Scientific Journal Impact Factor (SJIF) : 1.711
International Journal of Modern Trends in Engineering and Research
ISSN (ONLINE) : 2349 - 9745 ISSN (PRINT) : 2393 - 8161

# Knowledge Acquisition from Chemical Computation: An Initiative to Transfer Tacit Knowledge to Explicit Form

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**Abstract -** Knowledge derived from chemical computation is the initiative to transfer tacit knowledge to explicit form. Here in this paper researcher is identified computational problems from chemical domain to better understand existing chemical reaction approaches, actual experimental results and its corresponding efficient and effective solutions. During this process researcher contribute to this knowledge base by identifying the areas and locations where their knowledge Management is possible. Further this paper insight on development of chemical ontology and KM framework based on proposed ontology .Also this research paper focuses on software tools used to implement the novel solutions of computational problems in chemical reaction mechanism.
**Keyword** - Knowledge Management, Tacit Knowledge, Explicit Knowledge, Chemical Ontology

## I. INTRODUCTION

The science of computational chemistry carries many benefits to society. Chemistry helps to explain how the nature works, principally by exploring nature on the chemical molecule. Industry uses chemical reactions to make useful product. Chemical analysis is used to identify chemical properties of substances. The science of computational chemistry is unique in that it comprises the capability to generate new forms of compound by combining the elements and existing substances in new but controlled ways. The construction of new chemical compounds is the area from which knowledge generated and need to capture and preserve. Here, we explore the different types of chemical reactions, highlighting the reactions that have solution and implementation phases. So we consider computational chemistry to comprise the study of the structure, properties, and dynamics of chemical systems. The major activities in computational chemistry can be classified as molecular electronic structure, molecular dynamics and reaction dynamics. These are used to calculate the properties of molecules, chemical configurations and reaction trails for chemical reactions.

In such scenario computational chemists have been key users of computer software and software tools to produce and capture novel solutions to reduce the cost of performing the computations. We demonstrate here reaction mechanism, for that much of our current methodology is incapable of extending the accuracy of our description of molecular systems beyond what we can currently achieve, and that new methods must be sought (**Peter R. Taylor,02**).

## II. COMPUTATIONAL PROBLEMS-CHEMICAL DOMAIN

In a chemical reaction, compounds called reactants are changed into other compounds called products. You can't change one element into another in a chemical reaction — that happens in nuclear reactions. Instead, you generate a new substance with chemical reactions.

Following are the some problems identified from chemical domain where their chemical computation is required –

1. Reaction Mechanism
2. Molecular Modeling
3. Molecular Simulation
4. Chemical Properties Identification
5. Geometry Optimization
6. Molecule Structure Identification
7. Determination of Bond Energies

**1.Reaction Mechanism**

Chemical reactions involve the transformation of matter, the reactants, into different materials, theProducts.

**Problem Identified –**

How to represent chemical reactions using balanced chemical equations?
How to calculate the quantities of material involved in a chemical reaction?
The original reactants must contain atoms of which element?

Here three type of chemical reactions are carried out as-

**a. Combination Reactions**
**b. Decomposition Reactions**
**c. Displacement Reactions**

## III. SOLUTIONS FOR THE COMPUTATIONAL PROBLEMS

**Combination Reactions**

A combination reaction is one in which typically two or more reactants, usually compound or elements combine to form one product. In one type of combination reaction, two elements combine to form a compound.

For example, the elements hydrogen and oxygen combine to form water, giving out large amounts of energy in the process:

**2 H2(g) + O2(g) -›2 H2O(g)**
(Hydrogen) (Oxygen) (water vapor)

Other types of combination reactions include the combination of an element with a compound and the combination of two different compounds to form a new compound.

For example, oxygen reacts with sulfur dioxide to make sulfur trioxide.

**2 SO2(g) + O2(g) -›2 SO3(g)**

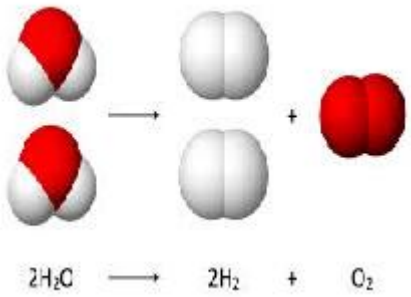
Sulfur trioxide and water undertake a combination reaction to form sulfuric acid.

