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Polymers of 4-Thieno[3,2-b]thiophen-3-ylbenzonitrile wit Anthracene and Biphenyl: Electronic and Optoelectronic Properties

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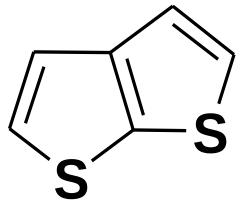
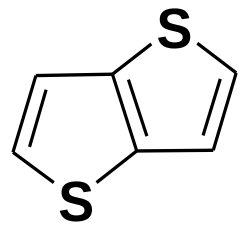
THIENOTHIOPHENES

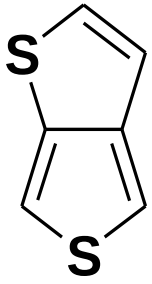
- Rich in sulfur
- Good electron donors
- Good electron delocalization
- Building block of many electronic and optoelectronic materials



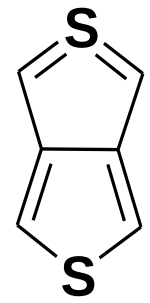
thieno[2,3-*b*]thiophene



thieno[3,2-*b*]thiophene

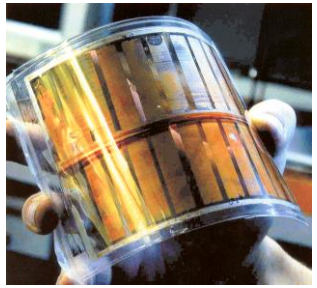


thieno[3,4-*b*]thiophene



thieno[3,4-*c*]thiophene

Applications of Thienothiophene Based Materials



• Photophysic
• Charge Transfer
• Photoconductivity

Solar Cell
Photodetector

Chemical
Biosensors

• Conductivity
• Redox Properties

OLEDs
Lasers

• Photophysics
• Luminesans
• Photoconductivity

• Electrochemistry
• Electronic Structure

Electrochromic
Devices

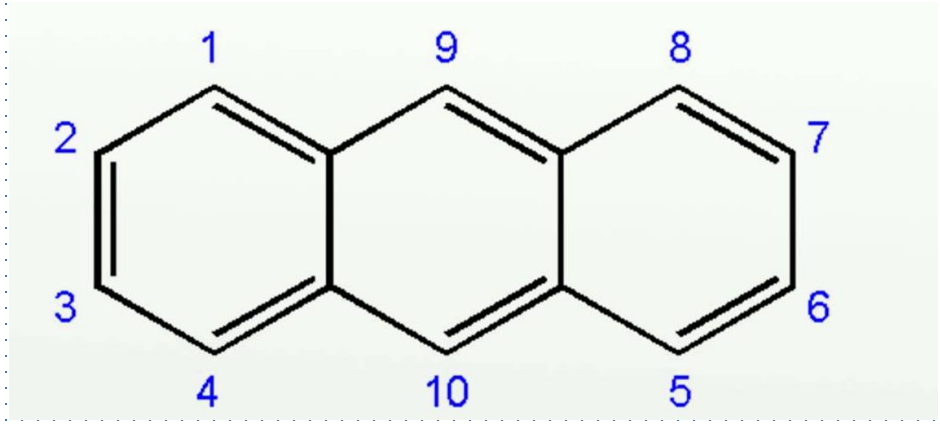
