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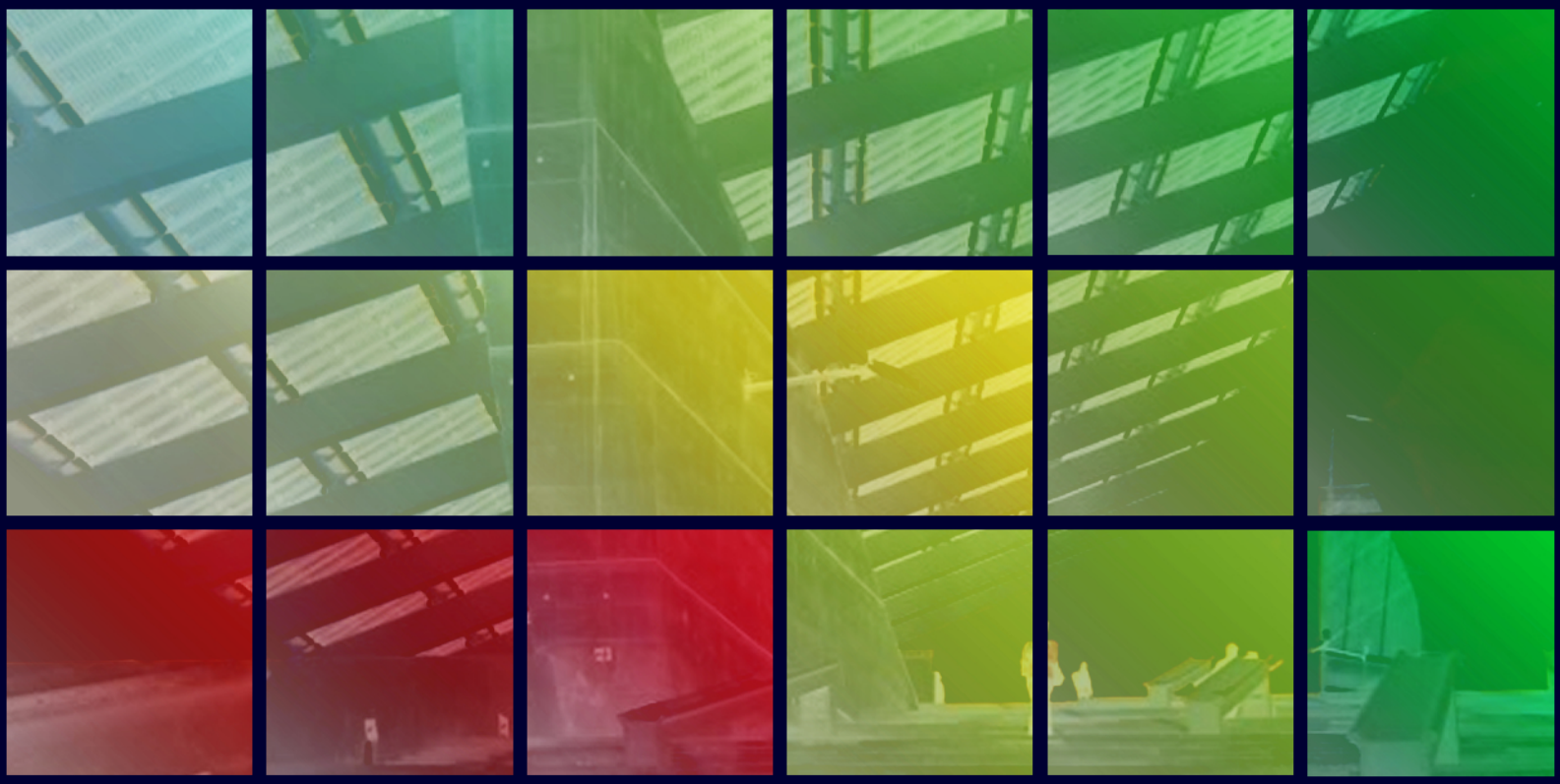

