Exploring the effect of computer-supported visualization on 2D and 3D chemical structural formulas identification

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Abstract: This study aims to explore how computer-supported visulaization affect how well students identify chemical structural formulas. To collect data for this study, a chemical structural formulas conceptual questionnaire, event-related potential experiments and interviews were administered to eighteen university students majoring in chemistry. The results showed that (1) students with strong visualization used more visual-spatial strategies to identify 3D computer models; (2) students with lower visualization often used similar imagery intelligence and strategies for identifying 2D chemical structures as 2D computer models; (3) most students used similar strategies to identify 3D computer models and 3D chemical structures. This study suggests that event related potential (ERP) technology could reflect the visualization of students and help further studies to explore the effects of visualization abilities on science learning.

Key words: chemical structures, event-related potentials (ERPs), visualization

1. Introduction

Chemistry is a difficult subject for students and one of the most important and difficult topics in chemistry is that of chemical structures (Korakakis, Pavlatou, Palyvos, & Spyrellis, 2009; Mayer, 2001). Learning about chemical structures must start with their identification. Some studies have suggested that computer-supported three-dimensional (3D) virtual chemical structures are more easily identified by students and could enhance their learning of chemical structures (Wu & Shah, 2004). However, other studies have indicated that people identified 3D models through visualization processing may lead to cognitive overload, making it more difficult to identify and learn chemical structures (Gerjects & Scheiter, 2003). Therefore, this study wanted to explore the effect of visualization on computer-supported 2D and 3D chemical structural formulas identification. The research question is based on the research goals.

Wang, Chiew and Zhong (2010) have suggested that many cognitive processes are difficult to explain verbally. Hence, it is insufficient to investigate the identification of 2D and 3D chemical structures simply using questionnaires and interviews. Previous neurophysiologic researches have suggested that humans will show similar trends, while responding to the same task, in elicited event-related potentials (ERPs) and in strategies, such as recognition, identification, thinking or problem solving (Lai, Lin, Liou, & Liu, 2010). Therefore, this study used ERPs to further strengthen previous research findings and investigate the application of visualization in the identification of chemical structures.
ERPs is a procedure used to collect data on the electrical activity of the brain through the skull and scalp. The averages of these corresponding electrical activities were integrated as

specific ERPs components (Coles & Rugg, 1995). In this study, there were two main sets of specific ERPs components. One is the early ERPs components N1, N2 and N250 (Caharel, Jiang, Blanz, & Rossion, 2009; He, Humphreys, Fan, Chen, & Han, 2008). Another is the score of correct responses, which is measured by the number of correct responses when participants manipulate the experiments.

The largest negative peak occurring between the latencies of 80-200ms is called the N1 component (Caharel et al., 2009; Jeffreys, 1996; Kasai et al., 2003). If the amplitude of the N1 component is larger, the participant has applied more visualization ability in the experiment (Caharel et al., 2009). The largest negative peak occurring between the latencies of 200-350ms is called the N2 component (Shedden & Nordgaard, 2001). A larger N2 amplitude was found when recognizing 3D figures rather than 2D figures (Shedden & Nordgaard, 2001). Based on previous studies (Caharel et al., 2009; Kasai et al., 2003), the N1 and N2 components were always found within the centre and occipital lobes (CZ, OZ, O1, O2 electrodes).

Past research mentioned that the ERP data of participants will show a larger N250 component when they identify the same contours of a face with different facial expressions or parts of the face, such as the nose or eyes, or different individual identity, emotional expression etc (He, Liu, Guo, & Zhao, in press). The N250 component occurs with a latency between 220-250 ms after stimulus onset (Caharel, Jiang, Blanz, & Rossion, 2009). According to the previous studies, the N250 component was always found in occipito-temporal electrode sites including TP7, TP8, T5, and T6. Students who had a greater recognition of the chemical elements within chemical structures would reveal a larger N250 amplitude compared to those who only noticed the figures of chemical structures. The amplitudes of N1 and N2 from CZ, O1, OZ and O2 were used to explore the influences of visualization on the identification of 2D and 3D figures and chemical structures. The amplitudes of the N250 component from TP7, TP8, T5 and T6 were used to investigate the influences of imagery intelligence on the identification of 2D and 3D figures and chemical structures. The results of this research offered the implication of learning and teaching strategies in identifying chemical structural formulas.

