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The Application Of The Contemporary Computational Graphics In Chemistry

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***Abstract*—In recent years, the use of images, photographs, diagrams, molecular models, graphics, specialized computer programs, and other visualization aids has grown significantly in chemistry instruction. To encourage visualization skills, the use of visual aids in chemistry instruction is essential. The relationships between the macroscopic, microscopic, and theoretical aspects may be imagined by students more easily. Movies and the dynamic interaction of molecules are significant multimedia components that help to develop spatial thinking abilities. The application of educational tools with excellent visual potential may be seen in several parallel instances. From the perspective of needed outputs, connections between the practical, visual, and numerical aspects demonstrate the learning content. The newly developing communication and visualization tools, which are aided by the development of computer graphics, animations, and simulated movements of the substances, are what are driving educators' increased interest in visual literacy. This essay's goal is to examine these applications and assess them in light of how they could be used going forward in chemistry training for basic chemical understanding. The demonstration gives students the opportunity to use their own data and conclusions in addition to applying several chemical education topics.**

Keywords—chemistry, computer laboratory, education, graphics

Introduction

The new group of undergraduate students is the one we taught (Fan et al., 2015). Young people frequently utilize books as resource in their educational endeavors. The representation of three-dimensional viewpoints for the real model is one of the major issues in literature. The fundamental difficulty in understanding stereochemistry as a branch of chemistry is three-dimensional viewpoints. All chemistry courses demand a lot of experience, as well as the ability to solve many types of issues and produce environmentally friendly processes, better pharmaceuticals, and new useful materials. The computational chemistry serves as the foundation for several chemistry-related professions. When a mathematical procedure is sufficiently developed to be automated on a computer, computational chemistry is utilized (Lee et al., 2011).

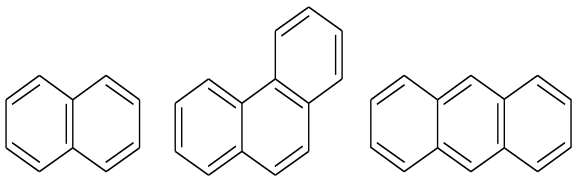
Chemical, mathematics, and computational abilities might be used to implement solutions to the chemical challenges. To help students visualize the lattice and maintain their interest, (Pekdag, Le Marèchal, 2010) employed computer graphics for the first time in chemistry when teaching about crystallography. It showed animation of the cubic crystalline structure. Giving pupils the chance to view things from a different perspective helps them to develop their abilities and deepen their comprehension of the chemical fundamentals. In order to provide meaningful chemical information based on dynamic molecular animation or to construct a dynamic display of how a piece of equipment was utilized, contemporary visuals are crucial (Tetko et al., 2005). The visualization in the chemical videos might be applied in a number of contexts, including experiment planning, lesson demonstration, and conceptual comprehension for building mental models (Pekdag, Le Marèchal, 2010). A variety of technologies, such as multimedia, contemporary computer graphics, and many chemistry software programs, should be available in the computer lab. This is crucial for helping students comprehend complex ideas like electron configuration and structural alteration as well as acquire general chemical knowledge. Modern computer graphics are used to improve structural visualization and to better comprehend stereochemistry, organic chemistry, binding bonds, and tridimensional arrangement (Jones et al., 2005). Due to the capabilities in computing graphics, it is possible to forecast a compound's reaction and calculate energy. Additionally, being

better prepared for making observations before doing the real tests aids chemists in their work.

I. COMPUTIONAL CHEMISTRY SOFTWARE

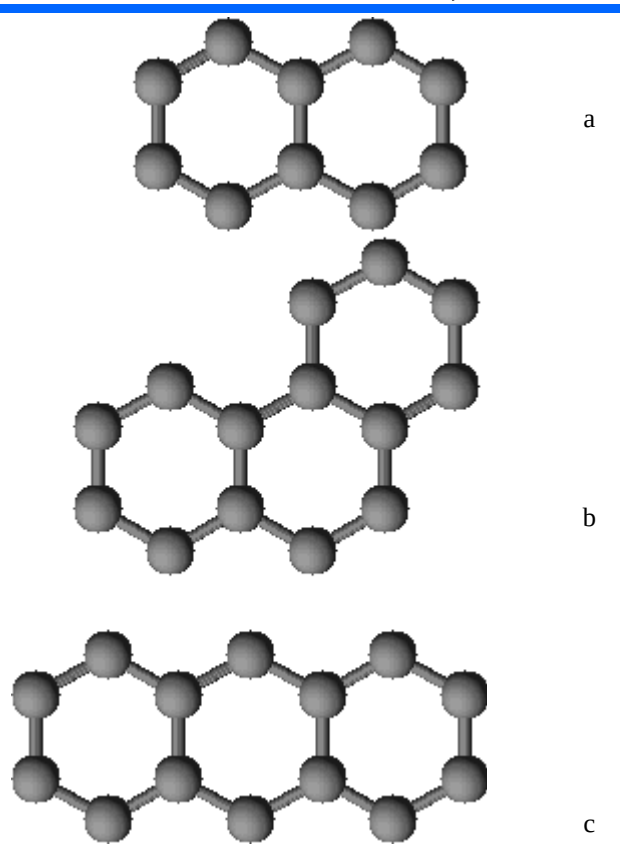
A. *Modeling structures*

Organic chemistry and biochemistry both need the capacity to depict molecules in three dimensions (He et al., 2011). Unfortunately, a lot of students have trouble resolving the structure in a variety of chemical topics since they are unable to visualize in space (Bottomley et al., 2006). The computer lab with various chemical software packages is crucial for learning the fundamentals of chemistry at a specific age. Students' ability to grasp bonds, isomerism, electrical configuration, as well as the atom arrangement in the specific molecule depends on their ability to depict structures in two or three dimensions (Nori-Sharga et al., 2005). Almost all chemical software programs, including ChemWindow, ACD/ChemSketch, and ChemDraw, are built around the modeling of chemical structures. Implementing theoretical knowledge in computers is the first step in helping students better comprehend the concepts behind the operation of the tiny world of atoms (Bottomley et al., 2006). Figure 1 shows the modeling of naphthalene (a), phenantrene (b), and anrtacene (c) in rendering with sticks (I) and sticks and balls (II). To better grasp atomic arrangements in three dimensions, this type of presentation is being used.