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INVESTIGATING THE EFFECTIVENESS AND EFFICIENCY OF THREE VISUAL REPRESENTATIONAL SYSTEMS FOR ASSIGNING CHEMICAL POLARITY

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Abstract

This study aimed to investigate students' assignment of chemical polarity using three visual modes representing electrostatic potential. The modes consisted of coloured lobes that indicate regions of negative (red) and positive (blue) potential, a colour gradient that maps the potential on the molecular surface and a novel representation that uses green surface(s) to show the interface between regions of positive and negative potential. Students' ability to assign polarity using the three visual modes was evaluated using a web-questionnaire. Mean scores indicated that students were able to successfully assign polarity to molecules using all the modes. However, students were less successful in identifying polar molecules in comparison with non-polar molecules using the map mode. A possible explanation for the lower scores for this mode is that the representational power of the map as a polarity assignment tool could be compromised by the visual complexity of the colour gradient, especially when a molecule is polar. The green surface representation was found to be a sensitive visual tool for assigning polarity to molecules, an encouraging finding since students were exposed to this visual mode for the first time. Given the possible perceptual constraints associated with the map mode, the results of this study might serve as a basis for uncovering the best conditions for pursuing a multiple representations approach to teaching chemical polarity.

Keywords: Visualization, Chemical polarity, Visual tools, Molecular representations, Web-based data collection, Teaching and learning, Chemical education.

1 INTRODUCTION AND AIMS

1.1 The importance of learning and teaching about chemical polarity

Predicting and assigning chemical polarity is often the gateway to providing chemists with important information pertaining to the physical characteristics of molecules. For instance, there is a direct relationship between molecular polarity and melting and boiling point properties. In addition, the deduction of bond and molecular dipole moments provides chemists with insight into predicting the 3D shape of different molecules.

Assigning molecular polarity calls on the ability to merge an interpretation of the overall shape of a molecule with the direction(s) of any dipole moments produced from the separation of charges within the molecule. Although understanding polarity provides students with chemical knowledge about fundamental properties of molecules such as solubility and intermolecular forces, science education research suggests that students often find predicting molecular polarity to be a demanding task (e.g. [1], [2] and [3]). Furió and Calatayud [1] showed that students' difficulties with molecular polarity might have its source in the perceptual challenges inherent in learners' interpretation of visualizations of chemical properties such as molecular shape. Interestingly, these authors revealed polarity to be a much more difficult concept for students to master than molecular shape, and in particular, learners struggled to apply knowledge of how bond polarity influences overall molecular shape. In work that, amongst other objectives, assessed learners' understanding of molecular polarity, Gonzalez et al. [2] uncovered that students battled to connect the symmetry of electron distribution to molecular polarity, could not distinguish between valence shell electron pair repulsion (VSEPR) theory and polarity, and confused bond and molecular polarity.

Given the potential learning difficulties associated with constructing knowledge about chemical polarity, some work in the literature suggests that polarity can be made more meaningful for novices by exploiting different visualizations of charge distribution (Fig. 1). For example, Jones [4] has pointed

out that visual representations such as electron density gradients can promote understanding of polarity. On this score, a study by Sanger and Badger [3] investigated how dynamic visualizations of electron density plots influenced students' understanding of molecular polarity and miscibility. One finding suggested that such visualisations of charge distribution assisted learners in acknowledging the influence of molecular shape on determining chemical polarity. The research also showed that viewing electron density plots improved students' conceptual knowledge of molecular polarity and intermolecular forces. Shusterman and Shusterman [5] have demonstrated how information about molecular polarity gained from interpreting electrostatic potential maps can be applied to understanding interactions between biological molecules. For example, this visual mode can be used to show how the alignment of guanine with cytosine occurs through three regions of opposite polarity in each molecule, allowing the biomolecules to associate through three hydrogen bonds. Similarly, students' application of knowledge gained from interpreting electrostatic maps to the importance of molecular polarity in the existence of intra and intermolecular forces in protein helices has also been illustrated by Sinex and Gage [6]. With respect to visualising molecular structural properties, Tuvi-Arad and Blonder [7] have recently shown how advanced chemistry concepts that are associated with polarity, such as continuous symmetry, can be cultivated through novel visualization tools.

