



AN INSIGHT TOWARDS CONCEPTUAL UNDERSTANDING: LOOKING INTO THE MOLECULAR STRUCTURES OF COMPOUNDS

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Abstract: The subject of molecular structures is one of the most important and complex subject in chemistry which a majority of the undergraduate students have difficulties to understand its concepts and characteristics correctly. To comprehend the molecular structures and their characteristics the students need to understand related subjects such as Lewis dot structures, molecular geometry, bond polarity, molecular polarity, resonance and hybridization. This study investigated the conceptual understanding levels and misconceptions held by university students about molecular structures subject. The sample of the study comprised of 88 undergraduate students enrolled in the Department of Mathematics and Science Education, Faculty of Education, Turkey. The participants responded to open-ended and interview questions regarding the subject. Students' responses were analyzed and their conceptual understanding levels were determined. The results indicated that students had lack of knowledge and misconceptions about the subject although they studied it in the university. Especially, they had poor knowledge about the molecular geometry, molecular polarity, resonance, and hybridization in molecular structures except for Lewis dot structures of molecules. Accordingly, implications have been made for more effective teaching approaches to ensure better understanding of the subjects.

Key words: Molecular structures, Lewis dot structures, molecular geometry, resonance, misconception

1. Introduction

It is the basic subjects in general chemistry that help students to improve their knowledge in other chemistry fields such as organic chemistry and biochemistry (Burrows & Mooring, 2015; Duis, 2011). Therefore, the specific basic chemistry concepts which underlie chemical systems, such as bonds, molecular structures, and reaction mechanisms and their characteristics, especially need to be learned (Fensham, 1975). The subject of molecular structures is a complex subject where students are expected to perceive and interpret symbolic representations in chemical bond structures and the formation of structures based on physical principles (Nicol, 2003; Taber & Coll, 2002).

1.1. The context of molecular structures

Molecular structures are identified by the effects of many factors such as bonds formed between atoms, the three dimensional layout of adjacent atoms around a center atom, and angles between bonds. These structures are the determinants of both the physical and chemical characteristics of the molecule. There are some theories that explain these structures. These theories are: the Valence Bond Theory, the Valence Shell Electron Pair Repulsion (VSEPR), the Ligand Close-Packing (LCP) Model, and the Molecular Orbital Theory (MOT). Explaining the same structure with many theories can cause students to experience confusion and misunderstanding in these subjects (Hurst, 2002).

Molecular structures are also the basis of the study of chemical bonding, which is one of the most important subjects in chemistry and which includes key concepts used in many other areas, particularly the structure of matter, change of state, chemical reactions, and thermodynamic and chemical reactivity

(Levy Nahum, Mamlok-Naaman, Hofstein, & Taber, 2010; Ünal, 2002). Because an atom, its structure, and its interaction with other atoms cannot be seen or experienced in daily life, the study of atoms, ions, molecules, and other subjects that include these concepts seems mostly abstract to students (Griffiths & Preston, 1999; Levy Nahum, Mamlok-Naaman, Hofstein, & Krajcik, 2007). In addition, many international studies state that the concepts of molecular structures and chemical bonding are abstract in nature and deal with the microscopic level of matter (Chittleborough & Treagust, 2008; Levy Nahum, Hofstein, Mamlok-Naaman, & Bar-Dov, 2004; Taber, 2013). However, students perceive matter as macroscopic in their daily life. Because of this, they explain the microscopic structure of matter with their macroscopic experiences and cannot understand the subject (Johnstone, 1991; Robinson, 2003; Stavridou & Solomonidou, 1998; Tsapalis, 1997). To teach chemical concepts effectively, both macroscopic and microscopic definitions and demonstrations should be given to students (Novick & Nussbaum, 1981; Taber, 2013). Due to the invisible structure of molecules, these structures constitute the microscopic and symbolic levels of matter. Both during high school and university education, most students have difficulties when they come across with concepts that include the mental manipulation of molecular structures (Copolo & Hounshell, 1995). Molecules should be perceived as three dimensional. However, molecular structures are shown with two-dimensional drawings in most lessons and textbooks. The perception of molecules as three dimensional will also help increase the comprehension of chemical reactions and molecular structures (Ferk, Vrtacnik, Blejec, & Gril, 2003; Rozzelle & Roserffeld, 1985; Wang & Barrow, 2013). In addition to comprehending the chemical behavior of matter, molecular structures should first be understood (Sarikaya, 2007).

Before determining molecular structures and their characteristics, students start with identifying the atom bond types in a molecule, valence electron numbers, its Lewis formula, and its Lewis dot structure depending upon these formulas. Based upon this dot structure, students identify atomic locations in the molecule according to the VSEPR theory. After this, students guess the polarity of the molecule based upon the attractive and repulsive forces determined by the electronegativity of its atoms. In this context, the molecular structures and the comprehension of their characteristics are directly related to Lewis dot structures, molecular shape, bond polarity, molecular polarity, and hybridization. By defining these concepts correctly and meaningfully, molecular structures and their characteristics can be perceived (Cooper, Underwood, & Hilley, 2012).

1.2. Students' conceptual understanding related to molecular structures

Conceptual understanding levels and misconceptions of students about molecular structures have been studied in national and international literature. These studies have shown that a significant number of college and high school students held alternative conceptions and had difficulties related to molecular structures (Burrows & Mooring, 2015; Cokelez & Dumon, 2005; Cooper et al., 2012; Dhindsa & Treagust, 2009; Furio & Calatayud, 1996; Meyer, 2005; Nakiboğlu, 2003; Peterson & Treagust, 1989; Peterson, Treagust, & Garnett, 1989; Purser, 1999; Sarikaya, 2007; Uyulgan, Akkuzu & Alpat, 2014; Wang & Barrow, 2013; Wu & Shah, 2004).

Some studies have been conducted where molecular structures, chemical bonding, and other concepts related to these subjects were examined together. Dhindsa and Treagust (2009) revealed that students have a partial understanding of the bond polarity of molecular structures, molecular shape, lattices, polarity of molecules, inter-molecular forces, and the octet rule, and they have some misconceptions about these concepts in their studies.

Wang and Barrow (2013) administered a diagnostic test to 159 students who attended a general chemistry lesson that included discussion of models of atomic structures and periodic variations, chemical bonding, and molecular shape and polarity. Forty-eight students of the students were then interviewed. These interviews showed that students have difficulties in comprehending VSEPR models and polarities. They also reported that molecular polarity has an important effect on learning the concepts of periodic variation (including models of atomic structure), chemical bonding, electronegativity, and molecular geometry.

Burrows and Mooring (2015) examined concept maps, using think-aloud applications during interviews with university students about their conceptual understanding of Lewis dot structure and bonding,

molecular geometry, and acids and bases. Their results showed that students showed a lack of knowledge and had misunderstandings about electronegativity, bond polarity, and covalent bonding.

Cooper et al. (2012) created a survey to study how university students attending general chemistry and organic chemistry lessons perceive molecular structures and their characteristics. Their results showed that general chemistry students made weaker statements about concepts related to molecular structures such as formal charge, resonance, and hybridization than organic chemistry students did.

