



**Conceptual integration of covalent bonds models by
Algerian students**

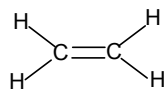
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Conceptual integration of covalent bonds models by Algerian students

Abstract: The concept of covalent bond is characterized by an interconnected knowledge framework based on Lewis and quantum models of atoms and molecules. Several researches have showed that the quantum model is one of the most difficult subjects to understand by students at all levels of chemistry learning. We try in this paper to analyze to what extent Algerian students, at the end of their training, have integrated covalent bonding theories based on quantum model of atom theory and are able to interpret Lewis structures with quantum model. Analysis of responses to a written questionnaire shows that this integration is not achieved by our students and that they are not able to describe correctly covalent bonds in Lewis structure using the concepts of quantum model. They have a "quantum box" conception of atomic or hybrid orbitals. This conception act as a "pedagogical learning impediment" to integrate the geometrical representations of atomic and hybrid orbitals, the conditions of their overlapping to give bonds and consequently the description of covalent bond using quantum model. So, students use an alternative conceptual framework based on the research of a Lewis model paired valence-electrons to form covalent bond that we have named: "electrons pair framework". In more, the denomination of covalent bond is restricted to the sharing of one electron (indifferently s or p and not sp) from each atom to give one "electron pair σ ", and the formation of σ bond occurs only in the case of a single bond.

Introduction

The usual representation of molecules is based on Lewis Model. The atoms, represented by their symbols, are connected by single, double or triple lines, supposed to represent the sharing of two, four or six valence electrons by the two bonded atoms. Let us consider the Lewis representation of ethene:



An experienced chemist is able to interpret this representation in terms of single and double covalent bonds, six bonding electrons pairs, and to make a link with the concepts and representations of atom and molecule quantum model (atomic or hybrid orbitals overlap to form σ and π bonds). As much abstract concepts that student must master to give the same meaning to such representations. It is therefore not surprising that they encounter difficulties in understanding the concepts and symbolism used to represent molecules (Taber, 2009).

Solving problems in organic chemistry requires articulation of these different models depending on the particular facts that we want to explain or predict (molecular geometry, inductive and mesomeric effects, reactivity, etc.). Without a correct understanding of the models and the meaning of the representations which are associated with them, students will have difficulty perceiving the implication of the structural aspects of a molecule in its

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3 reactivity. It is the coordination of these multiple representations that allows students to give
4 meaning in models and to favor the conceptual integration of the knowledge.
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6 7 **The theoretical framework for analysis**

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9 Consider again the Lewis representation of ethene. To interpret its reactivity it is necessary to
10 consider that the two dashes (or bonding pairs) between the carbon atoms do not symbolize
11 the bonds of the same type. To differentiate it is necessary to use the "Valence Bond Theory"
12 (VBT) quantum model. The two carbon atoms are sp^2 hybridized; one of the dashes
13 symbolizes σ bond resulting from an axial hybrid orbitals (HO) sp^2 carbons overlap, the other
14 symbolizes π bond resulting from a lateral overlap of the two carbon atoms AO p. This results
15 in a molecule of the planar geometry with angles of 120° between the links. To make this
16 reasoning, students must be able to link the concepts and representations of both models.
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23 Generally to give meaning to complex knowledge of this type, students will, from the
24 information received during the various teachings, perform their "conceptual integration"
25 (Taber, 2005a) by linking the different concepts involved and thus create a personal
26 "knowledge structure" (Champagne et al., 1981; Tsai, 1998; Nakiboglu, 2008; Taber, 2005b).
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31 One of the characteristics of science is that it produces a highly interconnected and mostly
32 coherent knowledge framework "(Taber, 2005a) (here the Lewis and quantum models). The
33 conceptual integration is seen as the source of our ability to give meaning (Turner, 2000). It
34 implements an integration mechanism which is based on a dynamic approach in which the
35 partial information or apparently contradictory insights can be reformulated so that these
36 elements can be combined into a harmonious piece of information, with more value
37 (Fauconnier and Turner, 1998). According to Taber (2005a), conceptual integration is "*the*
38 *knowledge structures of an individual are organized in such a way that there is strong linking*
39 *between different 'areas', and that, generally speaking, there is consistency between different*
40 *parts of the person's personal knowledge.*" A future teacher, at the end of his university
41 studies, should have built for himself an efficient knowledge structure that best reflects the
42 appropriation of the "target" knowledges set by teaching.
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51 Several researchers have noted that the covalent bonding theories based on the quantum
52 mechanical models are one of the most difficult subjects to understand by students at all levels
53 of chemistry learning (Gold, 1988; Zoller, 1990; Tsaparlis 1997, Taber, 2001, 2002a,b;
54 Tsaparlis and Papaphotis 2002; Papaphotis and Tsaparlis 2008; Nakiboğlu, 2003). The
55 concepts involved are complex and too abstract for many students. In this study our research
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questions are: To what extent have Algerian students integrated the concepts of Molecular Orbital Theory (MOT) to describe covalent bonding? To what extent do students link Lewis structures and concepts of Valence Bond Theory (VBT) when describing single, double or triple covalent bonds in terms of σ and π bonds?

Context of study

For Kouba (Algeria) Superior Institute of Education (Ecole Normale Supérieure in French), students intending to teach physical sciences, objects of our study, the covalent bond is taught during the first two years of common part of the preparation of a physical sciences bachelor degree curriculum, in the chapter relative to the chemical bond within the unit of general chemistry. It is first described using Lewis model and then the quantum model theories: VBT and MOT. The axial (σ bond or bonding MO σ) or lateral (π bond or bonding MO π) overlap of hybrid or atomic orbitals, will lead to another interpretation of the electrons sharing during the formation of covalent bonds. Note that in order to give a visual representation of the combination of orbitals and electron distribution (paired or not) resulting from the hybridization, it is used a representation of the hybridized and no-hybridized orbitals in quantum boxes, as shown in figure 1.

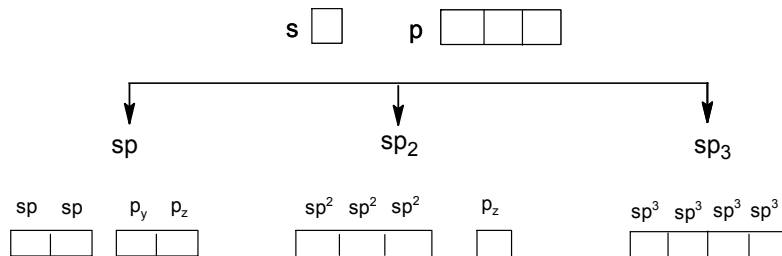
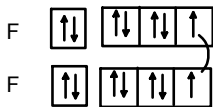
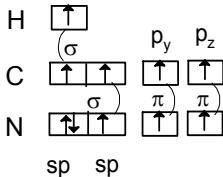
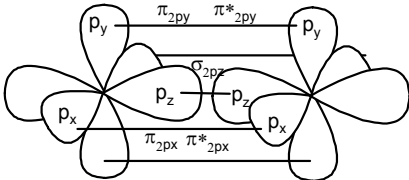
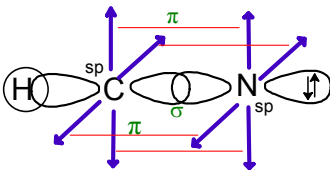


Fig. 1: Schematic representation of hybridization states using quantum boxes

The description and representation of organic structures will then be organized around the modeling of covalent bond involving the use of different concepts related to the Lewis model (shared or lone pair, electronic deficiency, covalence, octet or duet rule, etc.) as well as that of the quantum model (AO s and p, orbital overlap, hybridization sp^3 , sp^2 and sp , etc.) (see examples in Table 1). It is during their use in organic or inorganic chemistry that students will be asked to link the concepts of the different models.

