CHEMISTRY RULE-BASED SYSTEM (CRBS)

by

Kyi Kyi Tin

Submitted in Partial Fulfillment of
the Requirements for the Degree of
Master of Science
in Computer Science
Assumption University

March, 1999

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Thesis Approval

Thesis Title	Chemistry Rule-Based System (CRBS)
By	Ms. Kyi Kyi Tin
Thesis Advisor	Dr. Tang Van To
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The Department of Computer Science, the Faculty of Science and Technology of Assumption University had approved this final report of the twelve credits course, SC 7000 Master Thesis, submitted in partial fulfillment of the requirements for the degree of Master of Science in Computer Science.

Approval Committee:

(Dr. Tang Van To) Advisor	(Dr. Thitipong Tanprasert) Committee
(Dr. Pham Hong Hanh) Committee	(Dr. Boontee Kruatrachue) MUA Representative

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Faculty Approval

(Dr. Thitipong Tanprasert) Director	(Dr. Pratit Santiprabhob) Dean

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This paper is dedicated to my late beloved father who always tell me that **"It's never too late to learn"**.

ABSTRACT

This research was developed to enhance the process of teaching and learning chemistry by applying rule-based system. We try to derive rules how materials are combined and reacted together and implement it. The study emphasizes on formalizing and representing chemistry rules related to acid-base formation, combination of acids and bases to produce different salts and calculations concerning the mole concept are also intensively studied, implemented and evaluated.

The system will generate various acids and bases from a basis data set of atomic states. Then a data set consisting of many acid-base solution combinations, which can be used for preparing different salts, are generated. Different concentrations of acids and bases with related pH and pOH values will also be calculated. Being free of the tedious practical routines, virtual titration and the simulations process can be done on computer.

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Chapter 1

INTRODUCTION

1.1 Statement of the problem

Expert system is a computer program that acts as an expert. It can be run and give the advice where needed. Rule-based systems have been developed as MYCIN [20], XCON (R1) [14]. The approach, simple as it is, can well model the expert reasoning.

In this research, we try to develop a chemistry Rule-Based System (CRBS), which can enhance the process of teaching and learning Chemistry at ABAC. The author tries to derive rules of how materials are combined and react together and implement it. With such a CRBS that uses forward chaining, we can find out what can be the outcome when materials are combined. Backward chaining allows us to know how to produce a compound.

The study emphasizes how chemical rules are formalized and represented, and the implementation process of this is discussed. Due to the time constraints, only rules related to the acid-base formation, combination of acids and bases to produce different salts, calculations based on mole concepts, concentrations of acids and bases with pH and pOH will be intensively studied, implemented and evaluated. Finally virtual titration can be performed on the computer so that tedious practical routines can be avoided.

1.2 Objectives of the study

The objective of the study is to formalize rules, how materials are combined and implement them. The outcome of the system could be a part of CAI (Computer

Aided Instruction) for Chemistry. It can help students to understand how acids, bases, and salt are formed and the calculation involving mole concept, pH and pOH and performance of virtual titration. The computer knowledge will enable students to study Chemistry efficiently.

1.3 Scope of the study

This study covers the methodology, the realization of a CRBS, the implementation of the system, and the evaluation of the process that develops the system. We propose, therefore, an intensive study of how to derive rules, implement the rule based system for construction of acids, base compounds, formation of different salts and calculations based on mole concept, pH and pOH.

1.4 Outline of the system

The system will generate various acids and bases from a basis data set of atomic states. Calculation of the amount of products produced (i.e. acid, base and salt) from selected elements, and vice versa. The preparation of different salts from acid and base solutions will be generated. This will give a data set, consisting of many acid-base solution combinations, which can be used for preparing different salts. Different concentrations of acids and bases will be simulated. Related pH and pOH values of acids and bases will be also calculated.

The output will enable instant visualization of the construction of acid and base compounds, formation of different salts, without actually performing the experiments. Being free of tedious practical routines, many such simulations can be done within a short time, thus giving an overview, which will help develop insights into the real nature of construction process of the chemical compounds by applying CRBS.

Chapter 2

BACKGROUNDS AND CONCEPTS

As mentioned in chapter 1, this research aims to develop a chemistry rule-based system (CRBS) . It is necessary to review the related background of the chemistry and rule-based system before devoting to derive and implement a CRBS. In this chapter, the review of chemistry will be given in the first two sections, and the review of expert system and rule-based system will be given in the other two sections.

2.1 The periodic table

2.1.1 Modern version of the periodic table

The modern version of the periodic table tries to list elements in the same group when they have similar chemical properties and similar electron configurations. It is shown in Figure 2-1. Each group contains compounds with similar chemical properties. In most cases, the elements in a column also have similar electron configurations. The two most important exceptions are hydrogen and helium. On the basis of electron configuration, hydrogen ($1s^1$) should be in Group 1 (IA), along with lithium ([He] $2s^1$), sodium ([Ne] $3s^1$), potassium ([Ar] $4s^1$), and so on. But the other element in Group IA is metals, and hydrogen is not. Thus, it may be appropriate to include hydrogen in Group 7 (VIIA) of the periodic table, with the other nonmetals that have one less electron than a filled-shell configuration.

Similarly, helium ($1s^2$) should be placed in Group 2 (IIA) of the table, along with beryllium ([He] $2s^2$), magnesium ([Ne] $3s^2$), calcium ([Ar] $4s^2$), and so on. But the element in-group 2A is metals, and helium is not. Helium behaves more like the elements with a filled-shell electron configuration in the last column of the periodic table. Therefore includes helium among the elements in Group 8 (VIIIA).

2.1.2 Classification of elements

Elements are classified into five types depending on their outermost shell electron configuration.

1) Representative Elements (Group IA, IIA, IIIA ------>VIIA),

$ns^x\ np^y\ (x+y \leq 7)$

2) Transition Elements (Group IIIB -------> VIIIB, IB, IIB),

$ns^2,(n-1)d^x\ (x \leq 10)$

3) Noble or Inert gases (Group VIIIA), ns^2, np^6

4) Lanthanide series (Atomic Number 58 -----> 71)

5) Actinide series (Atomic Number 90 ------> 103)

2.1.3 Group IA : The alkali metals

The metals in Group IA include lithium (Li), sodium (Na), potassium (K), rubidium (Rb), cesium (Ce), and francium (Fr). These elements are called the **alkali metals** because they all form hydroxides (such as NaOH) that were once known as alkalies. Sodium and potassium are relatively common elements [4]. They are among the eight most abundant elements in the earth's crust. Discussions of the chemistry of alkali metals therefore focus on sodium and potassium.

2.1.4 Group IIA : The alkaline earth metals

The elements in Group IIA (Be, Mg, Ca, Ba, and Ra) are all metals, and all but Be and Mg are active metals. These elements are often called the **alkaline-earth**

metals. The term alkaline reflects the fact that many compounds of these metals are basic or alkaline. The term earth was historically used to describe the fact that many of these compounds are insoluble in water. These metals are less reactive than the neighbouring alkali metals.

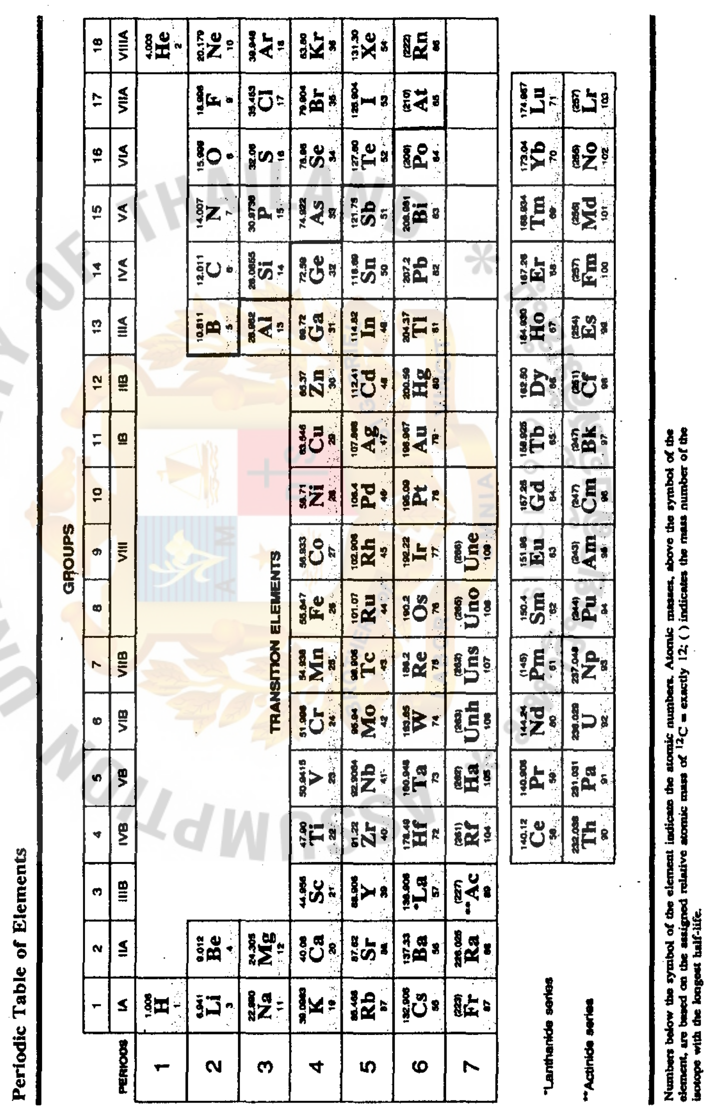


Figure 2-1 Modern version of periodic table (source: Fig. 7-4 [4])

2.1.5 The chemistry of nonmetals

More than 75% of the known elements have the characteristic properties of metals. They have a metallic luster; they are malleable and ductile; and they conduct heat and electricity. Eight other elements (B, Si, Ge, As, Sb, Te, Po, and At) are best described as **semimetals or metalloids**. They are brittle and semiconductors.

Once the metals and semimetals are removed from the list of known elements, only 17 are left to be classified as **nonmetals**. Six of these elements belong to the family of the noble gases in Group VIIIA, most of them is inert to chemical reactions.

2.1.5.1 Group VA : The chemistry of sulphur

Sulphur is below oxygen in the periodic table, therefore have similar electron configurations. There are four principal differences between the chemistry of sulphur and the chemistry of oxygen:

1) O = O double bonds are much stronger than S = S double bonds.

2) S - S single bonds are almost twice as strong as O - O single bonds.

3) Sulphur (EN = 2.58) is much less electronegative than oxygen(EN = 3.44).

4) Sulphur can expand its valence shell to hold more than eight electrons, but oxygen cannot.

Because sulphur is much less electronegative than oxygen, it is more likely to form compound in which it has a positive oxidation number. In theory, sulphur can react with oxygen to form either SO_2 or SO_3. Both of them dissolve in water to form sulphurous acid(H_2SO_3) and sulphuric acid(H_2SO_4).

$SO_2(g)$[1]+ $H_2O(l)$[2] --------------> $H_2SO_3(l)$

---

[1] g: stands for gas

[2] l: stands for liquid

$SO_3(g) + H_2O(l)$ ---------------> $H_2SO_4(l)$

2.1.5.2 Group VIA: The chemistry of nitrogen

The chemistry of nitrogen is dominated by the ease with which nitrogen atoms form double and triple bonds. A neutral nitrogen atom contains five valence electrons: $2s^2\ 2p^3$. A nitrogen atom can therefore achieve an octet of valence electrons by sharing three pairs of electrons with another nitrogen atom. At high temperatures, nitrogen reacts with oxygen to form nitrogen oxide:

$N_2(g) + O_2(g)$ ----------> $2NO(g)$

Nitrogen oxide is a colourless gas that reacts rapidly with oxygen to produce nitrogen dioxide, a dark brown gas:

$2NO(g) + O_2(g)$ ----------> $2NO_2(g)$

Nitrogen dioxide dissolves in water to give nitric acid and nitrous acid.

$2NO_2(g) + H_2O(l)$ ---------> $HNO_3(aq)$[3] $+ HNO_2(g)$

2.1.5.3 Group VIIA: The chemistry of halogens

There are six elements in Group VIIA, the next to last column of the periodic table. These elements have certain properties in common. They all form diatomic molecules (H_2, F_2, Br_2, I_2, At_2), and they all form negatively charged ions. When the chemistry of these elements is discussed, hydrogen is separated from the others and astatine is ignored because it is radioactive. The remaining four elements are called halogens because they are salt formers. They combine with hydrogen to form

---

[3] aq: stands for aqueous

hydrogen halides, colourless compounds and soluble in water to become mineral acids. $H_2(g) + Cl_2(g) \text{ -------------->} 2HCl(g)$

$$HCl(g) \xrightarrow{+H_2O} H^+(aq) + Cl^-(aq)$$

$$HCl(g) + H_2O \text{ -------------->} H_3O^+(aq) + Cl^-(aq)$$

2.2 Acids and bases

2.2.1 Discovery process of acids and bases

For more than 300 years, chemists have classified substances that behave like vinegar as acids. Substances that have properties like wood ash, on the other hand, have been classified as alkalis (or bases). In 1661 Robert Boyle summarized the properties of acids as follows:

1) Acids have a sour taste.

2) Acids are corrosive.

3) Acids change the color of certain vegetable dyes, such as litmus, from blue to red.

4) Acids lose their acidity when they are combined with alkalis.

5) Acids have pH value less than 7.

and he also summarized the properties of alkalis as follows:

1) Alkalis feel slippery.

2) Alkalis change the color of litmus from red to blue.

3) Alkalis become less alkaline when they are combined with acids.

4) Alkalis have pH value greater than 7.

Alkalis became known as bases because they serve as the "base" for making certain salts.

2.2.2 Definition of acids and bases

Arrhenius defined acids as a compound that ionize when they dissolve in water to give H^+ ions and a corresponding negative ion.

Example: HCl (Hydrogen Chloride) is an acid because it ionizes when it dissolves in water to give hydrogen (H^+) ions (or) hydronium (H_3O^+) ions and a corresponding negative ion.

$$HCl(g) \xrightarrow{+H_2O} H^+(aq) + Cl^-(aq)$$

$$HCl(g) + H_2O \longrightarrow H_3O^+(aq) + Cl^-(aq)$$

Arrhenius defined bases as a compound that either dissociates or ionizes in water to give (OH^-) and a positive ion. NaOH is an Arrhenius base because it dissociates in water to give the hydroxide (OH^-) ion and sodium (Na^+) ion.

$NaOH(s)$ ---in H_2O--------> $Na^+(aq) + OH^-(aq)$

2.2.3 Formation of acids and bases

Dissolving nonmetal oxides and hydrogen halides in water forms acids.

Example: NO_2, SO_2, SO_3, and HI dissolve in water to produce acids.

Nitrogen Dioxide + Water ——> Nitric Acid + Nitrous Acid

$$2NO_2(g) + H_2O(l) \longrightarrow HNO_3(aq) + HNO_2(aq)$$

Sulphur Dioxide + Water ——> Sulphurous Acid

$$SO_2 + H_2O(l) \longrightarrow H_2SO_3(aq)$$

Sulphur Trioxide + Water ——> Sulphuric Acid

$$SO_3(g) + H_2O(l) \longrightarrow H_2SO_4(aq)$$

Hydrogen Chloride* + *Water* ————> *HydroChloric Acid

$HCl (g) + H_2O (l)$ ---------------> $HCl (aq)$

Dissolving alkali metal oxides and alkaline earth metal oxides in water forms bases.

Example: Na_2O, K_2O, CaO, and MgO dissolve in water to produce bases.