There is a limited availability of studies in national field that examine students' misconceptions about levels of understanding of molecular structures. In these studies, the understanding levels of students on this subject were generally examined in terms of chemical bonding (Atasoy, Kadayıfçı, & Akkuş, 2003; Ünal, Coştu, & Ayas, 2010; Canpolat, Pınarbaşı, & Sözbilir, 2003; Yılmaz & Morgil, 2001). Yılmaz and Morgil (2001) used a diagnostic test to reveal second- and fourth-year university students' misconceptions about molecular polarity, VSEPR theory, Lewis structures, and molecular shape. In a similar study Canpolat et al. (2003) used a two-dimensional diagnostic test to reveal misconceptions of second (N=32), third (N=29), and fourth year (N=22) university students at Chemistry Teacher Training Program about bond polarity, molecular shape, attractive force among molecules, molecular polarity, and the octet rule. Ünal et al. (2010) studied eleventh grade high school students' conceptual understanding levels about chemical bonding. This study showed that students have a partial understanding with specific misconceptions when they determine Lewis dot structures and molecular polarity.

The above literature review suggests that students have misconceptions about the concepts associated with molecular structures: Lewis dot structures, molecule polarity, hybridization, molecular shape, resonance, and the octet rule. The studies above showed a preference toward using diagnostic tests to reveal misconceptions. The difference of this study from the other studies is revealing the misconceptions regarding the molecular structures subject and the reasons behind them through face to face interviews.

The main aim of chemistry education is to teach basic concepts and the connections among them, helping students obtain information for themselves rather than giving it all to them directly (Nakhleh, 1992; Raviolo, 2001). In accordance with this purpose, it is important to first determine students' chemistry knowledge and how they have made connections among different aspects of this knowledge (Ebenezer & Erickson, 1996; Taber & Coll, 2002). In this study, learning molecular structures accurately will have a positive effect on learning other subjects related to it. Therefore, it is important to determine when knowledge is incorrect or lacking, what misconceptions students may have, and what their understanding level of the subject is. This study contributes significant and deeply insight to the existing literature by identifying the misconceptions and conceptual understanding levels of undergraduate students on molecular structures subject.

1.3. Purpose of the study

In this study, we aimed at deeply examining undergraduate students' knowledge about concepts in molecular structures subject including Lewis dot structures of covalent compounds, VSEPR theory, hybridization, resonance, and polarity. The research questions addressed in this paper are:

- What are the undergraduate students' levels of conceptual understanding related to molecular structures subject including Lewis dot structures of covalent compounds, VSEPR theory, hybridization, resonance, and polarity?
- What are the undergraduate students' misconceptions related to molecular structures subject including Lewis dot structures of covalent compounds, VSEPR theory, hybridization, resonance, and polarity?

2. Method

2.1. Research design

In this study, a case study was used as a research method for examining undergraduate students' misconceptions and incorrect or lacking knowledge about the subject. A holistic single case study was used (Yin, 2003). The single case that was examined in the study involved molecular structures: examining the understanding levels of students about Lewis dot structures of covalent compounds, VSEPR theory, hybridization, resonance, and polarity. The case study method provides a close examination of research problems and provides in-depth information about the research (Bachor, 2000; Merriam, 1998). In a case study, a situation, relation, event, or process is examined at all points with a limited number of samples. Unlike many research methods, the case study method is a preferred method when it comes to asking what, how, and why questions about comprehension of subjects in education (Çepni, 2012).

2.2. Participants

The study participants were freshman students (N=94) in a public university's Department of Mathematics and Science Education in Turkey. Some students initially included in the study (N=6) could not participate in the study because of their absence. Therefore, the participation rate of the study was 93.6% (N=88).

The freshman students who participated in the study took General Chemistry during the fall semester. In this class, students first learned the concepts of formal charge and Lewis dot structures followed by molecular polarity, dipole moment, and electronegativity in covalent bonds, all concepts relating to chemical bonding. They then learned resonance, exceptions to the octet rule, repulsion of electron pairs, molecular geometry (VSEPR theory), hybridization, molecular orbital theory (MOT), and attraction forces between molecules. The students' basic knowledge about these subjects came from the high school ninth grade chemistry unit Chemical Interactions between Species in which students learned about molecules, ions, chemical bonding, interactions between molecules, and Lewis dot structures. In these lessons, Lewis dot structures are only shown for simple molecules (H_2 , Cl_2 , O_2 , N_2 , HCl , H_2O , NH_3 , CO , CO_2). In a later 12th grade chemistry unit, Introduction to Carbon Chemistry, students learned about inorganic and organic compounds, Lewis dot structures, hybridization, and molecular geometry. Expanded octet molecules are not taught within the context of this unit.

2.3. Procedure

Data was gathered in two stages in the study. First, students were asked open-ended questions. Second, students who had answered the questions were interviewed in depth to examine their knowledge about the subjects and concepts in the questions. Before the study, all the students were informed about the context of the study and how the results would be evaluated. An informed consent form was given to students for them to read. Students were free to choose whether or not to participate in the study (British Educational Research Association, 2011; as cited in Taber, 2014); therefore, all students in the study participated voluntarily. Because the aim of the study was to examine misconceptions and incorrect or lacking knowledge, data was collected from the students after they were taught the subjects at the university by a lecturer. Data collection tools were applied at the end of the fall semester.

2.4. Data collection tools

2.4.1. Open-ended questions

In the study, students were given open-ended questions in the form of a table chart where they were asked to fill in Lewis dot structures, bonding and non-bonding electron pair numbers, ball and stick models, molecular geometries, molecular polarities, central atoms, and hybrid types for eleven different molecules. An example was given of all the requested characteristics of a molecule (SF_4) (see Figure 1),

showing students that they were to show the structures of the molecules on a microscopic level in their drawings. In studies on conceptual understanding, student drawings are often used. Student drawings reveal conceptual understanding about a subject more clearly and transparently and do not limit students with words (Blanco & Prieto, 1997; Çalık, Ayas, & Ünal, 2006; Smith & Metz, 1996).

Molecule	Lewis dot structure	Bonding e ⁻ pair number	Non-bonding e ⁻ pair number	Ball-stick model	Molecular geometry	Molecular polarity	Center atom & Hybrid type
SF ₄		4	1		Distorted tetrahedral	Polar	S dsp ³
CO ₂	?	?	?	?	?	?	?

Figure 1. A sample section from the open-ended questions

An additional open-ended question asked students to determine the formal charges of each atom in three different molecules (SF₆, CO₂, and I₃⁻). Students were given 45 minutes to give the drawings and explanations in detail.

2.4.2. Semi-structured interviews

Semi-structured interviews consisting of questions about related subjects were conducted to determine students' understanding levels and misconceptions and the reasons behind these misconceptions. The researchers prepared four questions about the subject and its related concepts. To provide content validity to the interview questions, two chemistry faculty members were consulted and necessary editing was made in accordance with their recommendations. All students who answered to open-ended questions were invited to be interviewed by the two researchers. Each student's individual interview lasted 40-45 minutes. All students interviewed gave their permission to record the interviews on tape, and all interviews were completed in five days. The targets of the research questions are given in Table 1.

