

Research on Chemical Reaction Simulation Platform Based on Animation Model

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With the continuous development of computer technology and the popularity of network technology, virtual reality technology has also been rapidly developed. As an important branch of virtual reality technology, the simulation experiment is gradually applied in various fields according to its excellent three-dimensional expression and interaction characteristics, and has become an important part of computer assisted instruction, arousing widespread concern. The cognitive learning theory, media theory and constructivist learning theory are taken as the guidance to establish a set of simulation system about organic chemistry micro teaching, so that students can get rid of the limitation of time and space to explore the microscopic world movement law. The simulation experiment of the bromine electrophilic addition reaction mechanism is developed by using the virtual reality technology based on X3D standard development, simulating the whole process of the reaction mechanism. Through the development of the simulation experiment, the general modeling method and development process based on of X3D standard are mainly described, and the interactive mechanism and interaction of X3D standard are analyzed. With the further improvement of network bandwidth, the simulation experiment based on X3D standard not only simulates the abstract concepts and principal in teaching field by using its unique encoding and the interaction mechanism, but also can transmit conveniently on the internet. The virtual simulation technology based on Web becomes the future development direction. With the rapidly development and popularization of virtual reality technology, it will bring profound and extensive influence to the society and education field.

1. Introduction

The purpose of application of media technology in the teaching process is not to simply solve the expression of the teaching information, but to integrate a variety of information resources into an organic system ultimately. This system not only has the certain network and digital, but also have a certain intelligence and interaction function, playing teaching function of the teaching environment. The computer can even be use to replace the work part of teachers, and help teachers to impart knowledge and skills to the students, and provide services for students' learning through the interaction between student and computer. The media theory provides a constructive guidance for the research and provides the beneficial guarantee for the design of the interactive function of the virtual simulation experiment. The multimedia and computer network, especially the popularity of Internet network, provide a good condition for the development of learning environment which can embody the theory of constructivism. According to the constructivism learning theory, students can communicate with teacher or learning partners in real time and non real time by BBS, chat room module provided by Sakai course management platform. Combined with the advantages of network learning platform and the virtual simulation experiment developed by virtual reality technology, students can observe the chemical mechanism whenever and wherever through the expression of the three dimensional visual response, which not only can promote the learning effect but also stimulate interest in learning, and it is beneficial for students to extend knowledge.

2. Establishment of objects in the scene

2.1 Establishment of objects in the sub-scene

According to the analysis of the experimental data, the simulation of the $+Br_2$ (bromine water) electrophilic addition reaction mechanism involves the structural model of the Br_2 and the structural model of the ethylene hybrid orbital. According to the requirements of the previous chapter, we develop the virtual scene of sp^2 and sp^3 , SP hybrid orbit before the virtual simulation scene of the mechanism. The related sub scenes also include the electron transition sub scene formed by sp^2 and sp^3 hybrid orbitals.

2.1.1 Modeling of sp^2 hybrid orbitals

The modern theory of covalent bond think that the covalent bond is formed by overlapping of the atomic orbital where the bonding electrons exists (Michalski et al., 2016). S orbits is symmetrical around the spherical atomic nucleus, P orbit is symmetric dumbbell which takes the straight line through the nucleus as the symmetry axis. Three P orbits (in X axis, Y axis and Z axis) have the same energy, and their symmetry axes are perpendicular to each other. The sp^2 hybrid orbital model of carbon atom contains three hybridized p orbitals, and their symmetry axes are in the same plane, the angle between each other is 120° . One is not involved in the hybrid p orbit which is vertical with the plane of the axis of the three hybrid orbitals.

Firstly, the P trajectory model is established. Since the P orbit is symmetrical and involves the operation of the interactive part after modeling, only one half of the P orbit is established as the development unit. The 3DS MAX 2011 editing software is opened for modeling of the 3DS MAX custom unified cm. The specific modeling process is as follows: in the new scene is established in 3DS MAX, and the modeling is completed by opening the GridPoints in options and opening the command window.

