

3.091

Do yourself a solid.

3.091: Introduction to Solid State Chemistry
Fall 2018
Practice Problems D: Orbitals & molecules

The following problems sets are compiled from B. A. Averill and P. Eldredge, *General Chemistry: Principles, Patterns, and Applications*. License: CC BY-NC-SA. Source: [Open Textbook Library](#).

Reading: Averill 9.1-9.4

1. VSEPR

Averill Chapter 9, Section 1, Numerical Problem 1

Give the number of electron groups around the central atom and the molecular geometry for each molecule. Classify the electron groups in each species as bonding pairs or lone pairs.

- BF_3
- PCl_3
- XeF_2
- AlCl_4^-
- CH_2Cl_2

2. VSEPR

Averill Chapter 9, Section 1, Numerical Problem 2

Give the number of electron groups around the central atom and the molecular geometry for each molecule. Classify the electron groups in each species as bonding pairs or lone pairs.

- ICl_3
- CCl_3^+
- H_2Te
- XeF_4
- NH_4^+

3. VSEPR and 3D geometry

Averill Chapter 9, Section 1, Numerical Problem 5

What is the molecular geometry of ClF_3 ? Draw a three-dimensional representation of its structure and explain the effect of any lone pairs on the idealized geometry.

4. Identifying dipoles

Averill Chapter 9, Section 1, Numerical Problem 7

Predict whether each molecule has a net dipole moment. Justify your answers and indicate the direction of any bond dipoles.

- a) NO
- b) HF
- c) PCl_3
- d) CO_2
- e) SO_2
- f) SF_4

5. MO diagrams and bond order

Averill Chapter 9, Section 3, Numerical Problem 1

Use a qualitative molecular orbital energy-level diagram to describe the bonding in S_2^{2-} . What is the bond order? How many unpaired electrons does it have?

6. MO diagrams and bond order

Averill Chapter 9, Section 3, Numerical Problem 2

Use a qualitative molecular orbital energy-level diagram to describe the bonding in F_2^{2-} . What is the bond order? How many unpaired electrons does it have?

7. LCAO

Averill Chapter 9, Section 3, Numerical Problem 6

Sketch the *four* possible ways of combining two 2p orbitals on adjacent atoms. How many molecular orbitals can be found by this combination? Be sure to indicate any nodal planes.

8. MO diagrams and stability

Averill Chapter 9, Section 3, Numerical Problem 11

Draw a molecular orbital energy-level diagram for Na_2^+ . What is the bond order in this ion? Is this ion likely to be a stable species? If not, would you recommend an oxidation or a reduction to improve stability? Explain your answer. Based on your answers, will Na_2^+ , Na_2 , or Na_2^- be the most stable? Why?

9. MO diagrams, bond order, and stability

Averill Chapter 9, Section 3, Numerical Problem 13

Draw a molecular orbital energy-level diagram for O_2^{2-} and predict its valence electron configuration, bond order, and stability.

10. MO diagrams, bond order, and stability

Averill Chapter 9, Section 3, Numerical Problem 14

Draw a molecular orbital energy-level diagram for C_2^{2-} and predict its valence electron configuration, bond order, and stability.

11. MO diagrams and bond order

Averill Chapter 9, Section 3, Numerical Problem 17

Sketch a molecular orbital energy-level diagram for each ion. Based on your diagram, what is the bond order of each species?

- NO^+
- NO^-

12. Applying MO diagrams

Averill Chapter 9, Section 3, Numerical Problem 18

The diatomic molecule BN has never been detected. Assume that its molecular orbital diagram would be similar to that shown for CN^- in section 3 but that the σ_{2p_z} molecular orbital is higher in energy than the π_{2p_z} molecular orbitals.

- Sketch a molecular orbital diagram for BN.
- Based on your diagram, what would be the bond order of this molecule?
- Would you expect BN to be stable? Why or why not?

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