

## Rearrangements in Organic Chemistry: The Peircean semiotic modes and virtual representation on Chemistry Teaching

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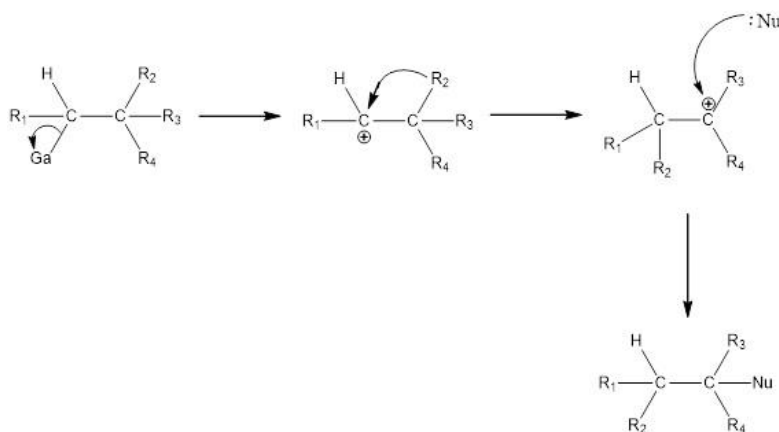
**Abstract:** In this paper, we report the construction of an application to aid in the understanding of an important content studied in organic chemistry disciplines, in higher education. We carried out a connection between the cognitive sciences and Peirce's semiotics, as a way to make inferences about the processes of appropriation of students, especially about the representations on the symbolic level that can be directly related to daily events. The application explains the potential of a virtual resource for learning rearrangement reactions, which implies in a complex degree of abstraction. The use of visuals, contributes greatly to the description of the procedures and semiotic artifacts that are used in the virtual plane to explain the occurrence of important chemical reactions, of the great importance in learning of many students in courses offered in higher education.

**Keywords:** chemistry education, learning, rearrangements, semiotics.

### I. Introduction

Cognitive sciences and Peircean semiotics may be used for understanding the difficulties faced by college students, particularly in organic chemistry disciplines. The similarities between these sciences allow the comprehension of which relationships can be established between the exposure of content, the thematic of organic chemistry and the perception and conceptualization of the student, from complex symbolic systems that allow the conceptual elaboration.

According to the theoretical assumptions listed for the preparation of this paper, the use of representations in Organic Chemistry, assumes a highly structured language that should be encoded by the student. During learning, the student prepares a series of symbolic systems involving the participation of images, schemes and diagrams. Particularly, in the context of organic chemistry various graphical structures are used to aid the student on the understanding of the chemical reactions considering the electron transfer (Scheme 1).



**Scheme 1:** General Mechanism of a organic reaction

Organic chemistry provides a great field for the study and understanding of the role of imagistic representations in scientific speech [1]. The diagrams are considered much more than heuristic auxiliaries to express or apply the functions of a linguistic theory, and among the various types of diagrams present in the organic chemistry language, structural formulas are the most important. The structural formulas can be considered as the result of the systematization evolution of knowledge, based on regulations and conventions, and develop important roles on the thoughts of organic chemist.

When Goodwin (2009) [2] assumes that the structural formulas are descriptive names, he refers to the chemical nomenclature according to the IUPAC system, because, through the names of the compounds it is possible to transmit enough information about its composition, connectivity. However, in several other cases, only the use of formulas - or written nomenclature - cannot transmit the molecular spatiality, requiring another means to convey knowledge such as three-dimensional representations. For the author, figures - molecular representations - may assume an important role in the process of argumentation, because as they explore the information from the context, they may contribute to the communication of propositions, playing an important role in premises and conclusions.

Some authors had already suggested that one of the problems in learning chemistry is the lack of establishment of relationships between the conceptual and visual components (such as images, schemes, diagrams or pictures more appropriate for that given situation) of the thematics presented to them [3].

