Spectroscopic Analysis of Photo-Degradation Process of PTB7-Th

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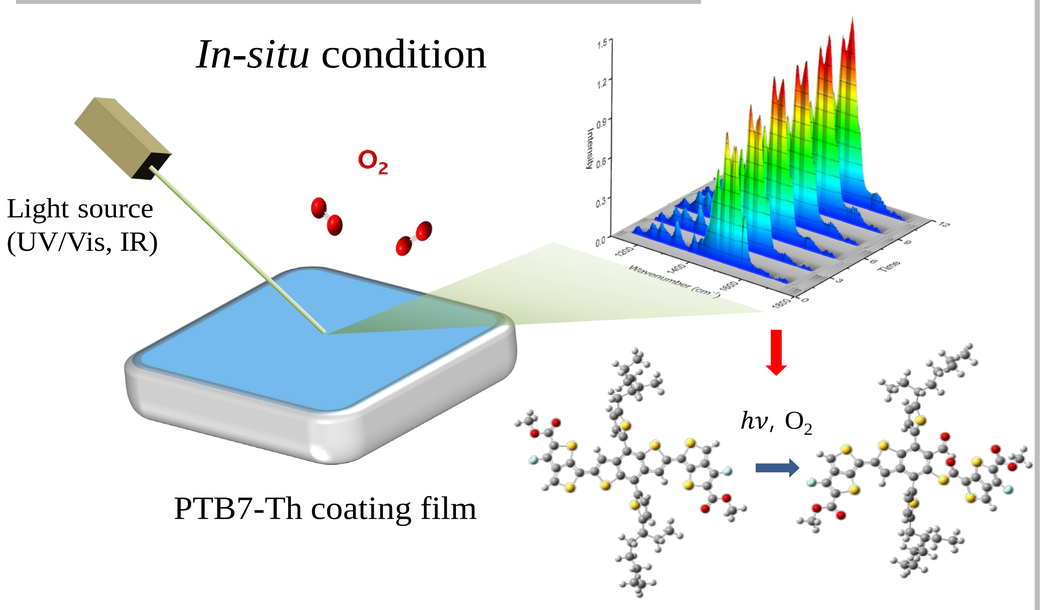
Abstract

There has been intensive interest in Organic photovoltaic (OPV) due to various advantages such as processability, flexibility, and low price compared with silicon based solar cell. In spite of these merits, due to its organic origin, there is an obstacle that OPV should overcome: Stability. There are various factors that affect the stability of OPV: Heat, air, light, etc. To reach commercialization level, it is crucial to understand the degradation phenomena at molecular level. There have been consistent efforts to elucidate the photo-oxidation of PTB7 which is one of the representative OPV components via Resonance Raman spectroscopy, and IR spectroscopy respectively. In this poster, the photo-oxidation of PTB7-Th whose structure is similar to that of PTB7 will be discussed via UV/Vis, IR, and Raman spectroscopies. Combined with calculation, photo-oxidation mechanism is suggested to explain the spectroscopic phenomena. We hope this research would be the clues to enhance the stability of OPV in future.

Introduction

In-situ condition

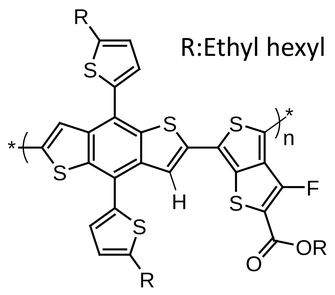


PTB7-Th coating film

Based on the spectroscopic data, mechanism could be proposed

Target

PTB7-Th



BDT (Donor, D) TT (Acceptor, A)

- Motivation

1. One of the representative polymer in OPV
2. To reduce the degradation initiating at side alkyl chain in PTB7

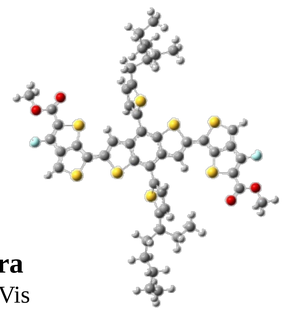
Calculation & Set up

- Calculation

Structure
A-D-A oligomer

Basis set
B3lyp/6-31g (d, p)

