Generating sound molecular cages

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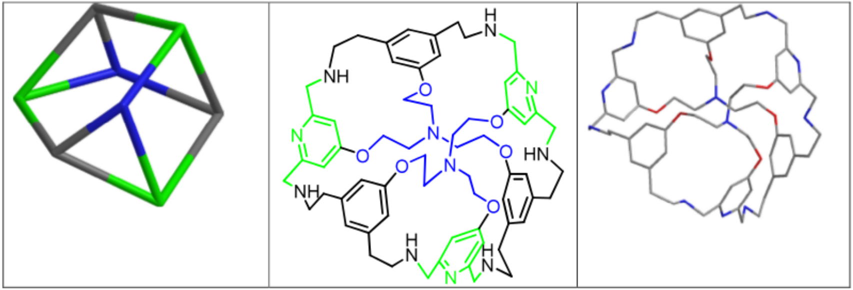
Introduction



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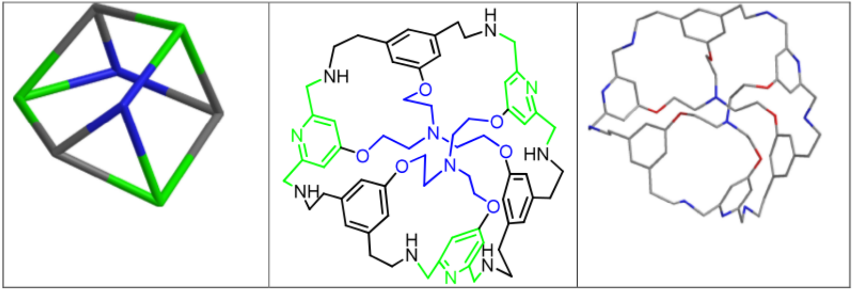

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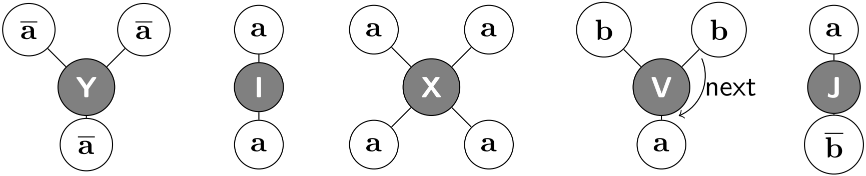
The motifs

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 $\mathcal{M}$

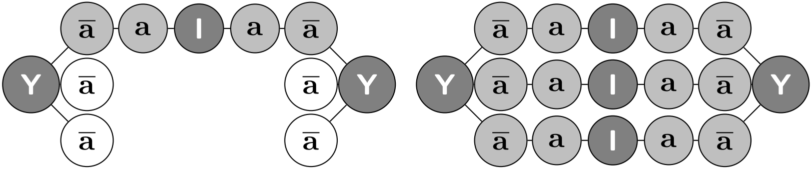


Figure : Example of two maps of motifs based on $\mathcal{M} = \{\mathbf{Y}, \mathbf{I}\}$, the first map is unsaturated while the second map is saturated.

Molecular map

Definition

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

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

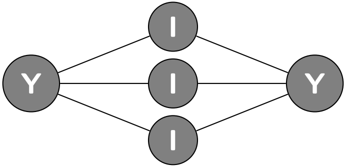


Figure : The molecular map corresponding to the saturated map of motifs in Fig. 1

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.

$$sparsity(S) = \frac{size(S)}{\min(|S_1|, |S_2|)}$$

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The problem

Enumeration problem

We want to generate, given a set of motifs $\mathcal{M}$ and a size n, all molecular maps based on $\mathcal{M}$ and of size n.

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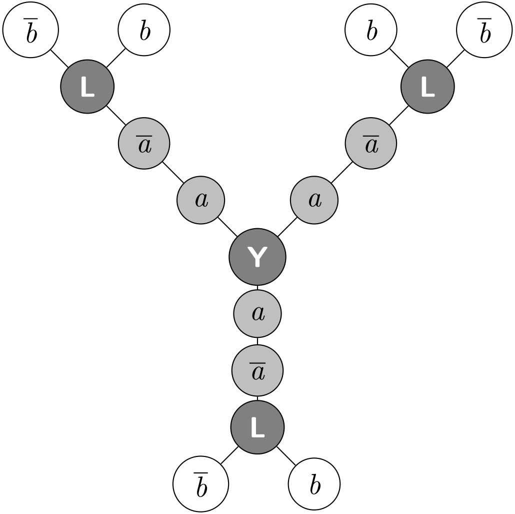