Table 1: Examples of descriptions and representations of bond formation

	F ₂	HCN
Description according to the Lewis model	A single bond (1 bonding electron pair) between the fluorine atoms and 3 lone pairs on each atom	A single bond (1 bonding electron pair) between hydrogen and carbon atoms + triple bond (3 bonding electron pairs) between carbon and nitrogen and one lone pair on nitrogen
Lewis representation	$ \overline{\text{F}}-\overline{\text{F}} $	$\text{H}-\text{C}\equiv\text{N} $
Description according to Quantum models	(MOT) 1MO σ_{2pz} (axial overlap of 2 p _z AO's) + MO's σ_{2s} , σ^*_{2s} , $\pi_{2px,y}$ and $\pi^*_{2px,y}$, globally nonbonding. This MO's correspond to the 6 lone pairs of Lewis representation	(VBT) 2 σ bond (axial overlap of H AO s with C HO sp and C with N HO sp) + 2 π bond (lateral overlap of 2 p AO's of C and N) + 1 nonbonding HO of the nitrogen atom
Representation of orbital in the form of quantum boxes		
Representation of the orbitals overlapping		

Previous research on the difficulties in understanding the covalent bonding models based on quantum model

The atomic orbital concept (AO)

Regarding the understanding of atomic orbitals, much confusion appear: the concept of atomic orbital is often considered equivalent to those of orbit, shell or sub shell, quantum box (Nakiboglu 2003; Cervellati and Perugini, 1981; Nicoll, 2001; Taber, 1997, 2002a; Tsaparlis and Papaphotis 2002; Tsaparlis and Stefani, 2009) or to an energy level (Cervellati and Perugini, 1981; Taber, 2002a; Nakiboglu, 2003).

Taber (2001) suggests that having learned the atomic structure in terms of electron shells may hinder learning in terms of orbital and that the emphasis in teaching on the rules of filling

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3 orbitals (s, p, d) is understood by students as a "puzzle" to achieve by not favoring
4 understanding of different concepts (Taber, 2002a). For example, Nakiboglu (2008) shows
5 that if the concept of atomic orbital is strongly linked to that of the electron, it is weakly
6 related to other concepts in the atom quantum model such as quantum numbers or designation
7 of the orbital types (s, p, d, f).
8
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10 11 **The hybridization concept**

12 For Taber (2002b), in the minds of students, the formation of hybrid orbitals takes place in
13 three steps: the starting point is the electronic configuration of the atom concerned in its
14 ground state, followed by seeking a new set of orbitals (electronic configurations) that are best
15 suited for recovery (hybridization), then they consider the formation of molecular orbitals or
16 bonds (Papaphotis and Tsaparlis, 2008b). In a previous study we showed that almost all of the
17 students involved in this study (Hazzi and Dumon, 2011), adopt the above reasoning to talk of
18 hybridization. It is, thus, the operation consisting of forming bonds between atoms by pairing
19 their single electron which is considered hybridization (the lone pairs are forgotten). If the
20 number of unpaired electrons does not allow the formation to the identified number of bonds,
21 then a state of hybridization by reorganization/ mixing or excitation of electrons has to be
22 considered, otherwise it is not useful. In more, the meaning of the hybrid orbitals symbolism
23 (sp , sp^2 , sp^3) is not understand. For example the carbon atom in CH_4 is sp^3 in conformity with
24 3 s_H - p_C bond pairs and not with the linear combination of orbital s respectively with 1, 2, or 3
25 orbitals p of the same atom.
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28 As already reported by other authors (Dumon and Sauvaitre, 1995 Taber, 2002; Stefani and
29 Tsaparlis, 2009), there is much confusion between (sp^n) hybrid equivalent orbitals formation
30 (AO combined belong to the same atom) and molecular orbitals formation (AO combined
31 belong to two different atoms) leading to bond formation. However, the σ and π bonds
32 formation is not directly related to the hybridization state of atoms but to the nature (single,
33 double or triple) of the bond to be formed. Moreover, as the lone pairs are not taken into
34 account when considering a hybridization state, it is systematically associated with a number
35 of σ bonds which can be formed: 4 σ bonds to sp^3 , 3 σ and one π for sp^2 , 2 σ and 2 π for sp .
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38 39 **The quantum models of covalent bond**

40 A significant proportion of students gives a rather poor definition of a molecular orbital ("*A*
41 *linear combination of atomic orbitals*") making the confusion between the mathematical
42 modeling of the MO formation based on approximations (LCAO method) and orbitals
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3 themselves (Dumon and Merlin, 1988; Dumon and Sauvaitre, 1995; Tsaparlis, 1997; Taber,
4 2002b). Dumon and Merlin (1988) and Dumon and Sauvaitre (1995) found that if the
5 formation conditions of σ MO by axial overlapping and π by lateral overlapping are well
6 discerned, however, in the AO overlapping schemes in polar representations, the relationship
7 between the wave functions signs involved in the linear combination represented in the lobes
8 and the bonding or antibonding character of the MO is not achieved. Cervellati and Perugini
9 (1981) signal that students tend to assimilate MO (or AO) to an energy level.

10
11 Understanding of what π bond represent seems to pose some particular problems for students.
12 Taber (2001) reports that some students consider π bonds as π hybridization, probably for the
13 reason that the considered atom is hybridized (sp^2 or sp) before the lateral overlap of
14 unhybridized p orbitals? For others, one π bond corresponds to two bonds (Taber, 2001,
15 2002b). This can be explained by the practice of orbital representation by probability
16 envelopes suggesting two unconnected areas of the presence probability (Taber, 1997).

25 **Methodology**

26 **Subjects**

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28 Undergraduate students from the Kouba (Algeria) Superior Institute of Education preparing
29 their physical sciences bachelor diploma are divided into three options (physic, chemistry and
30 technology) depending on their choice of branch of teaching and level to which they wish to
31 teach (high or secondary school). All students of physical and chemical option (intending to
32 teach in high school) where asked to participate in the study and have given their consent.
33 These are the same 140 third year students (98 girls and 42 boys, 21 or 22 years old) who had
34 followed the same course of physical (in two first university years) and organic (in third
35 university year) chemistry as those concerned by the study of hybridization (Hazzi and
36 Dumon, 2011). The period between end of the quantum model concepts teaching and the
37 collection of data, after teaching organic chemistry, is 8 months.

