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To what degree does handling concrete molecular model promote the ability to translate and coordinate between 2D and 3D molecular structure representations? A case study with Algerian students

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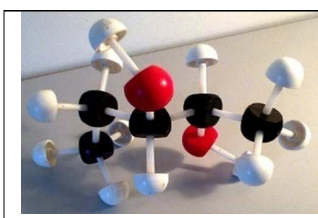
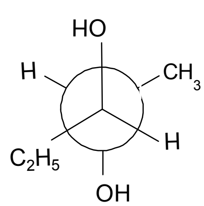
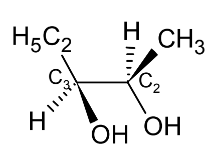
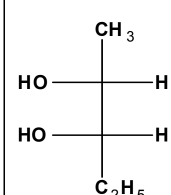
Abstract: This study aims to assess whether the handling of concrete ball-and-stick molecular models promotes translation between diagrammatic representations and a concrete model (or vice-versa) and the coordination of the different types of structural representations of a given molecular structure. Forty-one Algerian undergraduate students were requested to answer a pencil and paper questionnaire at the end of their training for a bachelor's degree in physical sciences to test their abilities to translate from Dash-Wedge or Newman representations to 3D ball-and-stick models (and vice-versa) of two molecular structures and from one concrete 3D model to the Fisher projection of the molecule. Our results show that concrete molecular models have the potential to be an effective spatial tool to promote visualization, orientation and rotation abilities. However, the handling of the concrete model did not have the same impact on all students and this effectiveness in promoting the spatial abilities required to translate and coordinate between representations was dependent on the representations: it was greater for Dash-Wedge diagrams than for Newman, and was inexistent for the Fisher projection. An implication of our research is that it may be necessary to work with a model over an extensive period of time to improve the mechanisms by which one translates between various representations when the conventions of these representations are varied in nature.

Introduction

Understanding models is an important aspect of the understanding of science, since models and modeling are considered to be the basis of scientific reasoning (e.g. Mendoça and Justi, 2014, Kênia et al., 2015; Gober et al. 2011). That is why their use to represent scientific information, explain and describe ideas, or provide means of visualising abstract scientific concepts is significant in science education (Mendoça and Justi, 2014; Gober et al., 2011 ; Warfa et al. 2014). All over the world, national science standard documents (e.g. USA, NRC, 2012; Québec, Ministère de l'Éducation, du Loisir et du Sport 2009: France, Ministère de l'Education Nationale, 2011) specifically call for students to be engaged in developing and using models, constructing explanations and participating in discussions. Scientists have developed different modes of representation of models with different degrees of abstraction (such as physical objects, photos, diagrams, graphs, texts) and different representational levels (such as macro, micro, submicro, and symbolic) (Kozma and Russell, 2005; Stull et al., 2012; Treagust and Tsui, 2013; Harlow et al., 2013; Roy and Hasni, 2014; Won et al., 2014). Having access to an assortment of representations helps connect various aspects of a phenomenon; builds a more complete, deeper understanding of science; and communicates scientific ideas more effectively (Ainsworth, et al., 2011). To be successful in science, students must therefore be able to understand, interpret, and readily translate among the different forms and types of representation, and also be able to choose the best representation for a given task. (Gilbert, 2010; Kumi et al., 2013). From the work of different authors (Keig and Rubba, 1993; Kozma & Russell, 1997; Ainsworth, 2006; Schönborn and Bögeholz, 2009) we can define translation between representations as the ability to move across, interpret, and, in a multi directional manner, link between representations of an underlying scientific concept, principle or process at a particular level of organization. However novices often have difficulty mastering the use of multiple representations in scientific disciplines, such as biology (e.g. Won et al, 2014; Ainsworth et al., 2011; Treagust and Tsui, 2013; Mulder et al., 2014), physics (e.g. Harlow et al., 2013; Jong et al., 2015), chemistry (e.g. Gilbert and Treagust, 2009; Taber, 2013; Olimpo et al, 2015) and biochemistry (e.g. Schönborn and Anderson, 2010). Like Ainsworth (2006), Cook (2006) and de Jong et al. (1998, p. 32, cited by Won et al., 2014), we can consider that the ability to integrate and coordinate multiple representations is a characteristic of expertise. The coordination of representations, was defined by Cook (2006, p. 1078) as *"the creation of referential connections between corresponding features of different representations"*. The coordination of representation is demonstrated, for example, by the capacity to understand and use the different types of structural representations of the same object reported in Figure 1 interchangeably (Head et al., 2005; Khanfour-Armale and Le Marechal, 2009, Stull et al., 2012).

Figure 1: Different representations of a given molecular structure

			
Concrete physical model	One Newman representation	One Dash-Wedge representation	The Fischer projection

The concept of model is omnipresent in chemistry teaching to represent abstract chemical ideas such as the nature of atomic and sub-atomic particles, molecular shapes, molecular polarity and other chemical concepts (e.g. Head et al., 2005; Chittleborough and Treagust, 2008; Jaber and Boujaoude, 2012; Head et al., 2005). Multiple representations of models have been used, for example, to highlight relationships across macro, submicro and symbolic levels of model representations (e.g. Jaber & Boujaoude, 2012; Becker et al; 2015; Kênia et al., 2015) or, in organic chemistry courses, to visualize the spatial arrangement of atoms in molecules (e.g. Stull et al., 2012; Kumi et al., 2013; Olimpo et al., 2015). This arrangement determines the identity of compounds, each of which has its own spatial individuality and uniqueness (Seddon and Shubber, 1984; Habraken, 2004). To represent this arrangement, organic chemists use, for example, concrete physical models that provide a tangible representation of 3D spatial relationships between atoms in the molecule and 2D iconic representations using certain conventions that are supposed to represent the 3D relations concisely on paper (Pribyl and Bodner, 1987; Hegarty et al., 1991; Hoffman and Laszlo., 1991; Wu and Shah, 2004; Jones et al., 2005; Stull et al, 2012; Graulish, 2015). Such 2D representations have been created for specific purposes during the history of chemistry (Hoffman and Laszlo, 1991; Goodwin, 2012; Dumon and Luft, 2008). Some well-known examples are the Newman projection to illustrate the energy change of a molecule with rotation around the internal carbon-carbon σ bond (concept of conformation), the Dash-Wedge representation to depict the spatial arrangement of substituents within a molecule and the Fischer projection to highlight the different stereochemical relationships between members of the same carbohydrate family (Stull et al, 2012; Olimpo et al, 2015). The widespread use of these stereochemical representations in the teaching of organic chemistry requires students to acquire competence in building, identifying, interpreting and coordinating these different representations (Shepard, 1978; Pribyl and Bodner, 1987; Kozma and Russell, 1997; Wu and Shah, 2004; Cook, 2006; Stieff et al, 2011; Stull et al., 2012; Olimpo et al., 2015; Graulich, 2015).

These competences involve spatial reasoning abilities. Spatial ability is the over-arching concept that generally refers to skill in representing, transforming, generating, and recalling symbolic, nonlinguistic information (Linn and Petersen, 1985). Psychologists have conducted many studies on the subject (e.g. Michael et al., 1957; McGee, 1979; Linn and Petersen, 1985; Lohman, 1988; Carroll, 1993; Voyer et al., 1995). Three major factors representing different kinds of spatial abilities have emerged from these studies: spatial visualization, spatial orientation and spatial relation. Definitions of these terms vary depending on the researcher and the specific study. The following definitions, consistent with usage by previous workers, have been adopted by chemists (Tuckey and Selvaratnam, 1993; Coleman and Gotch, 1998; Barnea, 2000; Ferk et al., 2003; Gilbert, 2010; Harle and Towns, 2011; Carlisle et al., 2015): 1) Spatial Visualization: the ability to understand three-dimensional (3D) objects from two-dimensional (2D) representations of them (and vice-versa); 2) Spatial Orientation: the ability to imagine what a three-dimensional representation will look like from a different perspective; 3) Spatial Relations: the ability to visualize the effects of the operations of reflection, rotation or inversion, or to mentally manipulate objects.