Table 1. The aims of the questions asked during the interviews

Questions	Aims
1	Defining of some concepts about molecular structures subject including Lewis dot structures of covalent compounds, VSEPR theory, hybridization, resonance, and molecular polarity
2	Understanding resonance structure of molecules
3	Understanding the exceptions to Lewis and VSEPR theory
4	Comprehension of Intramolecular bond polarity and molecular polarity

2.5. Data analysis

The students' answers and drawing given in response to the open-ended questions were evaluated into three categories: *correct*, *incorrect*, and *no answer*. A similar categorization system was used by Smith and Metz (1996). The frequency and percentage distribution of these categories, coded as 2, 1 and 0, respectively, were calculated using the SPSS 15.0 statistics program. A reliability analysis was performed using a coding key formed by writing different answers to each question as options. To determine the reliability of the coding, two researchers read and examined the answers given to the open-ended questions.

Content analysis was used to analyze the interview questions. The data obtained from the interview forms were transcribed using Microsoft Word. After the content analysis was performed to determine the conceptual understanding levels of the students, the students' answers were divided into five categories. These categories were *sound understanding*, *partial understanding*, *specific misconceptions*, *no understanding*, and *no response*. Similar categorization processes for determining students' levels of understanding are frequently encountered (e. g. Abraham, Williamson, & Westbrook, 1994; Özmen, Ayas, & Coştu, 2002; Ünal et al., 2010). The explanations of these categories are presented in Table 2. The answers given to these categories were evaluated by calculating frequency and percentage distributions.

Table 2. *The explanations of categories by coding criteria*

Categories	Coding criteria
Sound Understanding (SU)	Responses that include all components of the acceptable response
Partial Understanding (PU)	Responses that include at least one of the components of the acceptable response
Specific Misconception (SM)	Responses that include descriptive, incorrect, or illogical information
No Understanding (NU)	"I don't understand" or irrelevant responses
No Response (NR)	"I don't know"

Interrater reliability was calculated to provide reliability in analysis of open-ended questions and interview questions. The researchers independently placed all given answers into relevant categories by reading the documents belonging to each participant. *Agreement* and *disagreement* were determined by examining the categories of each coder (Kolbe & Burnett, 1991). The Cohen's kappa coefficient was used to measure interrater agreement for categorical variables. The Cohen's kappa coefficient for open-ended questions and interview questions between coders were respectively 0.92 and 0.84. These values reveal an almost perfect agreement (according to Landis & Koch, 1977).

3. Results

3.1. The results of open-ended questions

In this study, the students were asked to give the Lewis dot structures, bonding and non-bonding electron pair numbers, ball and stick models, molecular geometries, molecular polarities, central atoms and hybrid types for eleven molecules (CO_2 , SO_2 , H_2O , I_3^- , BF_3 , NH_3 , ICl_3 , CH_4 , XeF_4 , PCl_5 , and SF_6) in open-ended questions in a table consisting of eight categories. The students' answers in each relevant category for each molecule were analyzed as a total of frequencies. Figure 2 shows the frequency (f) distribution of answers given as correct, incorrect, and no answer in each category for the eleven molecules.

The answers given to the open-ended questions show that the most correctly answered categories from characteristics of molecules were bonding electron pair (f_c : 663; 68.5%), center atom (f_c : 590; 61.0%), and Lewis dot structure (f_c : 541; 55.9%) (See Figure 2). The most no answer categories were hybrid type ($f_{N/A}$: 480; 49.6%) and ball and stick model ($f_{N/A}$: 457; 47.2%). The most incorrectly answered categories were molecular geometry (f_{IC} : 322; 33.3%), molecular polarity (f_{IC} : 309; 31.9%), and hybrid type (f_{IC} : 306; 31.6%). The results show that students can identify Lewis dot structure, bonding/non-bonding electron pair numbers, and the center atom of molecule more easily than the other characteristics of a molecule. Though the students made correct drawings and gave correct answers, they could not identify molecular geometry and polarity correctly.

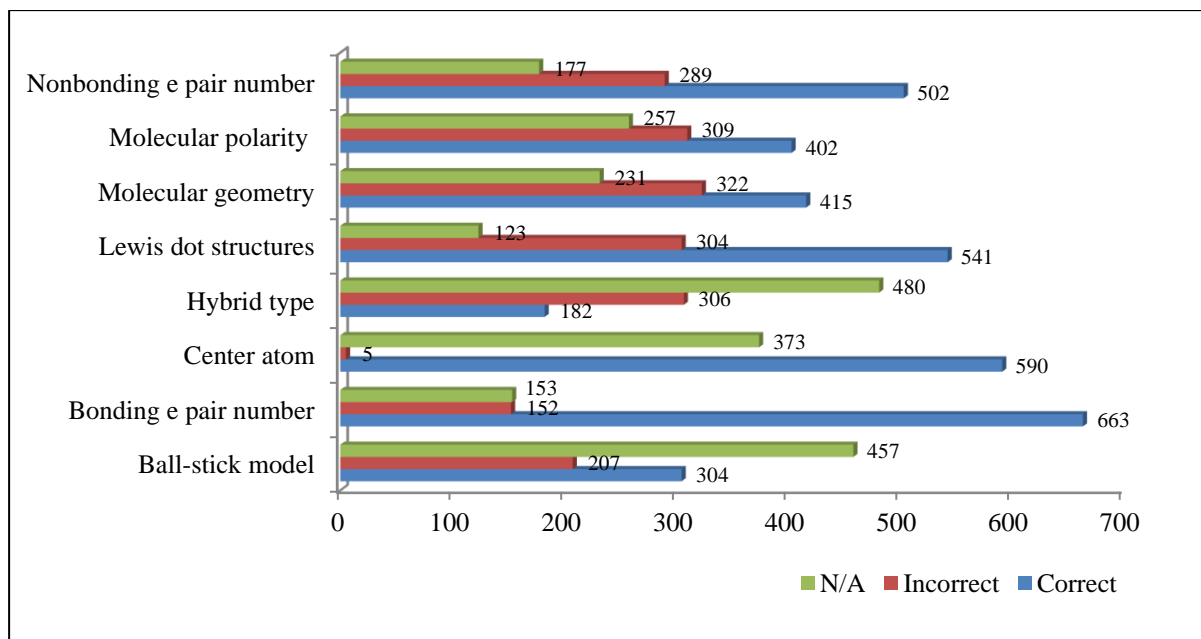
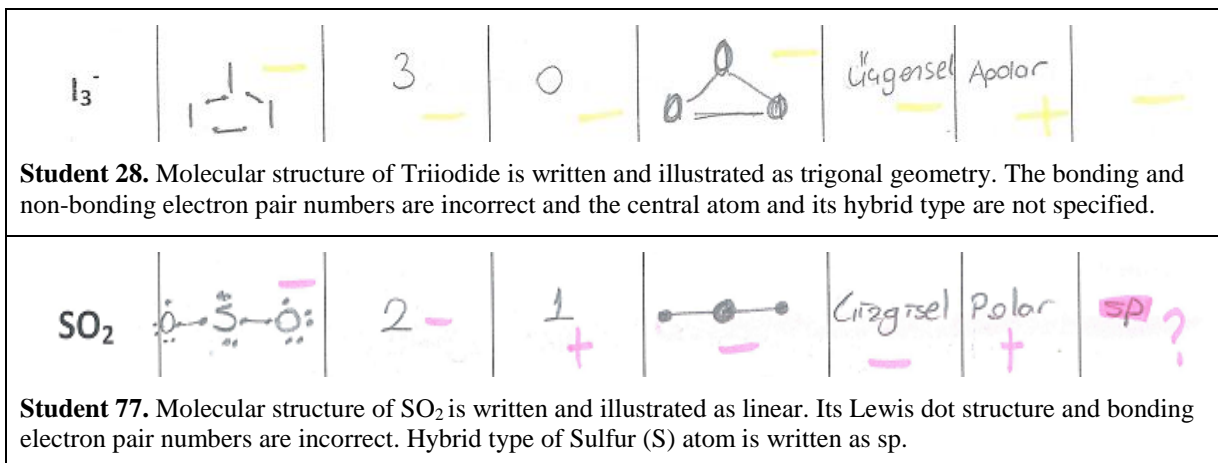