• Molecul Charge Transfer

Molecular
Electronics

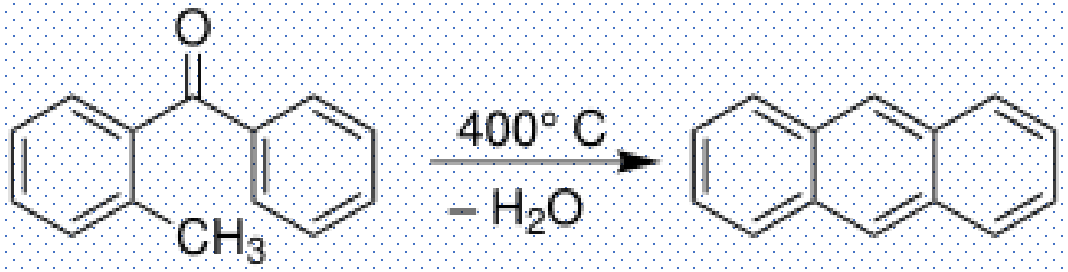
• Charge Transfer

Thin Film
Transistors

Anthracene



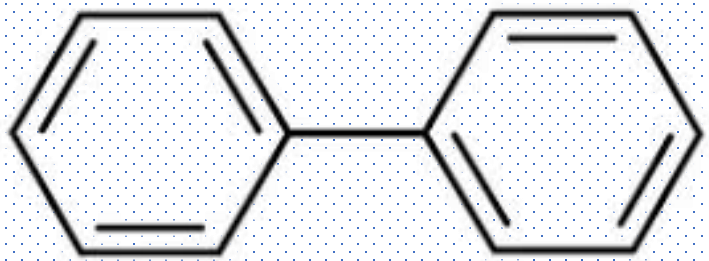
Chemical Structure of Anthracene



Synthesis of Anthracene by Elbs Reaction

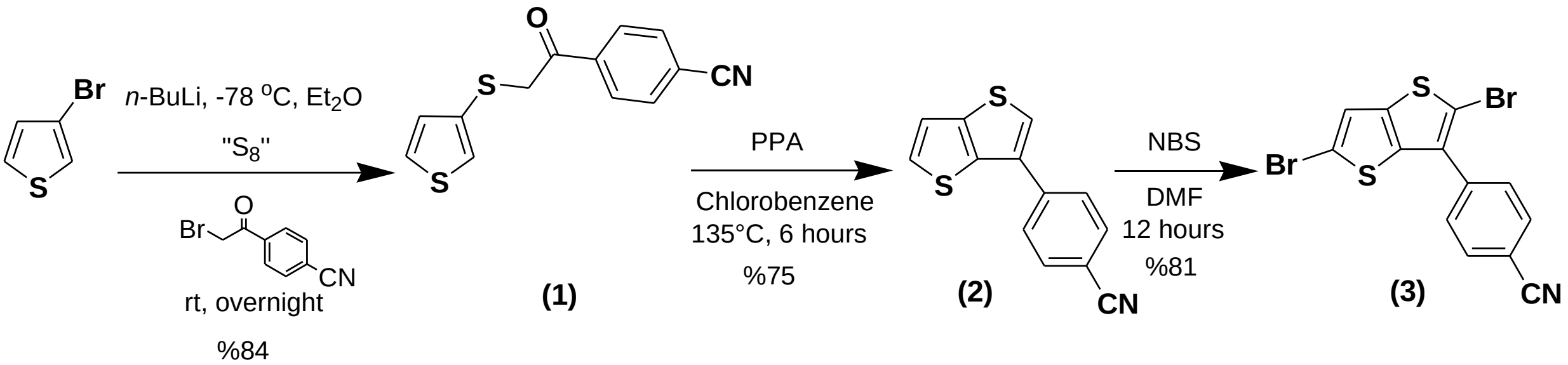
- Solid polycyclic aromatic molecule consisting of three fused benzene rings.
- Can tune the molecular packing and charge transport properties.
- π-electron-rich structure for electronic materials.
- Exhibits a blue fluoresence under ultraviolet light.

Biphenyl



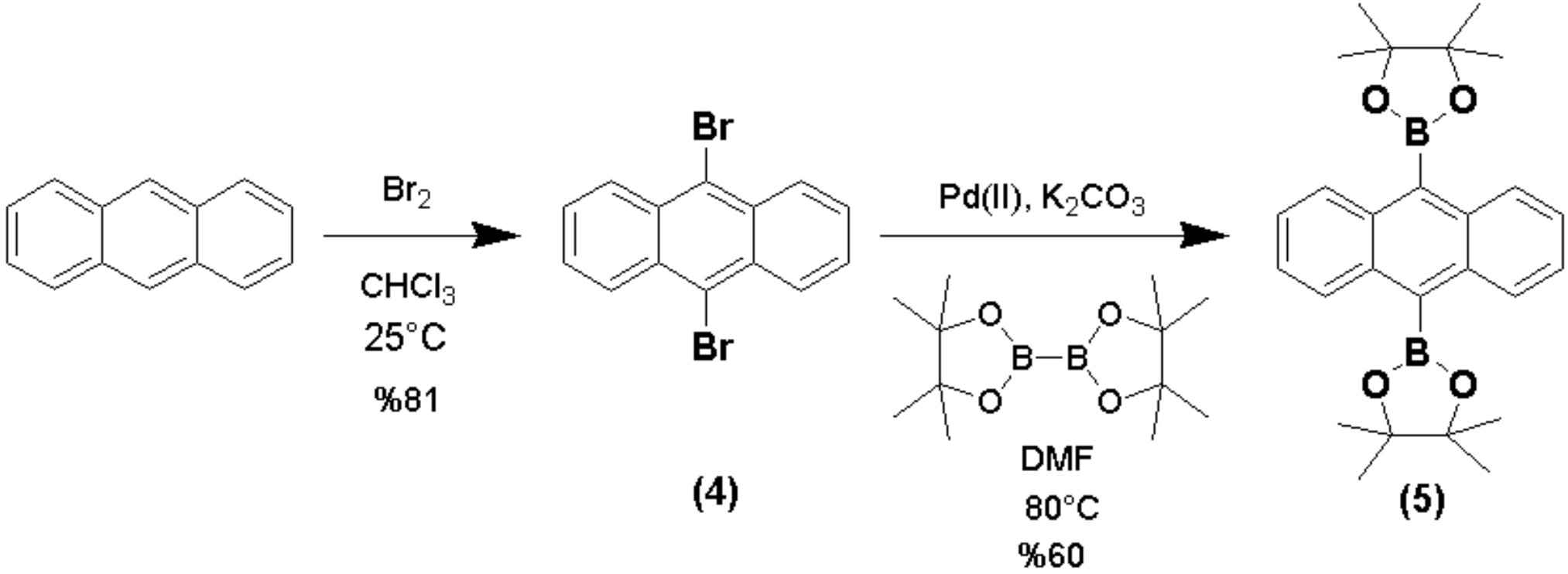
Chemical Structure of Biphenyl

- Good for conjugated and ordered packing.
- Has important roles as π - conjugated bridge and electron rich donor.
- Could be used for opto and electronic aplications.



Experimental

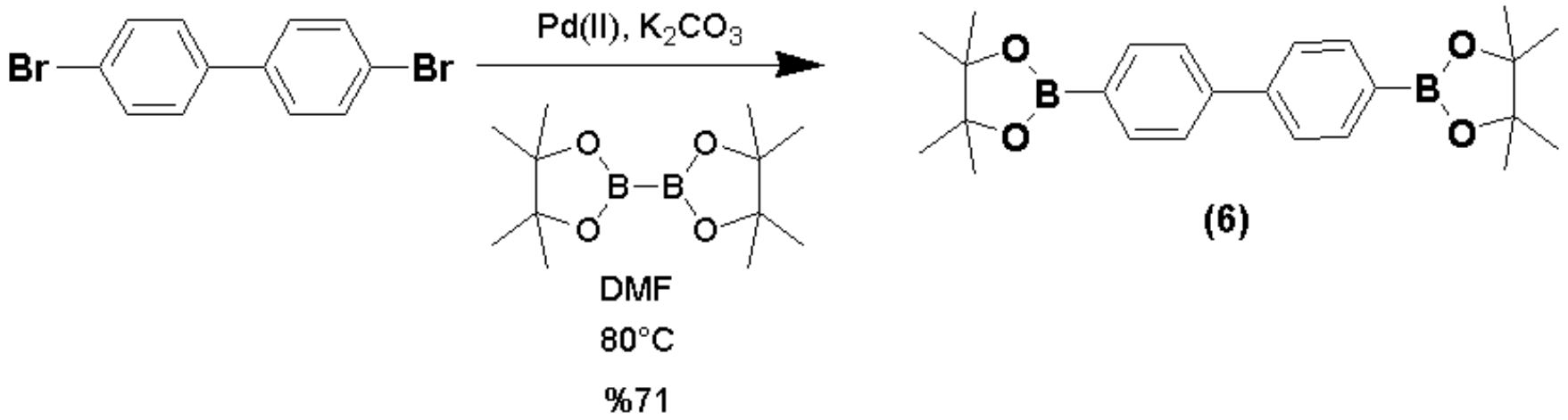
- Initially, the syntehesis of monoketone **1** was performed.
- Then, thienothiophene (TT) **2** ring was constructed through ring closure of **1**.
- Dibromination of the TT gave dibromo-TT **3**.