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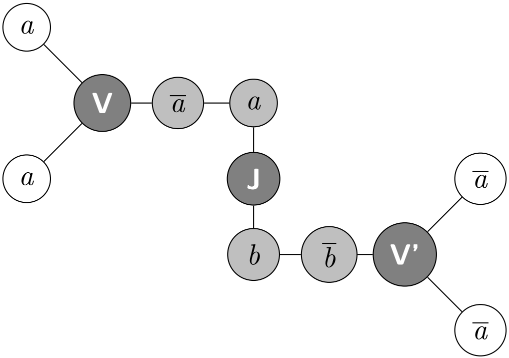

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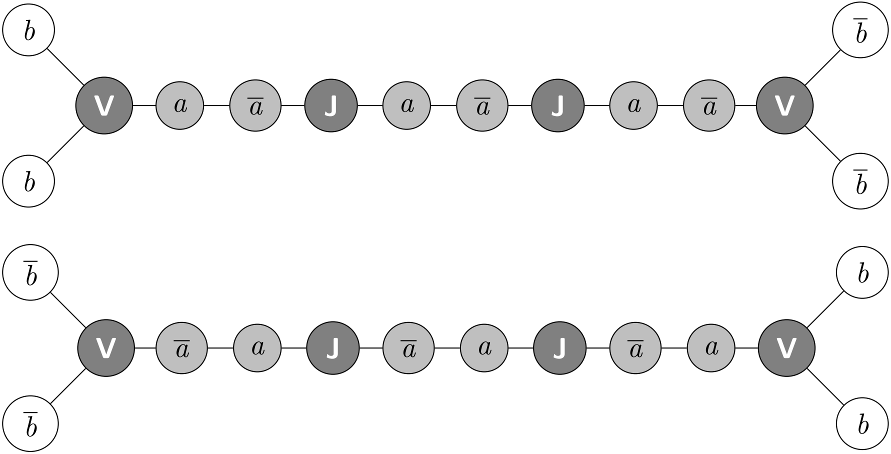

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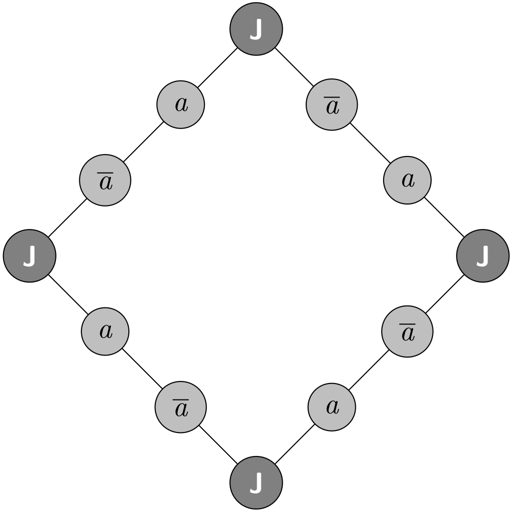
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Fold and outline

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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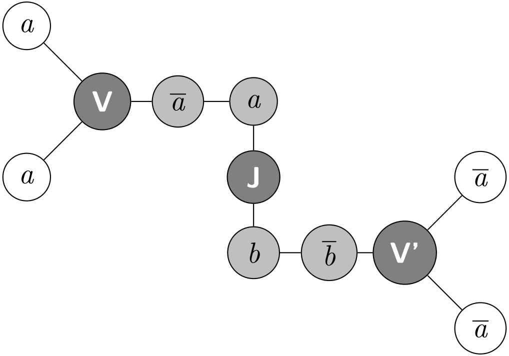

$$\text{outline} = \{a, \overline{a}, \overline{a}, a\}$$

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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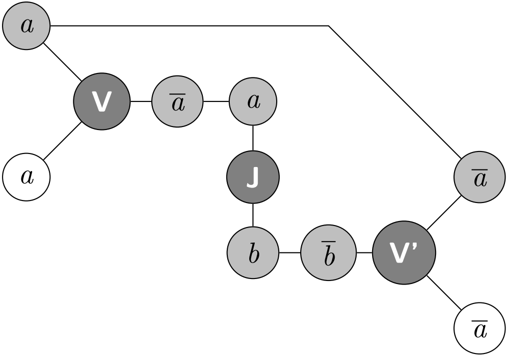

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The outline is a circular sequence of vertices. The fold remove two vertices of compatible colours.

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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Thanks!