So, interpreting how 2D diagrammatic conventions represent 3D space and providing the results of spatial transformations make a high cognitive demand on spatial working memory (Stull et al., 2012; Padakar and Hegarty 2014; Stull and Hegarty, 2015). Thus it is not surprising that understanding the spatial structure of organic molecules is a source of difficulties for many chemistry students (Dori and Barak, 2001; Lujan-Upton, 2001; Pellegrin et al., 2003; Jones et al., 2005; Kurbanoglu et al., 2006).

Students' understanding of the molecular structure representations: literature review

Many authors agree that students find it difficult to visualize the spatial structure of molecules from 2D iconic representations (e.g. Bodner and Domin, 2000; Wu et al., 2001; Ferk et al., 2003; Kuo et al., 2004; Appling and Peake, 2004; Wu and Shah, 2004; Head et al, 2005; Abraham et al., 2010; Kumi et al., 2013; Olimpo et al., 2015). Linking symbolic representations of molecules in two dimensions to the visualization of their three-dimensional aspect is a complex task that requires the spatial abilities defined previously (Kozma and Russell, 1997; Barnea, 2000; Wu and Shah, 2004; Jones et al., 2005; Graulich, 2015).

Furthermore, to visualize the three-dimensional aspect of 2D representations, students must firstly understand and interpret the different graphic conventions used to translate the 3D reality into a planar representation (Habraken, 1996; Pellegrin et al., 2003; Kuo et al., 2004; Wu and Shah, 2004; Jones et al., 2005; Head et al., 2005; Bucat and Mocerino, 2009; Stull et al., 2010; Padakar and Hegarty, 2014; Stull and Hegarty, 2015), conventions that are rather abstract and intangible in nature (Kuo et al., 2004; Olimpo et al., 2015). On the other hand, they must take the positioning of the observer relative to the observed molecular structure into account (Pellegrin et al., 2003; Head et al., 2005; Kumi et al., 2013; Carlisle et al., 2015), an activity termed “perspective taking” by Stieff et al. (2010) and Stull et al. (2010). The result is that students have difficulties translating between the different diagrammatic representations (Pribyl and Bodner, 1987; Wu and Shah, 2004; Boukhechem et al., 2011; Harle and Towns, 2011; Stull et al., 2010, 2012; Kumi et al., 2013; Koutalas et al, 2014 ; Graulich, 2015; Olimpo et al., 2015; Carlisle et al., 2015; Stull and Hegarty, 2015) and when they try to connect different representations, they often focus on surface-level features without being aware of the relevant underlying characteristics (Cook, 2006; Kumi et al., 2013; Olimpo et al., 2015).

To translate between the different diagrammatic representations, students can use various strategies (Stieff and Raje, 2010; Stieff et al., 2010; Stieff, 2011; Hegarty et al., 2013). One strategy can be named “imagistic”, as it involves creating mental models of diagrams and then carrying out internal spatial transformations (e.g. mental rotation, perspective taking, and rule-based strategy). The other strategy, named “algorithmic-diagrammatic», is used by manipulating the molecular diagram with heuristics or algorithms without invoking mental images (Stieff, 2011; Stieff et al., 2010). However, Stieff (2011) notes that students preferentially employ imagistic reasoning for translating between various molecular diagrammatic representations. For example to translate between the Dash-Wedge representation and the Newman projection of Figure 1, students tended to compare the spatial information depicted in the two representations of the same molecule and then execute mental rotation of the group of substituents around the carbon atom C_3 to adopt the conformation of the Newman projection.

Several authors have shown that many students find it difficult to view the atom positions after mental rotation of molecular structure (Tuckey et al., 1991; Head and Bucat, 2002; Stull et al., 2012.). Others report that it is the dynamic nature of the molecules that is forgotten when translating between the different diagrammatic forms (Grosslight et al., 1991; Stieff et al., 2005; Boukhechem et al., 2011; Kumi et al., 2013; Olimpo et al., 2015). This concerns the "spatial relation" ability, where the rotation is important but often not achieved. As a result, the students see the 2D diagrams in a fixed conformation and do not engage in the linking of different conformations of a molecular structure illustrated in a Dash–Wedge representation, a Newman projection, or the Fischer projection (Olimpo, 2013). For example, the translation from the Newman or Dash-wedge diagram to the Fisher projection of Figure 1 is a complex task. It involves a high cognitive demand to interpret how all 2D diagrammatic conventions (Newman, Dash-Wedge and Fischer) represent 3D space, then requires use of spatial visualization (imagine the movement or displacement of parts of a spatial figure relative to other parts), spatial relation (mentally rotate Newman or Dash-Wedge representation to obtain the C_2H_5/CH_3 pair of substituents in eclipsed conformation) and spatial orientation (imagine how the 3D object should be looked at to obtain the Fisher projection). The students can achieve these multiple transformations if they are able to coordinate the three diagrammatic representations. An illustration of the lack of such coordination of representations is that Fischer projections were always restricted to the simple projection, or “flattening”, of the representation in the plane (Boukhechem et al., 2011; Olimpo , 2013; Olimpo et al., 2015).

It is commonly accepted that handling concrete and/or virtual molecular models facilitates students’ understanding of the three-dimensional structure of molecules and is a means to help them identify spatial relations so as to understand 2D representations (see for example the most recent works: Kuo et al., 2004; Wu and Shah, 2004; Ferk et al., 2004; Appling and Peake, 2004; Habraken, 2004; Jones et al., 2005; Stieff et al., 2005; Cook, 2006; Kurbanoglu et al., 2006; Abraham et al., 2010; Kumi et al., 2013; Olimpo et al., 2015; Carlisle et al., 2015). By making it easier to visualize molecular structures from different viewing perspectives and/or to physically rotate the model around the carbon-carbon bond and observe the result rather than mentally rotating, these tools contribute to student’s understanding of the different representations (Copolo and Hounshell, 1995; Wu et al., 2001; Cook, 2006; Stull et al., 2012, 2013; Al-Balushi and Al-Hajrib, 2014; Olimpo et al., 2015). They can serve as “catalysts” (or “cognitive scaffolds”, Stull and Hegarty, 2015) thatenable students to make connections between 2D and 3D representations (Dori and Barak, 2001: Head and Bucat, 2002; Ferk et al., 2003; Stull et al., 2012). Some studies have shown that, by reducing the cognitive load, since “*the conventions of a diagram (for depicting the 3D structure of the molecule in the 2 dimensions of the page) do not have to be maintained in working memory”* (Stull et al., 2012, p. 408), the handling of a concrete model improved students’ performance in translating between different diagrams of molecules (Stull et al., 2010; Stull et al., 2012; Paddakar and Hegarty, 2014; Stull and Hegarty, 2015). However, it is important to note that placing the models in their hands did not have significant effects on their performance of spatial transformation tasks for all students (Stull et al., 2012; Kumi et al., 2013). For example, in a study by Stull et al. (2012), many students ignored the models and other studies have shown that some students have difficulties in building the molecular models from stereochemical representations (Ferk et al., 2003; Appling and Peake, 2004) or when they try to turn or rotate models while discerning structural properties (Copolo and Hounshell, 1995).

Research aims and methodology

In the some studies conducted in U.S. on the use of concrete molecular models during the translation process between Newman, Dash-Wedge and Fisher diagrammatic representations, students can use or not models as help or feedback. The aim of these studies is to examine how students use or not concrete models. In a different institutional and cultural context, our study looked into the question of whether the effective handling of a concrete molecular model by students promotes translation between diagrammatic representations and the concrete model (or vice-versa) and the coordination of the different representations of a given molecular structure. We make the hypothesis that the ability to coordinate 3D and 2D representations involves being able to translate both from the diagrammatic representations to the concrete model and from the concrete model to its representation in 2D diagrams (Head and Bucat, 2002; Al-Balushi, and Al-Hajrib, 2014). The evaluation of students' ability to coordinate the different representations will therefore be based on an evaluation of three translation processes between representations of two molecular structures (Al-Balushi and Al-Hajrib, 2014):

- Construct 3D concrete models from Dash-Wedge and Newman representations;
- Draw a Dash-Wedge and a Newman 2D representation of a 3D concrete molecular model after rotating it to a certain degree;
- Produce a Fischer projection of a molecule from a 3D concrete model or any other 2D drawings.