I

a b c



a

b

c

II

Fig. 1. Structural formulae of naphthalene (a), phenantrene (b), and anrtacene (c)

B. *Programs for quantum mechanics*

The flexibility to employ a variety of tools to address diverse chemical issues makes one software valuable as a component of a chemistry study program (Stone et al., 2009). Basic courses in theoretical organic chemistry, stereochemistry, and physical chemistry, particularly in crystallography, include quantum and classical mechanics, statistical physics, and thermodynamics. The determination of the electronic structure, geometry optimization, calculations of the electron and charge distribution, rate constants for chemical reactions, potential energy surfaces, molecular modeling with the focus on docking about the orientation of one molecule to the second, definition of transition structures, and reaction paths are just a few of the various aspects of chemistry that can be performed using modern computer graphics. *Ab initio*, semi-empirical, and molecular mechanics are the most significant numerical approaches (Jaskolski et al., 2007). There are several different types of specialist software packages that include tools for computing quantum features. The

HyperChem 7.0 software program enables the sketching and display of molecules in perfect replicas of their gas phase counterparts. Additionally, this tool may be used to do calculations for molecular mechanics, semi-empirical molecular orbitals, and ab initio (Gabriel et al., 2008). The program is made to depict the substance's structure so that certain calculations may be applied to a particular molecule. The block-diagonal (Newton-Rapson) approach is frequently used in conjunction with MM+ parameterization to optimize the drawn structures. The PM3 molecular orbital approach is frequently the foundation of semi-empirical computations. These computations' purpose is to ascertain if the experimental results may be used to quantum chemistry (Stone et al., 2009).

C. *Programs for drawing laboratory equipment*

The development of laboratory notebooks is one of the most crucial things for new researchers to do while tackling chemical issues (Fan et al., 2015). Understanding the equipment in the lab and correctly connecting it are crucial for doing various tests. There are a few components that must all be in place for the experimental portion of the analysis. Students should be aware of how effectively they depict certain pieces of equipment in their notebooks so they can accurately recreate it in the future. They must have good drawing skills and understand the value of the laboratory notebook in expanding their knowledge (Lee et al., 2011). There are several chemical applications with templates of many types of lab equipment, like ACD/ChemSketch and ChemDraw. A molecular modeling tool called Chemsketch is used to create and edit pictures of chemical structures. Understanding the structure of chemical bonds and the characteristics of functional groups is made easier by displaying molecules in two- and three-dimensional orientation. The application has sophisticated capabilities that let you rotate and color-code molecules to enhance visibility. The right flask, equipment for distillation or extraction, and the right drawing format may all be simply selected by the students. This is a fantastic chance for students to document the lab's visuals and improve their performance in chemistry experimentation (Pekdag, Le Marèchal, 2010).

The most common used laboratory equipment such as an Erlenmeyer flask (a), a funnel (b), a round-bottom flask (c), a separatory funnel (d), a volumetric flask (e), condensers: Liebig (f), Grahams (g), and Allihn (h) are presented in Fig. 2.

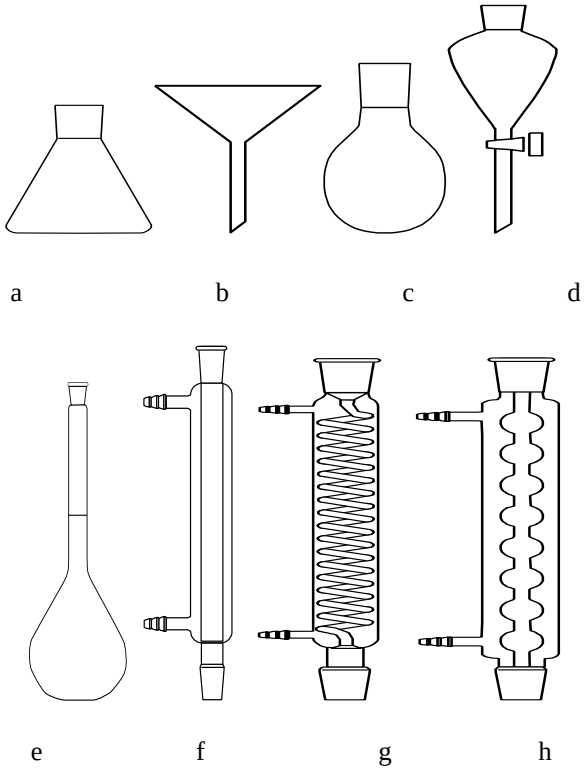


Fig. 2. Presentation of laboratory kit: Erlenmeyer flask (a), a funnel (b), a round-bottom flask (c), a separatory funnel (d), a volumetric flask (e), condensers: Liebig (f), Grahams (g), and Allihn (h)

II. CHEMISTRY EDUCATION

The responsibility of the instructor is to enhance the teaching techniques and introduce new methodological approaches. New trends in all courses, including chemistry, deal with the fact from the viewpoint of the students on how well they grasp chemistry (Wu, Shah, 2004). The difficulty with some sciences, such as chemistry, is that each stage of learning is crucial, starting with representations of equations, formulas, and structures on the one hand and connecting real-world laboratory experience to theoretical knowledge on the other. Chemistry principles are best understood via experimentation, process improvement, application of findings in other domains, and the use of less poisonous and irritating materials (Fan et al., 2015). Modern chemistry has many connections to fields like molecular biochemistry, medicine, and pharmacy.