46 **Collection of data**

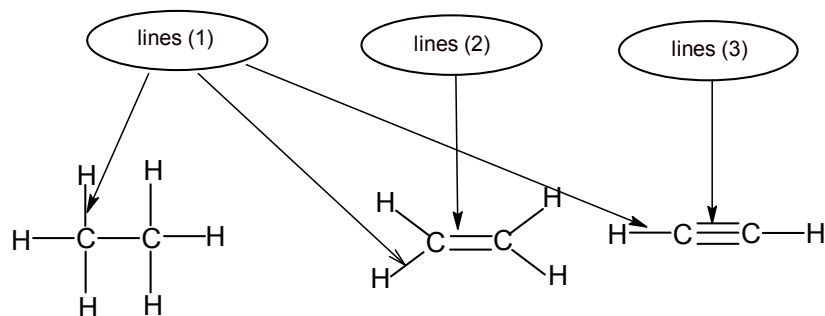
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48 Data were collected using a paper and pencil questionnaire on concepts taught during the
49 common part of the curriculum and frequently used in organic chemistry. The questions were
50 written out after dialogue between the two authors then submitted to two other chemistry
51 teachers to assess whether students are able to answer in view of teaching given. The
52 questionnaire was then tested with a group of 18 students (out of sample) to control that they
53 thought the questions meant, this has been the case. Their aim is to obtain the students'
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descriptions of single and multiple bonds formation using concepts of covalent bonding theories. In order to promote the emergence of knowledge having been integrated by students, we have chosen to propose two open questions (Table 2). The first question is to analyze to what extent students are able to use MOT concepts to describe formation of single covalent bonds in the case of simple polyatomic molecules (first research question). The second question concerns the description, using concepts of atom and molecule quantum model, of different Lewis representations of molecules containing two carbon atoms linked by single or multiple bonds (second research question). Note that, as students used them appropriately concepts of Valence Bond Theory (VBT) to answer at this question, and not those of MOT, it might sensible to revisit the inappropriate wording of question 2 if the work were repeated/developed. Students had to answer during a 30 minute session. The nature of the questionnaire was made clear to the students (it was anonymous, not used for assessment, seeking personal conceptions).

Table 2: Questionnaire

Q1: "Describe in terms of molecular orbitals (MO's), the formation of bonds corresponding to the different molecules H_2 , F_2 , HF . Specify in each case, with justification, the nature of the bond (σ , π , covalent, non-covalent, etc.)".

Q2: "Let ethane, ethylene and acetylene be molecules whose developed structural formulas are shown in the following figures:



Describe, in terms of molecular orbital, the bonds formation corresponding to lines 1, 2 and 3."

It should be noted that this students received a teaching in Arab language and that it is this language which was used for the collection of data. The questions and the answers were translated into French then into English for this report.

Data analysis

We expect that students describe the bonds formation by written sentences. If the covalent bonding theories based on quantum model of atom is correctly integrated, students should be able to write approximately the following sentences.

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3 *Question 1: Description of the H-H, F-F and H-F bonds (MOT):*
4

5 - The H-H bond is a single covalent bond. It is formed when an AO (s) of H overlaps with the
6 AO (s) of a second H atom to give an MO σ representing bonding electron pair.
7

8 - The bond F-F is a single covalent bond. It results from an axial overlap of $2p_z$ AO of two
9 fluorine atoms to give an MO σ_z representing bonding electron pair. Each of the two atoms
10 provides a single electron from its outer shell (eventually: others nonbonding electron pairs
11 correspond to lone pairs of the Lewis Diagram).
12

13 - The H-F bond is a single covalent bond. It results from the axial overlap of the H AO 1s
14 with fluorine AO $2p_z$ to generate an MO σ . Each of the two atoms provides a single electron
15 from the outer shell (eventually: others nonbonding electron pairs represent lone pairs of the
16 Lewis Diagram; possibly: the energy levels of the AO 1s (H) and 2p (F) being neighbors,
17 assuming that the z axis is the interatomic axis, both AO qualify for an axial overlap and the
18 formation of an MO).
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26 *Question 2: Descriptions of the different lines representing bonds (VBT)*
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28 Lines 1 represent one single covalent bond C-H (denoted σ). It results from the axial overlap
29 of hydrogen AO s with respectively: one carbon sp^3 HO (case of alkanes), one sp^2 HO (case
30 of alkenes) or sp HO (case of alkynes). This axial overlap generates σ bond representing
31 bonding electron pair. Each of the two atoms (C and H) provides a single electron from the
32 outer shell.
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37 Lines 2 represent one covalent double bond. The axial overlap of two HO sp^2 belonging to
38 each of the carbon atoms leads to the formation of σ bond representing bonding electron pair.
39 The lateral overlap of the two unhybridized p_y orbital of each atom leads to the formation of π
40 bond representing a second bonding electron pair (eventually: This lateral overlap is possible
41 only if their axes are parallel).
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46 Lines 3 represent one covalent triple bond. A σ bond is formed from axial overlap of two sp
47 HO of two carbon atoms and each containing one electron. Both π bonds are formed from the
48 lateral overlap of unhybridized p_x and p_y AO's present on each hybridized carbon and having
49 parallel axes (eventually: their symmetry planes are orthogonal and intersect at the bond axis).
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53 *Categorization of data*
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56 In the answers of students we note few written sentences (WS). They prefer use various
57 schematic representations to describe covalent bonds. We have classified these
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3 representations, retrospectively after reading responses, as: Quantum Boxes (QB), Atomic (or
4 hybrid) Orbitals Overlap (AOO) and correlation diagram of MO Energy Level (EL). That can
5 be explained by the fact that by drawing out such representations, the student reduces the
6 number of ideas and facts that they need to mentally manipulate before writing sentence.
7
8 These different representations can occur alone or in combination. After reading of the
9 answers, a categorization was made independently by the two authors on the following
10 principle:

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14 - for written sentences, identification of key words appearing in descriptions. These key words
15 can be these contain in expected sentence description above-mentioned or others significant
16 words. Note that key words can appear also in other written shorter traces (some words, Greek
17 symbols) accompany the various representations;

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20 - for other representations, identification of diagrams translating similar ideas.
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24 In the event of disagreement (in very little cases), a discussion with take place to arrive at a
25 common categorization. One answer is considered correct or acceptable if it is conform to the
26 teaching taught. The analysis of data will be compared in the discussion with the same type of
27 data obtain at different times for other topics (hybridization and drawing the orbitals
28 overlapping) of Hazzi thesis work (2012).
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33 34 **Results**

35 36 **Students' description of the single bonds formation (Question 1)**

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38 119 students (85%) respond to this question. The others students give no answer or answer
39 that are difficult to interpret. To describe the single bonds formation, students use the various
40 representations identified and, for 40 students (28%), they are accompanied by a Lewis
41 Representation of molecules (LR). In the description given by one student, multiples types of
42 representation can be used (see example table 3).
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47 We report in table 4 the total number of different categories of description identified in all students'
48 answers and, in italic, the number of others representation with whom they are associated.
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50 51 ***Descriptions in written form***

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53 Few students (10%) give the answer in the form of written sentences (see examples in table
54 3). These accompany other forms of representation (Quantum Boxes, or Atomic Orbital
55 Overlap). However, other written shorter traces appear in the various representations (see
56 example 3 in table 3).
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Table 3: some examples of multiples representation

1- QB + WS + LR		
	<p>The F – F bond is a σ bond formed by combination of two fluorine atomic orbitals</p>	
2- AOO + WS + LR		
	<p>The F-F bond is σ bond obtain by axial overlap of two fluorine p orbitals</p>	
3- QB + AOO + written shorter traces		
		<p>Axial overlap of two OA to form σ bond</p>
4- QB + AAO + WS + LR		
		<p>The σ-covalent bond F-F formed by a bonding electron pair is derived from axial fusion of two OA p_z which allows to surround each fluorine by one octet.</p>

Table 4 : The different categories of description identified

Categorization	WS	QB	AOO	EL	LR	NR+others
Number of representations	14 (with 10 QB, 4 AOO, 8 LR))	72 (with 10 WS, 14 AAO, 8 EL, 29 LR)	26 (with 4 WS, 14 QB, 4 EL, 3 LR)	32 (with 8 QB, 4 AOO, 6 RL)	40	21
Total students %	10	51	19	24	28	15

In Table 5 were summarized the frequencies and percentages of keywords found in all written bond descriptions given by the 119 students who responded.