Figure 2. Frequency distribution of student answers as categories

Similarly, the students could not make correct drawings by considering molecular geometry as three-dimensional in the ball and stick model category. Also, in the hybrid type category, where there are less correct answers than incorrect answers, the students seemed to lack information about hybrid type for which the center atom could bond. We concluded from the results obtained from open-ended questions that the students had specific misconceptions about some molecules. The analysis of the students' answers showed that they could not identify the molecular structures and characteristics of I_3^- , ICl_3 , and XeF_4 molecules. This result shows that the students could not understand compounds that the elements of VIIA and VIIIA formed. Also, some students stated that as the I_3^- molecule was a charged molecule, it was an ionic compound. A striking misconception in answers related to molecules is that since Xe in the XeF_4 molecule is in the VIIIA group, it cannot form a compound. Also, the students generally could not give the characteristics of PCl_5 and SF_6 molecules. We can infer that the students did not understand molecular structures with expanded octets. Additionally, our results show that the students stated that there were trigonal planar in BF_3 , NH_3 , and ICl_3 molecules. The students could not think about non-bonding electron pairs in NH_3 and ICl_3 molecules. Therefore, they stated that molecular structures were trigonal planar for every three molecules. Also, some students stated that every two molecules in CH_4 and XeF_4 molecules were in square planar geometry. Similarly, this result shows that non-bonding electron pairs were not considered. In CO_2 , SO_2 , and H_2O molecules, some students stated that molecule structure was linear in all molecules. Incorrect drawing examples given to this question are shown in Figure 3.



NH_3 5A 1A		3 +	1 +		Düzlem üçgen -	Apolar +	N (Azot) ?
CH_4		4 +	0 +		<div style="border: 1px solid red; padding: 2px;">Büyük düzey</div>	Apolar -	C (Carbon)
BF_3		3 +	1 -		Bozulmuş tetrahedral -	Apolar +	B sp^2 -

Student 72. Molecular structure of NH_3 is written and illustrated as trigonal planar, and hybrid type of Nitrogen (N) atom is not specified.

Student 63. Molecular structure of CH_4 is written as square planar, and hybrid type of Carbon (C) atom is not specified.

Student 49. Molecular structure of BF_3 is written as distorted tetrahedral and its Lewis dot structure is incorrect, and the hybrid type of Boron (B) atom is written as sp^2 .

Figure 3. Examples of students' incorrect answers

In another open-ended question, the students were asked to give the formal charges of the atoms in SF_6 , CO_2 , and I_3^- molecules. The answers that the students gave for this question were evaluated for each molecule, and the answer frequencies, categorized as correct, incorrect, and no answer, were gathered and are shown in Figure 4 for each molecule.

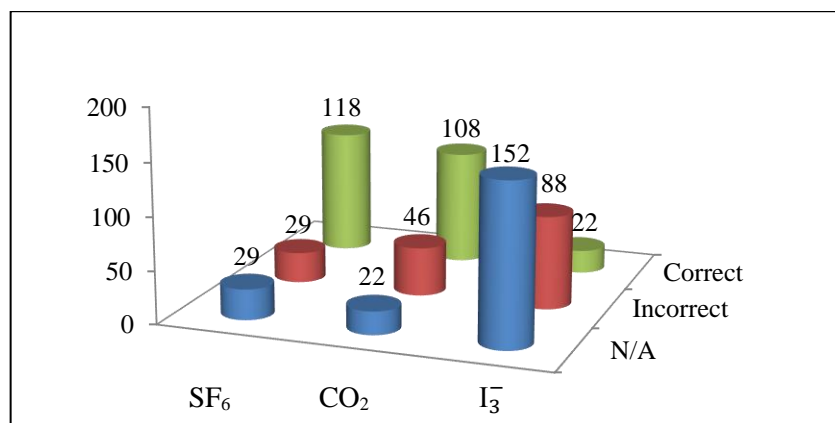
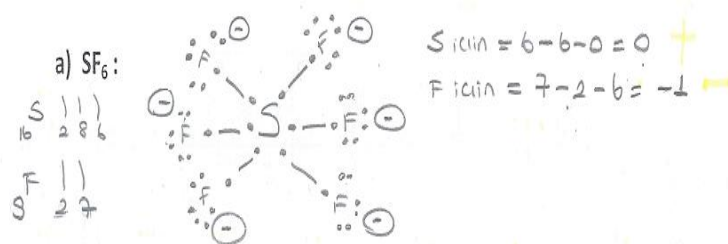
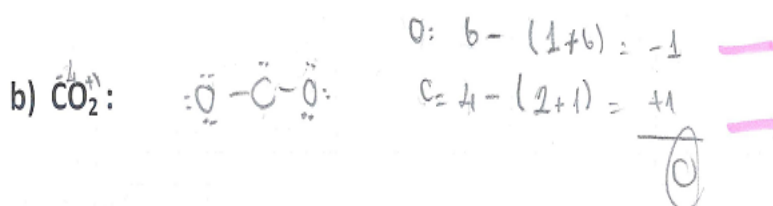


Figure 4. Student answer frequencies about the formal charges of atoms in each molecule

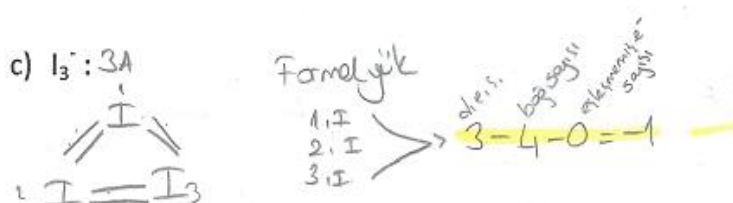
Figure 4 shows that the number of correct answers for the SF_6 and CO_2 molecules is high, while for the I_3^- molecule it is low. The students seemed to have difficulty in determining the formal charges of the atoms in the I_3^- molecule. Since many of the students could not identify molecular geometry in this molecule correctly, they also could not determine the formal charges correctly or they gave no answer. For molecules such SF_6 and CO_2 , which are commonly seen in textbooks and courses, they did not have any difficulty in determining formal charges. Examples of incorrect answers given to this question are shown in Figure 5.