Dealing with various challenges enables chemistry as a science to cope with unforeseen circumstances and be prepared to address issues at the molecular level. Even experienced scientists have trouble comprehending reactions and how atoms are arranged in many complicated structures, and beginners have trouble grasping the fundamental chemical ideas. Modern chemistry emphasizes the invention of novel medications, addressing the structure of substances, computations, and molecular modeling. Additionally, a lot of forensic cases, spectra data, and all contemporary laboratory apparatus are linked to computers. The representations of the laboratory data are significant topics for discussion, and the practice experience is the primary source of chemical knowledge. Both the data and the findings should be exact, accurate, and repeatable. The analysis needs to run as little as feasible and in real time (Kaushik, 2014).

A. Computers in chemistry education

Every contemporary chemistry lab is described as a location where students may put their theoretical knowledge into practice and improve their spatial and motor abilities (Kaushik, 2014). Different computer implementations are made in the lab. Some of these aid pupils with numerous computations and are utilized for mathematical calculations. In order to compare spectra, ascertain concentration, create the kinetics of the reaction, or even to draw various spectra with various instruments, other computers are components of the equipment with specialized software packages. On the other side, there are also programs that assist students in organizing their presentations and understanding molecular principles better. In chemistry education, it's crucial to define the issue before attempting to fix it. Chemical software programs are crucial to reducing computation times, visualizing molecular structures, solving structural issues, and being one of the most essential things in chemistry (Qiao et al., 2006).

B. Software packages

Numerous software programs, both free and paid for, are available and work with either Windows or Linux. The applications are useful because they are simple to install on computers and because they are relevant to a certain area of chemistry (Kaushik, 2014). The scientific field of chemistry includes a variety of subfields, including organic chemistry, stereochemistry, theoretical organic chemistry, and crystal chemistry. Drawing complicated structures, resolving spectral properties, and designing structures to safeguard reagents in actual experiments are the key components of all these chemical disciplines. All chemistry-related problems should be able to be resolved by computers. Modern ideas in chemistry are supported by computers and a particular software program that must be entered into the computer. Combining several chemistry programs makes it possible to forecast the behavior of certain substances and to portray the microscopic behavior of molecules more effectively. The application is suitable for use in chemistry instruction due to the orientation of the molecule and the utilization of information from certain fields. The major purpose of one program is to identify the target demographic of young researchers and the age of the population. It is important to understand if the programs are intended for elementary, secondary, or university students. Independent researchers have to be aware of the usual chemical program's correctness. The other thing in using modern graphics in chemistry laboratory is curricula of the program and the usefulness of some tools how well to be organized.

C. Methodological approaches in computational chemistry

The pupils anticipate complete clarity at all times. The idea of didactics is to gradually update one's broader understanding of chemistry. The fundamental idea is to go from well-known facts to unknown ones, from concrete to abstract, and from simple to harder level (Richardson and Richardson, 2002). Chemistry is one of the basic sciences, and understanding it is a valuable tool in many areas. Knowing spatial notions and how to identify structures in three-dimensional concepts is essential for understanding chemistry. The goal of contemporary computational chemistry is to discover novel connections between many domains of chemistry and science in general, as well as new techniques to enhance fundamental scientific notions (Stukowski, 2010). A subfield of chemistry known as computational chemistry produces information that supplements

experimental data on the structures, characteristics, and reactions of substances (Eller, 2006). All computations are based on ideas of symbolic computation, artificial intelligence, statistical theory, thermodynamics, and quantum and classical mechanics (Moll et al., 2005). It is nevertheless feasible to simulate the behavior without using quantum mechanics if a molecule is too large to be adequately studied using semi-empirical methods. The database utilized to parameterize a molecular mechanics approach is essential to the method's success. On the other hand, molecular dynamics enables the calculation of parameters for use in statistical mechanical treatment, such as diffusion coefficients or radial distribution functions. The accuracy in analytical chemistry is assessed using the standard deviation and a large number of similar observations. The identical action should provide exactly the same results in computational experiments. Comparing the quantity of related computations to the experimental results is the most effective technique to identify any type of inaccuracy. One of the biggest difficulties in dealing with many computations is the time commitment (Geng et al., 2016). The techniques that are employed for a certain sort of computation are crucial for reducing the length of the study. The main challenge is deciding which software will work best for your calculations. It's crucial to focus on approximation in calculations while dealing with theoretical approaches in chemistry. Gaussian and HyperChem are the two most used computer programs for computational chemistry (Leila et al., 2011). The process of exhibiting data in any kind of pictorial or graphical representation is known as data visualization. It is possible to deal with three dimensional representations or apply a colorization scheme to data using a variety of computer tools. The calculations are based on 1. the calculations of the global potential energy surface, which include equilibrium states, transition structures, and Van-der-Waals complexes. 2. Wave function, electronic charge distribution, and many other non-energetic features (such multiple moments, NMR parameters, etc.) are calculated. 3. The shape of molecules in their ground and excited states 4. Constants of rotation and vibration 5. Chemical reaction pathways and rate constants 6. Specifics of molecular collision dynamics 7. the thermodynamic characteristics. It is very beneficial for: Identifying features that are not available by experimentation 1. (2). Analysis of experimental results before beginning a computational chemistry project (lab), one must select an acceptable computational approach and the related software that fits the hardware constraints (memory, disk space, and CPU time) based on solid scientific evidence. The next step is to learn how to create an input file, execute the program, and evaluate the results using a few straightforward examples. After completing all of those procedures, the computation itself may begin (Levine et al., 2011). The strategy here is to employ a graphic user interface (GUI) that is currently in use, such as WebMO, Spartan, or GaussView, to reduce the steep learning curve of basis sets, functionals, techniques, and software. Therefore, rather of concentrating on the what to do and how to set up, the students may concentrate on understanding the chemistry and ideas. Semi-empirical techniques like PM3 and ZINDO [7] were utilized to save time. GaussView and Gaussian 09 were the programs utilized in this investigation (Bottomley et al., 2006). Compound geometries in the generated modules were enhanced using Pople's6-31G* basis set and the B3LYP functional (Stone et al., 2009). To comprehend real-world experiments and verify the predictions of theoretical models, computational models are crucial.