Sodium Oxide + Water ————> Sodium Hydroxide

$Na_2O(s) + H_2O (l)$ -----------> $2NaOH(aq)$

Potassium Oxide + Water ————> Potassium Hydroxide

$K_2O (s) + H_2O (l)$ ----------> $2KOH(aq)$

Calcium Oxide + Water ————> Calcium Hydroxide

$CaO(s) + H_2O (l)$ ---------> $Ca (OH)_2(aq)$

Magnesium Oxide + Water ————> Magnesium Hydroxide

$MgO(s) + H_2O (l)$ --------> $Mg (OH)_2(aq)$

2.2.4 Acidity (pH) and alkalinity (pOH)

In 1909, Danish biochemist S. P. L. Sorenson introduced acidity (pH) and Alkalinity (pOH) as follows:

$pH = - \log [H_3O^+]$

$pOH = - \log [OH^-]$

The relationship between the pH and pOH of an aqueous solution can be derived as:

$pH + pOH = 14 \quad ([H_3O^+][OH^-] = 10^{-14})$

This equation can be used to convert from pH to pOH , or vice versa, for any aqueous solution at 25°C, regardless of how much acid or base has been added to the solution.

2.2.5 Molarity

All concentration units have one thing in common: they describe the ratio of the amount of solute to the amount of solvent or solution. Chemist uses one concentration unit more than any other: **molarity** (***M***). The molarity of a solution is the number of moles of solute per liter of the solution. Molarity is calculated by dividing the number of moles of solute in the solution by the volume of the solution in liters.

$$\textbf{Molarity } (M) = \frac{molesofsolute}{litersofsolution}$$

Moles of solute can be converted from mass of solute as follows:

$$\textbf{Mole } (n) = \frac{massofsolute}{molarmassofsolute}$$

2.3 Quantitative analysis

2.3.1 Definition

Titrimetric analysis refers to quantitative chemical analysis carried out by determining the volume of a solution of accurately known concentration which is required to react quantitatively with the solution of the substance to be determined.

The solution of accurately known strength is called the **standard solution** .The process of adding the standard solution until the reaction is just complete is known as **titration**, and the substance to be determined is **titrated**. The point at which this occurs is called the **equivalence point** or the **theoretical** (or **stoichiometric**) **end-point**. The completion of the titration is detectable by some change, unmistakable to the eye produced by the standard solution itself (e.g, potassium permanganate) or more usually, by the addition of an auxiliary reagent, known as an **indicator.** After the reaction between the substance and the standard solution is practically complete, the indicator should give a clear visual change (either a colour change or the formation of a turbidity) in the liquid being titrated. The point at which this occurs is called the **end-point of the tritration**.

The term volumetric analysis was formerly used, but it has now been replaced by **titrimetric analysis,** since it is considered that the latter expresses the process of titration rather better, and former may be confused with measurements of volume, such as those involving gases. The reagent of known concentration is called the **titrant** and the substance being titrated is termed the **titrand.**

2.3.2 Concept for titrimetric analysis

Titrimetric analysis reaction must fulfill the following conditions:

1) There must be a simple reaction which can be expressed by a chemical equation
2) The reaction should be practically instantaneous or proceed with very great speed
3) There must be a marked change in free energy leading to alteration in some physical or chemical property of the solution at the equivalence point.
4) An indicator should be available which, by a change in physical properties (colour or formation of a precipitate), should sharply define the end point of the reaction.

2.3.3 Indicator

All the indicators indicate the end point by a change in colour. Indicators usually encountered are acid-base indicators (e.g, methyl orange ; phenolphthalein) redox indicators (e.g. ferrion, $KMnO_4$) and adsorption indicators (e.g. K_2CrO_4;KCNS).

2.3.4 Mole concept

The unit *mole* (abbreviated mol) can be applied to any particle. Before we can apply the concept of the mole, we need to be able to calculate the **molecular weight** of a compound, which is the sum of the atomic weights of the atoms in the molecules that form these compounds.

For example:

1 mol O atom = 16.0g   1 mol O_2 molecule = 32.0 g

The mass of a mole of any substance is often called the **molar mass**. The number of particles in a mole is called **Avogadro's number** or, more accurately, **Avogadro's constant** (6.02×10^{23}). The mole is a powerful tool, which enables chemist to convert grams into moles or vice versa. As an example, if Sodium (Na) metal reacts with Oxygen (O_2) to form Sodium oxide (Na_2O), the equation can be expressed in mole as:

$$4Na(s) + O_2(g) \longrightarrow 2Na_2O(s)$$

i.e 4 mole of Na atom + 1mole of O_2 molecule --------→ 2 mole of Na_2O

i.e (4 x 23) g of Na Atom + (16x2) g of O_2 molecule ----→ { 2[(23x2) + 16]}g of Na_2O

Atomic mass of Na = 23 amu, O = 16 amu. For calculations concerning titration, we apply the same concept. Suppose we titrate Sodium Hydroxide (NaOH) with Hydrochloric acid (HCl), then the chemical equation is written as:

Sodium Chloride + Hydrochloric Acid ----→ Sodium Chloride + Water

$NaOH(aq) + HCl(aq) \longrightarrow NaCl(s) + H_2O$

Mole Ratio of NaOH : HCl = 1 : 1

Molarity = mole / dm³

We can therefore calculate Molarity of base (or) acid as:

$M_A V_A = M_B V_B$

M_A = Molarity of Acid; M_B = Molarity of Base

V_A = Volume of Acid; V_B = Volume of Base

2.3. 5 Common apparatus for titrimetric analysis

1) Pipette
2) Burette
3) Erlenmeyer Flask
4) Funnel
5) Iron Stand and Plate
6) Burette clamp holder

As mentioned at the beginning of this chapter, the remaining of this chapter briefs concepts and issues of expert system, rule-based system and related issues.

2.4 Expert system

2.4.1 Definition of expert system

An expert system (ES) is a computer system (program/software) which acts as a human expert within a particular field of knowledge. The methodology of expert system plays an increasingly important role in future decision making. To remain competitive, the employment of expert systems become a necessity. ES embodies knowledge about one specific problem in this domain. ES can learn from mistakes and gain experience and able to explain the reasoning (the way) in which it has concluded. Expert system deals with knowledge rather than data and the files they used are often referred to as knowledge bases. The rules that the program uses are **IF-THEN-ELSE** type. A rule is made up of a list of **IF** conditions and lists of **THEN** and **ELSE** conditions or statements about the probability of a particular choice being the appropriate solution to the problem.

Expert systems determine what additional information it needs and how best to get the information. If possible, the program will derive information from other rules rather than asking the user. This ability to derive information allows the program to combine small pieces of knowledge to arrive at logical conclusions about complex problems.

2.4.2 Expert system structure

The structure of the expert system can be viewed as in Figure 2-2.

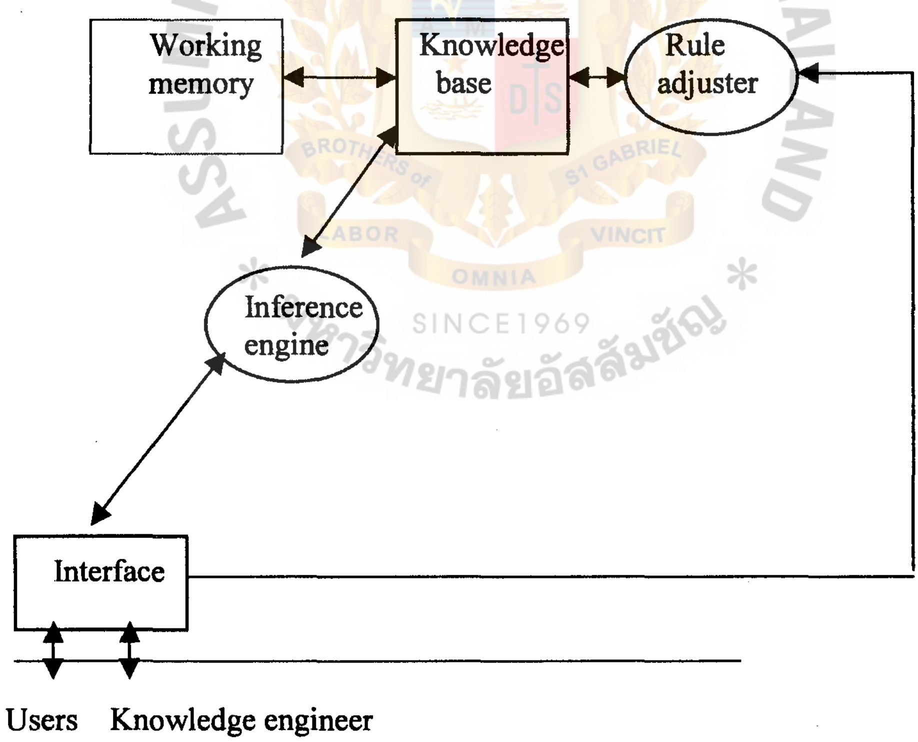


Figure 2-2 Structure of expert system (source: Fig.2-3, [8])

1) Knowledge engineer is the person responsible for placing the knowledge into the expert system's knowledge base and accomplishes this through the interface and the rule adjuster.

2) Users are individual who access to the expert system . The successful knowledge engineer must always keep in mind that the expert system is ultimately intended for the benefit of the user, not for that of the knowledge engineer or the domain expert.

3) Interface engine is employed during a consultation session, to examine the status of the knowledge base and working memory and to provide for the control of the session by determining the order in which inferences are made. The interface engine serves to merge facts with rules to develop, or infer, new facts.

4) Knowledge base is the heart of any expert system contain facts and rules.

5) Working memory consists of facts that change according to the specific problem at hand.

6) Rule adjuster serves as a rule editor by entering the rules specified by the knowledge engineer into knowledge base during the development phase of the expert system. The inference engine and knowledge base can be considered as a rule-based system, which will be discussed in section 2.4

2.4.3 Applications of expert systems

Expert System can be applied in a wide range of areas. Some typical expert systems are listed below as:

1) Codecheck (Computer Program Assessment) [17]

2) DENDRAL (Chemical Identification) [10]

3) DELTA/CATS (Maintenance of Diesel-Electric Locomotives) [3]

4) DustPro (Mine Safety) [14]

5) Expert System for Faster, Fast Food Operations [6]

6) GATES (Airline Gate Assignment and tracking Expert System) [4]

7) HERESAY (Speech Recognition) [16]

8) INTERNIST/CADUCEUS (Internal Medicine) [15]

9) Jonathan's Wave (Commodities Trading) [12]

10) MYCIN (Blood Infections) [18]

11) PUFF (Pulmonary Disorders) [1]

12) QMR (Medical Diagnostic Expert System) [9]

13) TOP SECRET (Security Classifications) [14]

14) XCON (R1) (Computer Configuration) [11]

The following areas are best suited to Expert System:

1)The field under study is able to be reduced into rules rather than mathematical formulae or equations.

2)The field under study should be well understood, so that rules can be well defined and formulated.

3)The field under study should not surround or include problems which takes too short time or too long time.

There should be general agreement among recognized experts in the field that these knowledge can be computerized.

- Number of rules must be large enough
- It should be built or involved by some experts.

2.5 Rule-based system

2.5.1 Definition

Rule-based system, also called production system, uses knowledge encoded in the form of production rules, that are **if...then** rules.

2.5.2 Rule-based system architecture

The last section described the expert system structure as being composed of five modules: knowledge base, inference engine, working memory, interface and a rule register. These five components comprise the heart of the system, but there are other subsystems that you will find in any real system. The complete architecture of a rule-based system is shown in Figure 2-3 as follows [5]:

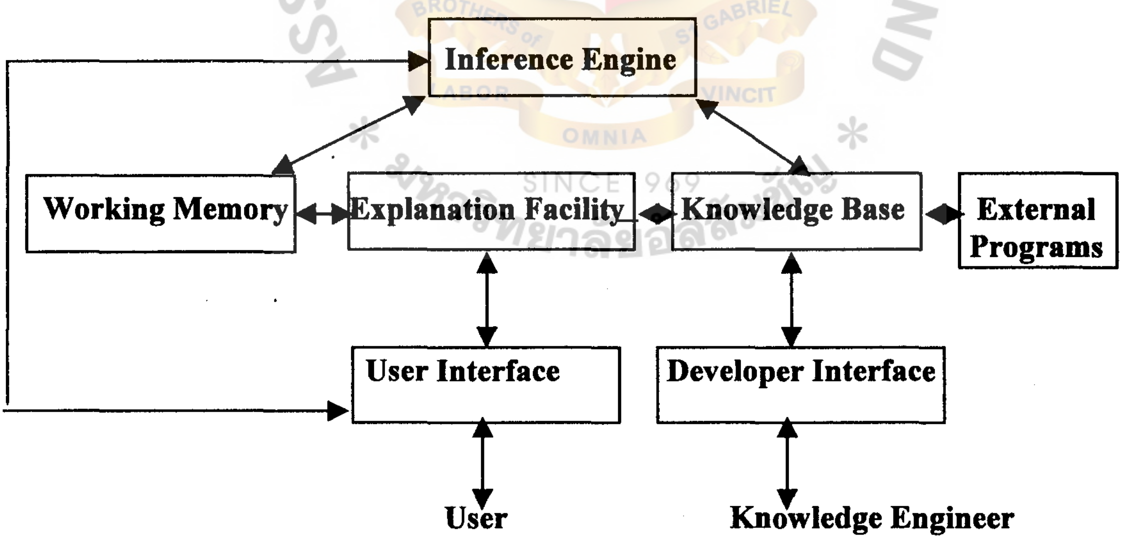


Figure 2-3 Rule-based system architecture

2.5.3 Reasons for selecting rule-based system

Rule-based Expert System is selected due to their popularity and widespread use such as:

1) Majority of existing Expert System employs rule bases.
2) Rule-based Expert System development packages are less expensive than other modes of representation
3) Knowledge engineer can focus attention on the knowledge base due to availability of rule-based expert system shells.
4) Takes less time to learn how to use and implement rule-based expert system.
5) Rules are transparent than frames and neural networks.
6) Easy to modify well - designed rule bases.
7) Ability to mimic most features of frame based representation scheme.
8) Validation is a simple process.

2.5.3.1 Development of rule-based system

Assume that our rule-based system is deterministic and we focus on just IF - THEN rules. That is condition - action or premise - conclusion comprising several premises and conclusion statements within a single rule. For example: Given the condition (or premise) that variable [Element] is "Sodium" or "Potassium" or "Lithium" or "Rubidium" and premise clause is "when combines with oxygen, we get the conclusion as:

(i) [Symbol] is Na

(ii) [Type] is Metal

(iii) [Atomic Mass] is 23.01 amu

(iv) assign [Symbol] as a [newsymbol]

(v) [product] is given the value [newsymbol] + "2O"

(vi) [Molar_Mas of oxide] is given the value ([Atomic_Mas] * 2 + 16)

Premise clauses may be connected by **AND** as well as **OR** operators and the conclusion clauses may only be connected by **AND** statements. It means that all of the conclusion clauses in a production rule must be true. Clauses connected by **AND** operators are called conjunctive classes and those connected by **OR** operators are termed disjunctive clauses. If we apply OAV triplet concept here..(O = Object , A = Attribute, V = Value), we can match Object to Element, Attribute to Name, and Value to Sodium (or) Potassium (or) Lithium (or) Rubidium.

