Spectrum of Zn Porphyrin Pair Under Translation and Rotation

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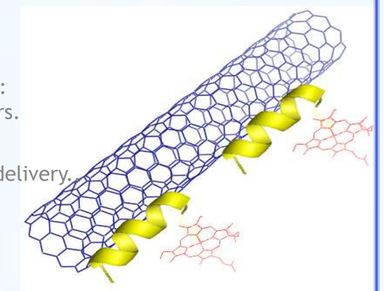
Abstract

- The spectrum for a pair of Zn-substituted Porphyrins (ZnP's) were calculated using a semi-empirical model.
- Spectrum was analyzed for various translations and rotations.

Motivation

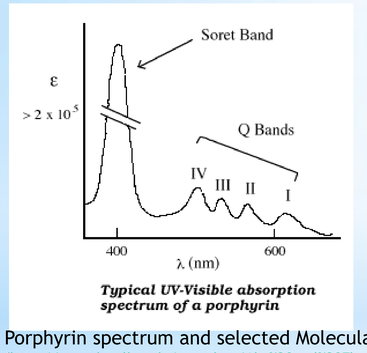
- Porphyrins
  - Central role in photosynthesis, oxidation and reduction, and oxygen transport (such as hemoglobin).
  - Excellent light absorbers. Can be used to harvest solar energy.
- Artificial Photosynthetic Nano-device
  - Zn-substituted Porphyrin (ZnP), embedded in polypeptide proteins : Harvest light, act as electron donors.
  - Carbon nanotubes (CNT's): Method for charge separation and delivery.
  - ZnP + CNT system: A module for larger scheme to generate electron separation for an H_2 producing device.

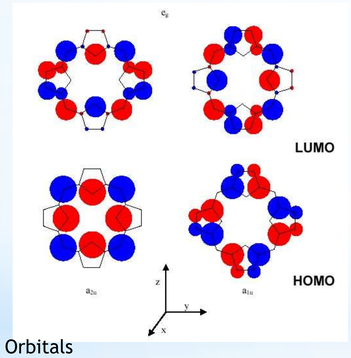


- Orientation-dependent ZnP Spectrum important.

Background

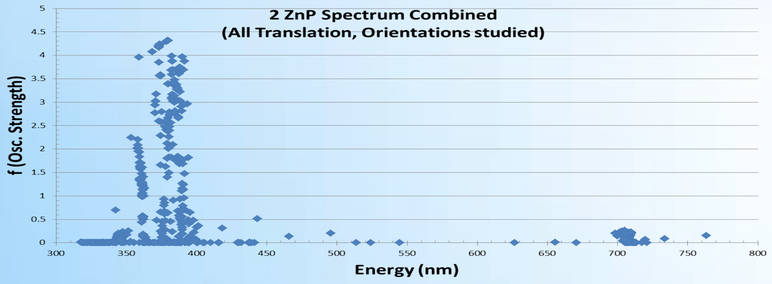
- Porphyrin- Gouterman 4-Orbital Model



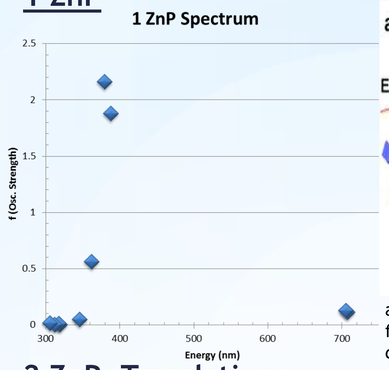


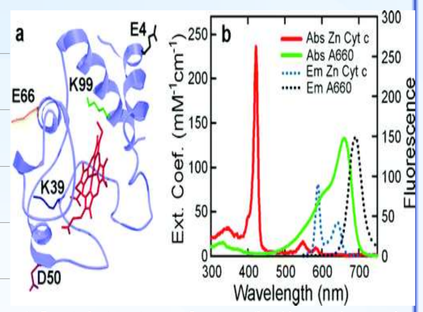
Porphyrin spectrum and selected Molecular Orbitals
(http://www.lasalle.edu/~prushan/Abs%20and%20Fluor%20of%20TPPH2.pdf)

- Semi-empirical Calculations
  - Software: Gaussian; Algorithm: "Zindo(Nstates=<x>,Singlets)".
  - Results: Excited states oscillator strength "f". (f<0.01 usually means dipole selection rule forbidden)
  - Oscillator Strength directly proportional to |Transition Dipole Moment|^2 . Hence, spectrum can be obtained.



