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FOLLOWING THE LOGIC OF STUDENT THINKING PATTERNS ABOUT ATOMIC ORBITAL STRUCTURES

Andero Vaarik, Mare Taagepera, Lembi Tamm

Abstract. *The aim of the present study was to follow the logic of student thinking patterns about atomic orbital structures on both the atomic model visualization and the corresponding symbolic representation levels. The students´ factual knowledge was measured by the percent correct answers with and without explanations, the misconceptions were documented, and the cognitive organization was analyzed using knowledge space theory. The study was carried out with 255 students studying chemistry at the 8th and 9th lower secondary school and 10th to 12th secondary school levels.*
The major findings included (1) the high proportion of correct answers on multiple-choice questions, without correct explanations, leading to false positive results which do not necessarily reflect understanding of the material; (2) the lack of a logic structure in students' thinking due mostly to the misunderstanding of symbols; and (3) misconceptions about what charges represent and the placement of electrons in ionic vs. covalent bonding.

Key words*: science education, knowledge space theory, visual representation, symbolic representation, misconception.*

Introduction

Interest in science has been investigated from different perspectives associated with student motivation (Teppo & Rannikmäe, 2003). A European wide survey again documented low student interest in science due to the perceived relevance and difficulty of the courses as well as perception of limited career opportunities (Teppo & Rannikmäe, 2003; Candidate Countries Eurobarometer on Science & Technology Education, 2002). Science would be less difficult and more understandable for students if it were presented with more emphasis on how students learn. Learning science involves understanding the principles that shape science, which requires conceptualization and visualization skills besides mathematical and problem solving skills (Drechsler & Schmidt, 2005).

Researchers have noted that even when students´ factual knowledge base increases, the cognitive organization of knowledge is weak and misconceptions persist (Taagepera & Noori, 2000). When too much factual information is presented there is little memory left for processing so that knowledge could be transferred from working to long-term memory (Johnstone, 1991; Baddeley, 1986, 1990). Since chemistry is taught at three different levels: microscopic, macroscopic, and symbolic, changing back and forth among these levels is part of what makes chemistry difficult to understand (Johnstone, 1997).

It is not always obvious when students have problems. One somewhat unexpected problem area for students is their inability to visualize atomic orbital models (the microscopic level) when given a representation at the symbolic level and vice versa. Espe-

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cially difficult seems to be visualizing ions from their symbols (Drechsler *et al.*, 2005; Robinson, 2003; Francisco *et al.*, 2002). Butts and Smith report the results of interviews with students who had studied chemical bonding. Some of these students consider sodium chloride to be molecular, suggesting that covalent bonds were present between sodium and chloride, but that ionic bonds between molecules were needed to create the full structure (Butts *et al.*, 1987). Taber suggests that students acquire this idea because they don not "share the framework of electrostatics knowledge" of teacher, and also because they are taught about the formation of ionic bonds in a way which promotes the molecular model (Taber, 1994).

The aim of the present study was to follow the logic of student thinking patterns about atomic orbital structures on both the atomic model visualization and the corresponding symbolic representation levels.

The students´ factual knowledge was measured by the percent correct answers with and without explanations, the misconceptions were documented, and the cognitive organization was analyzed using the *knowledge space theory*. (Taagepera *et al.,* 2002; 2004; Arasasingham *et al.*, 2005) developed by Falmagne (Doignon & Falmagne, 1999; Falmagne *et al.,* 2003; Falmagne, 1999).

Methodology of Research

This study was carried out with 255 students at the Tallinn Nõmme Gymnasium in the basic general chemistry understandings at 8th to 9th (ages 13 - 15) lower secondary school, 10th to 11th (ages 15 - 17) secondary school and 12th (ages 17-18) science class. A 9-question test with hierarchical ordering was constructed to follow the students´ understandings of chemistry by experts (three gymnasium teachers and students as well as university professors) who tend to visualize models for physical phenomena before assigning symbolic representations (Appendix 1, Figure 1). The students had access to the periodic table.

Three methods of analysis were used: the percent of correct answers for a particular multiple-choice question (with and without explanations), the use of knowledge space theory to determine the cognitive structure and the analysis of misconceptions. A trial test was given to university students and standardized before the test was used for analysis. The Knowledge Space Theory analysis was performed using the Hexagon Data Analysis software (hDA, 2002).

