COMPUTER SOFTWARE REVIEWS

RAIN—Reaction and Intermediates Networks, Version 2.0

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To propose a reaction mechanism for a relatively complicated reaction is not a trivial task. RAIN[1] is the first commercial software package of which I am aware that is attempting to address some aspects of this large problem. Based on user-defined constants, which include the types of bonds formed and/or broken, formal charges, ring sizes, etc., RAIN is able to generate all possible pathway connections from a set of reactants to the corresponding mass balanced products. A predefined stoichiometry must be provided in order to run the program. RAIN uses no knowledge base, no fixed set of transformations. The user must supply an extensive set of optional rules in order to generate the pathways, thus to form the network connection between reactants and products. RAIN does *not* specifically generate elementary steps in a reaction mechanism. It provides a complete set of pathways under the constraints defined by the user. On the one hand, this provides flexibility, but on the other it makes it difficult to use.

The 45-page user manual provides minimum information on the applications of the package. You need an IBM compatible PC with at least 505K Ram and a mouse to run RAIN. Since it is graphically operated, RAIN operates on a 286 machine painfully slowly. Some users will certainly feel that they could generate these pathways faster on a piece of paper with a pencil. I have loaded RAIN on different IBM-compatible machines (from 286 to 486), and they all worked fine. However, token ring software conflicts with RAIN. It must be unloaded before RAIN will run.

The five examples included in the tutorial provide only information on how to operate the package. They worked out, more or less, as described in the manual. Unfortunately, no explanation is provided on how or why the predefined constraints were set in the tutorial; therefore, the user must spend a great deal of time "learning the ropes". Furthermore, some important concepts in operating RAIN are introduced without clearly defining the terms used in the manual. For example, the network is formed by "the generation of reaction occurs in steps of so-called levels. Each level collects all molecules that have the same distance to the corresponding root molecules, when measured in reaction steps." Steps, levels, and distances are not clearly defined in the manual. The quoted part of the sentence is the only discussion using these terms. The user must thus make a guess in understanding what is the meaning of the obtained network. Even though I have read the manual many times, the information provided is just not enough for me to utilize the package comfortably! While it is very interesting to see the variety of pathways that could be generated between reactants and products from an academic point of view, this reviewer fails to see how useful information can be obtained efficiently from the package under the present setup. Another application of RAIN is to find all possible isomers of a certain elementary composition, with or without predetermined substructures in the isomers. This part could be used in an organic class to demonstrate the various types of possibilities in constructing the complete set of isomers.

RAIN is manual driven. The main menu provides options to open, copy, or erase a network. Once you give a name to a network, everything will be recorded by that name. They can be copied or erased as a whole. Besides information about the network, other items on the main menu are for operational purposes. They are described briefly below:

Molecules. This serves not only as a editor for input molecules but also is used for listing molecules in the network.

Substructures. This is a tool for entering, modifying, and listing substructures that are either forbidden or required in the generated molecules.

Elements. This is used to define all allowable conversions from one bond type to another for an atom. The "transition table" for each atom must be defined before the generating process can start.

Constraints. This menu provides user defined boundary conditions for generating a network, such as maximum number of reacting atoms, maximum number of reacting bonds, maximum change of bond order, and maximum number of rings, etc.

Networks. This menu is used to see the network generated by the program.

Generator. This produces reactions and structures according to user defined rules. The user can select the direction of generation to be forward, backward, or both alternatively.

Configuration. This menu is used to choose printer and atom display modes.

Of course, I recognize that a certain amount of personal preference is already interjected when evaluating software. Let me conclude this review by suggesting that the author of RAIN rewrite the users manual as the first step to improving the system.

REFERENCES AND NOTES

(1) RAIN, Version 2.0, is available from Dr. Eric Fontain, Organic Chemistry Institute, Technical University—Munch, Lichtenberg Street 4, D-8046 Garching, Germany. Phone: 49-89-3209-3378. FAX: 49-89-3209-3315. The cost is $50.00 for students, nonprofit organizations, and government labs. The cost is $200.00 for industrial companies.