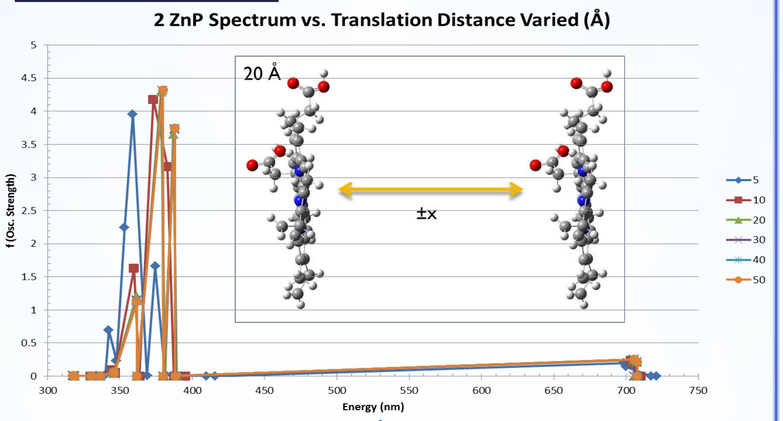
1 ZnP





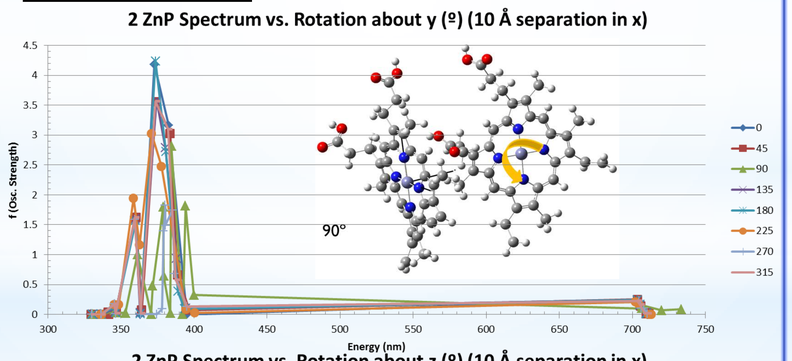
a) Crystal structure of cyt c. (b) Absorption and fluorescence spectra of Zn cyt c and free A660 dye. (Lee, et al. *J. of ACS* **132**, 1752 (2010).)

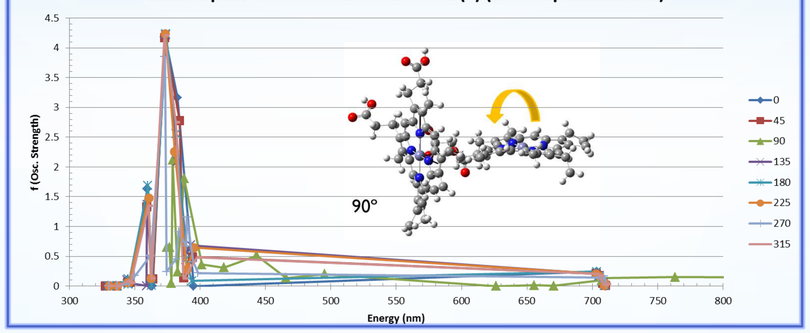
2 ZnP- Translations



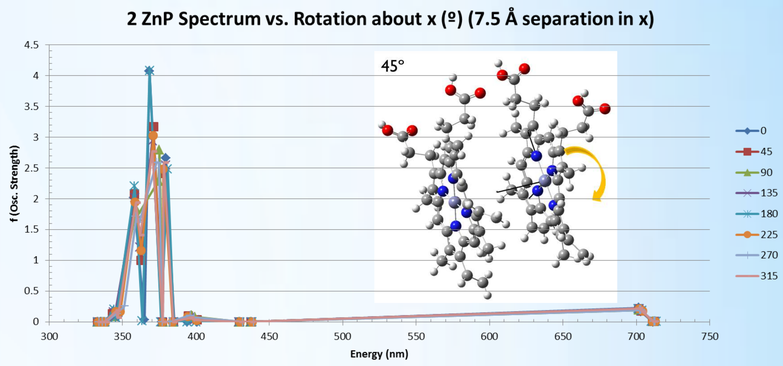
Noticeable spectrum changes for < 20 Å separation.

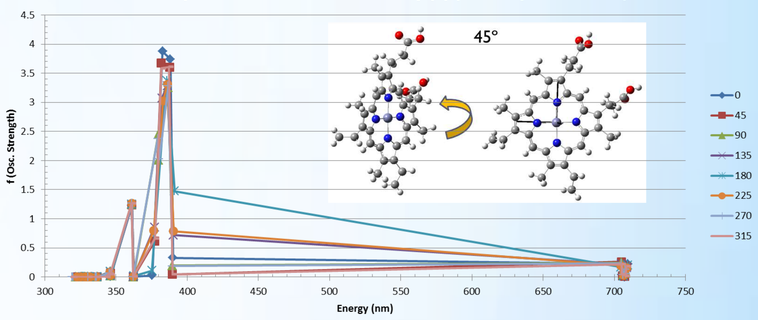
2 ZnP- Rotations

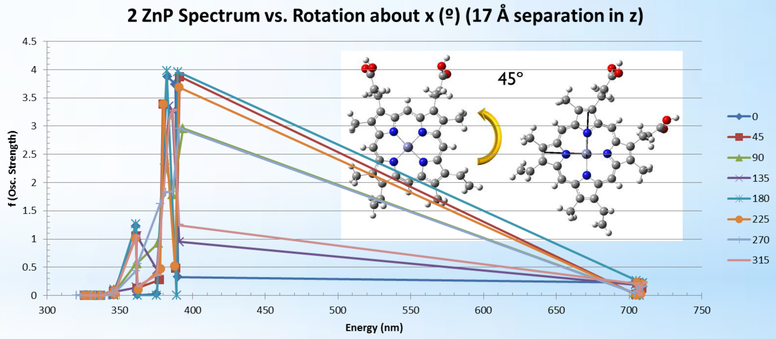


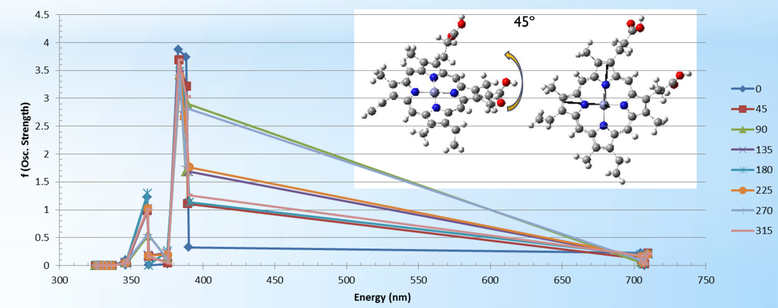


2 ZnP- Rotations









Acknowledgement

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