School of Engineering
Institute of Materials
Laboratory of Macromolecular
and Organic Materials

Organic Electronic Materials

Mock Examination

2025

____
Name

School of Engineering
Institute of Materials
Laboratory of Macromolecular
and Organic Materials

EPFL STI IMX LMOM
Prof. Holger Frauenrath
MXG 037, Station 12
CH-1015 Lausanne

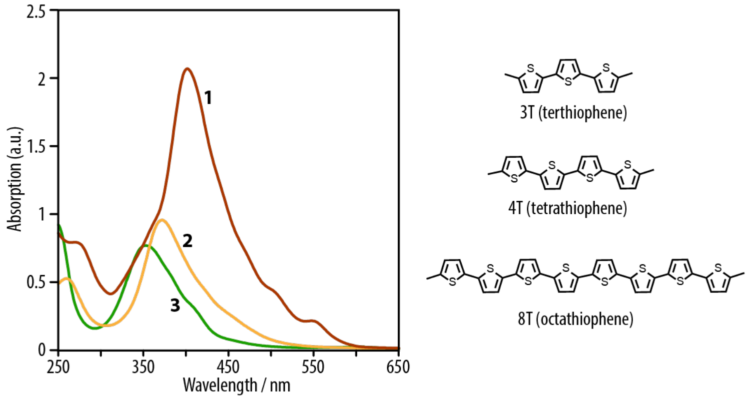
+4121 693 73 99
holger.frauenrath@epfl.ch
lmom.epfl.ch

Part 1 (X points)

1. Define and compare a semiconductor, a conductor and an insulator.
2. What types of organic molecules can exhibit semiconducting properties, and why?
3. Define the notion of the density of occupied states and explain how it can be determined.
4. In which hybridization state are the carbons involved in the naphtalene molecule? Draw the associated energy diagram as well as sketch of the shapes and orientations of the corresponding atomic/hybrid orbitals.
5. Is the naphtalene molecule stable? Why?
6. Let's consider you want to estimate the π-energy levels and the associated π-orbitals of naphtalene:
    a. Give a synonyme for the term "orbital" from a mathematical description point of view.
    b. What general equation should you try solve to get the energy levels and the associated orbitals? Use the braket notation. Name and give the physical meaning of this equation and the elements that appear in it. Which are the approximations you should you make to simplify the problem? Name the theory from which these assumptions come.
7. Define the notion of the density of occupied states and explain how it can be determined.
8. Why do most organic semiconductors have better conductivity than diamond at room temperature?
9. Distinguish the different possible transport mechanisms governing charge transport in organic materials and name the main physical effect by which each regime is dominated. For each case, indicate if majority of the charge carriers are localized or delocalized.
10. Qualitatively compare the MO energy level diagrams of ethylene, butadiene and octatetraene. Explain the evolution of the LUMO levels and optical gaps of these molecules.
11. Describe how charge transport occurs in the "multiple trap and release" model. Explain the two competing (in fact, opposing) effects of the temperature on the charge carrier mobility according to this model.

EPFL STI IMX LMOM
Prof. Holger Frauenrath
MXG 037, Station 12
CH-1015 Lausanne
+4121 693 73 99
holger.frauenrath@epfl.ch
lmom.epfl.ch

12. In the following graph the absorption spectra of three different oligothiophene derivatives (in dilute solution) are plotted. Which spectrum corresponds to which molecule? Explain the shift of the peak maxima of the absorption curves of the three molecules.



13. Explain on the example of two benzene molecules why face-to-face π-π stacking is never observed for regular aromatic molecules. What would happen if one of the two benzene molecules was perfluorinated?

Part 2 (X points)

14. We dissolve the following reactants in dry DMF under inert gas, and heat the flask to 80°C overnight (Figure 1).

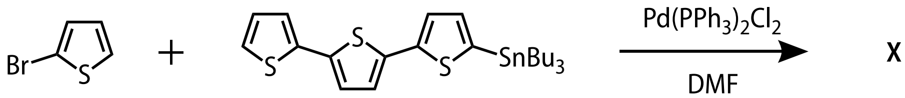


Figure 1 : Palladium-catalyzed reaction scheme

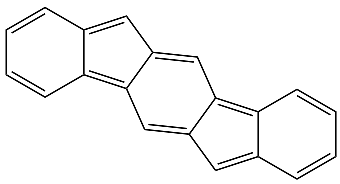
   a. What product do we obtain? What is the name of the reaction?

   b. Draw the detailed mechanism and name all individual steps.

   c. Why is the reaction above often replaced with other palladium-based reactions?

   d. What kind of molecular packing would be expected for the obtained product **X**? Explain briefly why.

15. What is the shape type of this molecule? How do you expect this molecule to pack?



16. Briefly define Keesom, Debye and London forces.

17. The absorption maximum of an asymmetrically substituted X in a thin-film is blue-shifted in comparison to its absorption spectrum in dilute solution (Figure 2). What is the reason for this blue-shift? Explain this effect with the help of an energy diagram.

