Design and Synthesis of Chiral Tetracyanoquinodimethane (TCNQ) derivatives to study CISS effect

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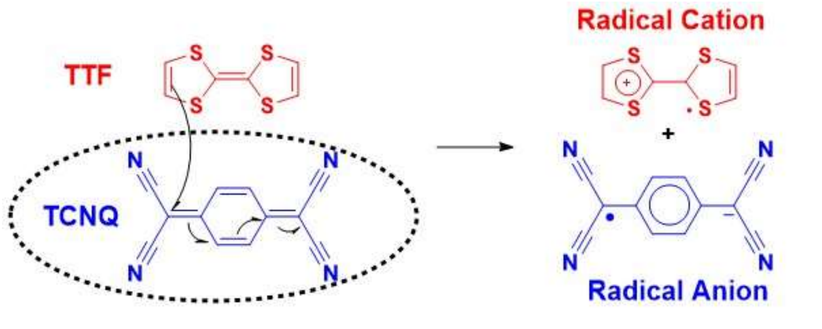
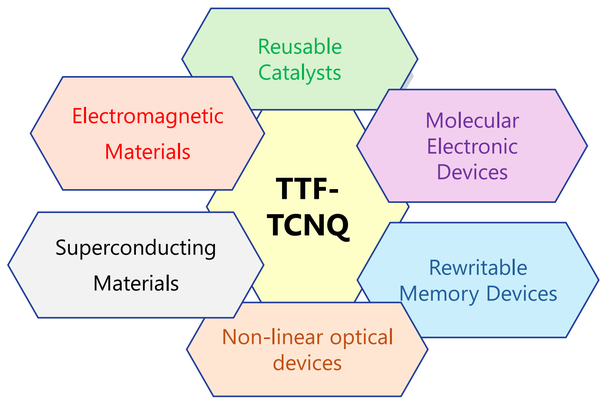
Introduction

- Chirality can be introduced in molecular semiconductors to study the role of **Chiral Induced Spin Selectivity (CISS)**[1-3] effect during charge transport. The electron acceptor **Tetracyanoquinodimethane (TCNQ)** forms highly conducting metal like organic charge-transfer complex (CT) with **Tetrathiafulvalene (TTF).**[4]

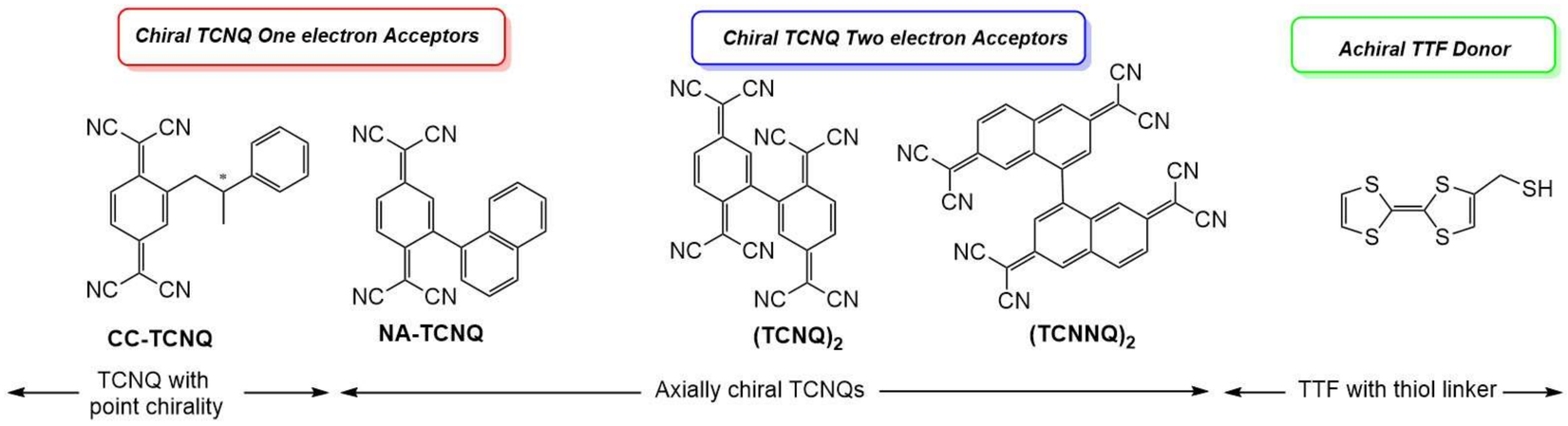


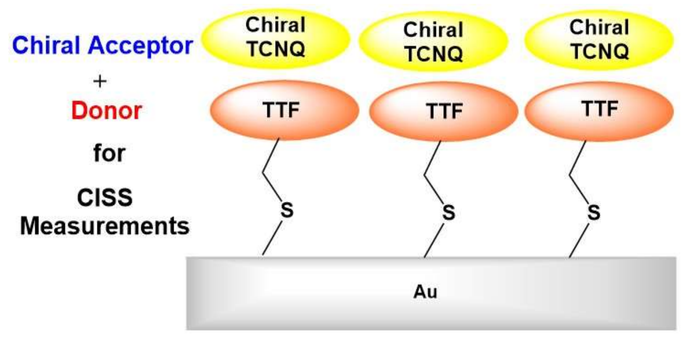
TTF-TCNQ Charge Transfer Complex and its applications



- To date, the CISS effect has been exclusively measured on closed-shell structures. We aim to design and synthesise **chiral TCNQs that can give open-shell monoradical and diradical anions** with TTF donors to increase the molecular diversity in understanding CISS effect.