Calculated spectra
Raman, IR, and UV/Vis



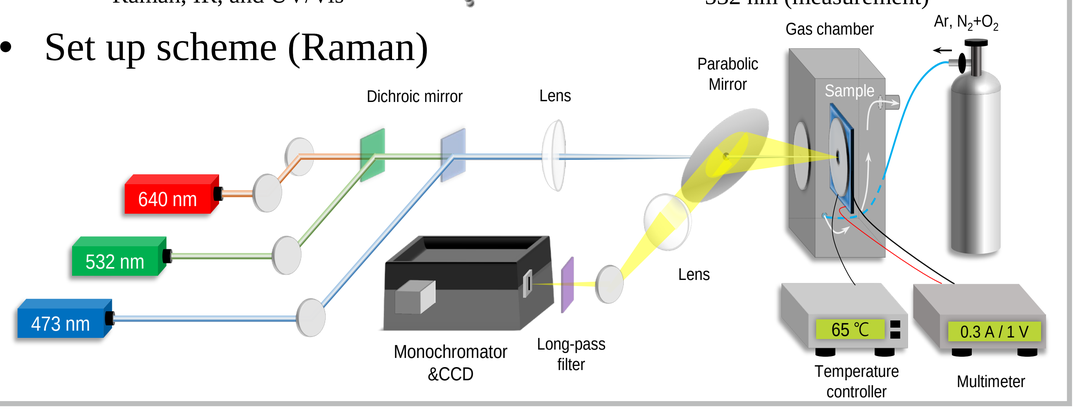
- Experiment condition

Substrate
CaF_2 (IR), Glass (Others)

Atmosphere
Ambient air, Ar gas

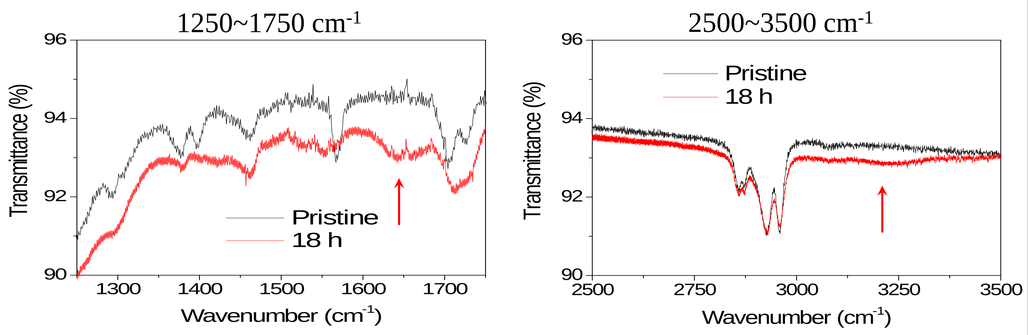
Light source (Raman)
640 nm (Degradation),
532 nm (measurement)

- Set up scheme (Raman)



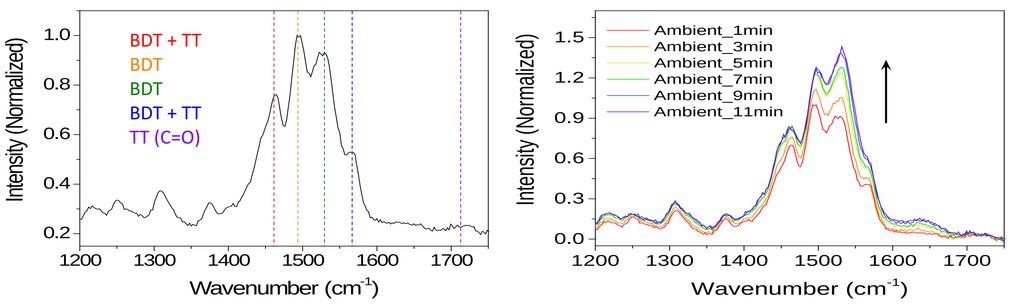
Results

- IR spectra



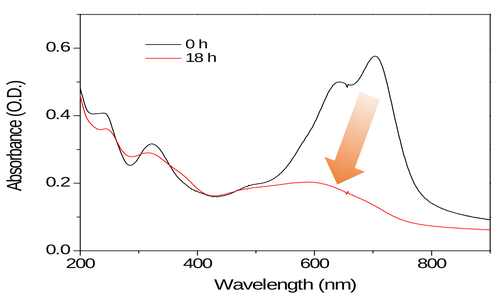
► Carbonyl and hydroxyl groups are generated

- Raman spectra



► BDT unit is affected during degradation

- UV/Vis spectra



► Conjugation bond is broken.