The chemistry is considered a complex science, both in terms of its understanding and its learning. One of the factors responsible for this fact is its unique language, used as a means to learn and communicate the chemical reality [4].

Chemistry evolved from a deep knowledge based on algebraic and verbal language, a feature of other sciences, to an international pictorial language in which the perception of the world of atomic particles, imagination and mental processing of visual information [5]. This is because many phenomena of chemistry are inaccessible through human senses, in some cases, even after the intervention of scientific instruments.

In Chemistry, the model is understood as "a symbolic transformation of reality". It is a process that is both figurative and linguistic. Figurative regarding the action of representing, and linguistic related to the extent of transmission of chemical knowledge. Representational processes have their historicity, while it is understood that the evolution of ways of representing molecular entities, contributing to the development of knowledge and theories of chemistry. Considering these representations, supported in scientific theories, they may be understood as a shared code of the 'subculture' of chemistry [6].

Habraken (2004) [7] discusses the hardships presented in learning chemistry, reinforcing the idea that the conceptual and logical-mathematical aspects, in many cases, have been favored at the expense of visual components, seeming to be among teachers, a consensus that signs (images, figures, diagrams) widely used in the communication of chemical knowledge, are reduced to mere illustrations.

It is important to note that nowadays there has been an increase in the concern of teaching approaches that exploit the potential of tools - whether is of viewing or from any other class - that can broaden the perception process of representational aspects in chemistry classes. Indeed, it is worth noting that the construction of knowledge occurs from the interaction between the various objects by means of linguistic expressions of conceptualizations. Thus, the perspective of Peircean semiotics enables analyses that permit better understanding of these relationships mediated by the content of the chemistry area as representation schemes in the symbolic level.

This article aims to discuss the construction of a virtual and free program that assists in learning process of the Rearrangement theme, in organic chemistry courses offered in higher education courses. Besides the construction, the objective is the analysis of how this program can be used and how semiotic tools may be enhancers, as theoretical assumptions the cognitive sciences and peircean semiotics.

## **II. The signs, semiosis and representation**

The Greek word *semeiotiké* was introduced in the philosophical field by John Locke (1632-1704), English empirical philosopher, as the designation of the doctrine of signs in general; doctrine postulated in his Essay on Human Understanding, dated 1690. This term was taken up in the twentieth century by the philosopher-mathematician-logician Charles Sanders Peirce (1839-1914) with its original meaning from the logic conceived as a scientific philosophy of language, and he devoted all his life to support the theories of this concept, namely the development of Semiotics, the science of signs.

Thus, semiotics existed for a long time, and reveals the ways in which the individual gives meaning to everything that surrounds him. It is, therefore, the science that studies signs and all languages and cultural events as if they were meaning producers phenomena. While disciplinary field, semiotics deals with concepts, ideas and investigates how these significance mechanisms are processed natural and culturally. Unlike linguistics, semiotics does not reduce their research to the verbal field, expanding it to any system of signs - Visual Arts, Music, Photography, Filmmaking, Fashion, Gestures, Religion, among others.

According to the definition of Peirce, the concept of semiosis, the activity of the sign, is characterized as an eminently evolutionary activity. His definition of sign leads to the center of the discussions developed in years of work, the foundation of the arguments of his pragmatism, the postulate of logical relationships that are interrelated in sign entity: the three sign elements: the representamen, the object and the interpretant. Santaella [8] analyzes the logical questions implicit in this Peircean concept, deepens the considerations of Peirce, and

defines the concept of logical engendering, as the primary function of the complex relationships that exist between the three elements of signic trichotomy.

A sign, or *representamen*, is what, under certain aspect or fashion, represent something to someone. It addresses to someone, that is, creates in the mind of that person an equivalent sign, or perhaps a more developed sign. The sign that is created is denominated interpretant of the first sign. The sign stands for something, its object [9]. It represents this object not in every aspect, but as reference to a kind of idea that I, sometimes, termed foundation of *representamen*.

