Simulating the spectra of phenolphthalein as a first step to predict the color of dye molecules

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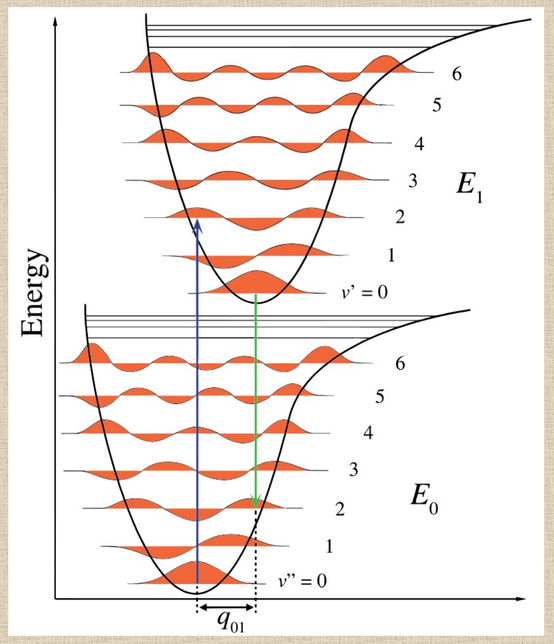
Introduction

Dyes provide color to many common items such as food, clothing, drinks, medicines, etc. More recently, researchers have replicated the process of photosynthesis for energy generation using dye sensitized solar cells which absorb specific wavelengths.

Dye molecules have complex structures which the arrangement of bonds contribute to the absorption of light and production of light that can be observed.

Franck Condon Principle

The Franck Condon Principle describes the absorption or emission of a photon. When an electron jumps from the ground state to an excited state, it will jump to a state where it has a high probability of being found. This "jump" is absorption; in terms of colors, the absorbed color is what we do not see, and we will see the complementary color.



https://chem.libretexts.org/Courses/Pacific_Union_College/Quantum_Chemistry/13%3A_Molecular_Spectroscopy/13.07%3A_The_Franck-Condon_Principle

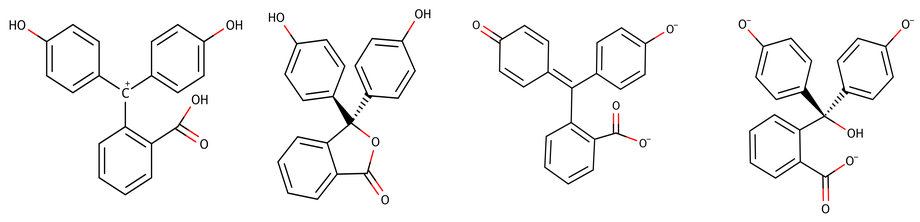
Methodology

Objective:

There are many software tools available today to explore molecular properties. Some require stronger computers or more resources not always available to the layperson. The goal is to find a method that is quick and inexpensive without sacrificing accuracy and precision.

Procedure

1) Phenolphthalein was selected due to prior extensive research on the molecule.
2) A series of calculations was run, and configurations were calculated for each structure.
3) Configurations were analyzed for the lowest energies, and repeat configurations were removed.
4) The configurations with the lowest energies had their UV-spectra calculated.



H3LN	H2LN	LN2	LNOH3
pH < 1	0-8.3	8.3-10.0	pH > 10
Red-orange	Colorless	Pink	Colorless

Results

Known Peak Values (nm)		Calculated Values	
Structure:		Gas	Water
H3LN	388	404	419
H2LN	275	253	249
LN2	555	448	472
LNOH3	298	410	410

The values of the calculated λ_{max} of each phenolphthalein structure in the gas solvent and water solvent were compared to known literature values. Different solvents were explored since they can affect the lambda max of a molecule.

Discussion

The calculation method selected for this study was more accurate to literature values for the H2LN structure compared to the other structures. There were also some problems in running some calculations since they would stall and not complete. It was not completely known as to what exactly caused the computation to stall but it was probably due to the complexity of the molecule and the lack of stronger resources in running these calculations.

Further research into other software tools will be required to study these dye molecules. One software tool being researched is QCHEM. This tool is much more user friendly and more accessible to all. The only issue is that there has not been much work done with this software, therefore, there could still be many issues that have been unaddressed.

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