D. Modern graphichs in chemistry computational laboratory

There are different kinds of computational packages which are used in the chemistry laboratory. Some of them can be applied for educational purposes such as ChemDraw, ACD/ChemSketch, and ChemWindow (Kaushk, 2014, Leila et al., 2011). ChemSketch is used to design and perform chemical equations, schematics, and templates of laboratory apparatus in addition to drawing chemical structures. The ability to translate from structure to name and vice versa is one of ChemDraw's primary features. Additionally, there are several templates that may be utilized for various circumstances, such as macromolecule presentations, particular laboratory components, and stereochemistry. Contrarily, ChemWindow is a good application for sketching two-dimensional structures that can recognize stereochemistry. Bond lengths, angles, and structural comparisons with databases are also

calculated (Kaushk, 2014; Leila et al., 2011). Modern graphics have solved the issues with the continuous depiction of the lines in chemical structures and have made it possible to better see three-dimensional representations of molecules. These graphics are utilized in chemistry software programs. The ability to display the global and local features of the molecule is one of the important applications of current graphics. Modern graphics now make it possible to display animations of chemical reactions and molecular processes (Levine et al., 2011).

Modern computational graphics in chemistry

Modern computational graphics make it possible to deal with and solve issues in a variety of chemistry-related areas, such as supramolecular chemistry, enzymatic processes, the structures and dynamics of biomolecules, coarse-grained simulations, and chemo- and bioinformatics (Craig et al., 2013).

E. ***Biochemistry***

Short peptides, proteins, enzymes, and short nucleic acid fragments are studied for their structure and behavior using a broad range of cutting-edge computational approaches. The key goal is to comprehend how these biomolecules are put together in space and how the relationship between their structure and function works. To forecast the architectures of protein-small molecule complexes, we employ molecular docking. Numerous methods, including molecular mechanics-based methodologies and extremely accurate quantum chemical simulations, are used to study interactions. Understanding reaction processes is a crucial first step in the logical design of potential drug-grade enzyme inhibitors. To identify the most likely reaction pathways, a hybrid quantum mechanics/molecular mechanics technique is used. In order to investigate complex potential (free) energy surfaces, many methods are applied. They range from simple approaches like single- and double-coordinate energy scans to sophisticated ones like Car-Parrinello dynamics and free energy calculations (Herráez, 2006). Nucleases, glycotransferases, glycohydrolases, and acetylcholine esterase enzymes are studied using developed methodologies. These procedures are essential for nanomedicine, toxicity, and drug delivery. The experimental conditions are the aim of passive endocytosis of ligand-coated particles over a zero-tension, receptor-rich, and phospholipid membrane with a variety of sizes, shapes, and coverage. These models are used to identify key variables that result in various aggregated morphologies, such as ribbons, bilayers, and other oligomers. There is currently a wealth of knowledge accessible on both small molecules (such as drug-like compounds, ligands, etc.) and biomolecules (such as DNA sequence and protein structure) (Singh, 2006). Processing of this data, which might provide information highly important in pharmacy, medicine, biotechnology, and other fields, is the major objective of bioinformatics and cheminformatics study. Advanced analysis of protein 3D structures, data processing from next-generation sequencing, and the prediction of the physic-chemical characteristics of organic compounds are the main areas of study at the lab. Molecular modeling methods, which combine quantum and molecular mechanics methodologies, are used to study the structural properties of substances as well as the stability and reactivity of supramolecular systems.

Amino acids are organic compounds containing (-NH_2) and carboxyl (-COOH) functional groups, along with a side chain (R group) specific to each amino acid. The main elements which are presented in amino acids are carbon, hydrogen, oxygen, and nitrogen.

Several amino acids drawn with ACD/ChemSketch are presented in Fig. 3.

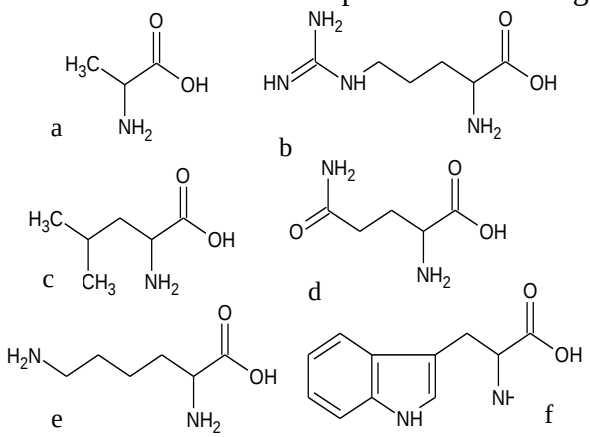


Fig. 3. Structural formulae of amino acids: alanine (a), arginine (b), leucine (c), glutamine (d), lysine (e), and tryptophan (f)

One of the main biochemistry substances are carbohydrates consisting of carbon, hydrogen, and oxygen atoms. The important sources are cereals, potatoes, fruits, and bread. In biochemistry, the simplest carbohydrates, monosaccharides are presented in three ways: the Fisher projection,

Haworth projection, and the chair conformation. The aldehyde or ketone group of a straight-chain monosaccharide reacts reversibly with a hydroxyl group on a different carbon atom to form a heterocyclic ring. Rings with five and six atoms are called furanose and pyranose forms, respectively, and exist in equilibrium with the straight-chain form.