Methodology

Subjects

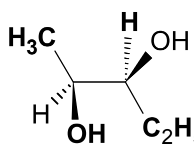
We administered a pencil and paper questionnaire to 41 undergraduate students at the Kouba (Algeria) Institute of Higher Education who were studying for a bachelor’s degree in physical science and who had volunteered to participate in the study. These students, predominantly female (37 women and 4 men), were also preparing to teach in establishments of a higher level than secondary school. They were divided into three options (Physics, Chemistry and Technology) depending on which branch of teaching they had chosen and the level they wished to teach. Whatever the option, the students received the same organic chemistry teaching during the third academic year, which included a course on stereochemistry where the conventions used to represent 3D space by 2D diagrams (perspective, dash-Wedge, Newman and Fisher), conformation, configuration, enantiomers and diastereoisomers were taught. For reasons of teaching organization, students of different options could not be interviewed at the same time. Students in the technology option were tested three months after taking the course whereas those in the fourth academic year of the chemistry and physics options were tested one year after teaching and those in the fifth year of the chemistry option, two years after the course. This delay ensured that the answers to our questions did not result from a simple memorization of recently learned knowledge. As students of the different options received the same teaching they were not differentiated in the results analysis.

Elaboration of questionnaire

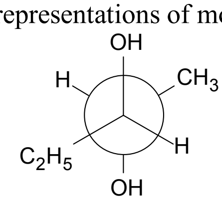
The three questions of the questionnaire (Table 1) were written after dialog between the two authors.

Table 1: Questionnaire

1- Consider the following Dash-Wedge and Newman representations of molecular structures:



(I)

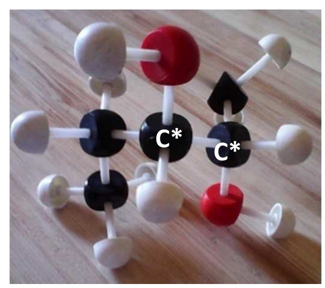


(II)

Build, and give a photograph of the concrete molecular model that corresponds to each representation

2- Consider the concrete model of structure (III):

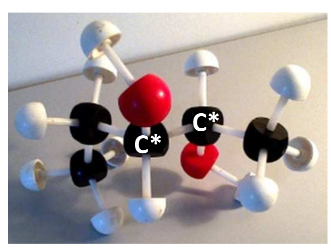
Photograph of structure III concrete model given to students



a-Draw the corresponding Dash-Wedge diagram and Newman projection for this structure.
b- Specify how you chose to position the observer relative to the C*-C* bond of the concrete model to obtain these representations. Number the two asymmetric carbons within the rules of the IUPAC nomenclature.

3- Consider the concrete model of structure (IV):

Photograph of structure IV concrete model given to students



a- Draw the Newman projection of the conformation that you think is the most stable. Specify how you chose to position the observer relative to the concrete model to obtain this projection.
b- Represents, using a concrete model, the molecular structure conformation according to the rules defined for drawing the Fischer projection and give a photograph of it.
c- Draw the Dash-Wedge diagram of this conformation and the Fischer projection of molecular structure IV.

The tasks of these questions were intended to evaluate students' abilities to coordinate the representations in translating from Dash-Wedge or Newman representations to 3D molecular models (and vice-versa) for two molecular structures and, for one molecular structure, to translate from the 3D molecular model in one staggered conformation to the Fisher projection.In the questionnaire, there was nothing that could orient students towards identifying that the structure I Dash-Wedge diagram was one Dash-Wedge diagram of the concrete model of structure III and that the structure II Newman diagram was one Newman representation of the structure IV concrete model.

Abilities to translate from the Dash-Wedge representation of structure I (≡ III) and the Newman representation of Structure II (≡ IV) to their representation by concrete (ball-and-stick) models were evaluated by the tasks of the first question. In other words, did the students make use of a spatial visualization ability related to their knowledge of the conventions used for 2D representations? The tasks of the second question assessed their abilities to translate from the structure III (≡ I) concrete model to these Dash-Wedge and Newman diagrammatic representations and thus concerned the abilities of visualization and spatial orientation, and a knowledge of the rules governing 2D representations (Dash-Wedge and Newman). The abilities evaluated with the tasks of the third question were: the ability to identify, by handling the 3D concrete model of structure IV (≡ II), the conformation for which interactions between substituents were minimal (spatial relationship ability); the ability to translate from this concrete model conformation to its Newman representation by specifying the position selected by observer (visualization and spatial orientation abilities); the ability to represent the molecular structure and conformation of structure IV (≡ II) respecting the rules to obtain the Fischer projection using the concrete model and then to draw these Dash-Wedge and Fisher representations (abilities in visualization, orientation and spatial relation related to the knowledge of conventions).

We think that the tasks students were expected to perform were valid. First, they are ecologically valid because these tasks could be used in the real organic chemistry classroom (Stull et al., 2012; Reiss and Judd, 2014). Then several reasons are related to their construct validity: 1) they tested the degree to which students understood how the different representations depicted the same molecules: (2S, 3S)-pentane -2,3-diol (Structures I and III) and (2R, 3S)- pentane -2,3-diol (Structures II and IV); 2) asking students to translate between different representations of the same molecular structure was a good indicator of their coordination of molecular representations; 3) the choice of two stereoisomers, with the distribution of substituents around asymmetric carbons,symmetrical or not, and the order and wording of the questions allowed us to evaluate the spatial visualization ability related to the knowledge of conventions used for 2D diagrammatic representations, spatial orientation, spatial relationship abilities and the capacity to combine these spatial abilities. This choice also enabled such abilities to be successively compared for two molecular structures.

Collection of data

The teachers supervising the students during their activities to answer to the questions were the organic chemistry teachers of the Kouba Institute of Higher Education. The questionnaire was distributed during a 90 minute session of chemistry practical work. Half of this time was devoted to this questionnaire, the other half to a questionnaire related to the students' understanding of stereochemical concepts. The nature of the questionnaire was made clear to the students (it was anonymous, not used for assessment, and was seeking personal conceptions).Given the constraints imposed by the insufficient number of ball-and-stick model boxes available, we divided the students into small groups of three or (rarely) four. After handling the model to visualize the three-dimensional spatial relationships of molecular structures, each student had to draw its molecular structures independently of the other members of the group under the watchful eye of an assistant teacher.

It should be noted that all the students had the opportunity to individually manipulate molecular models during their first academic year of general chemistry practical work and during one organic chemistry practical session in the third year to familiarize themselves with free rotation around a single bond, or breaking when a double bond was involved, and with the orientation of the substituents relative to the plane of a molecular structure. Nevertheless we assured ourselves that students were able to build and manipulate concrete models in two practical sessions concerning the spatial representation of molecular structures contained in the organic chemistry textbooks, prior to the assessment session.

Data analysis

For each question, an a priori analysis of the possible answers was carried out and the answers were encoded.

Translation concrete models ⇔Newman or Dash-Wedge diagrams

During the process of translating from Newman and Dash-wedge diagrams to concrete ball-and-stick model representations (and vice-versa), students could mentally or manually rotate the molecular structures around the C*-C* bonds to change their conformation. Also, during the translation process from concrete models to their Newman representations, the manipulation of the concrete model afforded the student complete freedom to orient the structure according to the axis C^*_2-C^*_3, or vice versa and to view the concrete model with carbon atoms C^*_2 or C_3^* at the front (see Tables 2 and 3).