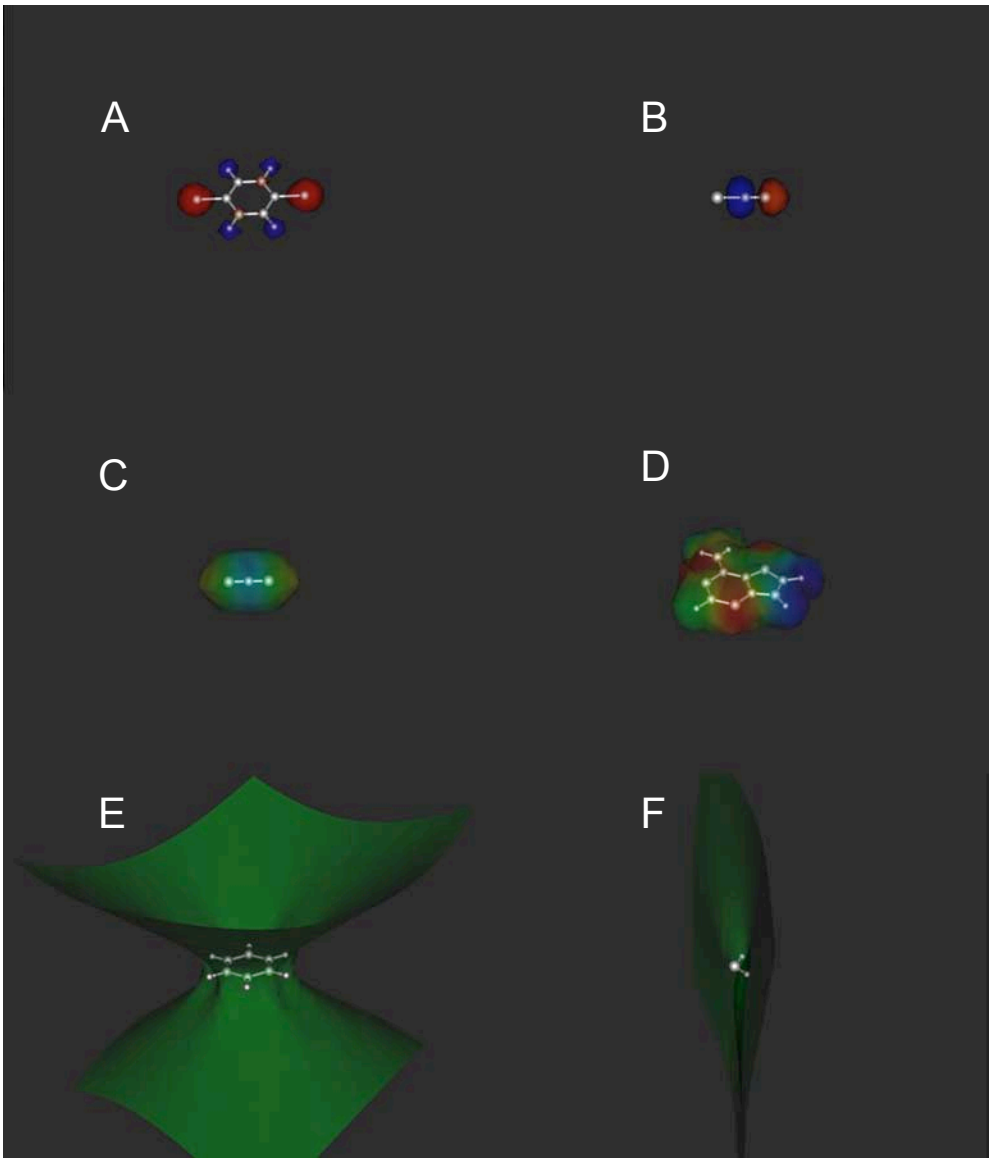

Fig. 1. Three representational systems for visualizing the chemical polarity of molecules. **A** and **B**: Regions of negative and positive potential represented as red and blue lobes (*RB*); **C** and **D**: An electrostatic map represented by a colour gradient showing electrostatic surface potential on a molecular surface (*MAP*); **E** and **F**: A novel representation that depicts a green interface between positive and negative regions around a molecule (*ISO*).

