

Research article

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Using electrostatic potential maps as visual representations to promote better understanding of chemical bonding

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Abstract: Static visual representations (VRs) of chemical structures are necessary for an understanding of chemical bonding, a topic which continues to lead to learning difficulties and misconceptions for many students. The efficacy and problems associated with the use of VRs of chemical structures and chemical bonding in the form of electrostatic potential maps resulting from accurate quantum mechanical calculations are the subject of this study, which involved a sample of first year, second semester students, studying the elective course “Science Education” ($N = 31$). Students distinguished between nonpolar and polar covalent bonding, however, they encountered difficulties with concepts related to ionic bonding. Most students did not employ multistructural thinking (in the sense of the SOLO taxonomy), when providing explanations about the variation of bond polarity. Persistence of a covalent-ionic bond dichotomy was apparent, while for some, ions can be involved in both ionic and covalent bonding. Many students preferred to use their established high school knowledge. On a positive note, many students were clearly affected by the information provided by the colored VRs. Finally, the minimal experience of our students with these VRs leads us to believe that a more systematic and extensive coverage would be likely to produce improved outcomes.

Keywords: chemical bonding; chemistry education; first-year undergraduate; misconceptions; quantum chemistry.

Introduction

The use of models and images (in general, of *visual representations*) are vital to our understanding of chemistry, with physical models of molecules providing tools for visualization of the molecular world for both learners and researchers. Such static images have become a *sine qua non* for chemistry textbooks. Visualization of a range of phenomena is clearly necessary for development of an understanding of chemistry (Ferk, 2003; Gkitzia, Salta, & Tzougraki, 2011; Kozma & Russell, 1997; Wu, Krajcik, & Soloway, 2001) so, in recent years, images, as a rule colored images, have taken up more and more space in textbooks. In addition, the use of technology, especially of personal computers and smart phones, has been increasingly important in enhancing both student interest and learning (Kelly & Akaygun, 2019). For instance, VandenPlas, Herrington, Shrode, and Sweeder (2021) developed and used online materials (simulations and screencasts) to support students’ learning of chemistry outside of a face-to-face classroom, with a focus on student understanding of the concepts of force and energy

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changes as they pertain to bonding and intermolecular attractions. Also, Isaloka and Dwiningsih (2020) produced 2D interactive multimedia to display special-visual orientations of polar and nonpolar covalent bonds, and evaluated their content validity, construct validity and practicality, while Brown, Whaley, and Hyslop (2020) compared the effectiveness of three methods (virtual reality, computer simulation, and traditional modeling) used in teaching molecular geometry to college chemistry students, and reported that while differences among the three methods were not significant, the results showed that the virtual reality method resulted in more enthusiasm and positive attitudes toward the topic among the students.

However, the mere use of images and technology does not guarantee their effectiveness in promoting learning and it may even contribute to the formation of misconceptions by students. Learning outcomes appear to depend on both the quality and the pedagogic content of the images and also on how the images and the technology are used (National Research Council, 2012). In particular, the speed with which a user can access different representations of molecules in a technology enabled environment can provide important benefits to cognitive development (Polifka, Baluyut, & Holme, 2021). Education research has definitively an important role to play here in assessing the outcomes and the effectiveness of these tools.

One topic where visual representations currently play a crucial role is that of chemical bonding, which is fundamental to the teaching of chemistry (Atkins, 1999; Gillespie, 1997; Holme & Murphy, 2012; Holme, Luxford, and Murphy, 2015; Taber & Coll, 2003). Chemical bonding is associated with the understanding of many chemistry concepts, such as chemical reactions and structure–property relationships, but continues to be difficult for teachers to organize and teach and for students to learn and understand. The initial focus here is on the teaching and learning of basic bonding concepts in upper secondary education (grades 10th to 12th). Prevailing approaches to teaching chemical bonding continue to lead to learning difficulties and misunderstandings for many students, with many of these misunderstandings proving resistant to instruction (e.g. Levy Nahum, Mamlok-Naaman, Hofstein, & Krajcik, 2007; Nicoll, 2001; Özmen, 2004; Taber & Coll, 2003).

Taber (1998) proposed an ‘alternative conceptual framework’ for chemical bonding, according to which the ‘octet rule’ is used by the students as an explanatory framework for chemical stability and reactivity, and he further identified the four key “pedagogical learning impediments” to the effective teaching and learning of chemical bonding (Taber, 2001): (1) an atomic ontology and the initial atomicity; (2) the over-generalization of the octet rule; (3) the dichotomous classification of bonding; and (4) the use of anthropomorphic language, with student explanations commonly phrased in terms of what an atom might ‘want’ or ‘need’ (Taber & Adbo, 2013, p. 348). Taber (1999) considered this framework as a largely coherent theory-like basis for thinking about chemical stability, change and bonding (for a review, see Taber, 2013). In addition, Taber (2001) introduced a curricular model of chemical bonding, which starts with metallic structures, then goes on to ionic structures, to giant covalent structures, and finally to simple molecular structures. The model emphasizes molecules and ions (rather than atoms) as the basic unit of matter, so as to avoid the assumption of initial atomicity, while the nature of bonding, structures, and properties of substances are explained in terms of electrostatic forces, but not the octet rule, nor the desires of atoms. Addressing bonding in terms of electrostatics could also serve as a good foundation for subsequently learning about electronegativity, bond polarity, hydrogen bonds, and solvent-solute interactions.

Levy Nahum et al. (2007) (see also Kronik, Levy Nahum, Mamlok-Naaman, & Hofstein, 2008; Levy Nahum, Mamlok-Naaman, & Hofstein, 2013; Levy Nahum, Mamlok-Naaman, Hofstein, & Taber, 2010) also developed “a new teaching approach for the chemical bonding concept aligned with current scientific and pedagogical knowledge”. A qualitative description that is conceptually consistent with quantum mechanics was adopted, providing an answer to the question “what really causes atoms to interact and form a chemical bond?” The authors suggested the ‘*bottom up*’ approach for teaching the bonding concept. The crux of the suggestion is that bonding should be taught based on elementary principles and by using the idea of a continuum of bond strengths, removing the artificial dichotomous division between different types of bonding.

In a preceding publication, we reviewed studies concerning students’ conceptual difficulties with the topic of chemical bonding, tested the knowledge of 10th-grade Greek students on certain key aspects of bonding and presented our findings from the use of an enriched teaching text on this topic (Tsaparlis, Pappa, & Byers, 2018). The enriched text started with covalent bonding between atoms of the same or different chemical elements and

the nature of the bonding but postponed the study of bond polarity (polar covalent bonds) until after discussing ionic bonding. It included a careful discussion about the octet rule, paid particular attention to features that characterize both the covalent and the ionic bond, and gave a more detailed coverage of electronegativity, stressing its importance to the understanding of the continuum between ionic and covalent bonding. The intervention introduced with the treatment group demonstrated mixed results, with statistically significant differences being detected for some concepts/knowledge elements, but not for others. Finally, in a follow up study to our previous one (Tsaparlis, Pappa, & Byers, 2020), we reviewed studies on student understanding and on teaching of bonding concepts and presented proposals for the teaching of chemical bonding at secondary level based on the findings of our own study (Tsaparlis et al., 2018). The proposals included a spiral curriculum spanning all three upper-secondary grades, plus a learning progressions approach, employing lower and upper anchors of relevant scientific knowledge and a proposed list of potential core concepts, lever concepts, and stepping-stones.

The net conclusion is that critical details and some sophisticated reasoning are required for an understanding of chemical bonding, for example the many types of bonding (metallic, ionic, covalent, polar and non-polar bonding, intermolecular bonding). It is crucial to have in mind that, because bonding is taught at both the (mainly upper) secondary and the tertiary level, there is an overlap of concepts, instructional tools and approaches between the secondary and the first-year undergraduate level. Although, complexity is present from the early stages, it deepens as we move from secondary to tertiary education.