**SO3(g) + H2O(L) -›H2SO4(aq)**

**Decomposition Reactions:**

The number of products is greater than the number of reactants. The reaction is basically the reverse of a combination reaction and typically results from the addition of electrical or thermal energy. Means breakdown of larger, unusual compound into smaller useful compound (**Chemical Interaction,10**).
For example, water is a very stable compound under typical conditions, but it can be made to decompose to its constituent elements by using electrical energy, a process called electrolysis.

**2 H2O(L) -›2 H2(g) + O2(g)**
(Water) (Hydrogen) (Oxygen)




Metal carbonates such as calcium carbonate, CaCO3, undergo decomposition when heated, giving out carbon dioxide gas as one of the products.
**CaCO3(s) -›CaO(s) + CO2(g)**

**Displacement Reactions:**
In displacement reactions, one atom or molecular fragment displaces another. Displacement reactions can be single or double reactions. Obtaining compounds of choice which are otherwise available with difficulty.**(Chemical Interation,10)**
For example, when a metal reacts with water. In the reaction of sodium metal with water, the metal displaces a hydrogen atom in water, forming sodium hydroxide
**H2O(L) + Na(s) -›H2(g) + NaOH(aq)**

The displacement reaction between sodium metal and water
The construction of new chemical may makes harmful waste products. Chemical reactants in catalytic converters make these waste products less harmful.

## IV. KM BASE IN PROBLEM, SOLUTION AND IMPLEMENTATION PROCESS

**KM generated from Combination Reactions**

- **"In n all combination reactions, the number of reactants is greater than the number of products"**
- **"Living things required chemical reaction"**

This combination reaction is used to generate power from the main engines in the space shuttle. The large fuel tank has separate compartments containing liquefied hydrogen and oxygen, which are vaporized prior to mixing.

**KM generated from Decomposition**

- **"The reaction is basically the reverse of a combination reaction and usually results from the addition of electrical or thermal energy."**
- **"Chemical reactions are used in Technology"**

The solution of large numbers of joined partial differential equations is necessary to analyze joined chemistry problems associated with many chemical systems (e.g. air pollution problems such as acid rain and photochemical smog, catalysis and reactor design, combustion).(**Valeriu Damian-05**)

**KM generated from Displacement Reactions**

- **"The reactions where the number of reactants is typically equal to the number of products."**
- **"Chemical reaction makes the tiny circuits that are used to run electric devices "**

## V. TACIT AND EXPLICIT SPECIFICATION FOR KM

Two entries from two different knowledge bases could be conditionally to relate to the same concept even if no such inference had been openly stated, through the chemical reaction mechanism. The integration of a large portion of chemical information into the linked open data, representing the usefulness of doing so with successfully fulfilled problems. Observed chemical phenomena are explained as subatomic particles and microscopic structure of atoms and molecules, agents, apparatus to construct explanation of the phenomena at the submicroscopic and to write equations which describes them.

During the balancing of chemical equation and classify the type of chemical reaction is the key area from which chemical knowledge base is identified as–

| Tacit Knowledge | Explicit Knowledge | Type of reaction |
|---|---|---|
| Complex relationships in-between states | explaining a chemical reaction | a. Combination Reactions<br>b. Decomposition Reactions<br>c. Displacement Reactions |
| Chemical configuration | Attributes and catalyst of entry element | |
| Microscopic chemical phenomena of molecules | Observed chemical phenomena of molecules | |
| Thinking, Experience, Competency, Commitment-about molecule | Data ,information ,record, Documents, files about substance | |
| Chemical configurations- know-how that are implied or indicated but not actually expressed | Codified vocabulary | |

## VI. IMPLEMENTATION BY USING SOFTWARE TOOLS

The concept of the paperless lab may never be a actuality, but the computer-free lab is definitely a thing of the past. Chemical experimental data output, high-throughput substances and chemical screening, and laboratory information systems are fast becoming part of the researcher's everyday life. Software packages such as word processors and spreadsheets are used for writing reports and analyzing data. The addition of molecular modeling to this gradually refined atmosphere is natural and almost unavoidable.

The advent of software chemical reaction mechanism and molecular modeling tools such as Materials GchemPaint, Jmol of IIT, Bombay covers the way for the future of computational chemistry. GchemPaint, Jmol is the first in what is bound to be a succession of high-quality software-based molecular modeling products. It runs on Linux, Windows, MacOS and Android as an Open Source there will be few commercial computational chemistry tools that run only on UNIX workstations.

