Generating sound molecular cages

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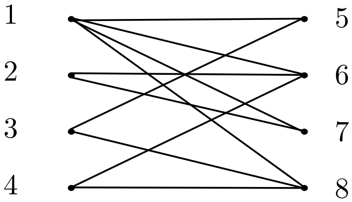
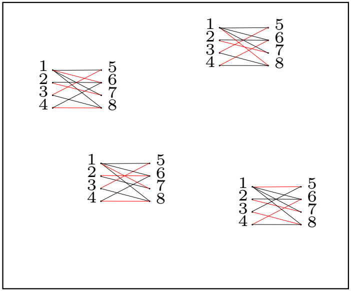
Enumeration problems

- Enumeration problems: list all solutions rather than just deciding whether there is one.

Perfect matchings:



Solutions :



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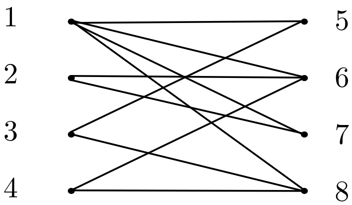

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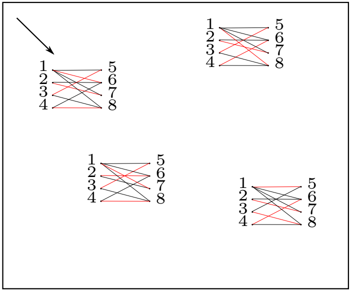

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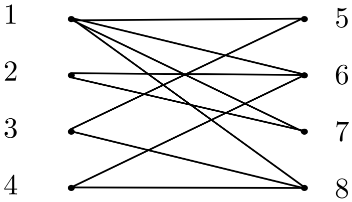

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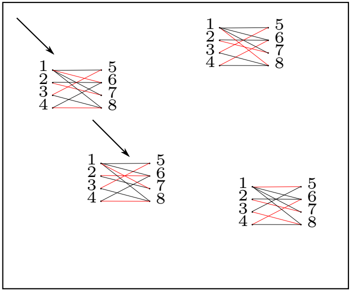

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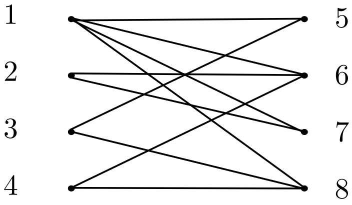

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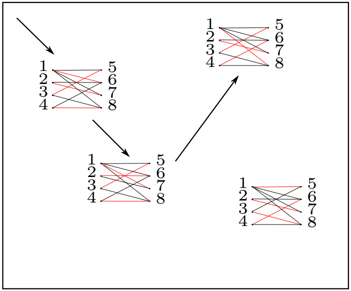

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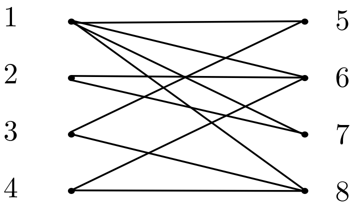

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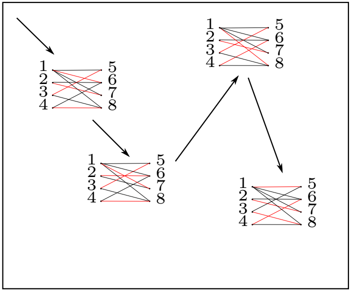

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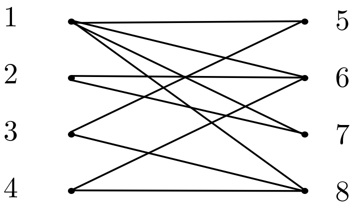

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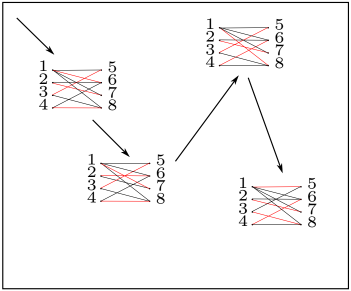

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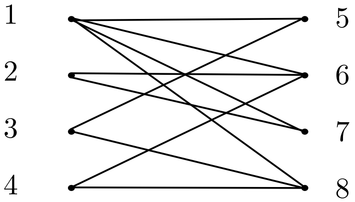