2.5.3.2 Attribute - Value pair properties

Each premise and conclusion clause contains attributes and values with implicit (or) explicit associated to object. AV pair is the fundamental building block of a premise or conclusion and also of a production rule. Associated with each AV pair is a set of properties such as:

1) Name (Name of the attribute)
2) Type (Class of values associated with attribute) . It may be symbolic, numeric or boolean values
3) Prompt : associated with certain attributes are user prompts , or queries. When necessary, the user replies to this prompt with a value for the attribute under consideration
4) Legal values: associated with every attribute is a set of legal , (or) acceptable values, for example: legal set of values for litmus colour might be red (or) blue
5) Specified values: Legal values simply represent the complete set of acceptable values for a given attribute . Specified values indicate the actual set of values that

are either to be tested against (i.e., in a premise clause) or that will be, or have been assigned (i.e., in a conclusion clause). Example in the case of a flower, the legal values may be red, white, yellow, and pink. However, some flowers may be multi-coloured. Specified flowers may be single or multiple.

6) Confidence Factors: When we deal with uncertainty in either conclusions or premises confidence factor is implied.

In order to clarify the above discussion, let us consider a following rule and how above attributes related to the rule's constituents.

Rule 1: If the name of the element is sodium

Then it is called metal

Referring to the **AV** pair of the premise of this rule, the associated properties are

1) Name: name of element
2) Type: symbolic
3) Prompt: "What is the name of the element?"
4) Legal values: sodium
5) Specified values: single (i.e., a given element has only a single name)
6) Confidence Factor: none

And refer to the conclusion clause of this rule, the properties of the **AV** pairs are

7) Name: element's status
8) Type: symbolic
9) Prompt: none (no prompts is required for conclusion clauses)
10) Legal values: metal or nonmetal
11) Specified values: single
12) Confidence factor: none

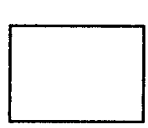
2.5.3.3 Rule properties

Concerning with AV pairs and clauses, there are certain important rule properties.

1) Name (the name of the rule)
2) Premise (the IF portion of the rule)
3) Intermediate conclusion (the THEN portion of the rule)
4) Notes (notes associated with the rule)
5) References (formal references associated with the rule)
6) Confidence Factors (a measure of confidence in the rule's conclusion)
7) Priority (a property used by the inference process)
8) Chaining preference (the normal or default mode of search used by the rule)
9) Status: active, inactive / discard , triggered, fired

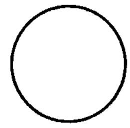
2.5.3.4 Inference networks chaining

Inference networks is a graphical approach to rule - base documentation that can be quite useful. The following conventions are employed in our inference networks.

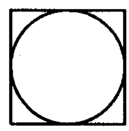


Assertion

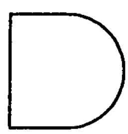
(i.e., The association of a premise attribute with a specific value)



Conclusion



Intermediate Conclusion



AND Node

OR Node

Rule 1: **IF** ([ELEMENT] = = " Lithium" || [ELEMENT] = = "Sodium" || [ELEMENT] = = "Potassium" || [ELEMENT] = = "Rubidium")

and When combines with oxygen

THEN called AlkaliMetalOxide

Its' inference network representation is:

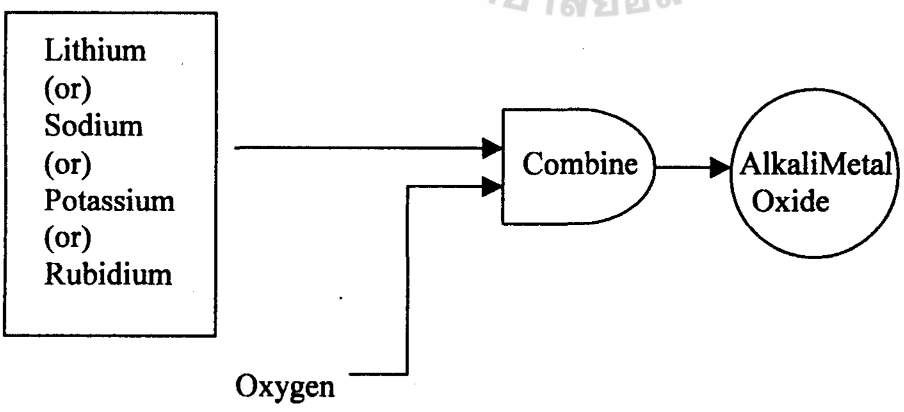


Figure 2-4 Inference network representation

Inference normally proceeds in either a forward manner (forward chaining) or backward manner (backward chaining). In reaching our final conclusion we move from left to right in the inference network - the direction used by forward chaining, which is data driven and apply the initial set of data to conduct the search. A backward chaining is moving backward from right to left, we want to know precisely what premises must be satisfied to reach the final conclusion.

Chapter 3

DESIGNING OF THE CHEMISTRY RULE-BASED SYSTEM

In this research, the CRBS (Chemistry Rule-Based System) is implemented under EXSYS, a rule - based system shell. In order to make the implementation well understood, the brief of EXSYS will be given in section 3.1.

3.1 EXSYS PROFESSIONAL

3.1.1 EXSYS: a Rule - based system shell

An expert system is a type of artificial intelligence program that emulates the interaction a user might have with a human expert encoded into rules to solve the problem. The user may answer by selecting one or more answers from a list or by entering data. Computer will continue to ask questions until reaching to a conclusion. The conclusion may be a single solution or a list of possible solutions arranged in order of confidence factors. The **EXSYS** can explain , **HOW** it arrived at its conclusion and **WHY** if user click at the corresponding button.

This rule - based system is developed under **EXSYS** for construction of any acid or base from an atomic set of elements. In **EXSYS** users deals with knowledge rather than data and the knowledge based files that helps the users to get rid of the complicated problems of computer knowledge.

The rules implied are **IF - THEN - ELSE** type rules. The computer determines what additional information it made and how it best to get the information. The program will derived information from other rules rather than asking the user. Therefore it can combine small pieces of knowledge to arrive at logical conclusion. The Rule Editor allows the rules to be easily modified, added or deleted.

Final goal is to select the most appropriate solution to a problem based on the data that has been input by the user. If more than one solution is possible the program will provide a list of the possible solutions arranged in order of confidence factors. The principal development tool in **EXSYS** is the **EXSYS Professional** Rule Editor, which enables you to generate your own expert knowledge bases. All available options are displayed on the screen.

EXSYS Professional also includes a rule compiler allowing you to create or edit rules with a word processor and then compile the rules for use with **EXSYS** Runtime or Editor. The Rule Editor is faster, easier and provides error checking. **EXSYS** offers the correct balance of power with ease of - use and it can be run by end user. The end user of the expert system can ask **HOW** the conclusions were reached or **WHY** the information is needed. The program will respond with a full explanation of the logic used to arrive at the conclusion, including backward chaining and external program calls for data. The developer can customise screen and derive what options are available to the end user.

3.1.2 EXSYS features

There are two versions of the **EXSYS** expert systems shell. The first is denoted as a **Standard** version while the second is termed as a **Professional** version. The features that both versions share in common are:

1) Support of IF - THEN – ELSE production rules
2) Support of both forward and backward chaining (backward is the default mode)
3) Automatic menu – driven user prompts
4) Several choices for rule confidence factors 0 or 1, 0 – 10, -100 to 100, etc.

5) Consultation session may be run, at any time, from within the rule editor
6) Bridges to external programs for either data acquisition or external program execution
7) Report generator and common language
8) Numeric and string variables
9) Support of various mathematical functions
10) Black boarding
11) Written in C

In the Professional version, there are some additional features:

12) An enhanced command language
13) A rule compiler that permits word – processor editing of the knowledge bases plus ease of movement of the rule bases of other shells into the **EXSYS** environment.
14) Development of custom screens
15) Custom formulas for confidence factors
16) A redesigned user interface
17) Hypertext

3.2 Methodology

3.2.1 Tasks for building CRBS

This research emphasizes on the methodology, therefore it is worthy to express it through a medium-sized real problem. The author intended to select the acid - base titration, which is the main part of the course "General Chemistry" at Assumption University, as an example to develop, implement, verify and evaluate derived methods and concepts. In order to achieve these goals, the following tasks are done forming:

1) Select from a list of elements, which are very common in acid-base titration, by clicking at the desired element.
2) Get corresponding physical properties and special characteristics (Name, Symbol, Type of Element, Outer Most Shell Electron etc.0 from database file.
3) Using information from database file and generate different compounds of strong acids and strong bases from a basis set of atomic states by implementing knowledge base consisting of a set of rules.
4) Calculate the amount of acid or base produced from the given amount of selected element and vice versa.
5) Design custom screens to ask questions of the user. The use of custom screens allows us to customize the user interface.
6) Generate different compound of salts, which will give a data set, consisting of any acid-base solution combinations.
7) Simulate pH, pOH for different concentrations of acid and base solutions.
8) Perform virtual titration on computer.

3.2.2 Typical rules

Rule 1: **If** selected element is Sodium and

When combines with oxygen

Then Retrieve the corresponding physical properties and characteristics of the selected element such as (symbol, type, oms electron, atomic_mass, etc..) from database and

Assign symbol as a new symbol (to aviod data conflict) and

Return product formed with related molar_mass of the oxide formed and Called alkali metal oxide.

Rule 2: **If** Alkali metal oxide combines with water

Then Compound formed is a (*newsymbol* + "OH") and Return molar_mass of that compound and Called AlkaliMetalHydroxide.

Rule 3: **If** Called AlkaliMetalHydroxide

Then Turns red litmus to blue, resulting compound is termed as Base and stored as a Compound 1.

Rule 4: **If** Compound 1 exists, and Input acid is hydrochloric acid (HCl)

Then Final product is (*newsymbol* + "Cl" and "H_2O")

Rule 5: **If** Mass of the given product formed (acid or base) is given

Then Calculate required amount of element

Rule 6: **If** Mass of the selected element is known

Then Calculate amount of product formed (acid or base)

Rule 7: **If** Volume of the solution (acid or base) is known

Then Calculate concentration (Molarity) of acid or base

Rule 8: **If** Molarity of acid or base is known

Then Calculate pH or pOH of the acid or base

Rule 9: **If** User is interested to see a *flow chart diagram* for all process

Then Click at "Yes" button

Rule 10: **If** Virtual titration of any strong acid and base is chosen

Then Animate *Virtual titration*

3.2.3 Implementation of rules in EXSYS

All the rules in English are implemented in **EXSYS** as follows:

Rule 1: **If** ([Element] = = "Lithium" || [Element] = = "Sodium" || [ELEMENT] = = "Potassium" || [ELEMENT] = = "Rubidium")and

When combines with oxygen

Then DB_GK(TEST.DBF,NAME.NDX,[N],SYMBOL, SYMBOL],OMS_E, [OMS_E],TYPE,[TYPE], ATOMIC_MAS, [ATOMIC_MAS]), and

[NEWSYMBOL] IS GIVEN THE VALUE [SYMBOL] and

[PRODUCT] IS GIVEN THE VALUE [NEWSYMBOL]+"2O" and

[MOLAR_MAS OF OXIDE] IS GIVEN THE VALUE ([ATOMIC_MAS] * 2 + 16) and

Called AlkaliMetalOxide

Rule 2: **If** Called AlkaliMetalOxide

and combines with water (H_2O)

Then [COMPOUND] IS GIVEN THE VALUE [NEWSYMBOL]+"OH"and

[MOLAR_MASSPRODUCT] IS GIVEN THE VALUE ([ATOMIC_MAS] + 16 + 1.008) and

Called AlkaliMetalHydroxide

Rule 3: **If** Called AlkaliMetalHydroxide

Then Turns red litmus to blue

and termed as Base – Confidence = 6/10

and [COMPOUND1] IS GIVEN THE VALUE [COMPOUND]

Rule 4: **If** [VOL] != 0

And [MASSOFELEMENT] != 0

Then [MOLARITY] IS GIVEN THE VALUE

(([MASSOFELEMENT] / [MOLARMASSPRODUCT]) / [VOL]) and

[AMTPRODUCT] IS GIVEN THE VALUE

(([MASSOFELEMENT]*[MOLARMASSPRODUCT]) /

[ATOMIC_MAS]) and [H] IS GIVEN THE VALUE [MOLARITY]

Rule 5: **If** [GIVENMASSPROD] != 0

Then [REQDELEMENT] IS GIVEN THE VALUE

([GIVENMASSPROD] * [ATOMIC_MAS]/[MOLARMASSPROD])

Rule 6: **If** [COMPOUND1] != " " and

([ELEMENT] = = "Sodium" || [ELEMENT] = = "Potassium") and

([M] = = "HCl" || [M] = = "HydrochloricAcid")

Then [FINALPRODUCT] IS GIVEN THE VALUE

((({NEWSYMBOL] + "Cl") + "+") + "H_2O") and

stop – Confidence = 5/10

Rule 7: **If** [MOLARITY] != 0

Then [pH] IS GIVEN THE VALUE – (LOG([H] / 2.303) and

[pOH] IS GIVEN THE VALUE 14 – [pH]

Rule 8: **If** User is interested to see a flow chart diagram for overall process

Then RUN (FLOW.EXE)

Rule 9: **If** Virtual titration of any strong acid and base is chosen

Then RUN (VIRTUAL.EXE)

3.3 Inference in rule-based system

The purpose of a rule - based system is to develop and recommend a proposed solution by conducting a *search* for the solution. It is the responsibility of the inference engine to perform this search in an efficient and effective manner. The two fundamental search strategies are forward and backward chaining.

3.3.1 Forward chaining

When the left side of a rule is instantiated first and if it is matched then THEN part of the rules is executed from left to right otherwise, the ELSE part is executed; such process is called forward chaining. This is also known as data-driven inference since input data are used to guide the direction of the inference process starting from starting state. Related to our Rule-based system, the forward chaining will form the element,

for example Sodium,

Sodium:	Na, metal, oms_e = 1, atomic mass = 23.01 amu
SodiumOxide:	Sodium, oxygen
SodiumHydroxide:	SodiumOxide, water
Base:	SodiumHydroxide, red litmus, pH > 7
Sodium Chloride:	Base, HydrocholricAcid

3.3.2 Backward chaining

Backward chaining is a goal directed solving mechanism. The way and the order in which facts, rules or parts of rules are used is called control structures and it is critical for an important and practical class of rule based system. It is also known as goal - directed reasoning. It starts from goal state and tries to find ways, how to make this goal to be achieved, which facts, rules should be used. If multiple conclusions are possible, backward chaining can try to prove the first, then try the second and so on. This process is Depth First search with back tracking. Related to our Rule-Based System, we are interested to construct acids and bases from atomic state and let them react together to produce corresponding salt and water by applying rule-based system.

