International Journal of Information Science and Computing 3(2): December, 2016: p. 91-97
DOI : 10.5958/2454-9533.2016.00011.9

Application of Information Science and Technology in Chemical Research

Bidyut Kumar Santra

Department of Chemistry, Raiganj University, Raiganj, Uttar Dinajpur, W.B., India.

Corresponding author: sntrab@gmail.com

Abstract

Information science and technology plays a very important role for the current chemical research activities. It has mainly two types of applications of which one is the computer connected advanced instruments for data collection and the other one is the software applications for modelling, molecular design, data searching and data analysis. Besides, theoretical chemists use computer programmes to calculate the structural properties of molecule such as quantum mechanics, molecular mechanics, simulation and conformational analysis. Chemical informatics used to solve chemical problems, management of data processing, information storage and searching of structures etc. Chemical Abstracts Service and ChemSpider are used as the source for chemical information. Cambridge Crystallographic Data Centre is providing all the structural information. Chemical drawing programmes such as ChemDraw, ChemSketch, WinPLT, MarvinSketch etc. are used for this purpose. Chemical informatics is widely used for molecular design and visualization and some of the programmes are Chemis3D**,** Chemissian**,** ChemWriter**,** IMol**,** Jmol, GIF Creator etc. Chemistry research work depends on the analytic computer based instruments such as NMR, IR, UV, Mass Spectroscopy etc. along with their respective chemical software such as ACD/NMR Predictors, ACD/NMR Workbook Suite, ACD/Structure Elucidator Suite, SpinWorks, Perch NMR Softwar, ACD/Spectrus Processor etc. Crystal structure determination is important for chemists and few crystallographic Software are Abscyl, Absen, Absorb Absorb-7 and Absorb-GUI, Dajust, Dash etc. The research activities are increasing in the fields of Cheminformatics.

Keywords: Chemical Information, Structural Database, Chemical Drawing, Molecular Modelling, Chemical Visualization, Chemical Software for NMR

Chemistry is a subject of understanding the atoms, molecules, electronic configuration and their properties which have wide application from chemical industries to agricultural sector. At present, the computer is just as important a tool for chemists as like test tube. Chemistry laboratories are using a wide range of software applications under different operating systems such as Windows, LINUX and Mac OSX. Information

technology is important for chemical research activities such as molecular modelling, chemical analysis, database searching etc.[1] In theoretical Chemistry, computational models and computational chemistry[2] are routinely used for prediction of molecular properties and also for testing of theory. Information technology based instruments have been developed for high-level research in Chemistry.[3] Several software have also been developed for molecular modelling and molecular mechanics.[4] Information science and technology is the key to new scientific and chemical research and developments.[5] How does information science and technology affect the research progress and why is it so important for chemical research purpose? In other words, this article intends to discover how different technologies and information are used during research in each step of the chemical research process. The purpose of this article is to highlight the importance of information science and technology in all aspect of research in Chemistry and without it Chemistry cannot move forward for high-level research work.

Discussion

Chemical Information

First of all, for research in Chemistry, primarily it is necessary to storage and retrieval of all the chemical information related to that area of research and the current research activities of articles published in various journals by using information science. From the chemical databases it is possible of searching the chemical structure, chemical nomenclature, molecular visualization, chemical reaction, spectral information, crystallographic structure, chemical patent, laboratory automation and instrumentation. Chemical Abstracts Service (CAS)[6] is a division of the American Chemical Society which is a source of chemical information. With the help of Chemical Abstracts Service over 700,000 new chemical substances are including each year in its database. It is a impotant source of chemical information that is a periodical index which provides summaries and indexes of disclosures in recently published scientific documents from approximately 8,000 journals, technical reports, dissertations, conference proceedings and new books in any of 50 languages. CAS also provides accurate chemistry content and quality-controlled by hundreds of scientists from around the world and a global team of scientists is continually adding substance information from the world's disclosed chemistry to CAS for chemical substance information. The two main databases that support the CAS are Registry and CAplus. The chemical information produced by CAS is prepared by the CAS Registry System which identifies each compound with a specific CAS registry number, index name and graphic representation of its chemical structure. Bibliographic information and abstracts for all articles in chemical journals worldwide and chemistry-related articles from all scientific journals, patents and other scientific publications are obtained from CAplus. CAS databases are available mainly from two systems which are SciFinder and STN. SciFinder is a database of chemical and bibliographic information which has a graphics interface and could search for chemical structures and reactions. SciFinder provides unlimited access from anywhere, anytime to the world. STN offers access to the world's scientific information including the authoritative chemistry content from CAS. ChemSpider is a database of chemicals and owned by the Royal Society of Chemistry. It proves fast text and structure search access to over 58 million structures from hundreds of data sources[7]