The carbohydrates α-D glucopyranose (a), galactopyranose (b), and fructopyranose (c) are presented in Fig. 4.

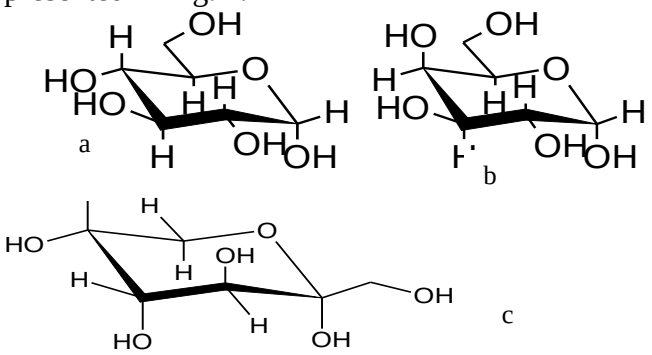


Fig. 4. Structural formulae of α-D glucopyranose (a), galactopyranose (b), and fructopyranose (c)

The class of biochemistry compounds which are vital nutrient and are required in limited amounts are called vitamins. The classification of the vitamins is based on their biology and chemistry activity and mainly grouped as vitamins dissolved in water or in oil.

Fig. 5 presents some common vitamins: A (a), B_1 (b), C (c), and D_2 (d). Vitamins B, and C are water dissoluble, while vitamins A and D is oil soluble substance.

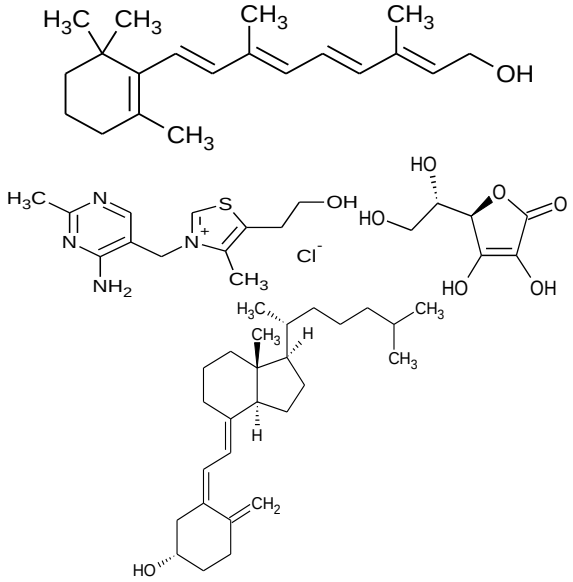


Fig. 5. Structural formulae of vitamins: A (a), B_1 (b), C (c), and D_2 (d)

Deoxyribonucleic acid (DNA) is presented in either a two-dimensional or three-dimensional form, which aids in comprehending the primary components of the molecule. The genetic instructions required for an organism's growth, development, operation, and reproduction are carried inside the molecule itself.

The main components of the DNA molecule such as base adenine (a), deoxyribonucleoside (b), deoxyribonucleotide (c), and chain form (d) are presented in Fig. 6.

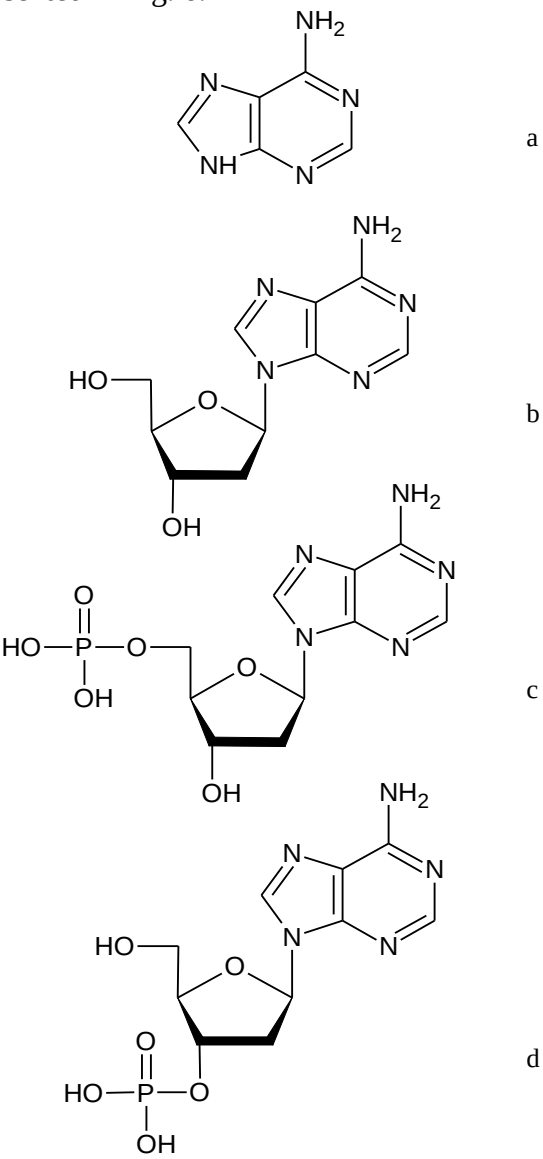
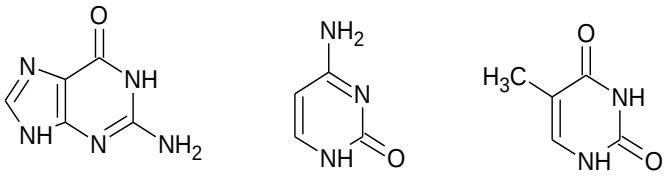


Fig. 6. Structural presentations of the DNA components: adenine (a), deoxyribonucleoside (b), deoxyribonucleotide (c), and chain form (d)

There are several bases consist in DNA structure besides adenine (Fig. 6, a), guanine (a), cytosine (b), and thymine (c) which are presented in Fig. 7.



a b c

Fig. 7. Structural formulae of guanine (a), cytosine (b), and thymine (c)

F. Organic chemistry

The model representations in organic chemistry are important due to the visualization of dots and lines describing chemical reactions and placement of electrons. The models often provide useful information in terms of explaining strange phenomena occurring in structures (Hanwell et al., 2012).

