

ICT TOOLS FOR TEACHING AND RESEARCH IN CHEMISTRY

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ABSTRACT

Chemistry is the discipline of study of atoms & molecules and their properties due to which chemistry have lot of applications from agricultural sector to the chemical industries. In present scenario, the computer is just an essential tool as the test tube for chemists. The employment of ICT for teaching and research is compulsory for the overall development in the field of chemical science. Now-a-days, chemistry laboratories are using a lot of softwares which run under the various operating systems like Windows, Mac, UNIX, and Linux. In this paper, some tools of ICT which are helpful to draw chemical structures, , to realize the structure of chemical bonds, molecular design and 2d & 3D visualization of chemical structural formula are discussed.

Keywords: Molecular Editor, Chemdraw, Chems sketch, Xdrawchem, Avagadro, ISIS/Draw.

I. INTRODUCTION

ICT is the key to novel scientific research and developments in chemical sciences. ICT tools & softwares help in better understanding of concepts of chemistry because it helps to visualize the chemical structures in 3D-way. It helps learners or researchers to understand practical meaning of chemistry. In today's world, ICT plays a very significant role for carrying out various activities and functions for chemical research. Chemists use a lot of computer programmes to explain chemical problems, compute the structural properties of molecule such as quantum mechanics, simulation, geometrical and conformational analysis. Cheminformatics is extensively used for processing of data, storage of information & searching of structures of molecules. Chemical & structural information can be retrieved by Chemical Abstracts Service and ChemSpider, Cambridge Crystallographic Data Centre. ICT softwares for chemical drawing such as ChemDraw, ChemSketch, Marvin, Chemwindow, ChemDoodle, XDrawChem etc. are used for teaching & research. Cheminformatics programmes like Chemis3D, ChemWriter, Jmol, etc. is extensively used for molecular design & visualization etc. A molecule editor is a computer program for making and transforming representations of chemical structures. Many softwares have also been made for molecular mechanics, simulation & molecular modelling. Molecule editors can control representations of chemical structure either in a 2D or 3D-way. 2D- output is used as illustrations or to query chemical databases. 3D- output is used to build molecular models, usually as part of molecular modeling software packages. ICT tools play a significant role in carrying out various chemical research activities such as molecular modeling, database searching, chemical analysis, simulation etc. Various ICT tools used for teaching & research in chemistry are discussed in this paper.

1. Various Software for Chemists

The Information technology is helping to design software tools & programmes for chemistry teachers & researchers. Few of them are discussed in this section.

(i) ChemDraw: It is the most widespread drawing tool used for chemistry research. It is a division of the ChemOffice suite & is accessible for Mac & Windows. This tool allows us to draw chemical structures & One can also use it to find out properties of chemicals & view 3D structures, etc. It generates accurate structures from the chemical names and offers precise IUPAC names for the chemical structures.

(ii) ChemDoodle: It provides advanced mechanism drawing tools to show lone electron, pair of electron, & arrow notation of bonds. It is the single chemical drawing ICT tool which has subscript & superscript merge formatting in text to simply generate atomic notations & chemical text.

(iii) ChemSketch: It helps us to draw chemical structures of organic chemistry, organometallics & polymers. It can compute molecular weight, density, molar refractivity, etc. It is used for viewing 2D and 3D structure. This is a molecular editing tool used to make & revise images of chemical structures. ChemSketch is a comprehensible molecular structure drawing tool having 20 lakhs users all over the world.

(iv) ChemWindow: It is a chemical structure drawing molecule editor published by John Wiley & Sons. It is used for 2D & 3D- visualization of structures, computation of bond lengths, angles etc. It is used by chemists for realistic process flow diagrams.

(v) Chem3D Pro: It is also a division of the ChemOffice suite. It permits drawing of chemical structures, visualization of 3D structures, studying molecular properties, like name, molecular weight etc. It runs on windows OS.

(vi) MarvinSketch: It is a desktop toolkit used to draw, alter, publish, import-export molecular structures. It also permits conversion of various chemical & graphical file formats. It is a molecular editor for making science accessible on every platform. It interprets chemistry into a digital environment & supports almost all normal chemical file formats.

(vii) BKChem: It is a free drawing program for chemists that is written in Python. It can simply create the basic structure of each element & its association with the symbols of that element. It is a cross-platform application & permits drawing for chemical compounds & molecular structures. It is used for bond-by-bond drawing, ready-to-use templates for molecular charts or graphs. It is useful for chemical researchers to represent complex diagrams by using BKChem.

(viii) JChemPaint: It is a molecule editor tool developed by Chemistry Development Kit for 2D chemical structures. It is freely accessible software written in Java & can run on the Windows, Mac OS, Linux, and UNIX. It is used to draw chemical structures & also to import -export data in plain-text formats.. Drawing & removal of various chemical bonds can be done easily by using JChemPaint. It is available free of cost. Ring templates having size between 3-8 atoms are available for use.

