

## DEVELOPING INORGANIC EXPERT SYSTEM TO AUTOMATE INORGANIC CHEMISTRY

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The Inorganic Expert attempts to reproduce the performance of human experts in the domain of Inorganic Chemistry. It is a rule-based system that predicts the behavior of the already known as well as the yet-to-be-discovered elements, on the basis of the Periodic Table, which illustrates the recurring (or 'periodic') trends in the properties of elements. This system would also keep track of the elements that show 'exceptional' behavior. Many expert systems have been put into practical use by the researchers in the domains of Mathematics (SAINT), Organic Chemistry (DENDRAL, No Electron Left Behind, Beaker, etc), Archeology (LITHAN), and so on. So, the aim of this paper is to give an idea about all currently existing expert systems and to present a proposed system named "INORGANIC EXPERT" to automate the inorganic chemistry.

Keywords: Expert System, Rule-based Systems, Inorganic Chemistry, Automation (of Inorganic Chemistry), Periodicity, Periodic Table, Balancing (of Equations) and Prediction (of Properties and New Elements).

### 1. INTRODUCTION

An expert system is defined as a software that attempts to reproduce the performance of one or more human experts, most commonly in a specific problem domain. It basically uses an inference engine connected to the knowledge base in its field as shown in Fig. 1. A wide variety of methods can be used to simulate the performance of the expert however common to most or all are:

- the creation of a so-called "knowledgebase" which uses some knowledge representation formalism to capture the Subject Matter Expert's (SME) knowledge;
- a process of gathering that knowledge from the SME and codifying it according to the formalism, which is called knowledge engineering.

Expert systems may or may not have learning components but a third common element is that once the system is developed it is proven by being placed in the same real world problem solving situation as the human SME, typically as an aid to human workers or a supplement to some information system.

The examples of Expert Systems are explained as following:

- MYCIN: To identify bacteria causing severe infections, such as bacteremia and meningitis, and to recommend antibiotics, with the dosage adjusted for patient's body weight.

- DENDRAL: Its primary aim was to help organic chemists in identifying structure of unknown organic molecules, by analyzing their mass spectra and using knowledge of chemistry.
- SAINT: To solve problems based on Integral Calculus, and eventually generate simpler expressions for complex functions.

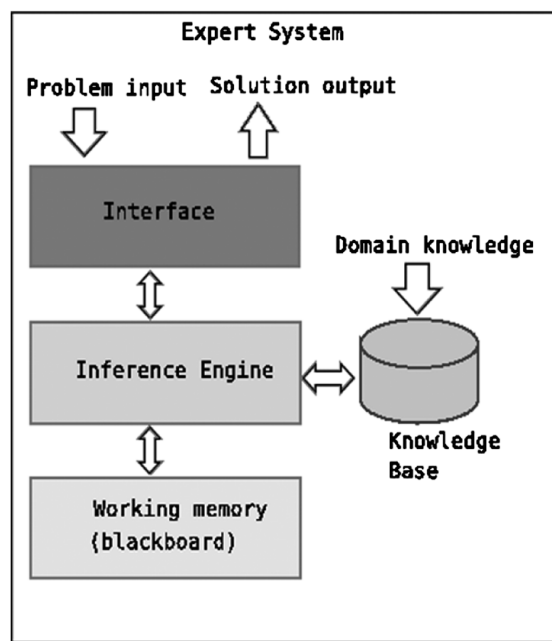


Fig. 1 Architecture of Expert System

A rule-based system is a system to store and manipulate knowledge to interpret information in a useful way. They are often used in artificial intelligence applications and

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research. Rule-based programming attempts to derive execution instructions from a starting set of data and rules, which is a more indirect method than using an imperative programming language which lists execution steps straightforwardly [1].

In Inorganic Chemistry, periodic trends are the tendencies of certain elemental characteristics to increase or decrease as one progresses along a row or column of the periodic table of elements [2].

## 2. RELATED WORK

In the past, there have been lots of developments in this field (Expert System) of Artificial Intelligence, so as to mechanically solve problems related to a specific domain, sometimes, even better than as solved by a human expert! Even today, there have been no popular and in-use expert system known that solves problems in the domain of Inorganic Chemistry.

The Inorganic Chemists still face some major complications, such as:

- Remembering the periodic properties (physical as well as chemical) of all the 117 elements known till date.
- Predicting the behavior of all these elements under different physical and chemical conditions.
- Predicting the properties of the unknown or yet-to-be-discovered elements.
- Remembering the names and properties of the elements that show 'exceptional' behavior.