Targets

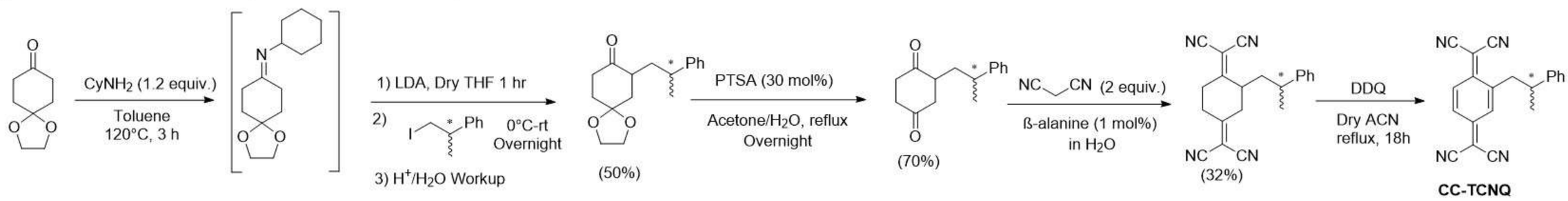


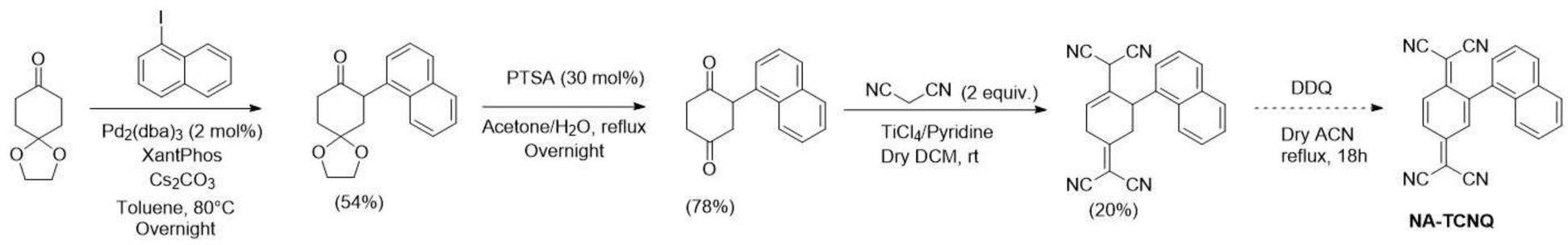


We have designed chiral TCNQs to make conducting CT complex with TTF based donor.[5] These novel chiral TCNQs are anticipated to behave as **redox active n-type semiconductor** that can contribute to the understanding of the **CISS effect in molecular semiconductors** and **organic materials in spintronic devices**.

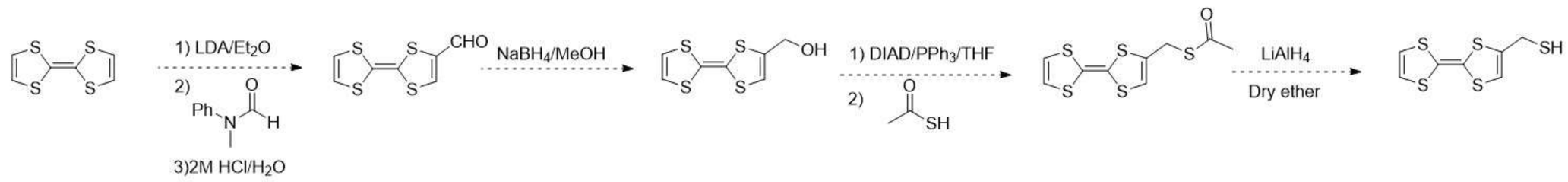
Synthesis

Synthesis of Chiral TCNQ One electron Acceptors:





Proposed Synthetic route to Achiral TTF with a Thiol linker:



Conclusion & Future Outlook

- We are currently developing a scalable route to synthesize Chiral TCNQ one-electron acceptors. Optimisations to other chiral TCNQ targets are underway in our laboratory.
- The charge-transfer properties of these chiral TCNQ-TTF complex will be studied. Further these **CT complexes will be fabricated onto Au surface for the quantification of CISS effect** by various complementary methods, including **spin polarized AFM, SQUID, Hall effect, and photoelectron spectroscopy with a Mott polarimeter**.

References

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