Organic Synthesizability

An examination of a strictly mathematical representation of the organic chemical synthesis

Short summary

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The organic synthesizability question for a finite set $\mathcal{R}$ of reaction step rules, a finite set C of organic compounds and an organic compound p is the question:

Does a synthesis of p from C exist whose steps follow $\mathcal{R}$?

A synthesis of p from C has in its initial stage only compounds in C and p in its final stage.

Given $n \in \mathbb{N}$, organic compounds are represented for a function d: $\{0, \ldots, n\} \to \mathbb{N}$ by n-multigraphs whose points of type $0 \leq i \leq n$ have degree $d(i)$, while a reaction step rule is represented, for only one operation, that I call *shift*, by an n-rule, which is an n-multigraph together with a sequence of its points, that establishes the points in an n-multigraph at which the operation can be applied. A theorem states that the shift has a property that justifies its role.

Translated back from the graph theoretical results the decidability results can be expressed in the following way:

> There is a finite set $\mathcal{R}_0$ of reaction step rules, a finite set C_0 of organic compounds such that the organic synthesizability question for $\mathcal{R}_0, C_0$ and an organic compound is not decidable (said differently, it is not decidable for an organic compound p, whether there is a synthesis of p from C_0 whose steps follow $\mathcal{R}_0$).
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> On the other hand I listed some conditions such that the organic synthesizability question for a finite set $\mathcal{R}$ of reaction step rules that fulfills one of the conditions, a finite set C of organic compounds and an organic compound p is decidable (said differently, it is decidable for $\mathcal{R}, C, p$ as above, whether a synthesis of p from C whose steps follow $\mathcal{R}$ exists).
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> This result is easy to prove for some of the conditions and less easy for the others.

The graph theoretical problems representing the organic synthesizabilty problems are in a natural way special cases of a model theoretical problem, since the finite sets of reaction step rules can be represented by model theoretical interpretations, once this concept is narrowed down to the right point.

Once the model theoretical representation is recognized, the organic synthesizability question can be reduced to the finite satisfiability question for sentences in a particular class. We can also for example conclude that for the previously described $\mathcal{R}_0$ and C_0 the class of all final stages of a synthesis from C_0 whose steps follow $\mathcal{R}_0$ is not first-order axiomatizable and not closed under ultraproducts.