Experimental

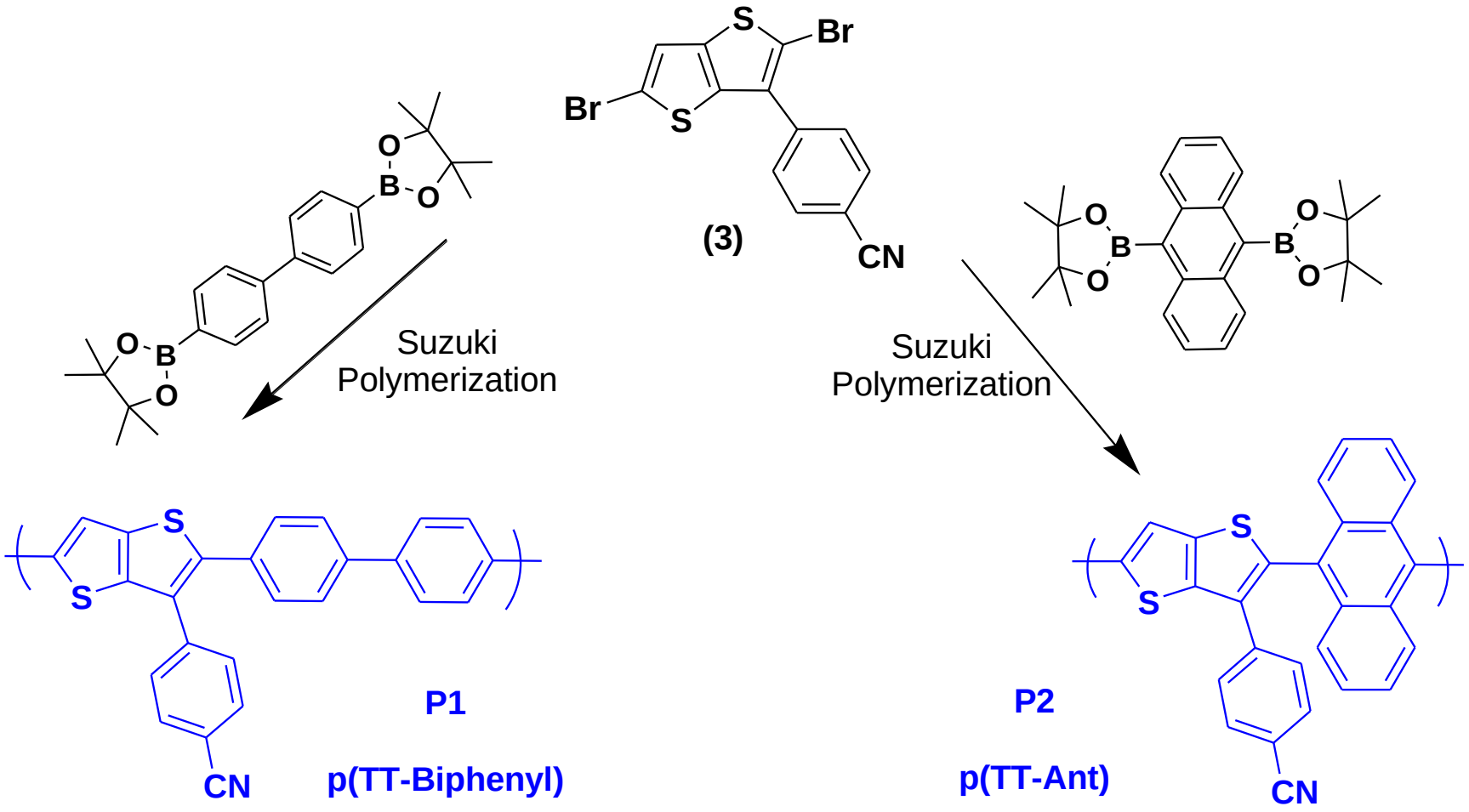
- Dibromination of anthracene yielded dibromoanthracene **4**. In order to make it ready for a Suzuki polymerization in the next step, it was borolated to obtain **5**.

Experimental



Similarly, dibromobiphenyl was borolayted to obtain **6** for Suzuki polymerization to obtain the second polymer

Experimental

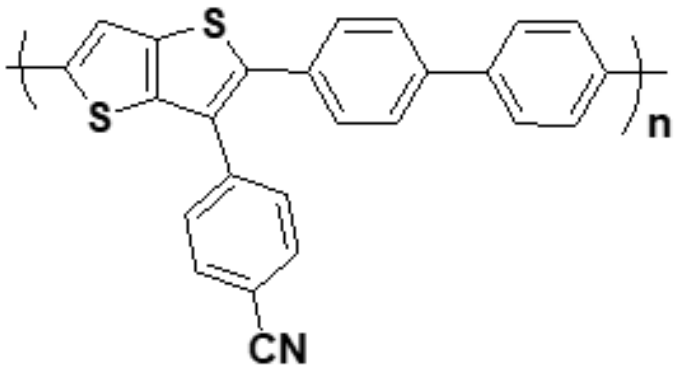


Two different polymers, including anthracene **P2** and biphenyl **P1** groups, were then obtained through Suzuki polymerization reaction.

