

Composition of Chemical Graph Grammar Rules

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Graph rewriting has been applied successfully to model chemical and biological systems at different levels of abstraction. To this end chemical reactions are modelled as graph transformations and in a generative fashion a hypergraph is expanded that allows for subsequent network flow analysis. A particularly powerful feature of rule-based models that are rigorously grounded in category theory, is, that they admit a well-defined notion of rule composition, hence, provide their users with an intrinsic mechanism for compressing trajectories and coarse grained representations of dynamical aspects. The same formal framework, however, also allows the detailed analysis of transitions in which the final and initial states are known, but the detailed stepwise mechanism remains hidden. To demonstrate the general principle we consider how rule composition is used to determine accurate atom maps for complex enzyme reactions. This problem not only exemplifies the paradigm but is also of considerable practical importance for many down-stream analyses of metabolic networks and it is a necessary prerequisite for predicting atom traces for the analysis of isotope labelling experiments.