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Virtual chemical education—novel teaching materials by means of the Internet*

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A proposal will be made to establish a global network for chemical education based on the Internet, tentatively named as Virtual Chemical Education. It is expected that such a system will innovate the style of chemical education, will solve geographical problems to some extent by creating a virtual classroom for anyone.

INTRODUCTION

The explosive development of the World Wide Web (WWW) has dramatically changed the computer network and international communications. Such recent progress of the Internet leads us to expect innovation in the traditional style of education [1]. The geographical restriction is no longer a serious problem, and teachers and students far apart from one another can communicate without difficulty.

In response to such an innovation, we would like to open and establish a new project, tentatively called Virtual Chemical Education (VCE), on a world-wide basis [2]. The concept is to use the Internet as a means of combining e-mail and multimedia to make a new educational tool.

In this VCE project, we are planning to develop a new educational tool to be constructed with the Hypertext Markup Language (HTML), Common Gateway Interface (CGI), Java and Virtual Reality Modeling Language (VRML) [3–5] techniques on the WWW. Information and software on the computer connected to the Internet can be easily operated by the WWW browser using these techniques and can be applied effectively to chemical education on a world-wide basis. Our proposal will provide a new concept in the distribution of education and distance learning of chemistry via the Internet.

We do not think that we are the first chemical educators who have thought of such a possibility. Rather, we believe that there are many others who are doing the same thing. The uniqueness of our proposal is mainly based on the fact that we are going to ask chemical educators all over the world to cooperate with IUPAC, the Committee on Teaching of Chemistry (CTC), not with us. IUPAC CTC has a long history, and has acted as the key organization for chemical education.

This proposal was made at the meeting of the CTC during the 39th IUPAC General Assembly held in Geneva, 1997 and an approval and support of CTC to this project was immediately given. Furthermore,

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some CTC members and observers showed interest in participating in this project. In line with the spirit of IUPAC, the project is open to the world. Cooperation from all over the world will be welcome.

The project will produce and develop the new style teaching and learning chemistry materials on the Internet as follows:

(i) *Hypertext teaching and learning materials*: HTML can describe the new type of textbook on the WWW.

(ii) *Multimedia teaching and learning materials*: The chemical education materials can be animated as MPEG movies and Macromedia Shockwave files.

(iii) *Interactive teaching and learning materials*: The interactive chemical education materials can be constructed by using the CGI and Java techniques.

(iv) *Virtual reality 3D graphics teaching and learning materials*: VRML presents the visualization of molecular models and molecular orbitals by using the WWW browser.

In this paper, we will first briefly report on the relationship between Internet and chemical education as well as the major forerunners in this field, and then show the whole picture of the VCE project.

INTERNET AND INFORMATION FOR CHEMISTRY TEACHING

The information provided through the Internet for chemistry teaching may be categorized as two major fields: (i) information related to chemistry and education [6] and (ii) education systems.

Internet as an information server

The first category, information related to chemistry and education, is further divided in three subcategories.

Chemical information: the results of research, including compounds data, theories, experimental techniques and results. Most information of this type, however, can be obtained from conventional media, such as books, dictionaries, or handbooks on chemistry. So the existing on-line databases in this category, although available on the Internet, such as CAS On-line, Gmelin, or Beilstein, would rarely be used by teachers. However, since an increasing amount of useful information is being accumulated on the Internet, collections of chemical information selected for teachers will become more and more available in due course.

Information related to education: including new teaching materials, new experimental materials for teacher's demonstration or students' practice, reports from research class, and tips on class teaching. These materials are devised in the classrooms, distributed, and utilized in other classrooms. Some of these products have been reported in journals on chemical education or in national or regional meetings on science education, but the number of teachers who can attend such meetings, or have access to the abstracts of papers for the meetings, is quite limited. The Internet will serve as a medium for providing collections of this kind of information on a world-wide basis, together with the searching system for the existing information.

Sub-textbooks for students' use: Formerly, this category was of limited importance in the class because the materials in this category have hitherto been used for self-learning by only limited number of students. The situation may, however, be changing in several countries since investigation-oriented curricula are introduced, aiming at identity and creativity of students, as in Japan where the 'project study' was introduced as part of the new course of study started in 1994 [7]. This kind of curriculum requires a vast amount of subtextbooks to cover the wide range of knowledge potentially required in the study by the students, which are almost impossible for one school library to prepare. The Internet may meet this kind of need, by providing on-line subtextbooks on various fields, each of which may be located in a separate server, and all of which are available from schools from which the Internet is accessible.

