Students' Use of three Different Visual Representations to Interpret whether Molecules are Polar or Non-polar

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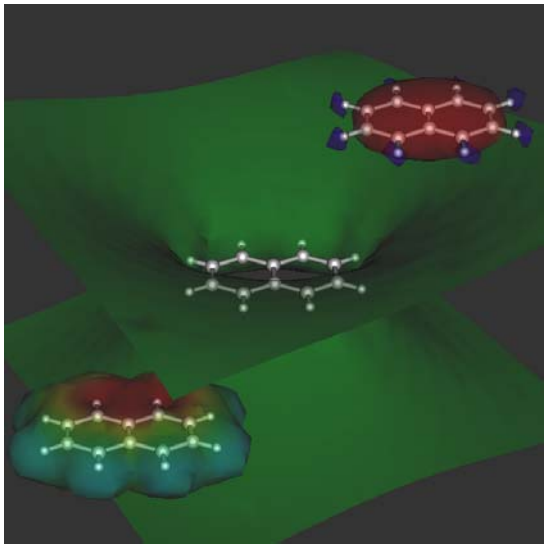
Abstract

Visualizing molecular properties is often crucial for constructing conceptual understanding in chemistry. However, research has revealed numerous challenges surrounding students' meaningful interpretation of the relationship between the geometry and electrostatic properties of molecules. This study explored students' (n=18) use of three visual representations of electrostatic potential to interpret whether molecules are polar or non-polar. The representations consisted of red and blue 'lobes' (termed RB) indicating regions of negative and positive potential, a color gradient mapping electrostatic potential on a molecular surface (MAP), and a rendering of the interface between regions of positive and negative potential (ISO). Data on students' accuracy, time-on-task and evaluation related to the three visual modes was collected via a web-questionnaire. ANOVA indicated that students were significantly more accurate in interpreting ISO, although more than half evaluated this mode the most difficult to use. Furthermore, students took significantly longer to interpret complex than simple molecules using ISO and RB. The results indicate that there may be possible pedagogical benefits in using unconventional visual representations that reduce visual complexity by making molecular relationships explicit. Hence, this has implications for future work on the role of cognitively mapping between different instructional visualizations in the development of fundamental chemical concepts.



Keywords:

Audience: High School / Introductory Chemistry; First-Year Undergraduate / General

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Introduction

Pedagogical importance of understanding molecular polarity

The internal (within the mind) and external (on the page or screen) visualization of relationships between molecular structure and properties are often at the forefront of a chemist's cognitive pedigree (e.g. (1)). Uncovering these relationships brings to bear the seminal notion of "representational competence", which Kozma and Russell (2) articulate as the set of skills associated with interpreting different representations to understand chemical phenomena. Representational competence captures the reciprocal relationship between the process of interpreting different representational systems to construct meaning, and how the acquired meaning is fed back into representational use.

Recent work in chemistry education has exploited different visual representations to teach fundamental concepts related to chemical polarity (3, 4). The process of predicting polarity requires chemists and learners to interpret physical characteristics of molecules, by combining information about bond and molecular dipole moments with 3D molecular shape (4). Assigning polarity requires *integration* of an interpretation of overall molecular shape and the direction(s) of any dipole moments arising from electrical charge separation within a molecule.

Although interpreting polarity provides conceptual understanding about central chemical properties such as solubility, melting, boiling, surface tension and intermolecular forces, research indicates numerous difficulties surrounding students' understanding of molecular polarity (e.g. (5, 6, 7, 8, 9, 10)). Students' difficulties with interpreting molecular polarity could be linked to the often cognitively demanding interpretation of molecular shape and associated geometry. In this regard, Furió and Calatayud (5) and Furió et al. (6) have demonstrated that one obstacle is applying knowledge about the influence of bond polarity on overall molecular shape, where students often reduce the prediction of molecular polarity either by attributing polarity to molecular shape or to bond polarity alone, and that students often lack the necessary procedural knowledge. Furthermore, Gonzalez et al. (7) have revealed that learners often struggle to associate the symmetry of electron distribution with molecular polarity, cannot discriminate between VSEPR theory and polarity, and often interchange the concepts of bond and molecular polarity.

According to Wang and Barrow (11), assigning molecular polarity requires the competence to perform mental operations on represented molecular information that involve the necessary 2D to 3D transformations. Given these mental requirements, research indicates that the concept of polarity can be made more meaningful by exploiting how the charge distribution within a molecule is visualized (Figure 1). For instance, Sanger and Badger (8) have shown that electron density plots of charge distribution can support learners' prediction of chemical polarity, and improve conceptual knowledge of the concept. Furthermore, Shusterman and Shusterman (12) have shown how electrostatic potential maps can assist in comprehending the alignment of guanine with cytosine in DNA.

