



## CHEMISTRY WITH JAVA

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**Abstract-** The Chemistry with java is an application which combines the Organic and the Inorganic world of Chemistry into a single application which can be accessed by users across all changes to promote the learning and the understanding of the subject by introducing visual aid to the subject. The application is developed basically with three levels The User Interface being built using the Swing framework is an API for providing Graphical User Interface across all platforms. The Intermediate level we implement Java Database Connectivity for SQLite3 implying that the underlying base layer we use SQLite3 as the database. For the Organic world of Chemistry we use an API named OPSIN(Open Parser for Systematic IUPAC Nomenclature) which converts the general name of the Organic Compound into the IUPAC name of the same compound along with its standard structure.

**Keywords:** Chemistry, Java, IUPAC Nomenclature.

### I. Introduction

This Java Based Application is an integration between the Organic and the Inorganic ecosystems of Chemistry. The Organic Ecosystem of the project lays its emphasis primarily towards adding a visual impact to the Periodic Table where every element on the table acts as a button which when clicked extracts all the information from the underlying database and displays the most prominent information about the specific element[1]-[10]. The other main branch of the application being the Inorganic Chemistry branch which when given with a common nomenclature to an organic compound returns the IUPAC Nomenclature of the compound along with the standard structure of the compound.

### II. Objective

A recent study showed the decline in the interest of the students into chemistry because of the lack of the visual aid in learning unlike the other branches of science which have excessive resources to learn and adapt your knowledge practically. This application is developed to provide visual aid to this aspect of science to spark better learning interests. Thus, this application works as a catalyst to the interest in students and also facilitates easier teaching and a better learning experience. This also provides the interested users with additional knowledge which does not necessarily come with the academics.

III. Literature Survey

[1] Open chemistry: RESTful web APIs, JSON, NWChem and the modern web application, Marcus D. Hanwell, Wibe A. de Jong, Christopher J. Harris, Journal of cheminformatics, 2017

This was a modern end-to-end system which was developed. It was a web based interface which only provided basic information about the elements in the periodic table. This development offered pragmatic learning experiences for the first time irrespective of the device being used and maintained a standard User Interface across various devices like mobiles, desktops, Laptops etc.

[2] Chemical Name to Structure: OPSIN, an Open Source Solution, Daniel M. Lowe, Peter T. Corbett, Peter Murray-Rust\*, Robert C. Glen, Journal of chemical information and modelling, March 2011.

OPSIN (Open Parser for Systematic IUPAC Nomenclature) is an open source parser which converts the chemical name into structure. This system interprets most of the chemical compounds to its respective structures fast and precise. This system works based on the regular grammar used for the conversion from the chemical name to the Structure. The grammar is used to guide the process of tokenization of the conversion from name to structure.

[3] M-Learning: Atomic Orbitals of Elements in Periodic Table using SPATO, AngL, Fauzi S, Mazlan Umi, Zhafran A, Najwa-Alyani M, Journal of Physics, July 2018.

SPATO is a mobile learning tool which was developed to inculcate interest in learning chemistry amongst the science students. A waterfall model was used in developing SPATO. It was well accepted by the users but the people were not familiar with the concept of mobile Learning limited their understanding. SPATO provided an excellent stepping stone for the rest of the M learning application world.

[4] A Java Chemical Structure Editor Supporting the Modular Chemical Descriptor Language, Sergei V. Trepalin, Alexander V. Yarkov, Igor V. Pletnev, Andrei A. Gakh, Multidisciplinary Digital Publishing Institute, 2006.

This is a Java Applet which only produces the SMILES and the InChI coordinates of an organic compound which produced simple organic structure and because the size of the

applet was around 200kb it became easier to implement it over various platforms. The editor also supported the MCDL format which could even specify the canonical bonds of the system and provide to the smallest specification of the bonds between the atoms and molecules.

[5] A Java Tool for the Management of Chemical Databases and Similarity Analysis Based on Molecular Graphs Isomorphism, Irene Luque Ruiz, Miguel Ángel Gómez-Nieto, 2008.

This paper primarily focussed on the management of the database which consisted of both elements and molecules and they also try to calculate the difference between the separate molecules using isomerism. This allows the user to store different custom molecules and analyses the similarity of already present molecules through a wide range of similarity indices.

[6] An algorithm to identify functional groups in organic molecules, Peter Earl, 2007.

An algorithm was developed which identified the 3080 unique functional groups. This algorithm used an iterative approach marching through atoms described in the molecules. Functional groups are divided based on their Spectrography reading, organic chemistry, medicinal chemistry and also their chemical nomenclature. This paper was an attempt to identify all the functional groups atomically using an iterative algorithm.

[7] Real-Time Interactive Simulation and Visualization of Organic Molecules. Heta A. Gandhi, Sebastian Jakymiw, Rainier Barrett, Harshita Mahaseth, and Andrew D. White, September 2020. ACS Publications.