In the present study, we examined the efficacy and problems associated with the use of static colored visual representations (VRs) of chemical structures and chemical bonding resulting from accurate quantum mechanical calculations (Jensen, 2010). The diagnostic part of our 2018 study led to the conclusion that many fundamental misconceptions were evident in our samples. We list below some selective misconceptions and conceptual difficulties that were discussed in the Tsaparlis et al. (2018) study, which are relevant to the present study:

- The ionic bond is referred to as just a transfer of electrons between separate atoms in order to acquire full valence shells and satisfy the octet rule.
- Covalent and ionic bonds are often presented in isolation, as bonds that share electrons and bonds that transfer electrons respectively.
- Bond polarity is directly linked to the covalent bond. As a consequence, students fail to realize the covalent-ionic bond continuum.
- Ions are involved in both ionic and covalent bonding (deriving from the knowledge that a polar covalent bond possesses some ionic character).

Rationale

In the final part of a previous paper, we considered the pros and cons of teaching a modern qualitative quantum mechanical approach to bonding (Tsaparlis et al., 2020). Despite the fact that the teaching of modern qualitative quantum mechanical descriptions of atomic and molecular structure at secondary level has been criticized by some chemistry educators (Bouayad, Kaddari, Lachkar, & Elachqar, 2014; Tsaparlis, 1997a, 1997b, 2013), there is no doubt that quantum mechanics can refine one's understanding about the submicroscopic world. Atomic orbitals, their physical interpretation, as well as electron configurations of atoms and monoatomic ions are often discussed in upper secondary school. Although molecular orbitals are not generally introduced, Lewis structures, possibly hybrid atomic orbitals, use of the VSEPR model to discuss molecular structure and consideration of electron clouds and their overlap in bonding are all likely to be beneficial to students' understanding. Pauling's proposal that beginning courses in chemistry should emphasize the simpler aspects of molecular structure in relation to the properties of substances is clearly of relevance here. According to Pauling (1992), concepts to be covered should include the electronic structure of the atom, with emphasis on the noble-gas structure, the shared electron-pair bond, the tetrahedral carbon atom, the electronegativity scale, the partial ionic character of bonds, and the idea of resonance as applied to the benzene molecule; but molecular orbitals should not be introduced at this stage.

Some researchers have encouraged early introduction of a quantum mechanical approach. For example, considering upper-secondary and first-year undergraduate students, Dhindsa and Treagust (2014) used the valence-bond model of bonding to explain covalent bonding in terms of the overlap of atomic orbitals on bonded atoms, while Nimmermark, Öhrström, Martensson, and Davidowitz (2016), based on data concerning Swedish undergraduate students, suggested that it is likely to be beneficial to the understanding of bonding (and especially the covalent bond) if secondary-school students have been introduced to at least a simplified quantum model of the atom. Although the physical interpretation of atomic orbitals and the electron configurations of atoms and monoatomic ions may be useful, molecular orbitals should certainly not be introduced at the secondary level, and only Lewis structures and the VSEPR model should be used to consider molecular structures at this stage. It appears that the teaching of certain aspects of the molecular quantum mechanical model in secondary education, such as electron clouds and their overlap in bonding, can be beneficial to students and should not be ruled out. However, modern quantum-chemical concepts should only be introduced, with great care (Dunstan, 1968; Tsaparlis, 1997a, 1997b).

The importance of static visual representations of chemical structures resulting from quantum mechanical calculations

It is known that conventional undergraduate courses on quantum chemistry tend to be strongly mathematically oriented and this poses a learning impediment to most students, making it hard for them to gain conceptual understanding of the relevant concepts (Tsaparlis, 1997a, 2013). On the other hand, qualitative approaches, which are based on the visualization of atomic and molecular orbitals and, as a rule, are employed in introductory general and inorganic chemistry courses, may also fail to provide a clear physical picture. For Barradas-Solas and Sánchez Gómez (2014), the use of graphical representations of orbitals have characteristics that fall into the category of alternative conceptions or misconceptions and this has even led to suggestions that these ‘chemical’ orbitals should be omitted from chemistry education altogether. In any case, to be effective, such approaches require great care (Tsaparlis & Papaphotis, 2009). Dangur, Avargil, Peskin, and Dori (2014) employed a qualitative visual-conceptual approach to teaching quantum chemistry (including bonding concepts, and emphasizing interdisciplinary real-life applications) and investigated the effectiveness of the approach on students’ visual and textual understanding of quantum mechanical concepts. According to their findings, the textual and visual understanding of quantum mechanical concepts and the ability to move across illustrations and explanations were significantly improved for high school honors and undergraduate chemistry students, who were exposed to this approach. Polifka, Baluyut, and Holme (2021) have used a “Variable Representation Assessment” tool, with which questions and responses are delivered via a web browser, and which can provide formative information about how students in a course are utilizing molecular representations to respond to questions about molecular properties that can be inferred from such representations. Using this tool, students in a US general chemistry course navigated among five different representation styles: (1) chemical formulas; (2) Lewis structures; (3) wedge and dash structures; (4) ball and stick structures; and (5) electrostatic potential maps. Results suggested that students needed to utilize a better balance among the various molecular representations. It was concluded that the preponderance of use of Lewis structures in many chemistry lessons might have led students to limit their use of a wider range of representations, while the students’ apparent lack of familiarity with electrostatic potential maps seems likely to have contributed to their relative aversion to using them.

Supplementary Material S1 discusses the concept of *electron probability density* (or simply *electron density*) (Jensen, 2010; Matta & Gillespie, 2001, 2002; Pilar, 1967), while Supplementary Material S2 describes the method of construction and interpretation of isodensity surfaces and electrostatic potential maps (Anslyn & Dougherty, 2006; Reed College, 2021). Note that this knowledge is supplied here for the benefit of the readers, but it was not part of the teaching and knowledge of the students in our study. Also, although electrostatic potential ranges were not included in the electrostatic potential maps used, it is important and useful to compare structures with the same electrostatic potential ranges (see Supplementary Material S2).

The present study – research questions

Taking into account that the students were not familiar with the static colored representations prior to the examination used in the present study, the main research question is:

- *How do students interpret colored VRs when presented with them for the first time? Or equivalently:*
- *Are students able to immediately decode and incorporate/synthesize colored VRs into their previous chemistry knowledge?*

The answer to this main research question will be derived from the answers to a number of subsidiary research questions, relating to students' use of static visual colored representations (VRs) of chemical structures and chemical bonding which have resulted from accurate quantum mechanical calculations, as follows:

- To what degree did the provided static colored VRs help the students to:

RQ1: deduce the type of bonding in various molecules?

RQ2: explain the variation of bond polarity in various molecules?

RQ3: exploit the difference in size between an atom and its corresponding ion?

RQ4: comprehend the concept of a continuum of bonding type and overcome the common misconception that bond polarity is only a feature of covalent bonds and not of ionic bonds? In addition:

RQ5: What types of static VRs for common covalent molecules, such as H_2 and H_2O , are the students already familiar with?

RQ6: How does the information that students can obtain from the colored VRs resulting from quantum mechanical calculations compare with the information that they can obtain from the VRs that they are already familiar with?

Method

Sample

The students of our study ($N = 31$) were in their first year, second semester (age 18–19), studying the elective course “Science Education” in the Department of Chemistry at the University of Ioannina, in the spring semester of the academic year 2018–19. The purpose of the course was to function as an introduction to content knowledge and pedagogic content knowledge which is relevant to the profession of a secondary school chemistry teacher. Students take this course because “Chemistry Education” is prescribed by the Greek Ministry of Education and by Greek law as one of the tests to be taken by secondary chemistry teacher candidates.

The lecturer, who was one of the authors of this paper (GP), is a secondary science teacher with a first degree in physics, and a holder of a M.Sc. and a Ph.D. in science education and was hired to teach this course within a project offering university teaching experience to recent Ph.D. graduates. Instruction was carried out in Greek and followed an in-class lecture format, with the instructor adopting an interactive approach, making efforts to engage the students in thinking, questioning and discussion during the lectures. The students (both male and female, with females outnumbering males: 19 vs. 12) were majoring in chemistry and used Greek science education textbooks (in Greek) that were recommended for this course by the instructor.