From a pedagogical point of view, it is important to expose learners to different representations of the same chemistry idea, so that they can construct a more integrated conceptual understanding (1, 2). If so, chemistry education research has a responsibility to empirically evaluate the representational usefulness of varying molecular visualization forms. One way of doing so is to conduct experiments that measure the cognitive processing perspectives of representational use (2). In this respect, it is not well known to what extent students' can successfully interpret different electrostatic visual formats, or the relative processing constraints involved. Determination of molecular polarity based on electrostatic potentials offers one context from which to investigate students' visual interpretations of a fundamental chemical concept, and serves as the basis of this study.

Electrostatic potential visualization systems for representing molecular polarity

Three examples of representational systems for visualizing molecular polarity are communicated in Figure 1. Two conventional forms (e.g. (13)) available to educators include RB (Figure 1A and B), and MAP (Figure 1C and D), perhaps the most widespread form. A novel system that we have reported in this *Journal* (14) visualizes the topography of the interface between negative and positive regions of electrostatic potential using an isovalue of zero for the electrostatic potential (ISO, Figure 1E and F).

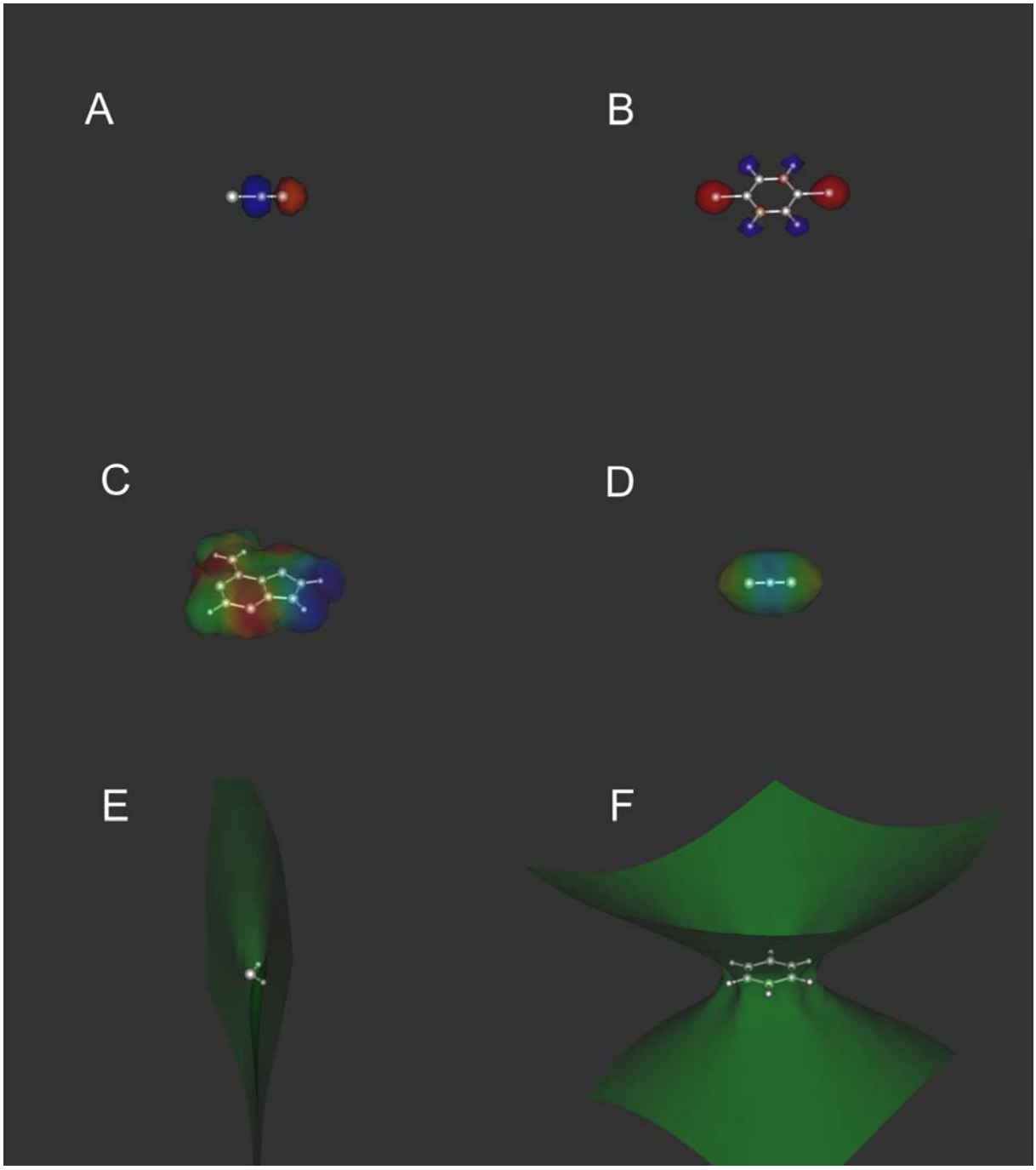

Figure 1. Visualizing molecular polarity using three representational systems. A and B: Red and blue 'lobes' represent regions of negative and positive electrostatic potential (RB); C and D: An electrostatic map in the form of a color gradient represents the electrostatic potential at the van der Waals surface (MAP); E and F: A representation (14) that visualizes the interface between positive and negative regions around a molecule using a green isosurface (ISO). The color ranges from red (negative potential) via green (zero potential) to blue (positive potential).

The ISO representation (Figure 1E and F) provides a visual indication of where the electrostatic potential 'changes sign' (actual signs of the electrostatic potential within the separated regions are not shown). Since the electric field is determined by the molecular charge distribution, the shape of the rendered surface can be interpreted in relation to the electric properties of the molecule. For example, with respect to polarity, the planar sheet-like shape generated by the water molecule (Figure 1E) reveals the molecule as polar since it indicates a charge separation within the molecule, with one positive (on the right of the

surface) and one negative end (on the left of the surface). In contrast, the closed and rotationally symmetrical surface arising from the benzene molecule (Figure 1F) indicates a symmetrical charge distribution, which infers a non-polar molecule. This visual reasoning has been expressed as the following set of 'rules' (14):

A molecule is non-polar if it yields:

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 yields:

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