A lot of works have been done in this field. The current work can be described in terms of Description of already developed EXPERT SYSTEMS as follows:

### MYCIN

MYCIN was an early expert system developed over five or six years in the early 1970s at Stanford University. It was written in Lisp as the doctoral dissertation of Edward Shortliffe under the direction of Bruce Buchanan, Stanley N. Cohen and others. It arose in the laboratory that had created the earlier Dendral expert system, but emphasized the use of judgmental rules that had elements of uncertainty (known as certainty factors) associated with them. This expert system was designed to identify bacteria causing severe infections, such as bacteremia and meningitis, and to recommend antibiotics, with the dosage adjusted for patient's body weight — the name derived from the antibiotics themselves, as many antibiotics have the suffix "-mycin". Mycin systems are also used for the diagnosis of blood clotting disease. The evolution of MYCIN Expert system is shown in Fig.2.

MYCIN operated using a fairly simple inference engine, and a knowledge base of ~600 rules. It would query the physician running the program via a long series of simple yes/no or textual questions. At the end, it provided a list of possible culprit bacteria ranked from high to low based on the probability of each diagnosis, its confidence in each diagnosis' probability, the reasoning behind each diagnosis (that is, MYCIN would also list the questions and rules which led it to rank a diagnosis a particular way), and its recommended course of drug treatment [1].

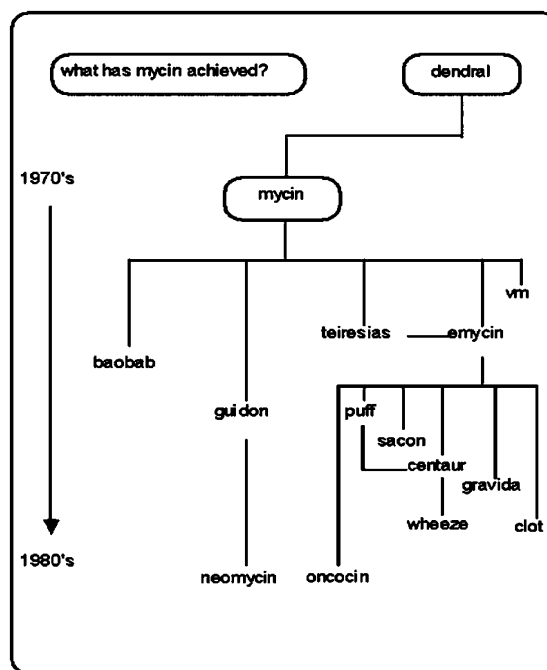


Fig. 2: Evolution of MYCIN Expert System

### Dendral

Dendral was an influential pioneer project in artificial intelligence (AI) of the 1960s, and the computer software expert system that it produced. Its primary aim was to help organic chemists in identifying unknown organic molecules, by analyzing their mass spectra and using knowledge of chemistry. It was done at Stanford University by Edward Feigenbaum, Bruce Buchanan, Joshua Lederberg, and Carl Djerassi. It began in 1965 and spans approximately half the history of AI research. The software program Dendral is considered the first expert system because it automated the decision-making process and problem-solving behavior of organic chemists. It consists of two sub-programs, Heuristic Dendral and Meta-Dendral. It was written in Lisp (programming language), which was considered the language of AI. Many systems were derived from Dendral, including MYCIN, MOLGEN, MACSYMA, PROSPECTOR, XCON, and STEAMER. The name Dendral is a portmanteau of the term "Dendritic Algorithm" [7].

### PUFF

PUFF is a program that interprets lung function test data and has become a working tool in the pulmonary physiology lab of a large hospital. Elements of the problem that paved the way for its success are examined, as are significant limitations of the solution that warrant further study [14].

### Blue Box

An early phreaking tool, the blue box is an electronic device that simulates a telephone operator's dialing console. It functions by replicating the tones used to switch long-distance calls and using them to route the user's own call, bypassing the normal switching mechanism. The most typical use of a blue box was to place free telephone calls - inversely, the Black Box enabled one to receive calls which were free to the caller. The blue box no longer works in most western nations, as modern switching systems are now digital and no longer use the in-band signaling which the blue box emulates. Instead, signaling occurs on an out-of-band channel which cannot be accessed from the line the caller is using (called Common Channel Interoffice Signaling (CCIS)). The blue box got its name because the first such device confiscated by Bell System security was in a blue plastic case [9].

### DELTA

An Expert System for Diesel Electric Locomotive Repair General Electric Company's Corporate Research and Development has applied expert system technology to the problem of troubleshooting and the repair of diesel electric locomotives in railroad running repair shops. The expert system uses production rules and an inference engine that can diagnose multiple problems with the locomotive and can suggest repair procedures to maintenance personnel.