The study utilized a final written in-class closed-book examination in June 2019. There were four sections in the examination paper, but only section D is relevant to this study and has been reproduced in English in Supplementary Material S3. The duration of the examination was 3 h, but the distribution of time to each section and question was left entirely up to the student.

The instrument

Section D of the examination consisted of four questions. Question D.1 (which addressed research question RQ5 and is also related to RQ6) asked the students to draw as many VRs as they knew about the hydrogen molecule (H_2) and the water molecule (H_2O). Question D.2 involved five parts and related to a set of colored static structures, in the form of electron potential density (EPD) surfaces, which have resulted from proper quantum mechanical calculations of high accuracy (Jensen, 2010). The electrostatic potential map for hydrogen fluoride was not included with the hydrogen halide molecules because its intense polarization, as shown through coloring, makes it very similar to the coloring of LiH, hence there was the fear that HF could be taken by the students as being essentially ionic (see Figure 1). Figure 2 shows the electrostatic potential maps used in the study.¹ Note that dipole moments, electronegativity differences and gas phase bond lengths were not supplied for the hydrogen halide molecules.²

For convenience of reference for the reader, the five parts of question D.2 are listed in Table 1, along with the research questions they were designed to address.

Question D.3 (which addressed research question RQ2) provided pictures of colored VRs for two organic molecules with similar structures (CH_3Li and CH_3Cl) (see Figure 3 and Supplementary Material S3), and asked students to identify and justify which structure corresponded to which molecule. Note that the diagrams used for question D.3 (which were taken from the internet) have certain drawbacks, such as the weakness of the blue and red coloring, as well as the sizes of the shown nuclei of the chlorine and the lithium atoms, which must have caused problems to the students. This was taken into account when marking the students' answers. Finally question D.4 (which addressed research question RQ6 and is also related to all previous research questions) was of a metacognitive nature and asked students to compare the VRs for the hydrogen molecule and the water molecule that they drew in answering question D.1 with the corresponding colorful quantum mechanical VRs.

Ethical considerations

Every effort was made to observe the rules of good ethical conduct for implementing a social research study with university students (Taber, 2014). The students answered the questions as part of their final examination in the science education course, that is, they were not given any choice over taking part. Institutional permission to use formal examination material in the research was not required, but the lecturer had to report on the course and the exam to a departmental professor. In addition, the students were informed that the particular questions would be used as part of an education research study and no objections were received. All students provided written consent to the use for their responses for the stated research part of the test. Although the students were required to provide their names, as the questions were part of the examination, with responses contributing to their course mark, their names were not to be revealed to any third parties.

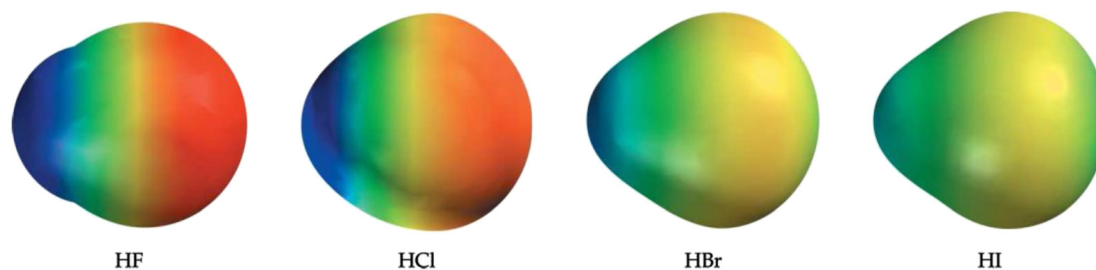


Figure 1: The electrostatic potential maps for the hydrogen halide molecules HF, HCl, HBr and HI, where the colors show differences in chemical bond polarity. The dipole moments μ (in D) are 1.86 for HF, 1.11 for HCl, 0.788 for HBr, and 0.382 for HI. The corresponding Pauling electronegativity differences are 1.78/0.96/0.76/0.46. Note that the shapes shown do not reproduce the relative actual molecular sizes: the gas phase bond lengths $D(H-X)$ (in pm) are 91.7 for HF, 127.4 for HCl, 141.4 for HBr, and 160.9 for HI.

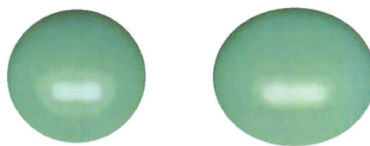
¹ Electrostatic potential maps resulting from quantum mechanical calculations of high accuracy by Jensen (2010), in black-and-white. The static colored figures were taken from website <http://www.flickr.com/photos/molmodbasics> (accessed 17-May-2021) and are used here with permission from the author.

² Although it is assumed that a lack of understanding of electronegativity may lead to a misunderstanding of polar covalent bonding (Burrows & Reid Mooring, 2015), we wanted to avoid the simple interpretation that if the electronegativity difference is large enough then ionic bonds will be formed. However, we know that it is not as simple as this, as the case of HF demonstrates.

Question D2. The following (electrostatic potential) maps are given:

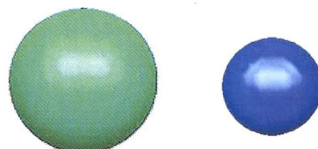
Maps (a)

Theoretical (quantum mechanical) calculation of the geometry of the H atom (*left*) and the H₂ molecule (*right*)



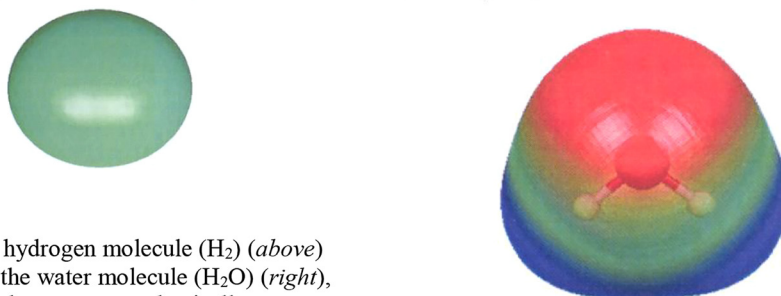
Maps (b)

Theoretical (quantum mechanical) calculation of the geometry of the lithium atom (Li) (*left*) and the lithium ion (Li⁺) (*right*)



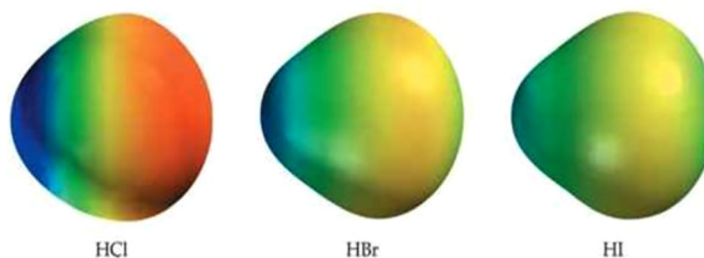
Maps (c)

The structure of the hydrogen molecule (H₂) (*above*) and the structure of the water molecule (H₂O) (*right*), as they are calculated quantum-mechanically.



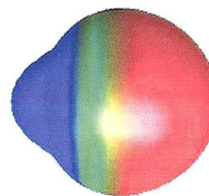
Maps (d)

The structure of the hydrogen halide molecules HCl, HBr and HI.



Map (e)

Geometry of the system which consists of one lithium atom and one hydrogen atom (*lithium hydride*, Li-H) as it is calculated quantum-mechanically.