The rules presented here are provided for the purpose of structuring the visual reasoning behind interpreting the ISO representation with respect to molecular polarity. They are *not* intended in this paper as specific goals for students' learning outcomes. In this regard, rote knowledge of the rules does not necessarily imply a conceptual understanding of the information communicated by ISO. As is the case for the MAP and RB forms, a meaningful educational application of the ISO representation should connect the visually represented information about molecular electrostatic potential to the underlying scientific concepts.

Research aims

In light of the importance of understanding the concept of polarity in chemistry through the interpretation of different electrostatic potential representations, the goal of this study was to investigate students' assignment of chemical polarity to molecules using two 'conventional' (MAP and RB) and one 'novel' (ISO) visualization system (Figure 1).

Atkins and Beran (15) define any molecule that has a non-zero electric dipole moment as a *polar* molecule, while a molecule with a zero electric dipole moment is defined as *non-polar*. Being able to use molecular information to determine whether a molecule is polar or non-polar is a fundamental step towards developing an understanding of other chemistry concepts related to polarity (e.g. (8, 12)). These related concepts include the direction of a dipole moment, relative dipole magnitudes, deducing polarity for the purpose of rationalizing physical properties such as miscibility, intermolecular interactions between dipoles, and varying semantic interpretations of the term (e.g. in chromatography).

We investigated students' performance on the task of *interpreting whether a molecule is polar or non-polar* by obtaining the following data: i) accuracy of assignment of polarity using each of the three representations (Figure 1), ii) the time taken to complete each polarity task (time-on-task), and iii) evaluations of each visual mode. The specific aims of the study were to:

- Explore any accuracy and time-on-task differences in students' use of the MAP, RB and ISO visual modes to interpret whether molecules are polar or non-polar.
- Investigate students' evaluations of the three visual modes with respect to perceived difficulty and time-on-task.
- Compare the measured accuracy and time-on-task data with students' evaluation data of the three visual modes.

Given the aims above, measuring students' accuracy of using different electrostatic visual modes to assign chemical polarity is related to the way students' mentally visualize and conceptualize communicated molecular phenomena. Also, measuring 'time-on-task' could

provide processing insight into the practical feasibility of utilizing different visual representations as instructional tools.

Methods

Design of a chemical polarity instrument

The designed instrument required students to assign polarity to a set of 20 molecules. The molecules consisted of 10 distinctly polar and 10 non-polar species, which, in turn, comprised of 10 'simple' and 10 'complex' molecules. Altogether, the 20 molecules encompassed 5 of each of *simple/polar*, *simple/non-polar*, *complex/polar*, and *complex/non-polar* species. Simple molecules contained a central atom and 7 constituent atoms or less, steric numbers ranging from 2-6, and molecular shapes that included linear, bent, trigonal planar, tetrahedral, trigonal bipyramidal and octahedral configurations. Complex molecules lacked a central atom but were composed of more than 7 constituent atoms. Applying 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).