Results

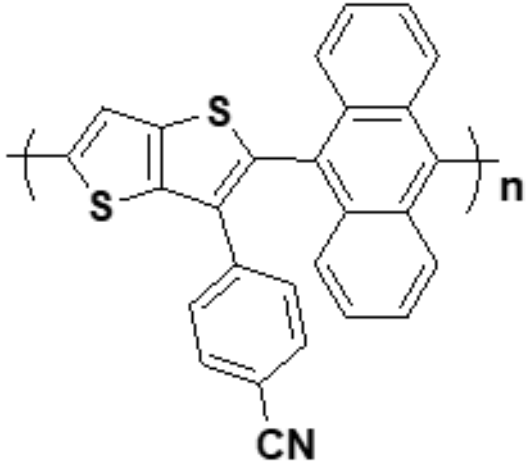
Obtained Molecules

Polymer of TT-Biphenyl



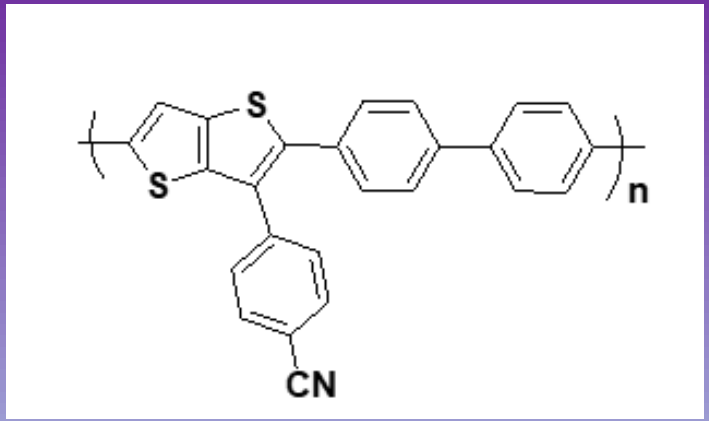
under uv light

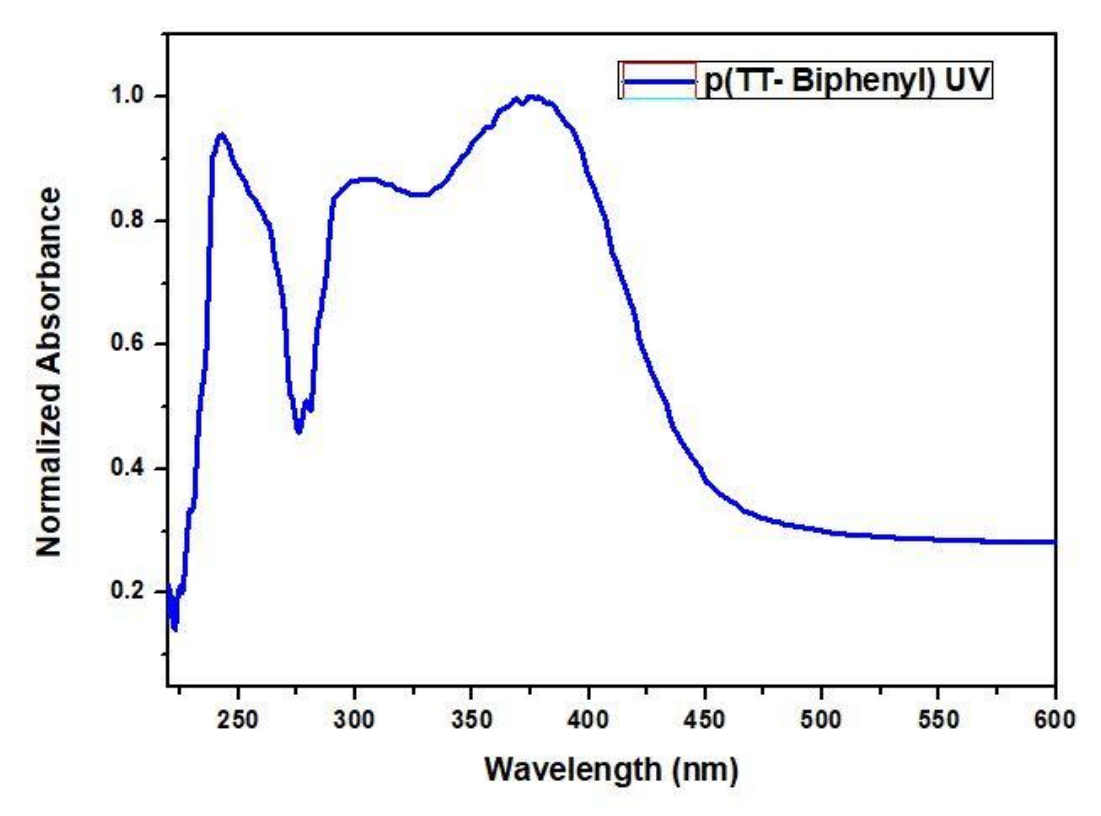
Polymer of TT-Anthracene

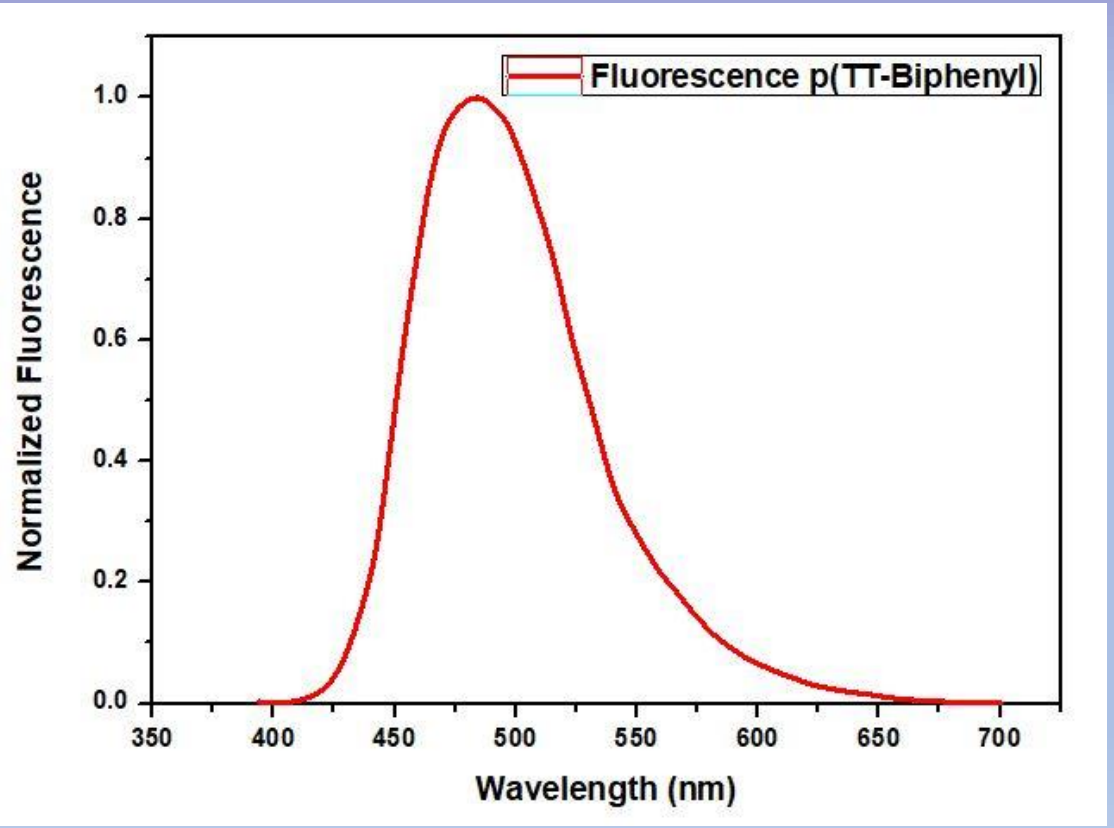


under uv light

Results

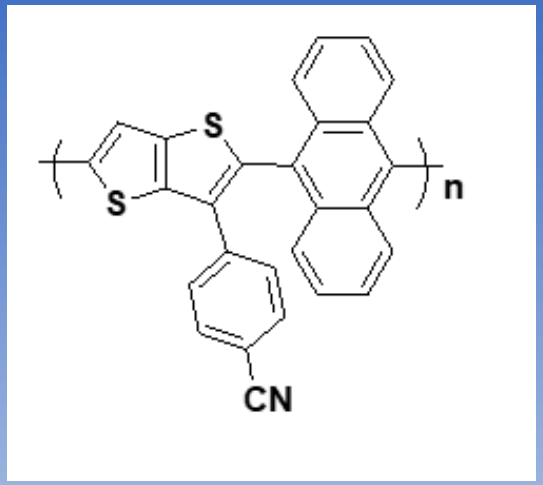


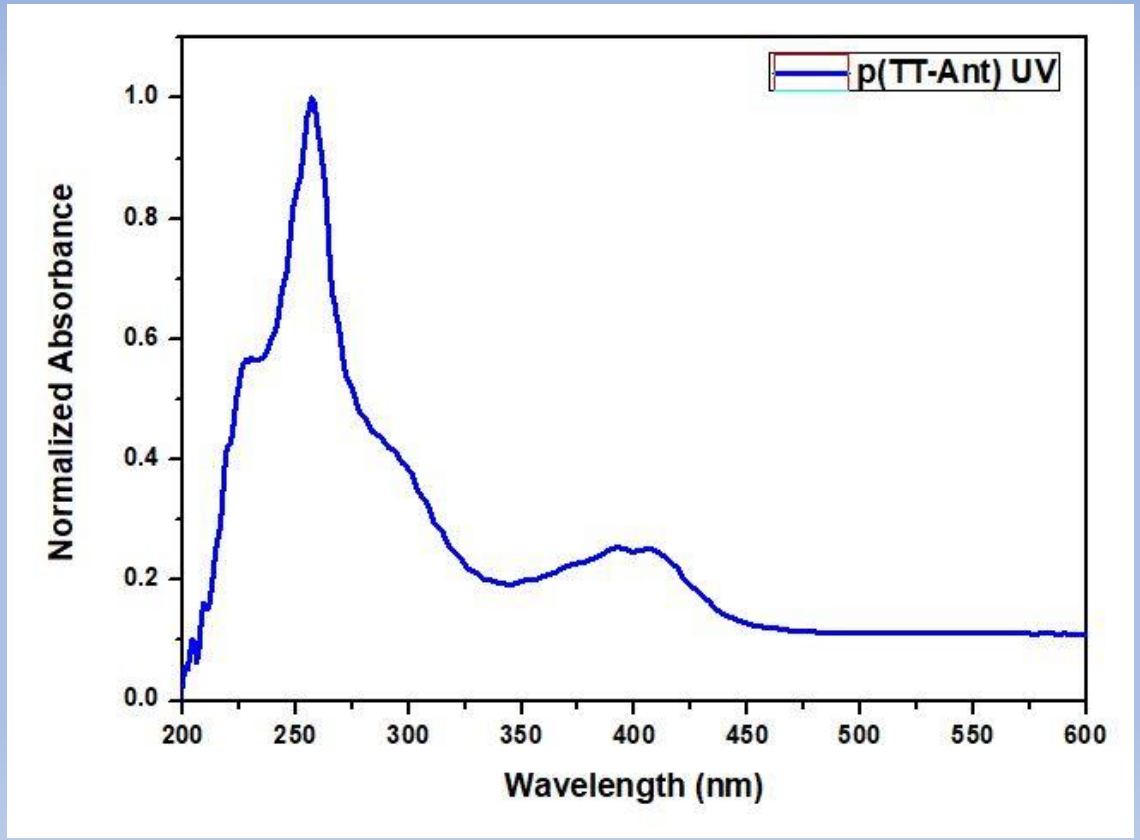


