

Kwansei Gakuin University

Report of Research Outcome

2020.02.21

To President

Department : Science and Technology

Position : Postdoctoral fellow

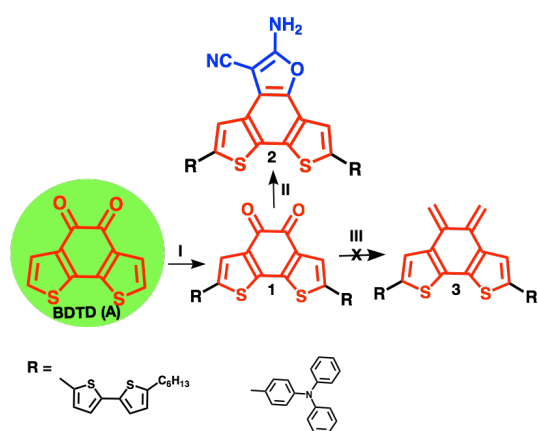
Name : BINOD BABU SHRESTHA

I report the outcome of the research as follows.

Name of the Fund/Program	<input type="checkbox"/> Sabbatical leave with grant <input type="checkbox"/> Sabbatical leave with no grant <input type="checkbox"/> KGU Joint Research <input type="checkbox"/> Individual Special Research <input checked="" type="checkbox"/> Postdoctoral fellow ※Please report by designated form as for "International Research Collaboration".
Research Theme	BDTD based π-extended derivatives
Research Site/Venue	Hamura lab
Research period	2019/04/01 ~ 2020/03/31 (12 month)

◆ **Summary of the research outcome** (approx. 2,500 words)

Please write down the outcomes in detail regarding the research theme above.



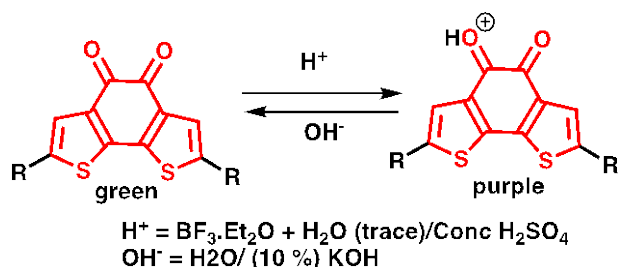
Scheme 1: Research outcomes of BDTD based π -extended derivatives

The donor-acceptor approach orbital mixing of donor and acceptor units in a π -conjugated compounds to decrease the electronic band gap has become one of the most powerful strategies. In order to tune up band gaps and their effects on physical properties, a new type donor and acceptor molecule is highly demanding such as Thiophene based-1,2 diones (BDTD, A, Scheme 1). This molecule offers various features for synthesizing attractive π -conjugated materials such as wide range of electronic properties offered by thiophene-unit, possibility of post derivatization on the thiophene rings (i.e., halogenation, borylation, stannylation, coupling reaction etc.) and further derivatization and co-ordination of alpha dicarbonyl group. However,

there are a few reports based on them. Here, we think that BDTD 1,2 diketone compound (1) in which diones can be its self good coordination site for electrophiles and metal.

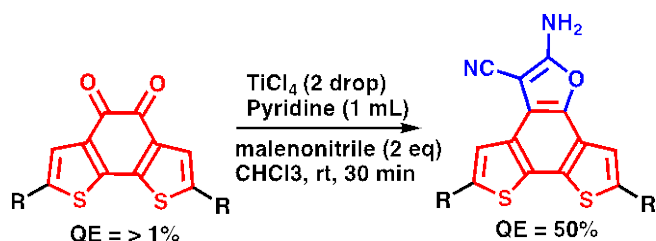
Hence, compounds (1) were synthesized by Stille coupling reaction from dibrominated derivatives of BDTD(A) compound. Coupling reaction was only proceeded after protection of dicarbonyl functional group. Without protection dicarbonyl group in dibrominated -BDTD compounds and corresponding Suzuki coupling reaction did not proceed.

I) Acid response color switching BDTD based 1,2 diketone, a donor and acceptor π -extended derivaives and its application to tune up Near Infrared Absorption.



New molecules that reversibly change their chemical or physical properties in response to external stimuli have received significant attention because of their potential versatility in applications related to molecular memory and switches. In this study, protonation-induced co-ordination of 1,2 diketone of compounds 1, produce stable cationic species which is delocalized over π -conjugated system and displaying a green to purple color when treated with bronsted acid such as sulfuric acid or in situ generation of $BF_3 \cdot H_2O$. This change might occur when the lowest unoccupied molecular orbital (LUMO) level is lowered in the protonated species. We aimed to synthesize protonation induced cationic species delocalized over the π -conjugation structure via chemical stimuli. Consequently, it will produce a remarkable molecular switching system. We found that the 1,2 diketone π -conjugated structure of 1 is regenerated from protonated species by the addition of water/10% KOH. In addition, a unique NIR-absorption properties of protonation species of 1 were observed and identified on the basis of DFT calculation. It is suggested that π - extended system stabilizes protonation of 1,2 diketone of cationic species that can reduce electronic band gap.

II) Synthesis of BDTD based highly fluorescent amine-functionalized benzofuran derivatives via one step cascade reaction



The fused polycyclic furan structure is a ubiquitous motif in naturally occurring organic compounds. However, they had been rarely seen in the literature of organic electronic research probably because of the lack of stability furan ring. Here, a synthetic route to novel amine functionalized benzofuran fused BDTD derivatives was achieved by $TiCl_4$ catalyzed one step cascade reaction and their emission properties was studied. These compounds showed high green fluorescence properties (QE = 50%), while corresponding 1,2 diketone based BDTD (1) showed very weak fluorescence (QE >1%). Preliminary results show that these derivatives can be used as green emitters for optoelectronic applications.

Deadline : Within two months after finishing the research period.

Sabbatical leave with grant: Submit this report to President with confirmation by the dean of school you belong to.

※ Postdoctoral fellow is required to submit this report with confirmation by the dean of graduate school before the end of employment period.

Where to submit : Organization for Research and Development and Outreach (NUC)

◆ We put this report on the web of KGU. If there is any problem about it because of difficulties on your research, please let us know.