A Categorical Approach to Synthetic Chemistry

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Retrosynthetic analysis

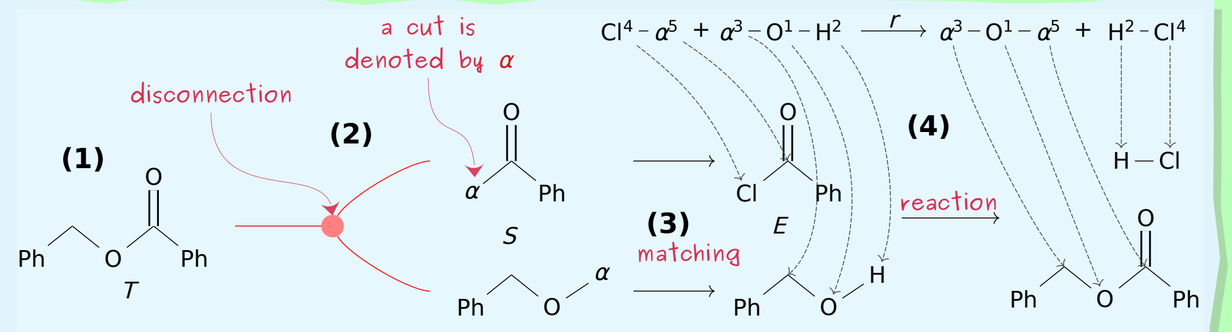
(1) Start with the target molecule(s) T

(2) Disconnect the target by "cutting" along some bonds, creating two or more *synthons* S

(3) Search for *synthetic equivalents* E: embeddings of synthons into molecular graphs

(4) Search for a known reaction whose reactants contain the synthetic equivalents E and whose products contain the target T

(5) Check whether the synthetic equivalents are known molecules: if yes, terminate, if no, return to **(1)** taking the synthetic equivalents as the new target: $E \mapsto T$

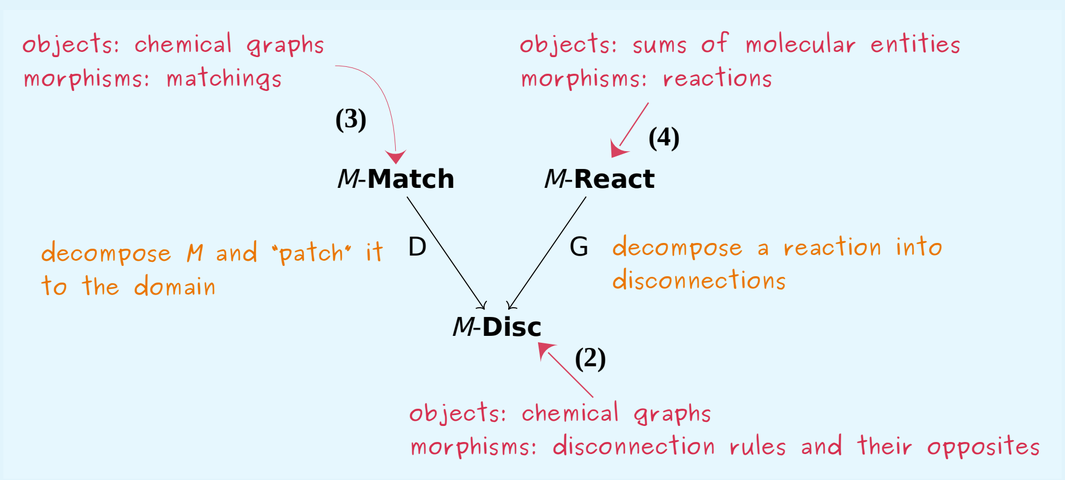


A layered prop for retrosynthesis

see for the definition of a layered prop

L. Lobski, F. Zanasi. String Diagrams for Layered Explanations. ACT 2022. arXiv:2207.03929.

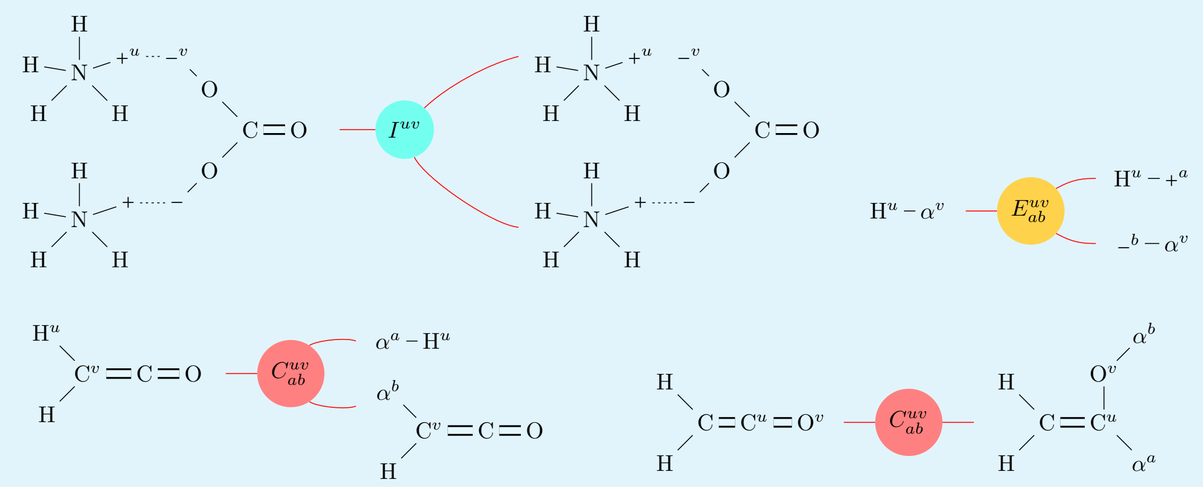
For a finite collection of molecular entities M, we generate the (monoidal) categories and functors below:



All of these are parameterised in M, representing an unbounded supply of molecules in the environment. The above diagram, together with inclusions between different choices of M, generates a *layered prop* in which retrosynthetic search can be expressed as "filling the gaps" of a given type. Below we represent formally one iteration of the search (left), the output of a successful search with n iterations (right), and an example of the kind of reasoning that the formalism allows (the 2-cell in the middle).

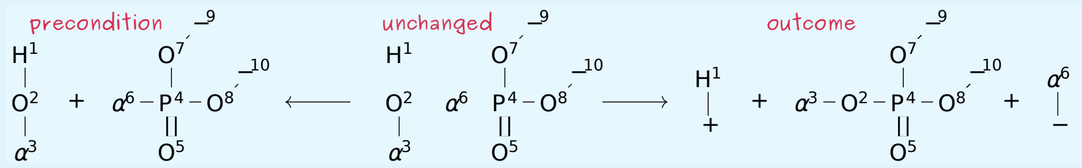
Disconnection rules

There are three kinds of disconnections: *electron detachment* E, *ionic bond breaking* I, and *covalent bond breaking* C:

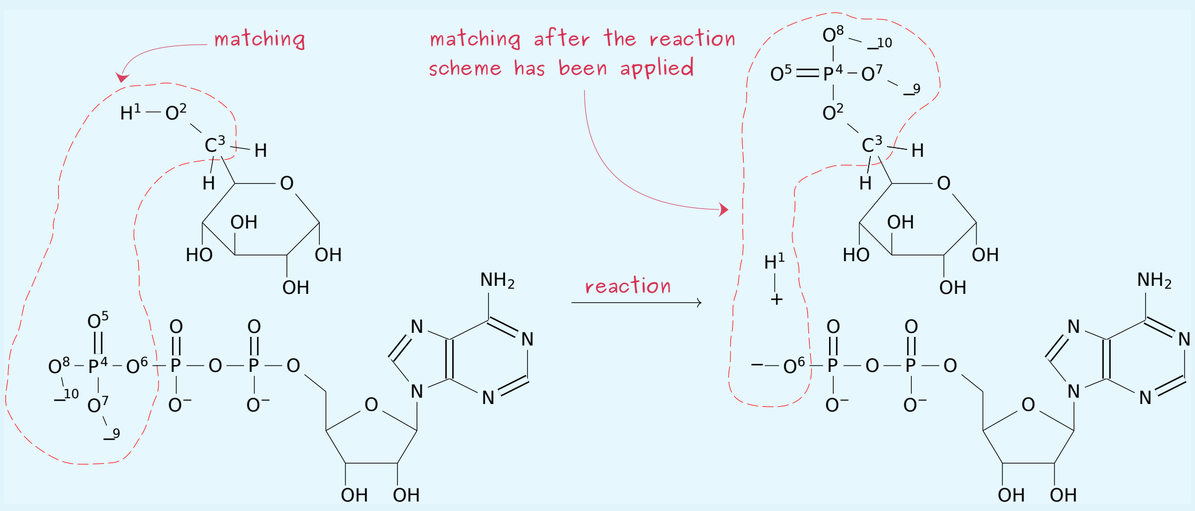


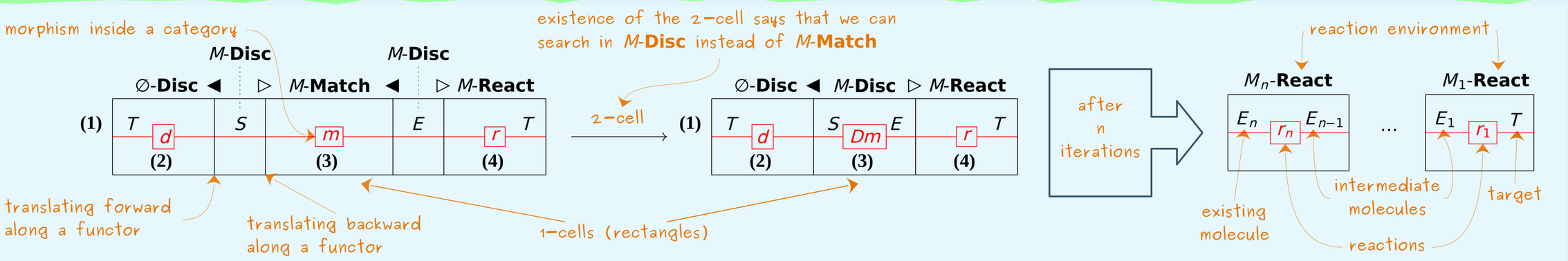
Reactions

Reactions are graph rewrites generated using *reaction schemes*:



by *matching* the left-hand side in a larger molecular entity:





References

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