The Test

The test was hierarchical proceeding from simple to complex questions which were based on understanding the previous question(s) in an effort to follow the logic structure which the students had or had not developed (Figure 1).

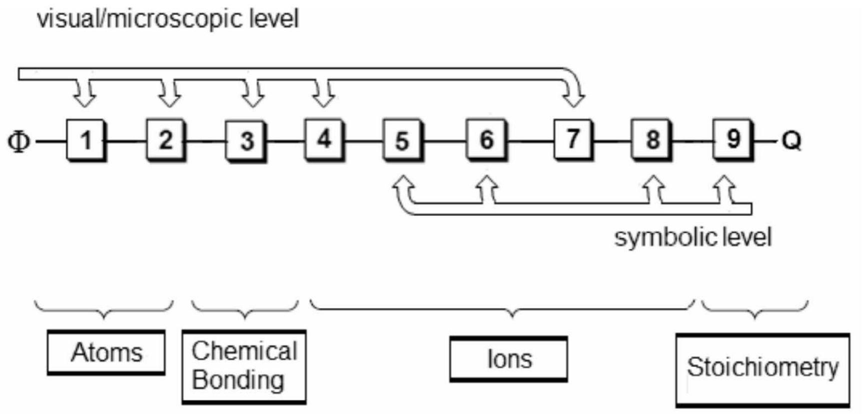

Figure 1. Hypothetical expert learning pathway.
* where Φ is the null state (no correct responses) and Q is the state where all questions are correct

Questions 1 – 4 and 7 are at the microscopic visual level representations and questions 5, 6, 8 and 9 use symbolic representations. In question 1 students had to determine the atomic structure from the information in the periodic table. In question 2 students had to draw the orbital structure from the atomic number. Question 3 requires understanding covalent and ionic bonding at the orbital level. Question 4 asks for a representation of an ionic structure, questions 5 and 6 ask for understanding of symbolic representation single ions and salts, respectively. Question 7 involves the formatting a salt at the microscopic level when electrons indicating charges need to be balance. Question 8 asks for the same information on a symbolic level. Finally, question 9 involves stoichiometry at the symbolic level

The Knowledge Space Theory (KST)

The hierarchical order of the test allows for the determination of conceptual understanding by constructing *knowledge structures* and a *critical learning pathway* which show the students´ cognitive organization of knowledge using the *knowledge space theory* (Doignon, Falmagne, 1999). KST depends on collecting student data from a set of questions that reflect different levels of conceptual development or their *response state* (list of correctly answered problems). The most highly populated response states of the students are used to construct a *knowledge structure* which is well graded or in other words, where each state is connected to a prior state by containing one more problem and a subsequent state by containing one less problem. The structure starts from the null state, (Ø), where no questions are answered correctly, to the full expert state, (Q), where all questions are answered correctly and achieved by successively mastering each question in the order consistent with a learning pathway (see Figure 1).

Our nine-question test can have 2^9 (512) possible *response states*. From all the possible student *response states*, KST recognizes a subset which is called the *knowledge structure* and major response states called *knowledge states* and represents the original response structure at least to $p = 0.05$ level of significance. The lucky-guess and careless-error parameters are estimated, usually at 0.1. Finally, from the highest probability knowledge states the most probable learning pathway is identified as the *critical learning pathway* consisting of response states which best define the classes or school. (Taagepera, Arasasingham, Potter, Soroudi, Lam, 2002).

Results of Research

A general pattern for all grades was analyzed. The % correct answers increased by grade level, the cognitive structure analysis by grade level will be the subject of a separate study. Table 1 presents the results of the multiple-choice test with and without explanations.

Table 1. Percent correct answers on the multiple-choice test.