Student 18.

Formal charge of Sulfur (S) atom is correctly identified, but all of the Fluorine (F) atoms' formal charges are identified as **-1**, so the total formal charge of the molecule is identified as **-6**.

Student 85.

The number of bonds in the carbon dioxide molecule is not correct; a non-bonding electron pair on the Carbon (C) atom is shown. Therefore, the formal charges of Carbon (C) and Oxygen (O) atoms are given incorrectly.

Student 30.

Molecular structure and bond numbers of Triiodide molecule are determined incorrectly. Formal charges are identified as **-1** for all of the Iodine (I) atoms. Iodine (I) is considered to be in the IIIA group element.

Figure 5. Examples of students' incorrect answers

3.2. The results of interviews

The interview questions asked to the students in the study were designed to examine their knowledge about resonance structure, polarity, hybridization, Lewis dot structures, VSEPR theory, and exceptions to these theories. We analyzed the interviews in detail, and the analysis was conducted separately for each question, with the findings for each question presented below.

In the first question, the students were asked to define some concepts related to molecular structures: non-polar molecule, dipole moment, electronegative atom, formal charge, hybridization, the octet rule, paramagnetism, and resonance. We analyzed the students' answers in terms of their conceptual understanding levels. Figure 6 shows the frequency distribution by student conceptual understanding level.

The findings show that the students had the most sound understanding level of the concepts of formal charge ($f_{SU}:46$; 52.3%) and the octet rule ($f_{SU}:73$; 83.0%), while the concepts the students had the most problems defining were dipole moment ($f_{NR}:46$; 52.3%), hybridization ($f_{NR}:27$; 30.7%), and paramagnetism ($f_{NR}:20$; 22.7%). The results showed few correct definitions of the dipole moment concept when identifying molecular polarity. A lack of understanding the dipole moment concept was

reflected in identifying molecular polarity. Similarly, we found out that not correctly understanding the hybridization concept led to incorrect or incomplete answers about the hybrid type of the center atom.

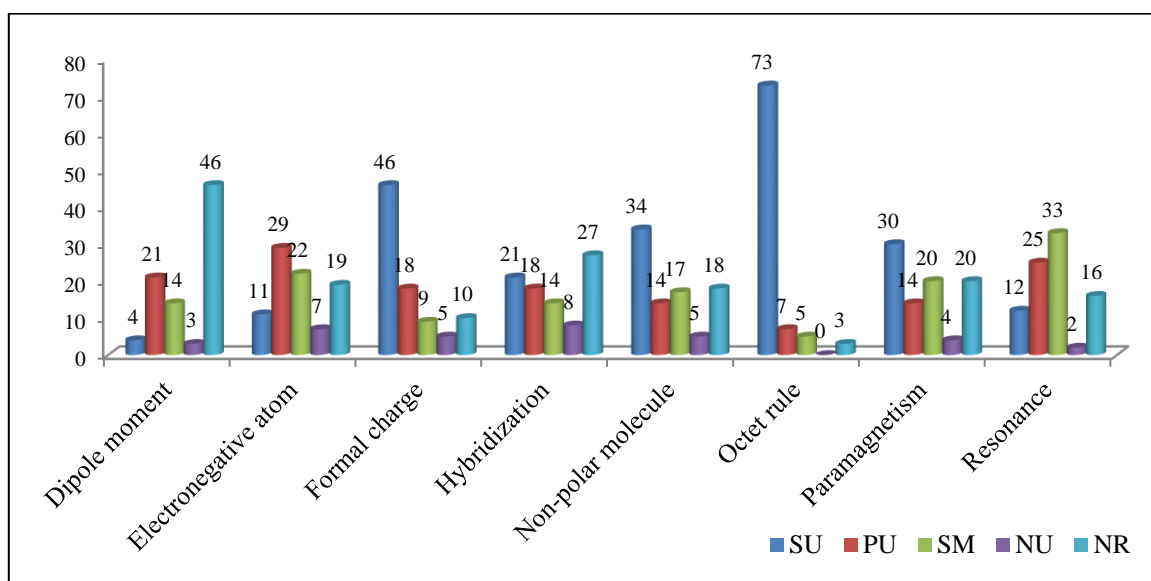


Figure 6. Frequency distribution by students' conceptual understanding levels

Additionally, the concepts of non-polar molecule ($f_{SM}:17$; 19.3%), electronegative atom ($f_{SM}:22$; 25.0%), paramagnetism ($f_{SM}:20$; 22.7%) and resonance ($f_{SM}:33$; 37.5%) were mostly determined to be misconceptions (see Figure 6). Examples from student answers that include specific misconceptions are shown in the Table 3.

Table 3. Examples of student answers including specific misconceptions(SM)

Concept	f	%	Some examples from students' SM responses
Dipole moment	14	15.9	Angle between two atoms (S5). It is seen in compounds with ionic bonds (S63).
Electronegative atom	22	25.0	Negatively (-) charged atom which has more electrons (S18). Atoms which have more electrons than protons (S28).
Formal charge	9	10.2	It is the electrical charge of an ion (S35). Excess or missing electrons in an atom that can form a bond (S38).
Hybridization	14	15.9	Location of electrons in terms of poles according to the doublet and octet rules (S28). It is used to determine which orbital the electrons are located in. They are located in orbitals such as s,p,d,f (S49).
Non-polar molecule	17	19.3	There are not any non-bonding electrons around atoms in non-polar molecule because all electron pairs form bond (S18). The molecular structures of compounds which only consist of the same elements (S25).
Octet rule	5	5.7	Atoms tend to complete the bond number to eight (S79). Having eight electrons in an element (S81).
Paramagnetism	20	22.7	Matter is attracted to magnets strongly (S70). Molecules are repulsed by a magnetic force (S65).
Resonance	33	37.5	Having a plurality of molecular geometry for a molecule (S25). Locating in different positions of atoms in molecules (S14).

The second interview question aimed at students' understanding of molecular resonance structure. We gave students three possible resonance structures for the N_2O molecule (See Figure 7) and asked to guess which one was the most representative: "Which of these possible resonance structures of the N_2O molecule is the representative resonance form? Please explain why you choose these structure/structures."

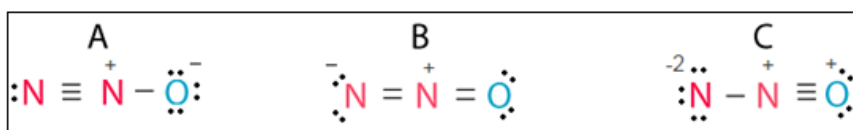


Figure 7. Resonance structures for the N_2O molecule

The distribution of the frequency and percentage of answers given to this question broken down by relevant reason is given in Table 4. The results show that 23.9% of students were able to give the correct reason when answering this question.