(ix) Jmol: It is a molecular viewer for 3D- chemical structures written in Java. It is cross-platform that runs on Windows, Mac OS and Linux/Unix systems. It can read a range of file formats, quantum chemistry program outputs & animation of multi-frame files.

(x) ChemWriter: It is the molecular editor used to design web applications & making 2D chemical structures. It is the greatest ICT tool for displaying & making chemical structures online.

(xi) XDrawChem: It is a freely accessible software program used for drawing chemical formulas, run for Mac OS and Unix. In Windows this program is called **WinDrawChem**.

(xii) ISIS/Draw: It is developed by MDL Information Systems. It contains a lot of file formats for the storing chemical information. It is primarily a 2D-drawing program but has some 3D-rotation attributes also. It has ample facilities, to symbolize relative or absolute configurations for stereochemistry and to show geometrical isomers to visualize double bonds.

(xiii) Avogadro: It is a 3D- molecular editor & visualizer, made for cross-platform and has lot of applications in computational chemistry.

These various types of softwares used by chemists for making their teaching interesting & effective and also to carry out research in chemical sciences along with their developers, licence, user interface & characteristic features are summarized in Table 1.

Table 1: Softwares used by Chemists for Teaching & Research

Software	Developer	Licence	Platforms	Features
ChemSketch	ACD Labs	Proprietary	Windows	Used to draw chemical structures of organic chemistry, organometallics & polymers. It can compute molecular weight, density, molar refractivity, etc. It is used for viewing 2D and 3D structure.

Chem3D Pro	CambridgeSoft	Proprietary	Windows	It is division of the ChemOffice suite. It permits drawing of chemical structures, visualization of 3D structures, studying molecular properties, like name, molecular weight etc.
ChemDraw	PerkinElmer	Proprietary	Windows Mac OS	It allows us to draw chemical structures & One can also use it to find out properties of chemicals & view 3D structures, etc. It generates accurate structures from the chemical names and offers precise IUPAC names for the chemical structures.
ChemWindow	John Wiley & Sons	Proprietary	Windows	It is used for 2D & 3D-visualization of structures, computation of bond lengths, angles etc. It is used by chemists for realistic process flow diagrams.
XDrawChem	Woodside Labs	GNU GPL	Windows, Unix and Mac OS	XDrawChem is used for drawing chemical formulas, run for Mac OS and Unix. In Windows this program is known as WinDrawChem .
Avagadro	Avogadro project team	GNU GPL	Windows, Unix and Mac OS	It is a 3D- molecular editor & visualizer, made for cross-platform & is extensively used in computational chemistry.
ChemDoodle	iChemLabs	Proprietary	Cross- platform	It is a drawing tool to show lone electron, pair of electron, & arrow notation of bonds. It is the single chemical drawing ICT tool which has subscript & superscript merge formatting in text to simply generate atomic notations & chemical text.
JChemPaint	Chemistry Development Kit (CDK)	GNU LGPL	Cross- platform	It is used to draw chemical structures & also to import - export data in plain-text formats.. Drawing & removal of various, chemical bonds can be made easily by using JChempaint. It is available free of cost.

ISIS/Draw	MDL Information Systems	Proprietary	Windows	It has ample facilities to show bond notations & to represent relative or absolute configurations and to recognize geometrical isomerism in double bonds.
JMol	JMol developers	Free open-source	Windows, Unix and Mac OS	It is a molecular viewer for 3D-chemical structures written in Java. It can read a range of file formats, quantum chemistry program outputs & animation of multi-frame files.
Marvin	Chemaxon	Free	Cross-platform	It is used to draw, alter, publish, import-export molecular structures. It also permits conversion of various chemical & graphical file formats. It generally supports almost all normal chemical file formats.
BKChem	Beda Kosata	GNU/Linux	Windows Mac OS	It is used for bond-by-bond drawing, ready to use templates of common rings, rotation of molecular fragments around bonds.

Besides the above discussed software tools/programs, a lot of ICT bases instruments like spectrophotometers, scanning electron microscope, flame photometer, X-Ray crystallography, ACD processors are extensively used by chemists to carry out various research in chemical sciences. Hence, integrating computer science with chemistry has lot of future prospects for chemists.

II. CONCLUSION

Information science and technology is the solution to novel research & developments in the field of chemistry. Without ICT, Chemistry cannot make its way for carrying out high-level research. Research laboratories in chemistry are constantly using lot of softwares for various research activities. These softwares are used for carrying out different chemical research activities such as molecular modeling, simulation, chemical analysis, 2d & 3d- visualization of chemical structures, searching databases for Computational chemistry and many more. IT based instruments like UV, IR, NMR, Mass Spectrometers, X-Ray Crystallography, Flame Photometry; Scanning electron microscope etc. have been developed for performing chemical research & latest developments in chemical sciences. The most remarkable success is the development of these ICT softwares for the drawing of chemical structures & storing the information through Chemical Abstract Services. ICT has paved the way for teaching & novel research in chemistry.

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