Experimental chemists will interact with molecular models on their PCs and work closely with computational chemists to advance chemical and materials research using every available software technological tool. Fetching the latest scientific computing resources to every researcher will have a reflective effect on the way researchers work. Chemical communication and the scope for individual creativity will be immensely enhanced and will open the gates to increased chemical innovation, the key to future scientific innovations and financial growth. Software based chemical reaction mechanism and molecular modeling, whether under Linux or Windows, will be the champion in the great platform thought.
Chemical reaction mechanism and Molecular modeling software is now available for a variety of computer platforms, opening the field to new users. Chemical reaction mechanism and Molecular modeling can be a computationally intensive activity. Ab initio quantum mechanical calculations, many-thousand-step molecular dynamics calculations, and the rendering of high-quality molecular graphics all require substantial computing power to make virtual experiments viable.

The below listed software packages are the some knowledge-based reaction prediction tools. Knowledge-based systems include reaction predictors like ROBIA (Reaction Outcomes by Informatics Analysis) to finding answers to chemical-related questions. Makes it possible to gain access to information hidden in complex equations and tables using analytical and search tools. Users can find data in its online reference collection and then extract, analyze and manipulate the data found in tables and charts for further analysis.

| Sr. No. | Software Name | Purpose | Software Features | Language Support |
|---|---|---|---|---|
| 1 | **ASAD**-Chemical Integration Software | To solve the chemical rate equations | • Understands common approximations such as chemical families and the steady state approximation.<br>• A reaction database is included for building your own chemistry schemes. | FORTRAN |
| 2 | **ThermoData** | supports evaluation of the thermodynamic properties of | • Implements an algorithmic | Open Source |

| | | | | |
|---|---|---|---|---|
| | **Engine** (TDE) | chemical reactions | approach to aid users in experiment planning based on the accumulated body of knowledge | |
| 3 | **CAMEO**-modular expert system | predicts the products of organic reactions given starting materials, reagents and conditions | • It is constructed as a modular expert system, each module dealing with a different reaction class<br>• Perform a number of other functions, such as three-dimensional structure minimizations, bond predictions, bond angle and length calculations | Mac, Solaris 5.7, IRIX 5.3 |
| 4 | **Cantera**-object-oriented software | To handle problems in areas such as combustion, molecular structure, detonations, electrochemical energy conversion, fuel cells etc. | • Reaction managers phases of substances<br>• Chemical Vapor Deposition | C++ |
| 5 | **CHIMP** | Tool for the modeling of chemical phenomena | • Chemical reaction modeling, molecular mechanics will be implemented, along with an easy to use graphical-user interface (GUI)<br>• Integrate the species balance and reactor design equations | Open Source |

## VII. PROPOSED ONTOLOGY FOR COMPUTATIONAL PROBLEM

Formal specifications (relational vocabulary) of chemical entities that describe chemical objects and their relationships are designed as proposed ontology for computational chemistry reaction mechanism problem, solution and implementation spaces. This enable the search across multiple data sources ontology for representing chemical information and descriptors. Problem-Solution and Implementation (PSI) is a general ontology that provides object relations and classes of various entities, including chemical and informational ones. The Problem-Solution and Implementation (PSI) Ontology for chemical reaction mechanism was developed with its component ontologies for descriptions of materials, chemical structures, reactions, material properties and experiments. There are numerous challenges in the prospect, which include the consideration of rates of reaction to control significance and evaluation of multiple measures of molecular comparison. Here each data source is individually mapped to the ontology (**Bert Coessens,03)**

Chemical equations show the reactants and products, as well as other factors such as energy changes, catalysts, and so on. With these equations, an arrow is used to indicate that a chemical reaction has taken place. In general terms, a chemical reaction follows this format:

**Reactants =➔ Products**

The obtained ontology is displayed as Ontology-Based Response Component

✓ **Chemical Entity(CheEnt)** – Reactants and Products

✓ **Data Descriptor(DatDes)** – Data item whose syntax and semantics conforms to some data format specification and provides information about chemical entities
✓ **Chemical configuration(CheCom)** – every attribute has in-built chemical configuration (reflection of the sum of the conditions that may change the value)
✓ **Number of Units(NumUni)–** Unit involve molecular weight and number of molecule taking part in reaction (parameters used in generating value)
✓ **Value Change (ValCha**)–output has its new identity
✓ **Reaction Class (ReaCla)–** Combination, Decomposition &Displacement Reactions

We insight on the concepts present in the chemical entities as ontology to assign general classes to the appropriate chemical entities.In order to enable intellectual and implication over this chemical information, each represented entity also has to be explicitly assigned to a class that is defined within a supporting ontology.