Table 2: Newman representations of the possible conformations of structure III

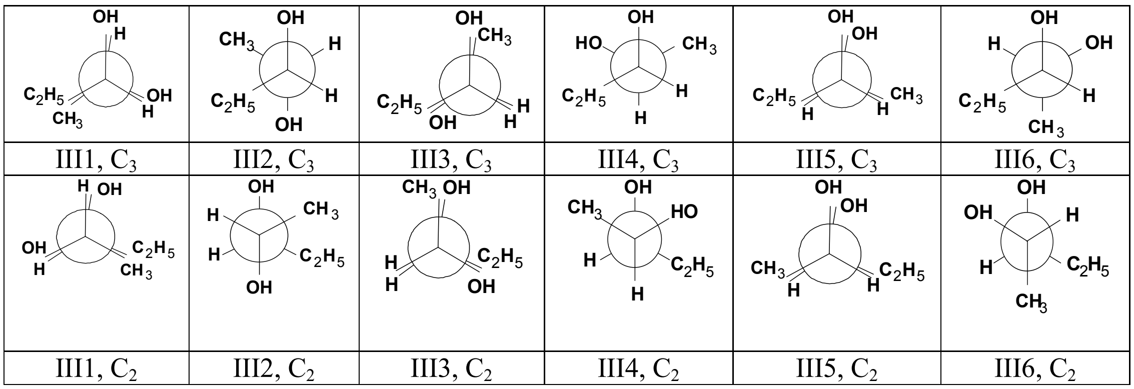
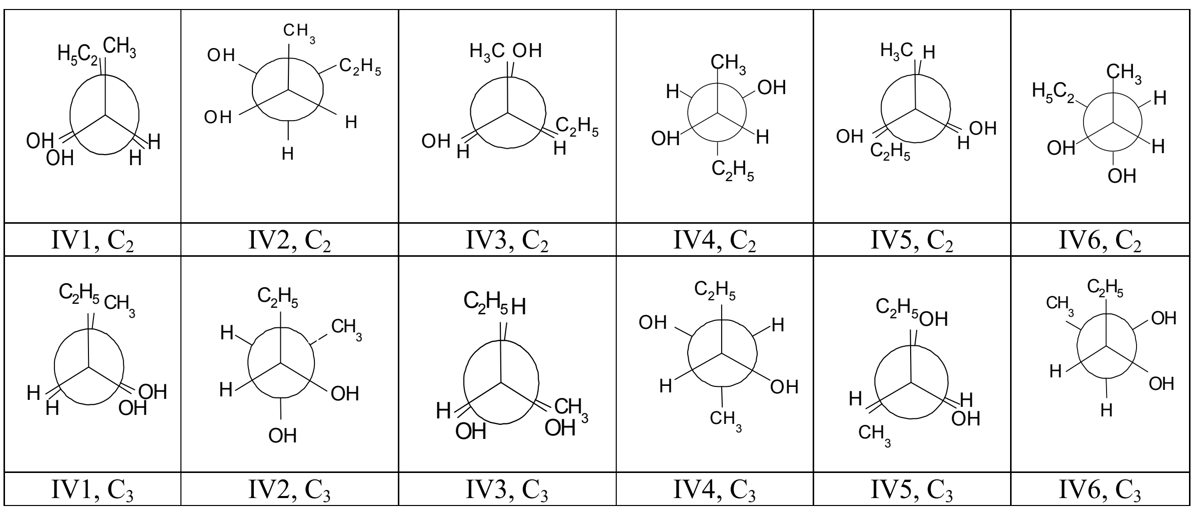
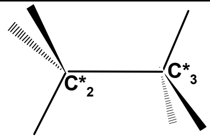
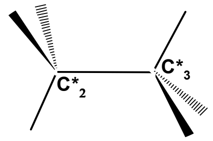
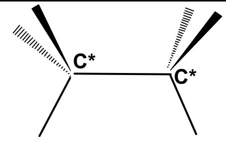
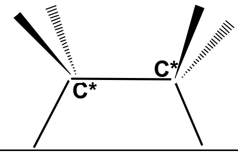
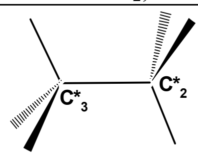
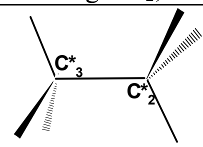
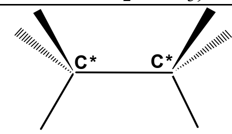
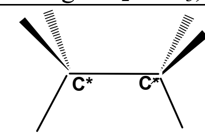


Table 3: Newman representations of the possible conformations of structure IV



To draw the Dash-Wedge diagram, students could orient the structure according to the axis C^*_2-C^*_3, or vice-versa, looking at: the asymmetric carbon 2 or 3 from a position slightly shifted to the left (L) or to the right (R), the concrete model in frontal position with respect to the C*-C* bond, in a position shifted slightly upward (U) or downward (D). Table 4 shows the coding of possible generic Dash-Wedge representations of staggered and eclipsed conformations of the molecular structures (limited to the orientation of the bonds, without indicating the nature of the substituents) according to the orientation of the structure and the position of the observer.

Table 4: Possible generic Dash-Wedge representations of staggered and eclipsed conformations and their coding

Staggered conformations		Eclipsed conformations	
			
Observer slightly to the left C_2, L	Observer slightly to the right C_2, R	Observer slightly to the left C_2 or C_3, L	Observer slightly to the right C_2 or C_3, R
			
Observer slightly to the left C_3, L	Observer slightly to the right C_3, R	Observer in front shifted downward C_2 or C_3, D	Observer in front shifted upwardly C_2 or C_3, U

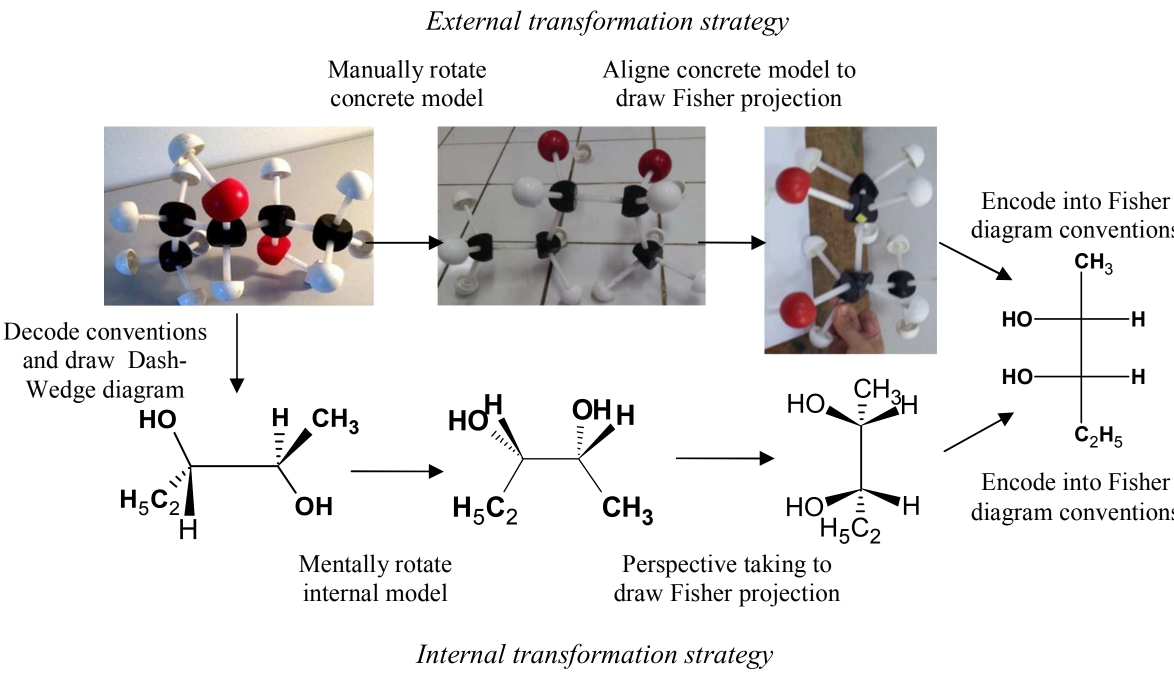
It should be noted that other drawings of these Newman or Dash-Wedge representations could be given if the observer rotated the entire concrete model to 120° or 240°.We indexed the representations as follows: structure number (III or IV), serial number in the energy - conformation diagram (1 to 6); carbon placed in front of the observer (C_2 or C_3), and the letter corresponding to the position adopted by the observer for Dash-Wedge representations (L, R, U or D). For example the conformation III1, C_2, U (see Table 8) corresponds to the eclipsed conformation with the maximal interaction energy between substituents; the structure was oriented according to the axis C^*_2-C^*_3; the observer looked at the concrete model from a frontal position with respect to the C*-C* bond, in a position shifted slightly upward (U).