A prototype system has been implemented in FORTH, running on a Digital Equipment PDP 11/23 under RSX-11M. This system contains approximately 530 rules (roughly 330 rules for the Troubleshooting System, and 200 rules for the Help System), partially representing the knowledge of a Senior Field Service Engineer. The inference engine uses a mixed-mode configuration, capable of running in either the forward or backward mode. The Help System can provide the operator with assistance by displaying textual information, CAD diagrams or repair sequences from a video disk. The rules are written in a representation language consisting of nine predicate functions, eight verbs, and five utility functions. The first field prototype expert system, designated was delivered in July 1983 and is currently under field evaluation [9].

### OncoLogic

OncoLogic is a Computer System to Evaluate the Carcinogenic Potential of Chemicals. EPA (U. S. Environmental Protection Agency) "What is an expert system? An expert system is a computer program that mimics the judgment of experts by following sets of knowledge rules that are based on studies of how chemicals cause cancer in animals and humans. An expert system, like OncoLogic, asks for chemical and use information from the user and following the knowledge rules incorporated into the system, uses the responses to construct an estimation of the most likely results" [18].

### LifeCode

It is a Deployed Application for Automated Medical Coding. This is based on the authors' presentation at the Twelfth Innovative Applications of Artificial Intelligence Conference (IAAI-2000). LifeCode is a natural language processing (NLP) and expert system that extracts demographic and clinical information from free-text clinical records [8].

### Ramp Activity Expert System

Ramp Activity Expert System is used for Scheduling and Coordination at an Airport. By user-driven modeling for end users and near-optimal knowledge-driven scheduling acquired from human experts, races can produce parking schedules for about 400 daily flights in approximately 20 seconds; human experts normally take 4 to 5 hours to do the same [10].

### An Expert System for Automotive Diagnosis

This 'expert in a box' will guide a human technician through the entire service process, from the initial customer interview at the service desk to the diagnosis and repair of the car in the garage [18].

## 3. PROPOSED WORK

Our main objective behind developing the EXPERT SYSTEM named as INORGANIC EXPERT would be to achieve its ability to automate Inorganic Chemistry. Keeping in mind the complications faced by the chemical researchers in the field of Inorganic Chemistry such as remembering the names and properties (physical and chemical) of all the 117 known elements of the periodic table and the varying trends in their properties along with their exceptional behaviors., the INORGANIC EXPERT, is being developed to achieve the solutions to such complications. This system would be able to carry out the following functions as shown in Fig.3:

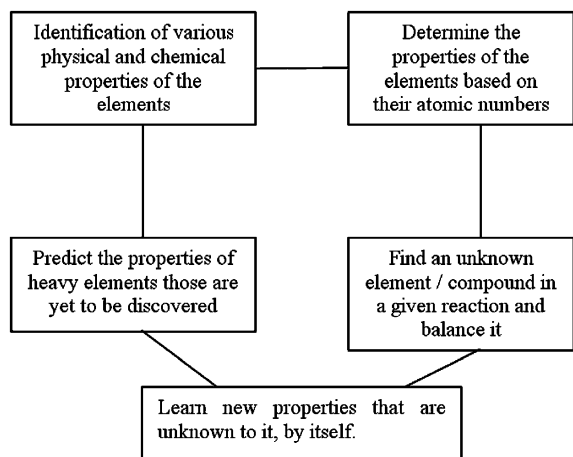


Fig. 3: Proposed INORGANIC EXPERT System

This system will be able to find the yet to be discovered elements/compounds and predict their properties or behavior under different physical and chemical conditions.

#### 4. CONCLUSION AND FUTURE SCOPE

All the previously developed Expert Systems were based on one of Organic chemistry, mathematical calculus techniques, diagnosis of a disease, evaluation of carcinogenic potential of chemicals, or medical coordination. Due to the fact that none of the already developed Expert Systems is related to inorganic chemistry, it became a need to develop such an expert system to give the history of expert systems, a new revolution. The INORGANIC EXPERT, aiming helping out almost everyone involved in the field of inorganic chemistry, defines a good future scope for itself as it solves majority of the complications, being faced by the researchers and students in the field of inorganic chemistry. These solutions primarily will constitute identification and determination of the properties of existing elements in the modern periodic table, assisting the chemical researchers by providing basic knowledge about existing elements and their various combinations, in a single click and achieving Computer-based learning in the field of Inorganic Chemistry. The system would also prove to be a great help in discovering

the yet-unknown elements or compounds and predicting their behaviors.

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