1.2 Different representational modes for visualizing molecular polarity

As inferred from results of the studies above, different representational modes of electrostatic potential can provide learners with visual information to support interpreting the polarity of a molecule (Fig. 1).

Examples of two representational systems available to chemists and educators for visualizing polarity include the following. Firstly, one type of visual mode uses coloured 'lobes' to indicate regions of negative (red) and positive (blue) electrostatic potential of the molecule (RB, Fig. 1 A and B). Secondly, in what is perhaps the most popular mode, a colour gradient is employed to map the electrostatic potential at the van der Waals surface (MAP, Fig. 1 C and D). In addition to these two modes, we have developed a novel representation [8] that visualizes the topography of the interface between negative and positive regions of electrostatic potential through a green isosurface(s), a visual surface produced by setting the isovalue to zero (ISO, Fig. 1 E and F).

With respect to the development of the visualization mode presented in Fig. 1 E and F above, we have deduced the following rules of interpretation for using the representational system to assign polarity to a molecule:

A molecule is non-polar if it generates:

I. one closed and rotationally symmetrical isosurface, and/or;

II. more than one isosurface, of which, each exhibits rotational symmetry with one or more of the other isosurfaces.

A molecule is polar if it generates:

III. any isosurface(s) that do not conform to either I or II.

Given the importance of understanding and visualizing the concept of polarity in learning chemistry, this study aimed to investigate students' assignment of chemical polarity using three different visual modes representing electrostatic potential. Specifically, the study raised the following research questions:

- Which of the representational modes will students use to assign polarity most effectively?
- Which of the representational modes will students use to assign polarity most efficiently?
- Are there any differences between the three modes with respect to combinations of simple/complex and polar/non-polar molecules?

2 METHODS

2.1 Design of the chemical polarity exercise

The exercise required students to assign polarity to a set of molecules. Molecules selected for the study consisted of 10 polar and 10 non-polar molecules which, in turn, comprised of 10 'simple' and 10 'complex' molecules. Together they comprised of 5 of each simple polar, simple non-polar, complex polar, and complex non-polar molecules. Simple molecules were defined as having a central atom and 7 constituent atoms or less. The selected simple molecules had steric numbers ranging from 2-6, with molecular shapes that included linear, bent, trigonal planar, tetrahedral, trigonal bipyramidal and octahedral configurations. Complex molecules were defined as lacking a central atom but consisting of more than 7 constituent atoms. Using this designation, an example of a simple molecule was carbon dioxide (CO_2, linear, steric number 2, 3 constituent atoms) while an example of a complex molecule was octagen ($C_4H_8N_8O_8$, eight-membered ring, 28 constituent atoms). Overall, the selection procedure ensured an equal representation with respect to both molecular polarity and structural complexity.

Images of the 20 different molecules were prepared in each of the RB, MAP and ISO modes (e.g. Fig. 1), with a transposed ball-and-stick figure to indicate molecular geometry, yielding a total of 60 images. Orientation of each molecule for presentation to students was deduced as follows: First, the largest plane in the molecule was aligned perpendicular to the plane of the screen. Second, where necessary, we identified the chemical group that was most unique (in terms of greatest molecular/atomic weight, and/or nature of constituent atoms) and aligned this group on the left. Third, we tilted the molecule downwards between 30 and 40 degrees (see Fig. 1). All of the images were constructed in the same scale. The images were integrated into a web-based platform for data collection.

