

# A Spectroscopic Approach to Photo Oxidized Degradation Process of PTB7 Polymer

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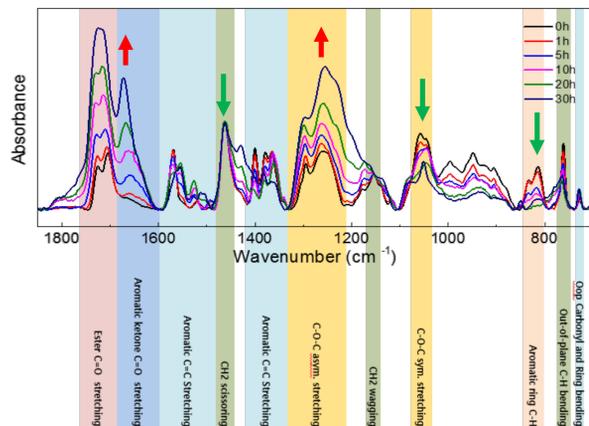
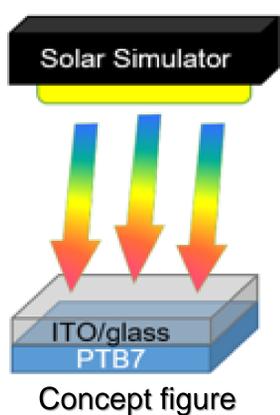
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## Abstract

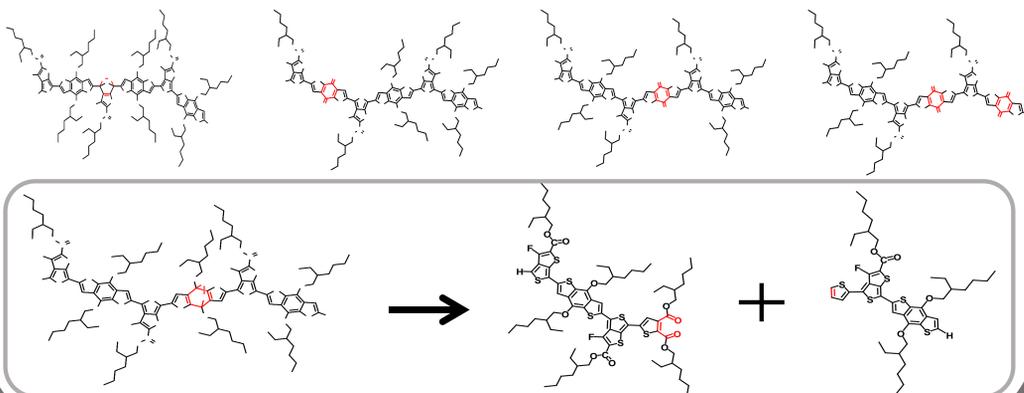
As power conversion efficiencies (PCE) of organic photovoltaics (OPVs) edge over 10%, lifetimes of devices are crucial for commercialization. In order to increase the durability, we need to prevent degradation of the polymer. Unfortunately, the degradation mechanism of photovoltaic materials has rarely been investigated. In this work, we investigate PTB7 polymer, which is widely used in OPVs, by FT-IR spectroscopy and DFT calculations. First, we record IR spectra of PTB7 while increasing the illumination time of solar simulator. We use DFT calculation to get vibrational frequencies of the proposed intermediates. To track photochemical degradation mechanism, we compare the experimental and the computational IR frequency values. We find the candidates experimental IR spectra that well matched with DFT calculations. Our findings provide clues as to where the molecule breaks apart and ways to make stable OPVs by modifying the molecule.

## Experiment



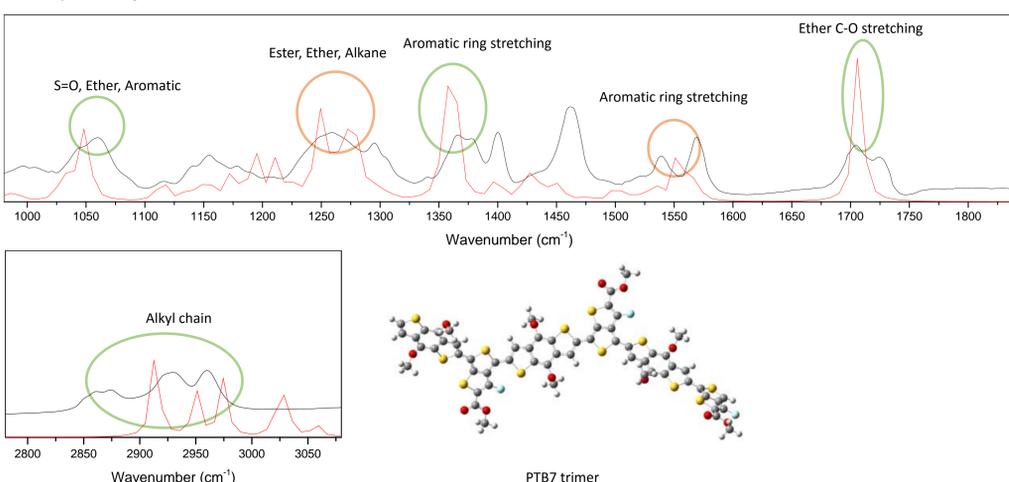
This data represents the change of FT-IR spectrum of PTB7 polymer with the exposure time. And arrows show the changes in peak intensities. 1 sun of sunlight is illuminated to the sample by Solar Simulator. Color shading indicate the motion of vibrational mode on that frequency