2. Methodology

2.1 Research Population and Instrument

This study was conducted at an urban university in Taiwan. Fifty university students majoring in chemistry (n=50, 31 males, 19 females; Mean age ± S.D. = 20.9 ± 2.0 years) participated in the study.

A questionnaire, developed by the authors and based on previous researches (Chiu & Fu, 1993; Frailich et al., 2009), was administered to the participators. The questionnaire (perfect scores = 100) involved ten questions (perfect scores for each question = 10). These questions were used for understanding the learning performances of students related to chemical structure. The questionnaire was constructed using the Delphi method and was determined by reaching consistency. The expert panel involved two science educators, two science teachers, one chemist and two psychologists. Then, the constructed questionnaire was tested by thirty university students majoring in chemistry to validate the content, reaching a Cronbach's α value of .935.

After the test, two science teacher graded the questionnaires. Based on the scores of the questionnaire, students with upper and lower 27% of total scores were grouped into the high score (HSG, n=9; Mean age ± S.D. = 20.7 ± 2.7 years) and low score (LSG, n=9; Mean age ± S.D. = 20.4 ± 1.9 years) groups respectively (Kelly, 1939). A prediction of the

sample size was generated by GPower 3.1 Software. With power=0.90 and α=0.05, the sample size, which involved 18 participants in the study, was deemed appropriate (Sokel & Rolf, 1981). All participants gave voluntary consent to participate in the ERPs experiments. This study conformed to The Code of Ethics of the World Medical Association (Declaration of Helsinki) and was approved by the ethics committee of the National Kaohsiung Normal University.

2.2 ERPs Experiments

Based on the research questions, this study designed four types of ERPs experiments, which included computer-supported 2D figures, 2D chemical structures, 3D figures and 3D chemical structures. Both computer-supported 2D and 3D figures were presented by a similar shape to 2D and 3D chemical structures but without any chemical elements inside (Figure 1(a)). Each experiment included a short guideline and 62 trials (Figure 1(b)). The participants were asked to respond by recognizing whether the pair of figures was matched or not by pressing the appropriate buttons (matched: press ○; mismatched: press ×).

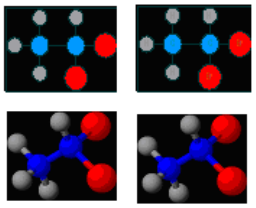
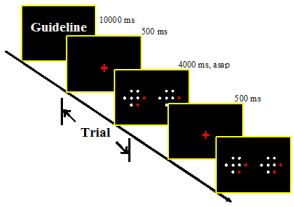
(a)  (b) 

Figure 1. (a) The examples of experimental tasks and (b)The meaning of "a trail" in ERPs

2.3 Data Collection and Analysis

The EEG was amplified (band pass, 0.01-40Hz) by the SynAmps/SCAN 4.4 hardware and software (NeuroScan, Inc., Herndon, VA); using the commercial electro-cap (Electro-Cap International, Eaton, OH) which was placed at 32 scalp locations based on the 10-20 International system. The electrode impedance was kept below 5 kΩ. The averaging epoch was 1024 ms, including 200 ms of pre-stimulus baseline. EEG channels were continuously digitized at a rate of 10000 Hz by a SynAmpTM amplifier. The signal was analogue filtered (0.1-200 Hz), A/D converted with a sampling rate of 10000 Hz and 14 bit precision, and digitally filtered in the range 0.1-30 Hz.

For the ERPs data, the N1 and N2 amplitudes were obtained from the CZ, OZ, O1 and O2 electrodes and the N250 amplitudes were obtained from the TP7, TP8, T5 and T6 electrodes (Caharel et al., 2009; Tanaka et al., 2006). The extracted data were analyzed by t-test (SPSS version 12.0).