The 20 different molecules were represented in each of the RB, MAP and ISO visual modes (e.g. Figure 1 and Supporting information) yielding a total of 60 images. A ball-and-stick model was transposed within each image to designate molecular geometry. Since the instrument intended to measure students' performance in assigning polarity with respect to the displayed electrostatic potential in each representational mode, constituent atoms were colored grey to limit inferences to any previous knowledge of molecular structures. The images were captured by taking screenshots of each visual mode generated using the Marching Cubes algorithm (16). Electrostatic potentials were calculated based on atomic partial charges. An isovalue of zero was used to generate ISO (14). For MAP, a van der Waals surface was generated upon which the electrostatic potential was mapped using a color scale ranging from red (negative values of electrostatic potential), via green (zero potential) to blue (positive values). A range of suitable isovalue magnitudes were used to generate RB (e.g. (13)). Although we used an in-house application, it should be feasible to generate all three modes using available molecular modeling software (e.g. Spartan (17)).

Orientation of each molecule on the presentation screen was standardized as follows. First, the largest 'planar arrangement' of interconnected atoms was identified and aligned perpendicular to the plane of the screen. For example, this planar arrangement corresponds to the plane formed by all atoms in benzene or water, and by the trigonal planar PCl_3 part of PCl_3F_2. Second, where required, the most 'unique' chemical group (e.g. in terms of highest weight or nature of constituent atoms) was aligned 'on the left'. Third, we tilted each molecule 'downwards' between 30 and 40 degrees (see Figure 1 and Supporting information). All of the images were identically scaled and incorporated into a web-based questionnaire.

The chemical polarity instrument was piloted with nine first-year university chemistry students in Sweden. The purpose of the pilot phase was to validate whether the electronic instrument functioned as intended and whether students were in fact able to respond to the tasks. The obtained data revealed that the instrument could be used to gather data as anticipated, and that students were able to execute the polarity tasks. Mean accuracy scores were approximately 0.8 for each of the three modes, and students spent a mean duration of approximately 5 s to assign polarity to each molecule.

Student participants and educational context

An invitation to participate in the main study was sent to students at a Swedish university enrolled in a *Basår*, a bridging-year program between secondary and tertiary levels that qualifies students with non-science backgrounds for a university science track. The students had recently covered the subject of polarity in their chemistry course. The entire cohort of 38 students were invited to participate in the study, of whom 18 (5 females and 13 males, median age 22) agreed to participate. Prior to data collection, participants were given a 15 minute introduction to polarity and the three visualization modes (Figure 1). The introduction provided a brief overview of the concept of polarity, and how it arises as a consequence of asymmetric distribution of electrons in covalent bonds. In addition, two examples of molecules (adenine and benzene) were displayed in the three visual formats, in conjunction with an oral explanation about how the visual information could be interpreted to assign polarity. The introduction was given in person by the first author to the whole class as part of one of their lectures, and the students were allowed to ask any questions regarding their interpretation and understanding of the visual representations.

Data collection

Following the introductory lecture, each student was electronically mailed a unique internet link (accessible once) to the instrument. Before commencing with the actual questionnaire, the instrument presented students with examples of each of the four classes of molecules across the three visualization systems (12 example images). For each example, the correct answer was provided to help students understand how the three visualization systems could be used to perform the task. The questionnaire then commenced with the same 12 examples one at a time in the same sequence for all participants. The purpose of this was to acquaint students with the instrument and at the same time confirm that they clearly understood what was required in the tasks. This was followed by presentation of the 60 test images one at a time. Students assigned the polarity to each displayed molecule by clicking a "polar" or "non-polar" box. Each student's response and time-on-task were logged automatically for each image.

Any potential presentation order effects of the 60 images based on representational mode, molecule size, and molecular polarity were minimized by applying randomization in three steps during preparation of the display sequences. Firstly, the images were divided into two 'blocks' (A and B), each consisting of 30 images, randomly assigned to the two blocks for each of the four molecule types and each representational mode. Thus, for example, three of the five images of simple non-polar molecules displayed in RB were assigned to the first block and the remaining two were assigned to the second block. Secondly, a large number of variants of each block were prepared, wherein the image sequence within each block was randomized. Thirdly, the presentation order of the two blocks (AB and BA) was randomized. As a consequence, each student received a uniquely-randomized sequence where any potential order effects (such as fatigue and practice effects) were essentially eliminated by ensuring that each image was equally represented in the first and second 'halves' of the 60-image sequence.

