THE USAGE OF A SIMULATION TO STUDY INTERMOLECULAR FORCES: SOME FINDINGS

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Abstract

The purpose of this research was to discuss and reflect about the use of a computer simulation in the learning of intermolecular forces. Simulations are dynamic representations of chemical processes or systems, and allow users to select values for input variables from within suitable ranges and observe the results on output variables. In this study we used free software named "Ligações Intermoleculares", from http://nautilus.fis.uc.pt/molecularium/pt/ligintermol/index.html. The goal of this activity was to help students build internal representations (mental models) for course content. The research is qualitative. We applied a pre-test and a post-test to a class of students (n=30) from a secondary school trying to find what these internal representations are like. The research indicates that students' pictographic representations of intermolecular forces improved substantially. These findings suggest that the use of this visual tool helped students to make a better connection between the chemical representations and the macroscopic phenomena presented during a mini-course about solubility.
Key words: *visualization, computer, simulation, chemistry*.

Introduction

The use of visualizations in chemistry education became a new field of research. In the last years, four very different groups of people (computer software specialists, scientists, educationalists and cognitive scientists) have promoted the development, the discussion and the use of visual tools in sciences instruction (Gilbert, 2007), nevertheless research evidences are only in the beginning. There are more questions than answers. The role of models and visualization in science and science education has been discussed in the last years in several studies: what to study, how to do so, what constitutes good practices, or how to evaluate the outcomes of that practice are some of the challenges that researchers have faced and will continue to face in the next years.

There is a central topic that often crosses these studies which is the definition of the term "visualization". According to Gilbert, Reiner and Nakleh (2008) there are two conventions, in convention 1, visualization is a verb (to visualize something is to mentally act on it), in convention 2 visualization is a noun (visualization is something in the public realm). Inevitably, there are also studies that cross the two conventions, for instance, studies about "visuospatial thinking".

Has been found literature approaching this issue in the sense of convention 1 that dealt with questions such as: how is a visual representation turned into knowledge? What are the mental processes that are involved in attaching a meaning to a representation? What mental and brain processes are involved in "seeing"? (Reiner, 2008). Other authors (Gilbert, 2007; Rapp & Kurby, 2008) also present their ideas about these concerns. Gilbert refers the importance of developing "metavisual capability" or "metavisualization", the acquisition of fluency in visualization and the making of meaning for any representation (Gilbert, 2008). This author suggests that this development could be done by general good practice in the use of representations by teachers and in textbooks and by the specific cultivation of the skills involved (Gilbert, 2007).

Like has been mentioned before, there is another trend of research that uses the term visualization in the sense of convention 2, a noun, something that has been placed in the public realm in either a material object, visual, verbal or symbolic form. Here has been found several studies (Wu, Krajcik & Soloway, 2001; Santos & Greca, 2005; Tasker & Dalton, 2006; Kozma & Russel, 2007; Arroio & Honório, 2008) that by using a different approach try to evaluate the use of different kinds of visualizations in chemical instruction. Most parts of these studies are only quantitative and through a series of specific tests they try to evaluate the pupil's apprenticeship and indirectly the effectiveness of the visualization used.

Problem of Research

Therefore, it began to encounter some studies where a component of qualitative research is introduced. The aim of this introduction is to obtain rich information of how pupils develop an understanding of chemical concepts while using visualizations as helping tools in learning. A great part of these tested visualizations are software with virtual 2D and 3D images and in a few cases animations and simulations or combinations of various representations (e.g. concrete three-dimensional models, virtual computer models, static two-dimensional computer models, stereo-chemical formulas). So, in this work we try to contribute with some insights of how students build internal representations from external representations (visualizations). This qualitative approach was used to get more information about what do students glean from external representations and how they internalize and express that information.

Simulation was chose to discuss the intermolecular force's concepts. Like has been mentioned before, simulations are dynamic representations of chemical processes or systems, and allow students to interact with this by changing input variables from within suitable ranges and observe the results on output variables. It is recognized their limitations, a simulation incorporates one or more rules to define a model. These rules are applied within some limited conditions, but when introduced carefully, a simulation is a good tool for exploration and learning. Kozma and Russell (2007), present an interesting investigation using five chemistry multimedia visualization projects using different approaches. The authors concluded that all five projects show an improvement in the learning of chemistry concepts and development of scientific investigative process skills.