Table 5: Keywords contained in all written forms

Keywords	H_2		F_2		HF		
	N	%	N	%	N	%	
covalent	79	66	85	71	21	18	
σ	54	45	53	45	40	34	
Overlap (s-s) and axial overlap (p-p and s-p)	37	31	42	35	32	27	
MO	2	2	2	2	2	2	
Other keywords	single	13	11	15	13	0	0
	bonding electron pair	18	15	15	13	9	8
	sharing a pair of e-	23	19	28	24	0	0
	duet/octet	18	15	40	34	4	3
	Hydrogen bond	7	6	0	0	3	3
Non-covalent	0	0	0	0	18	15	

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4 The first finding is that when students are asked to describe the bonds formation in terms of
5 molecular orbitals, nearly (98%) of the descriptions does not refer to them. Considering the
6 number of keywords occurrences it is possible to simulate the description of bonds made by
7 students. For H₂ and F₂ molecules the bonds between atoms are mainly covalent (about 69%),
8 of σ -type (45%), obtained by overlapping the hydrogen atoms s orbital or by axial overlap of
9 fluorine p orbitals (about 32%). In contrast, in the case of HF, the bond is σ type (34%),
10 obtained by axial overlap of the hydrogen s orbital and fluorine p orbital (27%). It is
11 considered by 18% as being covalent and non-covalent by others students (15%) due to the
12 difference in electronegativity between the two atoms constituting the molecule.
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20 According to the keywords in expected sentence description we note that:

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22 - The term single bond is little mentioned (by about 12% of students);
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24 - The nature of AO's involved and their symmetry overlapping is not always précised
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26 The reference to the Lewis model (Bonding electron pair, sharing a pair of electrons; duet or
27 octet rules) is present in some written forms (24% of keywords on average), principally for H₂
28 and F₂, associated with quantum boxes or AOO: for example, "*In hydrogen bond, each H*
29 *participates in the formation of the σ bond by an electron so as to respect the duet rule*"; "*F-*
30 *F bond: each fluorine participates with an unpaired electron to form σ bond respecting the*
31 *octet rule*"; "*Axial overlap of two fluorine AO p_z to form one bonding electron pair*
32 *representing covalent bond σ* ". These sentences show that these students have constructed a
33 hybrid model (quantum and Lewis).
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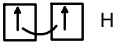
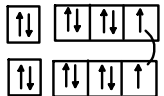
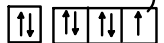
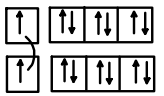
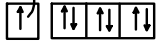

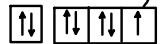

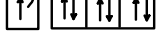
40 ***Descriptions using quantum boxes (QB)***

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42 The bonds description is mainly (51% of students tested) schematically represented in the
43 form of quantum boxes (QB) (Table 6) (35% alone and 16% in combination with AOO or EL
44 descriptions).
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48 ***Bond H-H***

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50 In all representations we note the connection between the H quantum box by a curved line (or
51 arrow). In more, the majority of students mention the participation of each hydrogen atom by
52 one electron in bond formation. The bonding pair is not mentioned, but it appears in the Lewis
53 structure that accompanies, in 29% of cases, the representation in quantum boxes. Finally, in
54 the written traces, the bond is called " *σ covalent because it is s-s type.*"
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Table 6: Descriptions in quantum boxes

H  H		NR
N = 72 (100% of the quantum box descriptions)		0
F  F 	F  F 	
N = 63 (87%)	N = 6 (8%)	3 (4%)
H  F 	H  F 	
N = 63 (87%)	N = 6 (8%)	3 (4%)

Bonds F-F and H-F

In the case of F₂ molecule representations in quantum boxes, 87% represent pairing between two electrons p in connecting the two unpaired p boxes by a curved line (or arrow). The participation of an electron from each atom in the bond formation is often invoked in parallel with this diagram. However, the valence shell of the fluorine atom is misrepresented by some, because it was represented schematically by only 3 p AO's. This suggests that they do not take into account the sub shell s, and this representation gives two lone pairs only to fluorine.

For some students (8%), the bond is called, as in H₂, '*σ covalent type s-s*'. To represent it schematically, they show by arrow the shift of an electron from the sub shell s to sub shell p in such a way as to have a single electron in the box s and a full sub shell p (some speak of 'hybridization sp'). Two electrons s of the two fluorine atoms are then paired. Thus, the term covalent seems to be qualifying of one (s-s) type bond as in H₂.

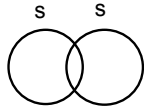
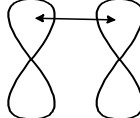
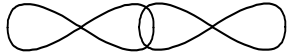
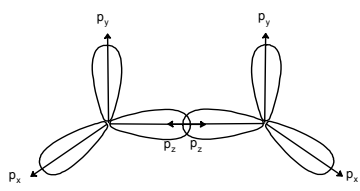
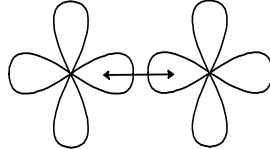
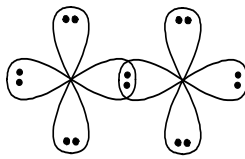
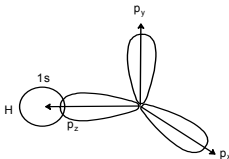
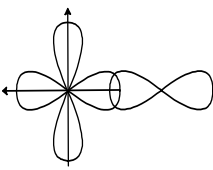
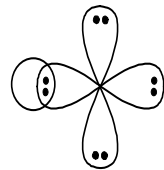
Descriptions in the form of atomic orbitals overlap (AOO)

Such schematic representations were proposed by 26 students (19%), either alone (8 students) or in combination with other representations (14 with QB and 4 with EL). These schematic representations were listed in Table 7.

Bond H-H

It is predominantly (22 out of 26) represented by the participation of two s AO's, schematized more or less correctly with spherical symmetry. But the four other schematic representations of the σ bond involve the overlap, either axial or lateral, of two s AO's with axial symmetry (p-type).

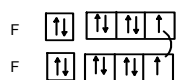
Table 7: Representation of orbitals overlap

H₂			
	N=22	N= 4	
F₂			
	N=5	N=3	N=13
HF			
	N=6	N=5	N=11

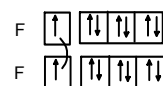
Bonds F-F and H-F

If in the case of HF, the s orbitals are mostly represented with spherical symmetry, none of the students represents p orbitals correctly. They are represented either by three half orthogonal atomic orbitals, or in most cases, by four identical pseudo orbitals arranged in a plane and in an orthogonal ways.