Following the polarity tasks, students responded to four evaluation items that asked participants to choose, with respect to assigning polarity, which of the images were considered most easy to use, most difficult, took the shortest time, and took the longest. During both design and implementation of the instrument, we adhered to a set of standards for internet-based experiments proposed by Reips (18).

Data analysis

The response data were analyzed with respect to accuracy, time-on-task (cf. (19)) and students' evaluation of the three systems (Figure 1). A statistical analysis was performed using SPSS version 19.

Students' use of the three visual modes to correctly assign polarity to molecules was assessed by analyzing accuracy scores. A score of one or zero was awarded to each correct and incorrect interpretation of polarity, respectively. For each student and each visual mode, the mean score for the twenty molecules was used as a measure of accuracy. In addition, mean scores for each student were calculated for each of the four molecule types across the three visual modes (i.e. a set of 4×3 scores for each student).

The time taken for students' to use each of the three visual modes to assign polarity was obtained from the automatically captured response times. The mean value across all molecules for each student and each visual mode was calculated as measures of time-on-task. Corresponding time-on-task values per visualization system for each of the four molecule types were also calculated for each student. Early analysis revealed that one student produced 19 outlier response time values (standardized scores in excess of 3.29) (e.g. (20)), most likely caused by not following the instruction to only take breaks between polarity assignments, and this student was consequently excluded from the analysis.

Any differences in accuracy and time-on-task between the three visual modes were investigated through ANOVA. For each of the dependent variables (accuracy score and response time) a 3 × 2 mixed ANOVA was conducted using representational mode (MAP/RB/ISO) as the within-subject independent variable and order of block presentation (AB/BA) as the between-subject independent variable. The order of block presentation was included to check for any order effects with respect to visual presentation sequence. No statistically significant interaction effects between representational mode and order of block presentation (accuracy: $F(1,16) = 0.453$, $p = 0.511$; time-on-task: $F(1,15) = 0.713$, $p = 0.412$) and no significant main effects for order of block presentation (accuracy: $F(1,16) = 0.312$, $p = 0.584$; time-on-task: $F(1, 15) = 0.312$, $p = 0.584$) were found, which indicate that the students' performance with the three visual modes was not affected by the order of block presentation. The ANOVA was followed by Bonferroni post-hoc comparisons between mean values (21, 22). For each visual mode, any differences with respect to the different molecule types were investigated through ANOVA. For each of the dependent variables (accuracy score and mean response time), a 2 × 2 ANOVA was conducted for each visual mode using polarity of displayed molecules (polar/non-polar) and complexity of displayed molecules (simple/complex) as independent variables. Similar statistical procedures are evidenced in various other educational studies that adopt repeated measures designs (e.g. (23, 24, 25, 26)).

The evaluation data was analyzed in two steps. Firstly, the responses to four evaluation items with respect to the three visual modes were considered across all participants across two dimensions, namely perceived relative time-on-task and perceived relative difficulty. Secondly, to connect these evaluation data to the task performance data, a ranking between the three visual modes was constructed for the time-on-task data and the accuracy data. Any associations between the evaluation data, and the accuracy and time measures in students' assignment of polarity were unpacked by constructing four cross-tabulations. Two of the cross-tabulations displayed a ranking of students' perceived relative difficulty versus ranked accuracy scores, while the remaining two presented a ranking of students' perceived relative time-on-task versus ranked response times.

Results

Students' accuracy and time-on-task using the three visualization systems

Results showed that all three visual modes (Figure 1) could be used by the students to assign polarity to the 20 molecules (Table 1).

Table 1. Mean accuracy scores and time-on-task values obtained from students' use of the three visual modes to interpret whether molecules are polar or non-polar.

	Accuracy score			Time on task	
	Mean	SD		Mean (s)	SD
RB	0.75	0.20	RB	7.0	7.5
MAP	0.69	0.13	MAP	5.8	3.1
ISO	0.81	0.19	ISO	7.4	5.8

ANOVA indicated a significant difference between the visual representation modes ($F(1,16) = 6.535$, $p = 0.021$, $\eta_p^2 = 0.29$). Bonferroni adjusted post-hoc tests (using a total α level of 0.05) revealed that the students achieved significantly higher scores using the ISO mode than either RB or MAP. No statistically significant difference was found between the RB and MAP modes.

Mean accuracy scores for students' use of the three visual modes to assign polarity to the four classes of molecules are indicated in Figure 2. An ANOVA revealed a statistically significant difference for ISO between complex (Estimated marginal mean = 0.78) and simple (Estimated marginal mean = 0.85) molecules ($F(1,17) = 5.390$, $p = 0$ .033, $\eta_p^2 = 0.24$). No statistical differences were found between molecule classes for MAP or for RB.

