Supporting Information

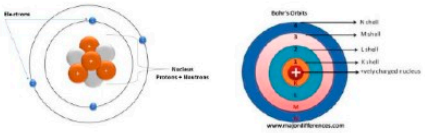
ASSESSING LEARNING IN AN IMMERSIVE VIRTUAL REALITY: A CURRICULUM-BASED EXPERIMENT IN CHEMISTRY EDUCATION

Supplementary Materials S1: Text-based content for 2D Test Group.

D) Text content for 2D group reading

Hybridization and Lewis Structures

Atoms are made up of electrons, protons, and neutrons. The protons and neutrons are in the nucleus of the atom. The electrons orbit the nucleus in orbitals. An orbital is defined as a region in space in which there is a high probability of finding an electron.



Bonding between atoms:

Bonding happens when two **valence** orbitals overlap and share their electrons to create a sigma bond. In valance-bond theory, electrons of two atoms occupy the same space. This is called overlap of orbitals.

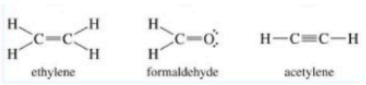
(1S + 1S) (1S + 2Px)

Hybridization:

Hybridization is the idea that atomic orbitals fuse to form newly hybridized orbitals, which in turn, influences molecular geometry and bonding properties. Hybridization is also an expansion of the valence bond theory. To explore this idea further, we can utilize three types of hydrocarbon compounds to illustrate sp^3, sp^2, and sp hybridization.

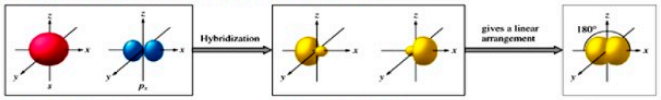
Lewis Structures:

A Lewis Structure is a very simplified representation of the valence shell electrons in a molecule. It is used to show how the electrons are arranged around individual atoms in a molecule. Electrons are shown as "dots" or for bonding electrons as a line between the two atoms. The goal is to obtain the "best" electron configuration, *i.e.* the octet rule and formal charges need to be satisfied.

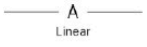


SP hybridization:

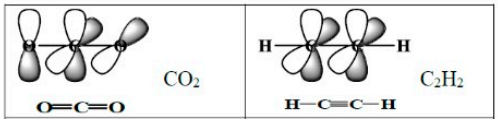
For molecules that have a **linear** (180 degree) geometry, the atoms use sp hybridization for bonding, and their orbital structures is as shown below:



Unhybridized SP hybrid orbitals Linear

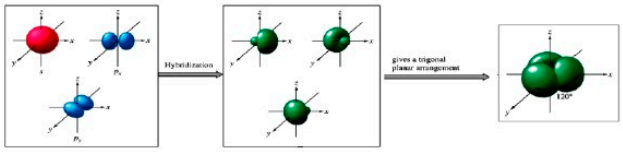


In this hybridization, one s atomic orbital of C combines with one p atomic orbital to create TWO equal energy sp hybrid orbitals lying along the x axis as shown above. Examples of such molecules are CO_2 and C_2H_2. In these carbon-containing sp-hybridized molecules, there are two unhybridized p atomic orbitals of the valence shell of C as shown drawn on the y and z axes, which are used to create the pi bonds in the structures of these molecules.

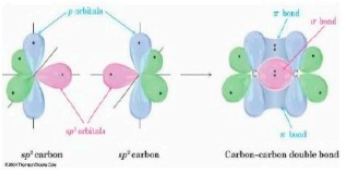


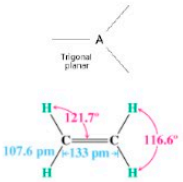
SP^2 hybridization:

For molecules that have a **trigonal planar** (120 degree) geometry, the atoms use sp^2 hybridization for bonding, and the orbital structure is as shown below:



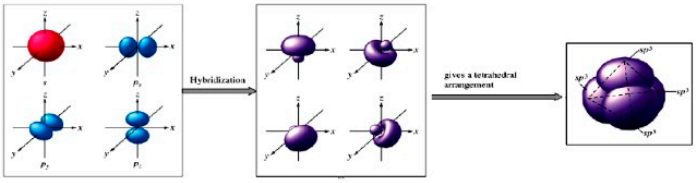
In this hybridization, one s atomic orbital of C combines with two p atomic orbitals of C to create THREE equal energy sp^2 hybrid orbitals lying flat on the plane of a paper as shown above. Example of such a molecule is ethylene (C2H4) shown below, where each C is sp^2 hybridized with one unhybridized p atomic orbital remaining on each C atom (shown in blue) that is used to create the pi bond in the structure:



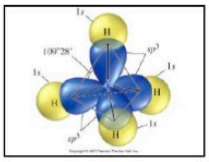


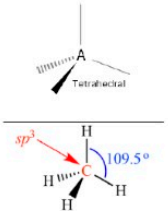
SP^3 hybridization:

For molecules that have a **tetrahedral** (109.5 degree) geometry, the atoms use sp^3 hybridization for bonding, and their orbital structure is as shown below:



In this hybridization, one s atomic orbital of C combines with all three p atomic orbitals of C to create FOUR equal energy sp^3 hybrid orbitals arranged in a tetrahedral shape, as shown above. Example of such a molecule is methane (CH4) shown below, where each C is sp^3 hybridized and there are no remaining unhybridized p orbitals. Thus, it does not contain any pi bonds unlike the sp2 and sp hybridization shown earlier.





Supplementary Materials S2. Study 2b

A) Post-experiment Questionnaire

1. Participant ID: [ ] * You have received this code from within the VR app.
2. Age:
3. Handedness:
    a. Left
    b. Right
4. Gender:
    a. Man
    b. Woman
    c. I prefer not to answer
    d. Something else. Specify if you prefer:
5. Which statement is true about your experience with Virtual Reality (VR):
    a. I am familiar with VR and have experienced it.
        i. Specify your experience type:
    b. I am familiar with VR but have never experienced it myself.
    c. I am not familiar with VR and have not experienced it.

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B) Knowledge test for all groups (A, B, C)

Question5
a) *Draw (or select) the **Orbital structure** of each compound $BeCl_2$ and annotate/show the correct angle.
b) Draw (or select) the **Lewis structure** of $BeCl_2$ Annotate/show the correct angle.

Question 6
a) Draw (or select) the **Orbital structure** of each compound BF_3, annotate/show the correct angle.
b) Draw (or select) the **Lewis structure** of BF_3, annotate/show the correct angle.

Question 7:
a) Draw (or select) the **Orbital structure** of each compound NH_4, annotate/show the correct angle.
b) Draw (or select) the **Lewis structure** of CH_4, annotate/show the correct angle.

Each question has 2 parts, a) for the orbital structure and b) for the Lewis structure

*Considering the limitation of the online-survey tool, students might not be able to "Draw" therefore we might ask the same questions using a multiple-choice question and provide them with **3 images to choose from**. If the experiment is done in person, students will be given a paper version of the knowledge test and will be asked to draw/ write the answers.

Question 8:
Rate the following question from 1 to 5 (1 strongly disagree 5 strongly agree)
This VR visualization helps to understand the SPS concept (angles) better compared to what I read in the textbook.

Question 9:
Which of the following statements is agreeable to you?
a) My test score would improve if I had a chance to complete the VR experiment before taking the knowledge test
b) Completing this VR experiment before the knowledge test would not help me to score better"

C) Usability Questions for VR groups B and C (both interaction types)

Question 1. On a scale of 1-5 (1 very negative and 5 very positive, rate your VR experiment related to each of the following criteria:

	1	2	3	4	5
Ease of use					
Memorability					
Learnability					
Pleasantness					
Clarity					
Visualization					
Overall satisfaction					

Question 2. Any other comments about your experiment in virtual reality?