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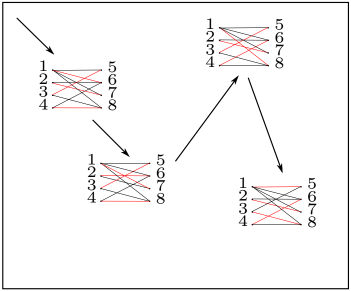
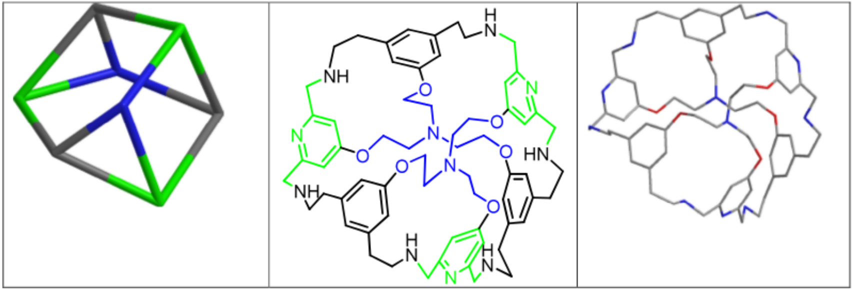


Introduction



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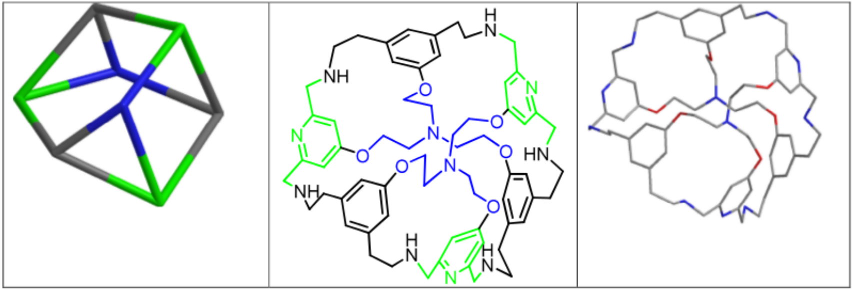

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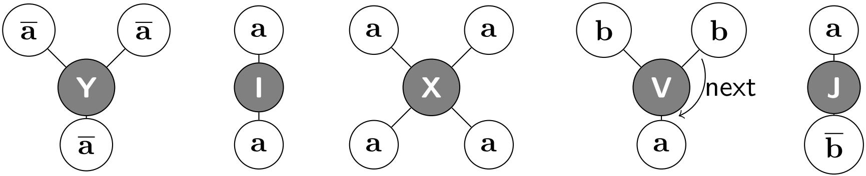
The motifs

Definition

A map $G = (V_c, V, E, \text{next})$ is a **motif** if

1. V_c contains only one vertex c called the center
2. each vertex in V is colored with a color in $\mathcal{A}$ a fixed alphabet
3. $E = \{(c, u),\ u \in V\}$
4. next gives an order on the edges of c



Map of motifs

Definition

A connected planar map $G = (V_c, V, E, \text{next})$ is a **map of motifs** based on $\mathcal{M}$ if,

1. each vertex in V is connected to at most one vertex in V, which is of the complementary colour.
2. when all edges between vertices in V are removed, the remaining connected components must all be motifs of $\mathcal{M}$

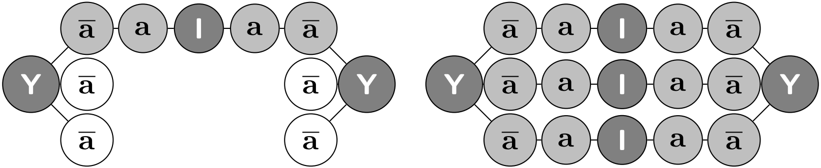


Figure: Example of two maps of motifs based on $\mathcal{M} = \{\mathbf{Y}, \mathbf{I}\}$, the first map is unsaturated while the second map is saturated.

Molecular map

Definition

Let $G = (V_\mathsf{c}, V, E_G, \mathsf{next}_G)$ be a saturated map of motifs based on $\mathcal{M}$, we define the **molecular map** $M = (V, E_M, \mathsf{next}_M)$:

1. $V = V_\mathsf{c}$
2. $(c_1, c_2) \in E_M$ if it exists a path (c_1, u, v, c_2) in G
3. $\mathsf{next}_M((c, c_1)) = (c, c_2)$ if it exists two paths (c, u_1, v_1, c_1) and (c, u_2, v_2, c_2) in G and $\mathsf{next}_G((c, u_1)) = (c, u_2)$

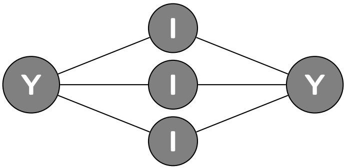


Figure: The molecular map corresponding to the saturated map of motifs in Fig. 1

The indices

Why is a molecular map a good representation of a molecula ?

