ASTROCHEMISTRY LIBRARY WITH ARTIFICIAL INTELLIGENCE FOR QUALITY CONTROL

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ABSTRACT. Libraries of reactions used in astrochemistry modeling have seen an explosive increase in size in recent years. Their quality control by manual effort is almost impossible. Expert systems with artificial intelligence are now needed to ensure the quality of large scale astrochemistry libraries.

1. PROBLEM DEFINITION AND SOLUTION CONCEPT:

Two decades ago, in early 70s, interstellar chemistry modeling used only modestly large reaction sets (e.g., 100 reactions involving 30 species). The beginning of the next decade saw a quantum leap in the size of the network with the publication in 1980 of Prasad and Huntress (1980) model. This model used 1423 reactions and 137 species. The new direction became popular, and the trend towards large scale models continued throughout the 1980s. The most recent publication in this class is the UMIST Ratefile (Millar et al 1991) with 2880 reactions and 313 species.

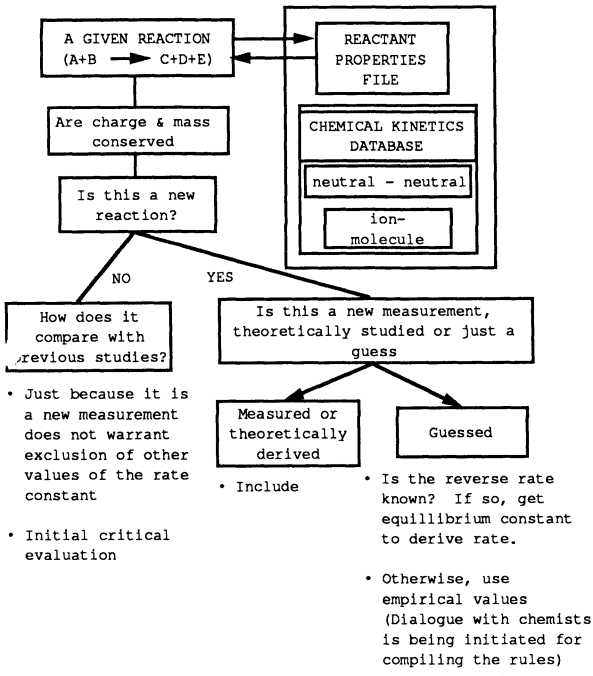
The problems now are: (i) How to guard against unavoidable human errors in the traditional way of assembling a library? or, (ii) How to deal with the difficulties of manually searching the literature adequately? "Expert systems" with artificial intelligence for quality control constitute the solution to these problems.

The quality control capabilities of "expert system" would originate from the current knowledge (both scientific and empirical) of human experts that are stored in computer subprograms queried by the master quality control program. Such "expert systems" are quite common in numerous fields (e.g., medical diagnosis). It is now time to consider its application in astrochemistry.

2. OUTLINE OF MINIMAL CAPABILITY "EXPERT SYSTEMS":

Quality controllers can be as sophisticated as we may wish them to be. But the toll on time and effort increases steeply with the intended sophistication. To begin with we may try to have at least the following capability for our systems: (i) ability to make charge and mass balance check, (ii) detect repetitions, (iii) consistency between forward and backward reactions, (iv) ensuring that endothermic reaction do have activation energies and that the reaction rates do not have alarming values due to human errors during data entry, (v) ensuring maximum scan of the published work, (vi) use of evaluated data when more than one study exist for a given reaction.

P. D. Singh (ed.), Astrochemistry of Cosmic Phenomena, 19–20.



These capabilities can be accomplished with an approach outlined in the Figure 1. We need to create a property file containing the following data for each reactant: charge, mass, atomic composition, heat of formation, and entropy. For the neutral partners of ion-molecule reactions, we must also include their rotational constants, dipole moments and polarizabilities. These would be needed to get the reaction rates at the very low temperatures (~10 - 20K). Preparation of the property file is now rendered easier due to the availability of computerized data bases for the various chemical and physical properties of atoms and molecules from national standards institutions. The required information may not be in the data base for many of the astrochemistry species. For them empirical rule may be used.

Chemical kinetics data bases on computer readable media are also available for both ion-molecule and neutral-neutral reactions. These and the property file become input to chemical reaction scrutinizer outlined in the figure 1.

Figure 1: Reaction scrutinizer expert system: an outline of its possible functions.

3. CONCLUDING REMARKS:

Building of "intelligent" expert systems is not easy. It certainly cannot be done by a single astrochemistry modeler. The purpose of the presentation at this symposium has been to expose the new opportunity due to the recent advances in data base technology, and to invite collaboration from interested modelers.

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