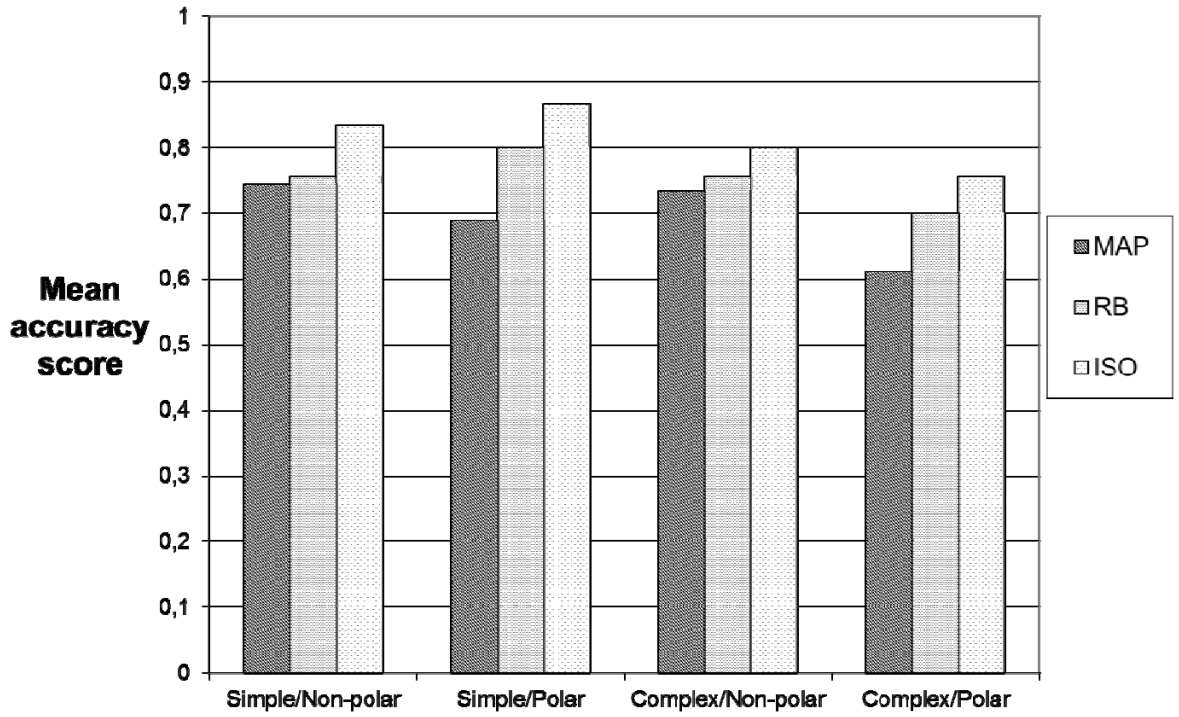

Figure 2. Mean accuracies for students' assignment of polarity to the four classes of molecules using three visual modes.

The mean time-on-task values for students' use of the three visual modes to assign molecular polarity are shown in Table 1. An ANOVA indicated that there was no significant differences between the visualization modes ($F(1,15) = 1.692$, $p = 0.213$).

Mean response times for assigning polarity to the four classes of molecules are indicated in Figure 3. A statistically significant effect of the complexity of the molecules was found for RB ($F(1,16) = 8.794$, $p = 0.009$, $\eta_p^2 = 0.355$), indicating a difference between simple (Estimated marginal mean = 4.0 s) and complex (Estimated marginal mean = 6.6 s) molecules. For ISO, a significant difference was found between simple (Estimated marginal mean = 5.3 s) and complex (Estimated marginal mean = 7.2 s) molecules ($F(1,16) = 16.744$, $p = 0.001$, $\eta_p^2 = 0.511$). For the MAP mode, no significant differences between molecule classes were found.

