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CONTENTS

Theoretical investigation of the isomerization of glucose into fructose within the scope of mathematical and quantum chemistry

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The isomerization of glucose into fructose (Lobry de Bruyne–van Ekenstein's rearrangment) has been investigated within the scope of mathematical chemistry (quasi-ANB matrices method and Shannon's modernized information entropy method) and quantum chemistry (the DFT method). Some peculiarities of this rearrangement are ascertained.

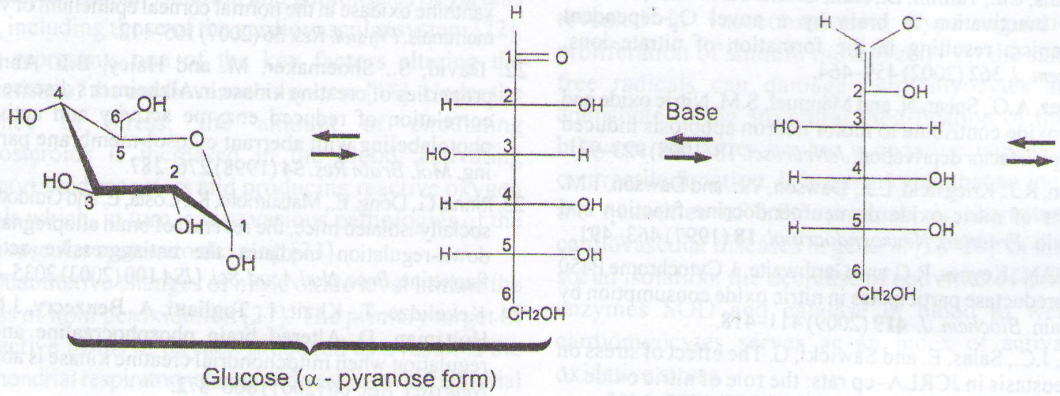
Keywords: DFT method, fructose, glucose, isomerization, quasi-ANB matrices method, Shannon's informational entropy method

1. INTRODUCTION

The complex and manifold reactions of the carbohydrates in alkali solution have fascinated organic chemists and engaged their attention for over a century. But despite extensive studies, knowledge of the interconversion and degradation reactions of carbohydrates in alkali solution is still incomplete [1, 2]. The action of alkali hydroxide solutions upon aldoses produces epimeric aldoses and ketoses; the action of concentrated alkali hydroxide solutions upon monosaccharides leads to various saccharinic acids [3].

The isomerization of glucose into fructose (Lobry de Bruyne–van Ekenstein's rearrangment) is a large-scale reaction for the production of high-fructose corn syrup and recently is under consideration as an intermediate step in a possible route from biomass to fuels and chemicals [4].

Studies using deuterated solvents have shown that bases (and enzymes) perform the aldose–ketose transformation through a mechanism involving a *cis*-1,2-enediol intermediate, whereby the bonding electron pair at C-2 moves through the carbon skeleton to C-1 (Scheme 1) [5, 6].



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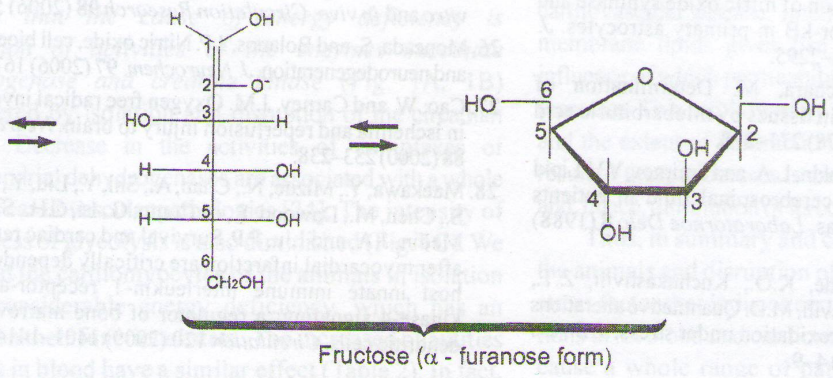

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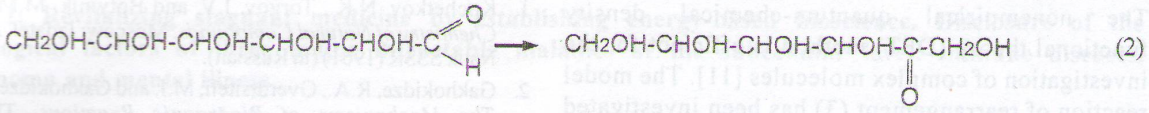
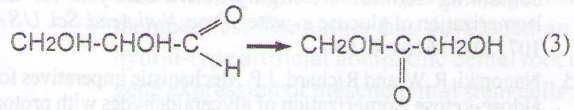


(2)

We have considered isomerization of 2,3-dihydroxypropanal into 1,3-dihydroxypropan-2-one as the model reaction:



(3)

2. MATHEMATICAL CHEMISTRY

The model reaction (3) was investigated within the scope of mathematical chemistry[1] on the basis of the quasi-ANB matrices method and Shannon's modernized informational entropy method [7–9]. The ANB matrix (atomic numbers–bonds) falls into the category of modified contiguity matrices of molecular graphs [10]. The diagonal elements of the ANB matrix are the atomic numbers of chemical elements; nondiagonal ones are the multiplicities of the chemical bonds. For an arbitrary XYV molecule the ANB matrix has the form:

$$\begin{Vmatrix} Z_x & \Delta_{xy} & \Delta_{xv} \\ \Delta_{xy} & Z_y & \Delta_{yv} \\ \Delta_{xv} & \Delta_{yv} & Z_v \end{Vmatrix} \quad (4)$$

where Z_x, Z_y and Z_v are the atomic numbers of the chemical elements X,Y and V, and Δ_{xy}, Δ_{xv} and Δ_{yv} represent the multiplicities of the chemical bonds between X and Y, X and V, and Y and V.