[Acid] + [Base] ----------> [Salt] + [Water]

Rule 1: **If** Acid combines with Base

Then products are salt and water

[Nonmetallic Compound] + [water] ---------> [Acid]

[Metallic hydroxide] + [water] ---------> [Base]

Rule 2.a: **If** Nonmetallic Compound combines with water

Then product is acid

Rule 2.b: **If** AlkaliMetalOxide or AlkalineEarthMetalOxide combines with water

Then product is base

[Alkali metal oxide] + [water] --------> [Metallic hydroxide]

(or)

[Alkaline Earth metal oxide] + [water] -----> [Metallic hydroxide]

Nonmetal oxide + water -----> Nonmetallic Compound

(or)

Hydrogen Halide + water ------> Nonmetallic Compound

Rule 3.a: **If** Alkali metal oxide (or) Alkaline Earth metal oxide

combines with water

Then product is Metallic Hydroxide

Rule 3.b: **If** Nonmetal oxide (or) hydrogen halide combines with water

Then product is Nonmetallic Compound

Nonmetal + Oxygen ----------> Nonmetal oxide

(or)

Nonmetal + Hydrogen ---------> Hydrogen Halide

Rule 4.a: **If** Nonmetal combines with oxygen

Then product is Nonmetal oxide

Rule 4.b: **If** Nonmetal combines with hydrogen

Then product is Hydrogen Halide

Metal + oxygen ------------> Metal oxide

Rule 5: **If** Metal combines with oxygen

Then product is Metal oxide

Metal (or) Nonmetal

Input: Name of element

Source: Database file

Rule 6: **If** the name of the element is known

Then Retrieve data from database file and products are Type, oms_electron,

Atomic_mass and symbol

Chapter 4

RESULTS AND DISCUSSIONS

4.1 Rules used in CRBS

In order to derive rules, first we need to determine the major goals and the ways these goals can be established. Next look for ways of acquiring information to support goal rules. After that inference network of the rules were drawn[5]. Inference network for our rule-based system shows the logical relationships between pieces of information that are presented in the system. Figure 4.1 shows the inference network for goal rules how acid and base are produced and how they are combined together to obtain salt and water. This inference network can be translated to rules. In order to reduce the number of rules, several steps can be combined into one rule, and if the steps involve several different atoms with different pattern of properties, it can be represented by several parallel rules. For example, referring to Figure 4-1, from getting an element, to determine type of its' element and combine with oxygen to get AlkaliMetalOxide can be presented by only one rule. (see Rules below)

Rule 1: **If** ([ELEMENT] == "Lithium" || [ELEMENT] == "Sodium" || [ELEMENT] = = "Potassium" || [ELEMENT] = = "Rubidium") and When combines with Oxygen

Then DB_GK (A:\TEST,DBF, A:\NAME.NDX, [ELEMENT], SYMBOL, [SYMBOL], TYPE, [TYPE], ATOMIC_MAS, [ATOMIC_MAS]) and [NEWSYMBOL] IS GIVEN THE VALUE [SYMBOL] and [PRODUCT] IS GIVEN THE VALUE [NEWSYMBOL] + "2O" and [MOLAR_MAS OF OXIDE] IS GIVEN THE VALUE ([ATOMIC_MAS] * 2 + 16) and

Called AlkaliMetalOxide

Rule 2: **If** ([ELEMENT] == "Magnesium" || [ELEMENT] == "Calcium" ||

[ELEMENT] = = "Beryllium" || [ELEMENT] = = "Strontium") and

When combines with Oxygen

Then DB_GK (A:\ TEST,DBF, A:\ NAME.NDX, [ELEMENT], SYMBOL,

[SYMBOL], TYPE, [TYPE], ATOMIC_MAS, [ATOMIC_MAS]) and

[NEWSYMBOL] IS GIVEN THE VALUE [SYMBOL] and

[PRODUCT] IS GIVEN THE VALUE [NEWSYMBOL] + "O" and

[MOLAR_MAS OF OXIDE] IS GIVEN THE VALUE

([ATOMIC_MAS] + 16) and

Called AlkalineEarthMetalOxide

Rule 3: **If** ([ELEMENT] == "Sulphur" and

When combines with Oxygen

Then DB_GK (A:\ TEST,DBF, A:\ NAME.NDX, [ELEMENT], SYMBOL,

[SYMBOL], TYPE, [TYPE], ATOMIC_MAS, [ATOMIC_MAS]) and

[NEWSYMBOL] IS GIVEN THE VALUE [SYMBOL] and

[PRODUCT] IS GIVEN THE VALUE [NEWSYMBOL] + "O3" and

[MOLAR_MAS OF OXIDE] IS GIVEN THE VALUE

([ATOMIC_MAS] + 16 * 3) and

Called NonMetalOxide

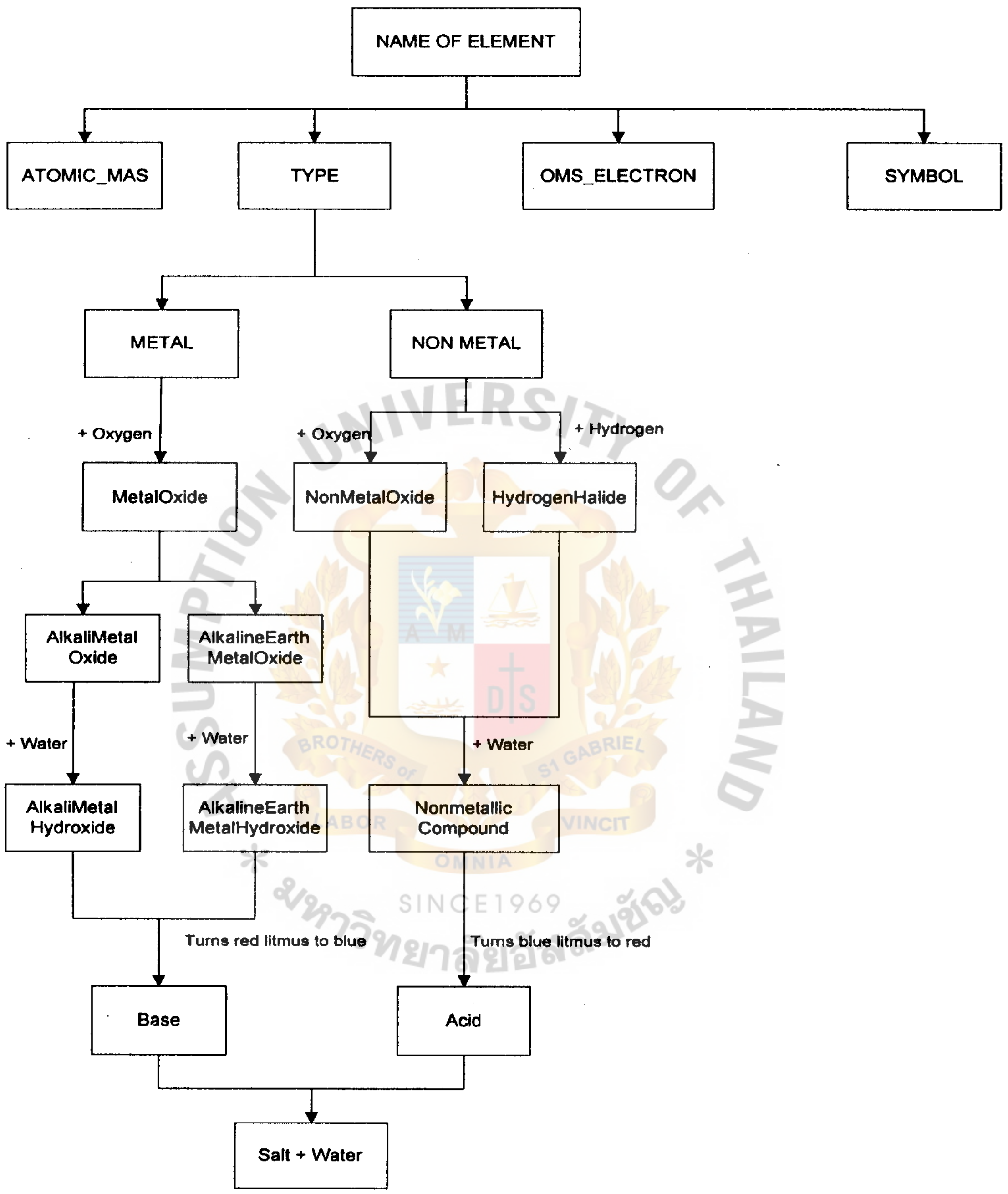


Figure 4-1 Inference network of CRBS

Rule 4: **If** ([ELEMENT] = = "Sulphur") and

When combines with Oxygen

Then DB_GK (A:\ TEST.DBF, A:\ NAME.NDX, [ELEMENT], SYMBOL, [SYMBOL}, TYPE, [TYPE], ATOMIC_MAS, [ATOMIC_MAS]) and [NEWSYMBOL] IS GIVEN THE VALUE [SYMBOL] and [PRODUCT] IS GIVEN THE VALUE [NEWSYMBOL] + "O2" and [MOLAR_MAS OF OXIDE] IS GIVEN THE VALUE ([ATOMIC_MAS] + 16 * 2) and

Called NonMetalOxide1

Rule 5: **If** ([ELEMENT] == "Nitrogen" and

([ELEMENT] != "Chlorine" || [ELEMENT] != "Sulphur") and

When combines with Oxygen

Then DB_GK (A:\ TEST.DBF, A:\ NAME.NDX, [ELEMENT], SYMBOL, [SYMBOL], TYPE, [TYPE], ATOMIC_MAS, [ATOMIC_MAS]) and [NEWSYMBOL] IS GIVEN THE VALUE [SYMBOL] and [PRODUCT] IS GIVEN THE VALUE [NEWSYMBOL] + "O2" and [MOLAR_MAS OF OXIDE] IS GIVEN THE VALUE ([ATOMIC_MAS] + 16 * 2) and

Called NonMetalOxide2

Rule 6: **If** ([ELEMENT] == "Chlorine") and

When combines with Hydrogen

Then DB_GK (A:\ TEST.DBF, A:\ NAME.NDX, [ELEMENT], SYMBOL, [SYMBOL], TYPE, [TYPE], ATOMIC_MAS, [ATOMIC_MAS]) and [NEWSYMBOL] IS GIVEN THE VALUE [SYMBOL] and

[PRODUCT] IS GIVEN THE VALUE "H" + [NEWSYMBOL] and

[MOLARMASSHALIDE] IS GIVEN THE VALUE

(1.008 + [ATOMIC_MAS]) and

Called HydrogenHalide

Rule 7: **If** Called AlkaliMetalOxide and

Oxides (or) Halides formed combine with Water (H_2O)

Then [COMPOUND] IS GIVEN THE VALUE [NEWSYMBOL] + "OH"

and [MOLARMASSPRODUCT] IS GIVEN THE VALUE

([ATOMIC_MAS] + 16 + 1.008) and

Called AlkaliMetalHydroxide

Rule 8: **If** Called AlkalineEarthMetalOxide and

Oxides (or) Halides formed combine with Water (H_2O)

Then [COMPOUND] IS GIVEN THE VALUE [NEWSYMBOL] + "$(OH)_2$"

and [MOLARMASSOF PRODUCT] IS GIVEN THE VALUE

([ATOMIC_MAS] * 2 +16 + 1.008) and

Called AlkalineEarthMetalHydroxide

Rule 9: **If** Called NonMetalOxide and

Oxides (or) Halides formed combine with Water (H_2O)

Then [COMPOUND] IS GIVEN THE VALUE

"H_2" + [NEWSYMBOL] + "O_4" and

[MOLARMASSPRODUCT] IS GIVEN THE VALUE

(2 * 1.008 + [ATOMIC_MAS] + 4 * 16) and

Called NonMetallicCompound

Rule 10: **If** Called NonMetalOxide1 and

Oxides (or) Halides formed combine with Water (H_2O)

Then [COMPOUND2] IS GIVEN THE VALUE

"H_2" + [NEWSYMBOL] + "O_3" and

[MOLARMASSPRODUCT] IS GIVEN THE VALUE

(2 * 1.008 + [ATOMIC_MAS] + 3 * 16) and

Called NonMetallicCompound1

Rule 11: **If** Called NonMetalOxide2 and

Oxides (or) Halides formed combine with Water (H_2O)

Then [COMPOUND] IS GIVEN THE VALUE

"H" + [NEWSYMBOL] + "O_3" and

[MOLARMASSPRODUCT] IS GIVEN THE VALUE

(1.008 + [ATOMIC_MAS] + 3 * 16) and

named NonMetallicCompound2

Rule 12: **If** Called HydrogenHalide and

Oxides (or) Halides formed combine with Water (H_2O)

Then [COMPOUND] IS GIVEN THE VALUE

[MOLARMASSPRODUCT] IS GIVEN THE VALUE

(1.008 + [ATOMIC_MAS]) and

Called NonMetallicCompound3

Rule13: **If** named AlkaliMetalOxide

Then TURNS RED LITMUS TO BLUE and

Termed as Base - Confidence=6/10 and

[COMPOUND 1] IS GIVEN THE VALUE [COMPOUND]

Rule 14: **If** [VOL] != 0 and

[MASSOFELEMENT]! = 0

Then [MOLARITY] IS GIVEN THE VALUE

(([MASSOFELEMENT] / [MOLARMASSPRODUCT]) / [VOL]) and

[AMTPRODUCT] IS GIVEN THE VALUE

(([MASSOFELEMENT]*[MOLARMASSPRODUCT]) /

[ATOMIC_MAS]) and

[H] IS GIVEN THE VALUE [MOLARITY]

Rule 15: **If** [GIVENMASSPROD]! = 0

Then [REQDELEMENT] IS GIVEN THE VALUE

([GIVENMASSPROD] * [ATOMIC_MAS]/[MOLARMASSPROD])

Rule 16: **If** [COMPOUND1]! = " " and

([ELEMENT] = = "Sodium" || [ELEMENT] = = "Potassium") and

([M] = = "HCl" || [M] = = "HydrochloricAcid")

Then [FINALPRODUCT] IS GIVEN THE VALUE

((({NEWSYMBOL] + "Cl") + "+") + "H_2O") and

stop – Confidence = 5/10

Rule 17: **If** [NEWNAME1]!= " " and

([ELEMENT] == "Sodium" || [ELEMENT] == "Potassium")

([M] == "Sulphuric Acid" || [M] =="H_2SO_4)

Then [FINALPRODUCT] IS GIVEN THE VALUE

((([NEWSYMBOL] + "2" + "SO_4") + "+") + "H_2O) and

stop - Confidence=6/10

Rule 18: **If** [MOLARITY] != 0

Then [pH] IS GIVEN THE VALUE – (LOG([H] / 2.303) and

[pOH] IS GIVEN THE VALUE 14 – [pH]

Rule 19: **If** User is interested to see a flow chart diagram for overall process

Then RUN (FLOW.EXE)

Rule 20: **If** Virtual titration of any strong acid and base is chosen

Then RUN (VIRTUAL.EXE)

After finished encoding all goal rules into the system, test the system using information specific to the new knowledge. Running the system several times for different combination of answers to make sure that all goals were tested and successfully established. The whole list of rules were developed and given in Appendix A.

4.2 Screen Design

Creation of custom screen to ask questions concerning with goal rules developments are implemented with a custom screen item on the KB file menu. Many screens are stored in a single file and are separated bt special commands that indicate the start of a new screen. Custom screen files usually contain many separate screen in a single file. This helps the user's interface friendly and easy to use. Typical screens are shown in the next section.