Ardac and Akaygun (2004), also present a study that evaluates the effectiveness of multimedia-based instruction on students' understanding of chemical change. The authors concluded that students who received multimedia-based instruction outperformed students from regular instruction group in terms of the resulting test scores and the ease which they could represent matter at the molecular level. They also mentioned that, results relating to the long-term effects suggest that the effectiveness of this type of instruction can be improved if instruction includes additional prompting to help students to do the correspondence between different representations of the same phenomena.

This multimedia effect is considered today to be very important in learning. Computer-based technologies provide powerful means for fostering molecular understanding, because they can represent the multilevel thought in chemistry. Theoretical and empirical evidence in-

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dicate the importance of multiple symbol systems in enhancing learning. Allan Paivio (1986), presents Dual Coding Theory (DCT), that provides the basis for using multiple representational systems in instruction. This theory suggests that information presented by way of verbal and imagery channels are processed separately, and it has been tested in several multimedia studies to explain how information presented as text and animated sequences interact to produce learning. Most part of these studies was conducted by R. Mayer and his collaborators (Mayer, 2001). These studies have shown that, as in a dual coding model, the combined use of text and animated graphics made the information more memorable, and that problem solving was improved when using software that paired animations with narration. These findings are also supported by Cognitive Load Theory (CLT) proposed by John Sweller (2003). Cognitive Load is a term that refers to the load on working memory during instruction. This theory differentiates between three types of cognitive load: intrinsic cognitive load, germane cognitive load, and extraneous cognitive load. This theory has broad implications for instructional design, because it allows instructional designers to control the conditions of learning, within an environment, or more generally within most instructional materials.

In another study, Tasker and Dalton (2006), discuss the use of animations and present a multimedia information-processing model for learning from audiovisual information. Once again, it's based on the theoretical models depicts above (DCT and CLT), and they concluded that animations and simulations can communicate many keys about the molecular level effectively, which is considered to be very important in chemistry apprenticeship. These authors also point out the need to build mental models, and that many student difficulties and misconceptions in chemistry result from inadequate or inaccurate mental models at the molecular level. On their research, they use the *Vischem Project*, which was founded to produce a suite of molecular animations depicting the structures of substances and selected chemical and physical changes that in contrast to textbook illustrations can show the dynamic, interactive, and multiparticulate nature of chemical reactions explicitly.

Research Focus

The understanding of the particulate nature of the substance is one of the central topics of sciences, in particular of chemistry, and, in accordance with Adadan, Irving and Trundle (2009), it involves the following aspects: the nature of particles for same them, the relative distance and the arrangement between them, the existence of electrostatic forces between particles (intermolecular forces) and the intrinsic movement of particles. Being this concept, for its nature, linked with the submicroscopic level of representation, it is opportune that if available to the student tools that the same facilitate the understanding of this concept, according others authors (Kozma, Chin, Russell & Marx, 2000; Wu, Krajcik & Soloway, 2001).

Methodology of Research

The purpose showed to the school's master was a mini-course about solubility. It was organized with the application of a structured experimental activity on the concepts of polarity and solubility of the substances and the usage of multimedia resources.

Participants of Research

This work was conducted with a class of 30 pupils, from the second year of a public secondary school in São Paulo city. This school has an informatics laboratory with 12 computers with broad band internet access. The majority of students had regular chemistry classes but some of them didn't have any chemistry lessons since the start of the school year. These students were organized in four groups, female and male.

Leaving from the planning, a prior informal surveying was done with the pupils with the purpose of find out what they knew about atoms, molecules, simple and compound substances, homogeneous and heterogeneous mixtures and solubility.

Instrument of Research

In this study, it was considered opportune to apply a questionnaire before the experimental activity and after the activity with the multimedia resource, so that the pupil has the chance to make registers, through the writing and drawing of its representations for the situations in study. In such a way, it will be possible to analyze which is its understanding on the macroscopic and submicroscopic levels, before the practical activity and the use of the multimedia resource, as well as later, promoting a scene where we wait to be able to evidence the occurrence or not of changes in its representations, what it will imply in possible changes in its mental models.

