**Hands-On H2O Molecular Orbital Construction: Applying Symmetry Principles**

**Objective:** To construct and interpret the Molecular Orbital (MO) diagram for the water molecule (H2O) using a whiteboard, markers, transparent orbital cutouts, and the C2v character table. You will demonstrate your understanding of MO theory, symmetry principles, and their application to predict molecular properties.

**Materials:**

* C2v​ character table
* Scissors
* Scotch tape
* Whiteboard
* Black, red, and blue whiteboard markers
* Transparent orbital printout sheets

**Instructions:**

**Part 1: Introduction to Molecular Orbitals**

* **Review Fundamental Concepts:** Begin by briefly discussing the core principles of molecular orbitals. Explain with your classmate how atomic orbitals combine to form molecular orbitals (MOs), distinguishing between bonding and antibonding interactions.

**Part 2: Symmetry Analysis for H2O**

* **Identify Atomic Orbital Symmetries:** Using the provided class PowerPoint slides as a reference, identify the symmetry designations (e.g., a1​, b1​, etc.) for the atomic orbitals (s, px​, py​, pz​) on both the oxygen atom and the hydrogen atoms using the C2v​ point group.
* **Determine Orbital Mixing:** Determine which oxygen and hydrogen atomic orbitals can combine into molecular orbitals based on their symmetry and energy. Remember, only orbitals with matching symmetry and similar energies can mix!

**Part 3: Deriving the H2O Molecular Orbital Diagram**

* **Prepare Orbital Cutouts:** Carefully cut out the atomic orbital shapes for oxygen and Ligand Group Orbital (LGO) sets representing the hydrogen atoms from the transparent sheets. On each cutout, write its correct symmetry label as determined in Part 2.
* **Construct Molecular Orbitals:** On the whiteboard, begin to combine the atomic orbital cutouts to visually represent the formation of molecular orbitals. Use tape to secure the cutouts together and to the whiteboard as you illustrate the orbital overlap.
* **Illustrate Bonding and Antibonding MOs:** Using the red and blue markers, draw the resulting bonding and antibonding molecular orbitals on the whiteboard. Use one color (e.g., blue) for bonding interactions and the other (e.g., red) for antibonding interactions. Ensure the nodal planes are clearly indicated for antibonding orbitals.
* **Label Molecular Orbitals:** Label each newly formed molecular orbital with its appropriate symmetry designation (e.g., 1a1​, 1b2​, etc.). Also, indicate whether it is bonding, non-bonding, or antibonding.
* **Fill MOs:** Based on the total number of valence electrons in H2O, fill the molecular orbitals according to the Aufbau principle, Hund’s rule, and the Pauli exclusion principle.

**Part 4: Analysis and Questions**

Once your whiteboard diagram is complete, take a photo of your work. This photo will be submitted along with your answers to the following questions.

* 1. Using your completed MO diagram, describe the nature of the bonding in the H2O molecule.
  2. If H2O were to lose an electron to form H2O+, what would be the new electron configuration? How would this affect its stability compared to H2O?
  3. How does the molecular orbital diagram you constructed explain why the H2O molecule has a bent shape rather than a linear one? Specifically, refer to the symmetry and occupancy of relevant molecular orbitals.
  4. Why would a linear H2O molecule be energetically unfavorable compared to the bent geometry? (Hint: Consider the overlap of atomic orbitals in a linear arrangement and how it would affect the energy of the MOs).
  5. Predict what might happen to the energy levels of the molecular orbitals as the H-O-H bond angle in H2O increases from its experimental value of approximately 104.5 degrees to 180 degrees (a linear geometry). Which orbitals would be most affected, and how?
  6. Would the molecular orbital diagram and the symmetry labels for the MOs be different if the H2O molecule were perfectly linear (180.0 degree bond angle)? Explain your reasoning, considering the point group symmetry change. What would the new point group be, and how would that impact the symmetry labels?
  7. Why is it crucial to consider the symmetry of atomic orbitals when constructing a molecular orbital diagram? What fundamental principle of quantum mechanics does this relate to?
  8. Could you form a molecular orbital from an oxygen 2px​ orbital and a hydrogen group orbital of a1​ symmetry? Explain why or why not.
  9. If you were to repeat this activity using SH2, which also has C2v symmetry, how would its MO diagram compare to the one you derived for H2O? Would the predicted bond angle in SH2 be closer to 105°, 90°, or 180°? Provide reasoning to support your answer.

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A diagram of a molecule

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