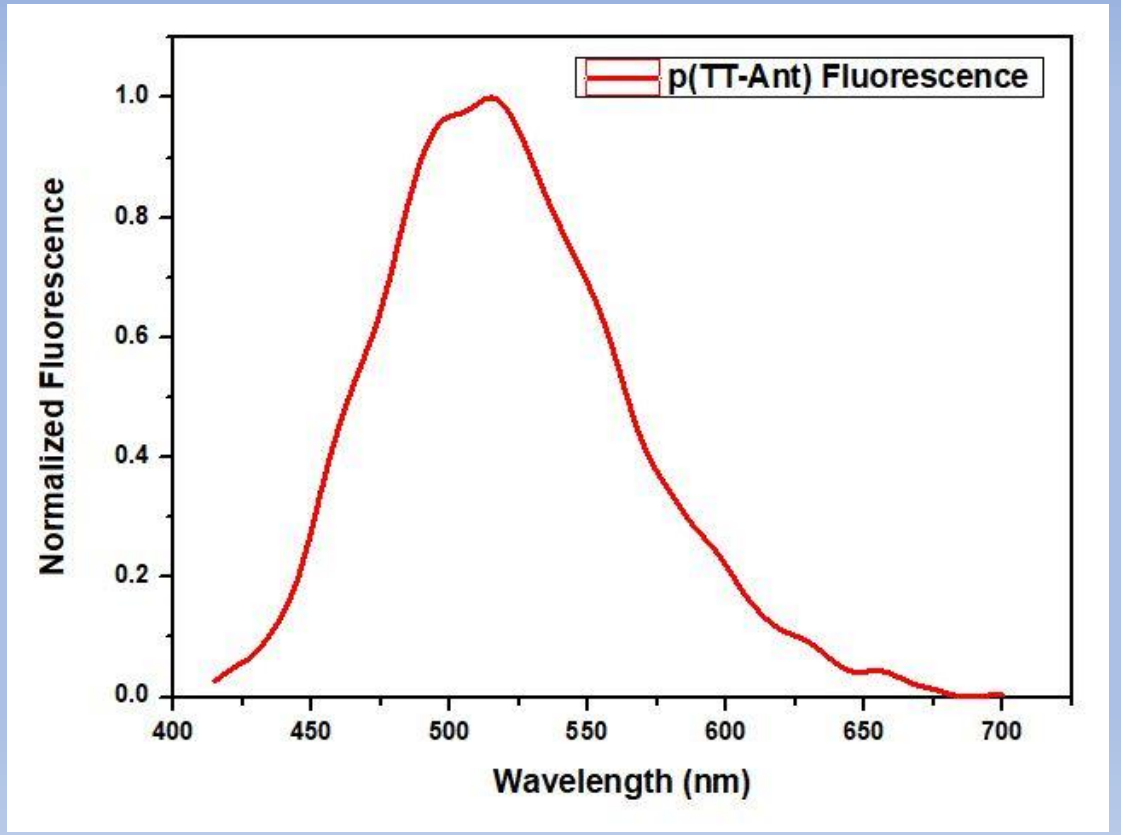


UV-Visible and Fluorescence of p(TT-Biphenyl) in THF

Results

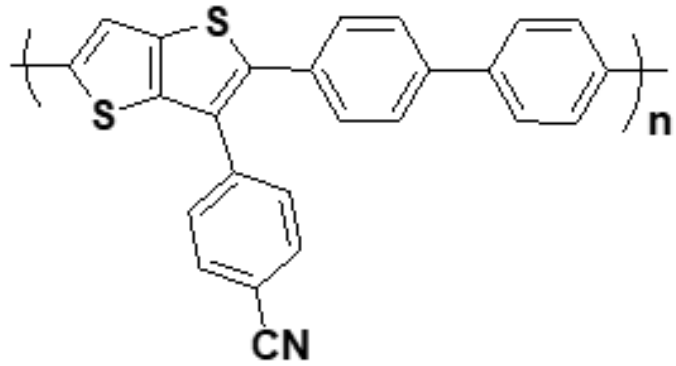


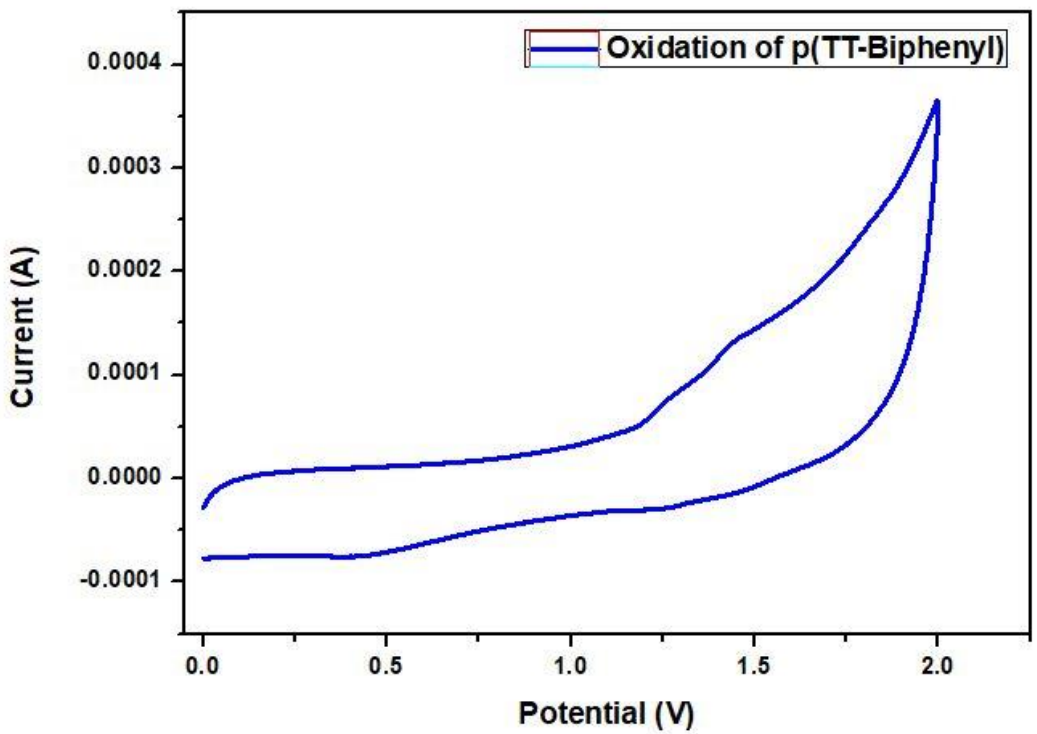


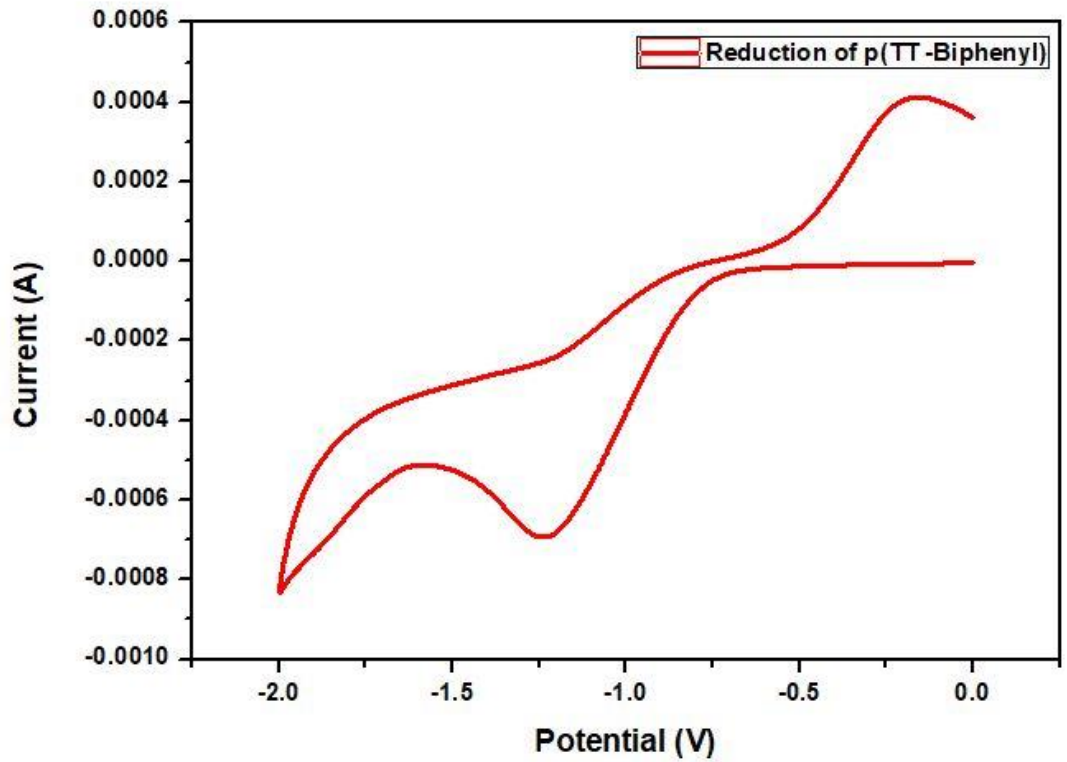


UV-Visible and Fluorescence of p(TT-Ant) in THF

Results

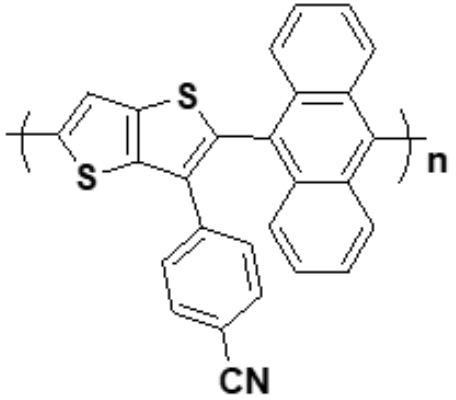


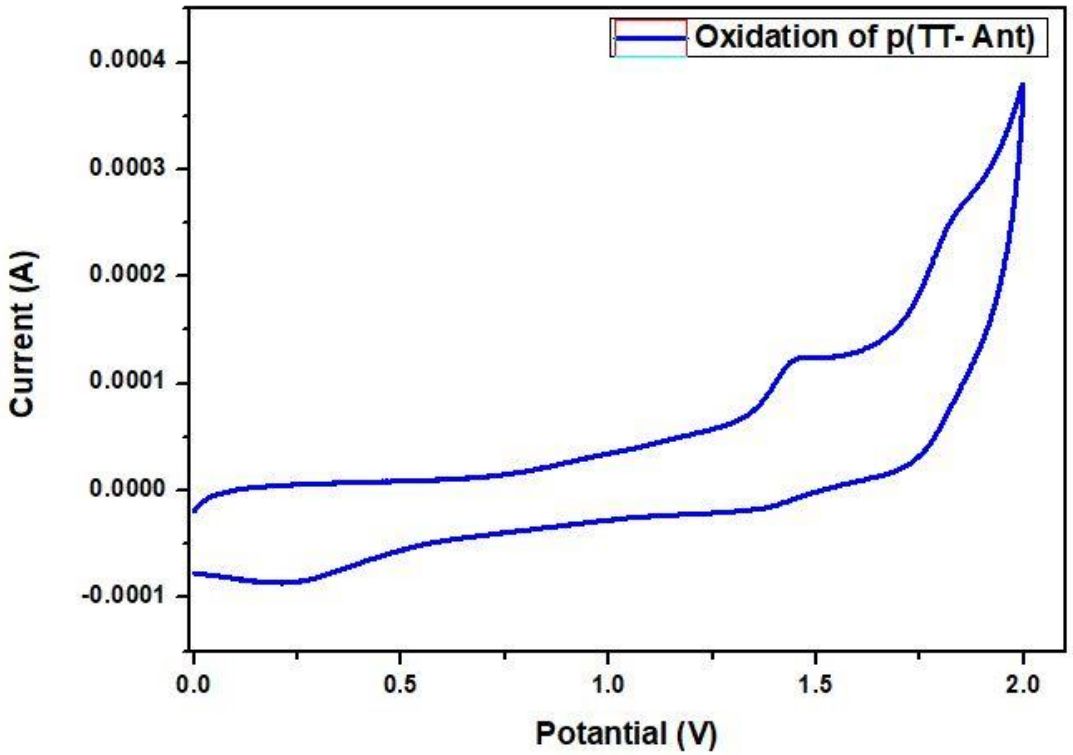