2.2 Participants and web-based data collection

Nine first year student volunteers (mean age 20, 7 females and 2 males) enrolled in an introductory university chemistry course participated in the study. All students had been exposed to polarity concepts as part of a preceding university course. The participants completed a chemical polarity web-based questionnaire that comprised of assigning polarity to the 20 molecules using the three visual modes (60 images). The potential risk of any image order effects were reduced by employing a randomized block design for image presentation with 2 blocks containing 30 molecules each.

Each student was sent a unique individual internet link that could only be opened once. By checking an appropriate agreement box, students consented to taking the test which activated the questionnaire. Before students commenced the test, they were exposed to examples of molecules in each of the four categories across the three visual modes (12 images). For each student, the test began with the 12 example images, followed by the 60 test images presented in a random sequence. Each of the 60 images appeared on the screen one at a time. The participants were required to assign polarity to each displayed molecule by clicking a “polar” or “non-polar” box. The response and the time (sec.) taken to assign polarity were logged automatically for each image. The instructions for the test allowed students to take breaks between assignment tasks if desired.

During design and implementation of the web-based questionnaire, we adhered to a set of standards for internet-based experiments composed by Reips [9]. Amongst other criteria, these included: ensuring that the platform was pretested for clarity of instructions, checking for configuration errors, preparing ‘filter’ questions by having the first 12 items of the test the same standard items across all respondents, ensuring that multiple submissions were impossible, and recording logs of respondents’ interaction with the platform such as mouse clicks and relevant keystrokes.

2.3 Data Analysis

The response data were analysed with respect to two parameters, namely *effectiveness* and *efficiency* (cf. [10]).

The effectiveness of using the three visual modes to correctly assign polarity was assessed by investigating the students’ accuracies. Each correct assignment was awarded a score of one, and incorrect assignments were awarded a score of zero. Students’ mean scores across the five molecules representing a specific combination of molecular properties (i.e. simple polar, simple non-polar, complex polar, and complex non-polar molecules) were calculated for the three visual modes. For each student, the corresponding mean values were used as measures of the individual student’s accuracy in correctly assigning polarity to that type of molecule using the different visual modes. Differences in students’ accuracies using the three visual modes were analysed by examining mean values and confidence intervals (CI) of the accuracy scores across the students for the entire set of possible combinations of molecular properties and subsets of such combinations (e.g. polar vs non-polar and simple vs complex).

Efficiency of using the three visual modes to assign polarity was investigated by analysing response times. For each student, the corresponding response times for assigning polarity to a molecule was used as measures of the individual student’s efficiency in assigning polarity to that same molecule using the different visual modes. Should a student have paused during an assignment task, an outlier response time would have been recorded. The data were inspected manually for any such outliers. Differences in response times when using the three visual modes were analysed by examining mean values and confidence intervals of the response times across the students for all molecules, and for subsets of the molecules corresponding to different combinations of molecular properties listed above.

3 RESULTS

3.1 Effectiveness

The overall effectiveness of using the three visual modes to assign polarity to molecules is shown in Table 1. All three visual modes could be used by the students to assign polarity with mean accuracies of approximately 0.8. The mean value for the electrostatic map mode (MAP) is slightly lower than for the red and blue lobes mode (RB) and the green surface representation (ISO), but the variance in the data indicates that no firm conclusions about which mode is most effective for assigning polarity can be drawn from this observed difference.

Table 1. Overall descriptive statistics for the effectiveness and efficiency of assigning polarity to molecules using three visual modes

	Effectiveness (accuracy scores)					**Efficiency** (response times) (sec.)				
	Mean (±95% CI)	Median	SD	Max	Min	Mean (±95% CI)	Median	SD	Max	Min
RB	0.86 ± 0.05	0.80	0.15	1.00	0.40	5.1 ± 0.6	3.5	3.9	26.1	2.0
MAP	0.80 ± 0.06	0.80	0.18	1.00	0.40	4.7 ± 0.5	3.4	3.3	21.9	1.6
ISO	0.84 ± 0.06	0.80	0.17	1.00	0.40	5.1 ± 0.5	3.7	3.7	20.4	1.7

Analysis of accuracy in assigning polarity to molecules with different molecular properties revealed a difference in students' assignment of polar and non-polar molecules using the MAP mode. Assignment of polar molecules using this mode was less accurate than assignment of non-polar molecules (Fig. 2). Furthermore, mean accuracy scores in assigning polar molecules using the MAP mode was lower than the mean accuracy scores for polar and non-polar molecules using the RB and ISO modes.