Internet as an education system server

What is expected for the Internet mentioned in the previous section may have been realized, although insufficiently, with the aid of conventional media such as books, and more conveniently as floppy diskettes or CD-ROMs. The second category, however, will only be achieved on the Internet. The world-wide, real-time, and two-way, features of the Internet are quite suitable for distant education in an interactive, sometimes real-time, manner.

The first subcategory, self teaching-learning systems, has been developed with the advance and personalization of computers. A number of well-programmed educational software on various subjects, earlier on text and more recently on graphic bases, have been reported. They will be more widely used if distributed on, or used through, the Internet or, more accurately, the WWW. This is because such educational systems usually work better when an appropriate instructor is involved. He/she does not have to stay at the side of the students but may be apart from them, even on the opposite side of the earth, when the systems are used through the Internet. The students will be able to engage in the system, communicating, as necessary, with the instructor by e-mail or even by chatting.

The second subcategory represents some kind of virtual classrooms, which will first be accomplished on the Internet. Well refined audio-visual systems built in or added on the WWW will enable class teaching between a teacher and students, each located apart from one another, in a real-time interactive manner, as if they were sitting together in a classroom. This kind of teaching system will be quite useful particularly in countries where school teaching is not easy due to geographical restrictions.

In addition, in the first case, and even in the second, the instructor (or teacher) might not have to be a human being; an elaborately programmed 'virtual' instructor might play his/her role, as if the students were communicating with a human instructor.

Environment for developing novel teaching materials and systems using the Internet

Standard data format. Under the present environment of the WWW, only the 'text' and 'graphic' (GIF or JPEG) materials are officially supported. The more sophisticated data such as sound, video, and animation are provided with the corresponding add-on softwares, which work under the relevant WWW browser environment, and each of which sometimes accepts only data of its own data format. This causes such a problem that there exist as many data formats as the number of add-on software. Establishment of the standard data format for each class of data will be required for the enhanced development and wide distribution of the teaching materials using such sophisticated data. The VRML [3], for instance, may be promising for the animation.

Developing tools for chemistry-teaching materials. Teaching materials are usually best developed by teachers themselves. However, they are not necessarily expert creators of the materials for the WWW. In addition, in teaching chemistry, some special materials are required, such as structural formulae or other graphic data. Animations will be quite effective in some stage. Thus, convenient tools for creating graphics, animation, or other class of data for chemistry-teaching are necessary for teachers who are not experienced in creating such data. Wide availability of such developing environment tools will contribute to the increasing number of teachers engaged in creation of novel teaching materials and systems and their enhanced development and distribution.

AN EARLIER EXAMPLE OF CHEMICAL EDUCATION ON THE INTERNET

There have already been a variety of examples of utilization of the Internet, or WWW in particular, for chemical education. Note that some of the example presented here are typical, but not necessarily representative nor advanced ones.

Internet as a communication media

Application of the Internet for global communication on chemistry and education developed with the development of the network, in particular, the WWW. In 1994, Rzepa at Imperial College started a forum called GIC (Global Instructional Chemistry), which was followed by Chemweb in 1995 [8]. He did this because he believed strongly in a global forum for creating new tools and mechanisms for helping the teaching of chemistry, and for disseminating best-practice in a rapidly changing environment. It was not associated with an explicitly funded project. He invited people to contribute examples themselves, and over the four years of operation it has received a regular, if not voluminous, set of contributions.

By now, a large number of forums and mailing lists like this are being developed in both national and international levels: some have been run under mutual cooperation while most of them appears to be working on independent basis.

Internet as a data source

The information-providing feature of the WWW servers led to its application for setting up a data server in various fields. For instance, The Macrogalleria [9] in the University of Southern Mississippi, started in 1995, provides working knowledge of polymers and related concepts to students, from secondary to graduate-level and the general public as well. It has been programmed as both informative and entertaining to both beginners and more advanced people, to the end of helping to create a more scientifically literate general public, receiving awards from numerous authorized agents on the Internet.