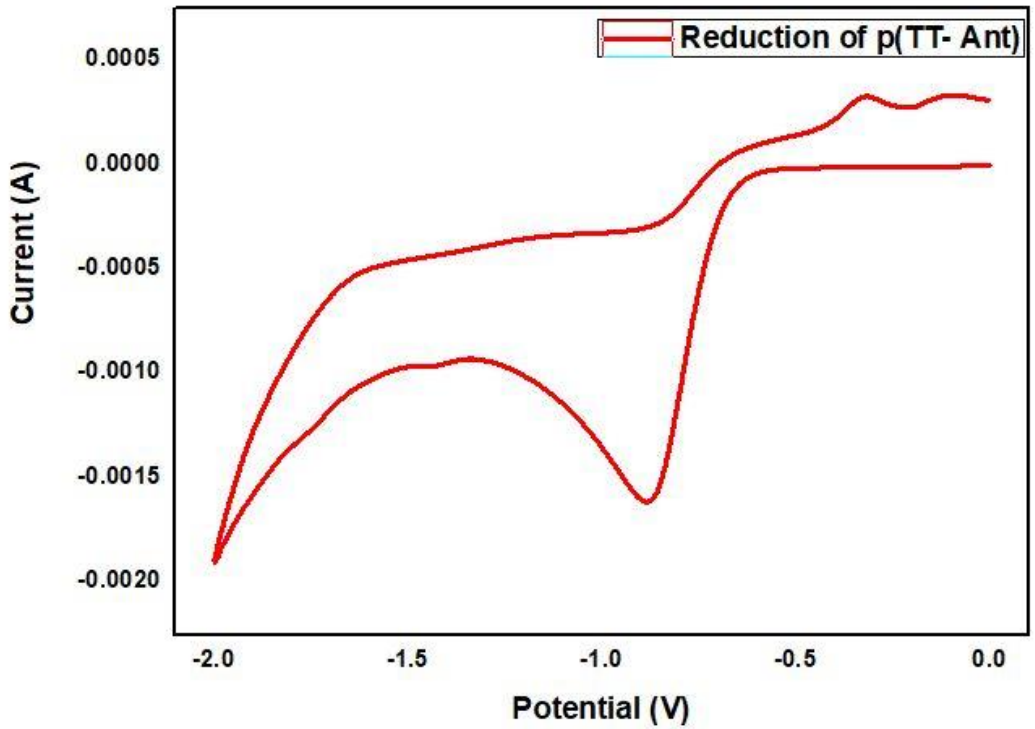


Electrochemical Proporties of p(TT-Biphenyl)

Results





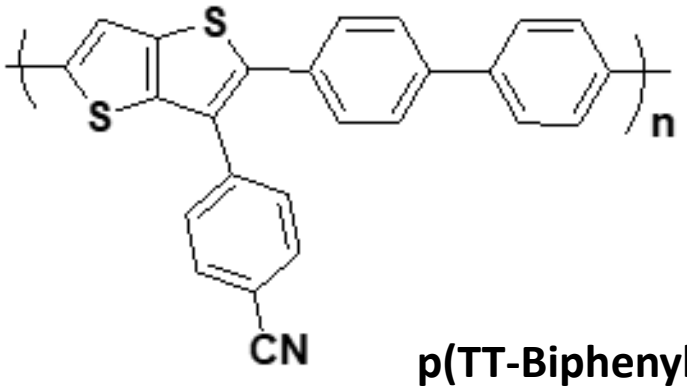


Electrochemical Proporties of p(TT-Ant)

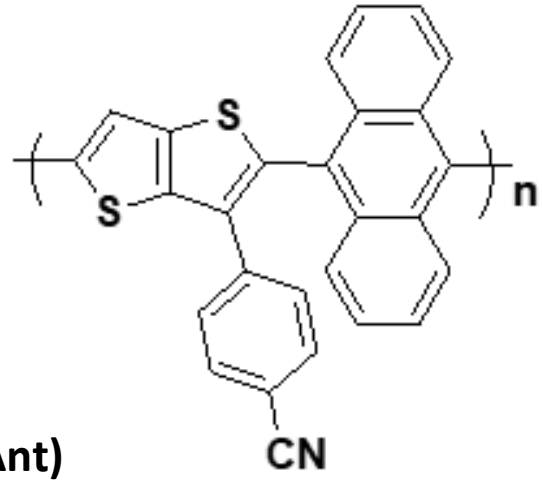
Results

Optical Proporties of P1 and P2

Polymers	λ_{max} – UV (nm)	λ_{max} – Floresans (nm)	E_{opt} (eV)
p(TT-Biphenyl) P1	380	480	2.64