In the case of F-F bond, for 13 representations out of 21, these orbitals are accompanied by two types of representations in quantum boxes:



9/13



4/13

As we can see for example 4 in table 3, these representations are generally accompanied by a written commentary making reference to the Lewis model. So, we can consider that the purpose of these representations is to show that, in accordance with the Lewis representation, the overlap of two orbitals leads to a bonding electron pair; each of the remaining orbital contains lone pairs. There are also eleven such representations in the case of the H-F bond. Although some students mention the overlap of p_z orbitals (see table 3, example 4), it seems that for these students the four “pseudo orbitals” represent in fact the four quantum box.

1
2
3 The F-F bond is σ bond and the axial overlap p_z/p_z between the two fluorine atoms is
4 represented in the majority of cases. For others, the description seems to be schematically
5 represented by axial overlap and lateral overlap of two p AO's (or 4 pseudo orbitals?), the
6 third is forgotten.
7
8

9
10 The H-F bond is called σ bond. In some representations ($N = 6$), the axial overlap s/p_z
11 between H and F is mentioned. In height other representations s AO have an axial symmetry
12 and fluorine only represented by two orthogonal p AO's (or 4 pseudo orbitals?). As in the
13 previous case the overlap between the orbitals is either axial or lateral.
14
15

16
17 *Descriptions in the form of energy level correlation diagrams (EL)*
18

19 Among the 32 students using such descriptions (24%), 28 represent the energy diagram of the
20 H_2 molecule, 26 that of F_2 molecule and 20 that of HF. Seven other students give only the
21 electronic structure of molecules. Examples of different kinds of typical representations are
22 summarized in Table 8.
23
24

25
26 - In the case of H_2 molecule, 11 out of 28 diagrams are represented correctly. For seven
27 representations, the energy level of the bonding MO is correctly positioned but antibonding
28 MO is not represented. We can consider this representation as partially correct. In contrast, 10
29 representations are incorrect because, either the energy level of the bonding MO is the same
30 as that of AO (so there is no stabilization by AO's overlap) or it is superior to it (thus
31 destabilizing the system). The principle of forming a bonding MO σ resulting in a stabilizing
32 nucleus-electrons attraction is far from being understood.
33
34

35
36 - There are, for F_2 , few correct representations ($N = 4$) of the type listed in the table. We note
37 second type of representation ($N = 5$), not totally correct because the energy level of the
38 bonding MO σ_z is not correctly positioned, has been identified. It may be due to an analogy
39 made by students with N_2 diagram for which there is an inversion of the energy level of the
40 bonding MO σ_z and that of MO π_x and π_y . There, these representations will be considered as
41 partially correct. In contrast, for the 17 other representations, the relative positioning of AO's
42 and MO's energy levels is totally incoherent.
43
44

45
46 - In the HF case, no representations are correct. For two representations, the hydrogen 1s AO
47 overlapping with 2p AO of fluorine is considered. However, the electrons pairs seem to be
48 placed on p AO's of fluorine which would be stabilized from an energetic point of view.
49 Another type of representation involves only the s AO's of the two atoms for the formation of
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MO's. This confirms the idea already encountered, that the bonds involving fluorine atom are of "s-s" type.

Table 8: Descriptions in the form of energy levels correlation diagrams

H₂		
<p style="text-align: center;">H H₂ H</p>	<p style="text-align: center;">H₂</p>	<p style="text-align: center;">H H₂ H</p>
N= 11	N=7	Diverse : N=10
F₂		
<p style="text-align: center;">F F₂ F</p>	<p style="text-align: center;">F₂</p>	<p style="text-align: center;">F₂ and other representations</p>
N= 4	N= 5	Diverse : N=17
HF		
<p style="text-align: center;">H HF F</p>	<p style="text-align: center;">H HF F</p>	<p style="text-align: center;">Type s-s : N = 4</p> <p style="text-align: center;">and other representations</p>
N = 0	N = 2	Diverse : N=18

Representations only in the form of electronic structures of molecules given by seven students are satisfactory only for H₂ (1σ)². In the case where the fluorine atom is involved, they are incorrect; for example for F₂, 1σ² 1σ*², 2σ² 2σ*², 2π_x² 2π_x*² (π_y² π_y*², π_z¹ π_z*¹) instead of (2σ)² (2σ*)² (3σ)² (or σ_{2pz}²) (π_x)² (π_y)² (π_x*)² (π_y*)². We note that students shall include the electrons of the internal shell which are not involved in the formation of bonds.

Several difficulties are noted in understanding the relationship between the σ bond formation and the energy levels associated with an OM formation. The positioning of the MO assumed to be bonding energy, unchanged or superior to that of AO's that overlap, shows that the principle of stabilization (bonding MO) or destabilization (antibonding MO) of the system is not taken into account. To this is added, in the molecules involving fluorine, the generally inconsistent positioning of the energy levels related to AO's and MO's and the lack of association of lone pairs of the Lewis representation with those present on the MO's σ , σ^* and π , π^* , generally nonbonding (F_2 case), or unchanged AO 2s and 2p of fluorine (HF case).

Description of the bonds formation corresponding to lines 1, 2 and 3 (Question 2)

For this question, the non-response rate is high (34%). Out of the 93 students who responded, 55 (59%) give a description in the form of quantum boxes and 38 (41%) represent it schematically in the form of AOO. These representations are sometimes accompanied by written traces.

Descriptions in written form

In table 9 were summarized frequencies and percentages of keywords noted in the written traces of descriptions accompanying the various representations of bonds given by students.

Table 9: Keywords contained in any written traces

Keywords	C-H		C=C		C \equiv C	
	N	%	N	%	N	%
Covalent	21	23	0	0	0	0
σ	14	15	0	0	0	0
$\sigma + n\pi$	0	0	10	11	13	14
axial overlap	25	27	44	47	46	49
<i>whose axial overlap (p-p or s-p)</i>	(25)	(27)	(27)	(29)	(32)	(34)
lateral overlap (p-p)	0	0	23	25	44	47
Other keywords	Single	05	5	0	0	0
	Sharing a pair of e-	02	2	0	0	0
	Hydrogen bond	06	6	0	0	0

The simulation of this description (carried out by 93 students) according to the percentage of keywords would be as follows:

- In ethane, the C-H bond is covalent (23%), obtained by axial overlap (s-p) of the H orbital s with C orbital p (27%), of σ type (15%). In contrast, this bond is not described in the case of ethylene and acetylene;
- In the description of multiple bonds, the term 'covalent' does not appear. Line 2 (C = C) is obtained by an axial overlap (47%) of type p-p or s-p (29%) and a lateral overlap between two

1
2
3 p orbital (25%) leading to a ($\sigma + \pi$) type bond (11%). Line 3 ($C \equiv C$) results from an axial
4 overlap (49%) of type p-p or s-p (34%) and a lateral overlap of two AO p (47%). It
5 corresponds to a ($\sigma + 2\pi$) type bond (14%).
6
7

8 According to the key words in expected descriptions we note that:
9

- 10 - If the term single bond is little mentioned for the C-H bond (by approximately 5% of
11 students), those of double and triple bonds are completely omitted;
12
13 - If the reference to the symmetry of axial overlap leading to the formation of σ bonds is
14 mentioned in the case of multiple bonds, the nature of AO (s/sp^n) and (sp^n/sp^n) involved is
15 not cited by students.
16
17

18 *Descriptions using quantum boxes*

19
20 The 55 students' responses for the various lines are classified into different categories and
21 reported in table 10. The representations are concrete cases representing the concerned
22 category. The number in parentheses indicates the number of students involved in the
23 response category.
24
25
26