Table 4. Distribution of frequency and percentage analysis of the second question

Reason	Options				Total		
	I don't know	A (Correct)	B (Incorrect)	C (Incorrect)	All	f	%
I don't know	13	11	3	1	0	28	31.8
Incorrect reason	0	4	16	11	8	39	44.3
Correct reason	0	21	0	0	0	21	23.9
Total	13	36	19	12	8	88	100.0

We inferred from the student responses that 44.3% of the students gave incorrect reasons and 31.8% both could explain why they had given the answer they did and had only guessed. Although these students guessed the correct option, they could not give an explanation about the resonance concept. Some examples of incorrect explanations students gave are shown in Table 5.

Table 5. Examples of incorrect explanations on the second interview question

Option	f	Some examples of incorrect explanations
A	4	A zero formal charge shows that this structure is possible (S3).
B	16	Because on the right and the left, there is only a double bond (S19). Nitrogen forms three bonds in A. Because of that it will be difficult to form two sigma bonds, so the most representative form is the B molecule, which forms two bonds with both of the atoms (S79). (+) and (-) charges balance each other, and the repulsion force of the bonds remain the same (S14).
C	11	Because the most electronegative atom in the structure is oxygen. That's why the one which forms more bonds should be the oxygen (S34). Because there should be triple bonds between nitrogen and oxygen (S51).
All	8	All of them are correct because of resonance structure. But it cannot be known which one is correct in reality (S18). All structures are suitable. All resonance structures are the same as each other. The formal charge of all of them is zero (S77).

Option A in the second interview question is the most representative form for the resonance structure of the N_2O molecule. The results show that some of the students (23.9%) choosing option A were able to explain this form correctly while 44.3% gave incorrect answers (Table 5). Students could not explain the resonance structure since they did not entirely understand bond number, total formal charge, and

ionic charge. The statements by students who chose form B mentioned making double bonds. These students stated that the nitrogen atoms and the other atoms needed to form double bonds, so they noticed that oxygen had to be uncharged and that the total number of bonds of the nitrogen atom had to be four. Some students who chose option C incorrectly stated that there might be triple bonds between nitrogen and oxygen. The students who stated that all options were correct could not explain formal charge and bonding between atoms.

The third interview question aimed at examining student understanding of exceptions to the Lewis and VSEPR theories. We asked students to explain the molecular structure of NO and NO₂ based on the Lewis and VSEPR theories: "How do you explain whether NO and NO₂ molecules are appropriate for the Lewis and VSEPR theories?" Students were given empty sheets to draw the molecular structures. Therefore, the students could reflect their ideas on these sheets. The frequency and percentage distribution of students' conceptual understanding levels by category are shown in the Table 6.

Table 6 shows that in this question a clear majority of the students (85.2%) did not state that NO and NO₂ molecules had a radical structure. Some students were able to use the radical conception in structures correctly and stated that such compounds could not be explained based on the Lewis and VSEPR theories (f_{SU} :13; 14.8%).

Table 6. Findings of the third interview question according to the conceptual understanding levels(CUL)

CUL	f	%	Some examples of students' responses
SU	13	14.8	<i>NO and NO₂ molecules are radical molecules, so we cannot explain molecular structures according to the Lewis and VSEPR theories (S16).</i>
PU	38	43.2	<i>NO and NO₂ molecules are not appropriate for Lewis structure because there is one non-bonding electron on the nitrogen atom (S81).</i> <i>Because bond numbers are 5/2 and 7/2 it cannot be explained with Lewis and VSEPR theories (S56).</i>
SM	25	28.4	<i>The two molecules are not appropriate. Because nitrogen can make a maximum of three bonds. It gets charged as +2 in NO and +4 in NO₂ molecules (S85).</i> <i>Like the NO molecule, there is not any molecular geometry like the AB form (S4).</i>
NU	9	10.2	<i>It is not represented by Lewis structure but it can be explained with VSEPR theory (S73).</i> <i>There is expanded octet, it is not appropriate for Lewis or VSEPR theories (S6).</i>
NR	3	3.4	<i>I don't know or no response</i>

In statements that showed partial understanding, the students were able to explain the inappropriateness of using bond numbers and electron numbers (f_{PU} :38; 43.2%). Some of the students had misconceptions (f_{SM} :25; 28.4%). One of these misconceptions was that nitrogen could make three bonds but not more or less. They had similar misconceptions about the oxygen atom. Some students were able to relate bond numbers with group numbers and thought bonds could be made by octet completion.

The fourth interview question aimed at understanding of Intramolecular bond polarization and molecular polarization. We asked students to explain bond and molecular polarization of CH₄, CCl₄, and CHCl₃ molecules: "How do you explain polarization of bonds and molecules in CH₄, CCl₄, and CHCl₃?" The frequency and percentage distribution of their responses is shown by conceptual understanding level in Table 7.

Table 7 shows that the number of the students who have a sound understanding of the bonds and molecular polarization in the molecules is low (f_{SU} : 12; 13.7%). In the partial understanding category, a clear majority of the students could explain bond polarity correctly but they did not make correct statements about molecular polarity (f_{PU} : 33; 37.5%). We can state that the students could not inductively understand by starting from bond polarity in the concept of molecular polarity. This result could also be associated with the failure to accurately answer questions about concepts such as dipole moment and non-polar molecules related to polarity.

Table 7. Findings of the fourth interview question according to the conceptual understanding levels(CUL)

CUL	f	%	Some examples of students' responses
SU	12	13.7	<p>Bonds in CH_4 are polar and the molecule is non-polar because repulsive and attractive forces of hydrogen atoms are equal.</p> <p>Bonds in CCl_4 are polar and the molecule is non-polar because repulsive and attractive forces of chlorine atoms are equal.</p> <p>Bonds in $CHCl_3$ are polar and the molecule is polar because repulsive and attractive forces of hydrogen and chloride atoms are not equal (S23)</p>
PU	33	37.5	<p>The bonds between C-H and C-Cl are polar because each atom is nonmetal (S28) (There is not any comment about the molecule).</p> <p>Intramolecular bonds and molecules are polar because each molecule consisted of different nonmetals (S27).</p>
SM	27	30.7	<p>Each of the three molecules is non-polar. There are not any non-bonding electron pairs in the center atom (S73).</p> <p>Bonds and molecules in CCl_4 and $CHCl_3$ are polar because, though the shape of the molecule is tetrahedral, non-bonding electron pairs make the structure polar (S11).</p> <p>The molecules are polar as they consist of different atoms (S48).</p>
NU	11	12.5	<p>In the periodic table, polarity increases to the right and it decreases to the bottom. $CCl_4 > CHCl_3 > CH_4$ (S38).</p> <p>It made II bond. The charge of the molecule is zero. Therefore it is polar (S82).</p>
NR	5	5.7	I don't know or no response

4. Discussion and conclusion

In this study, we examined the undergraduate students' conceptual understanding levels and their misconceptions about the subject of molecular structures and the concepts related to it. Open-ended questions and interviews were applied to determine student conceptual understanding and misconceptions related to molecular structures and their characteristics. The predominant categories as they appear in the findings were discussed under these headings: Lewis dot structure, bonding or non-bonding electron pair number, VSEPR theory, molecular geometry, molecular polarity, center atom, and hybrid type.

