ABSTRACT:
Herein is described an ongoing research project whose goal is the realization of so-called Automatic Deductive Systems capable of solving class problems of interest to the chemistry related disciplines. Such systems are easily used by researchers without mathematical or computer backgrounds to help design experiments and to process data. These systems will eventually be coded in a machine and configuration independent high-level language, called TPL, so that they then can be run without change on a wide variety of machines having different peripheral equipment, architecture and memory sizes.

Four systems (CURFIT, CRAMS, FRANS, and MATCHEM) have been conceived and two of these (CURFIT and CRAMS) are implemented. CURFIT is an automatic curve-fitting system that can be used to obtain unambiguous fits of data to linear or non-linear equations. CRAMS and FRANS have both predictor and data-processing capabilities. MATCHEM, which is based on the work of Dugundji and Ugi [1], will be
capable of solving a variety of chemical problems in a deductive manner, and devising new ways for synthesizing compounds.

In this paper we illustrate the use of CURFIT and CRAMS and describe principles that are used in all four systems.

I. INTRODUCTION

In experimental chemistry a research objective is generally realized by a procedure that involves the following steps.

(i) Identification of the phenomenon that is to be studied or the goal that is to be realized.

(ii) Hypothesis of a model, or the outline of procedures that can be used to design experiments.

(iii) Design or selection of the experiments that are to be performed. Here it should be noted that frequently there is a one to many mapping of (ii) to (iii).

(iv) Execution of the experiment(s) and collection of data.

(v) The data, frequently combined with data from other sources, are processed.

(vi) Conclusions are drawn. Parts of this procedure are repeated until the goal is realized.

The project that is described and demonstrated in this paper has as its goal the realization of automatic, general computer systems that can be widely and easily used by non-computer experts to help design experiments, Step (iii), and to process data, Step (v). Such systems must have the following properties:

(a) The user interface must accept questions and return answers in an easily understood chemical language. Thus it will be subject dependent.

(b) The main part of the system must be subject independent and:

1. Capable of generating all those combinations of input data that can be used to obtain successful solutions (if they exist) in the data-processing step, (v). This so-called predictor capability is needed to aid in the design of experiments (Step (iii)).

2. Have an automatic data-processing capability for analyzing information collected in experiments that were designed with or without use of the predictor capability. There is a unique relationship between the predictor and processing functions: The deductive system will provide (i.e. predict) all those combinations of data for which it can obtain solutions to the given problem, if input data for processing were provided.

(c) To insure the widest possible use of such systems they must be coded in a programming language that is independent of both the machine and its configuration. Moreover, because the systems are to be immediately usable, the compiler for this implementation language must itself be machine and configuration independent.