- 27
28 - A category we called "hybridization", where the redistribution of electrons corresponding to
29 different hybridization states of carbon is most often described in the form of 4 equivalent
30 quantum boxes, which, according to the teaching taught, is only correct for the sp^3 state ($N =$
31 23). It seems that for these students, what is important is to get in all cases the four unpaired
32 electrons necessary for the four bonds formation. However, two students give a representation
33 in quantum boxes conforming to the teaching taught: 3 equivalent boxes for sp^2 and a p
34 unhybridized box, two equivalent boxes for sp and two unhybridized p boxes;
35
36 - A category referred to as "carbon excitement s - p", where the hybridization state
37 corresponds to the transfer or the excitation of an electron from a subshell s to a subshell p
38 in such a way as to obtain a number of unpaired electrons in accordance with the tetravalence of
39 the carbon ($N = 23$ for ethane or ethylene and 26 for acetylene);
40
41 - A category referred to as "initial C structure", for which the representation of the carbon
42 electronic structure is not modified, because possessing two unpaired electrons ($N = 9$ then 6).
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52 *C-H bond (line 1) description*

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54 Regarding the "hybridization" category, the C-H bond is represented schematically by all only
55 in the case of ethane whereas carbon - carbon bonds are shown by all in ethylene and
56 acetylene representations.
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Table 10: Representation of the different bonds using quantum box

Hybridization	Carbon "excitement" s - p			Initial C structure
Ethane (Bond C - H)				
(23)	(23)	(11)	(2)	(9)
Ethylene (Bond C = C)				
(2)	(11)	(5)	(7)	(5)
(23)	(23)	(4)	(7)	(9)
Acetylene (Bond C ≡ C)				
(2)	(7)	(4)	(15)	(6)
(23)	(26)	(6)	(15)	(6)

For ethylene and acetylene, the C-H bonds formation by the overlap of a carbon $HO\ sp^2$ or sp with a hydrogen AO s is shown schematically only by the two students who gave a correct representation. It may be assumed that for others, such as ethane, the C - H bonds are obtained by sharing a hydrogen $1s$ electron with one electron from an unused "hybrid orbital".

In the case of carbon "excitement" s-p category, C-H bonds are represented for the three molecules as resulting from the pairing of a hydrogen $1s$ electron with either one carbon electron $2s$ (type s/s: 7 occurrences), or with one carbon electron $2p$ (type s/p: 12 occurrences). The same is true for the single C - C bond resulting from the sharing of one carbon $2s$ electron with one electron $2p$ from the other (10 occurrences).

1
2
3 Finally, when the representation in the form of quantum boxes of the carbon initial electronic
4 structure is kept, the C - H bond is represented by combining the 1s electron of hydrogen with
5 one unpaired electron in the subshell 2p of carbon. The carbon is not hybridized as having
6 unpaired electrons, and for these students, hybridization *"is the fusion between the s and p*
7 *AO's to give σ bond."* It is worth noting that in the case of ethane such representation does not
8 allow for the interpretation of the carbon tetravalence.
9

10
11
12
13 *Multiple bonds carbon - carbon (lines 2 and 3) description*
14

15 Among the 23 "hybridization" category representations, only two explicitly indicate the
16 formation of a σ bond between two carbon atoms by the overlap of HO's (sp^2 or sp) and one
17 or two π bonds by the overlap of unhybridized p AO's. The others ones represent the
18 formation of double and triple bonds using description in quantum boxes of the sp^3
19 hybridization state in the form of four equivalent AO's, each containing a unpaired electron.
20 From there they build bonds by pairing the electrons of the two carbon atoms; 2 electrons of
21 each of the carbon atoms are combined to form the C = C double bond and 3 to the triple bond
22 C \equiv C. This reflects a lack of mastery of the hybridization concept and its representation in
23 quantum boxes and a failure to take into account the overlapping conditions for the formation
24 of σ and π bonds.
25
26
27
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31

32 For 23 students (26 in the case of acetylene), hybridization is summed up in the excitation of
33 an electron in a subshell s to a subshell p, without distinction between the different possible
34 states. From the excited state of carbon 16 (case of C = C) or 11 (case of C \equiv C) among them
35 describe the formation of a bond of the kind "s/s" linking the 2s boxes of two carbon atoms
36 and bonds of the kind p_x / p_x (case C = C) and p_y / p_y (case C \equiv C) by connecting the unpaired
37 electrons of the two-carbon atoms p boxes. Although this appears explicitly in just a few
38 schematic representations, in written form ($\sigma+\pi$) for C = C and ($\sigma+2\pi$) for C \equiv C, we can
39 assume that for these students, the s/s type bond corresponds to a σ bond and p/p type bonds
40 to π bonds. The other 7 (case C = C) consider that multiple bonds are obtained only by the
41 sharing of electrons in the p subshells. The pairing between 1s (H) electrons and 2s (C) is
42 restricted to the formation of a C - H bond. In the case of acetylene, presumably because the
43 number of unpaired electrons p allows the interpretation of the tripe bond formation, 16
44 students adopt this point of view. Here too there is a misinterpretation of the overlapping
45 symmetry conditions (axial, lateral) leading to the formation of σ or π bond.
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56 Some students (9 for ethylene and 6 for acetylene) consider that carbon does not require to be
57 hybridized. They start with the electronic configuration of the two carbon atoms in their
58
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60

ground state. The schematic representation of bond formation is subsequently done using two methods: connect unpaired electron boxes p_x/p_x and p_y/p_y of two carbons by a curved line (4 students in the case of ethylene) to form the C = C double bond, forgetting the C - H bonds, involving dative bonds, the s pairs of one carbon is considered donor while vacant AO p_z of the other one is considered as acceptor (5 for ethylene and 6 for acetylene). In this case the C - H bonds are represented by pairing the hydrogen 1s electron and one carbon electrons 2p. The third bond for acetylene results from the sharing of two carbon electrons p.

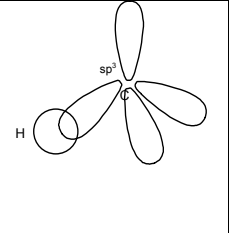
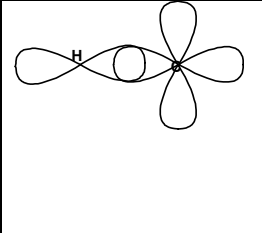
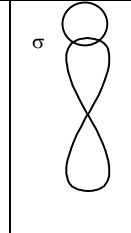
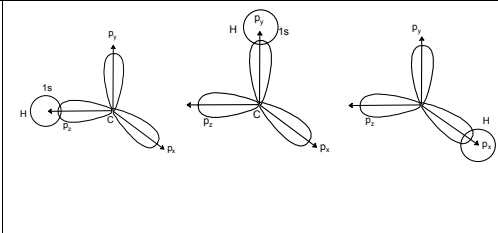
Descriptions in the form of orbitals overlap (AOO)

This mode of representation was chosen by 38 students, but not all have schematically represented the three bonds.

C - H bond (line 1)

The description of C-H bond appears in all representations given for ethane (table 11) and only in the six correct representations which explicitly mention the overlap between C HO and H AO s for ethylene and acetylene (see table 12).