Three Dimensional Visualisation of Organic Molecules using Virtual Reality in an emerging way technical. This working VR utilises Unity3D and works with ZEROMQ message passing service. All MD simulations are done in the HOOMD-blue simulation engine, and the graphics for the VR are rendered in Unity3D. This feature sets it apart because of the advancement in the technology apart from the other applications because of the actual advancement in 3D Virtual Reality. Allowing users to access the application in real time. This application is a useful tool for studying the thermodynamic applications of the Chemical Compounds and molecules.

[8]CheS-Mapper - Chemical Space Mapping and Visualization in 3D, Martin Gütlein, Andreas Karwath & Stefan Kramer, Journal of Cheminformatics, March 2012.

This tool acts more like a database management tool where the user uploads the database needed to visualise the molecules or atoms present on the database. The 3D mapping used here uses spatial arrangement which helps even identify various isomers of indicating the various . The user also has the modularity of selecting the required elements helping in identifying the various similarities involved with this tool. This system can calculate various similarities because of the spatial arrangement of the molecules which can be obtained using the spatial management. The further subsets also can be exported from this tool for further detailed analysis.

[9]Tasker R., Dalton R. (2008) Visualizing the Molecular World – Design, Evaluation, and Use of Animations. In: Gilbert J.K., Reiner M., Nakhleh M. (eds) Visualization: Theory and Practice in Science Education. Models and Modeling in Science Education, vol 3. Springer,

This is a stepping stone to the world as it is an introduction to the digital world with chemistry. A lot of hardships regarding the learning of chemistry would be solved. A selection of a number of misconceptions involving chemistry in the VisChemApplication. The effectiveness of this system was calculated taking into the effect the various reasons why lectures were failing because of the lack of visual aid. An animation is embedded as learning objects in learning activities. A variety of the confusions present because of the absence of any visual aids in teaching .

#### IV. Demonstration Methodology

##### A. Inorganic Chemistry

The periodic table is hosted in this wing of the application where each element of the periodic table is also a button this button on click leads us to all the essential information of the element that was clicked

##### B. Organic Chemistry

Organic Chemistry deals majorly with carbon and its compounds . It is the branch of chemistry that has an extensive

nomenclature and has a regular grammar based on which these rules are built . In this part of the project we try to use these rules and grammars to convert compounds with an IUPAC nomenclature to show the general structure of the compounds.

#### V. Implementation Methodology

In order to establish and create the Application we use an approach dividing the application into 3 major layers .

##### 1. Software Requirements

A. The database - The database we use for our application is SQLite3. SQLite3 is the most widely used database engine and it comes built into a number of mobiles and other devices. Moreover SQLite3 is an open sourced software. SQLite3 is an in process Library which makes it easy to implement and requires zero configuration.

B. The Database Connectivity - Once we have the data it is essential to connect this data to the front end of the system to make this data viewable. To establish this connection between the database and the front-end we use Java Database Connectivity(JDBC). JDBC is an Application programming Interface which defines how a database can be accessed by the client. It is available in the Java Standard Edition Platform.

C. The Front End - To develop the Graphical User Interface(GUI) we use Java SWING. Swing is a GUI widget toolkit which was built to provide a sophisticated GUI development environment in Java. It uses a single threaded programming model. This Library can be used for building Applications and Applets.

##### 2. The flow of data

The application is built on 3 levels so it's important to have a well designed flow of data through the application to ensure none of the pre-existing data about the Periodic table goes corrupt.

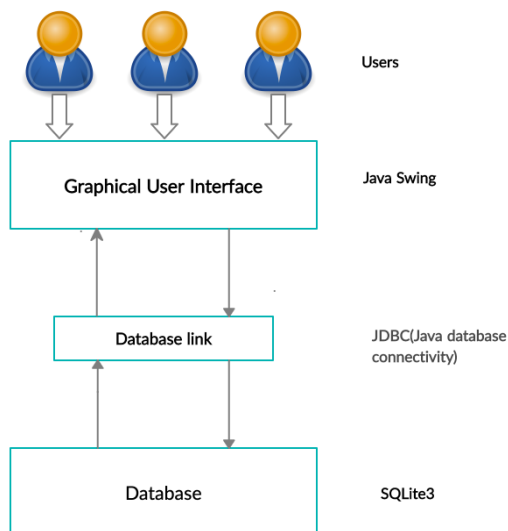


Fig 1. The data flow diagram

### 3. The Organic Chemistry API

In order to develop the Organic wing of the application we used the OPSIN API which followed the general rules to generate the standard structure of the organic chemical Compounds.

OPSIN API - the OPSIN API is a parser developed by cambridge university to follow the rules and grammar used to name the compounds to generate the structure of the compound.