Questions	Response (%)			
	A	B	C	D
Question 1: Which of the following boxes represents Li structure?	2	5	84*	9
			67**	
Question 2: Which of following boxes represents the orbital structure for an atom with the atomic number 9?	2	5	91*	2
			70**	
Question 3: Which of following boxes represents LiF ionic structure?	12	59	15*	14
			10**	
Question 4: Which of following boxes represents Na ionic structure and charge?	51*	40	6	3
	42**			

Questions	Response (%)			
	A	B	C	D
Question 5: Which of following boxes represents chloride ion charge?	6	91*	3	
		50**		
Question 6: Which of following boxes represents the potassium chloride structure?	95*	2	2	1
	40**			
Question 7: Which of following boxes represents the magnesium chloride structure?	11	18	71*	
			30**	
Question 8: Which of following boxes represents the magnesium chloride structure?	6	4	13	77*
				33**
Question 9: HCl + MgO. Write compounds and balanced the reaction	58*			
	18**			

* - represents the correct answer and ** indicates the correct answer with the correct explanation

Some general trends are noted. Students did well on questions #1 and 2 which asked about atomic structure. There was considerable confusion with questions #3 and 4 which referred to pictorial representations of ionic structures, but not with symbolic representations of ionic structure. Question #5 and 6 asked for understanding of symbolic representation single ions and salts or question # 7 and 8 involved magnesium chloride formatting on symbolic and microscopic level. The scores were much lower when justification was required. A lot of students said that the information was on the periodic table, but they used it incorrectly. This was not accepted as a correct explanation. A similar situation occurred in questions 5, 6 and 8.

In the first question 9% of students gave the answer (D), thinking that Li is a molecule. In the second question some of students said that all 9 electrons should be located in outer shell. The third question turned out to be the most difficult: 85% of students could not identify ionic bonding and 59% of students depicted LiF as a covalent compound (B) explaining that in order for a loss or gain of electrons the orbitals had to be close together. In the fourth question 40% of the students thought that the charges on the ion represent the number of electrons in the outer shell and lose the electron in the inner shell (B). In the fifth question most of students offered no explanation or said that the periodic table shows that the chloride ion has a formal charge where the oxidation number is -1 or that Cl is a diatomic molecule and therefore the formal charge is 0. In question 6 the students gave as an explanation that K and Cl ion formal charge should be same (both - or both +) otherwise they would not dissociate. The students have seemingly memorized the symbolic representation without understanding the atomic model in question 5 and 6 which the symbol represents. In the seventh question the students focused on the fact that "magnesium chloride" contains one Mg ion and two Cl ions not noticing that the Mg and Cl were interchanged and not ionic (B) or gave as an explanation that Mg loses one electron and Cl gains one electron because Cl ion did not have enough space to gain more electrons (A). The question 8 13% of students picked out drawing (C) and explained that Mg^{2+} and Cl^{2-} formal charges should be balanced because Mg loses two electrons and Cl gains two electrons. In question 9 most of students explained that the compounds are acids and alkaline oxides and balanced the reaction and didn't explain the answer. The common products were given as: H + MgCl, ClMgO + H_2, MgCl + H_2O, MgHCl + H_2O etc.

Discussion

1. Percent of correct answers with and without explanation

The results of the multiple-choice test with explanations were analyzed in terms of (I) the correct answers and (II) the correct answers with explanation (Figure 2). The analysis indicated that the results with the correct answers (without explanations) were much higher, on the average of about 30% higher (Mean = 63,6 SD= 25,7 for the correct answer and Mean = 35,2 SD.= 19,9 for the correct answer with explanation). If the student cannot explain why the answer is correct, then the student most probably does not understand the concept.

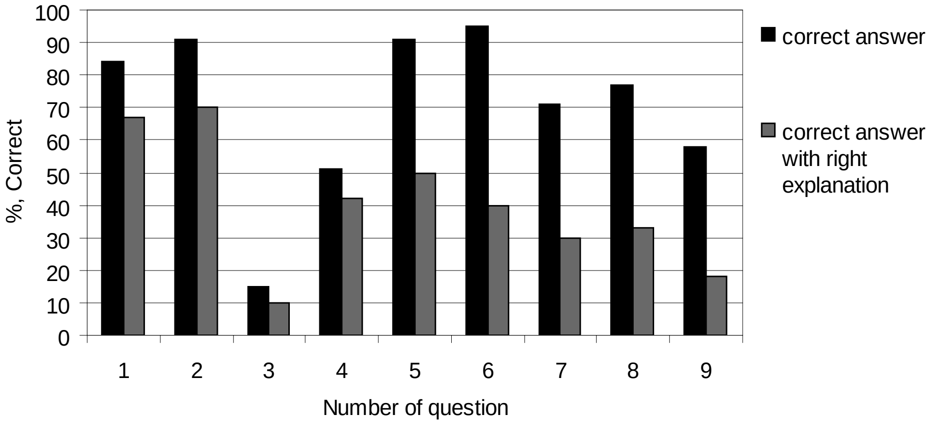

Figure 2. Comparison of the results of the multiple-choice test with and without explanations.

