Strategies and Requirements for the Automated Exploration of Complex Chemical Reaction Networks

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In recent years the computer based, automated exploration of reaction networks has seen a growing interest. A variety of different approaches have been proposed, implemented and used to explore a diverse set of chemical reactions[1–3].
All of these methods rely on a reasonably complete reaction network in order to allow for accurate predictions. A complete reaction network for a given area of interest consists of all thermodynamically relevant intermediates and all reaction paths that connect them. Already due to conformational diversity the reaction network generated for relatively simple chemical processes can be vast if they are to be complete.
The requirements for a software that strives to explore reaction networks in this manner will be highlighted using our own approach[4,5] as an example. Key steps in the exploration of networks, such as error control, as well as the final visualization and interpretation of generated data will be touched upon.

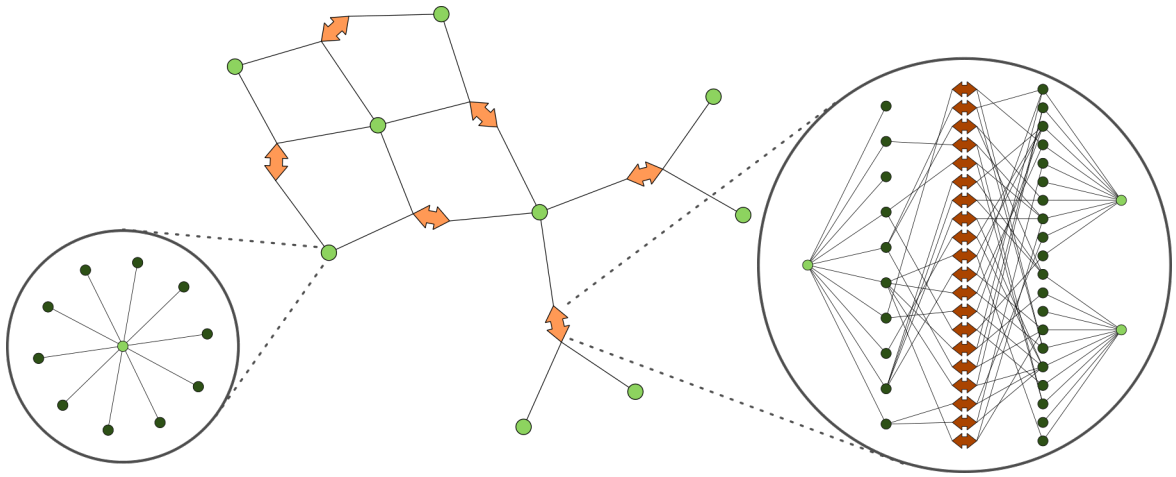

Figure 1: Example reaction network.

References

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