The quasi-ANB matrix $\left(\widetilde{\text{ANB}}\right)$ is a modernized form of the ANB matrix and can be constructed on the basis of molecular models [10]. Diagonal elements of the quasi-ANB matrix are the sums of the atomic numbers of the chemical elements that contain different structural fragments of the molecule. Nondiagonal elements represent the multiplicities of the chemical bonds between the chosen structural fragments. For the reaction (3) we can construct the simplest model reaction:

$$\text{A-B-D} \rightarrow \text{A-E-A} \quad (5)$$

where A ≡ CH_2OH, B ≡ CHOH, D ≡ CHO and E ≡ C=O.

The general representation of process (5) in the form of an $\left(\widetilde{\text{ANB}}\right)$ matrix is given as:

$$\begin{Vmatrix} Z_A & 1 & 0 \\ 1 & Z_B & 1 \\ 0 & 1 & Z_D \end{Vmatrix} \rightarrow \begin{Vmatrix} Z_A & 1 & 0 \\ 1 & Z_E & 1 \\ 0 & 1 & Z_A \end{Vmatrix} \quad (6)$$

or, in numerical form:

$$\begin{Vmatrix} 17 & 1 & 0 \\ 1 & 16 & 1 \\ 0 & 1 & 15 \end{Vmatrix} \rightarrow \begin{Vmatrix} 17 & 1 & 0 \\ 1 & 14 & 1 \\ 0 & 1 & 17 \end{Vmatrix} \quad (7)$$

Consider the expression:

$$\Delta_r = \Delta_f - \Delta_i \quad (8)$$

where Δ_i is the value of the determinant of the $\left(\widetilde{\text{ANB}}\right)$ matrix for the initial compound, Δ_f is the value of the determinant for the final compound and Δ_r is the change of the value of the determinant during the reaction. Calculations show that for the model reaction (5) $\Delta_r = -36 < 0$. If we consider the value of the determinant of the $\left(\widetilde{\text{ANB}}\right)$ matrix as a "parameter of complexity"[2] of the system, we can conclude that the complexity of the system (during the reaction) decreases.

Shannon's informational entropy can be calculated by the formula:

$$H = -\Sigma p_i \log_2 p_i \quad (9)$$

where p_i is the probability of some occurrence. This approach can be applied to chemical reactions. The expression

$$H_r = H_f - H_i \quad (10)$$

must be considered, where H_f is the informational entropy of the final system (the reaction product), H_i is that of the initial system and H_r is the change of H in consequence of the reaction.

Calculations on the basis of the model process (5) show that $H_r = -0.6598 < 0$. Thus the information content of the system (during the reaction) decreases.

[1] Mathematical chemistry is the field of modern theoretical chemistry that investigates molecules and their transformations on the basis of the mathematical categories of higher algebra (groups, graphs, matrices etc).

[2] In mathematical chemistry the parameter that shows the specific character of the chemical bond distribution in a molecule is called the "parameter of complexity" [10]. In the ANB matrices method the "parameter of complexity" is proportional to the value of the determinant of the corresponding ANB matrix.

3. QUANTUM CHEMISTRY

The nonempirical quantum-chemical density functional theory (DFT) method is efficient for the investigation of complex molecules [11]. The model reaction of rearrangement (3) has been investigated within the scope of the DFT method. The energy of the reaction ΔE = –59.0 kJ/mol. Thus, this rearrangement is exothermic. The activation energy E_A of this reaction equals 99.4 kJ/mol.

4. CONCLUSIONS

Considering the value of the determinant of the $\left(\widetilde{ANB}\right)$ matrix as a "parameter of complexity" of the chemical system, we can conclude that the complexity of the system during Lobry de Bruyne–van Ekenstein's rearrangment decreases.

Shannon's informational entropy for this process also decreases, implying that the informational content of the product is less than for initial compound. In other words, the initial compound can undergo more versatile transformations than the final compound (the initial compound is more "informative").

Quantum-chemical calculations show that this rearrangement is exothermic and has a comparatively low activation energy.