More recently, Rzepa *et al*. launched a virtual laboratory VChemLab [10] in 1996 for the storage, retrieval and display of information of chemical substances. This project has been developed in conjunction with another virtual reality project VChemLib [11], a 3D virtual chemistry library with a descriptive molecules database encoded in .pdb, .mol file and VRML formats—showing molecular properties and structural features. Both work under 2D and 3D graphic environments, and are being developed in conjunction with each other.

Internet as a teaching–learning system

The Internet and the WWW has the potential for extending the preceding interactive teaching-learning systems developed on the local area network (LAN) into a wide, even international, area. A variety of teaching-learning systems seem to have been developed and used in many fields and areas. The list of these together with some explanation is given in a site at Murdoch University, Australia [12].

One of those which has obtained prominent success is the WebCT developed in the Department of Computer Science at the University of British Columbia, Canada [13]. WebCT is actually a tool that facilitates the creation of WWW-based educational environments. The characteristic features of WebCT include: (i) multipurpose, not specialized to a certain subject or area, (ii) easy-to-use, designed for use by nontechnical users or noncomputer-programmers, and (iii) wide variety of tools provided, such as a conference system, student progress tracking, group project organization, student self-evaluation, and so on. More than 10 universities have introduced chemistry courses created on WebCT; the users are located not only in Canada but also in USA, UK and Australia.

THE VIRTUAL CHEMICAL EDUCATION (VCE) PROJECT

As described above, the explosive development of the WWW has changed the computer network and international communications dramatically. The HTML, CGI, Java and VRML techniques can be applied effectively to chemical education. In spite of these developments of technologies and voluntary attempts, no support has been provided by the international organizations for world-wide cooperation on chemical education via the Internet.

The proposed new project, VCE, will provide a new concept in the distributed education and distance learning of chemistry. This project is on a world-wide basis, authorized and supported by IUPAC/CTC, and will start with major collaborators in Australia, South Africa, the UK, and the USA. In addition, VCE will accept all who are engaged in an activity similar to or related to the VCE project from all over the world and are willing to collaborate under the banner of IUPAC/CTC.

The project will produce and develop the new style teaching and learning chemistry materials on the Internet as mentioned in the introduction. The project will also offer original chemical softwares for the creation of the virtual chemical education materials. For instance, it will support the following free softwares developed, or being developed, by our group. These examples will be demonstrated in detail in the next section.

Molecular modeling and graphics software. This software generates 3D molecular structures in VRML for the creation of the 3D graphics teaching and learning materials. The structures can also be drawn for electronic publishing on the Web.

Programmed study on stereochemistry. This is an application of self-learning system on the WWW, with graphical and animation functions, in the field of organic stereochemistry.

In addition, the materials created by collaborators all over the world will be offered.

The materials will be available on the WWW, at the World-wide Chemical Education Network page in the IUPAC/CTC Home Page [14]. This page will also provide an environment for communication and information exchange by the collaborators all over the world.

Molecular modeling program for creating teaching materials on the Internet

Three-dimensional (3D) graphics on the Internet have recently been developed and its new technique, VRML, presents the visualization of molecular models by using the VRML viewer. The 3D technique based on the VRML can be applied effectively in chemistry [4,5]. Our project is developing the original chemical software, MOLDA [15–18], which generates 3D molecular structures in VRML for the creation of the 3D graphics teaching and learning materials on the Internet.

Overview of MOLDA

Two types of *MOLDA* are provided by the project from our anonymous FTP server [15]. One is *MOLDA for Windows* and the other is *MOLDA Beans*. MOLDA for Windows was designed as a native program for Windows (Fig. 1). On the other hand, MOLDA Beans, which is written in Java, can work platform-independently if the Java virtual machine has been installed (Fig. 2–4). This means that MOLDA can run not only on the well-known platforms such as Windows, Macintosh and UNIX, but also on new platforms which will appear in the future.