The built track model is derived, the virtual scene file format is .Wrl after derived by 3D MAX. Because the coding ways of VRML and X3D encoding are different, and the whole module is developed by using the X3D standard, hence the X3D Editor 3.2 development tools is needed for the twice conversion, namely: the .Wrl file is transformed into .X3d file, and the converted file is named p.x3d.

Secondly, the established .X3d file will be cited and used by X3D's `<Inline>` inline nodes and `<Transform>` nodes in X3D Editor editing software to form the final P trajectory model.

Then sp^2 hybrid orbital model will be established. In the design of X3D program, when making X3D source program, the X3D source program is too long and too big because of the complex of the nodes' modeling, causing too much inconvenience for programming and debugging. Therefore, the `<Inline>` inline nodes are introduced in X3D standard, which make a large X3D source program be split into several small programs, making the frame of the whole program more structured and modular. After the introduction of the inline node to the X3D editing environment, and then the `<Transform>` node displacement, scaling and other attributes are used to modify the prototype.

The final sp^2 hybrid orbital model simulation screenshot is as follows:

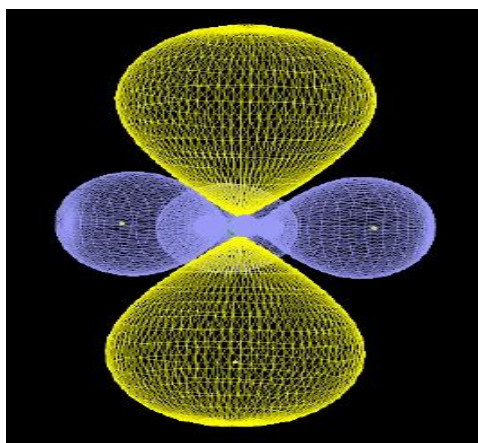


Figure 1: Sp^2 hybrid orbital

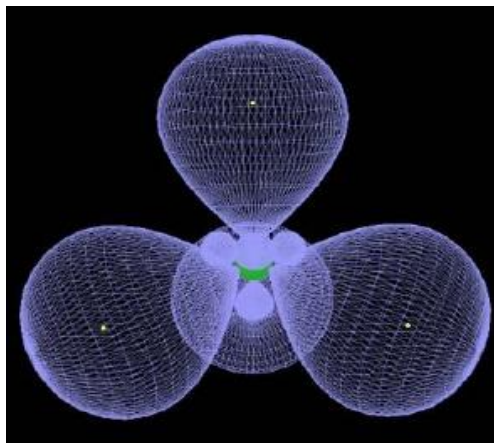


Figure 2: Sp^3 hybrid orbital

2.2 Main scene modeling

According to the script description, the pathway model of Br atom and H (hydrogen atom) can use the standard geometric sphere model as the prototype, and can be modeled directly in X3D Editor editing

environment; the molecular structure of ethylene is relatively complex, including two sp^2 hybrid orbital model and 4 H (hydrogen atom) model.

The specific modeling process is as follows:

First, the H atom and Br atom model is created according to the description of the experimental script. H atom and Br atom three-dimensional model is relatively simple, which can be directly coded by using the <Shape> sub node in the X3D document.

Second, the ethylene molecular structure is established. According to the sp^2 track in previous section, the <Transform> nodes in the main scene are used to complete the combination to form a CZH4 (ethylene) molecules.

The completed CZH4 molecular structure screenshot is as below:

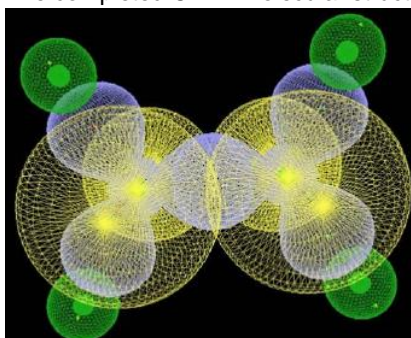


Figure 3: CZH4 molecular structure screenshot

The main scene screenshot of bromine electrophilic addition reaction mechanism is as follows:

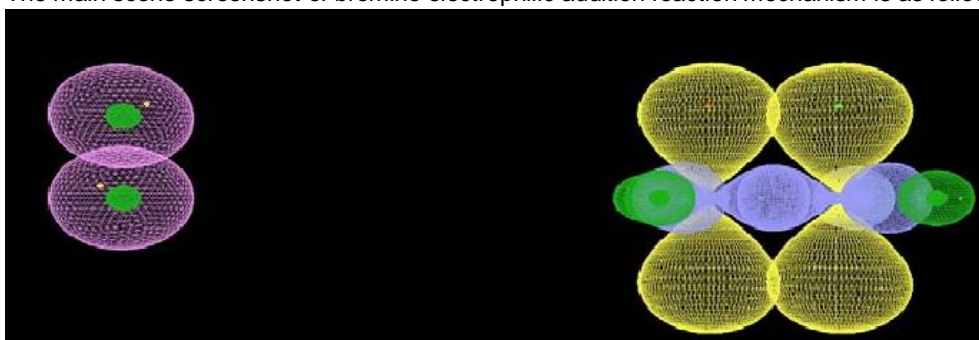


Figure 4: Scene screenshot of bromine electrophilic addition reaction

3. Realization of the interactive functions

3.1 Realization of the interactive functions in the main scene

The interactive implementation of the main scene is relatively complex. It is necessary to fully consider the structure of the scene and the details of each animation before setting the interaction. In the simulation scenario of the electrophilic addition reaction mechanism of Br_2 , the interaction parts are mainly the interaction between the scene object elements and the interaction between the user and the scene. The interaction between the user and the scene can be realized by the button function. The interaction in the scene includes both simple and complex interaction. As mentioned earlier, the simple interaction is achieved by relying on a variety of interpolation nodes as well as trigger nodes provided by X3D (Supalo et al., 2016), and the complex interaction depends on the new feature SAI interactive mechanism of X3D to achieve. The reaction mechanism is described as follows: nonpolar bromine molecule is polarized into dipolar molecules due to the influence of the ethylene π electronic or polar conditions and polarization. The addition reaction is divided into two steps: the first step: Br^+ with the positive charge in Br_2 will attack ethylene molecule to make the π bond between carbons weak, and the π bond between bromine also will be weak, generating a Br^- negative ion. Second step: the Br^- attacks carbon positive ions to form the addition of products.

According to the description of the reaction mechanism, the interaction between the user and the scene is realized by adding the trigger node. After the user clicks the start button, the simulation animation starts until the first step of the reaction is completed, when the step is completed, the user clicks the Br atom to start the

second step of the simulation until the animation is over. The scene will also provide an interactive button, and the entire reaction mechanism be observed in the new pop-up window when it is clicked. The following is a description of the interactive animation in the scene:

When the user clicks on the trigger, the Br_2 molecule begins to approach the ethylene molecule. In the process of approaching, the trajectory of the Br_2 molecule is irregular (Guo et al., 2016). When the Br_2 moves above the ethylene molecule, the electronic in Br_2 transfers from a Br atom to another atom, and the Br atom which is lack of electronic will combine with the π bond to form a three three-membered ring, the electrons in sp^2 orbitals will do no regular exercise in the three membered ring. The user clicks the separated Br ion, the Br with electronic will attack the below carbon ions, when the Br ion contact with carbon ions, the three membered ring occurs fracture again and electronic transfers again. The sp^2 hybrid orbital began to change into the orbit of sp^3 (Randall et al., 2016). In the end, the two Br atoms and ethylene will form the addition product. In order to display the functional groups in the adduct, we also designed the function of methyl rotation.

The new X3D standard is used to develop scene animation, which is in line with the modular programming features of modern software development. After careful analysis of the characteristics of the interactive animation, the simulation of the first step is divided into 3 modules: Br_2 attack, the movement of electrons in the scene, the transfer of electrons in the Br_2 molecule (Mehta et al., 2016). In the process of development, the three modules is corresponding to three time triggers, respectively, expressed as `clockjg\clockclz\clockclzzyi`. The three triggers are triggered by the same button. The second step simulation is divided into four modules: the attack of Br_2 , the deflection of P orbit, the change of sp_2 orbit and the rotation of methyl group. The four modules corresponds to four time triggers, which are represented as `clockBr2jg\clockppz-r\clocksp2bh\clockjjxz` (Michalski et al., 2017).