The questionnaire before the experimental activity, had six open questions where the intention was to survey which was the previous ideas of the pupils on models, the relation between model and reality, which idea they brought on animation and computational simulation, on the union between atoms and molecules, which the importance of this subject, what are the chemical bonds and if the atoms and its bonds are statics or dynamics. It also had one seventh question where was asked the pupil to represented, through drawings, the visual aspect and the organization of particles of the participant substances of the mixtures water/kitchen salt, water/copper sulphate II ($CuSO_4$), water/cleaning fluid, water/alcohol and water/kitchen oil. The questionnaire after the activity with the multimedia resource, had four open questions where the pupil would have a new possibility to register their ideas on the chemical bonds, if they are statics or dynamics, if the use of the simulation/animation made some difference in their learning on bonds and which was this difference, which the opinion of it on the mini-course, indicating positive and negative points and their suggestions. It also had a fifth question, that it was the same one of the previous questionnaire, where the pupil was asked to represented, through drawings, the visual aspect and the organization of particles of participant substances of the studied mixtures.

The multimedia resource together with the use of the technology was used to expand the meaning of the chemical phenomena, for the systems in submicroscopic scale and for the outside world. In accordance with Russel *et al* (1997),

> 'Visualizations of chemical phenomena and concepts linked to microscopic-level animations and to examples from the students' everyday life may aid the more visual learner and stimulate more students to achieve mastery-level understanding of chemical concepts.'

Some researchers, in its articles, refer the use of tools of visualization with the objective to facilitate the understanding of the particulate nature of the substance or to promote conceptual changes in the students on the particles' behavior (Snir, Raz & Smith, 2003; Kozma, Chin, Russell & Marx, 2000; Adadan, Irving & Trundle, 2009; Bowen, 1998; Yezierski and Birk, 2006; Sanger, Campbell, Felker & Spencer, 2007). Research involving the visual representations showed that the use of visual tools, such as livened up or static computerized molecular models, followed of verbal speech and writing, facilitates the construction of scientific conceptions (Kozma, Chin, Russell & Marx, 2000).

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Data Analysis

During the conceptual survey with the pupils, they had been organized in four groups, with approximately seven pupils in each.

The pre-questionnaire was supplied to the pupils. This questionnaire involving open questions and graphical register, took 10 minutes approximately to be answered by the pupils. After that, it was made the survey of the pupils' conceptions and the development of the experimental activity. On the ending of the experimental activity, the pupils had been directed for the informatics laboratory, in order to use the multimedia resource on intermolecular interactions and during this usage the pupils had a script structuralized with opened questions on the situations simulated for by the resource.

As the groups finished the activity in the informatics laboratory, a questionnaire after activity was given to them to being answered. In this, the question involving the macroscopic and submicroscopic visualization was repeated in order to create the chance of the pupils to modify or to complement its representations, in case that they wanted.

Results of Research

Previous Questionnaire

In the first question, the answers of the pupils identified the model as a drawing, a project, an idea that still schematizes an experience or a theory, being then a base for new experiences and/or theories. Some affirmed to be a representation of an idea, a suggestion, of theory or an experience, if thus becoming base for new experiences. It was explicitly replied that the model "is a form to demonstrate something", without leaving clearly what it would be this demonstration; if it would be a exemplifying or a representation of something.

The model understanding is in fact, for some pupils, as being an example, something specific, that it identifies a prompt situation; others as if the model were the proper reality, experience or theory and not a representation. However, it is important to detach that the expression "representation of theories" appears in some answers.

In the second question, some had strengthened the idea of that model represents the reality, that explains the reality. Others had affirmed that the model is an attempt to explain the reality, however that the same one is more complex. In this affirmation we perceive that pupil considers the distant model of the reality, as being a simplifying of the reality. In this context, the model has its value attributed to an incomplete, simplistic base, which it does not have the level of detailing and complexity that the reality brings in them. In such a way, it is a starting point, but it does not support, does not explain the reality. One of the answers affirms that "Model serves person to understand it as it would be…, the reality is more complex." One of the pupils affirms that "reality is what it is happening and the model is something that demonstrates what it can occur." showing that the model would have the function to predict facts or situations.