Lewis structures of ethanoic acid (a) and methane (b) are presented in Fig. 8.

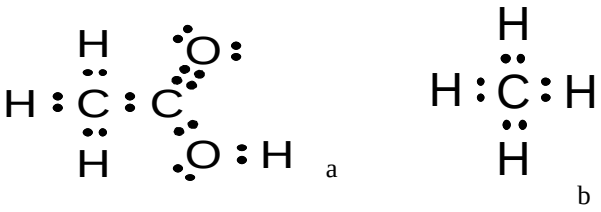


Fig. 8. Lewis structures of ethanoic acid (a) and methane (b)

The structures show the bonding between atoms of a molecule and a lone pair of electrons that may be present in the molecule. A Lewis structure can be drawn for any covalently bonded molecule and by adding lines between atoms is to be represented the shared pairs in a chemical bond.

The main bonds present in many structural substances are given in Fig. 9 with the chemistry program ChemWindow.

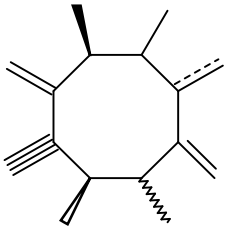


Fig. 9. Presentation of the typical chemistry bonds

As a result of their propensity to organize themselves in the most stable ways, atoms frequently complete or full their outermost electron orbits. Chemical bonds are the forces that bind groups of atoms together into molecules. Alkanes, alkenes, and alkynes often have single, double, and triple bonds. The bond is seen to be extending behind the plane of the drawing surface by the dotted line. The bond is shown to be sticking out from the drawing surface's plane by a prominent, wedged line. A solid line indicates that the bond exists in the plane of drawing surface. Unknown stereochemistry of the bond is shown by a wavy line. A dotted line denotes a partial bond, such as a hydrogen bond or a partially formed or broken link in a transition state, rather than a complete bond.

Drawing chemistry structures involves introducing functional groups which are important in understanding chemistry aspects of the certain substance (Lindahl et al., 2001).

Fig. 10 presents the structural formulae of organic compounds phenylalanine (a) diphenylphosphine (b), bicyclo[2.2.2]octane (d), bicycle[1.1.1]pentane (d).

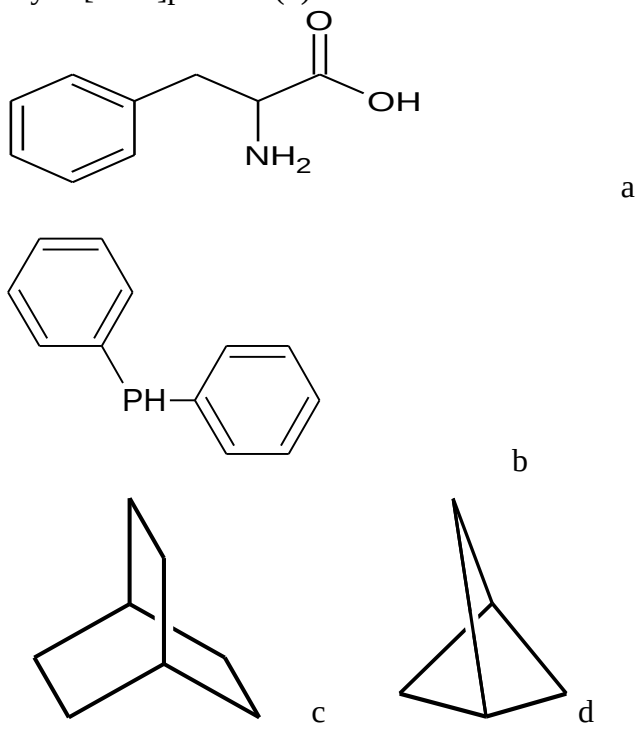


Fig 10. Structural formulae of diphenylphosphine, bicyclo[2.2.2]octane, bicycle[1.1.1]pentane

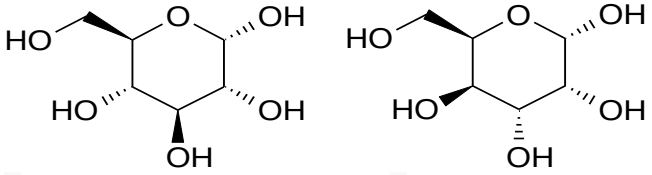
Functional groups can be drawn in chemistry programs and are important due to the addition of chemistry properties of organic compounds such as carboxylic, aldehyde, hydroxilic, and keto group.

G. ***Stereochemistry***

As a branch of chemistry, stereochemistry focuses on manipulating and studying the relative spatial arrangement of atoms that make up molecules. Stereochemistry research focuses on stereoisomers, which are compounds with the same formula but different three-dimensional atomic arrangements (Cieplak, Wisniewski, 2001).

The fundamental idea of organic chemistry is the three-dimensional orientation of molecules in space. Additionally, it contained techniques for identifying and characterizing connections between biology, organic, inorganic, physical, and supramolecular chemistry. Understanding the fundamentals of stereochemistry requires a knowledge of the chirality of the structures and optical activity. Some molecules and ions have a geometric characteristic that prevents them from superimposing on their mirror counterpart. One of the many structural characteristics that involve chirality in organic and inorganic compounds is the existence of an asymmetric carbon core. Enantiomers or optical isomers are the opposites of a chiral molecule or ion. Given that the majority of medications and biomolecules are chiral, the idea is extremely important in practice (Long et al., 2017).