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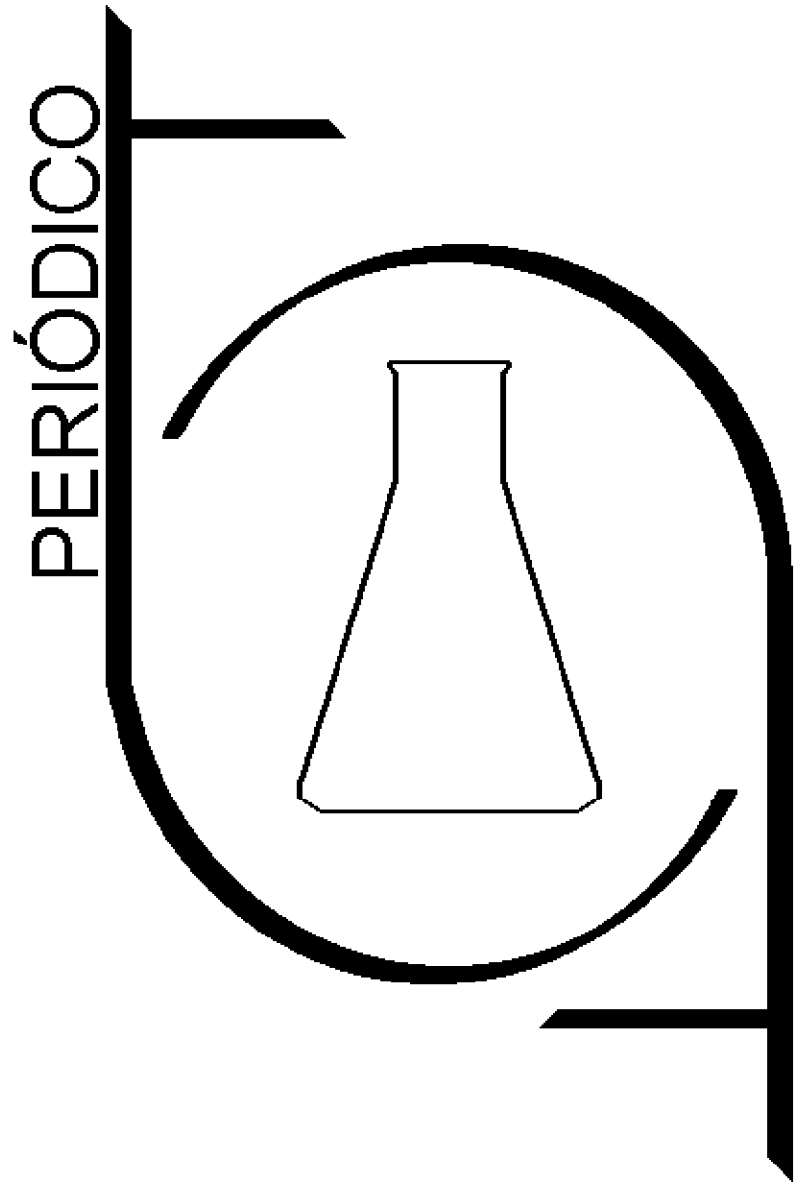

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Índice

COMO PREPARAR AULAS DE QUÍMICA MAIS FÁCEIS E COMPREENSÍVEIS (UM EXEMPLO DE PROGRAMA CONCRETO)

HOW TO MAKE LESSONS OF CHEMISTRY MORE UNDERSTENDING AND EASY (ON AN EXAMPLE OF CONCRETE PROGRAM)

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RESUMO

O presente manuscrito apresenta um curso de docência multimídia ministrado pela autora em um curso de Química escolar criado na Ilia State University. Os materiais de ensino são apresentados juntos com modelos dinâmicos visuais de processos químicos. As mudanças e informações adicionais podem ser apresentadas a qualquer momento devido à estrutura do curso. Portanto, o modelo contém os elementos de um estudo de caso. Os princípios de didática considerados são particularmente eficientes pelos programas de computação educacionais nas aulas de Química. A questão é acerca dos estágios do processo educacional durante os quais o professor pode, de maneira eficiente, usar tais programas. O artigo traz um panorama a respeito da situação de lecionar Química nos dias de hoje na Geórgia – problemas e caminhos para solucioná-los. O trabalho também apresenta os meios para integrar a Química com outras disciplinas como, por exemplo, Biologia, História e Artes.

Palavras-chaves: métodos e ferramentas de ensino, interface homem-computador, sistema multimídia, realidade virtual.

ABSTRACT

The article presents author's multi-media teaching course on school course chemistry, created in Ilia State University**.** Teaching materials are presented together with visual dynamic models of chemical processes. The changes and additional information can be introduced any time due to the structure of the course. Therefore, the model contains the elements of Case Study. Those principles of didactics are considered, realization of which are particularly efficient by educational computer programs on the lessons of chemistry. The question is about the stages of educational process, during which teacher can efficiently use such programs. In the article is overviewed the situation of teaching chemistry in Georgia nowadays- problems and the ways of solution of this problems. Is shown the ways to integration chemistry with other subjects, e.g. biology, history and arts.

Keywords: authoring tools and methods; human-computer interface; multimedia systems; virtual reality.

INTRODUCTION

Chinese sage was asked: what can we do in order that people live better. He answered, that it depends on period of time. If it is only one year, sow rice for the subsistence of people. If it is twenty years, than plant fruit trees, than people can delight with fruits. If you mean hundred years, educate the people and every problem will be solved.

It is indisputable truth. There is nobody stronger than educated man. Although, unfortunately some subject have the "privilege" to be "fearful" for school students. At the lessons of the "fearful" subjects school students come with sense of duty and they bring nothing from lessons. What is cause? They have not motivation.

In this case I mean the chemistry. Where are the roots of such attitude to chemistry? They must be searched in the process of teaching of chemistry, in the forms of its account and present to the school students. This form must have one aim – to go to the lesson of chemistry must be a little holiday and not obligation, because a pupil does not afraid this subject. To excite the curiosity of a pupil is very easy, especially to such "indocile", "capricious", "stimulant" science as chemistry. The points on the agenda are in what form present and discuss each chemical phenomenon.

So, how can we interest school students on the lessons of chemistry? Which principle of didactics is better to create merry and gripping lesson? –We accentuate on obviousness, on scientific character and availability (certainly it is our opinion and it is possible that others accentuate on different approach.

I want briefly review each principles (Uznadze, 1979; Woolfolk,2000). The *obviousness* principle is very important for the lessons in chemistry and other natural sciences. It is very difficult to imagine chemistry without experiment, which unfortunately is rarely carried out nowadays in Georgian schools; on account of the lack of laboratories, preparations or simply time (not enough hours and enormous material). Such experiments also exist, which need special rules of safety and teachers in justice try to avoid them. Different chemical mechanisms, which are very difficult to study for pupils, need special obviousness and not only simple static picture, which they can see in books or in educational posters.