Table 11: Representations of the C - H bond in the form of AOO for ethane

C - H bond for ethane			
			
N = 6	N = 22	N = 5	N = 2

In the case of ethane, only six students represent correctly the overlap of C HO sp^3 and H OA s.

In the category of representation chosen by 22 students, we find the representation identified in question 1 of 4 identical "pseudo orbitals" arranged in a plane and orthogonal. Are they supposed to represent them four carbon "hybrid" equivalent sp^3 , two orthogonal p AO's or the four quantum boxes? The C-H bond results from the overlap of any of these orbitals (or p AO $\frac{1}{2}$ lobe) with AO s of hydrogen. It is noted that the s orbital is represented as a p orbital with an axial symmetry.

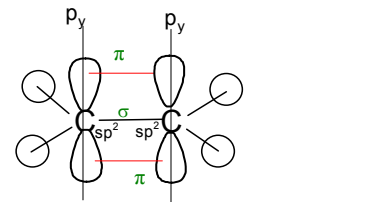
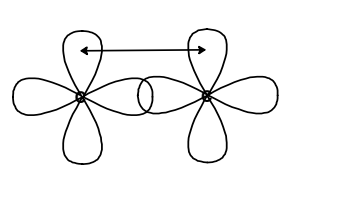
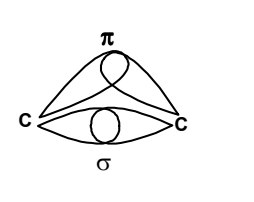
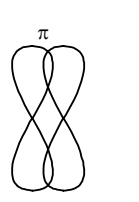
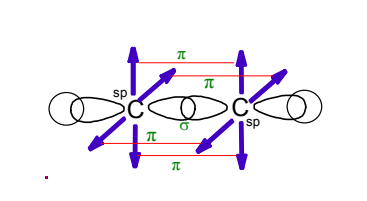
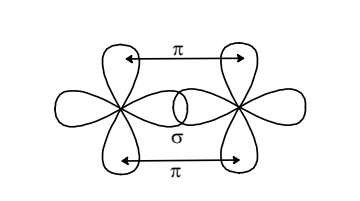
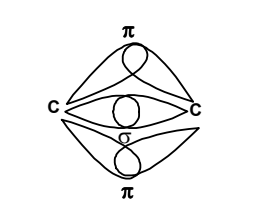
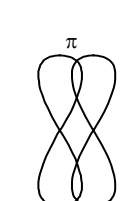
For five students, it seems that it is the axial overlap of an atomic orbital 1s with an atomic orbital p which leads to the formation of σ bond. The sp^3 hybridization of carbon is not taken

into account. So is same for both students who represent formation of σ bonds (C - H) by an axial overlap of the hydrogen AO s with carbon AO's p_x , p_y and p_z . One notices, as in the case of fluorine, that the orthogonal orbitals p are represented by only half a lobe and the carbon is schematically represented by three atomic orbitals (subshell s is omitted in the representation.) And therefore the fourth bond is ignored.

Multiple bonds carbon - carbon (lines 2 and 3) description

In 6 of the 38 representations given by students, overlapping are clearly identified (hybrid carbon HO sp^2 or sp and unhybridized AO p), correctly represented, and the axial overlap of HO leading to the σ bond formation and lateral unhybridized AO p to form π bonds are explicitly reported (Table 12).

Table 12: Representations of multiple bonds using AOO

C = C			
			
6	14	14	4
C ≡ C			
			
6	19	12	1

We find the representation category identified for the C-H and F-F bonds where the 4 equivalent AO's of carbon are shown as being orthogonal in a plane. Multiple bonds result from forming a σ bond by axial overlap of two pseudo orbitals and of one or two π bonds by lateral overlap of two half lobes supposed to represent p AO's. It seems that for these students the nature of AO's which overlap to form the covalent bond is of little importance (they can be hybrids as well as p or s). What seems important is that the axial or lateral overlap of two of these orbitals leads to the pairing of the two electrons required for the bonds formation ($\sigma + \pi$) and ($\sigma + 2\pi$), each of the remaining orbital contains then a single electron which can be paired with the s electron of hydrogen to form C - H bond. For ethylene, there results an

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3 incorrect representation of the angles between the σ bonds and therefore of the molecular
4 geometry.
5
6

7 In other representations (14 for $C=C$ and 12 for $C\equiv C$) the axial overlap leading to the
8 formation of σ bond, and the lateral overlap required for the formation of π bond are shown
9 schematically, but with a disrespect of the parallelism of the symmetry axes of p AO's.
10 Finally, some representations describe only the lateral overlap of two p orbitals for the π bond
11 formation. One may wonder whether these students confuse multiple bonds with π bond or
12 whether it is simply due to a misunderstanding of the question asked. If in the case of the
13 double bond this schematic representation limitation to only one bond may be explained (limit
14 line 2 to π bond), it is not the same for the triple bond which requires the formation of two π
15 bonds.
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22 **Discussion**

23 *Integration of atomic or hybrid orbitals concepts*

24
25 We can note an unsatisfactory integration of what an orbital represents. The majority of
26 quantum boxes representations used by students reflect a "quantum box" conception of AO's
27 or HO's. This conception has been already highlighted by other authors (Cervellati and
28 Perugini, 1981, Taber 1997, 2002a; Nicoll, 2001; Tsaparlis and Papaphotis 2002; Nakiboglu
29 2003; Tsaparlis and Stefani, 2009). Concerning hybrid orbitals of carbon, we find again the
30 conception according to which hybridization is an operation that consists of getting a new
31 electronic configuration of the carbon atom (transfer / excitation of an electron from an
32 subshell s in a subshell p) (Dumon and Sauvaitre, 1995; Taber, 2002b; Nakiboglu, 2003;
33 Stefani and Tsaparlis, 2009, Hazzi and Dumon, 2011) leading to a number of unpaired
34 electrons conforming to tetravalence of carbon in order to form σ and π bonds (Hazzi and
35 Dumon, 2011).
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46 If the s orbital is predominantly represented with spherical symmetry, several students
47 represent s AO with axial symmetry (p-type). A correct representation of p orbitals is rarely
48 performed. The few representations by three $\frac{1}{2}$ orthogonal orbitals demonstrates a
49 misperception of the fact that a p AO has two lobes of opposite signs oriented following axial
50 symmetry. More often, students draw representations that can be two orthogonal OA's p
51 (then the third is forgotten) or a representation in the form of four identical pseudo orbitals
52 arranged in a plane in an orthogonal way. This same representation is found predominantly to
53 represent four hybrid AO sp^3 in conformity to tetravalence of carbon. As this type of
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3 representation is often associated with a representation in quantum boxes (see table 3 and
4 analysis of the F-F bond description in the form of AOO), we can make the hypothesis that
5 this representation is connect with the "quantum box" conception of AO's.
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8 *Integration of molecular orbital concept*