3. Findings and Discussion

3.1 Students who performed a high visualization ability used more visual-spatial strategies to identify 3D figures

A paired t-test of the scores within both HSG and LSG groups showed that, for the students within the HSG group, the amplitude of N1 (t=6.0; P<.001; Cohen's *d*=2.799) and N2 (t=4.2; P<.01; Cohen's *d*=2.799) from the identification of 3D figures was significantly

larger than those from the identification of 2D figures. Likewise, for the LSG students, the amplitudes of N1 (t=3.6; P<.01; Cohen's *d*=1.951) and N2 (t=5.4; P<.01; Cohen's *d*=1.665) were significantly larger from the identification of 3D figures than those from the identification of 2D figures. Kasai et al. (2003) have suggested that the recognition and identification of 3D figures is not a simple perception task because students need to construct a 3D spatial representation of the external world. In other words, it is more difficult for a person to identify 3D figures than 2D figures. Our results additionally demonstrated that both HSG and LSG students used more visual ability, as indicated by brain activity, to identify 3D figures than 2D figures. Furthermore, the N1 and N2 components from the HSG and LSG students were analyzed by t-test (Table 1).

Table 1 The differences in N1 and N2 amplitudes between the HSG (n=9) and LSG (n =9) groups

Variable	Group	Mean ± S.D.	*t*	Cohen's *d*
N1 amplitude (3D)	HSG	9.6 ± 3.4	2.6*	1.206
	LSG	6.1 ± 2.3		
N1 amplitude (2D)	HSG	2.9 ± 0.6	0.9	0.339
	LSG	2.6 ± 1.1		
N2 amplitude (3D)	HSG	10.4 ± 6.2	2.8*	0.661
	LSG	7.2 ± 2.9		
N2 amplitude (2D)	HSG	4.1 ± 1.8	-0.1	-0.065
	LSG	4.2 ± 1.2		

* P<.05

Our results indicated that HSG students exercised more visualization ability than LSG students in the recognition and identification of computer-supported 3D figures (Nagamatsu, Liu-Ambrose, Carolan, & Handy, 2009). In contrast, there was no difference between the HSG and LSG students in the identification of 2D structures, demonstrating that both HSG and LSG students exercise similar visualization abilities in the identification 2D figures (He et al., 2008; Mathewson, 1999; Rafi et al., 2005). This study suggested that visualization ability is not likely to be the primary reason for the difference in learning performance between the HSG and LSG students.

3.2 Students who scored lower in the learning of chemical structure often used a similar imagery intelligence and strategies to identify 2D chemical structures and 2D figures.

We performed a paired t-test on data from HSG and LSG students and found that, for the HSG students, the N250 amplitude obtained from identifying 2D chemical structures was significantly larger than that from identifying 2D figures (t=11.6; P<.001; Cohen's *d*=2.953). However, for the LSG students, there was no statistic difference in N250 amplitude between 2D chemical structures and 2D figures identification tasks (t=-0.07; P=0.944; Cohen's *d*=-0.020). In other words, based on the definition of the N250 component used for this study, the HSG students needed to exercise more cognition ability to identify the contents of the chemical shapes (Caharel et al., 2009). This study suggests that the HSG students exercised different imagery intelligence when identifying 2D figure and chemical structures, while the LSG students used a similar imagery intelligence to complete these two experiments.

4. Conclusion

The results in this study indicated that students were better at identifying computer-supported 2D and 3D figures than 2D and 3D chemical structures. Hence, this study suggested that teachers could help students by practicing identifying 2D and 3D figures first. Second, many lower achieving students in this study thought that 2D chemical structures were the same as 2D figures because they had an alternative conception about ball and stick models of chemical bonding. As Boo (1998) mentioned, these students believe that a chemical bond is a real physical entity, and they did not understand the meaning of the 2D representation of chemical structures. Science teachers must avoid only introducing the ball and stick models when teaching chemical structures, and they need to emphasize the translation between 2D and 3D chemical structures through the use of multiple representations and analytical strategies. Finally, this study suggested that ERPs technology could reflect visualization abilities, as evidenced by brain activity, and we feel that the ERPs technology could help additional studies explore the effects of visualization ability and imagery intelligence on science learning.

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