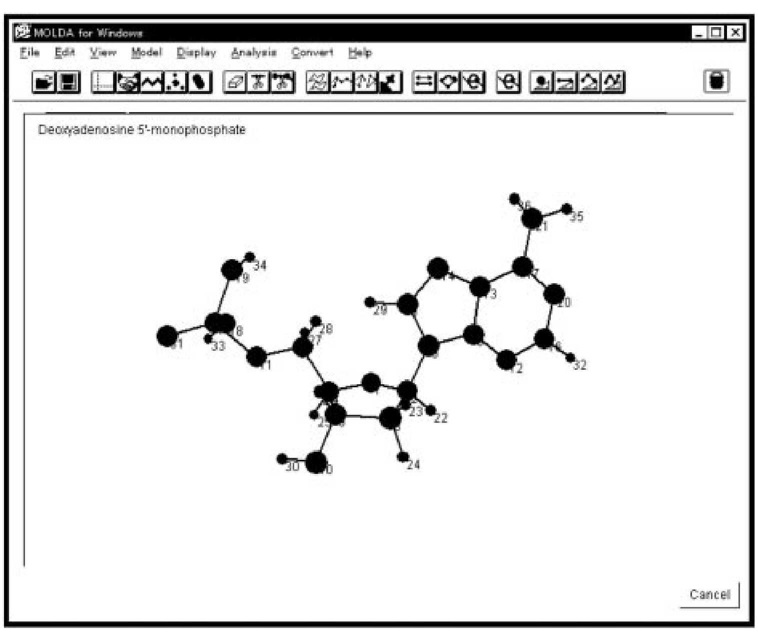

Fig. 1 MOLDA for Windows.

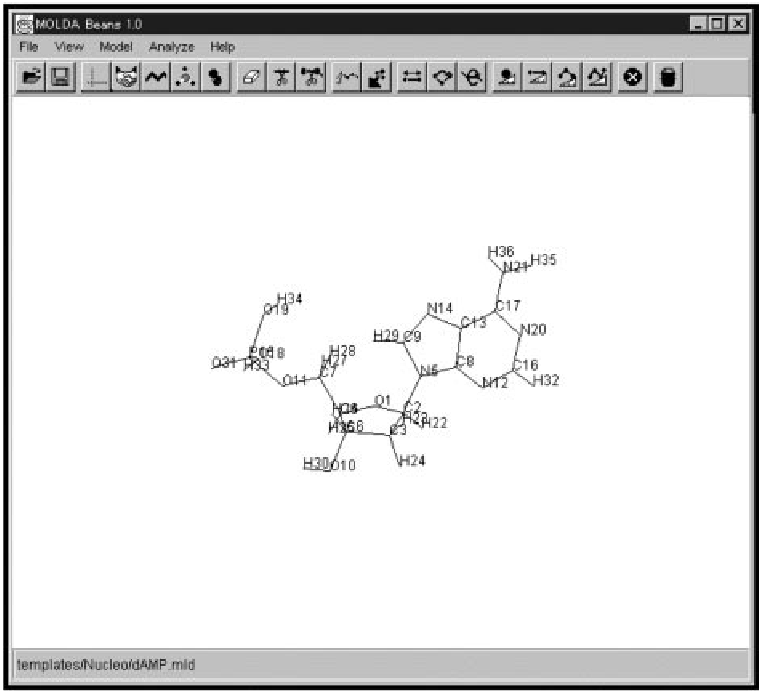

Fig. 2 MOLDA Beans on Windows.

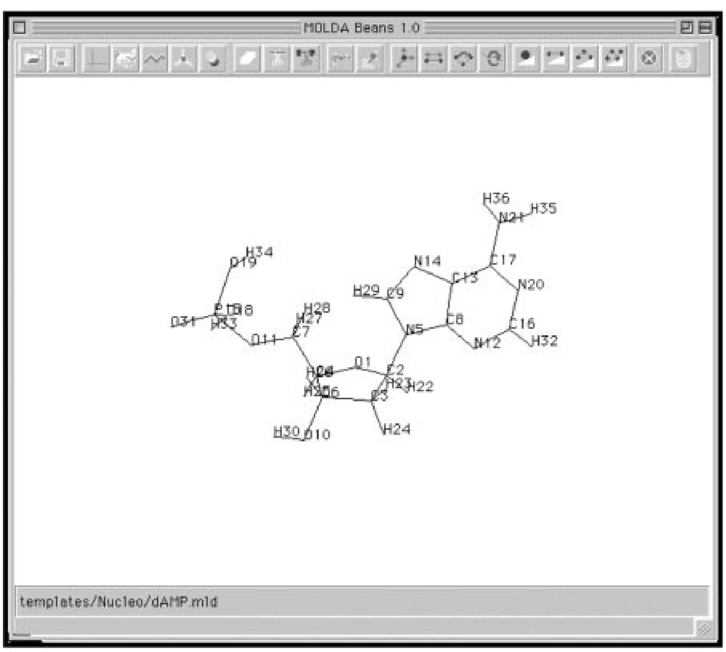

Fig. 3 MOLDA Beans on MacOS.