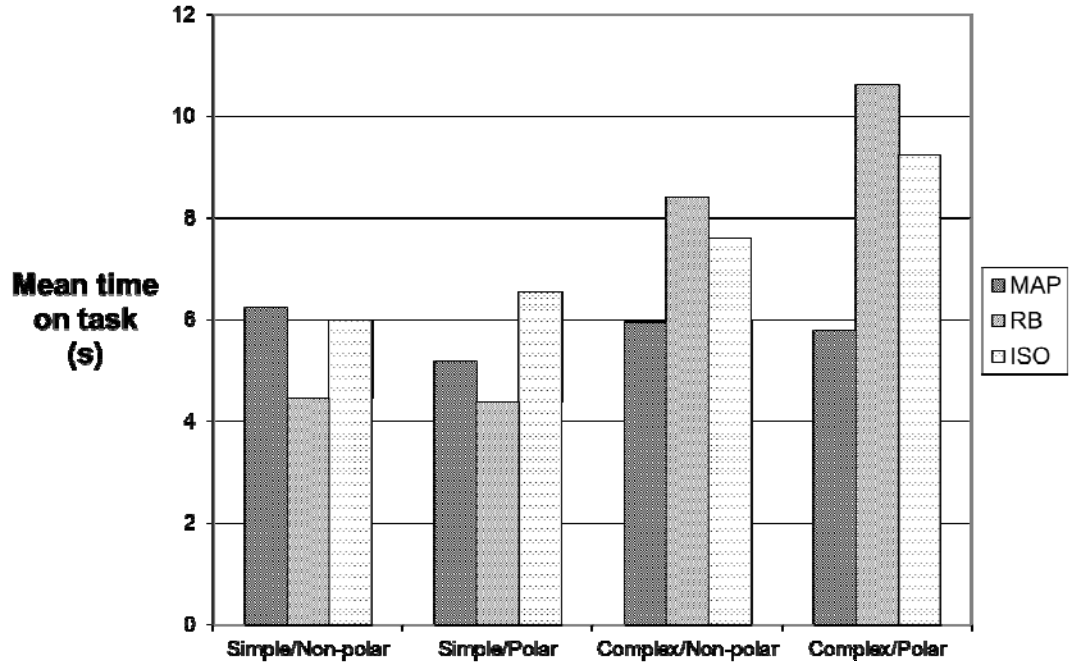

Figure 3. Mean response times for students' assignment of polarity to the four classes of molecules using three visual modes.

Students' evaluation of the three visualization systems

As shown in Table 2, most students (12/16) considered RB the easiest mode for performing the polarity tasks, while half the student sample (8/16) felt ISO to be the most difficult. A similar pattern was attributed to students' evaluation of the perceived relative time-on-task. Here, 11 students evaluated RB as requiring the shortest time to assign polarity, and 10 students judged ISO to be associated with taking the longest time.

Table 2. Students' evaluation of the three visual modes for assigning molecular polarity.

Which of the three types of image:	MAP	RB	ISO	No answer
was the most difficult to use for assigning polarity?	6	2	8	2

was the most easy to use for assigning polarity?	2	12	3	1
took you the longest time to assign polarity with?	6	1	10	1
took you the shortest time to assign polarity with?	2	11	4	1

With respect to accuracy, cross-tabulations of evaluation data with task data showed that participants scored the highest using ISO in eleven cases but evaluated RB to be the most easy to use (Table 3). The majority perceived RB to be the easiest, although ISO was in fact the most successfully used. Furthermore, although nine students ranked ISO to be the most difficult, in only one case did this mode deliver the lowest accuracy. Overall, students' evaluation of perceived relative difficulty was often inconsistent with the accuracy scores.

Table 3. Cross-tabulations showing comparisons of students' ranked accuracy and time-on-task data with their evaluation of visual mode difficulty and perceived time requirements.*

		Highest accuracy		
		MAP	RB	ISO
Evaluated as most easy	MAP	1	1	0
	RB	0	2	11
	ISO	1	1	2

		Shortest time-on-task		
		MAP	RB	ISO
Evaluated as taking shortest time	MAP	1	1	0
	RB	1	6	3
	ISO	1	2	1

		Lowest accuracy		
		MAP	RB	ISO
Evaluated as most difficult	MAP	5	2	0
	RB	1	0	1
	ISO	5	4	0

		Longest time-on-task		
		MAP	RB	ISO
Evaluated as taking longest time	MAP	1	2	3
	RB	0	0	1
	ISO	1	1	7

* The data excludes a student that did not respond to all the evaluation items. In cases where rankings were equal, both were counted.

There was consistency between what visual mode half of the students perceived to require the shortest time and the mode that actually was responded to in the shortest time. A similar trend was observed for perceptions of what mode took the longest time. Seven of the eleven students that took the longest time processing ISO evaluated it as taking the longest to interpret.

Discussion

The ISO visualization system was used significantly more accurately than both MAP and RB for assigning polarity, and ISO was used significantly more accurately for deducing the polarity of simple molecules compared to complex molecules. From a pedagogical point of view, this may indicate the potential representational power of introducing formats such as ISO into early learning about electrostatic phenomena. In terms of an instructional design perspective, the finding that students were both significantly more accurate and took significantly shorter to assign polarity to simple versus complex molecules using ISO may mirror a lower processing demand required for integrating the visual information representing a simpler electrostatic field. Overall, the finding that task times were not significantly different between the three modes could indicate that introducing even unconventional representational formats such as ISO into the classroom may be practically feasible.