The percent of correct answers for problems which deal with symbols, visual representations and the combined total are given in Table 2. The questions which deal with symbols only (#5, 6, 8, 9) show almost a 3-fold difference between the answers given with and without explanations. The problems which require visualization (#1, 2, 3, 4, 7) show a much wider spread of answers and appreciable overlap. The main reason for this is the particularly low score on question #3 where ~60% of the students indicated that LiF had a covalent bond. Vanessa Kind has also reported that students find ionic bonding hard to describe and learn (Kind, 2004)

Table 2. Statistical analysis of percent correct answer.

	Symbolic	Visual	Total
Correct answer no explanation (Mean)	87.3	52.9	63.6
Standard deviation (SD)	9.5	30.6	25.7
Correct answer with explanation (Mean)	33.2	35.8	35.2
Standard deviation (SD)	7.5	25.3	19.9

The combined total of symbolic and visual questions again shows an almost 2-fold difference between the answers given with and without explanations. This indicates a problem with false positive results in multiple-choice tests. The significant difference between correct answers only between symbolic (Mean = 87.3 SD = 9.5) and visual (Mean = 52.9 SD = 30.6) representations showed that students preferred to learn in symbols rather than in visual representations. This could possibly result from the teachers themselves, who preferred to teach with greater emphasis on symbolic representations and weak links to visual representation of atomic orbitals. There was no significant difference between the % correct answers for symbolic (Mean = 33.2 SD = 7.5) and visual (Mean = 35.8 SD = 25.3) representation for the students, who understood the chemical concept as shown by a correct explanation.

2. Knowledge Space Theory Analysis of the Cognitive Structure

All 255 students were assigned a response state. For instance, if a student answered questions 1 and 2 correctly, the student is in a response state [1, 2]. If after optimization the response state contributes to the knowledge structure, it becomes a knowledge state.

Students with correct answers on the multiple-choice tests without explanations displayed a maximum of 64 response states and in multiple-choice tests with explanations displayed a maximum of 87 response states. Optimization of all sets of data gave well-defined knowledge structures with 12 and 22 knowledge states. The overall knowledge structures with knowledge states are given in Figure 3 where the bold line indicates the major critical learning pathway.

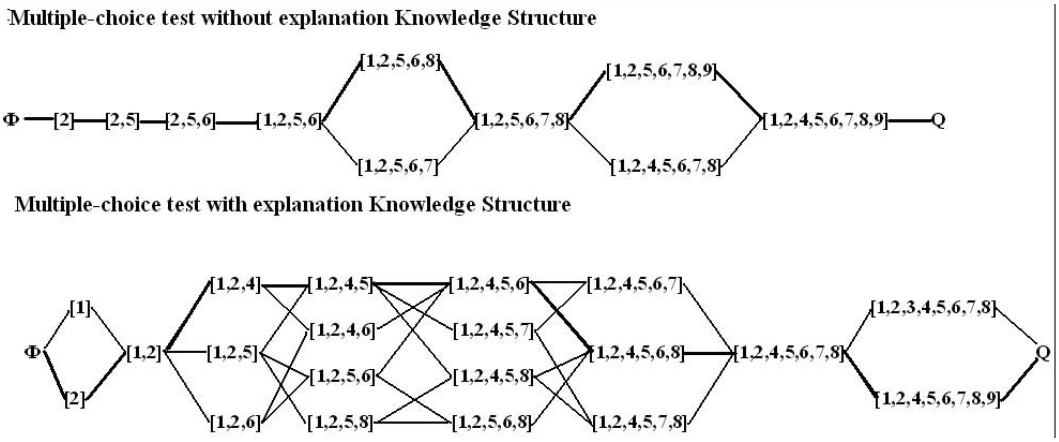

Figure 3. KST knowledge structures (the bold line indicates the major critical learning pathway).

The knowledge structure for the correct answers without correct explanations was less complex (containing 12 versus 22 knowledge states) since students apparently have similar superficial understanding of the material (Figure 3).