Features of molecular modeling

MOLDA is a molecular-model building program and has the following features:

1 Molecular file formats are MOLDA, XMol [19], Chem3D [20] and Protein Data Bank [21].

2 Some fundamental organic and biological molecules (amino acids, nucleotides and sugars) can be used as template molecules.

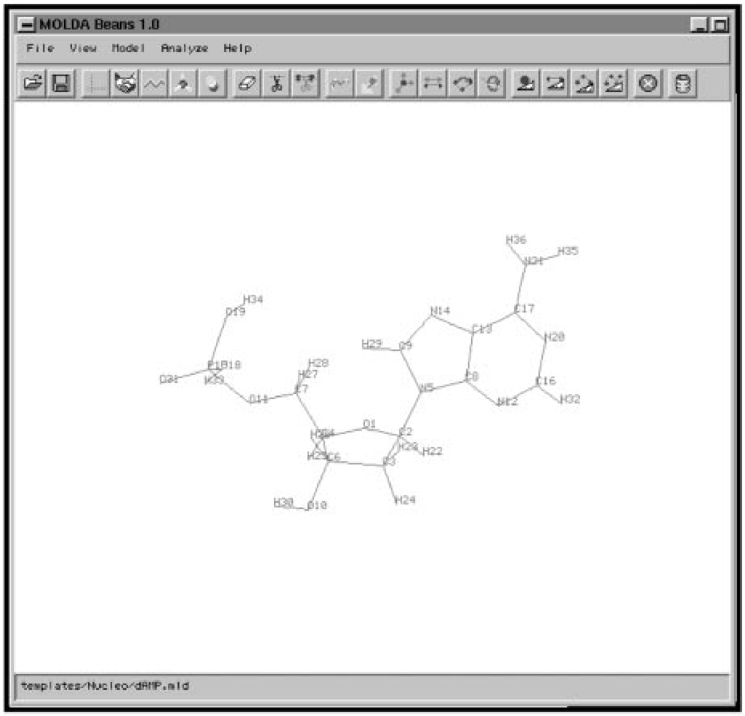

Fig. 4 MOLDA Beans on Linux.

3 MOLDA also provides the organic molecular structure database and the search engine for obtaining molecular coordinates which you are interested in.

4 Cartesian coordinates of atoms, atomic numbers, and atom connection lists are input from a keyboard.

5 Structural parameters (bond lengths, bond angles and dihedral angles) can be changed by dragging a mouse.

6 The all-*trans* conformation of *n*-alkane can be generated in a one-step operation.

7 Hydrogen atoms are automatically added when the carbon skeleton is constructed.

8 A specified atom may be replaced by another atom.

9 Any molecule made by MOLDA can be connected with each other in several modes (a specified spatial arrangement, a substitution, a ring fusion, a bridged ring-connection, and a spiro ring-connection) by mouse operation. New substituent can be registered by users.

10 A symmetry operation may be done by inputting the symbol Cn, m, i or Sn.

11 MOLDA can make input data for molecular mechanics (MM2 [22]), semiempirical MO (MOPAC6 [23]) and *ab initio* MO calculations (Gaussian94 [24]), and read output geometries obtained by MM2, MOPAC6 and Gaussian94. Vibrational spectrum and vibrational modes obtained by MOPAC6 and Gaussian94 can be also visualized.

Features of molecular graphics

After creating molecular models by using MOLDA, 3D molecular structures in VRML format can be generated. These molecular structures can be viewed in 3D using a VRML viewer (such as Netscape Navigator with Cosmo Player) and demonstrated on the WWW. At present, Dreiding-sticks (Fig. 5), ball-and-stick models (Fig. 6) and space-filling spheres (Fig. 7) are available. The molecular models written in VRML can be easily operated by the VRML viewer not only by local users but also by remote users, who can use terminal computers connected to the Internet. Moreover, the molecular models can be viewed

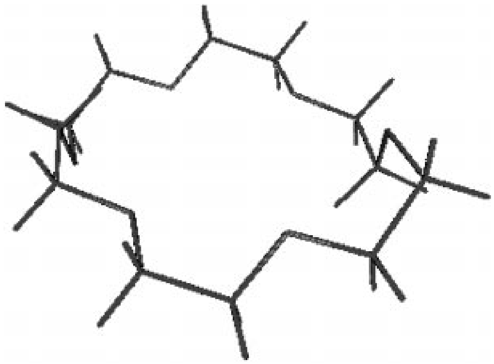

Fig. 5 A Dreiding-stick model of 18-crown-6.