Translation concrete model → Fisher projection

To represent the molecular structure conformation leading to the Fischer projection it is necessary to know the conventions used for this representation: the main carbon chain defined in the nomenclature is represented vertically; the carbon having the highest oxidation number is placed on top of the vertical axis; CH_3 and C_2H_5 substituents in eclipsed conformation are behind the observation plane and those on the horizontal axis are in front of this plane, which corresponds to a position of the observer over the C*-C* bond of the concrete model, thus seeing groups OH and H above the plane and the alkyl groups below. Two strategies can be used to translate between the concrete model and the Fisher projection (Figure 2): an external strategy using manipulation of an external concrete model, and an internal strategy employing mental imagery (Stull and Hegarty, 2015).

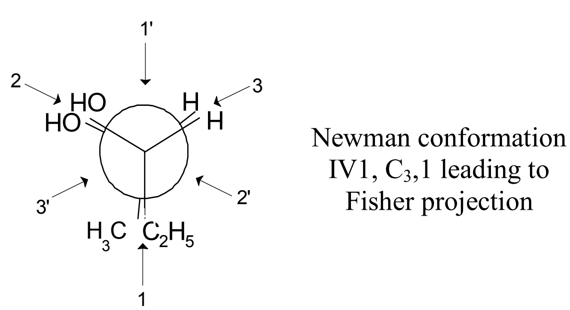
Using the external strategy suggested by question 3b of the questionnaire, the student should first manually rotate the concrete model in staggered conformation IV4 to obtain the C_2H_5/ CH_3 pair of substituents in eclipsed conformation IV1. Second, s/he should select the observer position relative to the C*$_2$-C*$_3$ bond to observe this concrete model conformation (shifted slightly upward, coded U, or downward, coded D) and the model orientation in conformity with the Fischer representation. But various model photographs (and Dash-Wedge diagram) of the eclipsed conformation IV1 were possible depending on the position selected by the observer and the model orientation.

Figure 2: Illustration of translation strategies between concrete model and the Fisher projection



We have represented these different orientations in the Newman diagram of the conformation IV1, C$_3$ of Figure 3. The C_2H_5/CH_3 pair can be set back (orientation 1) or forward (orientation 1') of the observation plane as can pairs OH / OH (orientations 2 or 2') and H/H (orientations 3 and 3 ')

Figure 3: The coding of the different possible model orientations



For the answer to each task, we also analyzed the different kinds of spatial reasoning abilities (spatial visualization, spatial orientation, and spatial relation) implemented by the students.

Results

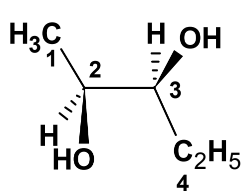
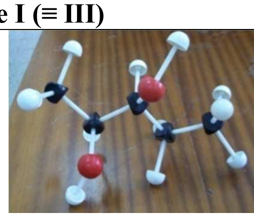
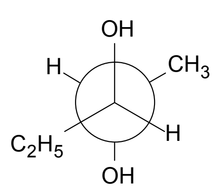
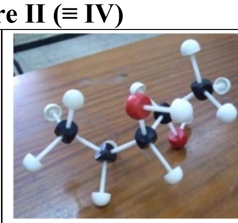
We considered that students were able to translate between molecular structure representations of the same object if they correctly represented diagrammatic representations by their concrete models or drew correct (or acceptable) diagrammatic representations from the concrete models. Therefore, we will initially seek to identify, for the two proposed molecular structures, whether students knew the conventions used for different representations and whether they gave correct representations (concrete model, 2D diagrams) or not. If a student was able to represent or use the different types of structural representations of the same object correctly, we considered that s/he had the capacity to coordinate these different representations. To evaluate the students' spatial orientation and spatial relationship abilities we complemented the analysis of representations by watching the conformation adopted for the different representations of these structures and the position relative to the C^*_2 - C^*_3 (or C^*_3 - C^*_2) bond chosen by students to observe molecular structures.

Translation of diagrammatic representations (Newman and Dash-wedge) → concrete models

Expected answers

If students maintained the conformations and orientations of the given Dash-Wedge and Newman molecular structure representations, the answers expected for the building of concrete models of the first question were those listed in Table 5. However, models representing this structure with other conformations could also be considered as correct.

Table 5: Photographs of the expected concrete models of structures I and II

Structure I (≡ III)		**Structure II (≡ IV)**	
			

Students' answers

Table 6 records the number of ball-and-stick models of different types constructed by students from the two representations: the Dash-Wedge representation of structure I (N.I) and the Newman representation of structure II (N.II).

The majority of students (26 i.e. 63%) succeeded in building a correct concrete model from structure I (≡ III) Dash-Wedge representation, either with conformation identical to the proposed molecular structure (18), or with another conformation obtained by free rotation around the C *-C * bond. The incorrect models built by other students mainly did not respect the position of the substituents, either on one of the asymmetric carbons (6 to C^*_2 and 5 to C^*_3) or on both (3).

Table 6: Quality of concrete models built from representations of structures I (Dash-Wedge) and II (Newman)

Quality of concrete model		N.I	N.II
Correct model	Conformation ≡ to diagram	18	19
	another conformation	08	12
Incorrect model	Positioning error of the substituents on one or both C *	14	8
	Other: Model with 6 carbons	01	0
No reply		00	2
Total students		41	41

A slightly larger number of students (31 i.e. 76%) built a correct concrete model from a structure II (≡ IV) Newman representation, either with an identical conformation to the proposed one (19) or with a different conformation (12). The incorrect concrete models built by students (8) showed an inversion of the arrangement of substituents on C^*_2.

Twenty-three students (56%) built correct models from both representations and only 7 (17%) proposed incorrect models for two representations. Of the remaining students, 8 seemed to find it easier to build a concrete model from a Newman than from a Dash-Wedge representation, and 3 found the opposite.

The above results show that, in carrying out these tasks of translating 2D diagrams into 3D concrete molecular models, the majority of students used spatial visualization ability related to a knowledge of the conventions (76% Newman, 63% Dash-Wedge and 56% both). It should be noted, firstly, that the visualization of the position of functional groups in space, was favored by the Newman representation for some students, while some showed a spatial relation ability (rotation around the C*-C* bond) during the building of concrete molecular model.

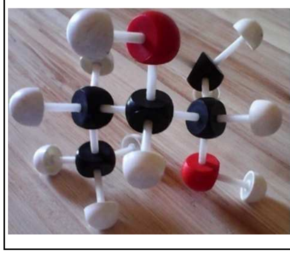
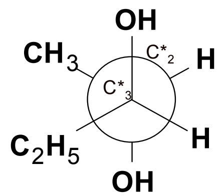
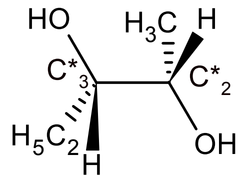
Translation of 3D ball-and-stick model diagrammatic representations (Newman and Dash-wedge)

For structure III (≡ I) (Q2)

Expected answers

The Dash-Wedge and Newman representations expected in answer to the second question, and corresponding to the conformation and orientation of the given concrete model were those drawn in Table 7**.**

Table 7: Expected Newman and Dash-Wedge representations of structure III

<table>
<tr><td>The concrete model given to students</td><td>Newman representation of its conformation</td><td>Its Dash-Wedge representation</td></tr>
<tr><td></td><td>
</td><td>
</td></tr>
</table>

To produce these drawings, the students had to place the observer in front of C^*_3 to achieve the Newman representation and in a position slightly shifted to the left to obtain the Dash-Wedge representation, respecting the sequence and orientation of the substituents and the conventions governing each representation.

Students' answers

Dash-Wedge representations of structure III

Of the 41 representations of the concrete molecular model given to students (staggered conformation III2, C_3), 34 (83%) were considered as acceptable: 18 were entirely correct and 16 approximately correct (sequencing of the substituents around each atom C* was correct, conventions for representing bonds were adopted, but the drawing was defective: the positioning of the bonds in space or bond angles were incorrect). For the other 7 representations, the sequencing and/or the conventions to represent bonds were not respected.

Table 8 reports the number of the different conformations identified in the 34 acceptable representations.

