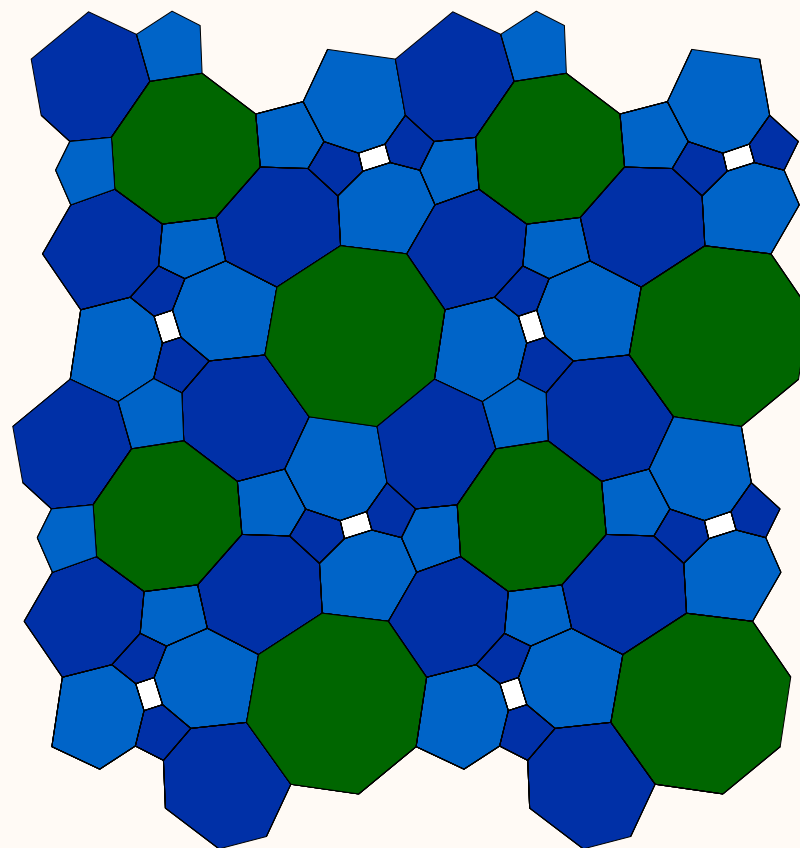
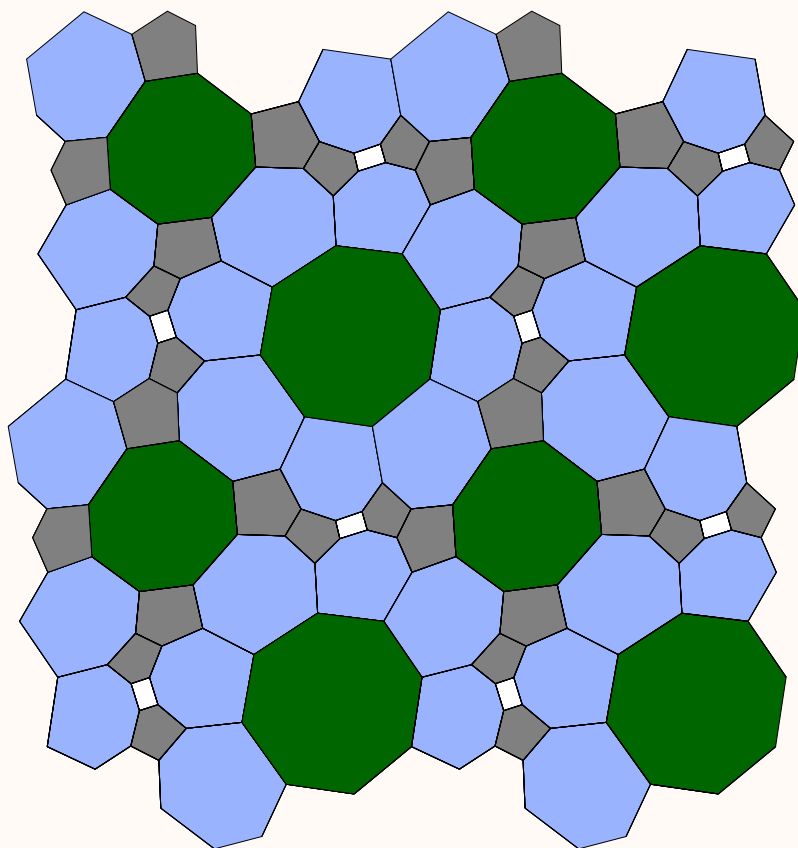
Marked vs. Unmarked