4.3 CRBS Features

The following scenario of running CRBS gives us what are the features of CRBS. When you run CRBS the first screen is displayed as:

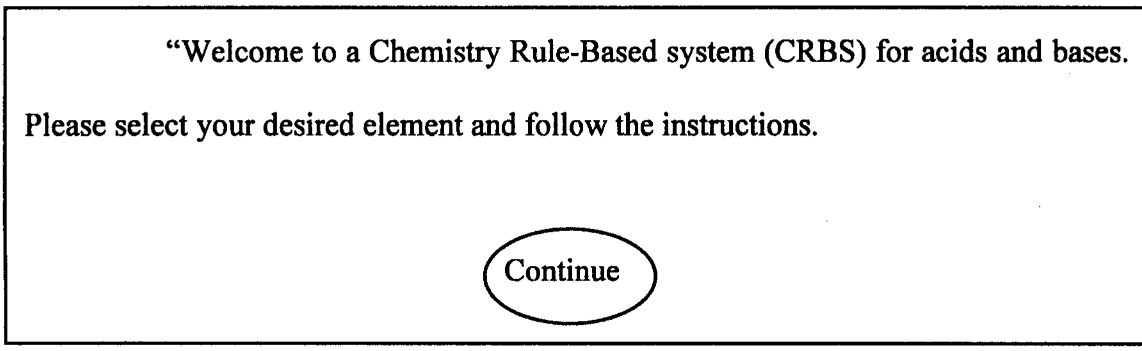


Figure 4-2 Description of a program

After reading the screen, click on the continue button. The CRBS will display the second screen as:

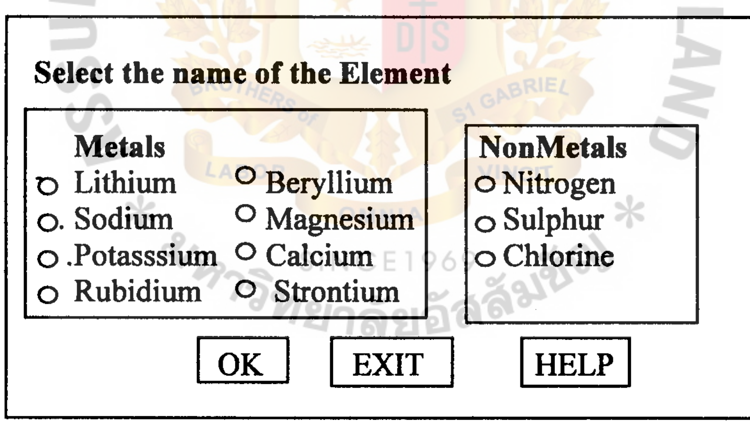


Figure 4-3 Selection of element

After selecting the desired element and click on the OK button, CRBS takes data from various sources and uses rules to interact with user to derive to the conclusions. The sequenceof screens will be appeared one by one as given in Figure 4-4 to Figure 4-13.

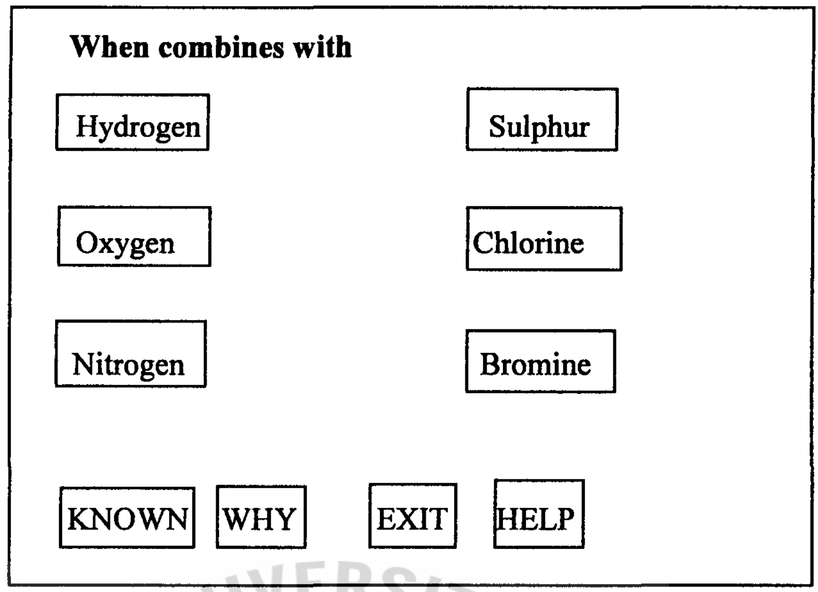


Figure 4-4 Selection of combined elements

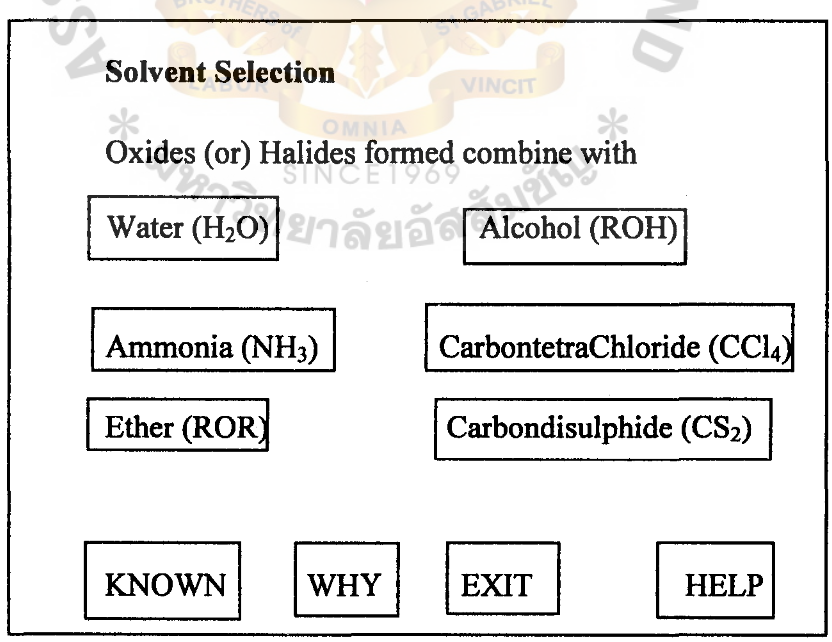


Figure 4-5 Selection of solvent

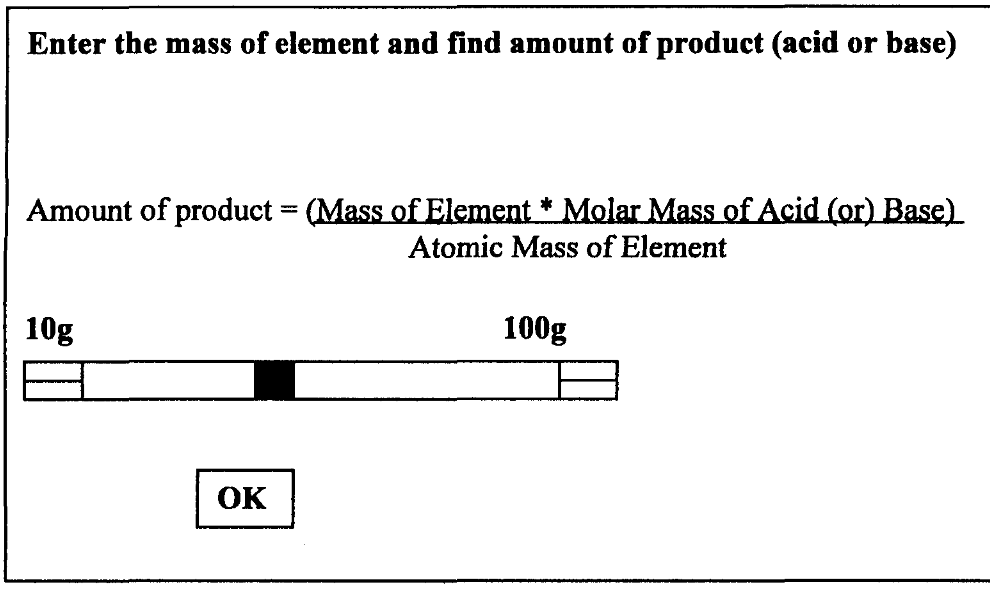


Figure 4-6 Calculation for amount of product produced (acid or base)

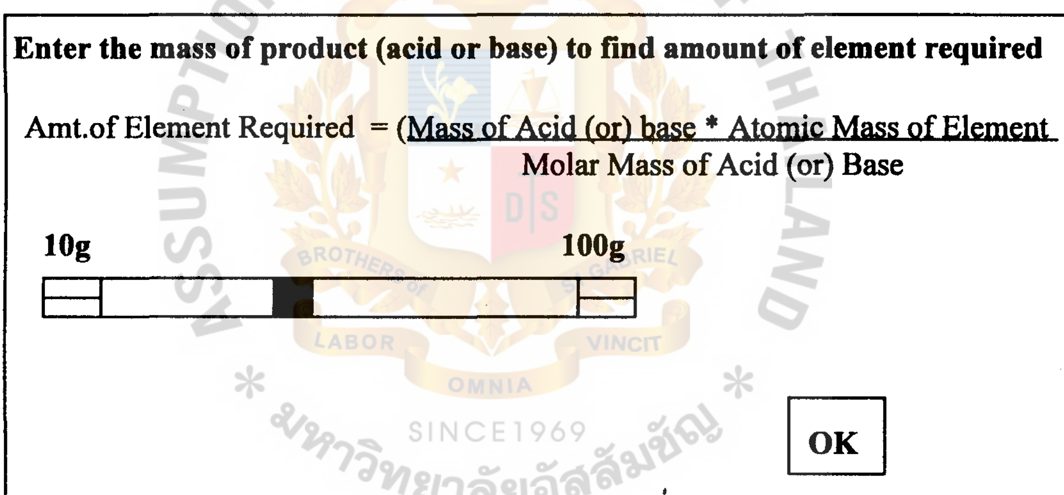


Figure 4-7 Calculation for required element

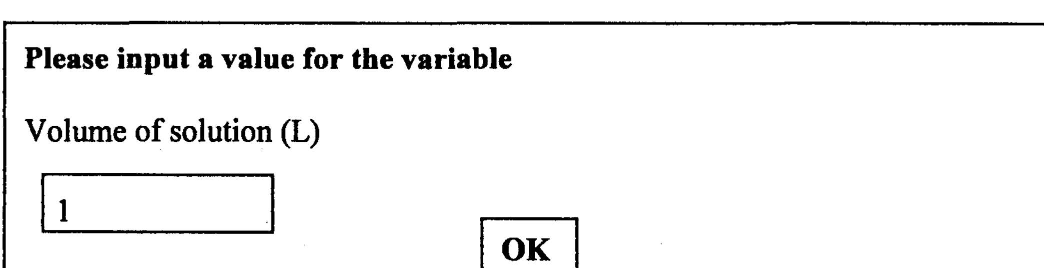


Figure 4-8 Calculation for molarity

Select one of the Followings:

For NonMetals

O Hydrocholoric Acid (HCl)
O Sulphuric Acid (H_2SO_4)
O Nitric Acid (HNO_3)

For Metals

O Sodium Hydroxide (NaOH)
O PotassiumHydroxide (KOH)
O Calcium Hydroxide ($Ca(OH)_2$)
O Magnesium Hydroxide($Mg(OH)_2$)

KNOWN | WHY | EXIT | HELP

Figure 4-9 Selection of acid / base to prepare salt

Select one or more values

What would you like to observe?

1. Flow Chart

2. Virtual Titration

Figure 4-10 Selection of choice

When screen designing is completed, run the program by following instructions given and finally results will appear like this:

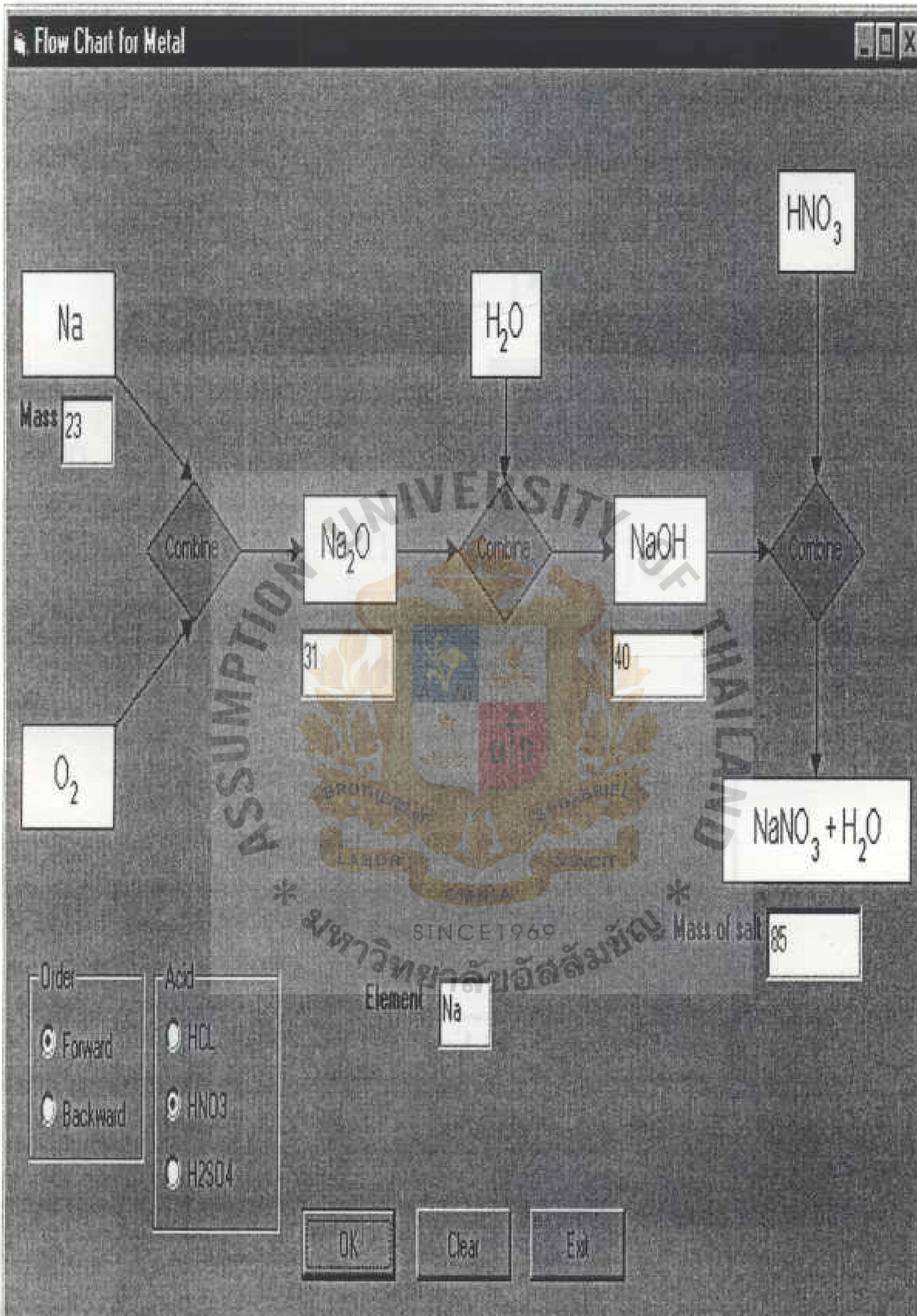


Figure 4-11 Flow chart diagram

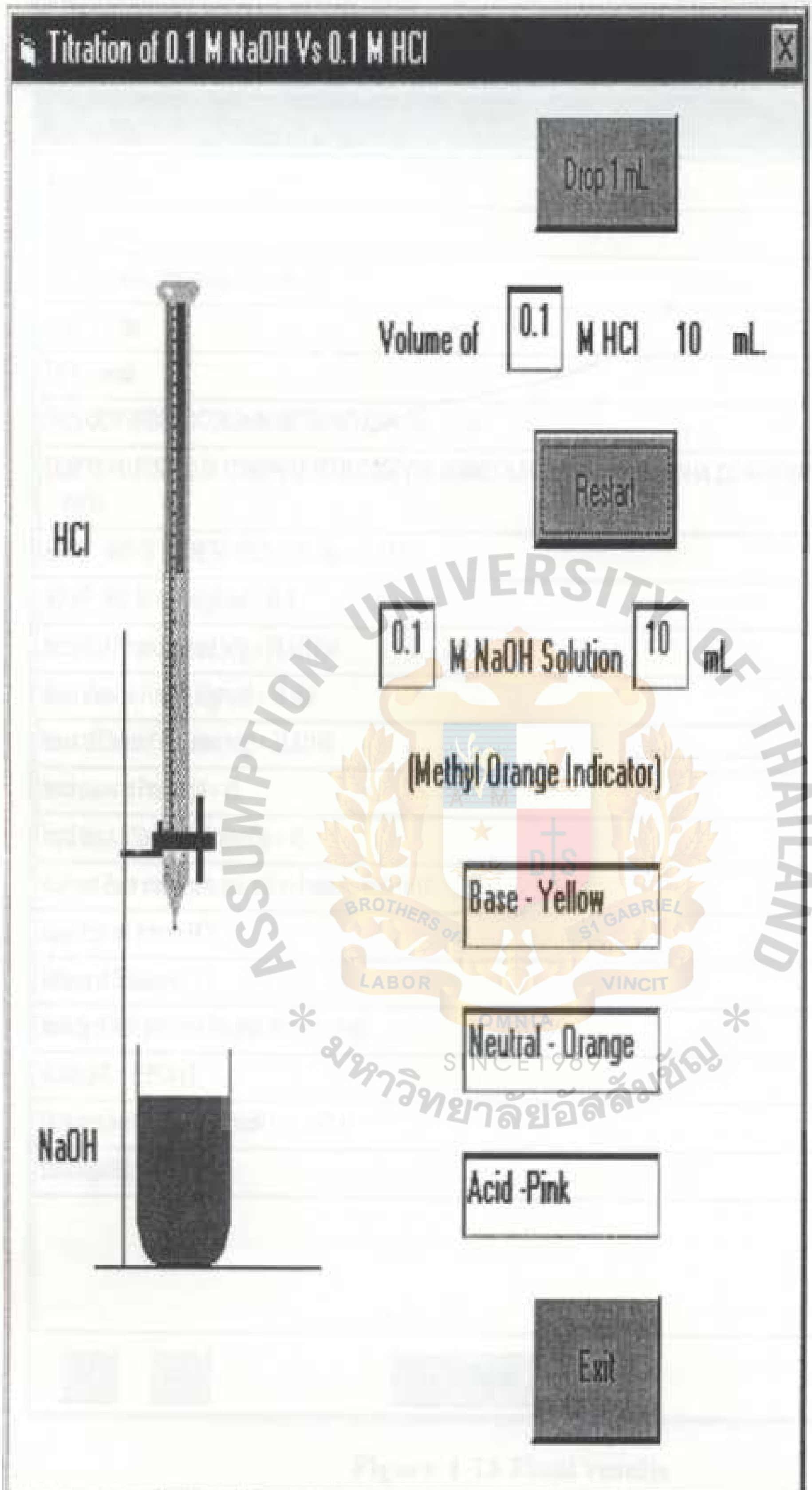


Figure 4-12 Virtual titration

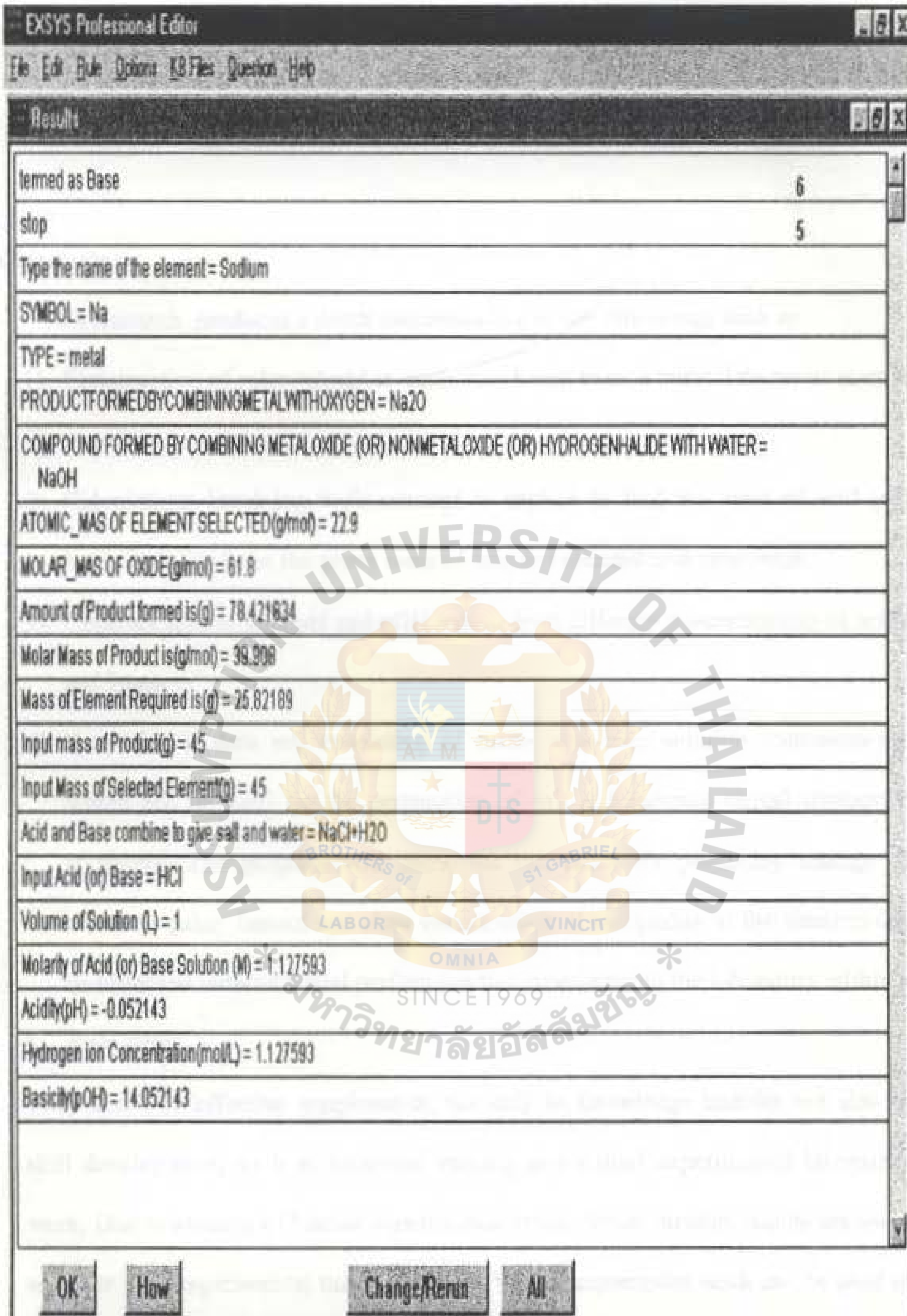


Figure 4-13 Final results

Chapter 5

CONCLUSION AND RECOMMENDATION

5.1 Conclusion

This research produces a depth understanding of the followings such as:

1) Construction of rules related to acids and bases from a basis data set of atomic states
2) Calculations involving mole concept is applied to find the mass of acid (or) base produced from the given mass of selected element and vice versa
3) Generation of related pH and pOH values from different concentrations of acids and bases
4) Producing a data set, consisting of many acid-base solution combinations, which can be used for the preparation of salt and running virtual titration o computer. The program will show the end-point, by producing change of indicator color. Instant and clear visualization of the quality of the titration can be observed without actual performing the experiment in the laboratory within a short time.

They could be effective supplements, not only to knowledge transfer but also to skill development, such as technical training and virtual experimental laboratory work. Due to absence of human experimental error, virtual titration results are more accurate than experimental titration results. Virtual experiment work can be used to replace the real work in a training process to make the trainees more or better understanding when they perform the real experiment, avoiding hazardous chemical effects, and at the same time saving financial resources also. Furthermore, the concepts, rules, and knowledge base developed in CRBS, can be a kernel of Computer Aided Instructions (CAI) system which embedded in artificial intelligence technology and offers more flexibility and greater effectiveness than traditional teaching methods.

Students learning with this method can expect to become more proficient at manipulating chemical equations, basic characteristics of elements, calculations involving mole concept and lastly titrimetric analysis which is one of the fundamental topics in General Chemistry laboratory techniques. This study can also provide with an opportunity for interactive practice of the General Chemistry while receiving helpful guidance in dealing with this program.

5.2 Recommendation

Since the present study covers only the titration method involving a single step titration, it would be of great interest beneficial to extend further works consist of a two steps double titration method in titrimetric chemical analysis.

For further continuation of the research works in this field, it is highly recommended to undertake more research works on:

1) Chemical compounds construction from the atomic states
2) Titrimetric methods involving various types of acids and bases with different concentrations by using relevant indicators
3) Redox, Iodometric, and Complexometric titrations to increase knowledge efficiency in chemistry for students.

APPENDIX A

Rules

Rule number 1

IF:
([ELEMENT] = = "Lithium" || [ELEMENT] = = "Sodium" ||
[ELEMENT] = = "Potassium" || [ELEMENT] == "Rubidium")

and When combines with Oxygen

THEN:

DB_GK(a:\TEST.DBF, a:\NAME.NDX, [ELEMENT], SYMBOL, [SYMBOL], TYPE, [TYPE], ATOMIC_MAS, [ATOMIC_MAS])

and [NEWSYMBOL] IS GIVEN THE VALUE [SYMBOL]

and [PRODUCT] IS GIVEN THE VALUE [NEWSYMBOL]+"2O"

and [MOLAR_MAS OF OXIDE] IS GIVEN THE VALUE ([ATOMIC_MAS] * 2+16)

and Called AlkaliMetalOxide

Rule number 2

IF
([ELEMENT] = = "Beryllium" || [ELEMENT] = = "Magnesium" ||

[ELEMENT] = = "Calcium" || [ELEMENT] == "Strontium")

and When combines with Oxygen

THEN:
DB_GK(a:\TEST.DBF, a:\NAME.NDX,[ELEMENT], SYMBOL,[SYMBOL],TYPE,[TYPE], ATOMIC_MAS,[ATOMIC_MAS])

and [NEWSYMBOL] IS GIVEN THE VALUE [SYMBOL]

and [PRODUCT] IS GIVEN THE VALUE [NEWSYMBOL]+"O"

and [MOLAR_MAS OF OXIDE] IS GIVEN THE VALUE
([ATOMIC_MAS] +16)

and Called AlkalineEarthMetalOxide

Rule number 3

IF:
[ELEMENT]=="Sulphur"

and When combines with Oxygen

THEN:
DB_GK(a:\TEST.DBF, a:\NAME.NDX,[ELEMENT],
SYMBOL,[SYMBOL],TYPE,[TYPE],
ATOMIC_MAS,[ATOMIC_MAS])

and [NEWSYMBOL] IS GIVEN THE VALUE [SYMBOL]

and [PRODUCT] IS GIVEN THE VALUE [NEWSYMBOL]+"O3"

and [MOLAR_MAS OF OXIDE] IS GIVEN THE VALUE
([ATOMIC_MAS] + 16 * 3)

and Called NonMetalOxide

Rule number 4

IF:
[ELEMENT] == "Sulphur"

and When combines with Oxygen

THEN:
DB_GK(a:\TEST.DBF, a:\NAME.NDX, [ELEMENT],
SYMBOL,[SYMBOL],TYPE,[TYPE],
ATOMIC_MAS, [ATOMIC_MAS])

and [NEWSYMBOL] IS GIVEN THE VALUE [SYMBOL]

and [PRODUCT2] IS GIVEN THE VALUE [NEWSYMBOL] +"O2"

and [MOLAR_MASOXIDE2] IS GIVEN THE VALUE ([ATOMIC_MAS] + 16 * 2)

and Called NonMetalOxide1

Rule number 5

IF:

[ELEMENT] == "Nitrogen"

and When combines with Oxygen

THEN:

DB_GK(a:\TEST.DBF, a:\NAME.NDX, [ELEMENT], SYMBOL,[SYMBOL],TYPE,[TYPE], ATOMIC_MAS,[ATOMIC_MAS])

and [NEWSYMBOL] IS GIVEN THE VALUE [SYMBOL]

and [PRODUCT] IS GIVEN THE VALUE [NEWSYMBOL] +"O_2"

and [MOLAR_MAS OF OXIDE] IS GIVEN THE VALUE ([ATOMIC_MAS] + 16 * 2)

and Called NonMetalOxide2

Rule number 6

IF:

[ELEMENT]=="Chlorine"

and When combines with Hydrogen

THEN:

DB_GK(a:\TEST.DBF, a:\NAME.NDX, [ELEMENT], SYMBOL, [SYMBOL], TYPE, [TYPE], ATOMIC_MAS, [ATOMIC_MAS])

and [NEWSYMBOL] IS GIVEN THE VALUE [SYMBOL]

and [PRODUCT] IS GIVEN THE VALUE "H"+[NEWSYMBOL]

and [MOLARMASSHALIDE] IS GIVEN THE VALUE
(1.008 + [ATOMIC_MAS])

and Called HydrogenHalide

Rule number 7

IF:
Called AlkaliMetalOxide

and Oxides (or) Halides formed combines with Water(H_2O)

THEN:
[COMPOUND] IS GIVEN THE VALUE [NEWSYMBOL]+"OH"

and [MOLARMASSPRODUCT] IS GIVEN THE VALUE
([ATOMIC_MAS]+16+1.008)

and named AlkaliMetalHydroxide

Rule number 8

IF:
Called AlkalineEarthMetalOxide

and Oxides (or) Halides formed combines with Water(H_2O)

THEN:
[COMPOUND] IS GIVEN THE VALUE
[NEWSYMBOL] + "$(OH)_2$"

and [MOLARMASSPRODUCT] IS GIVEN THE VALUE
([ATOMIC_MAS] * 2 + 16 + 1.008)

and named AlkalineEarthMetalHydroxide

Rule number 9

IF:

Called NonMetalOxide2

and Oxides (or) Halides formed combines with Water(H_2O)

THEN:

[COMPOUND] IS GIVEN THE VALUE
("H" + [NEWSYMBOL] + "O_3") + "+" +
("H"+ [NEWSYMBOL] + "O_2")

and [MOLARMASSPRODUCT] IS GIVEN THE VALUE
(1.008 + [ATOMIC_MAS] + 16 *3) ||
*(1.008 + [ATOMIC_MAS] + 16 *2)*

and named NonMetallicCompound2

Rule number 10

IF:

Called NonMetalOxide

and Oxides (or) Halides formed combines with Water(H_2O)

THEN:

[COMPOUND] IS GIVEN THE VALUE
"H_2"+[NEWSYMBOL]+"O_4"

and [MOLARMASSPRODUCT] IS GIVEN THE VALUE
(2 * 1.008 +[ATOMIC_MAS] + 4 * 16)

and named NonMetallicCompound

Rule number 11

IF:

Called NonMetalOxide1

and Oxides (or) Halides formed combines with Water(H_2O)

THEN:

[COMPOUND2] IS GIVEN THE VALUE [COMPOUND]

and [COMPOUND2] IS GIVEN THE VALUE "H_2"+ [NEWSYMBOL]+"O_3"

and [MOLARMASSPRODUCT] IS GIVEN THE VALUE (2 * 1.008 +[ATOMIC_MAS] + 3 * 16)

and named NonMetallicCompound1

Rule number 12

IF:

Called HydrogenHalide

and Oxides (or) Halides formed combines with Water(H_2O)

THEN:

[COMPOUND] IS GIVEN THE VALUE "H"+[NEWSYMBOL]+"(Aq)"

and [MOLARMASSPRODUCT] IS GIVEN THE VALUE (1.008 + [ATOMIC_MAS])

and named NonMetallicCompound3

Rule number 13

IF:

named AlkaliMetalHydroxide

THEN:

TURNS RED LITMUS TO BLUE

and pH value is > 7

and termed as Base - Confidence=6/10

and [COMPOUND1] IS GIVEN THE VALUE [COMPOUND]

Rule number 14

IF:

named AlkalineEarthMetalHydroxide

THEN:

TURNS RED LITMUS TO BLUE

and pH value is > 7

and termed as Base - Confidence=5/10

and [COMPOUND1] IS GIVEN THE VALUE [COMPOUND]

Rule number 15

IF:

named NonMetallicCompound

THEN:

TURNS BLUE LITMUS TO RED

and pH value is < 7

and termed as Acid - Confidence=7/10

and [COMPOUND1] IS GIVEN THE VALUE [COMPOUND]

Rule number 16

IF:

named NonMetallicCompound1

THEN:

TURNS BLUE LITMUS TO RED

and pH value is < 7

and termed as Acid - Confidence=7/10

and [COMPOUND1] IS GIVEN THE VALUE [COMPOUND2]

Rule number 17

IF:

named NonMetallicCompound2

THEN:

TURNS BLUE LITMUS TO RED

and pH value is < 7

and termed as Acid - Confidence=7/10

and [COMPOUND1] IS GIVEN THE VALUE [COMPOUND]

Rule number 18

IF:

named NonMetallicCompound3

THEN:

TURNS BLUE LITMUS TO RED

and pH value is < 7

and termed as Acid - Confidence=7/10

and [COMPOUND1] IS GIVEN THE VALUE [COMPOUND]

Rule number 19

IF:

[MASSOFELEMENT] != 0

and [SOLUTIONVOL] != 0

THEN:

[AMTPRODUCT] IS GIVEN THE VALUE
(([MASSOFELEMENT]*[MOLARMASSPRODUCT][ATOMIC_MAS])

and [MOLARITY] IS GIVEN THE VALUE
([AMTPRODUCT] * [MOLARMASSPRODUCT]) / [SOLUTIONVOL]

and [H] IS GIVEN THE VALUE [MOLARITY]

Rule number 20

IF:

[GIVENMASSPROD] != 0

THEN:

[REQDELEMENT] IS GIVEN THE VALUE
([GIVENMASSPROD] * [ATOMIC_MAS]/MOLARMASSPRODUCT])

Rule number 21

IF:

[COMPOUND1] != " "

and ([ELEMENT] = = "Lithium" || [ELEMENT] = = "Sodium" ||
[ELEMENT] = = "Potassium" || [ELEMENT] = = "Rubidium")

and ([M] == "HCl" || [M] == "HydrochloricAcid")

THEN:

[FINALPRODUCT] IS GIVEN THE VALUE
((([NEWSYMBOL] + "Cl") + "+") + "H_2O")

Rule number 22

IF:
[COMPOUND1] != " "

and ([ELEMENT] = = "Lithium" || [ELEMENT] = = "Sodium" || [ELEMENT] = = "Potassium" || [ELEMENT] = = "Rubidium")

and ([M] == "H_2SO_4" || [M] == "Sulphuric Acid")

THEN:
[FINALPRODUCT] IS GIVEN THE VALUE
((([NEWSYMBOL] + "$_2$" + "SO_4") +"+") + "H_2O")

Rule number 23

IF:
[COMPOUND1]!=" "

and ([ELEMENT]= ="Lithium" || [ELEMENT]= ="Sodium" || [ELEMENT] = = "Potassium" || [ELEMENT] = = "Rubidium")

and [M]== "H_2SO_3" || [M]== "Sulphurous Acid"

THEN:
[FINALPRODUCT] IS GIVEN THE VALUE
(([NEWSYMBOL]+"$_2$"+"SO_3") +"+") + "H_2O"

Rule number 24

IF:
[COMPOUND1] != " "

and ([ELEMENT] = = "Beryllium" || [ELEMENT] = = "Magnesium" || [ELEMENT] = = "Calcium" || [ELEMENT] = = "Strontium")

and ([M] == "HNO_3" || [M] == "Nitric Acid")

THEN:
[FINALPRODUCT] IS GIVEN THE VALUE
((([NEWSYMBOL] + "$(NO_3)_2$") +"+") + "H_2O")

Rule number 25

IF:

[COMPOUND1] != " "

and ([ELEMENT] = = "Lithium" || [ELEMENT] = = "Sodium" || [ELEMENT] = = "Potassium" || [ELEMENT] = = "Rubidium")

and ([M] == "HNO_3" || [M] == "Nitric Acid")

THEN:

[FINALPRODUCT] IS GIVEN THE VALUE
((([NEWSYMBOL] + "NO_3") +"+") + "H_2O")

Rule number 26

IF:

[COMPOUND1] != " "

and ([ELEMENT] = = "Beryllium" || [ELEMENT] = = "Magnesium" || [ELEMENT] = = "Calcium" || [ELEMENT] = = "Strontium")

and ([M] == "HCl" || [M] == "Hydrochloric Acid")

THEN:

[FINALPRODUCT] IS GIVEN THE VALUE
((([NEWSYMBOL] + "Cl_2") +"+") + "H_2O")

Rule number 27

IF:

[COMPOUND1] != " "

and ([ELEMENT] == "Magnesium" || [ELEMENT] = = "Calcium" || [ELEMENT] = = "Beryllium" || [ELEMENT] == "Strongtium")

and ([M] == "H_2SO_4" || [M] == "Sulphuric Acid")

THEN:

[FINALPRODUCT] IS GIVEN THE VALUE
((([NEWSYMBOL] + "SO_4") +"+") +"H_2O")

Rule number 28

IF:

[COMPOUND1] != " "

and ([ELEMENT] =="Magnesium" || [ELEMENT] =="Calcium" || [ELEMENT] = = "Beryllium" || [ELEMENT] == "Strongtium")

and ([M] = = "H_2SO_3" || [M] == "Sulphurous Acid")

THEN:

[FINALPRODUCT] IS GIVEN THE VALUE
((([NEWSYMBOL] + "SO_3") + "+") + "H_2O")

Rule number 29

IF:

[COMPOUND1] != " "

and ([ELEMENT] == "Sulphur")

and ([N] == "NaOH" || [N] == "Sodium Hydroxide")

THEN:

[FINALPRODUCT] IS GIVEN THE VALUE
(((("Na_2" + [NEWSYMBOL]) +"O_4") + "+") + "H_2O")

Rule number 30

IF:

[COMPOUND1] != " "

and ([ELEMENT] == "Sulphur")

and ([N] == "NaOH" || [N] == "Sodium Hydroxide")

THEN:

[FINALPRODUCT2] IS GIVEN THE VALUE
(((("Na_2" + [NEWSYMBOL]) +"O_3") + "+") + "H_2O")

Rule number 31

IF:

[COMPOUND1] != " "

and ([ELEMENT] == "Chlorine")

and ([N] == "NaOH" ||[N] == "SodiumHydroxide")

THEN:

[FINALPRODUCT] IS GIVEN THE VALUE
((("Na" + [NEWSYMBOL]) + "+") + "H_2O")

Rule number 32

IF:

[COMPOUND1] != " "

and ([ELEMENT] == "Chlorine")

and ([N] == "KOH" || [N] == "Potassium Hydroxide")

THEN:

[FINALPRODUCT] IS GIVEN THE VALUE
((("K" + [NEWSYMBOL]) + "+") + "H_2O")

Rule number 33

IF:

[COMPOUND1] != " "

and ([ELEMENT] == "Sulphur")

and ([N] == "KOH" || [N] == "Potassium Hydroxide")

THEN:

[FINALPRODUCT] IS GIVEN THE VALUE
((("K_2" + [NEWSYMBOL]) + "O_4" + "+") + "H_2O")

Rule number 34

IF:

[COMPOUND1] != " "

and ([ELEMENT] == "Sulphur")

and ([N] == "KOH" || [N] == "Potassium Hydroxide")

THEN:

[FINALPRODUCT2] IS GIVEN THE VALUE
((("K_2" + [NEWSYMBOL]) + "O_3" + "+") + "H_2O")

Rule number 35

IF:

[COMPOUND1] != " "

and ([ELEMENT] == "Nitrogen")

and ([N] == "KOH" || [N] == "Potassium Hydroxide")

THEN:

[FINALPRODUCT] IS GIVEN THE VALUE
((("K" + [NEWSYMBOL]) + "O_3" + "+") +"H_2O")

Rule number 36

IF:

[COMPOUND1] != " "

and ([ELEMENT] == "Nitrogen")

and ([N] == "NaOH" || [N] == "Sodium Hydroxide")

THEN:

[FINALPRODUCT2] IS GIVEN THE VALUE
((("Na" + [NEWSYMBOL]) + "O_3" + "+") + "H_2O")

Rule number 37

IF:

[MOLARITY] != 0

THEN:

[PH] IS GIVEN THE VALUE -(LOG([H]) / 2.303)

and [POH] IS GIVEN THE VALUE 14 - [PH]

Rule number 38

IF:

[ELEMENT] == "Nitrogen"

THEN:

RUN("A:\PROJEC~2.EXE")

and RUN(A:\TITRA-nitrogen.EXE [N])

Rule number 39

IF:

[ELEMENT] == "Sodium"

THEN:

RUN("A:\PROJEC~2.EXE")

and RUN(A:\TITRA-metal.EXE [element] [M])

Rule number 40

IF:
[ELEMENT] == "Magnesium"
THEN:
RUN("A:\PROJEC~1.EXE")

and RUN(A:\TITRA-metal.EXE [Element] [M])

Rule number 41

IF:
([ELEMENT] == "Chlorine")

THEN:

RUN("A:\CHLORINE.EXE")

and RUN(A:\TITRA-Chlorine.EXE [N])

Rule number 42
IF:
([ELEMENT] == "Sulphur")

THEN:
RUN("A:\SULPHUR.EXE")

and RUN(A:\TITRA-sulphur.EXE [N])

Rule number 43

IF:
([ELEMENT] == "Potassium")

THEN:
RUN("A:\PROJEC~1.EXE")

and RUN(A:\TITRA-metal.EXE [element] [M])

Rule number 44

IF:
([ELEMENT] == "Calcium")

THEN:
RUN("A:\PROJEC~1.EXE")

and RUN(A:\TITRA-metal.EXE [element] [M])

Rule number 45

IF:
[COMPOUND1] != " "

and ([ELEMENT] == "Nitrogen")

and ([N] == "Ca(OH)$_2$" || [N] == "CalciumHydroxide")

THEN:
[FINALPRODUCT] IS GIVEN THE VALUE
("Ca" + "(" + [NEWSYMBOL] + "O$_3$" + ")" + "$_2$" + "+" + "H$_2$O")

Rule number 46

IF:
[COMPOUND1] != " "

and ([ELEMENT] == "Sulphur")

and ([N] == "Ca(OH)$_2$" || [N] == "Calcium Hydroxide")

THEN:
[FINALPRODUCT] IS GIVEN THE VALUE
("Ca" + "(" + [NEWSYMBOL] + "O$_3$" + ")" + "+" + "H$_2$O")

Rule number 47

IF:
[COMPOUND1] != " "

and ([ELEMENT] == "Sulphur")

and ([N] == "Ca(OH)$_2$" || [N] == "Calcium Hydroxide")

THEN:
[FINALPRODUCT] IS GIVEN THE VALUE
("Ca" + "(" + [NEWSYMBOL] + "O$_4$" + ")" + "+" + "H$_2$O")

Rule number 48

IF:
[COMPOUND1] != " "

and ([ELEMENT] == "Chlorine")

and ([N] == "Ca(OH)$_2$" || [N] == "CalciumHydroxide")

THEN:
[FINALPRODUCT] IS GIVEN THE VALUE
("Ca" + "(" + [NEWSYMBOL] + "$_2$" + ")" + "+" + "H$_2$O")

Rule number 49

IF:
[COMPOUND1] != " "

and ([ELEMENT] == "Chlorine")

and ([N] == "Mg(OH)$_2$" || [N] == "Magnesium Hydroxide")

THEN:
[FINALPRODUCT] IS GIVEN THE VALUE
("Mg" + "(" + [NEWSYMBOL] + "$_2$" + ")" + "+" + "H$_2$O")

Rule number 50

IF:
[COMPOUND1] != " "

and ([ELEMENT] == "Sulphur")

and ([N] == "Mg(OH)$_2$" || [N] == "MagnesiumHydroxide")

THEN:
[FINALPRODUCT] IS GIVEN THE VALUE
("Mg" + "(" + [NEWSYMBOL] + "O$_4$" + ")" + "+" + "H$_2$O")

Rule number 51

IF:
[COMPOUND1] != " "

and ([ELEMENT] == "Sulphur")

and ([N] == "Mg(OH)$_2$" || [N] == "MagnesiumHydroxide")

THEN:
[FINALPRODUCT] IS GIVEN THE VALUE
("Mg" + "(" + [NEWSYMBOL] + "O$_3$" + ")" + "+" + "H$_2$O")

Rule number 52

IF:
[COMPOUND1] != " "

and ([ELEMENT] == "Nitrogen")

and ([N] == "Mg(OH)$_2$" || [N] == "Magnesium Hydroxide")

THEN:
[FINALPRODUCT] IS GIVEN THE VALUE
((("Mg" + "(" + [NEWSYMBOL]) + "O$_3$" + ")" + "$_2$" + "+") + "H$_2$O")

Rule number 53

IF:

([ELEMENT] = = "Sodium" || [ELEMENT] = = "Potassium" ||
[ELEMENT] = = "Magnesium" || [ELEMENT] = = "Calcium" ||
[ELEMENT] = = "Sulphur" || [ELEMENT] = = "Nitrogen" ||
[ELEMENT] = = "Lithium" || [ELEMENT] = = "Rubidium" ||
[ELEMENT] = = "Beryllium" || [ELEMENT] = = "Strongtium")
and When combines with Hydrogen

THEN:

Show Error message

Rule number 54

IF:

([ELEMENT] == "Chlorine")

and When combines with Oxygen

THEN:

Show Error message

Rule number 55

IF:

([ELEMENT] == "Lithium")

THEN:

RUN("A:\PROJEC~2.EXE")

and RUN(TITRA-metal.Exe [element] [M])

Rule number 56

IF:
    ([ELEMENT] == "Rubidium")

THEN:
    RUN("A:\PROJEC~2.EXE")

    and RUN(TITRA-metal.Exe [element] [M])

Rule number 57

IF:
    ([ELEMENT] == "Beryllium")

THEN:
    RUN("A:\PROJEC~1.EXE")

    and RUN(TITRA-metal.Exe [element] [M])

Rule number 58

IF:
    ([ELEMENT] == "Strontium")

THEN:
    RUN("A:\PROJEC~1.EXE")

    and RUN(TITRA-metal.Exe [element] [M])

APPENDIX B

Data file (Test.dbf)

Record #	Name	Symbol	Oms_e	Type	Atomic_No	Atomic_mas	E_config	Valence
1	Hydrogen	H	1	NMetal	1	1.008	1	1
2	Lithium	Li	1	Metal	3	6.941	2.1	1
3	Beryllium	Be	2	Metal	4	9.012	2.2	2
4	Nitrogen	N	5	NMetal	7	14.006	2.5	3
5	Oxygen	O	6	NMetal	8	15.999	2.6	2
6	Sodium	Na	1	Metal	11	22.989	2.8.1	1
7	Magnesium	Mg	2	Metal	12	24.305	2.8.2	2
8	Sulphur	S	6	NMetal	16	32.066	2.8.6	2
9	Chlorine	Cl	7	NMetal	17	35.452	2.8.7	1
10	Potassium	K	1	Metal	19	39.098	2.8.8.1	1
11	Calcium	Ca	2	Metal	20	40.078	2.8.8.2	2
12	Rubidium	Rb	1	Metal	37	85.467	2.8.18.8.1	1
13	Strontium	Sr	2	Metal	38	87.62	2.8.18.8.2	2