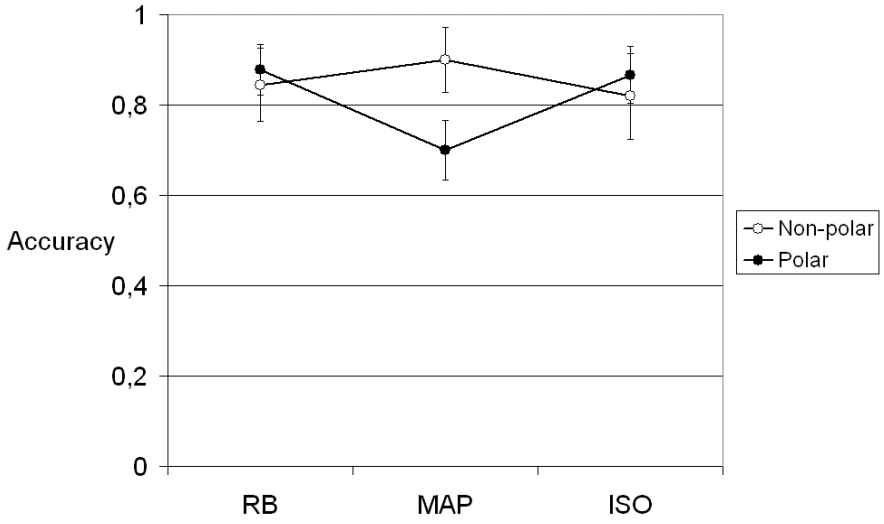

Fig. 2. Mean accuracies for the students (n=9) in assigning polarity to polar and non-polar molecules using the three visual modes. The vertical bars indicate 95 % confidence intervals

3.2 Efficiency

During initial inspection of the data, it was observed that on one occasion a student spent a significant time on an image. The response time for this image was six times larger than the second longest recorded response time. This was interpreted as an indication that the student paused during the assignment task, and therefore, the corresponding data point was considered an outlier and excluded from the analysis.

The overall efficiency of using the three visual modes to correctly assign polarity to molecules is shown in Table 1. The lowest mean and median response times for assigning polarity were observed for the MAP mode. In addition, the range of response times for the MAP mode was comparable to the ISO mode, and lower than the RB mode. Thus, the MAP mode can be interpreted to be the most efficient visual mode in assigning polarity, although the variance in the data warrants caution.

Analysis of mean response times for assigning polarity to different subsets of molecules indicated a difference in students' efficiencies of assigning polarity to simple and complex molecules (Fig. 3). For all three visual modes, the mean response times were lower for simple molecules than for complex molecules, indicating a higher efficiency in assigning polarity to simple molecules.