Semiosis is usually defined as a characteristic activity process of human inborn capacity of production and understanding of signs of various natures. Danesi [10] in his "Messages and Meanings" notes the fact that signs depend of simple physiological systems, systems that reveal the high complexity of symbolic structuring at stake in the interrelation process of physiological systems with the human capacity of abstraction. It is noteworthy that through the gradual acquisition of a symbolic system, the man discovers a way to adapt to the environment, transforming all the human life. This abstraction capacity, responsible for formalizing a whole symbolic universe, is a unique ability of man, different in kind from any other organism.

The philosopher Ernst Cassirer (1977), aware of this point of view, corrects and expands the classical definition of man as a rational animal, designating it in its specific difference, defining it as a symbolic animal. Semiosis as a process, begins with the transformation of the physical world, that is, the perceived reality. The phenomenon that is apprehended, perceived, becomes a mental world, psychological, transported to a reflected reality; so it is characterized its eminently symbolic feature, or in terms of Peirce, semiotics.

Signs can be considered something that has some representation for someone, perceived in some of its aspects. The mediation of meaning production process (interpretants) accepted by certain scientific community starts from the consideration of factors related to the interpreter (student): knowledge of content (perceive), rules and ability to establish relationships between sign-referent and sign-interpretant (relate) to be able to assign meanings (conceptualize) [9]. The Peircean Semiotics can be considered a solid theoretical framework for understanding the representations of chemical knowledge, especially from the content hosted in virtual environments.

In the post-structuralist view, representation is designed solely on their significant dimension, that is, as a system of signs, as pure material brand it considers that representation is expressed through a painting, a photograph, a diagram, an equation, a formula, a text or an oral expression. Therefore, in this conception, representation is never a mental or internal representation. Representation is, in this conception, always a visible and external mark or trace [11].

In this context, the teacher can be considered a mediator of speech; students as the discursive community; and the semiotic representations as teaching and learning tools. Besides that, in the classroom, teachers and students generate an exchange of ideas through language, which embodies a particular symbology, thus creating a system of representations. One can summarize the relationship between the semiotic triad as a pedagogical triad involving Perceiving (firstness), the ratio (secondness) and Conceptualization (thirdness) [9].

Access to chemical entities within the meaning of Peircean Semiotics, is always a mediated process and limited by relativism imposed by their very nature. Empirical evidences - including those made possible by instruments - act as signs that show specific and restricted aspects of the objects to which they refer.

It should also be considered that the proposal of a scientific theory, for example, involves various moments of firstness (perceive), secondness (relate) and thirdness (conceptualize), which may lead to different dynamic interpretants (emotional, energetic and logical) whose intellectual synthesis possibly produce a consensus on certain logical interpretant (concept, law or theory) is believed to be closer to the scientifically acceptable knowledge [12].

The educational dimension of the teaching processes and chemistry learning, which involves the constant manipulation of phenomena, symbols and models, makes the ability of handling and understanding the different sign systems a crucial point not only in the construction process of chemical knowledge, but also in their enculturation process by students. As regards, more specifically, the issue of representation in Chemistry Teaching, Alex H. Johnstone, professor in the Department of Chemistry at the University of Glasgow, in several articles [13] [14] was one of first researchers that proposed a model for the representation of chemical knowledge, which subdivides into three different levels associated by the notorious triangle of Johnstone. Essentially, the Johnstone model proposes: a sensory or perceptual level (macroscopic level), a molecular or exploratory level (submicroscopic level), and a third level, the representational (symbolic level) that articulate the dimensions of chemical knowledge.

In apprehension of chemical knowledge, the same understanding brought by Hoffmann [6], Goodwin [1] points out that the structural formulas and contribute positively to the construction of arguments and explanations in organic chemistry, are used in the teaching of this science, whereas through these it is possible to seize and communicate information about the molecular world using different symbols.