Availability principle and *scientific* character are also very important. Teacher must try to interest , motivate pupils with the subject (in our case - chemistry). Teacher must be in permanent search to find interesting chemical histories and join it with them. By means of interesting chemical events and curiosities he can scientifically discuss the theme. For example, pupils may be don't know that the "reason" of "Titanic" 's going down was hydrogen bonds, because it had run into iceberg. The firmness of iceberg (ice) is caused by hydrogen bonds. The density of iceberg (ice) is less than of water and it can float on the surface of water. It will be interesting to discuss the nature of bonds, which had ruined legendary "Titanic".

End now we want to discuss the problem of the form of presentation of different questions, about what we had spoken above. One of the most effective form (among other forms) of the presentation of material to pupils is the educational computer program, which gives possibility to realize above-mentioned all three principles.

The *obviousness* principle in such programs can be realized very efficiently, because it can not be only static and planar, but dynamic and practical, decorated with different effects, among them-sound effect. It can be hyper textual with complex labyrinths, from where we can pass to another logically connected obviousness.

The modeling of the experiments in such programs can be represented by different spectrum, (among them for the experiments which need special rules of safety), if we carry them in real time in the process of lesson.

There are a lot of possibilities in this programs to realize the rest two principles.Such computer-educational programs are also called "Author's programs", because they represent the view of given author or the group of authors, which are unique and never be repeated. In spite of this, it is inadmissible that such program was turned into the electron version of any textbook.

When creating educational courses, we

must take into consideration, that they must not be transformed into electric version of textbooks (without any novelty). Such courses (they can be called "Author's courses") must reflect the view of the teacher (or the group of teachers) which created them, about the optimum teaching of the correspondent subject. The author's courses are created on the basis of the knowledge, methodical and didactic finds of the teacher (or the group of teachers).

The main aim of creating electric programs is to establish the model of the process of teaching concrete course. In this case it is important not only the specific character of the subject, but the individual habitus of the creator of the course, it is also important the establishment of the general methodic with general methods and general instruments. Such methodic contain the description of the content of the course on the basis of semantic nets, which are connected in definite limits by variable succession from the simple to the complex. They can be founded fractal-layer by layer. This layers create the skeleton and on its basis the whole process is formed. The visualization will be static, dynamic and spatial. The teacher, on each stage of the teaching, can apply to the resources of the illustration which he needs.

The content of educational material must coincide to the national educational plan, but it must be enriched by more information, by concrete examples and with corresponding commentary (Kupatadze, 2005;). Some of the topics will be teaching by axiomatic method and information will be represented in the form of graph- the unity of concrete and declaration teaching will be realized. Each topic will be connected with the knowledge of a pupil. The content will be in accordance with modern state of the sciences.

In Georgia, to overcome the "fear" to natural subjects (in this case-chemistry), to interest pupils and to create motivation is very actual.

MATERIALS AND METHODS

The application of new technologies makes it possible to show the dynamic nature of reactions. It is especially effective for illustrating processes such as organic reaction mechanisms which are traditionally illustrated with static figures. A dynamic illustration with the ability to stop and start the dynamics at any time, according to student's wishes can provide a more effective demonstration. If the mechanism consists of discrete steps, the transfer from one step to another can be performed when student wishes (by clicking through with a mouse). If the process or mechanism that is illustrated is general, then it can be linked to other processes or mechanisms. The frames of the animated fragments are connected to each other by efinite succession, though each frame is independent. Such animations should not be overloaded by text. Educational information offered in a visual context is fascinating, easily assimilated, and fixed in memory for a long time. The lesson acquires active form.

Using a computer to animate processes gives the opportunity to present vivid, eminent, and convincing illustrations about those events that are connected to various chemical transformations. The process is reflected in dynamics of the computer multimedia demonstration.

A narrative by the teacher is also attached to the process which helps create the mood of the multimedia environment, which, in turn, enhances student readiness for studying and learning the material.

We have created a computer teaching package in Inorganic and Organic chemistry http://cvl.iliauni.edu.ge/start.html which is done in Adobe Flash and includes all types of animations to connect organic chemistry with other sciences.

I want to point out one circumstance. There are many free educational computer programs in chemistry (we have seen many of these on the internet or on CD), also internet-sources, but in these sources didactic principles are realized very poorly. The aim of this program is less text and a lot more dynamic illustrations and use of different methods to stimulate a pupil's motivation. It is known fact that for teaching two main factors are obligatory: teaching school students with refined methodic and motivation for the study of presented information.

I mean to introduce such heading as: "May you will be interested", "May be you try",

"Now let us amuse our self". I mean to find a lot of chemical curious (to create animation about this curios). To make musical background to the created chemical clips. Musical backgrounds can different from each other. For example, in already created program we have "Chemical theatre" were elements go out on Shtraus' march, make the acquaintance with pupils and present very interesting information about themselves (figure 1) In other clips there is folklore (figure 2) and even though rock, why not! On the whole we shall get motivated school students and this is our aim.

According to D. Uznadze conception mood is created in simultaneous figurative conditions of two factors, with the demand of a person in the suitable environment of the given figurative conditions. If one of these factors isn't given the mood won't be created. A person will get into mood with the fulfillment of the activity of the specific situation based only on to the suitable requests (D. Uznadze. "The Psychology of Mood") [1].

Computer gives the opportunity to get vivid, eminent and convincing illustrations about those events, which are attached to this or that chemical process.

The process is reflected in dynamics on the screen of the computer together with the selected colors and according to the multimedia. The live word of the teacher is also attached to the process and so we can see two necessary factors for creating the mood, which causes student's corresponding activity-readiness for gaining and studying the material firmly. It must also be mentioned that "the mood gaining once, never looses and stays with the person, as the new readiness of actualization, in the new corresponding cases".

This program has been spreading in all Georgian schools were had been used in chemistry lessons.