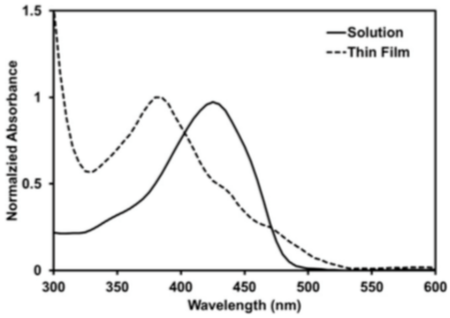
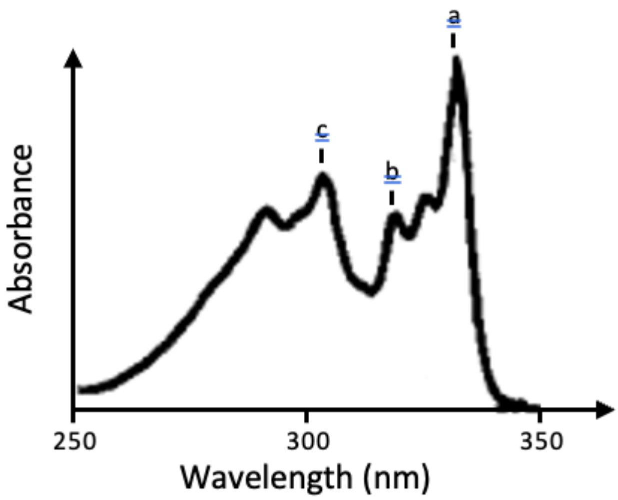
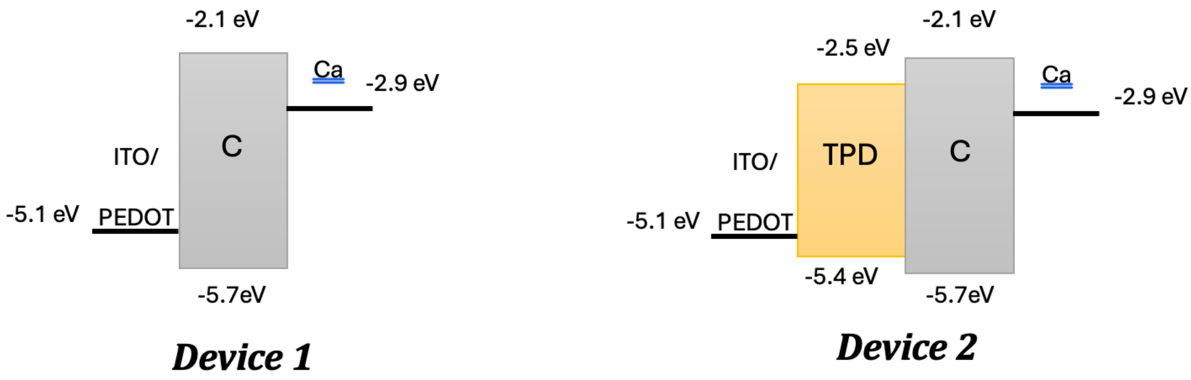


Figure 2 : Absorption spectrum of an asymmetrically substituted X in a thin-film (dashed) and in solution (plain)

18. The absorption spectrum of a molecule is presented on the graph below. To which transitions do "a", "b" and "c" correspond to?



19. Device number 2 presented below was created to improve the performance of device number 1. However, the second device led to poorer results. Explain what was the idea behind the addition of the TPD layer and why it actually reduces the efficiency?



20. Oligothiophene derivatives can be used as an active semiconducting layer in thin film transistors. On Figure 3, two different characteristics (curves) are shown. Name these characteristics (curves) and describe briefly how you obtain them. What kind of important parameters can you extract from the first characteristic? Name them, briefly explain their meaning and how you can determine them.

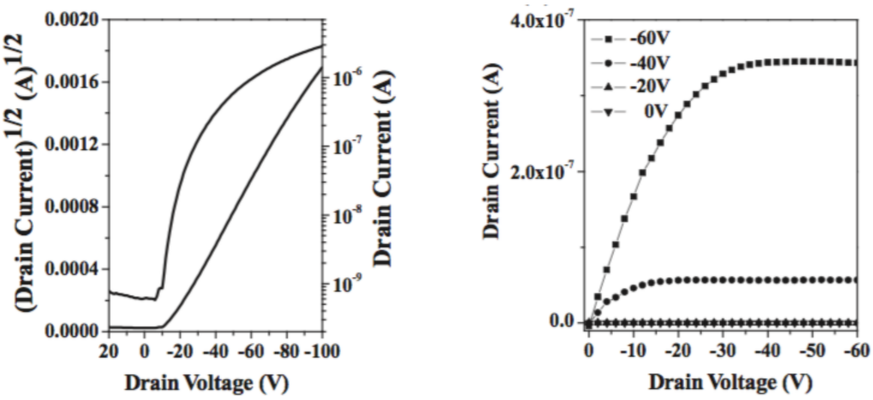


Figure 3 : Characteristics of an oligothiophene-based thin-film transistor.

21. Poly(phenylene) can be doped with either an oxidant or a reductant to improve its semiconducting properties. Give an example of a reductant used in this case and formulate the molecular structure as well as the energy diagram of the resulting doped state.

EPFL STI IMX LMOM
Prof. Holger Frauenrath
MXG 037, Station 12
CH-1015 Lausanne
+4121 693 73 99
holger.frauenrath@epfl.ch
lmom.epfl.ch