In general, in the discipline of organic chemistry, the rules depend on the conceptual framework and relevance of ontology in the physical world description process so that is possible to think and act on it. Thus, the Peircean Semiotics is a way of looking at the concept development process in organic chemistry and think about it.

### **III. Rearrangements in organic chemistry**

Rearrangements are part of an outstanding class of reorganization processes of bonds, which have many applications in organic chemistry. Applications that can be seen in the industrial sector, as in the production of acetone and phenol or in the cracking process to produce gasoline, among other processes [15].

The chemical usefulness of rearrangements is unquestionable; however, because it is a highly complex subject, its approach in higher education has been restricted to the use of lectures, with low use of virtual resources and dialogical tools.

In this paper, we present a novel fashion, the creation of an application that allows you to explore the various dimensions of this content, enabling multiple relationships between forms of symbolic representation of chemical knowledge, highly desirable to learning.

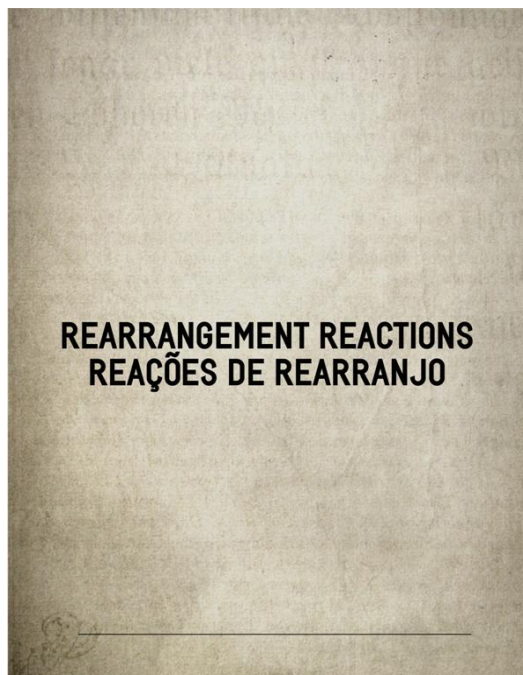
### **IV. Building the application**

This study, performed during a stage of a course of Organic Chemistry II taught to undergraduate students in chemistry of a Brazilian public university (Federal University of Santa Catarina) explains the potential of a virtual resource for learning the content Rearrangements Reactions, which implies a complex degree of abstraction.

The methodology was designed as an alternative to help the teacher to guide the study of rearrangement reactions, with the aim of understanding from interactive images. Among the set of reactions in the context of organic chemistry, the reactions that were chosen are the pinacol, Wagner-Meerwein, the Favorskii rearrangements and Baeyer-Villiger oxidation.

The application was developed from two tools. The first tool was built from the "Easel.ly" (<http://www.easel.ly>), which features models of infographics and an instrument that allows the modification and creation of new images. The second tool is the program Microsoft Office PowerPoint 2007 from Microsoft Corporation used to organize images and infographics and perform hyperlinks between each image and content. It was used this program to promote easy handling and distribution on the Internet. After the application download, it is no longer necessary to use the internet to run the program, only for the access of complementary materials, which maximizes the use conditions of this application in formal and non-formal education setting.

At the start of execution of the application, an opening page is presented, as Fig. 1.



**Figure 1:** Opening page of the application Rearrangement Reactions.

After opening the first page, the user will be directed to page 2 (Fig. 2) for the selection of the study language.