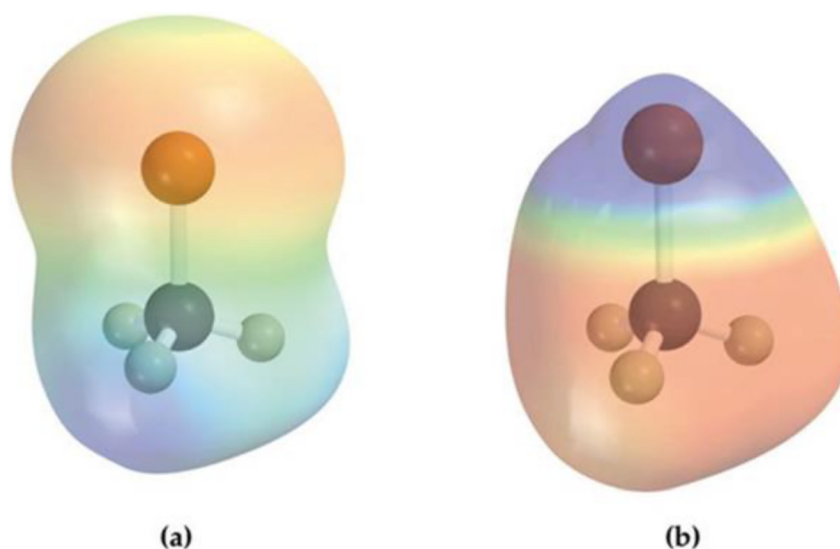
A color code scale for the *polarity of electrostatic potential* is also provided:



Figure 2: The electrostatic potential maps used in the main study, including a color code scale for the polarity of electrostatic potential.

Table 1: The five parts of question D.2 and the corresponding research questions (see also Figure 2).

Part of D.2	Tasks	Research question
D.2a	Compound lithium hydride is ionic (it is a crystalline solid, for which the melt is a conductor of electricity). (i) Which are the cation and the anion in this compound? (ii) With the aid of: maps (a) (left), maps (b) and map (c), explain why this compound is ionic.	RQ1, RQ3
D.2b	What do the color differences of the HCl, HBr and HI hydrogen halide molecules show? [maps (d)]	RQ2
D.2c	Which of the structures of maps (c), (d) and (e) show a chemical bond polarity?	RQ2
D.2d	State in which one of the maps (a), (b), (c), (d) and (e), the structures demonstrate the continuity between the covalent and the ionic bond, and why.	RQ4
D.2e	Mention two features that the color visual representations (VRs) help us understand.	RQ1, RQ2, RQ3, RQ4

**Figure 3:** Visual representations of chemical structures referring to chloromethane (CH_3Cl) and methyllithium (CH_3Li) from question D.3. (Students were asked to identify and justify which one corresponds to CH_3Cl and which to CH_3Li and why?).

Method of analysis

A variety of assessment approaches was adopted for marking the scripts. Three of the authors agreed on the assessment approaches to be used. Question D.1 was marked on the basis of a sequence of expected VRs for the H_2 and H_2O molecules. In the case of H_2 , half of the marks were assigned for the inclusion of the ellipsoid isodensity surface (a ‘flattened sack’) for H_2 [see maps (a) right in Figure 2, and the top right shape in the answer of student #18 in Figure 4]. The marking is evident from the answers provided by the two best students, as shown in Figures 4 and 5. Question 4 was of a metacognitive character and its marking was based on a list of expected points of view. In the cases of question D.2 (with the exception of part D.2e) and question D.3, the SOLO taxonomy was considered most appropriate. SOLO stands for “*Structure of Observed Learning Outcomes*”, and is suitable for open-ended questions where the complete answer involves many factors; it may, in addition, require relational and abstract thinking. More specifically, it classifies students’ responses into five levels of understanding from the simplest to the most complex: (1) pre-structural, (2) uni-structural, (3) multi-structural, (4) relational, and (5) extended abstract (Biggs, 1999; Biggs & Collins, 1982). Extended abstract understanding is essential for complex conceptual situations and for real problem solving. Further information about the SOLO taxonomy and the marking scheme employed can be found in Supplementary Material S4. In our case, we first considered what should be expected as a complete answer for each question, and then

judged the SOLO level that was required. Using this approach, we concluded that all questions were relatively straightforward, so extended abstract thinking was not required to answer any of them. Two parts (D.2b and D.2c) required only multi-structural thinking, while a further two parts (D.2a and D.2d) were more complex requiring relational understanding in addition to multi-structural thinking. Part D.2e required students to mention two features that the colored visual representations (VRs) help us to understand, so declarative and partly procedural knowledge were likely to be sufficient here, making the marking of this question relatively straightforward.

Reliability of the marking of the scripts was ensured on the one hand by the students' scripts being subjected to three rounds of marking by one author (GT) according to a pre-determined marking scheme. The correlations between markings were positive and very strong. For example, the Pearson correlation coefficient between the second and the third marking for question D.2a was $r = 0.851$, while the corresponding Spearman coefficient was $\rho = 0.835$; also the Pearson correlation coefficient between the second and the third marking for question D.3 was $r = 0.936$, while the corresponding Spearman coefficient was $\rho = 0.878$. In addition, ten of the student scripts were marked by another author (EP) according to the set marking scheme. After the dissolution of discrepancies by discussion, the Pearson correlation coefficients between the two markers ranged from 0.831 to 0.980, and the Spearman correlation coefficients (with one exception: 0.583) ranged between 0.766 and 0.969.

In addition to descriptive statistics, quantitative data were subjected to an inductive analysis, employing nonparametric statistics tests, as follows: the Friedman test for comparing multiple measures and the Wilcoxon signed-ranks test (with a Bonferroni correction applied) for carrying out paired comparisons. Nonparametric statistics was adopted because of the limited sample size and the non-conformity of the data to normal distribution in most cases. Statistical analyses were made using the SPSS package. However, the main

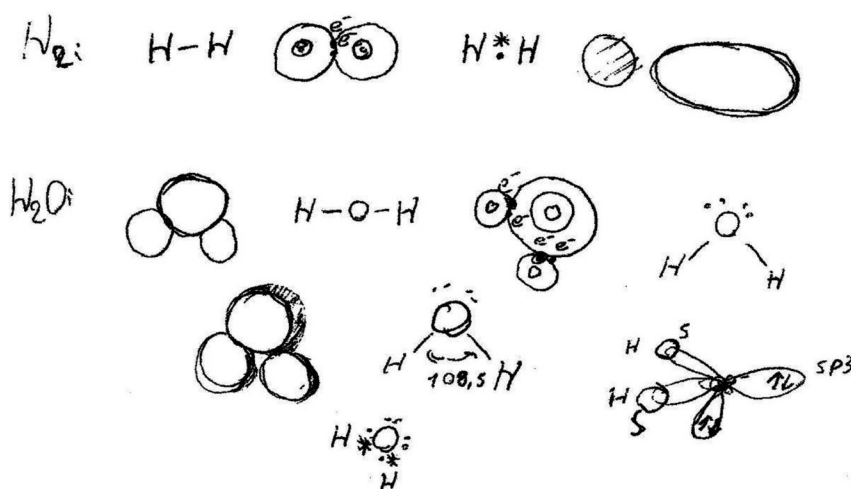


Figure 4: Student #18's drawings in response to question 1. This student was marked 100% for the structures for H_2 and 96% for the structures of H_2O .

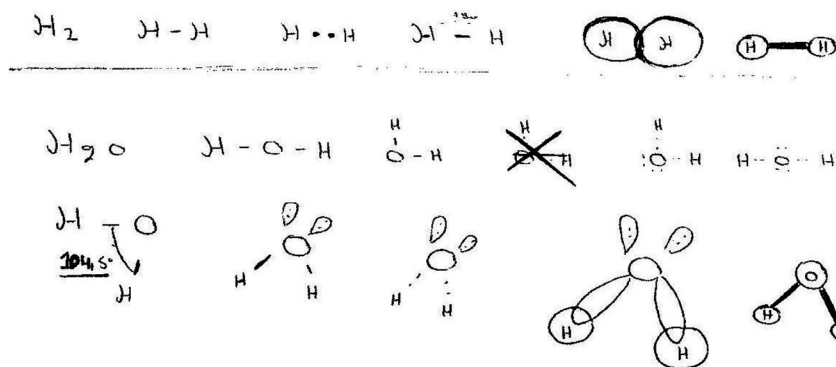


Figure 5: Student #16's drawings in response to question 1. This student was marked 50% for the structures for H_2 and 93% for the structures of H_2O .

emphasis of our reported results is on qualitative conclusions based on students' written justifications of their answers. The examination paper and students' written responses were in Greek. Accuracy of translation into English was checked by back translation of the English version into Greek by one of the authors (GT). The two Greek versions (original and back-translated) were then compared, some changes to the English version were made and the final text in English was checked by another author (BB) (Brislin, 1970, 1986).

