Investigating chemistry students’ skills to mentally manipulate (rotation & reflection) 2D symbolic molecular representations

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Abstract

The use of two-dimensional (2D) symbolic representations for describing, communicating and reasoning about phenomena and concepts is a common practice in Chemistry. Many researchers have shown that there is a positive correlation between visuospatial ability and fluency with chemical representations. The aim of this study is the exploration of chemistry students’ skills to visualize and mentally manipulate molecular structures. In this paper the results of the implementation to chemistry students of the computerized version of the Purdue Spatial Visualization Test: Rotation and two purposely designed and developed prototype «visualization» instruments dealing with rotation and reflection of 2D symbolic molecular representations are presented.

Keywords: molecular visualization; chemical representations; two-dimensional symbolic representations; visuospatial skills

1. Introduction

Fluency with Chemistry representations is closely related to molecular visualization ability and particularly the recognition of diagrammatic or graphic conventions, the perception of spatial information and the manipulation of spatial relations in molecular representations. Figure 1 shows examples of Chemistry tasks requiring students’ ability to mentally rotate or reflect molecular structures by the observation of their 2D symbolic representations. Researchers have shown that in Chemistry there is a significant correlation between students’ visual spatial ability and understanding of the underlying meaning of chemical representations (Bodner & Guay, 1997).

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However, several researchers have found that rotation and reflection transformations of 2D molecular representations are particularly troublesome for students (Wu, Krajcik, & Soloway, 2001).

Fig. 1. Example of spatial tasks, including visualization, rotation and reflection required in comparison of chiral (a) and achiral (b) molecules

1.1. Aim and objectives

The aim of this study is the investigation of chemistry students' skills to visualize and mentally manipulate molecular structures with specific geometries as these displayed in Figure 2.

Fig. 2. Two dimensional (2D) dash and wedge representations of molecules with square pyramidal (i, ii), octahedral (iii, iv) and triangular bipyramidal (v) geometry

The objectives to reach the aim are as follows: the evaluation of freshmen Chemistry students' general visual spatial ability, the evaluation of Chemistry students' ability to apply rotation and reflection transformations on 2D dash and wedge molecular representations and the examination of the relationship between students’ ability to apply rotations and reflections on 2D molecular diagrams and their general visual spatial ability.

2. Materials and methods

For the purposes of this study we designed, developed and implemented to chemistry students in the Department of Chemistry at Aristotle University of Thessaloniki a computerized version of the Purdue Spatial Visualization Test: Rotations (PSVT: R) by Bodner and Guay, (1997) and two prototype “visualization” instruments dealing with rotation and reflection transformations of 2D dash and wedge molecular representations.

2.1. The purdue visualization test of mental rotations, PSVT:R

The original PSVT:R test is a widely used 20 item spatial test and it is strictly timed at 10 minutes in order to restrict analytical processing (Bodner and Guay, 1997). In Figure 3, a representative item from its computerized version is displayed. In each item of the PSVT:R test students have to study how the object in the top line of the item is rotated, then to picture in their mind what the object shown in the middle line of the item looks like when rotated in exactly the same manner, and finally to select from among the five drawings given in the bottom line of the item the one that looks like the object rotated in the correct position.
The 20 items of the test are presented to all participants in the same order. There is shuffle within the five alternatives of each item. A 10 minute countdown and automatic termination of participants' attempt are among the main features of the computerized version of PSVT:R test. Multiple attempts are not allowed and for each participant a log file is recorded.

2.2. The mental rotation test of 2D symbolic molecular representations, MRot test

The MRot test aims to investigate students’ ability to perform rotation in molecules with certain geometry and orientation in space, by the observation of 2D dash and wedge symbolic representations. The test consists of 36 items and the available time to complete the test was defined to 20 minutes. A version of the test without time description has been also applied. A representative item from its computerized version is displayed in Figure 4a. There is shuffle within the six alternatives of each item. Multiple attempts are not allowed and for each participant a log file was recorded containing the correctness of their selection and the response time (RTs) per item in milliseconds.

In each item the participants are required to study how the initial stimuli in the top line of the item is rotated, imagine the effects of the same rotation on the second examined stimuli in the middle line and select among the six 2D representations the one that is identical with the examined 2D representation rotated through the proper axis (Figure 4a).
The three molecular geometries presented in the test as initial and examined stimuli are square pyramid, octahedron from two different perspectives and triangular bipyramid (Figure 2). All the examined 2D symbolic representations are 90° and 180° rotated molecular structures around the three Cartesian axes x, y and z (Figure 5).

2.3. The mental reflection test of 2D symbolic molecular representations, MRef test

The MRef test has been designed and developed in a similar manner with the MRot test. A representative item from its computerized version is displayed in Figure 4b. It consists of 18 multiple choice items that examine reflections of the same as above 2D molecular dash and wedge representations through Cartesian planes xy, zx and yz (Figure 5). The available time to complete the test was defined to 10 minutes.

3. Results and discussion

The participants in this research were 37 freshmen chemistry undergraduates at Aristotle University of Thessaloniki, during the academic year 2010/11. The three tests were initially given to 24 students (Group I) and then to other 13 students (Group II). The first group received versions of the MRot and the MRef test without time restriction while the second group received time restricted versions of the tests.