RESULTS AND DISCUSSION:

The use of computer teaching programs were accompanied by the different stages:

The aim of the first stage is the forming of the student's motivation towards the learning topic (material); At this time it is important to prove the necessity of the topic, to display its important features, juxtaposition of the other subjects (connection of different subjects); The whole class will be involved in this process and it would be right if the teacher used the most interesting illustrated computer materials of the topics which would be studied.

Though at this stage the suggested visual aids mustn't contain the deep contents of the materials which would be studied as this point is the main task of the next stages.

The aim of the record stage is to discuss studying material consecutively and deeply. While teaching the new material it is necessary to use the illustrated materials.

In this case the advantage has goof computer learning programs with the help of which it is possible to keep an aye on the development of the dynamic process of the studying material and in different scales. E.g. The development of different chemical mechanisms on the micro and macro levels of course the continuation of the reactions must be put into the computer models, the performing of which is difficult or impossible for many conditions in the laboratory circumstances. On the third stage there is a process of perception of already explained material.

It is very important the scientific language of the given subject, the learning of main terms and concepts. It is also suitable (on this stage) to use the multimedia models which contain especially difficult theoretical concepts. Together with it there must be taken into consideration student's interactive relation towards the studying material in the program maintenances.

Verbal methods are used on the *fourth and the fifth stages*. In this case there also must be used computer illustrated material showed on the second stage. Which must be filled with findings of kindred subjects. The elements of this program must be discussed, debated in the lecture- room.

The last the *sixth stage* is proposed for testing the studied theme. The teacher tests not only the general contents of the material, but the ability of the pupil to join this information with

other sciences and use it (the new information) for the solution of the new problems.

Also, I must underline, that in our program chemistry is connected with history of chemistry. We have reviewed periods, when the famous scientists was discovered they openings. Some of the subjects are connected with arts. For example, before studding Structures of Molecules the pupil introduce to "Cubism", where artists use geometrical figures- square, triangle, hexagon. Picasso is the famous representative of "Cubism". The pupils will meet such kind of geometrical figures, when they study Structures of Molecules.

Or, let us speak about *water*. What is water? According to the words of Saint-Exupéry "The basis of life", which has special chemical activity. For visualization consider its action with metals. It reacts very actively with lithium and sodium, potassium burns when touching with water. From what it contains? From hydrogen and oxygen. Both have wonderful chemical biography. The nature water is a part of man's body (cellular and intercellular). It plays different vital roles and its amount depends on the man's age, on the content of fat. Dehydratation sometimes may be mortal for man.

We have spoken about hydrogen and oxygen which are the parts of water. Hydrogen was discovered in 1766 in London by Cavendish. Oxygen was discovered in 1774 by Priestly and Sheele in towns Lids-Upsala. In the block of history the situation in England and Switzerland and the situation in Georgia will be discussed- what was happening in Georgia at that time, which problems (among them-scientific) were to be solved. This lyrical digression help us to make motivation in pupils (Kask, Rawn, 2000; Freemantle, 1991).

For example, the opinion of some teachers and pupils are adduced about computer-educational program in chemistry for basic schools (the originals of forms are kept in working-room of our group).

Teachers:

"I want to ask you to create such programs for high classes". The chemistry teacher of 16th public school Kh. Nozadze;

"You must continue your work!!! To show animated experiments is very useful, especially in such schools, where they have not laboratories, but have computer." The chemistry teacher of 165th public school N. Nadiradze;

"I had adopted your uncommon idea with great pleasure. I am delighted, I like it very much! I hope you will contact with me after innovations." The chemistry teacher of 2th public school Kh. Bregadze;

"I greet this innovation, I shall always have desire to use it." The chemistry teacher of 100th public school Msvenieradze;

7th class

"When studding the classes of chemical compounds we use computer program. It is very interesting. Afterwards we ask teacher and he carried out the experiment between sulfuric acid and sugar. It was identical to what we had seen in program. It is nice, if it will continues in such a way, we shall become chemists. Such lesson is very interesting and we want more lessons."

"The teacher had taken us to the informatics room. She had explained the properties of water and we had watched chemistry program. I like "You are vineyard", bubbles of soap. At home I had done it myself".

"Show it again. We had understood it. I had remembered how to construct and represent chemical formula. The Georgian dance between Fe and S is bright. I am interested what I had seen in computer."

"I had understood well and remembered mixers, the methods of their division on components. We often can't carry out the experiments, therefore I wont to study chemistry by this program."

8th class:

"I think such lessons must be held in every classes. It is one of the way to give knowledge to the child, which is not interested in chemistry. Even though the minimum from the whole information".

"In my opinion, the CD with such themes must be in every schools, to excite the curiosity of more pupils."

"I have learned very much about chemical elements, the Periodic Table, famous chemists.

Especially interesting were video materials and clips. You see everything obviously and get pleasure. I like that the mater is written clearly and it is easy to understand. I think that the CD is perfect for all ages and professions".

"More material must be created in future, to interest pupils and pleasure them by studding chemistry".

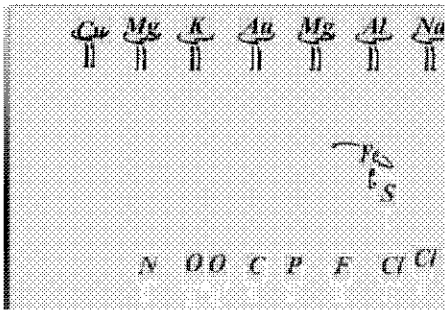

Figure 1. *The reaction with Georgian national dancing*

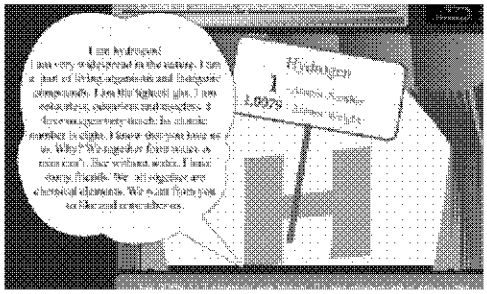

Figure 2. *Chemical Theater*

CONCLUSIONS:

With the introduction of new technology, school sstudents have become more interested in chemistry. After these lessons we receive a motivated school sstudent, who likes chemistry and is surprised, because s/he believed chemistry was a "terrible and dull" subject. Motivation does not fade. For every subsequent lesson, their motivation gets stronger. Brief extract with description of program you can see at the following link

http://www.youtube.com/watch?feature=player_embedded&v=JiXSb4Qlaag

http://www.youtube.com/watch?feature=player_embedded&v=D2RPOfn2j8g

http://www.youtube.com/watch?feature=player_embedded&v=hPxCb1g-DAY

http://www.youtube.com/watch?feature=player_embedded&v=D2RPOfn2j8g

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Giornale di Didattica e Cultura della Società Chimica Italiana

SPECIALE

CnS

LA CHIMICA NELLA SCUOLA

22nd ICCECRICE 11th

July 15- 20, 2012 ROME, Italy

PROCEEDINGS

IUPAC International Union of Pure and Applied Chemistry

European Association for Chemical and Molecular Sciences

Sapienza Università di Roma

coordinated by its DIDACTICS DIVISION Società Chimica Italiana

Dipartimento di Chimica

For the first time, the two major conferences on Chemical Education respectively by IUPAC and EUCHEMS have joined under the same roof, that of Rome, the eternal City: we were really proud for this.
Chemical Education is constantly undergoing major changes and developments which are also connected to the changing role of Chemistry in Society and the way this science is perceived; as it always more becomes a Science where social, scientific, cultural and didactic aspects interact with each other and with other emerging disciplines such as Museology, Ethics, Communication Science.
We hope that the Rome Conference will be remembered in the future for its contribution to the growth of the quality in Chemical Education. We have worked hard to assemble a high-level scientific program of which the present ACTA as special issue of CNS (Chemistry in the School) are profitable and enjoyable test.

Scientific Committee and Advisory Committe were constituted by prestigious names of Chemical Education such as Peter Childs, Morton Hoffman, Peter Mahaffy, Ilka Parchmann,Uri Zoller, Natalia Tarasova and many others

The Topics of ICCE ECRICE 2012 are reflected in the contributions here published

• *Communicating Chemistry*
- Teaching and learning Science and Chemistry
- History and Philosophy of Chemistry in teaching fundamental concepts
- Promoting the Globalization in Chemical Education

• *Didactics of Third Level Chemistry*
- Problem solving in Chemistry: Skill development and assessment
- Applications of Systemic Approach to Teaching and Learning in Chemistry
- Chemistry and Civil Society

• *ICT and Multimedia in Teaching Chemistry*
- The new educational software in Chemistry and science education and ways of improving Chemistry education with computers
- Inquiry-Based Student-Centered Instruction

• *Didactics of Second Level Chemistry*
- Pre-service training of Chemistry teachers
- In-service training of Chemistry teachers
–PCK and Chemistry teaching

• *Laboratory Work in Teaching Chemistry*

- Building active learning environments

Some conclusions can be drawn about the Conference and they well emerge from the communications present in this on line issue of CNS

- Chemical Education has gained during last years a globalized interest and content and this field has stimulated the chemical communities of the third world countries as well as those ones of the industrialized world.This enthusiasm must drive to a continuous increase in international support to the weakest situations
- Laboratory activities are fundamental for Chemical Education,but they need very careful attention to the choice of the proposed experiments
- Chemistry must absolutely not be confused with magic:it is a scientific discipline
- Electronic and informatic support are wellcome but they must remain an instrument and not the essence of the chemical education

Luigi Campanella
Conference Chairman

Information Technologies in Service of Chemistry Teaching (On an Example of concrete Program)

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Abstract
The article presents author's multi-media teaching course on school course chemistry, created in Ilia State University. Teaching materials are presented together with visual dynamic models of chemical processes. The changes and additional information can be introduced any time due to the structure of the course. Therefore, the model contains the elements of Case Study.
Those principles of didactics are considered, realization of which are particularly efficient by educational computer programs on the lessons of chemistry. The question is about the stages of educational process, during which teacher can efficiently use such programs. In the article is overviewed the situation of teaching chemistry in Georgia nowadays- problems and the ways of solution of this problems. Is shown the ways to integration chemistry with other subjects, e.g. biology, history and arts.

Author Keywords: authoring tools and methods; human-computer interface; multimedia systems; virtual reality.

Chinese sage was asked: what can we do in order that people live better. He answered, that it depends on period of time. If it is only one year, sow rice for the subsistence of people. If it is twenty years, than plant fruit trees, than people can delight with fruits. If you mean hundred years, educate the people and every problem will be solved.
It is indisputable truth. There is nobody stronger than educated man. Although, unfortunately some subject have the "privilege" to be "fearful" for children. At the lessons of the "fearful" subjects children come with sense of duty and they bring nothing from lessons. What is cause? They have not motivation.
In this case I mean the chemistry. Where are the roots of such attitude to chemistry? They must be searched in the process of teaching of chemistry, in the forms of its account and present to the children. This form must have one aim – to go to the lesson of chemistry must be a little holiday and not obligation, because a pupil does not afraid this subject. To excite the curiosity of a pupil is very easy, especially to such "indocile", "capricious", "stimulant" science as chemistry. The points on the agenda are in what form present and discuss each chemical phenomenon.
So, how can we interest pupils on the lessons of chemistry? Which principle of didactics is better to create merry and gripping lesson? –We accentuate on obviousness, on scientific character and availability (certainly it is our opinion and it is possible that others accentuate on different approach.
I want briefly review each principles [1-2].