Results and discussion

Descriptive statistics

The mean mark obtained by the 31 students on section D was 52.9% (s.d. 16.2%), reflecting a moderate performance. There were seven students (22.6% of all students) who achieved a mark >70% (students # 18, 8, 27, 16, 9, 12, and 4, with student #18 achieving the highest mark 77.4%). Table 2 shows descriptive statistical data for each of the four questions and the total mark for section D. We note that the highest mean mark was for question D.2 (57.9%) and the lowest for questions D.1 (37.3%).

Inductive statistical analysis I: comparison of the individual questions D.1, D.2, D.3 and D.4 of section D

The Friedman test statistic is $\chi^2(3) = 8.089$, which is significant ($p = 0.044$). Table 3 shows the statistical comparisons between pairs of questions D.1, D.2, D.3 and D.4, according to the Wilcoxon signed-ranks test. It is seen that question D.1's differences from questions D.2, D.3, and D.4 are statistically significant (for D.1–D.2, and D.1–D.3, $p < 0.01$; for D.1–D.4, $p < 0.05$), while D.2 and D.3, as well as D.2 and D.4 and D.3 and D.4 are not differentiated between themselves. It is concluded that while D.1 proved the most difficult question, the performances on D.2, D.3 and D.4 were all similar.

Table 2: Results of descriptive statistics: Percent achievement on the individual questions and overall performance on section D.

Question (contribution)	D.1 (20 marks)	D.2 (60 marks)	D.3 (10 marks)	D.4 (10 marks)	Section D, total
Mean	37.3%	57.9%	55.0%	51.8%	52.9%
s.d.	22.7%	18.1%	26.9%	31.3%	16.5%
Max	97%	89%	80%	93%	77%
Min	10%	7%	0%	0%	15%
Median	30.0%	59.6%	70.0%	60.0%	54.9%

Table 3: Paired comparisons of questions D.1, D.2, D.3 and D.4 on the basis of the Wilcoxon signed-ranks test. Values of z statistic, with 2-tailed significance level (p) within parenthesis.

Question	D.1	D.2	D.3	D.4
D.1	–	–3.626 ^a (<0.0001)	–2.957 ^a (0.003)	–2.343 ^a (0.019)
D.2	–	–	–0.353 ^b (0.724)	–1.009 ^b (0.313)
D.3	–	–	–	–0.546 ^b (0.585)

^aBased on negative ranks. ^bBased on positive ranks.

Question D.1: visual representations of the hydrogen and water molecules

Question D.1 showed the poorest achievement (37.3%), and this was the case for both its parts (see Table 4), dealing with VRs for the hydrogen and the water molecule respectively. The poor results resulted from the fact that many students used only simple structural formulas: H–H and linear and/or bent H–O–H, plus the corresponding Lewis structures. Many also used ball & sticks models. Very few included the value (104.5°) for the angle in H₂O. Several students used models of atoms in molecules, such as two touching and/or overlapping circles for H₂. Very few used the ellipsoid isodensity surface for H₂ (see Figure 4) or the *sp*³ hybrid orbitals model for H₂O (see Figures 4 and 5).

Figures 4 and 5 show the best two answers (97 and 80% respectively) to question D.1, which were submitted by students #18 (Figure 4) and #16 (Figure 5). Note that student #18 was ranked first with a mark of 77.4% and student #16 was ranked fourth with a mark of 73.4 overall on section D.

Question D.2: using electrostatic potential maps as visual representations

We will now focus on question D.2 and its five parts (see Table 1 and Figure 2), which is particularly relevant to the present study. Table 5 shows the descriptive statistics. Students performed well on parts D.2e and D.2c (82.7 and 73.2% respectively). D.2e asked for two features of the colored VRs that help us to understand chemical bonding and most students provided good answers, while part D.2c asked about polar structures among the colored figures. The remaining three questions showed lower mean performances of around the 50% mark. Part D.2a asked for an explanation of the highly polar bond (approaching ionic) displayed in the compound LiH, Part D.2b concerned the color differences displayed by the hydrogen halides HCl, HBr and HI, while D.2d involved the continuity between ionic and covalent bonding. For a complete explanation, all three of these parts required multi-structural SOLO thinking, that is, employment of more than one feature or property was needed. In addition, parts D.2a and D.2d, where a complete answer requires a relational dimension of the SOLO taxonomy, in addition to the multi-structural elements were considered particularly demanding. For this reason, we chose to assign a higher contribution to these two parts in comparison to the other three parts of question D.2 (see Supplementary Material S3).

Table 4: Percent achievement on the parts of question D.1.

Part (contribution)	D.1a (6 marks)	D.1b (14 marks)
Mean	39.8%	36.3%
s.d.	33.0%	22.5%
Max	100%	96%
Min	0%	7%
Median	16.7%	28.6%

Table 5: Percent achievement in the five parts of question D.2.

Part (contribution)	D.2a (15 marks)	D.2b (10 marks)	D.2c (10 marks)	D.2d (15 marks)	D.2e (10 marks)
Mean	47.9%	50.2%	73.2%	46.3%	82.7%
s.d.	25.1%	24.7%	25.4%	30.8%	24.7%
Max	85%	100%	100% (nine times)	85% (three times)	100% (16 times)
Min	0%	10%	0%	0% (six times)	0%
Median	50.0%	45.0%	75.0%	50.0%	100

Table 6: Paired comparisons of the five parts of question D.2, on the basis of the Wilcoxon signed ranks test. Values of z statistic, with 2-tailed significance level (p) within parenthesis.

Part	D.2a (15 marks)	D.2b (10 marks)	D.2c (10 marks)	D.2d (15 marks)	D.2e (10 marks)
D.2a	–	–0.347 ^a (0.729)	–4.027 ^a (<0.0001)	–0.304 ^b (0.761)	–4.229 ^a (<0.0001)
D.2b	–	–	–3.667 ^a (<0.0001)	–0.758 ^b (0.448)	–4.330 ^a (<0.0001)
D.2c	–	–	–	–3.764 ^b (<0.0001)	–1.923 ^a (0.054)
D.2d	–	–	–	–	–4.251 ^a (<0.0001)

^aBased on positive ranks. ^bBased on negative ranks.

Inductive statistical analysis II: statistical comparison of the parts of question D.2

The Friedman test gives the test statistic $\chi^2(4) = 42.064$, which is significant at $p < 0.001$. Table 6 has the results of *post hoc* comparisons with the Wilcoxon signed-ranks test. It is seen that the easiest parts D.2c and D.2e are not differentiated between themselves, and the same is true concerning the by pair comparisons between the hardest parts D.2a, D.2b, and D.2d. On the other hand, the differences between D.2a–D.2c, D.2a–D.2e, D.2b–D.2c, D.2b–D.2e, D.2c–D.2d, D.2d–D.2e are statistically significant ($p < 0.01$).

Qualitative analysis

Ionicity of the compound LiH

Part D.2a asks for a justification of compound lithium hydride being considered ionic on the basis of the electrostatic potential maps (a) (left), (b) and (e) in Figure 2. The acceptable answer should include that the marked decrease in size of the Li atom (being similar to the size of the Li^+ ion shown in map (b) right) and its large positive charge indicate that LiH can be essentially thought of as ionic (Li^+H^-). This means that the bonding electron pair is not shared but rather belongs almost entirely to H^- . The calculation models an isolated LiH molecule in vacuum.