Fig. 11 presents the structures of two types of sugars in their three-dimensional configuration.



α-D-Glucopyranose α-D-Gulopyranose

Fig. 11. Stereo projections of α-D-glucopyranose and α-D-gulopyranose with ACD/ChemSketch

It's common to categorize individual enantiomers as right- or left-handed. Sugars are dextrorotatory (D) while the majority of amino acids are levorotatory (L). Racemic mixtures of optically active isomers and their enantiomers have zero net rotation of plane-polarized light because each (+) form's positive rotation is perfectly balanced by the (-) form's negative rotation. For instance, just one of a drug's enantiomers frequently produces the intended physiologic effects, whereas the other enantiomer is inert, less active, or perhaps even responsible for undesirable consequences. Because of this finding, medications made up of only one enantiomer (referred to as "enantiopure") can be created to increase pharmacological efficacy and occasionally get rid of some negative effects. The ability of the molecules to rotate plane-polarized light makes them useful for chirality research. Contrarily, diastereomerism happens when two or more stereoisomers of a compound do not mirror each other and have distinct configurations at one or more (but not all) of the equivalent (related) stereocentres. Epimers are two diastereoisomers that vary from one another solely at one stereocenter. Each stereocenter generates two distinct configurations, resulting in a two-fold increasing in the number of stereoisomers. Enantiomers are pairs of stereoisomers that are mirror copies of one another and differ in all stereocenters, as opposed to stereomers, which are pairings of stereoisomers. Diastereomers of the other stereoisomers of a molecule with more than one stereocenter that are not its mirror image are also enantiomers of the compound. Diastereomers differ from enantiomers in terms of both physical characteristics and chemical reactivity (Long et al., 2017).

Students' awareness of atom configurations in space aids them in developing their comprehension of the fundamentals of stereochemistry. This course examines the circumstances in which specific molecular processes have a direct impact on the macroscopic behavior of objects. Chemistry students can benefit from computational graphics, thus it's critical to employ the most recent gear and software. Additionally, stereo specificity is a characteristic of a reaction mechanism that causes various stereoisomeric reactants to yield various stereoisomeric reaction products (Long et al., 2017).

Fig. 12 presents stereoisomer structures of ketoconazole. According to the presence of two chiral centers, there are four isomers of ketoconazole.

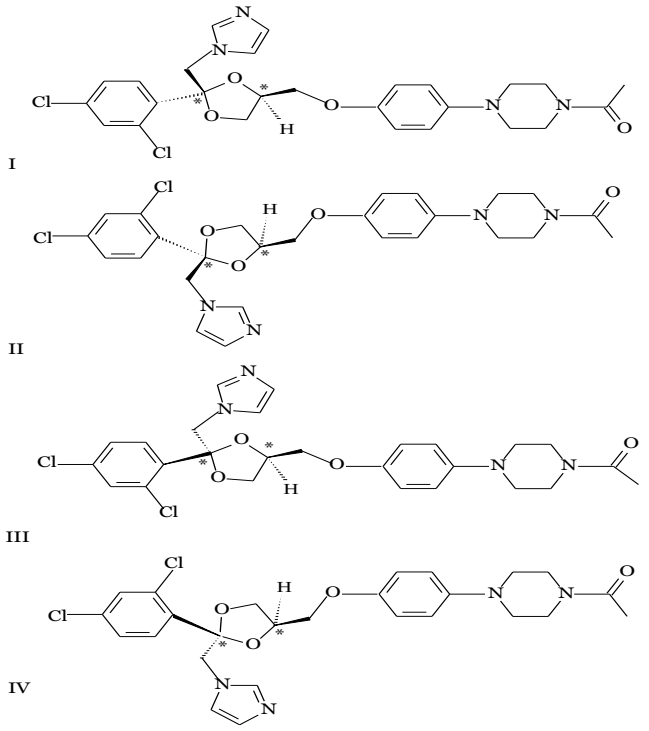


Fig. 12. Stereoisomer structures of ketoconazole

Geometric isomerism (also known as *cis/trans* isomerism or *E/Z* isomerism) is a form of stereoisomerism. In order to determine an absolute configuration, it refers to the spatial arrangement of the atoms of a chiral molecular entity and the descriptions of *R* and *S*. The approach in labeling the nomenclature is an important nomenclature system for denoting enantiomers. An enantiomer can be named by the direction in which it rotates the plane of polarized light. If it rotates the light clockwise (as seen by a viewer towards whom the light is traveling), that enantiomer is labeled (+). Its mirror-image is labeled (−). The (+) and (−) isomers have also been termed *d*- and *l*-, respectively (for *dextro*rotatory and *levo*rotatory). Naming with *d*- and *l*- is easy to confuse with D- and L-labeling and is therefore discouraged by International Union of Pure and Applied Chemistry (IUPAC).

H. ***Crystalochemistry***

The computational graphics plays important role in the crystal chemistry to understand the principles in the organization of the crystal structures. In this study it is important to notice the description of structure property in solids. The responsible of many physical properties are result in the effect of crystal structure (Vázquez et al., 2006).

In Fig. 13, the crystal lattices with ACD/ChemSketch chemical program are presented. Each crystal, lattice system and crystal family refer to one of space groups.