## Proposed Intermediate

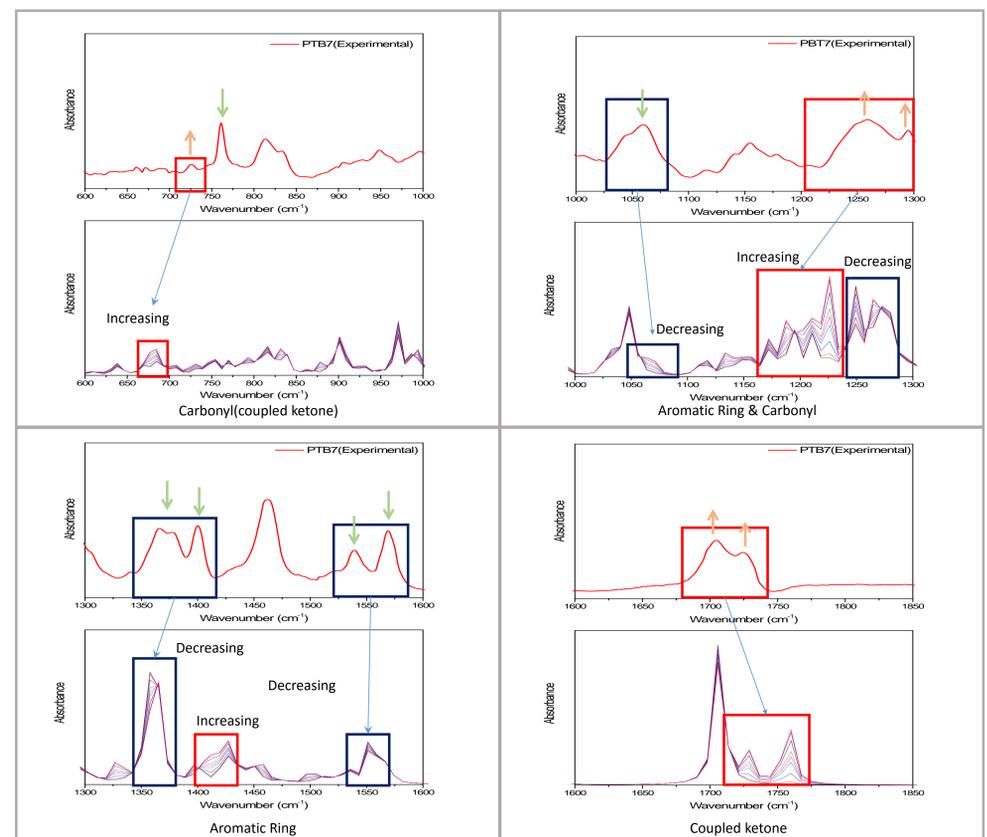


## Computational Method

In this research, Density Function Theory calculation provided by Gaussian 09 package was used and the molecules were described in 6-311G(d,p) basis set. To show how this calculation method matched well with experimental data, we compared FT-IR data of PTB7 and calculated frequency of the trimer.



## Result



Above spectra show the comparison between experimental data of PTB7 and calculated IR spectra of the oxidized intermediate. Red line corresponds to that IR spectrum of undamaged PTB7 polymer. Red and green arrows indicate increase and decrease in peak intensities respectively with change in exposure time. Below the red line there is calculated IR spectrum of the oxidized intermediate. To show the peak intensity increase or decrease, compare to reference, undamaged PTB7 trimer calculation data are shown. The functional group, confirmed by calculation, are indicated below each figure. Characteristically one can see the decomposition of aromatic ring and formation of coupled ketone peak caused by sunlight exposure.

## Conclusion & Future works

Here, we show that one of the proposed intermediates matches well with our prediction. Breakage of aromatic ring and formation of ketone cause significant changes to IR spectra as anticipated. A direct evidence of degradation is the decline of sunlight absorbance. Therefore comparing these results with time dependent UV-Vis spectra will be useful. Unfortunately, the change of IR spectrum is too large to sense the subtle change of UV-Vis spectra. To overcome this obstacle, we plan to record Raman spectra which will allow discovery of new vibrational modes which can not be seen in IR spectrum.

## Acknowledgment

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