# Investigation of Para-Aminobenzoic Acid's Photodegradation in Different pH Environments under UVB Light

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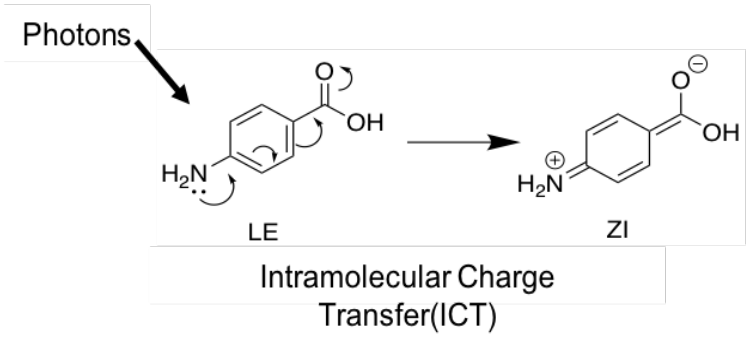
## Introduction

The wide use of UV-filters has been related to many recent environmental issues, including coral bleaching and inhibition of aquatic organisms' light-dependent metabolic functions. Para-aminobenzoic acid (PABA) and its derivates are common sunscreen active ingredient that have been widely studied. Past studies have shown that polarity and pH of the solution environment are able to affect PABA's intramolecular charge transfer process. Thus, PABA's kinetic behavior under UVB irradiation at different pHs were studied in this research. By applying mathematical modeling to the reaction, experimental absorbance spectrum were deconvoluted to trace changes in the solution composition throughout irradiation, and different reaction pathways were assessed to fit the data. At the end of the research, degradation pathways were obtained for PABA's degradations at pH 2, 7 and 10.

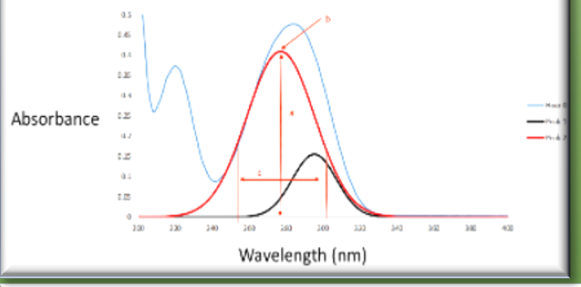



PABA may undergo an ICT depending following photoexcitation leading to a zwitterionic product.

## Methods

- Absorbance spectrum were fit to Gaussian peak(s) to represent each species
- Changes in the peak area represent changes in concentration and are modeled based upon kinetics
- MATLAB was used to assess the mechanism that best fits the data and determine rate constants

### Absorbance Spectrum Fitting

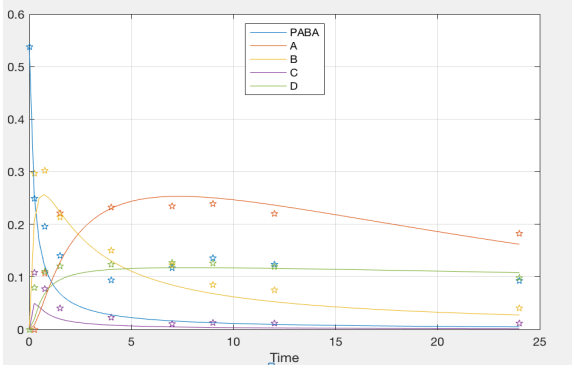



### Sample Rate Law

$$A \xrightarrow{K} B$$

$$\frac{d[A]}{dt} = -K[A]$$

### Data Fitting in MATLAB




Absorbance over time for PABA and degradation products (A-D), showing the fit (line) and experimental data points.

## Results

- Best fit mechanisms at pH 2, 7, 10

| pH | Optimal Mechanism |
|---|---|
| 2 | PABA $\xrightarrow{0.07443\ hr^{-1}}$ A $\xrightarrow{0.15674\ hr^{-1}}$ ?; PABA $\xrightarrow{0.03154\ hr^{-1}}$ B $\xrightarrow{2813.64436\ hr^{-1}}$ ? |
| 7 | 2PABA $\xrightarrow{6.44966\ M^{-1}hr^{-1}}$ B+B $\xrightarrow{1.65361\ M^{-1}hr^{-1}}$ A $\xrightarrow{0.04323\ hr^{-1}}$ ?; 2PABA $\xrightarrow{2.08754\ M^{-1}hr^{-1}}$ C+C $\xrightarrow{52.90249\ M^{-1}hr^{-1}}$ D+D $\xrightarrow{0.07041\ M^{-1}hr^{-1}}$ ? |
| 10 | 2PABA $\xrightarrow{1.81426\ M^{-1}hr^{-1}}$ A+B+C $\xrightarrow{5.14057\ M^{-5}hr^{-1}}$ ? |

- 1st order at pH2 and 2nd order at pH7 and 10
- PABA's degradation is slower or less favorable at lower pH, when it cannot undergo ICT
- It is hypothesized that the ability to undergo ICT and form the unstable ZI state of PABA leads to faster degradation at higher pH

## Future Work

- Use HPLC to experimentally trace the individual species
- Apply weightings to fitting to better fit all traces
- Characterize photoproducts of the degradation

## Acknowledgement

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