In the third question, the understanding about animation is about images in movement, with acceleration, as some answers. Some compare the computational animation with a livened up drawing, movements and speak, passing the idea of separation of the reality, as if the animation did not have linking with the real. Already the simulation, "tries to imitate" a situation, represents or interacts with the reality through the computer, transmitting the perception to that the simulation is next to the reality, has an aggregate value of fidelity with the reality biggest that the animation. This idea is shared by another pupil who answers that "animation is something surreal and computational simulation is something of the reality carried through in the computer." The idea of that the "animation is the livened up drawing that you only see" we denote low valuation of the animation as learning resource, as if its reading was not possible, to its interpretation. The animation does not allow the interaction as the simulation, the alteration of variable, with intention to understand and/or to foresee a behavior.

In the fourth question, where the pupil was asked to explain the union between atoms, the interaction between molecules and which the degree of importance of this topic, some pupils had not answered, leaving a blank space, or had written "do not know" or "we forget". Others, had answered on an evasion form, as "the union is very important, therefore help to create things" or "a thing leads to another one, believing that everything is on, forming something. The importance is our survival, to understand our formation…" They had explanation attempts where the pupil displays the union between atoms as "junction between particles of positive and negative components,…" probably a allusion to protons and electrons or that "the union between atoms and the interaction between molecules if must the electron union, protons and neutrons", demonstrating difficulty in the approach of more specific concepts to chemistry, without distinction between which the responsible particles for the bonds between atoms and as the same ones interfere with the interaction between the molecules. Still it had had answers where do not appear explanation attempts but the direct affirmation of that "union between atoms → molecule", demonstrating to a possible difficulty of interpretation of the question or an attempt to answer to show the pertinent knowledge of something to the subject or not to leave the question without reply.

The same it happens in the fifth question, with regard to the absence of answers. Some pupils, when answering, had affirmed that the chemical bonds are substances, that if mixing, can become another substance or that it is the mixture of two substances. These answers show the absence of the understanding of the concept and the confusion with regard to the formation of mixtures and the occurrence of chemical reactions.

In the sixth question, the majority of the pupils affirmed that the atoms and its bonds are dynamic and the explanation was that "they are moved, if mixes and if they transform" or something into this direction. It's possible to verify that the pupils explain the dynamism for the perception of the mixture and the transformation here, for the action to mix materials and the involved action in this situation, the agitation of the materials.

In the seventh question, the drawings of the pupils, with regard to the visual aspect, differentiate the homogeneous mixtures of the heterogeneous ones, however the same it does not happen in the representation of the organization of particles. In the mixtures water/salt of kitchen and water/copper sulphate II, only two pupils represent the systems in the same way that in the visual aspect (Figure 1). The remains, when drawing these two systems, if concern in representing, as much the kitchen salt how much the copper sulphate II, as points in watery way and consider the water as a continuous substance (Figure 2). The difficulty in visualizing the water particulate's nature is perceived there, assuming that the same one is a continuous substance, what is assimilated by its senses in the day. The other systems are all represented without distinction of particles, in the same way that in the visual aspect (Figure 3). A factor that could have contributed to the distinction of the drawings of the systems with kitchen salt and copper sulphate II to the others systems, it is that both of the substances had been used in the solid state, therefore, the pupils had transferred a macroscopic characteristic to the submicroscopic level. Valley to detach that one of the pupils, when drawing the mixture water/alcohol in microscopic level, it used representation of the symbolic level for the water (molecular formula H_2O), showing that the same it had not understood what was to be made or that the requested representation (organization of particles) was not a part of its repertoire.

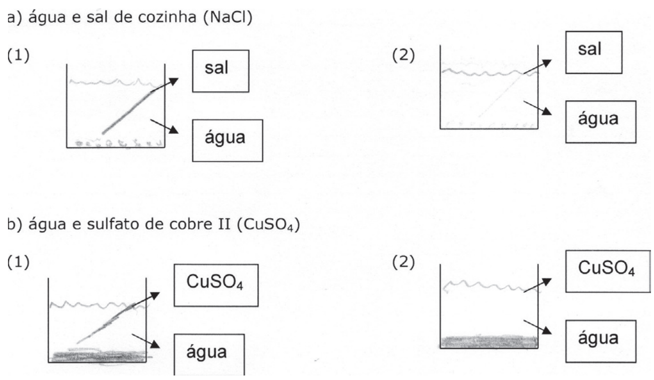

Figure 1. **Representation of the visual aspect (1) and the organization of particles (2) of the mixtures water/salt of kitchen and water/copper sulphate II.**