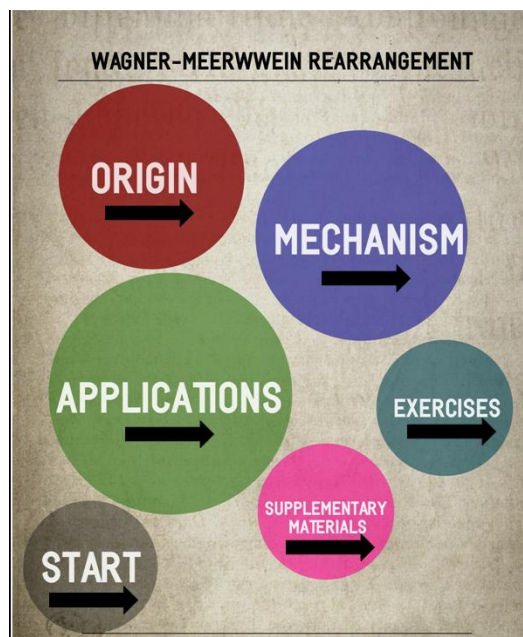
**Figure 2:** Initial image of selection of language of the application Rearrangement Reactions.

After choosing the language, the student gains access to Pinacol, Wagner-Meerwein, Favorskii and Baeyer-Villiger rearrangement reactions, as Fig. 3 by clicking on the indicative arrows.



**Figure 3:** Selection of rearrangement of the application Rearrangement Reactions.

Starting the presentation of a specific reaction, there is the possibility to study a little about the origin of each reaction, its reaction mechanism, its practical applications, some complementary materials and exercises, as can be seen in Fig. 4.



**Figure 4:** Selection of content of the application Rearrangement Reactions

From the option Origin, the student has the possibility to know the researchers who developed the rearrangement and their initial study, as shown in Fig. 5.

**WAGNER-MEERWEIN REARRANGEMENT**

Discovered in 1899 by Georg Wagner, a Russian chemist, and later studied and improved by Hans Meerwein, a German chemist.

Wagner- Meerwein Rearrangements are extensively studied in the class of natural products, because of they several rearrangements in the class of terpenes .

The rearrangements:  
In reaction there is the migration of an alkyl group to a cationic center by acid catalysis .

Isoborneol  $\xrightarrow{H^+}$  Camphor (Canfeno)

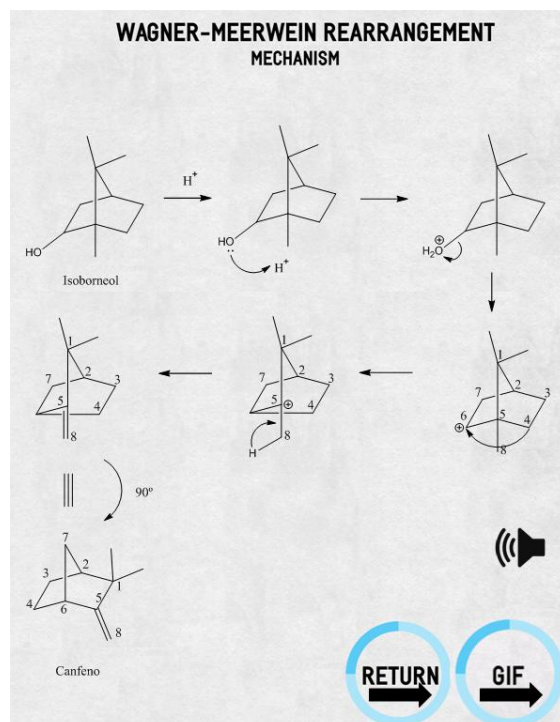
RETURN START

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**Figure 5:** Content “Origin” of the application Rearrangement Reactions

In the option Mechanism, the student can view the complete reaction mechanism of a rearrangement reaction, moreover, you can check this reaction in gif format and listen to an explanatory audio of the mechanism, as outlined in Figure 6. The intention of the audio is to make the application more interactive, assisting students with visual impairment. The application as a whole can be used in conjunction with a processing software and speech synthesis and Braille keyboards, which brings the possibility to visually impaired to use the application without difficulty.





**Figure 6:** Content “Mechanism” of the application Rearrangement Reactions.

The content "Applications" aims to contextualize the reaction, bringing at least one everyday example or of industrial compounds, which use rearrangements in its production. In this content as well as on the home page there is a question mark. By clicking on this button the student accesses an explanatory text related to the compound, clicking on this button again the text box fades from the home screen, as shown in Figures 8 and 9.