Structures deposited in CCDC (Cambridge Crystallographic Data Centre)[8] are made publically available for download at the point of publication or at consent from the depositor. It is also scientifically

enriched and included in the Cambridge Structural Database (CSD). The Cambridge Crystallographic Data Centre (CCDC) is a crystallographic organisation based in Cambridge, England. Target structure of the CSD is also freely available for support teaching, research and other activities in Chemistry. Any data can be uploaded to the CCDC for inclusion in the Cambridge Structural Database and can be viewed and retrieve structures from the Cambridge Structural Database. It has primary role in the compilation and maintenance of the Cambridge Structural Database. It also performs analysis on the database for the benefit of the scientific community and writes and distributes computer software to allow others to do the same. The Cambridge Structural Database is the world's repository for small-molecule organic and metal-organic crystal structures and has become an essential resource to chemists around the world. It contains over 800,000 entries from X-ray and neutron diffraction analyses and also made a unique database of accurate 3D structures. Each database entry is enriched with bibliographic, chemical and physical property information and continually updated with new structures each year and with improvements to existing entries.

Software for Molecular Modelling

The Information technology is helping to design more effective modelling programs over the years. Chemical drawing programs such as ISISDraw, ChemDraw, ChemSketch, WinPLT, MarvinSketch etc are used successfully for this purpose.[9] Outline of the programmes are given below.

A. ChemDraw: It is used by chemists to work quickly and effectively for drawing molecules, reactions and biological entities. It can be used to search databases, generate accurate names from structures and to predict properties and spectra. It is used as molecular editor , chemical structure to name conversion, chemical name to structure conversion, NMR spectrum simulation (^{1}H and ^{13}C), mass spectrum simulation and structure cleanup process.

B. ChemSketch: It is a molecular modeling program used to create and modify images of chemical structures. There is a software in this programme which allows molecules and molecular models to display in two and three dimensions, to understand the structure of chemical bonds and also to see the nature of the functional groups. It offers some advanced features which allow the molecules to rotate and apply colour to improve visualization. It has several templates with ions and functional groups with the possibility to add text. Using this programme it is possible to write and perform chemical equations, diagrams and chemical structures of various entities.

C. WinPLT: It is a general-purpose plotting utility for Microsoft Windows that can draw curves and surfaces presented in a variety of formats. It can generate both 2D and 3D plots of functions and sequences. It can also animate these plots using up to 23 variables and their corresponding sliders. It also has various export options such as EPS, SVG, PiCTeX, Metafile and simple copying to the Windows clipboard. It has notable ability to plot graphs such as implicit functions, slope fields, and intrinsic curves. Several standard calculus operations can be done on the functions, including generating graphs of cross-sectional solids, tracing trajectories on slope fields given an initial point, calculating line and surface integrals.

D. MarvinSketch: It is an advanced chemical editor for drawing chemical structures, queries and reactions. It is used to quickly draw molecules through basic functions on the GUI and advanced

functionalities such as sprout drawing, customisable shortcuts, abbreviated groups etc. It has a support for atom and bond properties and can be used to assign stereochemistry, charge, valence, radicals and isotopes to each atom. It has support to draw single, double, triple bonds and aromatic forms and to draw single step reactions by placing a reaction arrow in any position with pointing in any direction in relation to reaction products.