We know of course that discrete molecules of genuine ionic compounds do not exist, with ions only being found in condensed phases. This is supported by the quantum mechanical optimization of the structure of the system consisting of two lithium and two hydrogen atoms, which favors the formation of a dimer, leading to a lattice structure (a crystal) This should be contrasted with the optimization of the geometry of four hydrogen atoms, which leads to the formation of two distinct covalently bonded H_2 molecules (Jensen, 2010, p. 110).

Clearly, part D.2a can be considered particularly demanding, because a complete answer requires consideration of both bond polarity and the sizes of ions, with reference to maps (a), (b) and (e), on the question paper (see Figure 2), and this requires both multi-structural and relational dimensions of the SOLO taxonomy.

Students were asked to identify the cation and the anion in the compound lithium hydride. Surprisingly, six students suggested that H^+ was the cation and Li^- the anion, although one of these reverted to H^- and Li^+ , when subsequently providing an explanation. It seems likely that these students were very familiar with the H^+ ion (which is present in aqueous chemistry) but had not encountered the lithium ion, which (being a metal ion) will clearly be the cation.

Only four students, plus another who came close, were able to provide a satisfactory explanation for the ionicity of lithium hydride, with the aid of the provided colored VRs. Performance was moderate (mean of 47.9%) on this part. Complete or nearly complete explanations were expected to include mention of both the plus and minus polarities and the relative sizes of the two ions (with Li^+ being much the smaller partner). We provide below an example of a nearly “complete” explanation:

Student #23: “Li lies lower (than H) in the periodic table, so it is less electronegative, therefore H has a larger tendency to attract electrons. Consequently, H is the anion and Li is the cation. From maps (b) it is seen that the Li cation is smaller since it loses one electron, and its color is blue ... and acquires a positive charge. On the other hand, H, which acquires a negative charge, becomes red. Therefore, with the formation of ionic bond between them, the representation in map (e) results” [*Note that this student, and also many others, were exact in their response to the first subquestion and just stated which is the cation and which the anion, without referring to their actual charges (Li^+ and H^-). Several other students, however, did write the Li^+ and H^- ions*].

It is true that this student’s answer to the first subpart of D.2a was based on noting trends in electronegativity related to placement within the periodic table. This allowed the student to deduce that H would be the anion and Li the cation. This information was then mapped onto the VR to deduce which side is lithium and which side is hydrogen. Although most students utilized the color coding and electronegativity difference and/or the bond polarity, few made reference to the size of the two bonded entities:

Student #3: “ Li^+ , H^- . Ionic is the compound in map (e) because, as we see from the colors, the compound contains one blue color (the cation) and one red color (the anion)”.

Student #1: “From the colors [the color scale] for electronegativity, we see blue and red colors in Li–H, which means that there is a large difference in electronegativity, therefore the bond is much polarized, so that the elementary charges become nearly unity and we have an ionic compound (Besides, Li is a metal, so it does not make covalent bonds)” (*Note the more elaborate answer here*).

It is noteworthy that 10 students did not refer to the color coding for bond polarity at all, but instead used various arguments concerning the “mechanism” for ionic bond formation (the “history conjecture”, including anthropomorphic elements) (Taber, 2013):

Student #26: “It is about an ionic compound because as Li has one electron, which is ... donated to H, which has already one electron and wants to fill a He noble-gas structure. In map (e) we see that the bond is ionic because of the polarity difference, which is considerable” (*Note, the reference to the large bond polarity seems likely to have been deduced from the color differences observed*).

This argumentation is consistent with the approach taught in the upper secondary education (10th grade) chemistry lessons for these students (see Tsaparlis et al., 2018).

The polar character of the bonds in hydrogen halides and its chromatic interpretation

Part D.2b asked students to identify what the color differences of the HCl, HBr and HI hydrogen halides in maps (d) show. A complete answer required reference to both bond polarity and the difference in electronegativity among the three halogen atoms, as well as an explanation for the variety in the coloring. Most students used just one feature, and answers were often very short or vague. This accounted for the poor performance (mean of 50.2%) on this part.

Student #11: “[The color differences] show the difference of electronegativity between HCl, HBr, HI” [Similar: #12].

Student #17: “[It shows] where the charge is displaced”.

Student #10: “The color difference of the HCl molecule shows that from positive becomes negative, for HBr shows that from positive becomes neutral, while HI is a neutral molecule”.

Several students referred to ionic bonds or to ions, especially in the case of HCl:

Student #13: “[The color difference] shows the polarization of the ionic bond”.

Student # 23: “The stronger the ionic bond, the more intense and distinct the colors are in the quantum mechanical structures. Therefore, the color differences show the reduction of the electronegativity from Cl^- to I^- ”.

Student # 6: “They show the larger overlap of the H⁺ atom by the anions, because of their size and their electronegativity. [In terms of size] the case is that $I^- > Br^- > Cl^-$ ”.

Student #4: “The color differences of these molecules show the difference in electron density, and in this way we realize the ionic nature of the molecular bond and that there is a difference in electronegativity. The last molecule, HI, could even have a covalent bond because the electrons are nearly evenly distributed”.

Student #15: “The color differences show the difference in polarization of the atoms that make up each molecule; in short, they show the kind of the bond, which tends to ionic bond and which [tends] to covalent bond. Accordingly, HCl makes an ionic bond, where Cl pulls the common electron pair; HBr, where Br pulls a little the electrons; and HI makes covalent bond and shares the electrons”.

Note the elaborate wording of students #4 and #15, despite their conceptual deficiencies. Others referred to ‘ionicity’, meaning apparently the varying ‘ionic character of the (covalent) bond’:

Student #3: “The color changes show the difference of electronegativity between Cl, Br, I; that is, HCl is more ionic compound, while HBr and HI are not so ionic”.

Finally, we quote the best and three other very good answers to part D.2b (according to our marking):

Student #8: “The color difference show the change in bond polarity ($HCl > HBr > HI$). The larger the electronegativity difference, the more polarized the bond is: HCl, large difference, → much polarized; HBr, moderate difference, → little polarized; HI, small difference, → the least polarized [Similar: #9 and #26].

Student #22: “[They show] that because, in terms of the electronegativity, $Cl > Br > I$, ... the particular coloring happens, because Cl causes a larger polarity than Br, and Br than I” [Similar: #26].

Student #18: “They show how much polarized each bond is, because of the electronegativity difference”.

Student #14: “The color difference shows bond polarity, that is, [an] electronegativity difference between the two atoms of the molecule. The more electronegative the atom is ($Cl > Br > I$), the more red is the color of the atom that is joined to H”.

Structures with a chemical bond polarity

Part D.2c asked which of the structures given in maps (c), (d) and (e) show polarity in a chemical bond. Nine students achieved a 100% and 2/3 of the students included in their answer an essentially ionic structure for LiH, which is encouraging, leading to a satisfactory performance (mean mark = 73.2%):

Student #12: “In maps (c), the water molecule is a polar chemical bond because oxygen attracts electrons toward it. In maps (d), HCl shows the largest polarity, and then follow HBr and HI, with much smaller (nearly zero) polarity. In map (e), LiH is a polar chemical bond”.

Student #8: “maps (c): H₂O; maps (d): HCl, HBr (slightly), HI (almost not); map (e): LiH”.

On the other hand, apparently or implicitly, some students assumed that the LiH bond was nonpolar (Students #3, 25, 28 and 30). “In LiH we cannot talk about (bond) polarity” (Students #28 and 30). This is a known misconception: “Polarity occurs only in covalent bonds but not in ionic bonds” (Tsaparlis et al., 2018). One student (#3) did not include HCl among the polar bonds because (s)he assumed that it was ionic. Actually, several students assumed HCl to be ionic as was found from their responses to part D.2d: # 3, 4, 12, and 16 (for #3 and #4, “it is clearly ionic”). Hydrogen chloride is of course encountered by students as a strong acid, in its ionized form as an aqueous solution, and this seems likely to contribute to the above misconception. However, we have also observed an unfortunate side-effect of the colored representations that appeared to confuse several students: the intense/“thick” blue and red colors were taken as an indication of ionic bonding. This was the case more often with HCl (as compared to HBr and HI) but was also found with H₂O in some cases. The responses of students #23 and #25 were particularly notable:

“In maps (c), the continuity among bonds is apparent, because the form on the left (H_2) shows the covalent bond, while the form on the right (H_2O) (shows) two ionic bonds” (#23).