**PINACOL APPLICATIONS**

INSECTICIDE

RETURN

Rouchaud, J. and Meyer, J. (1982), Synthesis of the fungicide [<sup>14</sup>C]triadimefon. J Label Compd Radiopharm, 19: 111–116. doi: 10.1002/jlcr.2580190113

**PINACOL APPLICATIONS**

INSECTICIDE

THE PINACOLONE IS PRODUCED FROM PINACOL REARRANGEMENT. THE PINACOLONE IS AN INTERMEDIATE FOR SYNTHESIS OF A FUNGICIDE CHAMDO TRIADIMEFON , USED IN AGRICULTURE FOR CEREAL PROTECTION MOLD AND RUSTS .

RETURN

Rouchaud, J. and Meyer, J. (1982), Synthesis of the fungicide [<sup>14</sup>C]triadimefon. J Label Compd Radiopharm, 19: 111–116. doi: 10.1002/jlcr.2580190113

**Figures: 7** (on the left): Option “Applications” of the application Rearrangement Reactions. **8** (on the right): Functioning of the button “Question Mark” of the application Rearrangement Reactions.

In the option "Complementary Materials" (Figure 9), the application provides links that lead to materials that assist the student in understanding the content, among them there are links of the reactions in three-dimensional models (Figure 10), video lessons and databases.

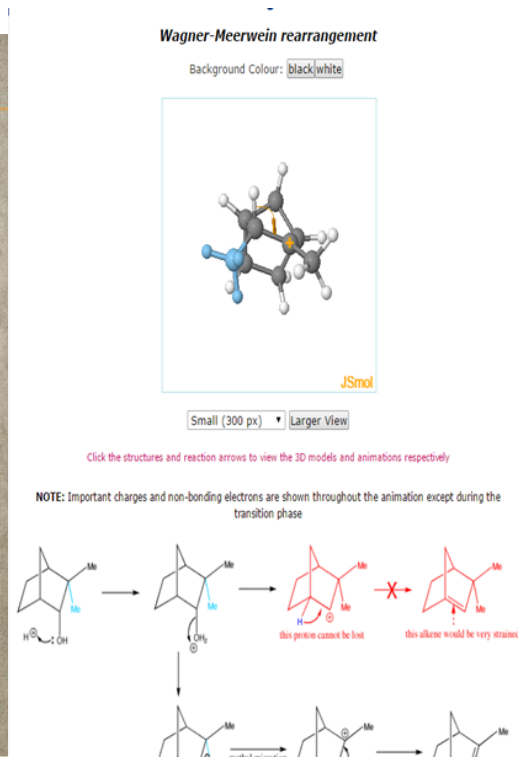
**PINACOL REARRANGEMENT SUPPLEMENTARY MATERIALS**

**PINACOL REARRANGENT IN 3D**  
<http://www.chemtube3d.com/Rearrangements-Pinacol.html>

**DESCRIPTION AND MATERIALS:**  
<http://www.organic-chemistry.org/namedreactions/pinacol-rearrangement.shtm>

**VIDEO :**  
 Part 1: <https://www.youtube.com/watch?v=qxPyEJIMYcc>  
 Part 2: <https://www.youtube.com/watch?v=ye5kj2Q4xf4>  
 Part 3: <https://www.youtube.com/watch?v=Wae2rC5nmbQ>

**RETURN** **START**

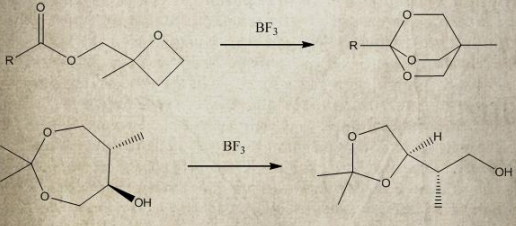


**Figures:** 9 (on the left): Content “Complementary Materials” of the application Rearrangement Reactions. 10 (on the right): PrintScreen of the link of 3D reaction in the Content Complementary Materials.