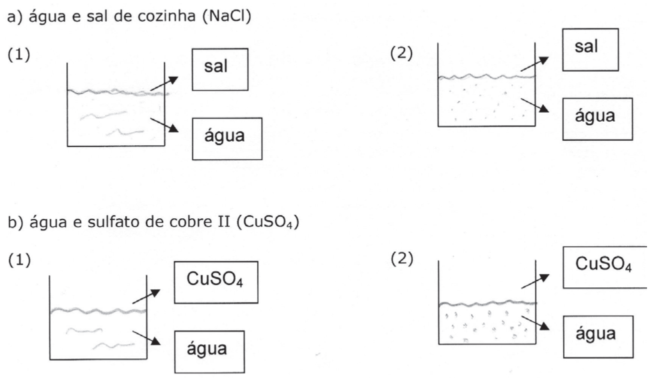

Figure 2. **Representation of the visual aspect (1) and the organization of particles (2) of the mixtures water/salt of kitchen and water/copper sulphate II.**

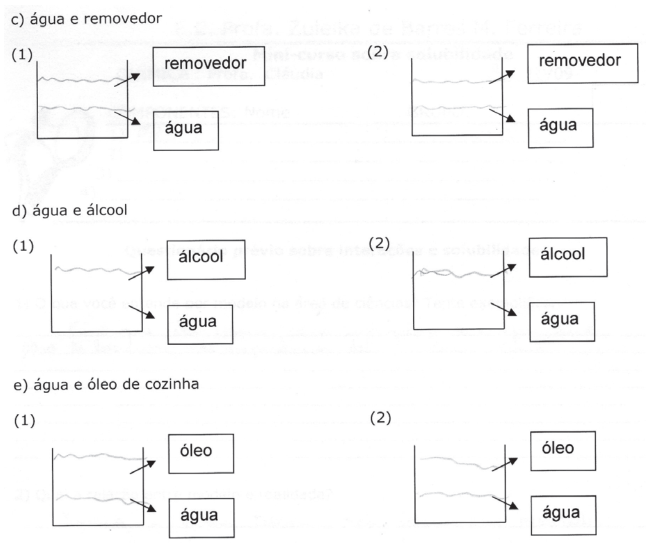

Figure 3. **Representation of the visual aspect (1) and the organization of particles (2) of the mixtures water/cleaning fluid, water alcohol and water/kitchen oil.**

Post Questionnaire

In the first question, the pupils had pointed the chemical bonds as dynamic, being that some had not justified the affirmation. Between that, they had justified that they had stories as "therefore they are always interacting with other elements.", "therefore they put into motion themselves and if they transform" or "because she has movement in particles when interacting two similar substances". These justifications show that the pupils had not differentiated atoms and molecules, from the existing bonds between the same ones, attributing pertinents characteristic's bonds to particles. That is confirmed from the justification of two pupils who tell "They are dynamic. Always the molecules' movement." Still in this question, two groups formed by three pupils each, had affirmed that the chemical bonds are static, because they involve the statics, if relating the electricity static. We perceive here the difficulty of understanding of the meaning of the used concept, therefore the same word possess distinct meanings, in accordance with the context that the same one is used.

In the second question, some pupils affirm that, with the multimedia tool they had been able "to see" what really he happens with loads gifts in objects, probably an allusion to the experimentation with the pen and water thread. Others had affirmed that "it was more clearly the comments made in laboratory" or despite "we can have a notion of how the alterations occurs". However, these affirmations are vacant, not being possible to affirm if really it had a change in the elaboration of the concept of bonds.