We note that, although the concrete model given to students presented a staggered conformation, many of them (22/34) chose to represent an eclipsed conformation, mainly conformation (III1), for which the interactions between the substituents are maximum. Conversely, conformation (III4), in which the interactions are weaker, predominated in the staggered conformations (9/12).

Table 8: Numbers of the various conformations identified in Dash-Wedge acceptable representations

	Identified conformations					
	Eclipsed		Staggered			
Observer position	III1	III3	III2	III4	III6	N

in front of	C_2	C_3	C_2	C_3	C_2	C_3	C_2	C_3	C_2	C_3	
L	0	0	0	0	1	0	3	0	0	1	5
R	1	1	0	0	0	0	3	3	1	0	9
U	8	4	5	2	0	0	0	0	0	0	19
D	1	0	0	0	0	0	0	0	0	0	1
total position	*10*	*5*	*5*	*2*	*1*	*0*	*6*	*3*	*1*	*1*	
total conformation	*15*		*7*		*1*		*9*		*2*		34

Letters L, R, U, D correspond to the position adopted by the observer (see Table 4)

Note that no student represented the expected conformation (III2, C_3) corresponding to the concrete model as it was presented to the students. While the concrete model was presented to them from left to right along the axis C^*_3-C^*_2, the majority of students (23/34) oriented the structure from left to right following the axis C^*_2-C^*_3 and observed it by placing themselves in front of this bond and in an upward shifted position (19/34). Note that the students worked standing up, which certainly affected their way of observing the model.

Newman representations of structure III

Table 9 reports the number of different conformations identified in the 40 students' Newman representations (correct or incorrect) of the concrete model given to them (staggered conformation III2, C_3).

The data in Table 9 show an equality of structure III concrete model representations in eclipsed or staggered conformations.

Table 9: Numbers of the various conformations identified in Newman representations

Representation	Identified conformations										N
	Eclipsed				Staggered						
	III1		III3		III2		III4		III6		
	C_2	C_3	C_2	C_3	C_2	C_3	C_2	C_3	C_2	C_3	
correct	7	2	5	0	1	1	1	0	0	0	17
incorrect	4	1	0	1	0	0	7	5	0	5	23
total position	*11*	*3*	*5*	*1*	*1*	*1*	*8*	*5*	*0*	*5*	
total conformation	*14*		*6*		*2*		*13*		*5*		40

We note that only 17 students drew correct representations, primarily those in eclipsed conformations (14/17). For the others, a reversal of the position of substituents was found on one or (rarely) both asymmetric carbons. Concerning the conformation adopted we observe an equality of structure III concrete model representations in eclipsed or staggered conformations and, as for the Dash-Wedge representations, a preference for the eclipsed conformation (III1) and staggered conformation (III4). Finally, a majority of students (25/40) chose to position the observer in front of C^*_2 (25/40) to obtain Newman representations.

Results of translation of structure III concrete model → Dash-Wedge and Newman representations

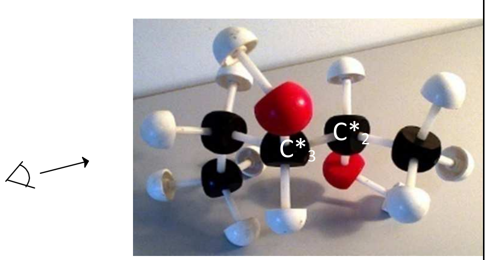
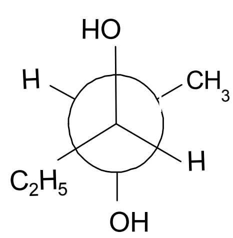
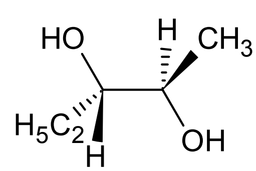
A significant proportion of students (31 i.e. 83%) gave an acceptable Dash-Wedge representation respecting substituent sequencing and conventions for representing bonds of the molecular structure III in and out of the plane of the sheet (spatial visualization ability and knowledge of conventions). To achieve these representations, the students all subjected the molecular structure to a rotation around the carbon-carbon bond, the majority (22, i.e. 54%) choosing the eclipsed conformation. A majority (23, i.e. 56%) oriented the structure in a direction different from that of the given model (C^*_2-C^*_3 instead of C^*_3-C^*_2), and 19 (46%) observed the structure from in front of the carbon-carbon bond in an upward shifted position. Orientation and spatial relation abilities were implemented.

The proportion of students giving a correct Newman representation respecting conventions and sequencing of substituents around the asymmetric carbon was significantly lower (17, i.e. 41%). Again the representation of the concrete model, whether correct or not, was performed after rotation around the carbon-carbon bond but with an equal choice of conformations between eclipsed (generally correct: 14/20) and staggered (generally incorrect: 17/20). The majority of students (25, i.e. 61%) chose to view the structure from in front of the C^*_2, and positioning errors of the substituents by students usually occurred on the C^*_3.

For structure IV (≡ II) (Q3)

Table 10 shows a photograph of the concrete model as presented to the students with its Newman and Dash-Wedge representations.

Table 10: Photograph of the concrete model and its Newman and Dash-Wedge representations

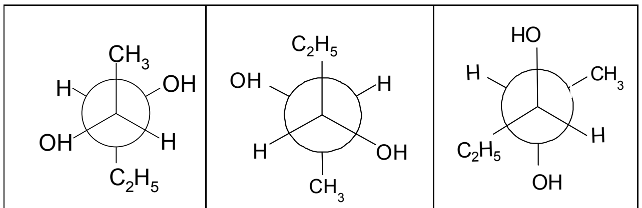
		
The concrete model as presented to students	Its Newman representation: IV4, C_3	Its Dash-Wedge representation: IV4, C_3 (G)

Translation of structure IV concrete model → Newman representation of the most stable conformation

Expected answers

To achieve the Newman representation of the most stable conformation, students had to know that this was the conformation for which the interactions between the substituents were minimal, that is to say the staggered conformation where the substituents with large steric requirements were farthest apart. Its representation depends on the position of the observer with regard to the molecular structure (in front of C^*_2 or C^*_3), as in the representations below (Figure 3) or other representations derived from them by a rotation of the entire structure through an angle of 60°, 120°, 180°, 240° (as other representation IV4, C3 in figure 3) or 300°.

Figure 3: Examples of the structure IV Newman representations of the most stable conformation



IV4, C_2	IV4, C_3

Students' answers:

Table 11 shows the numbers of the various conformations identified in the different Newman representations drawn by the students.

As regards the position of the observer relative to the concrete model for these representations, only 30 students gave an explicit response. We completed these responses using the data of Table 11. That is, whatever the nature of the response, the observer was positioned in front of carbon C^*_2 which was predominantly selected (24/41).

Table 11: The number of different conformations of Newman representations drawn by students

	Identified conformations								N
	Eclipsed				Staggered				
	IV1		IV5		IV4		IV6		
	C_2	C_3	C_2	C_3	C_2	C_3	C_2	C_3	
Structure IV acceptable Newman representations	2	0	0	1	15	10	1	0	29
Structure IV incorrect Newman representations		0	0	0	5	4	0	0	9
Other representations, totally incorrect or incomplete									3

The data in Table 11 show that the majority of students (29, i.e. 71%) made use of their spatial relation and visualization abilities to draw an acceptable Newman representation of structure IV respecting the sequencing and location of substituents around carbon atoms. Moreover, although 34 students (83%) represented structure IV in staggered conformation according to the most stable conformation (IV4), fewer of them (25, i.e. 61%) were able to draw the expected correct representation (15 IV4, C_2 and 10 IV4, C_3)for which interactions between substituents were minimal (spatial relation ability). It should be noted that only one student justified his correct representation of the most stable conformation by drawing the figure representing the different energy states of the molecule based on its conformation. For the other 9 representations, we noted an inversion of the positions of the substituents H and OH on one or two asymmetric carbons. Finally, a comparison of the relatively high non-response ratio for the position of the observer and the high proportion of acceptable conformations suggests that not all students felt the need to specify the observer's position when looking at the 3D molecular structure and projecting it onto a plane (spatial orientation ability); yet this is an important parameter for applying all elements of the rules governing the translation from one representation to another.