Chemical Informatics

Chemical informatics is solving chemical problems using computer. It is integrated information in which all aspects of chemical research and development can be done systematically. Chemical informatics is helping to organize and analyze scientific data and to share chemical information. It is also used to develop novel compounds, materials and processes. Chemical structures can be used as search keys in such systems and also unknown properties and spectra can be predicted with a high degree of accuracy using chemical informatics tools and techniques. Chemical informatics[10] is widely used for molecular design and visualization and some of the programmes are mentioned below.

A. Chemis3D: It is a Java Applet which makes virtual 3D molecular models within a web document. It is specially designed for open interactive molecular visualization on the internet.

B. Chemissian: This is a quantum chemistry software to analyze and visualize Gaussian outputs, plotting molecular orbital energy level diagrams, CIS/TDDFT-calculated and experimental spectra, electron density or spin maps. It can compute contributions of atoms and molecular fragments to MOs and draw them directly on the MO diagram.

C. ChemWriter: It is the 2D chemical structure maker and editor which designed for web applications. Lightweight and feature-rich, ChemWriter is the best choice for displaying and creating chemical structures on the web.

D. IMol: It is a molecular visualization application for Mac OS X operating system. The program is an important tool for chemists.

E. Jmol: It is a Java molecular viewer for three-dimensional chemical structures. It is cross-platform, running on Windows, Mac OSX and Linux/Unix systems. There are some features for reading a variety of file types, output from quantum chemistry programs, animation of multi-frame files and computed normal modes from quantum programs.

F. GIF Creator: Computer-generated GIF and PNG images of chemical structures for www pages etc. from the 2D or 3D input files.

Chemical Analysis

Advanced Chemistry research work depends on the analytic instruments such as NMR, IR, UV, Mass Spectroscopy etc. along with their respective chemical software.[11]

A. ACD/NMR Predictors : This software can work quickly and accurately to predict 1D and 2D NMR spectra, chemical shifts, and coupling constants for ^{1}H, ^{13}C, ^{15}N, ^{19}F, ^{31}P nuclei.

B. ACD/NMR Workbook Suite: It can be used for synchronize peak-picking among related spectra, powerful structure assignment tools and complete project management including databasing capabilities. It is the ultimate software tool for structure characterization by NMR.

C. ACD/Structure Elucidator Suite : This is a complete software package to help in the elucidation of unknown structures and for providing results. Experimental data can be to carry out a full elucidation resulting in a list of all possible structures that fit the data of a proposed structure and let the software predict the 1D and 2D NMR spectra and propose alternative structures.

D. SpinWorks: It is 1D and 2D NMR processing and simulation package.

E. Perch NMR Softwar: It is used for NMR processing, NMR prediction, spectral analysis, structure verification and quantification.

G. ACD/Spectrus Processor : This can be used to process and interpret all analytical data in one common interface, including LC, GC, UV, MS, IR etc. It also assists for routine structure verification and access to spectral databases.

Scanning Electron Microscope

SEM is a type of electron microscope that produces images of a sample by scanning it with a focused beam of electrons. The electrons interact with atoms in the sample and produce various signals that contain information about the sample's surface topography and composition. The SEM equipment includes a variable pressure system capable of holding wet and/or non-conductive samples with minimal preparation. The EDS has the features of a silicon drift detector (SDD) that offers superior speed and energy resolution compared with traditional SiLi detectors. The system is powered by the new TEAM software package that facilitates material characterization via methods such as spectral analysis, line scans and element mapping.[12]

Crystallographic Software

Crystal structure determination of new made molecule is very important for chemists and few crystallographic software are mentioned below.[13]

A. Abscyl: This is used for absorption correction for cylinders.

B. Absen: It is used to study and display of crystal structures, thermal ellipsoid plots, mouse based interactive editing of Shelx files with auto atom sort. RASTEP and RENDER have been added to the system which gives realistic 3D pictures from the same view as ORTEX direct from Shelx.INS files.

C. Absorb: It helps for Brennan-Cowan X-ray absorption, reflection and dispersion calculation. Calculates f' and f" based on theoretical work of Cromer and Liberman calculates Rayleigh and Compton cross-section based on McMaster.