In the X3D standard, a number of Interpolator nodes are used to control the animation, which are designed for linear key frame animation. A set of key values are used in the domain fields of these nodes, and each key value corresponds to a state. The browser generates a continuous animation based on these states. According to the different type, the interpolator nodes are divided into: color interpolator, coordinate interpolator, normal interpolator, orientation interpolator, position interpolator interpolator and scalarInterpolator.

According to the test script, in the simulation process of the first step, the interpolators used include position interpolator, orientation interpolator and scalar interpolator, which control the position, orientation and internal electronic transparency of the bromine water molecules. The interpolator nodes are controlled by the same time trigger.

In the design of the simulation in the second steps, when the user clicks on the bromide ion, Br ion coordinate position can be set by position interpolator node, which will stay below a p track; then the position interpolator is used again to set the upper P and Br ion (Han X., 2016) in its orbit to make the position to have deflection, and the three membered ring will fracture; then the orientation interpolator, scalar interpolation and position interpolator will be used to make P track deflecting, and at the same time, its size and location are changed, and the transparency of electron below the p orbital has also changed from the original transparency to the opacity. The hybridized orbital of sp^2 transformed into sp_a hybridization; finally, the methyl at both ends will be set by using orientation interpolator to make it rotate along the X axis.

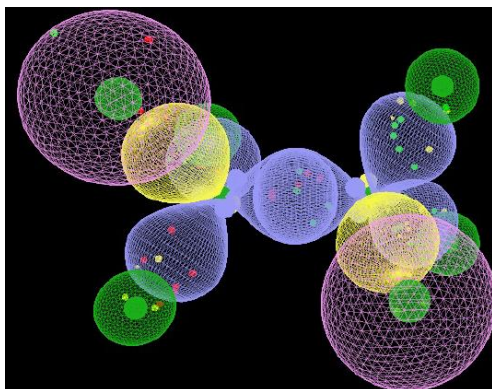


Figure 5: Scene screenshot at the end of the second phase

At this point, the module function divided before has been achieved. At this time, a few time triggers just set should be connected, in order to achieve continuous animation effect. A Javascript function (Smeal et al., 2017) will be set up according to the each time trigger cycle to control the convergence between the various

modules. The purpose of this function is to automatically trigger the next time trigger after the user clicks the start button for 10 seconds to start the animation in the second stage. Script source code is as follows:

```
<Script DEF="time1">
  <field name="touchTime" accessType="inputOnly" type="SFTIME"/>
  <field name="startTime" accessType="outputOnly" type="SFTIME"/>
  <![CDATA [avascript:
    function touchTime(timevalue)
      startTime=timevalue+10;
    ]]>
</Script>
```

The route that links to this node are as follows:

```
<ROUTE fromNode="qcmn" fromField="touchTime" toNode="time1"
toField="touchTime"/>
<ROUTE fromNode="time1" fromField="startTime" toNode="clockdzyi"
toField="startTime"/>
```

X3D provides a Anchor node, and the purpose is to link another animation or a valid network address in a three-dimensional scene. It has the hyperlinks function. When the user clicks on the entire simulation button in the three-dimensional scene in, it will pop up another three-dimensional scene. Examples of Anchor nodes are as follows:

```
<Anchor url="Br2 adds .x3d" parameter="target=_ blank">
  <Transform DEF="seven" translation="21-13.5 0">
    <Shape>
      <Appearance>
        <Material diffuseColor="0 1 0" shininess=" 1.0"/>
      </Appearance>
      <Text string="watching the whole simulation" solid="true">
        <FontStyle horizontal="true" size=" 1.0" style="true"/>
      </Text>
    </Shape>
  </Transform>
</Anchor>
```

At this point, the interactive function of the entire main scene has been developed.