Translation of structure IV concrete model Dash-Wedge representation of conformation leading to the Fischer projection

Expected answers

The conformation corresponding to the eclipsed position of the C_2H_5/CH_3 pair (conformation IV1, 1) was the expected answer, which was to be represented by a Dash-Wedge diagram (see Figures 2 and 3). A 180° rotation of the Dash-Wedge representations was possible (conformation IV1, 1'). The observer had to be placed below the C*-C* bond to obtain a correct Fischer representation.

Students' answers

The numbers of various conformations identified in the students' Dash-Wedge representations are reported in Table 12.

Table 12: The numbers of different conformations identified in the students' Dash-Wedge representations

Conformation / Representation	IV1, C_2 ou C_3, 1 ou 1'	IV1, C_2 ou C_3, 2 ou 3	IV4	other	N students
acceptable	5	3	15	3	26
substituent inversion on a C *	0	1	6	1	8
totally incorrect					5
no answer					2

The data in Table 12 show that a majority of students (26 i.e. 63%) made use of their spatial visualization ability to provide an acceptable Dash-Wedge representation of structure IV. Although the expected response to the question corresponded to an eclipsed conformation of the structure, it was the staggered conformation of the original model given to students that was proposed by the majority (21 i.e. 51%). Only 9 students (22%) made use of their spatial relation (rotation) ability to obtain the C_2H_5 / CH_3 pair in eclipsed conformation and only 5 (12%) drew the expected representation (IV1, C_2 or C_3, 1 or 1') correctly. The other students did not use their spatial relation ability, presumably because they forgot the rules leading to a Fischer projection. We can add that the majority of the identified representations (20/34) were, as in the case of structure III, oriented the direction C^*_2-C^*_3 with the position of the observer slightly shifted to the left.

Comparative study of translation of structure III and IV concrete models Dash-Wedge and Newman representations

Table 13 records the number of students who gave an acceptable answer for the translation representation(s) → concrete model(s) and concrete model(s) → representation(s). Concerning the structure IV Dash-Wedge and Newman representations drawn by students according to the concrete model, it was the number of acceptable representations of this structure identified in students' answers that were counted, regardless of whether the representations agreed with the expected answers.

Table 13: Number and percentage of students who represented structures III and IV correctly by a concrete model or a diagram in 2D

	Concerte model building	Model → Dash-Wedge	Model → Newman	Model → Dash-Wedge and Newman	Coordination representations ↔ models
Structure III (≡ I)	26(63%) (Dash-Wedge →Model)	34 (83%)	17 (41%)	16 (39%)	22 (54%)
Structure IV (≡ II)	31 (76%) (Newman→Model)	26 (63%)	29(71%)	18 (49%)	21 (51%)
Structures III and IV	23 (56%) (representations →models)	22 (54%)	10 (24%)	5 (12%)	12 (29%)

The data in Table 13 show a difference between structures III and IV for translations between 3D model and 2D representations. For structure III, the percentage of students giving a correct Dash-wedge representation (83%) was higher than for structure IV (63%). On the other hand, the opposite was true for the Newman representation: 41% for structure III and 71% for structure IV. It follows that, globally the ability to translate from 3D models to 2D representations was better for structure IV: 49% against 39%. In addition, the percentage of students able to correctly translate the concrete models representing the two structures into 2D representations was larger for the Dash-Wedge representation (54%) than the Newman ones (24%). Thus the handling of concrete models seems to promote the mobilization of visualization, orientation and spatial relation abilities more when translating a 3D structure towards this Dash-Wedge representation than towards its Newman projection.

Coordination molecular model ⇔Dash-Wedge and Newman diagrams representation.

To assess how handling a concrete model helped students to coordinate 2D and 3D representations (pass from concrete model to its diagrammatic representations and from diagrams to concrete model), we intersected the correct answers of each student about translation of the Dash-Wedge or Newman diagrams in the concrete model with those given for the translation of structure III concrete models in the Dash-Wedge representation and of structure IV in the Newman representation. The data appear in the last column of Table 15. They show that the majority of students were able to coordinate both a Dash-Wedge representation (structure III: 54%) and a Newman representation (structure IV: 51%) with their respective concrete models. However, only 29% of students had the spatial reasoning abilities to coordinate diagrammatic representations in 2D (Dash-Wedge and Newman) of the two molecular structures with their 3D concrete model.

Translation of structure IV concrete model Fischer projection

The translation from the model presented to students to its Fischer projection is a complex task that requires spatial visualization, spatial rotation and spatial orientation abilities (see Figure 2).

Representation with concrete model of the structure IV conformation leading to Fischer projection

Various photographs of the eclipsed conformation model were possible depending on the position according to the C^*_2-C^*_3 bond selected by the observer to view this concrete model conformation and the model orientation (see Figure 3).

The students took photographs of the model by adopting the different conformations shown in Table 14.

Table 14: Numbers of conformations represented by students using the concrete model to obtain a Fischer projection

Conformation represented	N
Eclipsed conformation IV1, C_2 or C_3, 1 or 1 '	9
Initial model conformation (IV4)	23
Other eclipsed conformations	7
No answer	2
Total students	41

Only 9 students manually rotated the concrete model around the C*-C* bond in order to obtain a conformation where the C_2H_5/CH_3 pair was in an eclipsed position. Other students either contented themselves with photographing the model in its initial conformation (23 students), sometimes by placing the model in a vertical position, or executed rotations leading to a variety of other eclipsed conformations.

Fischer representation of structure IV concrete model

To draw the Fischer projection, students, should not only have rotated the concrete model around C*-C* bond (external strategy, Figure 2) to obtain eclipsed conformation IV1, C_2 or C_3, 1 or 1' but also have oriented the concrete model to respect diagram conventions ("perspective taking") before projecting it onto the plane of the sheet (the main carbon chain defined in the nomenclature is represented vertically; the carbon having the highest oxidation number is placed on top of the vertical axis; CH_3 and C_2H_5 substituents in eclipsed conformation are behind the observation plane and those on the horizontal axis are forward of this plane (conformation IV1, $C_{3,}$ 1). Table 15 reports the numbers of the various categories of representations of the Fischer projection drawn by students.

Table 15: Categories of students' representations of Fischer projection

<table>
<tr><td colspan="3">Categories of representations</td><td>N</td></tr>
<tr><td colspan="3">Correct Fischer projection of conformation IV1, C_3, 1</td><td>4</td></tr>
<tr><td rowspan="3">Flattening of other IV1 conformations</td><td rowspan="2">With main carbon chain vertically but perspective taking incorrect</td><td>CH_3 at the top</td><td>2</td></tr>
<tr><td>C_2H_5 at the top</td><td>8</td></tr>
<tr><td>Other</td><td></td><td>2</td></tr>
<tr><td rowspan="3">Flattening of IV4 conformations</td><td rowspan="2">With main carbon chain vertically</td><td>CH_3 at the top</td><td>12</td></tr>
<tr><td>C_2H_5 at the top</td><td>4</td></tr>
<tr><td>Other</td><td></td><td>5</td></tr>
<tr><td colspan="3">Flattening of other conformations</td><td>3</td></tr>
<tr><td colspan="3">Totally incorrect</td><td>1</td></tr>
<tr><td colspan="3">Total number of representations</td><td>41</td></tr>
</table>

Only 4 students drew a correct Fisher representation. The analysis of the strategies used to obtain these representations showed that one student used the external strategy of Figure 2 and one other student used the internal strategy of Figure 2 by representing the Dash-Wedge diagram of the initial model (conformation IV4) then mentally rotating the structure around the C*-C* bond to obtain conformation IV1 (without diagram) before projection. For the other two students, the strategy was mixed: after manually rotating the concrete model, they represented the Newman projection and used this representation to obtain the Fisher projection.

We note that the great majority of students (36/41, i.e. 88%) simply drew the projection (or "flattening") onto the plane of molecular structure in various conformations, depending on their observer position relative to the model. We can also say that the rules leading to a Fischer projection were only partially known by our students. Although a significant proportion of students (30/41, i.e. 73%) remembered that the main carbon chain defined in the nomenclature should be upright, only 18 (44%) placed the carbon having the smallest index in the carbon chain at the top of the vertical axis and 16 (31%) knew that the molecular structure must be in a particular eclipsed conformation to obtain a Fischer projection. Finally, only a few students remembered the "perspective taking" necessary to obtain the Fischer projection of one molecular structure.