The multiple-choice tests with explanations were more similar to the experts´ critical learning pathway (Figure. 1 – expert learning pathway). When students understand the material as shown by the correct explanations, their thinking pattern starts to resemble that of the experts (teachers).

The major difference in the critical learning pathways for the students and experts was that the experts usually visualize the atomic structure first before giving it a symbolic representation (Figure 1 – expert learning pathway), while the students have seemingly memorized the symbolic representation without understanding the atomic model which the symbol represents (Figure 4). Robinson has also indicated that students have problems connecting symbols that describe chemical processes with the quantitative information which the formulas provide (Robison, 2003).

There were particular problems with ionic structures (questions 3 and 4, which appeared at the end of the critical learning pathway). Students thought that the charge on the ion (negative or even positive) represents the number of electrons in the outer shell (question 4). Thus in order to form an ion, an electron from an inner shell has to leave. The other major misconception was in question 3 -- the structure of LiF. It seems to be the most difficult question for the students because most of them explained that the atoms need to be close together for the transfer of electrons - close enough to form

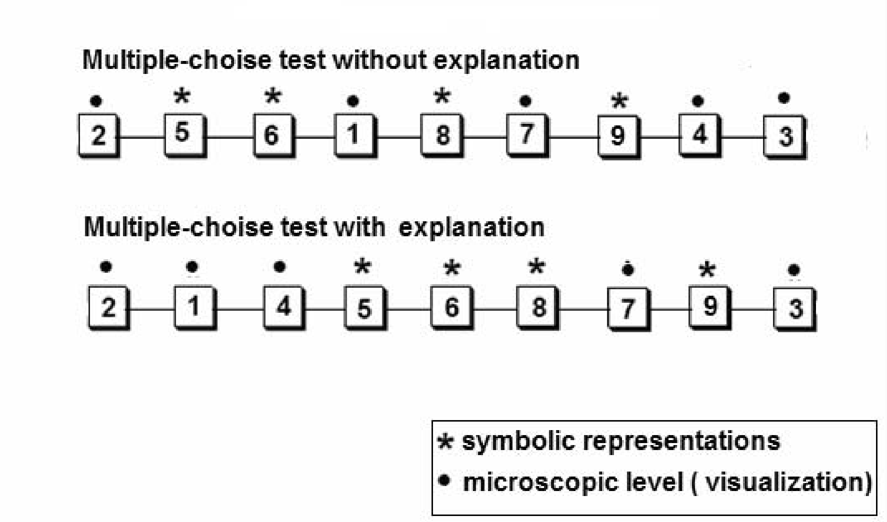

Figure 4. **Students´ critical learning pathways.**

a covalent bond (!) (Table 1, answer B).

In an effort to overcome the problem of visualizing orbital structures, which are reflected in the percent correct answer as well as the KST analysis, it would be helpful to: (1) have more well designed orbital drawings or visualization in the textbooks and the problem assignments; (2) use computer simulations which would allow the student to have more practice in visualizing the structures; and (3) spend more time making the connections between symbols and the visualized microscopic orbital models starting with students' pretest results.

Conclusions

The percent correct analysis indicated that the multiple-choice test results with just the correct answers (without explanations) was higher, on the average of about ~30% higher. It is therefore possible to get false positive results from a multiple-choice test, which does not necessarily reflect understanding of the material. The *knowledge state analysis*, reflecting the cognitive structure, indicated that the major difference in the *critical learning pathways* for the students and teachers (experts) was that the experts usually visualize the atomic structure first before giving it a symbolic representation. The knowledge structure for the correct answers without correct explanation was less complex (containing 12 versus 22 knowledge states) since students apparently have the same superficial understanding.

In an effort to overcome the problem of visualizing orbital structures, which are reflected in the percent correct answer as well as the KST analysis, it would be helpful to: (1) have more orbital drawings or visualization in the textbooks and the problem assignments; (2) use computer simulations which would allow the student to have more practice in visualizing the structures; and (3) spend more time making the connections between symbols and the visualized microscopic orbital models.