3.2 Realization of the function of "HBr (hydrogen bromide) electrophilic addition reaction mechanism"

The reaction mechanism of HBr is similar to that of the electrophilic addition reaction mechanism of Br. In the simulation of the scene, most of the scene features are consistent with the previous one. The difference is that one of the a Br atom in the Br molecule is replaced by a H atom. The range of the electron motion in the H atom also changes accordingly. Here is a screenshot of the key steps:

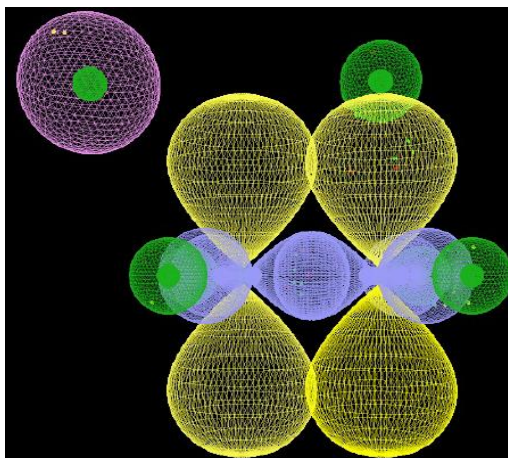


Figure 6: H ion attacks sp^2 orbital

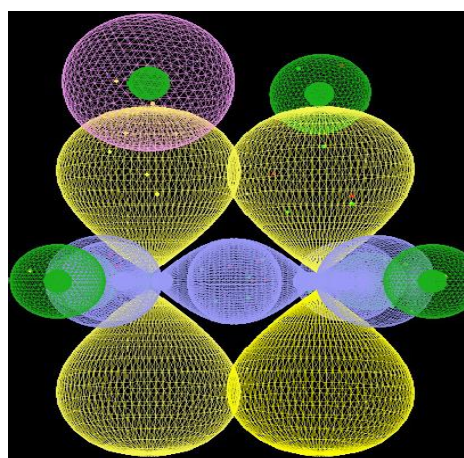


Figure 7: Br- attacks sp^2 orbital

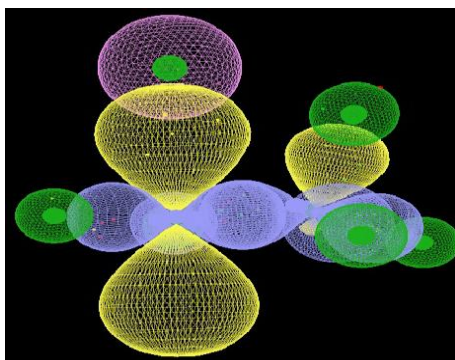


Figure 8: Sp^2 transforms into sp^3 with H

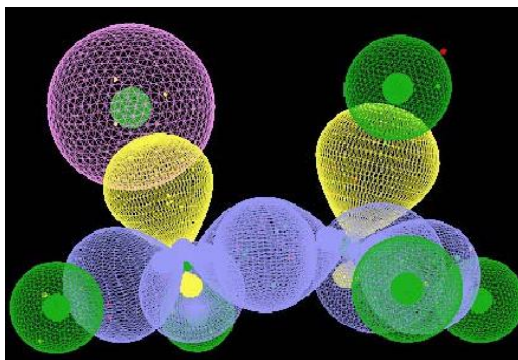


Figure 9 Sp^2 transforms into sp^3 with Br

So far, the entire virtual scene is finished.

3.3 Chapter summary

This chapter introduces the general method of scene modeling and the development process of scene animation. The interaction mechanism and interaction method of X3D are analyzed. The mechanism of electrophilic addition reaction of bromine water is taken as a case, the interactive design and implementation of the virtual scene are described in detail, and a more detailed development steps and the corresponding source are given.

4. Conclusions

This paper discusses the application of virtual reality technology based on X3D in the teaching of organic chemistry, especially in the simulation of molecular level in microscopic field. Through the analysis of the current research status of virtual reality technology in the teaching of organic chemistry, the Flash or 3DsMAX software are used in most researches on the micro level to make the video to show the molecular structure and its changes during the reaction. The simulation in this way is either lack of three-dimensional representation or lack of interactivity. In this subject, the simulation animation based on X3D standard can more intuitively express related teaching content in the micro structure. Students not only can observe various molecules but also can observe the transformation of different molecular electronic in the reaction process. It play a very good effect for the understanding of the concept and nature of reaction mechanism.

Reference

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