The *obviousness* principle is very important for the lessons in chemistry and other natural sciences. It is very difficult to imagine chemistry without experiment, which unfortunately is very rarely carried out nowadays in Georgian schools; on account of the lack of laboratories, preparations or simply time (not enough hours and enormous material). Such experiments also exist, which need special rules of safety and teachers in justice try to avoid them. Different chemical mechanisms, which are very difficult to study for pupils, need special obviousness and not only simple static picture, which they can see in books or in educational posters.

Availability principle and *scientific* character are also very important. Teacher must try to interest , motivate pupils with the subject (in our case - chemistry). Teacher must be in permanent search to find in-

teresting chemical histories and join it with them. By means of interesting chemical events and curiosities he can scientifically discuss the theme. For example, pupils may be don't know that the "reason" of "Titanic" 's going down was hydrogen bonds, because it had run into iceberg. The firmness of iceberg (ice) is caused by hydrogen bonds. The density of iceberg (ice) is less than of water and it can float on the surface of water. It will be interesting to discuss the nature of bonds, which had ruined legendary "Titanic".

Or… Everybody had felt that after thunder-storm air is very fresh. Why? Yes, ozone forms in atmosphere, which is unstable and decomposes with the isolation of oxygen. What are ozone and oxygen to one another? And what is oxygen, oxygen- which we breathe?

End now we want to discuss the problem of the form of presentation of different questions, about what we had spoken above. One of the most effective form (among other forms) of the presentation of material to pupils is the educational computer program, which gives possibility to realize above-mentioned all three principles.

The *obviousness* principle in such programs can be realized very efficiently, because it can not be only static and planar, but dynamic and practical, decorated with different effects, among them-sound effect. It can be hyper textual with complex labyrinths, from where we can pass to another logically connected obviousness.
The modeling of the experiments in such programs can be represented by different spectrum, (among them for the experiments which need special rules of safety), if we carry them in real time in the process of lesson.
There are a lot of possibilities in this programs to realize the rest two principles.
Such computer-educational programs are also called "Author's programs", because they represent the view of given author or the group of authors, which are unique and never be repeated. In spite of this, it is inadmissible that such program was turned into the electron version of any textbook.
When creating educational courses, we must take into consideration, that they must not be transformed into electric version of textbooks (without any novelty). Such courses (they can be called "Author's courses") must reflect the view of the teacher (or the group of teachers) which created them, about the optimum teaching of the correspondent subject. The author's courses are created on the basis of the knowledge, methodical and didactic finds of the teacher (or the group of teachers).
The main aim of creating electric programs is to establish the model of the process of teaching concrete course. In this case it is important not only the specific character of the subject, but the individual habitus of the creator of the course, it is also important the establishment of the general methodic with general methods and general instruments. Such methodic contain the description of the content of the course on the basis of semantic nets, which are connected in definite limits by variable succession from the simple to the complex. They can be founded fractal-layer by layer. This layers create the skeleton and on its basis the whole process is formed. The visualization will be static, dynamic and spatial. The teacher, on each stage of the teaching, can apply to the resources of the illustration which he needs.
The content of educational material must coincide to the national educational plan, but it must be enriched by more information, by concrete examples and with corresponding commentary [3-4]. Some of the topics will be teaching by axiomatic method and information will be represented in the form of graph- the unity of concrete and declaration teaching will be realized. Each topic will be connected with the knowledge of a pupil. The content will be in accordance with modern state of the sciences.
Program created in Adobe "Flash" casing and it gives additional advantages, in particular it can be used in network teaching.

In Georgia, to overcome the "fear" to natural subjects (in this case-chemistry), to interest pupils and to create motivation is very actual. This problem exists, and it is proved by the fact that in 2008, on national examinations, there were only few pupils, which wanted to go in for an examinations in natural sciences. The Country can't develop without chemists, biologists and physicists.

For example, the opinion of some teachers and pupils are adduced about computer-educational program in chemistry for basic schools (the originals of forms are kept in working-room of our group).

Teachers:

"*I want to ask you to create such programs for high classes". The chemistry teacher of 16th public school Kh. Nozadze.*

"*You must continue your work!!! To show animated experiments is very useful, especially in such schools, where they have not laboratories, but have computer." The chemistry teacher of 165th public school N. Nadiradze.*

"*I had adopted your uncommon idea with great pleasure. I am delighted, I like it very much! I hope you will contact with me after innovations." The chemistry teacher of 2th public school Kh. Bregadze.*

"*I greet this innovation, I shall always have desire to use it." The chemistry teacher of 100th public school Msvenieradze.*

7 th class

"*When studding the classes of chemical compounds we use computer program. It is very interesting. Afterwards we ask teacher and he carried out the experiment between sulfuric acid and sugar. It was identical to what we had seen in program. It is nice, if it will continues in such a way, we shall become chemists. Such lesson is very interesting and we want more lessons."*

"*The teacher had taken us to the informatics room. She had explained the properties of water and we had watched chemistry program. I like "You are vineyard", bubbles of soap. At home I had done it myself."*

"*Show it again. We had understood it. I had remembered how to construct and represent chemical formula. The Georgian dance between Fe and S is bright. I am interested what I had seen in computer."*

"*I had understood well and remembered mixers, the methods of their division on components. We often can't carry out the experiments, therefore I wont to study chemistry by this program."*

8th class:

"*I think such lessons must be held in every classes. It is one of the way to give knowledge to the child, which is not interested in chemistry. Even though the minimum from the whole information".*

"*In my opinion, the CD with such themes must be in every schools, to excite the curiosity of more pupils."*

"*I have learned very much about chemical elements, the Periodic Table, famous chemists. Especially interesting were video materials and clips. You see everything obviously and get pleasure. I like that the mater is written clearly and it is easy to understand. I think that the CD is perfect for all ages and professions."*

"*More material must be created in future, to interest pupils and pleasure them by studding chemistry."*

I want to underline one circumstance. Different education foreign (free) computer programs in chemistry exist (many of them we had seen by internet or on CD), also internet-sources (for example, Wikipedia - the free encyclopedia), but in this sources above-mentioned didactic principles are realized very poorly. I can't find the full dynamic obviousness in them. In some of them it was represented, but very poorly. The aim of such program is less text and a lot of dynamic obviousness and different methodic- ways for the pupil's motivation. It is known fact that for teaching two main factors are obligatory: teaching pupils with refined methodic and motivation for the study of presented information.