## VIII. DESIGN OF KM FRAMEWORK BASED ON ONTOLOGY

If a chemist is dealing with solutions of certain chemicals; he may need access to information like atomic properties of an element, solubility, heat of solution, etc. He can extract the data, he find in the online reference collection for further analysis from the framework. Any tables from KM database you export always come with a reference source for verification, making it possible to preserve an information source for future documentation and reference.
This framework will assist you for the reaction mechanism of computational chemistry problems. This KM framework needs to encourage chemist to codify their experience, to share their knowledge and to develop an energetic attitude towards using the chemical reaction mechanism system.
This framework has two pillars shown like titration beakers –one for reactants defect tacit knowledge and another beaker for product defect explicit knowledge. The same was shown in fig.2.

- Formal model of shared knowledge
- Mapping to effects that exist (ontological commitments)

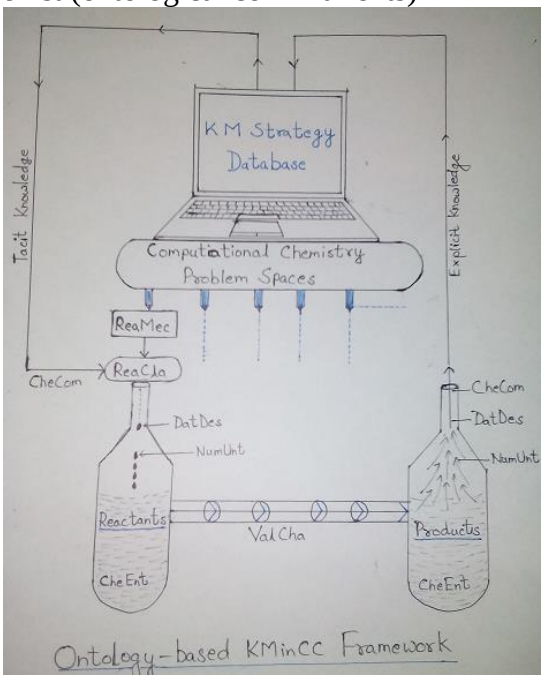



*Fig.2 KMinCC Ontology based Framework for Chemical Reaction Mechanism*

With the help of this illustrated **KMinCC** frameworks chemists and researchers can certainly find basic chemical information through these resources. KM database also offers certain interactive features that are not found in old-style chemical properties resources. These include providing conception of data points and the ability to calculate and plot additional data values as functions of variables, such as temperature, concentration, and pressure, search, and sort and filter capabilities, permitting for easy assessment and comparison of data after any chemical reaction.

This type of framework is a knowledge flow measurement which can help identify important topics within a collaborative knowledge portal [**D. T. Lee,01].** Tracking these measures with KMinCC helps in the identification of active subjects, which may take the form of problems, solutions, implementations, and accessible resources within the KMinCC knowledge framework .The complete process of tracing, managing, using and developing technical knowledge within.

## IX. CONCLUSION

Life and industry depends on chemical reactions. Chemical product design and development issues become more composite, chemists and researchers will need to have instant and consistent access to technical information along with advanced reaction calculators and modeling tools. A powerful knowledge management system gives users those tools and technology to access critical information. More access to this information gives users a better understanding and that frequently leads to greater innovation. Without a knowledge management system, you will be much more limited to what you can do during the early stages of chemical product development.

We conclude that there is a need to characterize a chemical knowledge resources in a more comprehensive and integrated manner than has heretofore been the one case of reaction mechanism. In order to promote a common understanding of Knowledge Management in Computational Chemistry (KMinCC), it is essential to organize and unite knowledge manipulation activities in a way that not only describes each activity clearly and completely, but also identifies their interrelationships. Similarly, it is important to recognize the influencing factors in a comprehensive and integrated way. Preferably, all of this can be accomplished in the creation of a new KMinCC framework that achieves association both within and across each of the chemical scopes. The frameworks designed and described here can serve as a starting point for creating a generic framework that unifies KMinCC concepts for reaction mechanism computational problem from chemistry domain. It should deliver a through basis for reviewing, assessing, and inventing various prescriptive KMinCC frameworks. Creating a generic expressive framework of knowledge management would benefit from a synthesis of the descriptive framework obtainable here, favorable and direct inputs from KMinCC experts and scholars.

A move to software- based reaction mechanism and molecular modeling will make computational chemistry more accessible in terms of the entry point in chemical domain. All the study may further apply to describe the discovery of novel reaction mechanism and molecular modeling knowledge of which might help to build powerful chemical software knowledge-base in the future.

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