Coordination of concrete model, Dash-Wedge and Fischer representations of structure IV

By intersecting the students' answers to questions 3b and 3c, we noted that of the 9 students who photographed the molecular model with the pair C_2H_5/CH_3 in eclipsed position (conformation IV1), 4 drew a Dash-Wedge representation according to the conformation leading to the Fischer projection (IV1, C_2 or C_3, 1 or 1'), two drew a Dash-Wedge representation of the conformation IV1 but with an incorrect orientation, two represented the initial conformation IV4, and one gave a totally incorrect Dash-Wedge representation. The connection between the correct Fischer representations and the various students' representations of the concrete model and Dash-Wedge diagram reveals that, of the 4 students concerned, 3 represented the concrete model with the conformation IV1 but without drawing a satisfactory Dash-Wedge representation and one gave a IV4 conformation representation for the concrete model and its Dash-Wedge representation. This suggests that handling the concrete molecular model did not promote understanding of what the Fischer projection of molecular structure represents. It led to "flattening" of various molecular structure conformations as a Fischer projection.

Discussion

Our results show that, during the translation process of Dash-Wedge and Newman diagrams to concrete ball-and-stick models (and vice versa) the majority of students made use of their spatial visualization ability related to knowledge of the conventions used for representing the 3D configuration of a molecular structure in 2D. Even if students did not feel the need to specify the observer's position when looking at the 3D molecular structure, the spatial orientation ability was identified in the majority of students' answers with the modification of the direction of giving the molecular structure (C^*_2-C^*_3 instead of C^*_3-C^*_2). Finally, spatial relation ability (rotation around the C*-C* bond) was implemented by numerous students.

So, it seems that handling a concrete molecular model promotes the translation process. But the manipulation of a concrete model seems more favorable to the mobilization of visualization, orientation and spatial relation abilities when translating a 3D structure to a Dash-Wedge representation than to Newman projection. This finding can be linked to the work of Stull et al. (2012) and Olimpo et al. (2015) that showed that students encountered difficulties in translating Dash-Wedge to the Newman representations. Olimpo et al. (2015) believe these difficulties can be attributed to a lack of clear understanding of what a Newman projection represents in three-dimensional space and/or a failure to recognize the dynamic nature of the molecules. However, it is apparent from the analysis of our results that this was not the case for a high proportion of students in our sample. So, how should this difference in performance in the translation concrete model–Dash-Wedge representation and concrete model–Newman representation be interpreted? First of all, it can be attributed to the fact that the Dash-Wedge representation is itself a very explicit 3D representation that can easily be identified with the 3D concrete model (Kumi et al., 2014; Olimpo et al., 2015): visualization, orientation and spatial relation abilities are made easier. Then, it can be attributed to greater difficulty with spatial relations consisting of mentally manipulating a 3D object to represent a Newman diagram in 2D. A frequently encountered error was an inversion of the H and OH substituents position on one (or rarely two) asymmetric carbons. According to Stull et al. (2012, p. 425) we think that this common error "… *in which the molecular substituents were configured correctly on one side of the molecule but not on the other side is suggestive of a piecemeal strategy in which the same transformation was not applied consistently".* The fact that the proportion of correct Newman representations was higher for structure IV may be explained by a symmetrical configuration of substituents around the two asymmetric carbons, which promotes a uniform application of the transformation process to both sides of the representation.

In the case of structure III, where translation did not require changing conformations, like Stull et al. (2012) we note that reconfiguring the models by rotating substituents around bonds within the models was observed more often when translating to a Dash-Wedge diagram than to a Newman projection. From a staggered conformation of the model, such reconfiguring led to an eclipsed conformation. When translation began with the Fischer projection, Stull et al. (2012) observed the inverse: eclipsed → staggered. In the case of translation from the structure IV concrete model in staggered conformation to the Fisher projection that required adopting a conformation where the C_2H_5/ CH_3 pair of substituents was in eclipsed conformation, we noted that, contrarily to the observation by Stull et al. (2012), few students changed conformation: they kept the staggered conformation of the original model. In addition, they misaligned the observer with respect to the substituents and the great majority adopted a "flattening" strategy of the model representation of molecular structure, strategy identified in the case of diagrammatic translations (Boukhechem et al., 2011; Olimpo, 2013; Kumi et al. 2013; Olimpo et al., 2015). Like Olimpo et al. (2015) we believe that this inappropriate combination of representational skills utilized by students indicates that students do not appreciate the conventions represented by the horizontal and vertical lines in the Fischer projection. They focus on surface-level features without being aware of the relevant underlying characteristics (Cook, 2006; Kumi et al, 2013; Olimpo et al, 2015). From this we can conclude that the manipulation of a concrete model does not favor the mobilization of visualization, orientation and spatial relation abilities during the translation from the model presented to students to its Fischer projection.

Finally, does handling a concrete molecular model promote the coordination of the different representations of a given molecular structure? Our results show that the coordination of each Dash-Wedge and Newman representation with their 3D structure was achieved by a majority of students. However, the students who coordinated these two representations with models were not the same in both cases, probably because of the difference of substituent distribution in the two structures. The result was that only a minority of our students showed spatial reasoning abilities allowing them to coordinate diagrammatic representations in 2D (Dash-Wedge and Newman) of the two molecular structures with their 3D concrete model. This can be explained by the difficulties encountered by students in respecting the atom positions after mental rotation of the molecular structure (Tuckey et al., 1991; Head and Bucat, 2002; Stull et al., 2012). Concerning the coordination of the concrete model with Dash-Wedge and Fischer representations of structure IV, the high degree of difficulty students had in understanding the conventions of the Fisher projection (Olimpo, 2015) led to the result that no students coordinated these representations after handling the concrete molecular model.

Conclusion

Our results show that, during the translation tasks, concrete molecular models have the potential to be an effective spatial tool to promote visualization, orientation and rotation abilities. However, their effectiveness is different for the different representations. These abilities are implemented more for Dash-Wedge than for Newman diagrams, and not at all for

Fisher projections. These differences can be explained by the fact that, during organic chemistry teaching, teachers place more emphasis on the Dash-Wedge representation than the Newman or Fisher projections. To echo Stull et al.: “*The imbalance of familiarity by students may have had an influence over the results”* (Stull et al., 2010, p. 343). Furthermore, although the spatial visualization ability related to knowledge of the conventions used for 2D representations (Dash-Wedge and Newman) was used by a majority of students to build a concrete model, effective use of the model required them to do more than establish the correspondence between the diagrams and concrete models. The manipulation of a 3D molecular structure did not have the same impact of promoting the visualization of the substituents’ distribution around asymmetric carbons for all students. This impact appears to vary according to the conformations (greater for the eclipsed than for the staggered conformation) and the distribution of substituents around asymmetric carbons (greater for symmetrical distribution).

This research implies that working with concrete models should be effectively encouraged in the teaching of organic chemistry. To help students visualize the relationship between multiple representations of the same molecular structure, particularly when the conventions of these representations are varied in nature, considerable teaching time should be devoted to an explicit discussion of these diagrams and the mechanisms by which one translates between representations (Stull et al., 2012; Kumi et al., 2013; Olimpo et al., 2015). The teacher can:

- include examples of molecules depicted in various conformations and different examples of perspective-taking during classroom instruction, offering students extensive opportunities to practice working with each of these representations of a molecule, so that they can gain a better understanding of the relationship between diagrams (Olimpo et al., 2015);
- give opportunities for students to draw and describe 2D diagrammatic representations using a concrete Ball-and-Stick model and vice-versa (Head and Bucat, 2002; Harle and Towns, 2010; Stull et al., 2012, 2013; Al-Balushi, and Al-Hajrib, 2014; Stull and Hegarty, 2015; Olimpo et al., 2015);
- propose translation tasks with the opportunity to generate self-feedback using concrete models(Padalkar and Hegarty, 2014): *“using models as feedback is a particularly effective way of inducing students to engage with models and experience their benefits”* (Stull and Hegarty, 2015, p. 15).

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