APPENDIX C

Flow chart diagrams

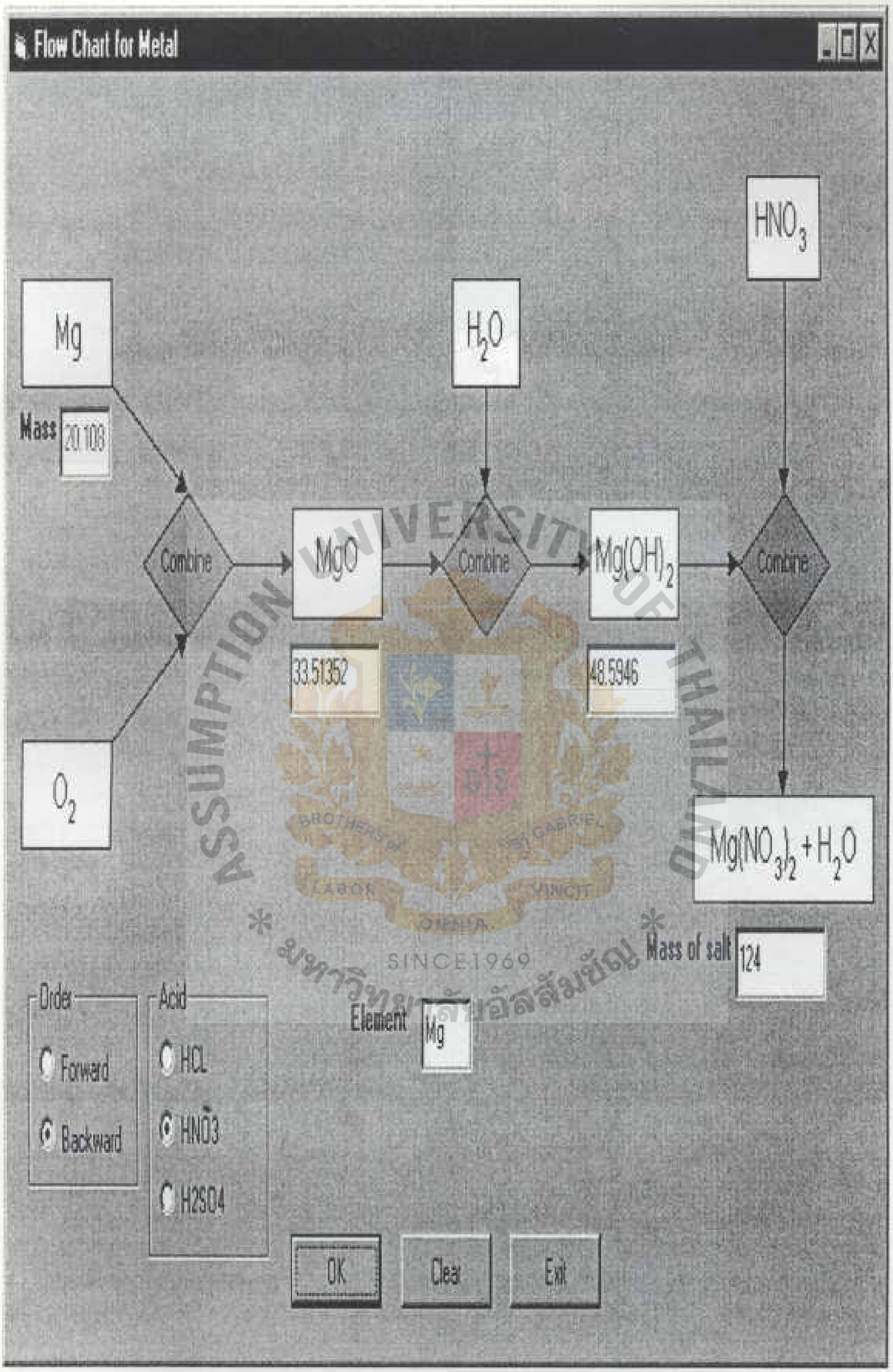


Figure 4-14 Flow chart diagram for Magnesium (Alkaline Earth Metal)

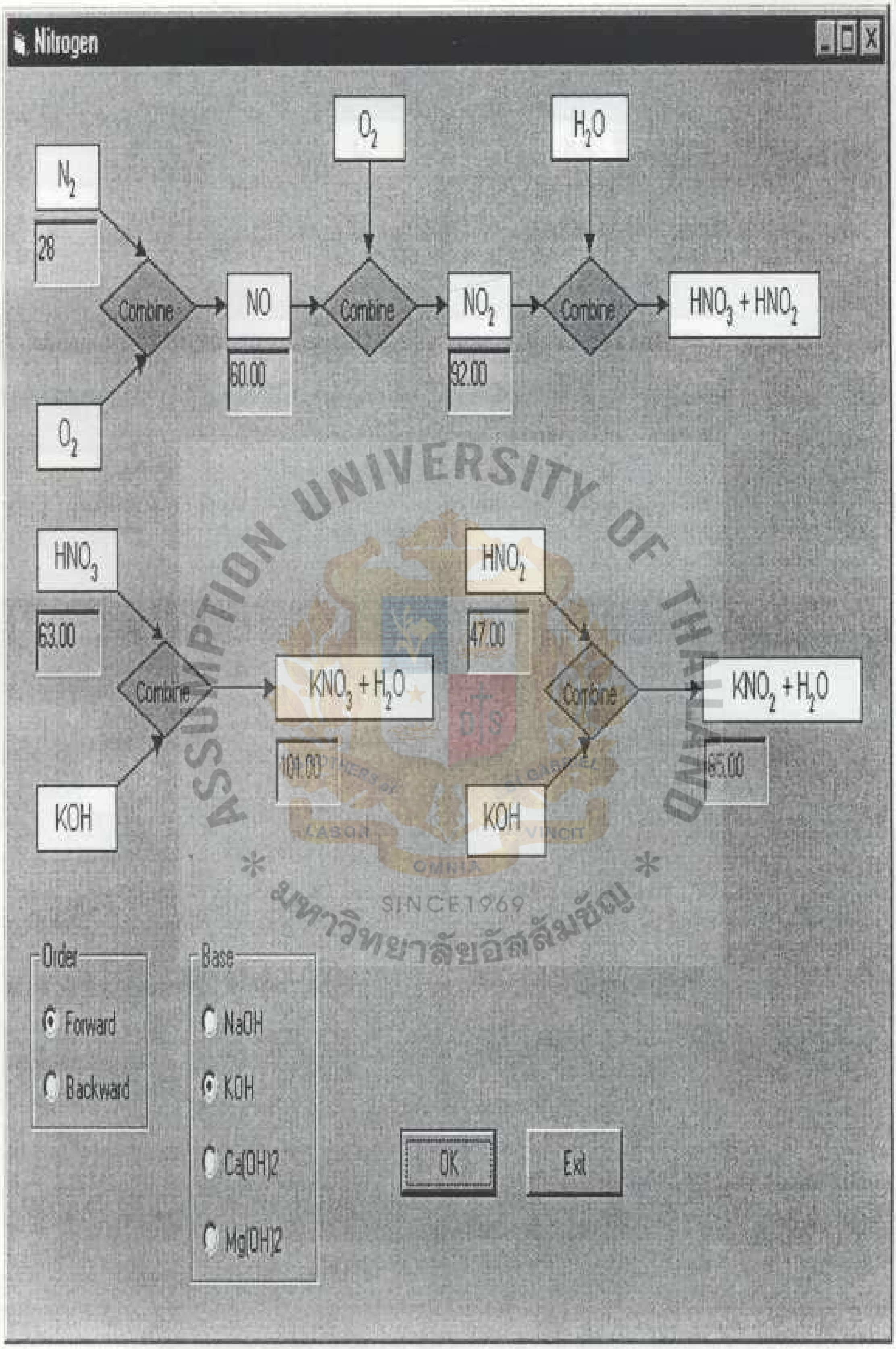


Figure 4-15 Flow chart diagram for Nitrogen (Non-Metal)

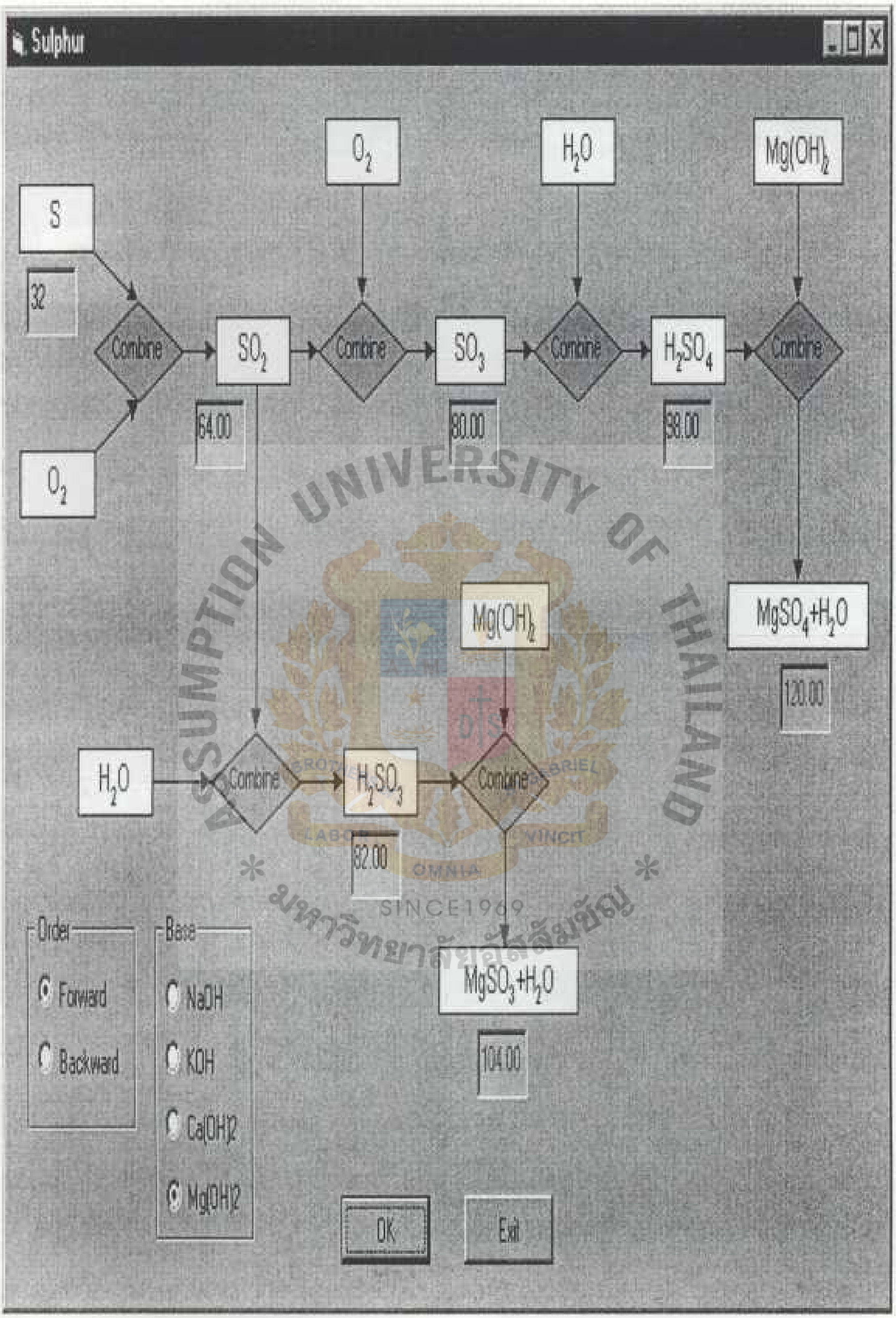


Figure 4-16 Flow chart diagram for Sulphur (Non-Metal)

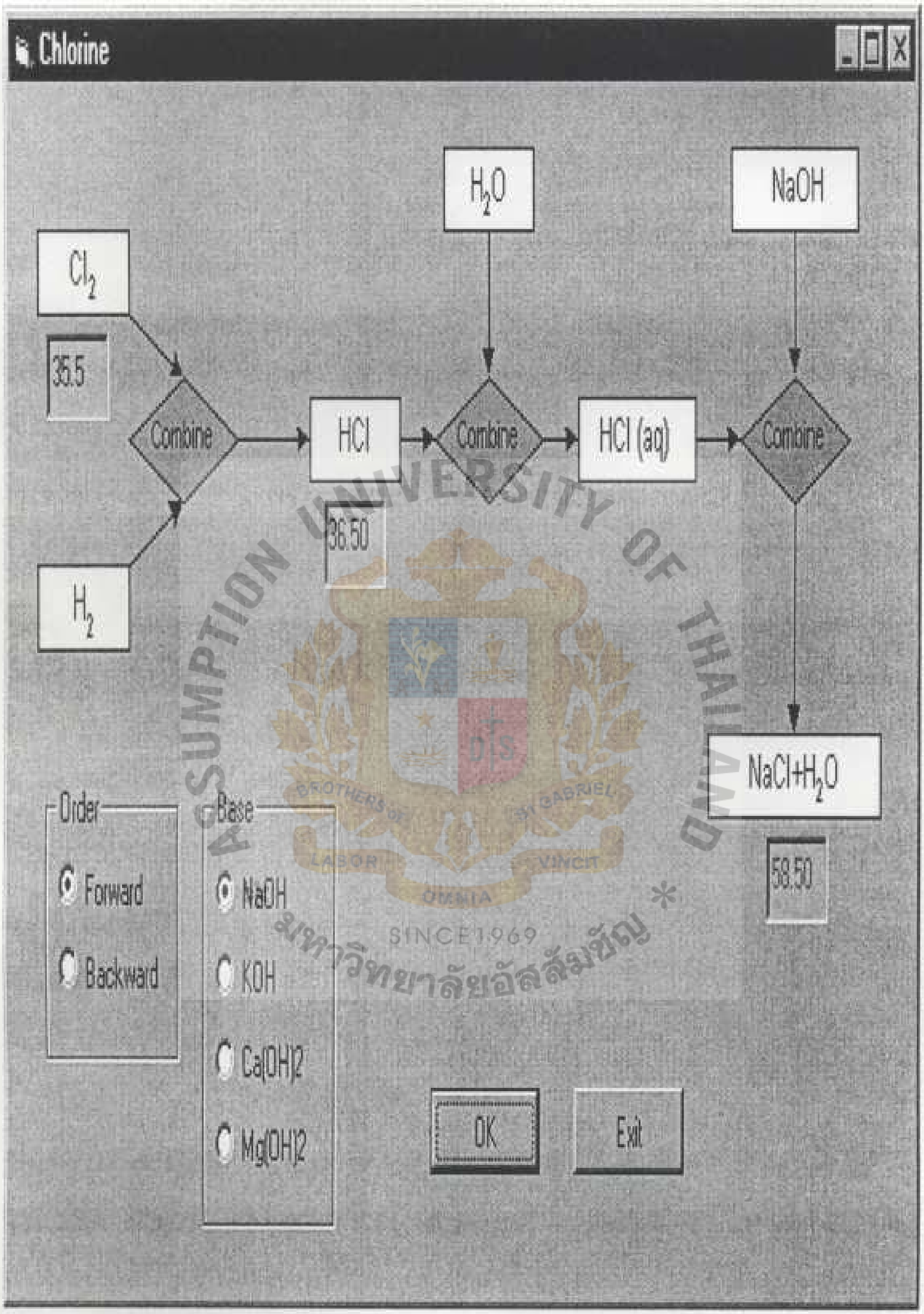


Figure 4-20 Flow chart diagram for Chlorine (Non-Metal)

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