

Organic Electronic Materials

Exercise 1

1. Explain three potential advantages of organic electronic devices over conventional ones!
2. What is the difference between a metal, a semiconductor, and an insulator? Briefly explain the differences in their electronic structure! Clarify the distinction between conductivity and mobility!
3. Give the Schrödinger equation in its most general form, briefly name/define all parameters/variables that appear in it, and paraphrase the meaning of the Schrödinger equation! Why is it actually a differential equation?
4. What is an atomic orbital? What is the valence shell? Why are noble gases particularly stable?
5. Explain the concept of “hybridization” of atomic orbitals means and what it is useful for. Detail the case of carbon atoms in different states of hybridization, including AO energy level diagrams and pictorial representations of the derived hybrid AO!
6. The hybridization concept and the construction of molecular orbitals both use linear combination of atomic orbitals. Give a simple answer what is the difference between the two?
7. What approximations are at the basis of the construction of molecular from atomic orbitals and why are they needed ? Briefly explain!
8. Draw a schematic MO energy level diagram as well as pictorial representations of the resulting MO for the interaction of two helium atoms! Name the AO and MO and add the electrons! Explain the terms “bonding” and “antibonding” MO. Explain why He₂ is not stable, and give a quantitative expression for the destabilization energy of He₂ compared to two He atoms!

Reading suggestions:

Organic Chemistry, Clayden, Greeves & Warren 2012 – Chapter 4 – Structure of molecules (or the corresponding chapter in any other organic chemistry book)

Physical Chemistry, Atkins & de Paula -Chapter 8– Quantum Theory: Introduction & Principles

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Exercise 2

1. Draw the MO energy level diagram of the C=C double bond in ethene. Start by briefly explaining which atomic orbitals or hybridized orbitals are involved in the double bond and why the chosen hybridization is required. Briefly explain the difference between σ -bonds and π -bonds, and draw graphical representation of the molecular orbitals.
2. Give the exact formula for the energy values of linear π -conjugated systems according to the Hückel theory! Draw the MO energy diagram of the π -system of 1,3,5-hexatriene as an example! Give the exact energy values of the different MO levels! Include simplified graphical representations of all MO (hint: consider the node planes)!
3. Draw a single MO energy level diagram (just the MO, not the constituting AO) comprising the π -systems of ethene, hexatriene, and the “realistic” limiting case of poly(acetylene). Why does poly(acetylene) not strictly follow the Hückel theory?
4. Give the Hückel matrices for a linear and a cyclic π -system with four carbon atoms. Why are they different? Draw the MO energy level diagram of the cyclic system! Why is it not considered an “aromatic” system?

Reading suggestions:

Clayden, Greeves & Warren, *Organic Chemistry*, **2012**; “Chapter 7 – Delocalization and Conjugation”.

Nordholm et al., “The Mechanism of Covalent Bonding”, *J. Chem. Ed.* **2007**, *84*, 1201.

Fox et al., “Electronic Structure in π -Systems”, *J. Chem. Ed.* **1985**, *62*, 367 (just the first two pages).