1. Constraint on the edges: possible chemical connections
2. The *size* of a cut $S = (S_1, S_2)$ is the number of edges with one end in S_1 and the other in S_2.

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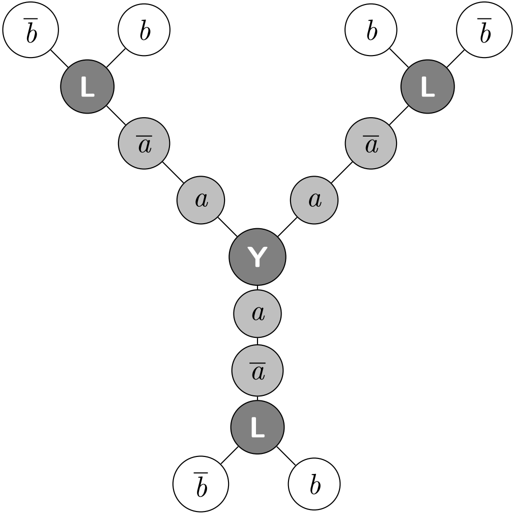

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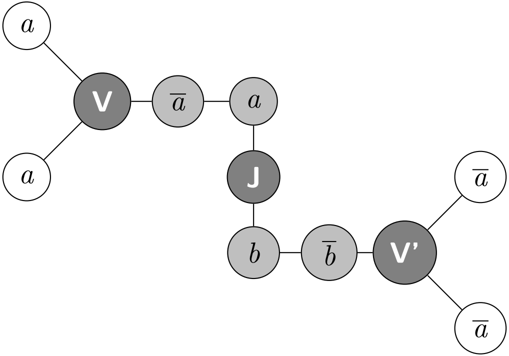

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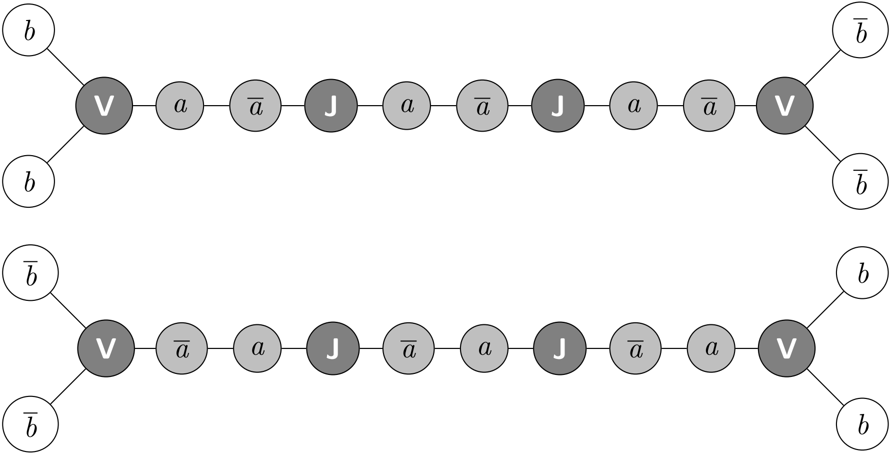
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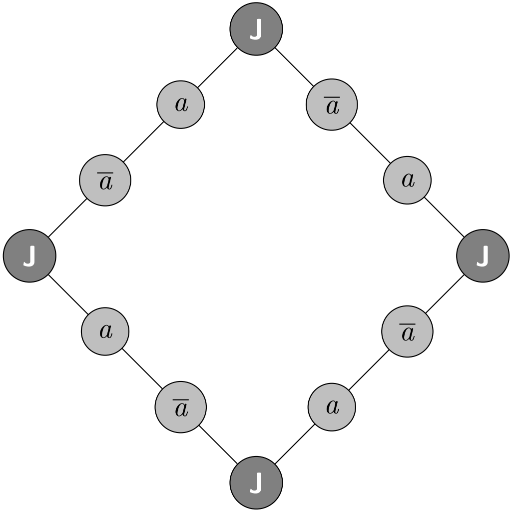
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Fold and outline

The fold operation on the vertices u and v is adding the edge (u, v) to G. Valid when u and v are:

1. free
2. of complementary colors
3. in the same face of G

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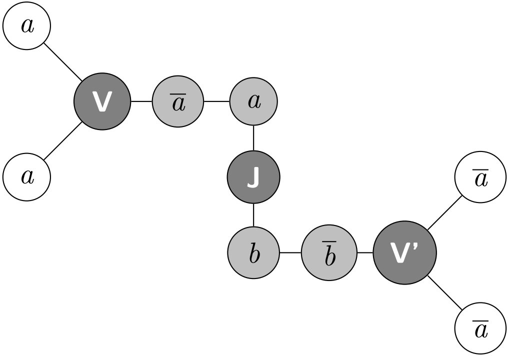

outline $= \{a, \overline{a}, \overline{a}, a\}$

Figure: A map of three motifs on $\mathcal{A}_M = \{\mathbf{V}, \mathbf{V}', \mathbf{J}\}$ and its outline before a fold operation.