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10 To describe single covalent bonds in the case of simple polyatomic molecules, students don't
11 use the MO concept. They have only retained that σ bond involve the pairing of electrons s
12 and/or p and result from an axial overlap of AO's.
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16 In the case of quantum boxes representations, this pairing is illustrated by curved lines linking
17 the quantum boxes s or/and p of the two bonded atoms. In the descriptions of bonds
18 represented schematically in the form of atomic orbitals overlap, it seems that for many
19 students the overlap of two atomic or "pseudo-orbital" leads to the pairing of two electrons
20 (see examples of representations in table 3 and 7). We can think that for those students, the
21 two electrons required for the bonds formation are localized in atomic orbitals. This is close to
22 the observation made by Taber (2005b) in another context: for students the bonding electrons
23 are in atomic orbital rather than molecular orbital.
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30 The use of energy levels correlation diagrams in place of MO description by some students set
31 in evidence, as it has report by Cervellati and Perugini (1981), that students have a tendency
32 to assimilate an MO (or AO) to an energy level. That probably results from the teaching
33 which gives too much importance to the correlation diagrams of energy levels and their
34 utilization (Dumon and Sauvatre, 1995). Moreover, incorrectness encountered in the relative
35 positioning of AO's and MO's energy levels in the energy level correlation diagrams shows
36 that the stabilization (bonding MO) or destabilization (antibonding MO) principles of the
37 system are not considered.
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43 *Connection between Lewis model and concepts of covalent bonding theory VBT*

44
45 When asking students to describe the various bonds figured in Lewis representations, what
46 seems important for us is to show, in accordance with the Lewis representation, the formation
47 of electrons pairs in using quantum boxes representation of orbitals (s, p or "pseudo hybrid")
48 or atomic orbitals overlap representations.
49
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51
52 In the case of σ bond, when the nature of orbitals is specified, they are only s or p, even in the
53 case of multiple bonds where overlapping of type s/spⁿ or spⁿ/spⁿ are mentioned by very few
54 students. Regarding the formation of π bonds, the lateral overlap of orbitals is simply seen as
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3 the overlap of two “half-orbital” (they can be p or “pseudo-orbital”) regardless of their
4 orientation, It should be noted that similar behavior was noted when it was explicitly asked at
5 another population of students to schematize the Lewis structures in the form of orbital
6 overlap (Hazzi, 2012). Students seen don't know the overlapping symmetry conditions
7 leading to the formation of bonds. As point out by Taber (2001, 2002b) they have not
8 integrated that π bond is represented by two lobes, separated by a nodal plane, resulting from
9 the overlap of two p orbitals of axial symmetry whose axes parallel.
10

11
12 So, it seems that for these students the nature of orbitals which overlap to form the various covalent
13 bonds is not important (they can be hybrids, p, s or “pseudo orbital). What seems important, as it has
14 already been highlighted in a previous study on the hybridization (Hazzi and Dumon, 2011),
15 is that the axial or lateral overlap of two orbitals leads to the pairing of the two electrons required for
16 the bonds formation. Then, we can made the hypothesis that students have not integrated the
17 covalent bond models but that they have elaborated an hybrid model mixing quantum and
18 Lewis models.
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20
21 It should be noted that the single bond term is little used and only for describe bond between
22 two identical atoms. For many students, this bond is σ bond obtained by axial overlap of
23 orbitals which the nature is not always specified and the formation of σ bond occurs only in
24 the case of a single bond.
25

26 27 28 29 30 31 32 33 34 *Integration of covalent bond concept*

35
36 We find the conception according to which the denomination of covalent bond is restricted to
37 the sharing of an electron from each atom to give a bonding pair σ in the case of H – H, F – F
38 and C-H bonds. It is a conception already highlighted in studies concerning the description of
39 line 1, 2 and 3 using Lewis model made by Cokelz and Dumon (2005) with high school
40 students and Hazzi et al (2011) with university students. In more, for some students, a
41 covalent bond is termed “s-s type”. Double and triple dashes are in no way associated with the
42 term covalent, nor with two or three bonds of different natures and characteristics. They are
43 simply $(\sigma + \pi)$ or $(\sigma + 2\pi)$ bonds.
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50 51 **Conclusion**

52
53 The fact that the spherical symmetry of the s AO is not considered by some students, that the
54 two lobes of opposite signs of p AO seems to be absent from the minds of students, that some
55 have associated with quantum boxes, whatever their nature, identical orbitals, shows that the
56 concepts of atomic and hybrid orbitals are not integrated by many students. In more, the AOO
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3 representations show poor control of the linking of the orbitals symbolization (s, p; or hybrid
4 sp^n) with their directional aspect (Zoller, 1990).

5
6 Concerning the conceptual integration of covalent bonds models, this study shows that our
7 students have neither integrated the molecular orbital concept nor establish correct connection
8 between Lewis model and covalent bonding theories (VBT and MOT). They have only built
9 piecemeal of knowledge (Taber, 2005b) without making the link between them, which leads
10 them to make a mix between Lewis model and quantum models.

11
12 In absence of atomic and hybrid orbitals concepts integration, they have used to describe
13 covalent bonds an alternative knowledge structure, a "quantum box" conception of orbitals.
14 We can consider that this knowledge structure result from the idea of sharing a pair of
15 electrons in the Lewis model of covalent bond. So, students search to form electron pairs, it
16 doesn't matter much where the electrons come to form this pair. An alternative conceptual
17 framework that, in study relative to hybridization (Hazzi and Dumon, 2011) we have named:
18 the "electron pair framework".

19
20 As "octet framework" (Taber, 1999) from which it follow, we can consider that this
21 framework is a "pedagogical learning impediment" (Taber, 2005b) in the sense that this idea
22 present in cognitive structure derive from the visual representation of the atomic electronic
23 structure in each HO and AO in quantum boxes, used in Algerian teaching. The linear
24 combinations of AO to form MO, the overlapping of orbitals to form MO or bond σ and π , the
25 symmetry condition of overlap are not present in this representation; it promotes the idea of
26 electron pairs formation to make bonds.

27
28 To improve the conceptual integration of covalent bonding theories (MOT and VBT) based on
29 quantum model of atom theory, in first it is necessary to not use in teaching the representation of
30 atomic or hybrid orbitals in quantum boxes that can only promote the development of
31 "quantum box" conception of orbitals. In more, in this form of representation, the sharing of
32 two valence electrons represents the covalent bond formation, which can only conduce to the
33 development of "electron pair framework". Next, the focus should be much more on the
34 meaning given to model by providing a clear explanation of the nature of the concepts
35 involved. On the other hand, in order to prevent students from falling into the mechanical and
36 superficial learning of models, students should be encouraged to think about the links between
37 concepts and proceed at once to distinguish between different models.

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39 For example:
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3 - by making a clear differentiation between the overlap of two atomic orbitals which lead to
4 the formation of σ or π molecular orbitals, bonding and antibonding (MOT), and overlap of
5 hybrid orbital with another hybrid or atomic orbital to form σ π bond according to type of
6 orbital (VBT);
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9
10 - by setting an relationships between the shared and lone electron pairs of Lewis model with
11 the occupation of OM energy level by electron pairs. For example, in the case of H-F, the
12 electron pair of bonding OM σ can be associated to the shared electron pair and the three
13 electron pairs of nonbonding orbitals $2s$, $2p_x$ and $2p_y$ to the three lone pairs surrounding F
14 atom.
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18 - by insisting on the symmetry condition of orbitals overlap to form MO's or bonds.
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20
21 In more, it would be interesting to use, as Frailich et al. (2007) to enhance the concept of
22 chemical bonding, a web-based learning environment combined with cooperative learning to
23 enhance the conceptual integration of covalent bonding theories.
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27 Finally, to complete this study, we envisage to submit the questionnaire to another population
28 of students and to interrogate some of them with a semi-structured interview to confirm our
29 hypothesis on students' knowledge structures.
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