D. Absorb-7 and Absorb-GUI: It is a program to calculate and apply absorption corrections to single-crystal X-ray intensity data. reconfigured to allow it to be called directly from external data processing programs. ABSORB-GUI has been developed to allow much easier specification of standard experiments.

F. Dajust: It is the generic name of a software package for powder diffraction formed by the core programs AJUST and SGAID. AJUST performs whole-pattern matching (cell-parameter refinement, profile fitting and intensity extraction), SGAID provides a list of the most probable space groups.

G. Dash: User-friendly graphical-user-interface-driven computer program for solving crystal structures from X-ray powder diffraction data, optimized for molecular structures.

Future possibilities

The future direction of chemical research activities are increasing in combining the fields of chemistry with computer science and information science which is the chemical informatics[14] or cheminformatics. Cheminformatics is the use of computer and informational techniques applied to a range of problems in the field of chemistry such as to improve the understanding of biological functions, development of life-saving drugs and minimize the impact of chemical environmental and data analysis for various industries like paper and pulp, dyes and such allied industries. Besides, the application of cheminformatics is in the storage, indexing and search of information relating to compounds. Several journals such as Cheminformatics (ACS), Journal of Chemical Information and Modeling (ACS), Journal of Cheminformatics (Springer) etc. are publishing research articles in this area.

Conclusion

Chemistry laboratories are continuously using several software applications for the research purpose. Information technology is very important for chemical research activities such as molecular modelling, computational chemistry, chemical analysis, database searching etc. Chemical Abstracts Service and ChemSpider are used as the source for chemical information. Cambridge Crystallographic Data Centre is providing all the structural information. Chemical drawing programs, molecular design and visualization programmes are used for the purpose research in Chemistry. Information technology based instruments have been developed for high-level chemical research work and for new scientific developments. For chemical analysis computer based instruments such as NMR, IR, UV, Mass Spectroscopy, X-Ray Crystallography, SEM etc are used. The most noteworthy achievement is the development of software for the coding and retrieval of chemical structures. This has resulted in ways of searching and associating with real information about chemistry which utilize for research in chemistry and for the chemical structures. The special techniques of chemical informatics are also used to solve complex chemical problems. Thus, research activities are gradually increasing in the fields of chemical informatics.

Acknowledgement

I am grateful to Dr. P. K. Paul, Department of Computer and Information Science, Raiganj University, for providing his valuable suggestion to complete this paper. Special thanks to Professor Dipak Chatterjee, Vice Chancellor, Seacom Skills University, for his support to this work.

References

1. P. von R. Schleyer, N. L. Allinger, T. Clark, J. Gasteiger, P. A. Kollman, H. F. Schaefer, P. R. Shreiner,

(Eds.). *Encyclopedia of Computational Chemistry*, Vol. 5, Wiley, Chichester, 1998.

2. Oscar N. Ventura and Martina Kieninger, "Computational chemistry as an analytical tool: thermochemical examples in atmospheric chemistry", *Pure & Appl. Chem*., 1998 Vol. 70, No. 12, p. 2301-2307.
3. Herman Skolnik, "The Role of Chemical Information Science in Computer-Assisted Chemical Research" *J. Chem. Inf. Comput. Sci.*, 1977, Vol. 17 (4), p 234–238.
4. Rama Rao Nadendla, "Molecular Modeling: A Powerful Tool for Drug, Design and Molecular Docking", *Resonance*, 2004, p 51-60.
5. S. P. Perone, "Computer applications in the chemistry laboratory. Survey", *Anal. Chem.*, 1971, Vol. *43* (10), p 1288–1299.
6. https://www.cas.org
7. www.chemspider.com
8. https://www.ccdc.cam.ac.uk
9. https://en.wikipedia.org/wiki/Molecule_editor
10. Johann J. Gasteiger, (Eds.), *Handbook of Chemoinformatics: From Data to Knowledge*, Vol. 4, Wiley-VCH, 2003.
11. www.acdlabs.com/resources/freeware/nmr_proc/
12. www.digitalsurf.fr/en/mntsem.html
13. www.iucr.org/resources/other-directories/software
14. Robert Glen, "Developing tools and standards in molecular informatics." *Chemical Communications,* 2002, 23, 2745-2747.