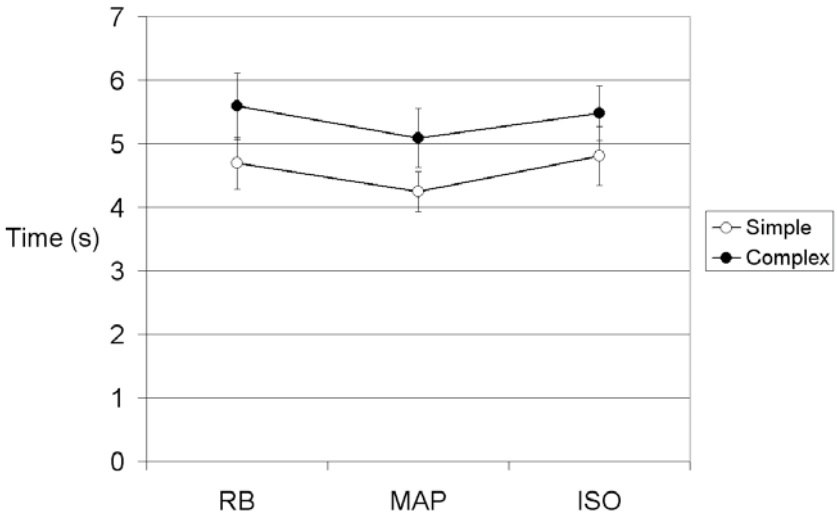

Fig. 3. Mean response times in students' assignment of polarity to simple (n=10) and complex (n=10) molecules using the three visual modes. The vertical bars indicate 95 % confidence intervals.

4 DISCUSSION

Based on the results of this study, the electrostatic map (MAP) appears to be a less effective visual tool for assigning polarity compared with the other two modes. This was most clearly shown for the assignment of polar molecules (Fig. 2). In a study by Sanger and Badger [3], it was showed that students were more successful at using electron density plots (synonymous with MAP in our study) to identify polar molecules than non-polar symmetric molecules. Specifically, results from these workers revealed that students who interpreted electron density plots were better at assigning symmetric molecules with polar bonds as being non-polar. With respect to the latter, our data suggest that from the three modes evaluated here, the MAP mode appears to be the most unfavourable for identifying polar molecules.

Although the relatively high efficiencies displayed for the MAP mode indicate that students did not find assigning polarity using this representation challenging, it nevertheless emerged as the least effective of the three for polar molecules. One possible hypothesis for the lower scores for this mode is that the representational power of the map as a polarity assignment tool could be compromised by the graphical detail of the colour gradient, especially when the molecule is polar. Using the map mode to assign *overall polarity* of a molecule may be a greater cognitive challenge than doing so using the other two modes, because students have to align molecular polarity with the asymmetry of the colour gradient (also, see [2]). From a cognitive perspective, when it comes to interpreting the ISO and RB modes, a reduction of visual complexity may reduce extraneous processing, which in turn, may free up working memory capacity for engaging generative processing, and ultimately, meaningful learning [11]. An implication of this finding is that whereas conventional methods (e.g. RB and MAP) for assigning polarity require students to integrate the relative positions of positive and negative regions, assignment of polarity via interpretation of an interfacial surface could place less strain on available perceptual resources.

As might be expected, the data revealed that students were able to assign polarity more efficiently to simple molecules than complex molecules using the three representations. This result is likely to be a reflection of the higher processing demands required for integrating the visual information from molecules with a more complex electrostatic field corresponding to charge distributed across a larger number of atoms in the structure. On average, students assigned polarity to simple molecules approximately one second faster than they did to complex molecules. Taken together, a possible hypothesis that could warrant further investigation is that complex and polar molecules represented in the MAP format require explicit explanation when used in introductory educational settings.

There is recent evidence in the literature suggesting that there is a benefit in reducing visual complexity and using multiple linked representations when teaching concepts associated with polarity (e.g. [7]). In support of this movement, one possible application of this study is to use multiple representational systems to display elements of charge distribution during teaching by actively comparing the three visual modes dealt with here.

5 CONCLUSIONS

Overall, this study has shown that students were effective and efficient at using all three representational systems to assign chemical polarity. It was also encouraging to note students' success at using the novel green interface system that they had encountered for the first time. Nevertheless, the data indicates that students may be less effective in assigning polarity using the map representation, especially when it comes to polar molecules. Hence, teachers should be aware of the potentially cognitively challenging nature of this conventional display as a tool for depicting molecular polarity. In turn, the results support using other representations including unconventional visual forms such as the green electrostatic interface representation for teaching about polarity.

The results of this study warrant further evaluations of the effectiveness and efficiency of different representational systems for communicating chemical polarity. In this regard, future work will be concerned with obtaining data from larger samples for the purpose of statistical generalisation as well as comparing student groups with varying levels of prior knowledge.

6 ACKNOWLEDGEMENTS

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