Table 1: Students’ performance in PSVT:R test

<table>
<thead>
<tr>
<th></th>
<th>Mean Time Completion (min)</th>
<th>S.D.</th>
<th>Mean Total Score (% success)</th>
<th>S.D.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group I (N=24)</td>
<td>9.6</td>
<td>0.7</td>
<td>10.8 (53.8%)</td>
<td>3.5</td>
</tr>
<tr>
<td>Group II (N=13)</td>
<td>9.9</td>
<td>0.1</td>
<td>10.9 (54.3%)</td>
<td>4.0</td>
</tr>
<tr>
<td>Group I+II (N=37)</td>
<td>9.6</td>
<td>0.6</td>
<td>10.8 (53.8%)</td>
<td>3.7</td>
</tr>
</tbody>
</table>

Table 2: Students’ performance in MRot test

<table>
<thead>
<tr>
<th></th>
<th>Mean Time Completion (min)</th>
<th>S.D.</th>
<th>Mean Total Score (% success)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group I (N=24)</td>
<td>28.8</td>
<td>4.1</td>
<td>28.8 (80.0%)</td>
</tr>
<tr>
<td>Group II (N=13)*</td>
<td>18.3</td>
<td>1.7</td>
<td>29.5 (82.1%)</td>
</tr>
</tbody>
</table>

Fig. 5. Rotation and reflection transformations of square pyramid representation used in (a) MRot and (b) MRef tests respectively.
A time limitation of 20 min is imposed by the application of the MRot test

Table 3: Students' performance in MRef test

<table>
<thead>
<tr>
<th></th>
<th>Mean Time Completion (min)</th>
<th>S.D.</th>
<th>Mean Total Score (% success)</th>
<th>S.D.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group I (N=24)</td>
<td>12.5</td>
<td>2.6</td>
<td>12.1 (67.1 %)</td>
<td>3.3</td>
</tr>
<tr>
<td>Group II (N=13)*</td>
<td>8.0</td>
<td>1.5</td>
<td>14.2 (78.6 %)</td>
<td>2.5</td>
</tr>
<tr>
<td>Group I+II (N=37)</td>
<td>10.8</td>
<td>3.2</td>
<td>12.8 (71.0 %)</td>
<td>3.2</td>
</tr>
</tbody>
</table>

* A time limitation of 10 min is imposed by the application of the MRef test

The three tests were distributed to both groups in the same order: PSVT:R, MRot and MRef. The log data from each test were analyzed within the two groups of students and within the categories of stimuli. The total score, the total time of completion (min), the number of wrong answers, the response time in each item (msec) and the participants’ choices in each item were gathered and analyzed in this study.

In Table 1, participants’ mean total score indicates that all groups obtained relatively poor performance in the PSVT: R test. Data from, Table 2 and Table 3, show that students of Group II, who completed the time restricted MRot test and MRef test were faster and more accurate than students of Group I. The findings of this study were also derived from the correlation analysis which was performed in order to investigate the relationships among students' performance in the three distributed tests.

The correlation analysis shows that Group II mean score on PSVT:R test was strongly and significantly related \[r(13) = 0.713, 0.006\] to their mean score on MRot test. Furthermore, a moderate but significant relationship \[r(13) = 0.586, 0.035\] between Group's II spatial ability as measured by PSVT:R test and achievement on MRef test was found. The data for Group I does not show statistical correlation between participants' total score on PSVT:R test and MRot test as well as between their total score on PSVT:R test and MRef test.

Additionally, for both groups there were a statistically significant positive correlation \[Group I, r(24) = 0.606, p < 0.001 and Group II r(13) = 0.639, p < 0.001\] between the mean score on MRot test and MRef test (Figure 6).

A further analysis of students' responses using two-way ANOVA in items of the MRot test indicates that there was a significant interaction effect of the examined rotation axis (x, y or z) and the rotation angle (90° or 180°) on students response times (Group I, F(2, 863)=124.51, p < 0.001 and Group II, F(2, 454)=8.22, p=0.038) as well as on students' score (Group I, F(2, 863)=11.73, p = 0.021 and Group II, F(2, 454) = 11.90, p = 0.021).

In the MRef test a similar analysis shows that the examined plane of reflection (xy, yz or zx) and the geometry of the initial stimuli, facilitated or impeded Group I students' response times (F(2, 431)=8.33, p = 0.038), whereas this
is not the case for Group II \( F(2,431)= 4.175, \ p = 0.105 \). Moreover the same analysis indicates that there wasn’t significant interaction effect of the examined factors on students score (Group I, \( p > 0.05 \) and Group II, \( p > 0.05 \)).

A planned comparisons analysis for each examined rotation axis and each examined rotation angle were also conducted. The later analysis shows that students in Group I responded faster to items dealing with 180° rotation than with items dealing with 90° rotation for all axes \((x\text{ axis}: t(2) = 6.015, p = 0.027, y\text{ axis}: t(2) = 10.360, p = 0.009 \) and \( z\text{ axis}: t(2) = 9.208, p = 0.012 \). On the other hand, students from Group II responded relatively faster to items dealing with 90° rotation than with items dealing with 180° rotation around the y axis \((t(2) = 3.185, p = 0.086)\).

4. Conclusions

The significant correlation between Group II scores on PSVT:R and time restricted versions of MRot and MRef test indicates that the time pressure impels students to employ visuospatial strategies rather than analytical strategies to apply rotation and reflection transformations on 2D molecular diagrams. In addition, the existence of significant correlation between the performance on MRot and Mref tests indicates that students applied similar strategies to the tasks which examine rotations and reflections. Furthermore, analysis revealed that the examined rotations and reflections seem to have specific effect on students' selections and response times in the items of both the MRot test and MRef test respectively.

Acknowledgments

This research has been co-financed by the European Union (European Social Fund – ESF) and Greek national funds through the Operational Program "Education and Lifelong Learning" of the National Strategic Reference Framework (NSRF) - Research Funding Program: Thales. Investing in knowledge society through the European Social Fund.

References