“Maps (c) show continuity between covalent and ionic bond because on the basis of the [shown] polarity scale it passes through both stages in the formation of H_2O ” (#25).

What appears to have happened in these cases is that students have naively adopted the ionic-covalent bond dichotomy and failed to appreciate the difference between highly polar covalent and ionic bonding.

The covalent-ionic bond continuity

As we reported earlier, part D.2d which dealt with the continuity between covalent and ionic bonds, had the lowest mean mark (46.3%) among all five parts of question D.2. A complete answer involves both the third (multi-structural) and fourth (relational) dimensions of the SOLO taxonomy. It is noticeable that performance in this question was similar to that for D.2a (47.9%), the only other question requiring the relational level. Four students did not answer the question at all, one merely referred to “map (e)”, while a number of others provided only irrelevant explanations at the pre-structural SOLO level:

Student #6: “Map (e), because none atom dominates, but the charges are different”.

Student #14: “In maps (c), the structures show the difference between ionic and covalent bond, because H_2 does not show polarity (same color everywhere), while in H_2O a difference in color appears, therefore it is a polarized molecule, that is, it forms a covalent bond”.

A serious problem reflected in several students’ responses to this question (which we referred to earlier) was that of misinterpreting the characteristic contrast between the blue and red colors as an indication of ionic bonding. This could also be a consequence of the fact that most students did not appear to pay attention to the change in size upon formation of ions and use this as a feature of ionic bonding. It is true that maps (d) alone do demonstrate the change of bond polarity on moving from HCl to HI, and these maps were used by most of the students, but map (e) (with the more polar LiH) and maps (c) (with H_2 and H_2O) provide further support, so a complete answer should employ all maps (c), (d) and (e). We quote below two good answers employing only maps (d):

Student #24: “It [the continuity of bond type] is demonstrated in maps (d) because from the left to the right the difference in electronegativity appears to lessen, and eventually it appears that the electrons appear to be shared equally”.

Student #30: “Maps (d) shows the continuity between ionic and covalent bond because it is evident that the difference in electrochemical potential decides the bond”.

Some students did employ all three sets of maps (four students) or two of these sets (c) and (d) or (d) and (e) (another three students). The best response and another interesting one are reproduced below:

Student #27: “The structures that demonstrate the continuity between ionic and covalent bond are those of LiH, HCl, HBr, HI, H_2O , because [starting] from LiH where we have very strong charges (the red and blue colors dominate), we move to H_2O where it [the blue vs. the red coloring] starts diminishing and we arrive at HI, where we have mainly green color in the ends and in the middle. Therefore we do not have polarity as large as in the previous [cases]”.

Student #11: “The continuity between ionic and covalent bond is evident in maps (c), (d) and (e) because of the alternation of colors – appearance of blue-green-red – and as shown in the (color) scale, this change of color explains the above [observations].

Contribution of the colored visual representations to understanding

Part D.2e asked students to refer to two features of the colored VRs that helped them to understand chemical bonding and a mean mark of 82.7% was obtained on this part. Sixteen students’ responses were awarded

100%, and satisfactory answers were submitted by many other students. The few poor answers made reference to only one feature. On the other hand, placing a limit of two features probably restricted the students from referring to the many issues associated with these VRs. Features reported included the extent of polarization of the bonds, the evidence for electronegativity differences, the type of bond formed, the size of atoms/ions and/or the size and form of molecules. There were both short and lengthier good responses:

Student #25: “It helps us deduce the type of bonding, as well as how polarity changes within the molecule”.

Student #8: “(1) The electronegativity of each element (and) consequently the polarity of its bonds. (2) The shape of the electron density in a compound”.

Student #27: “One feature is the existence of ionic, polar covalent and nonpolar covalent bond, [as deduced] from the color scale which shows ... the polarity of the bond. Also we realize which atom has the negative and which has the positive charge in the compound”.

Question D.3: an application – visual representations of organic molecules

Question D.3 presented students with colored VRs for two organic molecules which have similar structures, CH_3Cl and CH_3Li ,³ (see Figure 3) and asked for the identification with justification of the two VRs (which belongs to which molecule). The mean mark was 55.0%. A complete answer should involve not only bond polarities (on the basis of the colorings) but also a comparison between the larger electron cloud of Cl [in structure (a)] as compared to that of Li [in structure (b)]. The following is a good attempt to use both bond polarities and atomic sizes, however, it also refers to Li^+ and to an ionic bond in CH_3Li :⁴

Student #9: “Cl has larger size than Li, and this follows from how the charge is distributed around the molecule. Also the bond [in CH_3Cl] will be covalent, and therefore it will have a smaller polarity. In [the case of] CH_3Li the bond will be ionic and this follows from the polarity of bond, but also by the fact that Li^+ , which has a smaller size in comparison to C or to Cl because it has lost one electron”.

Bond polarities in the C–Cl and C–Li bonds respectively, with Cl being electronegative and Li electropositive, as judged from the coloring, were used as a criterion for the explanation, for 17 out of the 31 students. An example:

Student #2: “Structure (a) corresponds to compound CH_3Cl . Cl is more electronegative than C, so when they are bonded between themselves, the fraction of negative charge shifts toward Cl, so it acquires a red color in the above representation” [And similarly for structure (b)].

Question D.4: features and comparisons of various visual representations

Question D.4 asked for a comparison between the VRs for the hydrogen molecule and the water molecule that students had drawn when answering question (1) and the corresponding colored quantum mechanical VRs. In particular, the features and the advantages of the two visual representations were required. Although six students did not answer this question at all, many students provided more or less extensive answers, covering various aspects and views. Many students were supportive of the quantum mechanical colored VRs, although

3 Chloromethane (CH_3Cl), also called monochloromethane and methyl chloride, is a colorless, odorless, flammable gas, soluble in water. **Methyl lithium** is the simplest organolithium reagent with the empirical formula CH_3Li . It is a highly reactive compound, and, because it is highly reactive toward water, it is used as a solution in ethers.

4 CH_3Li can be thought of as being source for the CH_3^- ion: $\text{CH}_3\text{Li} \rightleftharpoons \text{CH}_3^- + \text{Li}^+$ (with CH_3^- being the conjugate base of the very weak acid CH_4 ($K_a = 1 \times 10^{-49}$), so CH_3^- is the strongest base ($K_b = 1 \times 10^{35}$).

several realized that they have limitations and are just complementary to the traditional VRs. Some students suggested that they are likely to be more suitable for older students and one student even suggested that they were inferior to the traditional ones:

Student #27: “In VRs [of question 1] we have the elements represented with symbols, and these are more understandable, and also they show better the elements that combine. Also, in these VRs, there is the possibility to represent electrons symbolically around the atoms, and this makes the concept of bond and electron sharing more understandable. Finally, from these VRs we obtain information about the orbitals and the geometry of the molecules (e.g. the angles). On the contrary, in the case of the maps of Figure 2, we have the electron density and [bond] polarity by means of a color scale. This facilitates understanding about which bond is polar or not, which atom has positive or negative charge in the bond, as well as how this charge is distributed along the bond”.

Student #9: “The simple VRs [of question 1] help simply in understanding of the bond in the molecule, [but] they don’t show clearly the nature of the bond, its type or its polarity. ... [On the other hand], the quantum mechanical, color representations offer more information about the bond that is formed, the size of the participating atoms, as well as how polar in this bond”.

Student #28: “In maps (c), the VRs are better because they include color, the H_2 molecule appears in color in the form of a flattened sack. In [the case of] H_2O , we have color that shows that it has a dipole moment, since the red [color] is on the side of oxygen and the blue on the side of hydrogen ...”

