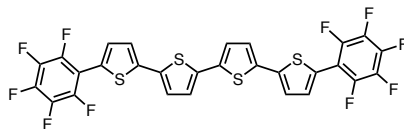


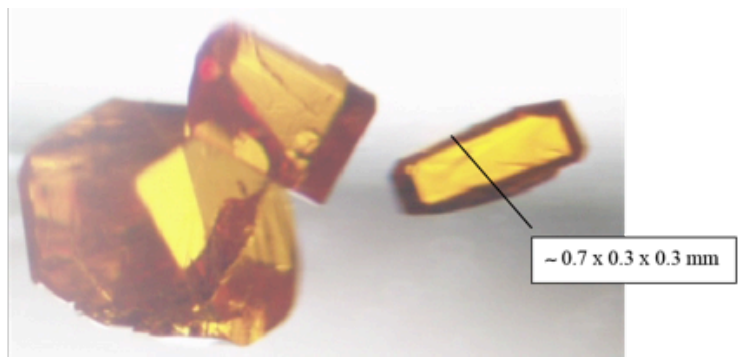
Organic Electronic Materials

Exercise 3

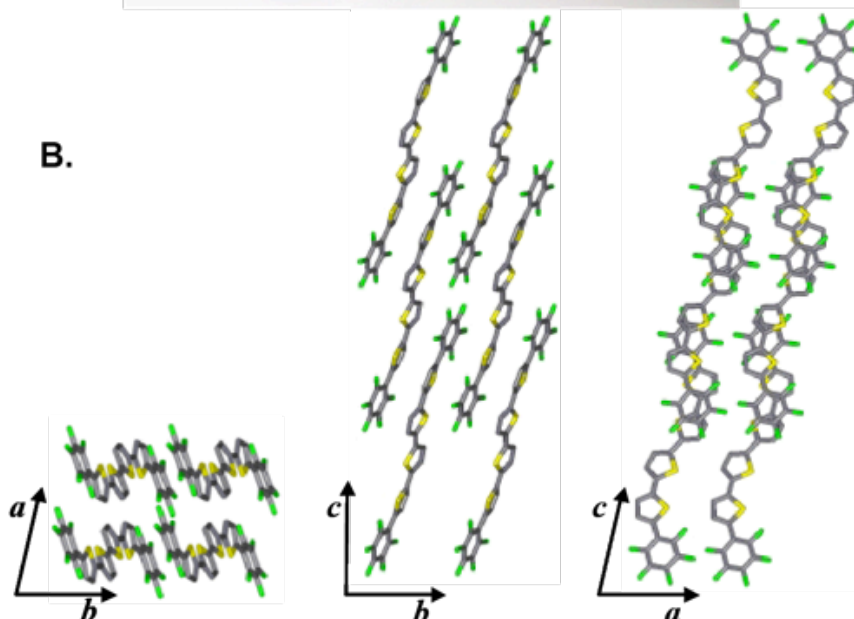
1. In an aromatic system such as benzene, the replacement of a hydrogen with a different atom or functionality affects the electron density of whole the π -system. In this context, explain what is the difference between mesomeric (M) and inductive (I) effects, and give on example for each.
2. Explain on the example of two naphthalene molecules why face-to-face π - π stacking is never observed for regular aromatic molecules! What would happen if one of the two naphthalene molecules were perfluorinated.
3. The crystal structure of the perfluorophenyl-substituted quaterthiophene is shown below. Describe typical features that you recognize in the molecular packing and speculate why a herringbone arrangement may be disfavorable!



A.



B.



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Exercise 4

1. The molecular orbital contribution to π - π stacking interactions is not energetically favorable; explain why π - π stacking is still observed. Explain why the HOMO-LUMO gap of closely packed aromatic molecules is narrower than that of the individual molecule.
2. Formation of a C-C bond between two aromatic rings commonly requires the help of a catalyst. Generally speaking, what is the function of a catalyst in a reaction?
3. Formulate the general reaction mechanism (catalytic cycle) of palladium-catalyzed carbon coupling reactions and name the important steps! Nickel, palladium, and platinum belong to the same element group; why is palladium a better catalyst than nickel and platinum for this type of reaction? Give the electron configurations of nickel, palladium, and platinum, and explain why are they called “transition metals”.
4. The use of sterically demanding ligands is found to be beneficial for the palladium-catalyzed cross-coupling. Try to give a brief explanation for this observation. By contrary, what disadvantage do you expect in the case of *very* bulky ligands?

Reading suggestions:

Organic Chemistry, Clayden, Greeves & Warren 2012 – Chapter 48 – Organometallic Chemistry