Students' evaluations provided a window into their use of the visual representations as problem-solving tools, divorced from task performance alone. With regard to the cross-tabulations, there was a relatively large degree of consistency between the evaluated and measured time-use. It appears that students made reasonable judgments with respect to the time-on-task dimension, but there was a discrepancy between the evaluated difficulty and actual accuracy. From the position of learning chemistry, a visual representation that students consider most challenging to use may still effectively communicate the intended molecular phenomenon.

Whereas interpreting molecular polarity using RB and MAP requires students to integrate the relative positions of positive and negative regions, interpretation of the interfacial surface offered by ISO could place less strain on available perceptual resources (e.g. (27)). Given Furió et al.'s (6) finding that students struggle to simultaneously interpret bond polarity and molecular shape in deducing polarity, ISO may support the visual communication that polarity is a function of both properties because the mental operation of "summing the dipole moments" with respect to the symmetry of a molecule is portrayed inherently in the visual mode. Although this may be a potential cognitive benefit, this work makes no assertion about the influence of any of the modes on mastering the 'standard procedure' for assigning polarity, the physical factors that determine polarity, nor the potential conceptual consequences of misinterpreting polarity.

Given the limited number of volunteers in this study (n=18), we paid careful attention to pursuing a high degree of internal validity by stringently randomizing the order of presented images across a range of polar/non-polar molecules that varied in complexity (statistical analysis did not reveal any order effect). Employing a within-subjects experimental design where each participant was exposed to *all* images would have countered any self-selection effects. Nevertheless, we acknowledge that results might have differed if students had used 3D interactive visualizations rather than static 2D representations (as presented in hardcopy textbooks), and we have not formally considered the influence of other variables, such as existing prior chemical knowledge, on task performance. Lastly, strengthening the generalizability of the statistical findings could be achieved by replicating the experiment with more students in other contexts. Overall, these findings can be viewed as a precursor to a potentially larger investigation that obtains data from more respondents, and formally considers the conceptual attributes and consequences of processing each representation.

Conclusions and Implications

This study has found that out of the three investigated modes (i.e. ISO, RB and MAP), students were significantly more accurate at interpreting the ISO representation of the interface between positive and negative electrostatic potential to decide whether molecules are polar or non-polar. The reason behind the differential processing success of interpreting ISO may be that it communicates electrostatic information in a way that reduces the extraneous processing attributed to other modes (27).

A recent assertion by Harle and Towns (28) states that "teaching and learning of chemistry between students and faculty is mediated by representations of molecules...", and recent literature suggests that there is a benefit in reducing visual complexity, making relationships explicit and using multiple linked representations to communicate molecular properties (4, 29). In this regard, educators should not shy away from the potential processing benefits of novel/unconventional visualizations. For example, Laverman (30) has rendered innovative visualizations relating to the varying of electrostatic potential in space, while Tuvi-Arad and Blonder (29) have depicted 3D molecular symmetry in novel ways. In the case of the ISO representation, the results of this study do not imply that ISO should now be viewed as the

superior or preferred visual medium for communicating molecular polarity, but rather that it could complement existing visual forms. In the spirit of pursuing representational competence amongst learners, we advocate the supplementation of empirically-evaluated innovative visual tools to support the interpretation of fundamental chemical properties, such as molecular polarity.

Based on the findings of this study, possible practical implications for teachers are as follows:

- Expose students to *different* visual forms (e.g. RB, MAP and ISO) for cognitively *mapping* between constructs of electrostatic properties, molecular shape, and polarity.
- Actively compare the three visual modes of representing electrostatic potential during teaching to engender conceptual discussions about polarity.
- Supplement traditional visual representations with the visual modes explored in this study to support learners' holistic understanding of the concept of polarity.

Further research is required to investigate the role of the visual representations dealt with in this inquiry as learning tools *per se*, which should include qualitative explorations of students' conceptual knowledge as they perform the task. Such rich data could be gathered through open-ended items on the electronic survey as well as individual clinical interviews probing relationships between interpretation of the visual information and the associated conceptual knowledge. In this way, a thorough qualitative component would be pivotal to getting more at the 'why' and the 'how' of students' interpretation of the visual forms. Doing so will allow for a better understanding of how similarities and differences between the visual representations impact understanding of concepts related to polarity, which could help inform real classroom practice. Furthermore, given the 3D capability of most molecular modeling software, investigating students' learning with electrostatic representations using interactive systems would be a compelling future research avenue.

Supporting information

A supplementary file containing all images used in the polarity instrument is provided as online supporting information accompanying this article.

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