In the topic Exercises, the student has access to activities selected from the book Organic Chemistry (Clayden et al, 2000) with their resolutions (Fig.11 and 12).

**EXERCISES**

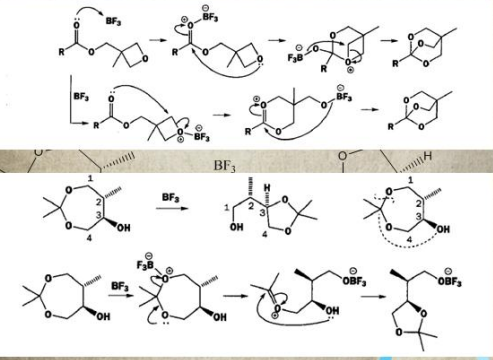
**1** Rearrangements by numbers. This problem is just to help you acquire the skill of tracking down rearrangements by numbering. There are no complicated new reactions here. Just draw a mechanism.



**ANSWER** **RETURN**

**EXERCISES**

**1** Rearrangements by numbers. This problem is just to help you acquire the skill of tracking down rearrangements by numbering. There are no complicated new reactions here. Just draw a mechanism.



**ANSWER** **RETURN**

**Figure:** 11: Content “Exercises” of the application Rearrangement Reactions. 12: PrintScreen of the link of 3D reaction in the Content Complementary Materials.

After interact and enjoy all the options of the selected rearrangement, the student can choose the option Return to start a new rearrangement.



## V. Conclusion

The appreciation of mediation aspects (pedagogical triad: perceive, relate and conceptualize) in organic chemistry classes may help to overcome some methodological and epistemological difficulties related to chemical entities (Ontological items), not only regarding its existence but also to their assertion consequences that the molecular reality is the cause of the phenomena, and not an explanation for them.

Semiotic representations, in turn, are productions made by the use of signs belonging to a system of representation, which have their own difficulties of meaning and functioning [16]. The writing in natural language, the chemical language, symbols, chemical equations, graphs and schemes are examples of semiotic representations. Such representations are external and conscious to the individual and perform inseparably functions of objectification and treatment.

As you can only see part of the object through the mediation of signs, it has only a partial perception (immediate object) of it [8]. This approach contributes to the understanding of scientific activity as a process of permanent construction, interpretation and signification, influenced by context. Thus, from the perspective of Peircean Semiotics, the perception of the chemical knowledge construction process allows to overcome some ontological problems related to the representation of chemical entities. As from the perspective of semiotics, the reality is mediated by interactions between signs (sign, object and interpretant), there is no involvement of equivalent plans of argument or representation: in other words, the sign is the object; the object determines the sign, and the interpretant is determined immediately by the sign and, mediately, by the object.

This is how reality (dynamic object) and represented reality (immediate object) have a necessary connection, which impels us to see them as interlinked.

The use of mediational objects in the classroom leads to the development of specific skills. The mediational objects have the Intent to provide students with the development of skills needed for the appropriation of scientific concepts and this happens through mediated action. The "mediated action" is the mental action that employs "mediational means" or "cultural tools", which are available in a particular sociocultural setting. Therefore, in this study we understand that the mediational objects have significant implications for the Chemistry Teaching, since, learn chemistry involves various forms of human action, such as: observe, describe, compare, classify, analyze, question, plan, evaluate, generalize, among others [17]. All these forms of mediated action involving cultural tools / mediational objects that are resources and restrictions.

The virtual representation using the previously described application, allows better understanding of the terms used in teaching rearrangements in organic chemistry. The use of visuals, contributes greatly to the description of the mechanisms and semiotic artifacts that are used in the virtual plane to explain the occurrence of important chemical reactions, desired to the learning of many students in courses offered in higher education.

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