Student #8: “It is better to use the color structures when teaching elder students, who have already understood concepts such as chemical bonds, charge, electronegativity of the elements, because while [these] demonstrate very well polarity, bond strength, [and] electron cloud, they do not show clearly the existence of electrons, the existence of bonds, and the presence of individual elements. On the contrary, the structures of question 1 make very distinctively apparent the existence of bonds and of elements [(s)he means atoms], the electrons of each element, and the electrons that participate in each bond. However, they do not show the difference in electronegativity, bond polarity, [or] the electron cloud. In conclusion, there is not a single representation which is better than another – we just consider which one is suitable for its purpose.

Student #31: “The [various] VRs present [various] advantages. Concerning the representations of question 1, they show the elements which form the compound, the bonds that connect them, the ‘free’ [non-bonded] electrons, their geometry in space. On the other hand, the color representations show the type of bond, [bond] polarity, the difference in electronegativity ... In my opinion, the representations of question 1 show more information about a chemical compound and many details ...”

Conclusions and implications

At the outset, we should point out that chemistry teaching in Greek secondary schools has traditionally been carried out with the aid of the chalkboard and textbooks, with particular attention being paid to the symbolic level of chemistry (writing molecular and structural formulas and chemical equations) and to solving computational exercises. Greek students’ experience of physical models of atoms and molecules tends to be limited to the pictures in their secondary-school textbooks, as no attention tends to be paid to them during the teaching. Note also that the chemical knowledge of these students was still immature, as they were just freshman students (at the end of their first year at university), so their responses should be judged taking this limitation into account. Let us first consider the answers to the individual subsidiary research questions posed in this study:

(RQ1): *To what degree did the provided VRs help the students to deduce the type of bonding in various molecules?*

The situation regarding nonpolar and polar covalent bonding appears encouraging. Part D.2c, which asked which of the structures of maps (c), (d) and (e) in Figure 2 show a chemical bond polarity, got a relatively high mean mark (73.2%). Consideration of LiH (part D.2a), however, where bonding starts to approach ionic caused difficulties (mean mark: 47.9%): only four students, plus another who was very close, provided complete or nearly complete multi-structural and relational explanations, which included mention of both the plus and minus polarities and the relative sizes of the two ions.

(RQ2): *To what degree did the provided VRs help the students to explain the variation of bond polarity in various molecules?*

When it came to providing explanations (part D2.b), the mean mark dropped from 73.2% (see above) to 50.2%, suggesting that students found difficulty in employing multi-structural thinking, often instead restricting themselves to considering only a single factor, aspect or feature.

(RQ3): *To what degree did the provided VRs help the students exploit the difference in size between an atom and its corresponding ion?*

The answer here is that only a minority of students appeared to understand the significance of size. It appears that the color scale marking different bond polarities as well as electronegativity differences played a dominant role in students' impressions about the VRs provided, with size of atoms and ions attracting only limited attention.

(RQ4): *To what degree did the provided VRs help the students to comprehend the concept of the continuum of bonding type and overcome the common misconception that bond polarity is a feature of covalent bonds only and not of ionic bonds?*

The relevant part (D.2d) got the lowest mean mark (46.3%) among all parts of question D.2, showing persistence in the covalent-ionic bond dichotomy in the thinking of many students. It appears that students readily relapse into a dualistic position when considering highly polar bonds, which is again consistent with the approach taken in the upper secondary education (10th grade) chemistry lessons for these students (see Tsaparlis et al., 2018). It is therefore likely to be important to continue to stress the continuum between a non-polar covalent bond and an ionic bond with the latter extreme never being achieved in practice.

Regarding the common misconception that bond polarity is only a feature of covalent bonds and not of ionic bonds, it is difficult to provide a definitive answer because there were cases where students did appear to hold this misconception. In addition, some students appeared to believe that ions can be involved in both ionic and covalent bonding (deriving from the use of blue and red colors to mark bond polarity in both covalent and ionic structures).

(RQ5a): *What types of static VR for common covalent molecules, such as H_2 and H_2O , are the students already familiar with?*

The findings from question D.1, which had the lowest mean mark (37.3%) among all questions, suggest that few students had available and were familiar with a satisfactory collection of VRs for these common molecules. Here many students drew only the H–H and linear and/or bent H–O–H, plus the corresponding Lewis structures, and/or ball & sticks models. Very few included the H_2O angle. Although, several students used models of atoms in molecules, such as two touching and/or overlapping circles for H_2 , very few used the ellipsoid isodensity for H_2 or the sp^3 hybrid orbitals model for H_2O (see Figure 4).

(RQ6): *How does the information that students can obtain from the colored VRs resulting from quantum mechanical calculations compare with the information that they can obtain from the VRs that they are already familiar with?*

On an optimistic note, the students worked with the colored quantum mechanical VRs and many of them expressed positive views about their features, as shown by the range of answers to question D.4 and the high mean mark (82.7%) obtained for part D2.e. Students referred to features such as the extent of polarization of the bonds, the evidence for electronegativity differences, the type of bond formed, and to a lesser extent the size of atoms/ions, thus suggesting that the students were able to appreciate that these colored VRs were able to provide information not available from the VRs that they were already familiar with. On the other hand, several students pointed out limitations of the colored VRs, considering them as merely complementary to the traditional VRs, and considered them as likely to be more suitable for older/more experienced students. The

mean performance over the whole of section D, which was only moderate (52.9%, s.d. 16.5%) can be justified by the fact that many students preferred to use their established knowledge, such as the process for ionic bond formation or simple rules such as a bond between a metal and a non-metal is ionic, while a bond between non-metals is covalent, rather than to employ new knowledge involving the colored VRs.

Finally, the fact that the representations used result from quantum mechanical calculations of high accuracy is clearly an asset, which adds to their importance and usefulness. However, it was noteworthy that almost none of the students mentioned this characteristic, probably because the students were not yet familiar with quantum mechanical calculations. In general, students were somewhat uncomfortable with these VRs due to their lack of previous exposure to them. A more systematic and extensive coverage would be expected to lead to better outcomes. Emphasis should clearly be paid not only to color scaling (as this is related to bond polarity), but also to the size and forms of atoms, ions, and molecules. The inclusion of the bond-and-stick model or the tube model inside these electrostatic potential maps could be very helpful in providing a helpful bonding picture within the potential map, thus connecting the classical with the modern picture of bonding.

In conclusion and importantly, the main research question for the present study was: *How do students interpret colored VRs when presented with them for the first time?* Or equivalently: *Are students able to immediately decode and incorporate/synthesize colored VRs into their previous chemistry knowledge?* As stated, a substantial limitation of this study was that the students had not encountered the quantum-mechanical colored VRs prior to the examination. Although the students were certainly able to work with the VR maps, it was not clear whether they were actually using the colored VRs to inform their understanding, or, whether they were instead resorting to previous knowledge and other heuristics to map onto the VRs. Further, students found difficulty in employing multi-structural thinking or simply did not feel a need to do so, and restricted themselves instead to considering only a single factor, aspect or feature. So it is not really clear to what extent the VRs helped these students to make the required deductions. It is expected that with exposure to these VRs and the method of constructing them, that students will become familiar and comfortable with their various features and uses.

It is hoped that the findings of the present study will be of interest to teachers looking to improve the teaching and learning of chemical bonding. We believe that these VRs can help in deepening students' conceptual knowledge of relevant structural matters, and in avoiding the formation of misconceptions derived from deficient knowledge and careless use. It is important that teachers stress the advantages of the colored VRs and provide advice to students on how best to use them. These VRs are not intended to replace other more common VRs but rather to synergistically supplement them by providing a simple new and different picture of the polarization in chemical bonds. Students will of course need practice to learn how best to use these VRs alongside other representations that they are already familiar with. These VRs provide information not only by using color but also through their representation of the size of the atomic cores. While the students in this study, by and large, tended to ignore or pay little attention to the latter factor, it seems reasonable to expect that with practice this should improve.

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