The results show that the students did not have difficulty in understanding Lewis dot structures, center atoms, and bonding electron pair numbers and generally they gave correct answers in these categories. Although the students wrote Lewis dot structures correctly, they had difficulty in determining molecular geometry, ball and stick model, molecular polarity, and hybrid type.

4.1. Lewis dot structures of the molecules

The results in this part of the study indicate that more students had a more sound understanding (52.3%) of the formal charge concept. Some students (10.2%), however, had misconceptions about the formal charge concept. In these misconceptions, the students confused the concepts of formal charge and ionic charge. In their study, Vaarik, Taagepera, and Tamm (2008) stated that the students could determine the ionic charge in a molecule but they were not able to determine the formal charge. The other significant concept in our results was the octet rule. We found that most of the students had a sound understanding level about this concept (83.0%). The fact that the students' conceptual understanding about these two concepts is high made it possible for them to give correct answers on questions about Lewis dot structures. Also, the students were able to easily identify bonding/non-bonding electron pair numbers by using their knowledge about the octet rule. Similarly, Nicoll (2003) stated that undergraduate students could correctly identify Lewis dot structures while forming molecular structures. In contrast, however,

the study showed that the students had difficulty in showing molecules' Lewis dot structures and determining their center atoms and non-bonding electron pair numbers (Furio & Calatayud, 1996).

In a study related to chemical bonding, Luxford and Bretz (2013) found that students had some misconceptions about the representation of Lewis dot structures and they pointed out that these misconceptions might stem from not understanding non-bonding electron pair locations in the molecule. They also stated that some of the students never struggled with constructing and interpreting the Lewis dot structure of molecules.

In the open-ended questions, while there were fewer incorrect answers about structures that were appropriate for octet rule, the students were not able to determine the molecular structures in the molecules such as PCl_5 and SF_6 using the expanded octet rule. Also, some students thought that these molecular structures were not possible as they were not appropriate for the octet rule. Students learn molecule geometry in 12th grade of high school and in the first year in the university. In 12th grade, molecular structure examples which expand the octet rule are not taught. Our results show that molecular structure examples with an exception to octet rule should be given in both the high school and university curriculum. Also, covering covalent structures such as AX_5 and AX_6 can decrease errors in this subject. Ünal et al. (2010) stated that the reason that students could not understand the molecular structures of polyatomic covalent compounds is that the students encounter only compounds generally comprised of two (H_2 , O_2 , HCl , or HF) or three atoms (H_2O , CO_2 , or H_2S) in their textbooks or lectures.

4.2. Geometrical organization in molecular structures

Students need to understand VSEPR theory after they learn Lewis dot structures in order to determine the geometrical organization of molecules. Our results show that the students have a lack of knowledge in drawing molecular geometry (23.9%) and ball and stick models (47.2%). Although most of the students could define Lewis dot structures, they could not determine the spatial dimension of the structure. As the students did not think the molecular structure was three dimensional, they incorrectly identified the molecular polarity. However, the three dimensionality of molecular structure should be taken into consideration. Most student experiences with these structures are two dimensional in their textbooks and lectures (Ferk et al., 2003; Coleman & Gotch, 1998). Therefore, the students may lack knowledge about the geometrical organization of molecular structures. Although Yılmaz and Morgil (2001) showed students the molecular structure of CF_2Cl_2 , they could not explain its structure as tetrahedral. In our results, the students used a planar square statement for the CH_4 molecule. A similar error was seen in drawing the NH_3 molecule as T-shaped. We revealed that the students were able to explain the geometry of the molecule only with Lewis dot structure but they were not able to conceptualize the structure as three dimensional. Similarly, Wang and Barrow (2011) revealed that the students could understand VSEPR structures but they could not understand the three-dimensional structure of the molecules in mental models. They stated that this problem would be solved by visualizing three-dimensional structures. These studies show that courses should be taught using three-dimensional models of molecular structures (Furio & Calatayud, 1996; Uce, 2015; Wu & Shah, 2004).

The students' answers to the open-ended questions in our study confirmed that the students had some misconceptions in identifying molecular structures. An example of these misconceptions is that some students thought that the XeF_4 molecule is not possible because Xe is in the VIIIA group. Some students also thought that the BF_3 , NH_3 , and ICl_3 molecules could all have a trigonal planar structure. Similarly, they said that all of the molecular structures of the CO_2 , SO_2 , and H_2O molecules were linear. Considering these answers, we can state that the students thought that non-bonding electrons in the molecule do not have an effect on molecular geometry. Some studies have indicated similar misconceptions in undergraduate students (Atasoy et al., 2003; Peterson & Treagust, 1989; Taber, 2002). In their study with high school students Atasoy et al. (2003) gave a misconception from student answers: "The geometry of the SCl_2 molecule is linear. Because of the linear direction of the two Cl-S bonds, the Lewis structure becomes Cl-S-Cl." In their study, Birk and Kurtz (1999) encountered a misconception in 27% of graduate students that "the shape of molecules is due only to the repulsion between non-bonding electron pairs." There are studies which show similar misconceptions (Nicoll, 2001; Yılmaz & Morgil, 2001).

In the interview question related to NO and NO₂ molecules, which are radical compounds, some students (14.8%) were able to identify these molecules as being radical. A clear majority of the students (43.2%) were able to determine that the molecules were not appropriate for Lewis and VSEPR theories but they did not mention the radical concept due to the fact that simple molecular structure examples appropriate for the theories are taught during their courses. However, students should be exposed to the situations contrary to these theories, such as radical compounds, in order to be able to construct these concepts correctly. From the students' misconceptions we found out that they could form bonds in specific numbers based on the octet rule for nitrogen and oxygen atoms. The students said that a nitrogen atom could form three bonds and an oxygen atom could form two bonds. Because of this, they could not determine the molecular geometries of the molecules. Taber (2002) revealed that the students considered only the octet rule in the formation of chemical bonds. In this context, during chemical bond formation the students had misconceptions such as "because atoms wanted to obtain full electron shells".

When the answers for the NO molecule were analyzed, there were not any explanations which mentioned MOT. These results show that students' understanding related to MOT is very poor. Malvern (2000) indicated the reason for this was that it was difficult for students to understand MOT as it is a mathematical and theoretical model. Hanson, Sam, and Antwi (2012) obtained similar results for the NO molecule. Students' explanations of the concept of paramagnetism, which is an important concept for MOT, were also examined in the interviews. Though some students (34.0%) were able to give correct answers for this concept, others (22.7%) could not give any answers. In addition, we concluded that the students had misconceptions about the concept such as "Matter is attracted to magnets strongly." This statement shows that the students could relate the concept of magnetization to paramagnetism in terms of the concept of magnetism.