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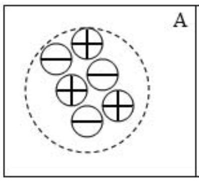
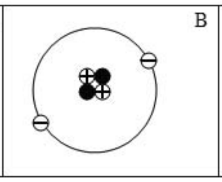
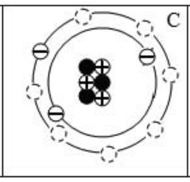
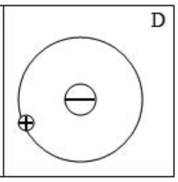
Appendix 1

Question 1 - Which of the following boxes represents Li structure? Mark the correct answer with X









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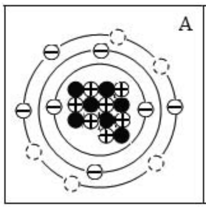
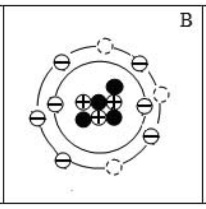
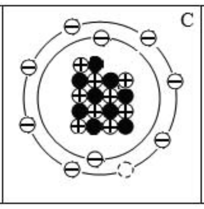
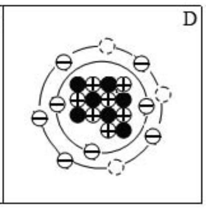
Question 2- Which of following boxes represents the orbital structure for an atom with the atomic number 9? Mark the correct answer with X









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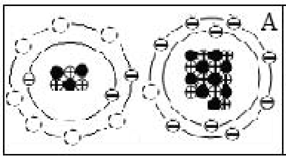
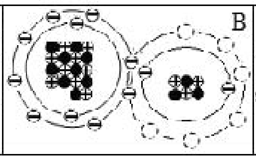
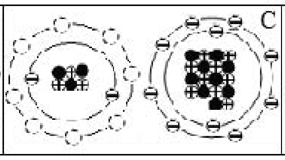
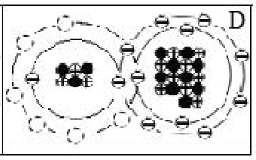
Question 3- Which of following boxes represents LiF ionic structure? Mark the correct answer with X









Explain ....

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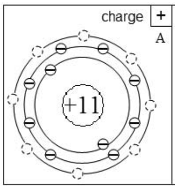
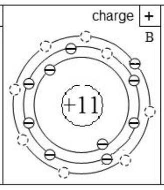
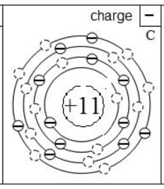
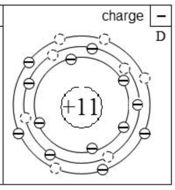
Question 4- Which of following boxes represents Na ionic structure and charge? Mark the correct answer with X









Explain ....

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Question 5 - Which of following boxes represents chloride ion charge? Mark the correct answer with X

A	B	C
Cl^0	Cl^-	Cl^+

Explain ....

....

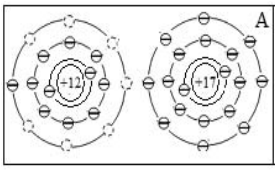
Question 6 - Which of following boxes represents the potassium chloride structure? Mark the correct answer with X

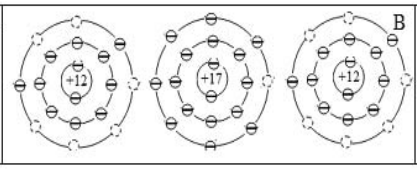
A	B	C	D
K^+Cl^-	K^-Cl^-	K^0Cl^0	K^+Cl^+

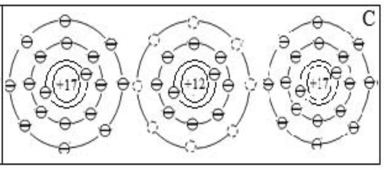
Explain ....

....

Question 7- Which of following boxes represents the magnesium chloride structure? Mark the correct answer with X







Explain ……………………………………………………………………………………

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Question 8- Which of following boxes represents the magnesium chloride structure? Mark the correct answer with X

A	B	C	D
$Mg^{+}Cl^{-}$	$Mg^{-}Cl^{-}$	$Mg^{2+}Cl^{2-}$	$Cl^{-}\ Mg^{2+}Cl^{-}$

Explain ……………………………………………………………………………………

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Question 9. Write compounds and balanced the reaction.

HCl + MgO

Explain ……………………………………………………………………………………

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