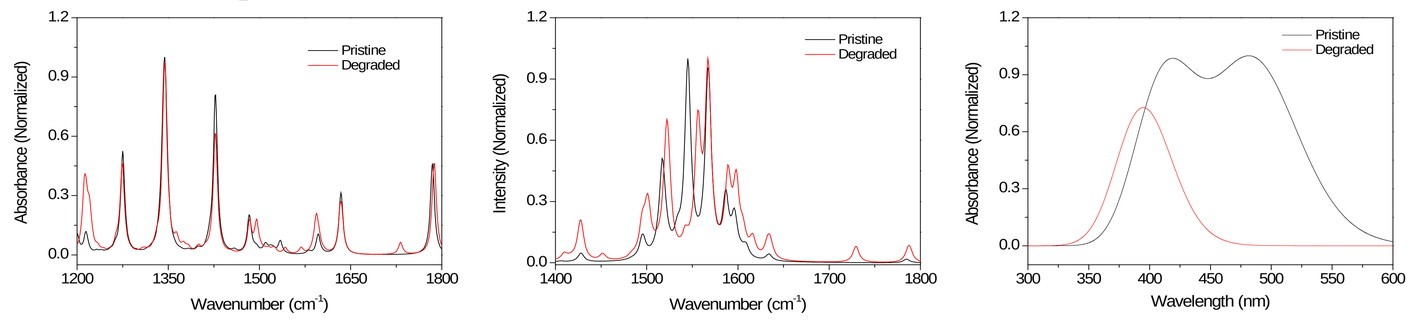
➢ Summary

- Conjugate bond dissociation
- BDT unit is vulnerable to degradation
- After degradation, carbonyl and hydroxyl bond are formed

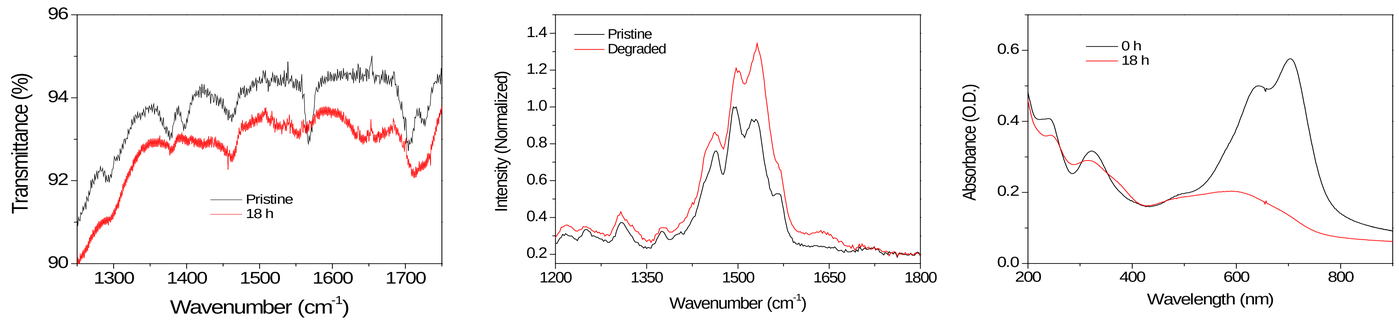
Proposed mechanism

A Comparison of Calculation and Experiment

- Calculated spectra



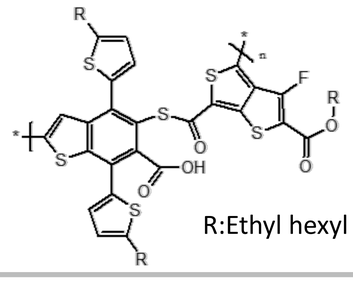
- Experimental spectra



► There is consistency between calculated and experimental spectra.

Conclusion

- In initial degradation process, oxygen is the major factor.
- The degradation product is generated via ring opening reaction.
- Conjugate bond in backbone is broken during degradation process.



Reference

1. *J. Mater. Chem. A*, **2014**, 2, 20189-20195.
2. *J. Am. Chem. Soc.*, **2011**, *133* (6), pp 1885–1894

Acknowledgment

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