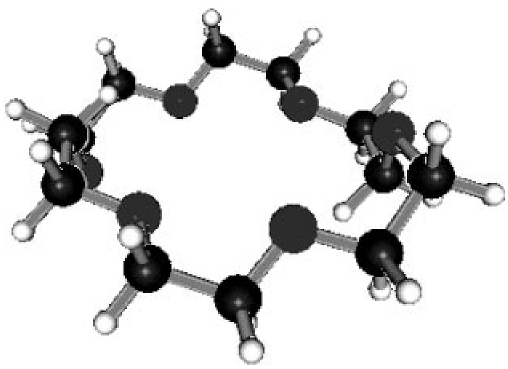

Fig. 6 A ball-and-stick model of 18-crown-6.

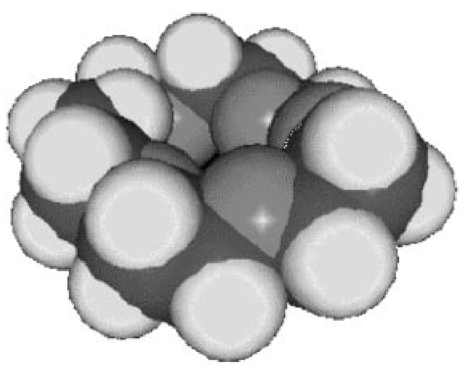

Fig. 7 A space-filling model of 18-crown-6.

platform-independently; in other words, they can be displayed on the DOS/V, Macintosh and UNIX machines. By the use of MOLDA, reliable molecular structures can be readily visualized on every platform. It may be utilized as a versatile tool in chemical education on the Internet.

Programmed study on stereochemistry

Although the programmed study is a conventional system for self-learning, it may be, with the aid of computers, designed as a pseudo-interactive learning system; depending on the answer by the students to a given question, the system will lead them to the next question or take them back to the review explanation relevant to the question. The questions and review explanations may be made up both on text and graphic bases. The system can even be designed to be interactive if it is developed to run on the Internet.

As a primary attempt to develop a programmed learning system used over the Internet, we selected a curriculum for an important field of organic chemistry, namely stereochemistry [25]. The 3D graphic and animating function (VRML) of the WWW will first enable us to illustrate the three-dimensional and dynamic feature of the materials of stereochemistry as realistically as possible. This project is now in progress and a prototype version is available now.

World-wide chemical education network—collaborating environment

What the Internet can provide is not limited to the environment for mutual distribution of completed teaching materials and systems and the media for distant education. It can also serve as the media for exchanging the systems on the way of development and for exchanging information among creators and users on the problems faced during their activity, on the global basis.

The VCE project is fundamentally based on international collaboration: in addition to the major members located in Australia, South Africa, UK and USA as well as in Japan, there will be numerous coworkers all over the world who are engaged in an activity similar to this project. In order for this kind of collaboration to work effectively, a certain environment will be required under which communication and information exchange is smoothly achieved.

This kind of environment is now established on the WWW, with the support of IUPAC/CTC. In the World-wide Chemical Education Network menu of the IUPAC CTC Home Page [14], the corner for Virtual Chemical Education Project is launched [2]. We hope that, via this corner, all the materials and information on the VCE project will be accessible which are available on the Internet—software with anonymous FTP and information and education systems with the WWW—so that everyone can have easy access to every product.

We hope that the efforts of numerous people living in various countries and working in various kind of fields in chemical education will be joined together in this project under the banner of IUPAC/CTC to contribute to the development of chemistry and its education.

CONCLUSION

We believe that the reader now fully understand our intention. We believe now that education at school is important but not almighty. There are many children who have a geographical problem; there are many students who feel that the pace of lectures are rather too rapid. On the other hand, there must be many bright students who are not necessarily satisfied with classroom lectures. For all these, Virtual Chemical Education can be a solution; not a complete solution, but a good solution, anyway.

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