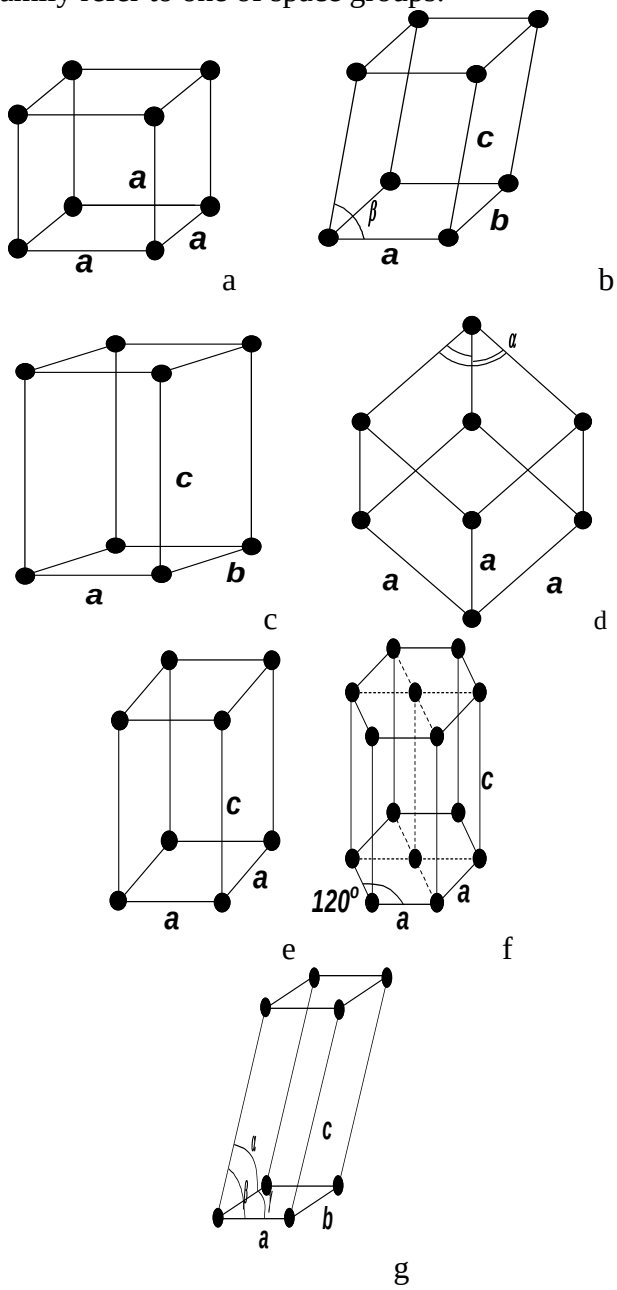


Fig. 13. Presentations of crystal lattices: cubic (a), monoclinic (b), orthorhombic (c), rhombohedral (d), tetragonal (e), hexagonal (f), triclinic (g)

The atomic details are made possible by knowing how certain chemical and physical traits relate to crystal structure and microstructure. To examine chemical bonding, phase diagrams, crystal systems, Miller indices, bond lengths and radii, theoretical density, as well as to identify key raw materials and chemistry formula names, specialized computer graphics are utilized in

chemistry labs. For interactive representations of inorganic structures, crystallographic modeling is frequently used. It might be used to modify the structure's specifics while keeping the original symmetry. Rotation of atom groupings is affected by the ability of translation. The goals of this discipline are focused on recognizing significant raw materials and minerals, along with their names and chemical formulas, defining significant materials' crystal structures, and figuring out their atomic composition. In crystallography, Miller indices serve as a notational method for planar (Bravais) lattices (Marcae et al., 2008). The organized configurations of atoms, ions, or molecules in a crystalline substance are referred to as the crystal structure. In order to create symmetrical patterns that recur in the main directions of three-dimensional space in matter, ordered structures naturally arise from the intrinsic nature of the component particles. The unit cell of the structure is the smallest collection of particles that makes up the repeating pattern in the material. The whole crystal lattice, which is constructed by repeatedly translating the unit cell along its primary axes, has a symmetry and structure that are entirely defined by the unit cell. The primary axes or edges of the unit cell's lengths and their angles make up the lattice parameters. A material's unit cell can be used to characterize the crystal structure of that substance. The unit cell is presented as a box containing one or more atoms that are grouped in three dimensions. By applying symmetry operations to the asymmetric unit, it is possible to compute the locations of the atoms inside the unit cell. The lowest feasible occupation of space within the unit cell is what is meant by an asymmetric unit, on the other hand. The idea of space groups may be used to characterize the crystal's symmetry characteristics. All symmetric configurations of particles in three-dimensional space are described by 230 space groups. Many physical features, including cleavage, electronic band structure, and optical transparency, are strongly influenced by the crystal structure and symmetry. Optical characteristics including the refractive index, absorption and reactivity, microstructural flaws, and plastic deformation all have an impact on how the crystal behaves. Chemical and physical processes take place at or close to surface atoms or molecules. The density of nodes affects these events. Depending on the density of the surface, an interface's surface tension changes. Straight grain boundaries that follow higher density planes are typical of pores. Commonly, greater density planes are parallel to the phenomena of cleavage. In plastic deformation, the dislocation glide preferentially occurs parallel to greater density planes. a disturbance caused by a dislocation traveling in a dense direction. Less deformation of the crystal lattice is required for the shift of one node in a denser direction.

The symmetry of the crystal structure defines some directions and planes. One particular axis, commonly referred to as the major axis, exists in the trigonal/hexagonal, rhombohedral, monoclinic, and tetragonal/hexagonal systems and has better rotational symmetry than the other two axes. In these crystal systems, the plane that is perpendicular to the primary axis is known as the basal plane (Daiyasu et al., 2002, Painter and Merritt, 2005).

CONCLUSION

Understanding the underlying principles of chemical issues and ensuring the long-term viability of many chemistry fields depend on the utility of contemporary graphics in computational chemistry labs. Modern graphics were created to help people comprehend the fundamental concepts at the molecular level and provided chances for visualization to advance. Students can be able to think independently better and easy to handle a variety of chemical problems as a result of the connections between chemistry and other disciplines.

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