- 4
- 5
- 6
- 7
- 8
- 9
- 10



Marked vs. Unmarked

- 4
- 5
- 6
- 7
- 8
- 9
- 10



Translation only

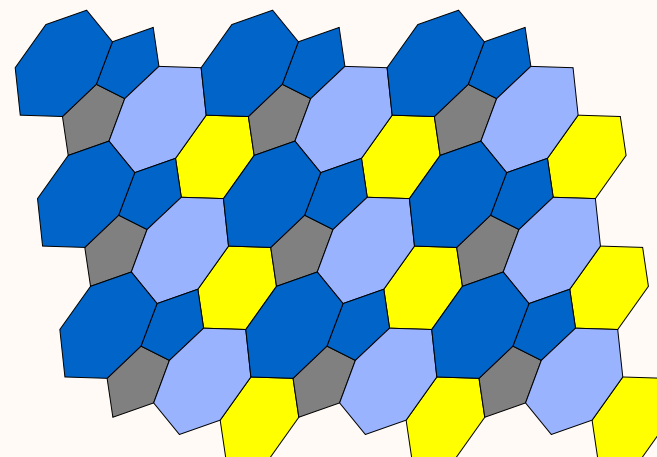
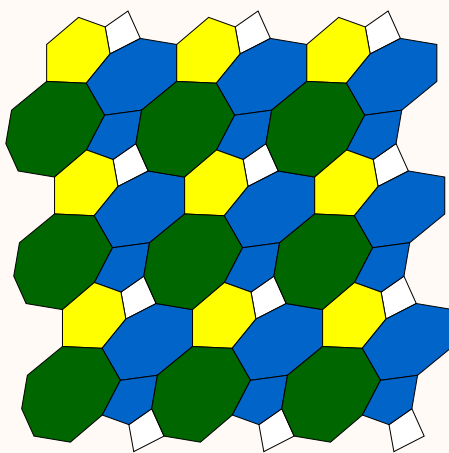
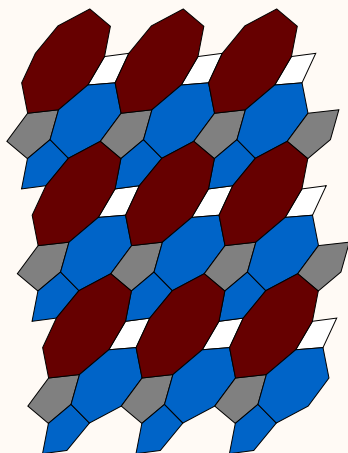
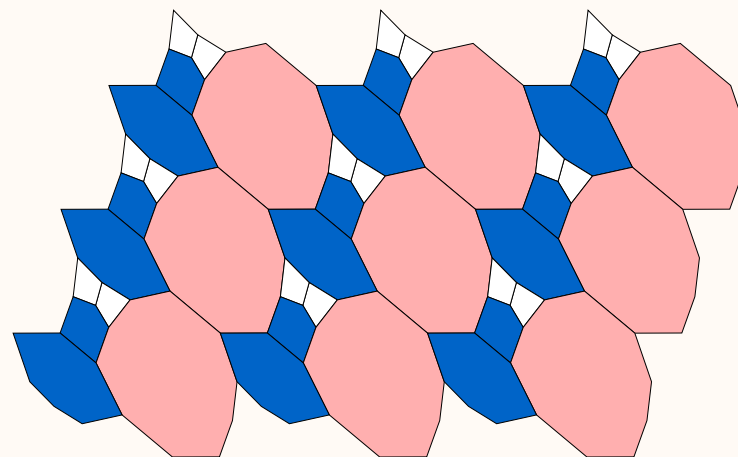
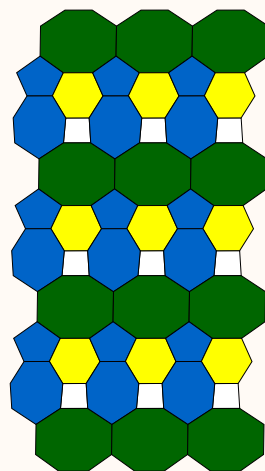
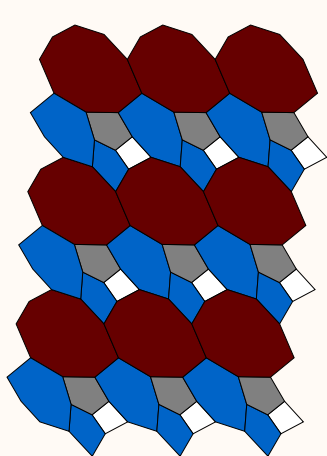
one orbit of azulenes under the subgroup of translations

or

all the azulenes have the same orientation

Translation only

- 4
- 5
- 6
- 7
- 8
- 9
- 10



End

Thanks for your attention!