

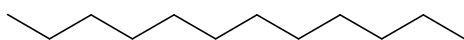
# Molecular Photonics

## Exercise 2

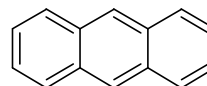
Give answers to six out of the seven questions below:

- What is the general trend that connects the size of a molecule, its polarizability and its ability to absorb light?

- Dodecane (**A**) is much longer than anthracene (**B**). Which one has a higher extinction coefficient ( $\epsilon_{\max}$ )? Explain.



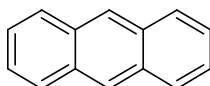
**A**



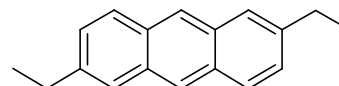
**B**

- What is Kasha's Rule and what is its cause? Please explain, and give a sketch.

- Which one of the following molecules has a lower fluorescence quantum yield? Explain.

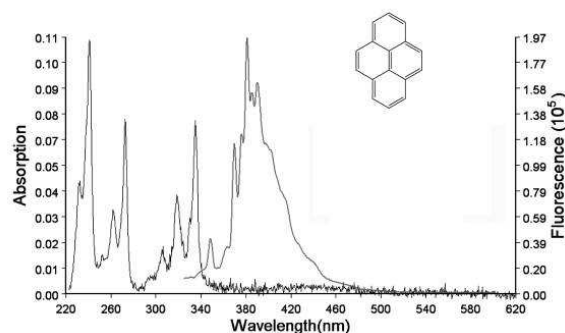


**C**

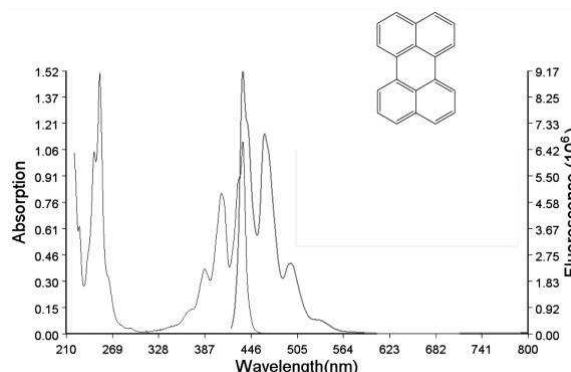


**D**

- The spectra below describe the UV-vis absorbance and the fluorescence of pyrene (**E**) and perylene (**F**).

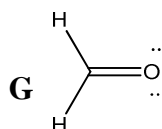


**E**

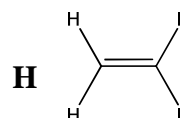


**F**

- Name the main transitions observed in the spectra.
  - What is Stokes shift and what can we learn from the Stokes shifts in the spectra of **E** and **F**.
  - What additional characteristic in the fluorescence spectra may help us strengthen the conclusion we come to after answering question b?
- Draw a scheme that describes the transitions of the valence electrons in formaldehyde (**G**) and ethylene (**H**). Why in the case of **G** intersystem crossing is efficient and in the case of **H** it is not?

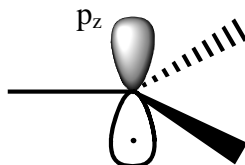


**G**



**H**

5. Momentum changes in an isolated system are not allowed. Explain how a change may become possible for the orbital momentum of the electron in the  $p_z$  orbital of  $\text{CH}_3^\bullet$  without any external interference.



6. Explain shortly using simplified diagrams the principle of spin-orbit coupling. How this coupling is connected to “heavy atom” effect?
7. Triplets are lower in energy than singlets in the excited state. Why? (see uploaded file - HundsRule.PDF) What did Mulliken say regarding calculations and concepts?