p(TT- Ant) P2	260, 400	515	2.61



p(TT-Biphenyl)
P1

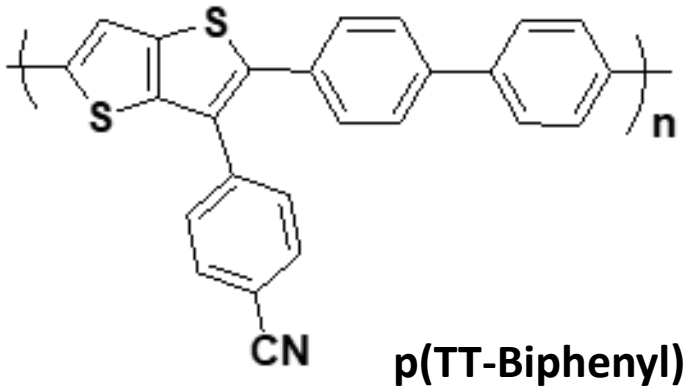


p(TT-Ant)
P2

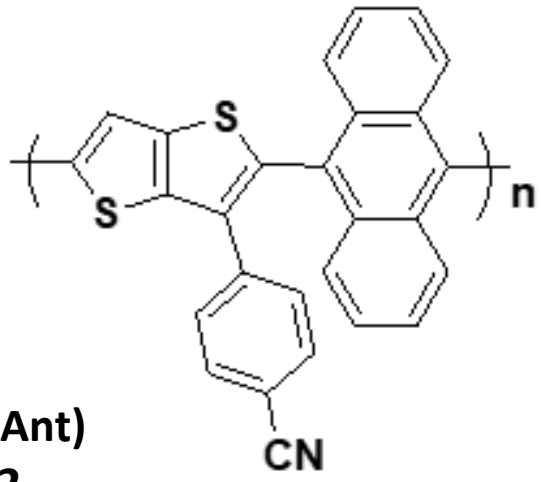
Results

Electrochemical Proporties of P1 and P2

Polymers	Oxidation Potential (V)	Reduction Potential (V)	$E_{electronic}$ (eV)
p(TT-Biphenyl) P1	1.28	-0.75	2.03
p(TT- Ant) P2	1.42	-0.64	2.06



p(TT-Biphenyl)
P1



p(TT-Ant)
P2

Conclusion

- In this work, two novel polymers, containing thienothiophene, anthracene and biphenyl groups, were designed and synthesized by Suzuki polymerization.
- Electronic and optical properties of the resultant polymers were investigated.
- UV, emission and CV values indicated that **P1** and **P2** are suitable materials for electronic and optical applications.