### 4. The working Output

Since the application has Two major wings a toggle screen to switch between the sections is incorporated for easy access. We also have user interface with a minimalistic design which is easy on the eyes

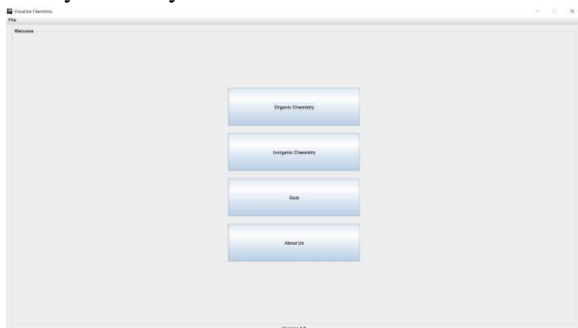


Fig 2. Screen to select the learning Option

The opening screen to select between the earning options available along with a brief area to test your understanding which you can take up.



Fig 3. The Periodic Table

The periodic table depiction where each of the elements is a button which redirects you to the page with all the in detail information about the selected element.

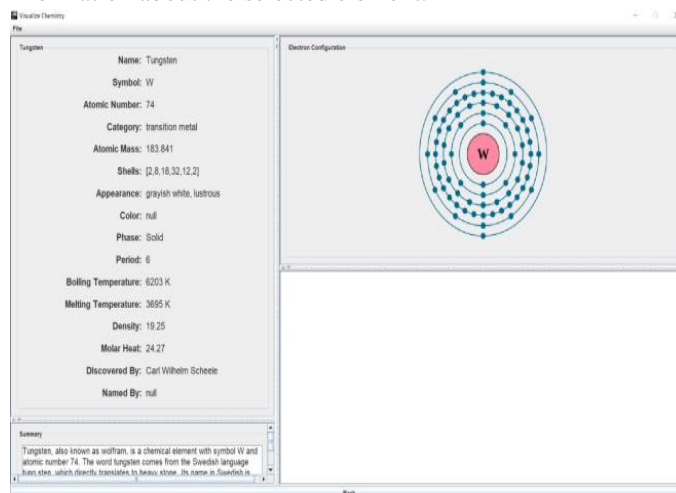


Fig 4. The Element detail

The left panel we use to put up the facts about these elements which are selected along with a detailed summary of the element. The top right panel shows the structure of the atom and helps us visualise how the atoms are different from one to another. The bottom right panel is a text area for the user to put down a few points while studying or write down a few clarifications.

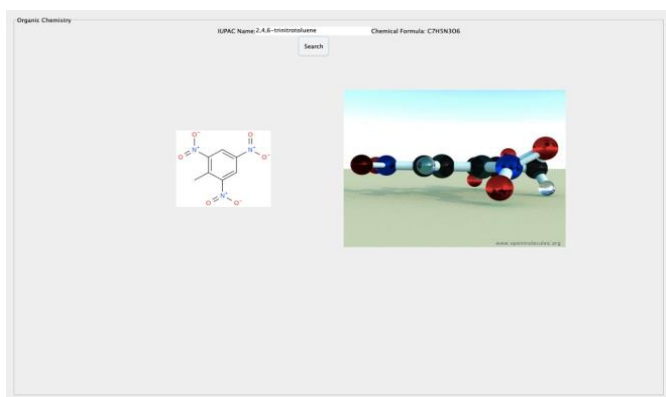


Fig 5. The organic compound structure generation

We use a text area to take an input of the name of the compound and it converts the name of the elements to a standard IUPAC structure and also mentions the chemical composition of the system along with the spatial arrangements of the various bonds in the molecule.

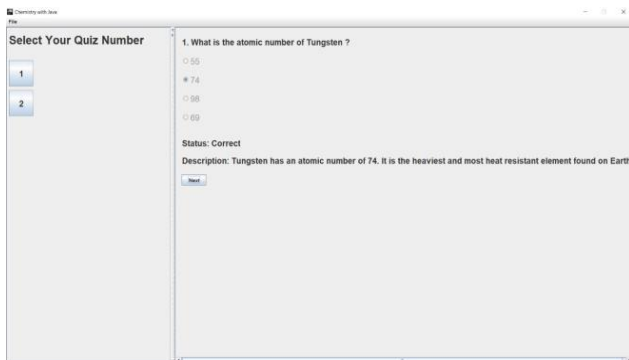


Fig. 6 The quiz section

The quiz section offers a platform to test your understanding on the basis of chemistry. It also offers a single line debrief of the answer which can also serve as flash cards.

## VI. Future Enhancements

As described the main purpose of this application was to develop a self paced learning application for appreciating the basics of chemistry. Hence, the large scale implementation of this application to android, iOS devices can also increase the reach of this application to the outside world. The application in the future can also be incorporated with an interactive video interface where the content can be produced at the tailor made pace of the users learning capability.

## VII. Conclusion

The Chemistry with Java, a learning application is a transformation we are seeing into the world of learning chemistry digitally. This makes it available to the fingertips of the user in a single application without having the hassle to look around the internet for similar information. The application developed with a very mild design language is easy and pleasing to use and the size of the application being less than 20MB is not memory intensive or needs no special requirements and can run on a daily system.

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