The third question was the same one of the previous questionnaire, which requested to the pupils the representations of the visual aspect and the organization of particles. The drawings made for the pupils show that great conceptual changes in the particulate representation of the substance had not occurred. In the referring drawings to the visual aspect, the representations were very seemed the facts in the previous questionnaire. However, in the referring drawings to the organization of particles, the mixtures water/cleaning fluid and water/kitchen oil had had its represented substances as points, restricted the phase identified for the substance, being the represented water still of continuous form (Figure 4). This occurred in 4 of the 11 scripts answered in group. In the mixture water/alcohol, 4 answered scripts of the 11, being 3 of the pupils of the cited situation previously, had presented drawings of this mixture where the alcohol was represented by points spread in the water, being this also represented of continuous form (Figure 4). Moreover, in 3 answered scripts of the 11, the water was represented of hybrid form, with points and also as continuous substance, disclosing the difficulty of the pupils in accepting the representation particulate for the water (Figure 5). It had change in the representation of substances, in submicroscopic level, identified through the done registers that indicate the occurrence of one better conceptual elaboration.

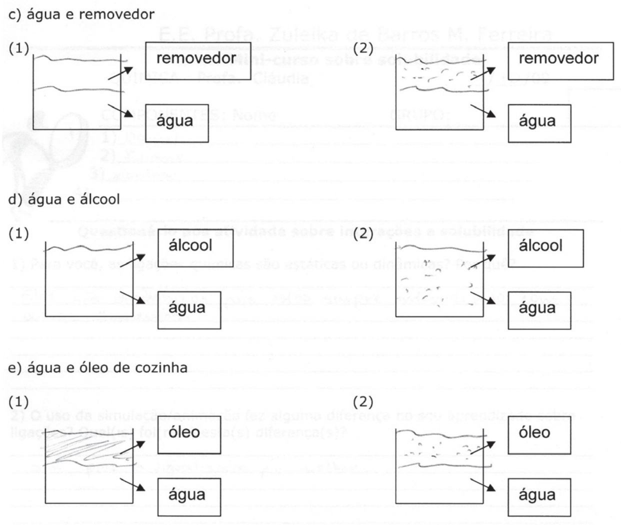

Figure 4. Representation of the visual aspect (1) and the organization of particles (2) of the mixtures water/cleaning fluid, water/alcohol and water/kitchen oil, being cleaning fluid, oil and alcohol with particles.

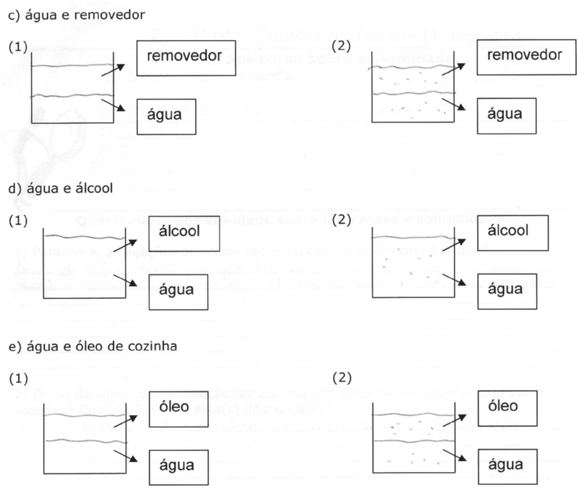

Figure 5. Representation of the visual aspect (1) and the organization of particles (2) of the mixtures water/cleaning fluid, water/alcohol and water/kitchen oil, with differentiation between (1) and (2) in all substances.

Discussion

Previous Questionnaire

The pertinent questions to the submicroscopic level had been the ones that the pupils had presented greater difficulty in answering, therefore do not know what to write, as to describe particles that are not part of its sensorial repertoire. This difficulty is evidenced by the representations of the organization of particles, where the representation of these practically does not appear. This difficulty to describe what it is not tangible for the directions is observed by Ben-Zvi, Eylon, and Silberstein (1986).

Post Questionnaire

In the first question we perceive as the fact of the pupil not to share of the language of a scientific community can implicate it difficulties in the conceptual elaboration. The words can have diverse meanings in accordance with the way where they are used and this absence of proximity with the one meanings determined area, they can take to a very different elaboration of concepts of what it was intended in the action, as the ideas of Lemke (1997).

Conclusions

Comparing the images of the representations of the pupils, before and after the use of the resource, it has indication of improvement in the representation of the particulate nature of the substance, what it can be reflected of a development in the mental model of the pupils on the worked systems.

These findings suggest that the use of this visual tool helped students to make a better connection between the chemical representations and the macroscopic phenomena presented during a mini-course about solubility

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