I mean to introduce such heading as: “May you will be interested”, “May be you try”, “Now let us amuse our self”. I mean to find a lot of chemical curious (to create animation about this curios). To make musical background to the created chemical clips. Musical backgrounds can different from each other. For example, in already created program we have “Chemical theatre” were elements go out on Shtraus’ march, make the acquaintance with pupils and present very interesting information about themselves. In other clips there is folklore and even though rock, why not! On the whole we shall get motivated pupil and it is our aim.
It is known in psychology that a person absorbs 90% of information of the surrounding environment, from vision 9% from hearing and 1% from touching [2].
Also “teenager” gains latentively more material, he/she uses in a specific reason, though there may not be the question of remembering of material” .
To remember something latentively is depended upon the emotional mood to the material which should be remembered.
Is a student indifferent towards the subject he /she remembers it superficially.
Everything which causes emotional feeling leaves the deep track in the mind and is fixed firmly.
In this case it is very important to make students interested in studying material. Such interest may be risen by using computer learning programs and the lectures given according to it rise students ‘remembering mechanism of reachiness and mood towards the learning material.
According to D. Uznadze conception mood is created in simultaneous figurative conditions of two factors, with the demand of a person in the suitable environment of the given figurative conditions. If one of these factors isn’t given the mood won’t be created. A person will get into mood with the fulfillment of the activity of the specific situation based only on to the suitable requests (D. Uznadze. “The Psychology of Mood”) [1].
Computer gives the opportunity to get vivid, eminent and convincing illustrations about those events, which are attached to this or that chemical process.
The process is reflected in dynamics on the screen of the computer together with the selected colors and according to the multimedia.
The live word of the teacher is also attached to the process and so we can see two necessary factors for creating the mood, which causes student’s corresponding activity-readiness for gaining and studying the material firmly.
It must also be mentioned that “the mood gaining once, never looses and stays with the person, as the new readiness of actualization, in the new corresponding cases”.

The use of computer teaching programs contains the following stages of perception process [5]:

The aim of the first stage is the forming of the student’s motivation towards the learning topic (material); At this time it is important to prove the necessity of the topic, to display its important features, juxtaposition of the other subjects (connection of different subjects); The whole class will be involved in this process and it would be right if the teacher used the most interesting illustrated computer materials of the topics which would be studied.
Though at this stage the suggested visual aids mustn’t contain the deep contents of the materials which would be studied as this point is the main task of the next stages.
The aim of the record stage is to discuss studying material consecutively and deeply. While teaching the new material it is necessary to use the illustrated materials.
In this case the advantage has goof computer learning programs with the help of which it is possible to keep an aye on the development of the dynamic process of the studying material and in different scales. E.g. The development of different chemical mechanisms on the micro and macro levels of course the continuation of the reactions must be put into the computer models, the performing of which is difficult or impossible for many conditions in the laboratory circumstances.
On the third stage there is a process of perception of already explained material.
It is very important the scientific language of the given subject, the learning of main terms and concepts.

It is also suitable (on this stage) to use the multimedia models which contain especially difficult theoretical concepts. Together with it there must be taken into consideration student's interactive relation towards the studying material in the program maintenances.
Verbal methods are used on the *fourth and the fifth stages*. In this case there also must be used computer illustrated material showed on the second stage. Which must be filled with findings of kindred subjects. The elements of this program must be discussed, debated in the lecture- room.
The last the *sixth stage* is proposed for testing the studied theme. The teacher tests not only the general contents of the material, but the ability of the pupil to join this information with other sciences and use it (the new information) for the solution of the new problems.
Also, I must underline, that in our program chemistry is connected with history of chemistry. We have reviewed periods, when the famous scientists was discovered they openings. Some of the subjects are connected with arts. For example, before studding Structures of Molecules the pupil introduce to "Cubism", where artists use geometrical figures- square, triangle, hexagon. Picasso is the famous representative of "Cubism". The pupils will meet such kind of geometrical figures, when they study Structures of Molecules.
Or, let us speak about *water*. What is water? According to the words of Saint-Exupéry "The basis of life", which has special chemical activity. For visualization consider its action with metals. It reacts very actively with lithium and sodium, potassium burns when touching with water. From what it contains? From hydrogen and oxygen. Both have wonderful chemical biography. The nature water is a part of man's body (cellular and intercellular). It plays different vital roles and its amount depends on the man's age, on the content of fat. Dehydratation sometimes may be mortal for man.
We have spoken about hydrogen and oxygen which are the parts of water. Hydrogen was discovered in 1766 in London by Cavendish. Oxygen was discovered in 1774 by Priestly and Sheele in towns Lids-Upsala. In the block of history the situation in England and Switzerland and the situation in Georgia will be discussed- what was happening in Georgia at that time, which problems (among them-scientific) were to be solved.
This lyrical digression help us to make motivation in pupils.

Acknowledgements
The author would like to express her appreciation to Rustaveli Fondation for financial support to making educational program in chemistry.

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