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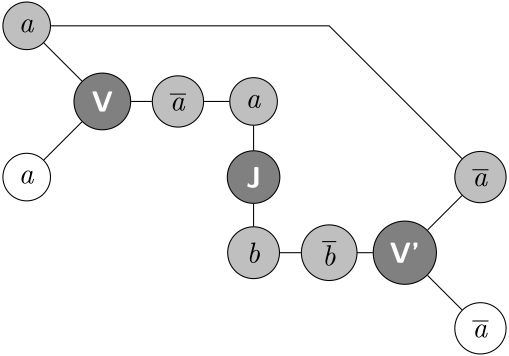

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When is a map foldable?

The outline is a circular sequence of vertices. The fold remove two vertices of compatible colours.

Enough to work with the sequence of colours of the vertices. In the previous example $a\bar{a}\bar{a}a$.

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How to avoid non foldable maps?

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A map is almost foldable if for every letter in $a \in \mathcal{A}$, there are as many vertices labeled with a and $\bar{a}$.

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$\{I, V1, V2\}$ of size 18:

- $179,896,320$ paths in 78.7s
- $1,277,952$ almost foldable paths in 0.63s.

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Seems large, but small with regards to the C^n paths.
$\{I, V1, V2\}$ of size 18:

- $179,896,320$ paths in 78.7s
- $1,277,952$ almost foldable paths in 0.63s.

How to fold a map?

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Problem: given a word, we want to generate the results of all sequences of reductions which yield an empty word.

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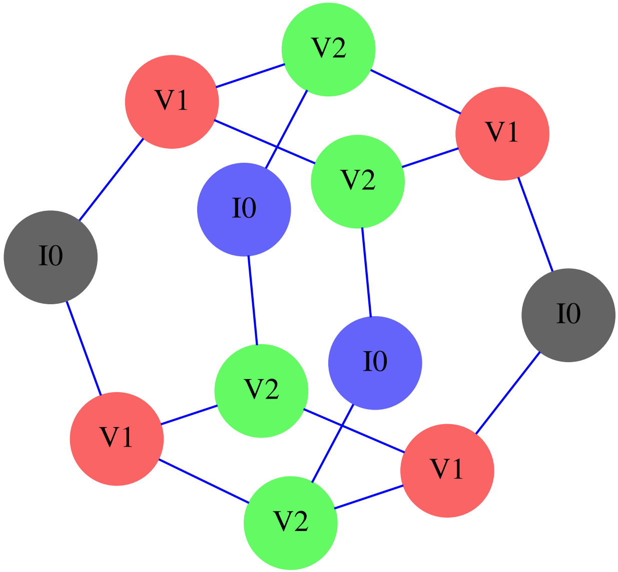

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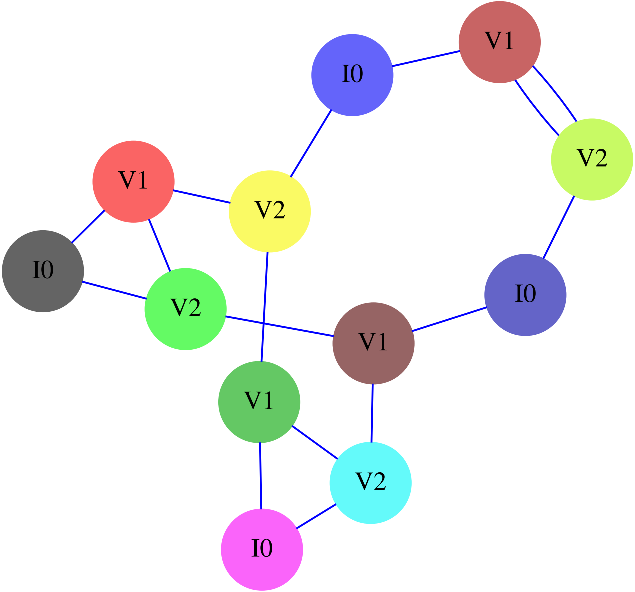

Dealing with duplicates

The algorithm generates many duplicates.
$\{I, V1, V2\}$ of size 18: $1,658,070$ maps produced but only $23,901$ unique maps

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