4.3. Polarity in molecular structures

The three-dimensional forms of molecules and their charge distributions are effective characteristics in identifying the polarity of a molecule. Depending on the electronegativity among the atoms, molecular polarity is specified as a result of the dipole moment. Therefore, the students should be able to identify the three-dimensional geometry of the molecule and understand the dipole moment concept correctly in order to learn molecular polarity (Linenberger, Cole, & Sarkar, 2011; Sarıkaya, 2007). As all these concepts are related to each other, incorrect knowledge in any of them will affect the others.

Our results showed that the students could not determine molecular geometry and identify molecular polarity. Also, when the concept definitions of some students (15.9%) are considered, it was seen that they had misconceptions in dipole moment concept. These misconceptions show that the students confused the dipole moment concept with dipole-dipole interaction and ionic bonds. Concepts such as negative and positive poles in dipole moment and partial charge remind students of ionic bond concept. Some students (19.3%) had misconceptions about the concept of non-polar molecules, which are related to molecular structures and polarity. In these misconceptions, some students thought that non-polar molecules would consist of the same elements and that a molecule consisting of different elements would not be non-polar. Giving H₂, N₂, and O₂ as examples of non-polar molecular structures in courses and textbooks can lead to misconceptions. Hanson (2015), in his study conducted with chemistry student teachers, stated that 49% had misconceptions such as all covalent compounds are non-polar.

Our results from the interview question about the polarity of molecules and bonds in the CH₄, CCl₄, and CHCl₃ molecules point that the students lack knowledge and have misconceptions about molecular polarity. These results correspond to the results obtained from the open-ended questions and concept definitions. The students need to consider many concepts, such as bond polarity, dipole moment, and molecular geometry, in order to answer this question correctly. However, we found out that the students could not determine the geometrical structure in these molecules and gave incorrect answers about polarity of the molecules. Taagepera, Arasasingham, Potter, Soroudi and Lam (2002) stated that this inability stemmed from the fact that electron density was not mentioned while learning about Lewis dot structures. Therefore, the students could not identify where electron density would be and they could not combine this with geometrical structure. Although a clear majority of the students (37.5%) stated that each molecule would be polar they could not identify geometrical organization and dipole moment.

Because of this, they stated that the bonds between the atoms in CH_4 , CCl_4 , and CHCl_3 were polar covalent bonds. These student statements show that they have misconceptions about bond polarity and molecular polarity. This could be caused by their generalization of these concepts. In their study, Birk and Kurtz (1999) stated that the students had misconceptions about the polarity of a molecule such as a molecule is polar because it has polar bonds. There are similar studies that show that students cannot distinguish molecular polarity from bond polarity (Hanson, 2015; Yılmaz & Morgil, 2001). In the partial understanding category of our study, even though there are many correct answers about the CH_4 and CCl_4 molecules, the students had difficulty with the CHCl_3 molecule and they could not give any answers. Student misconceptions related to this question showed that they considered non-bonding electron pairs of the atoms while identifying molecular polarity.

4.4. Resonance in molecular structures

In our study, we asked students which structure of the resonance formulas of N_2O molecules is the most representative form. The results show that the students lacked knowledge and had misconceptions about resonance structure. The students' incorrect answers revealed that they thought that double-bonded structures were more stable than the other structures, nitrogen atoms were more electronegative than oxygen atoms, and a triple bond was necessary between nitrogen and oxygen atoms. The students also stated that all structures were appropriate. However, even though the resonance structure in Option C is impossible in many respects, some students (13.6%) stated that this structure was possible. We determined that a clear majority of the students could not comprehend and explain resonance structures correctly. In addition, answers to interview questions about the definition of the resonance concept also showed that the students had misconceptions. The students' misconception about resonance concept was that they confused delocalization of electrons and bond delocalization. Similarly, Coll and Treagust (2002) found that undergraduate and graduate students have poor conceptual understanding about the notion of delocalization regarding resonance structure in benzene ring. Also, in resonance formulas, the students made statements that account for the fact that the atoms will move and the structure of the molecule will change. In a study with organic chemistry educators, Duis (2011) found misconceptions about the resonance concept such as electrons flow toward negative or uncharged sites, resonance is a fast exchange of electrons, and resonance is equilibrium.

In identifying resonance structure in molecule structures, the other effective concept is electronegative atoms. Based on their misconceptions, we concluded that the students thought that negatively charged ions were electronegative atoms. The students could not define this concept correctly and thought negatively charged atoms were electronegative atoms. Similar misconceptions such as this may cause students not to understand resonance structure correctly.

4.5. Hybridization in molecular structures

In this study, the hybridization concept was analyzed in open-ended and interview questions. In the open-ended questions, we asked students about the hybrid type of the center atom in the molecules. Some students (49.6%) were not able to give the hybrid type of the center atom in the molecules while other students (31.6%) gave mostly incorrect answers, showing that the students had difficulty in identifying the hybrid type. Also, responses to interview questions showed that students had misconceptions about hybridization. In their answers, the students were not able to state that hybrid orbitals occur as a result of overlapping of orbitals. The results of Hanson et al.'s study (2012) confirm these results.

Moreover, the students stated that hybridization was related to electron configuration, location in orbital and atomic orbital. These errors are supported by the fact that the students could not identify the hybrid type. In a study about hybridization and atomic orbitals, Nakiboğlu (2003) stated that the students could not identify hybrid types or define the hybridization concept. In his study, Zoller (1990) stated that the students confused the hybridization concept with electronic orbitals and could not really define it. Also, he suggested that hybrid orbitals should be taught with schematic statements which take into consideration electronic orbitals in order to make the hybridization concept more easily understood.

Taber (2001) revealed that the students thought that electrons in hybrid orbitals were the s, p, d atomic orbitals and they stated that hybrid orbitals were similar to atomic orbitals.

5. Recommendations

Molecular structure is a basic subject in university chemistry as well as in other areas and its basis is provided in ninth grade curriculum. Therefore, misconceptions which occur early become hard to correct at the university level. While teaching molecular structures, the use of three-dimensional materials may help students to structure their mental models. For example, molecular structures can be taught with ball and stick models using play dough and simple materials (straw, ping pong balls, toothpicks, etc.). In these representations, mentioning non-bonding electron pairs over the center atom can help students understand how molecular geometry will be affected by the angles in the structure. Since molecular structure is microscopic, it is an abstract and hard subject to understand. Activities such as computer-based learning, animation, and simulation may be used to help students concretize this subject. Visualization helps concretize the microscopic dimension of the molecules. Concrete materials about molecules presented in detail on a computer prevent students from adding physical characteristics into molecular structures.

Teaching step by step from the simplest (AX_2) to the most complicated (AX_6) molecule form may provide an induction to the subject. Giving examples from the simplest structures to the most complex may enable the expanded octet rule to be understood more easily.

When teaching subjects that are interconnected with each other, such as molecular geometry, molecular polarity, and bonds among molecules, a new subject can be introduced after identifying student misconceptions about that subject in order that misconceptions which occurred in a prior knowledge context can be prevented in advance. This study is instructive for teachers and researchers who are interested in doing research about teaching concepts and preventing misconceptions in this field. In future studies, learning-teaching activities that are beneficial for the students can be arranged to effectively teach molecular structures so that possible misconceptions and misunderstandings can be prevented.

6. Notes

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