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

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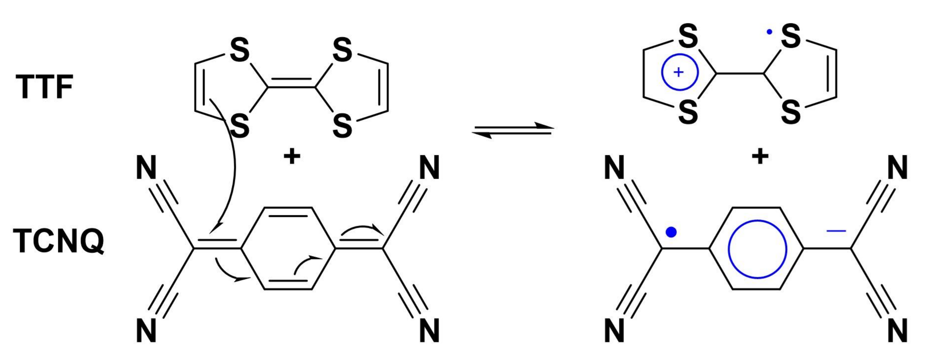
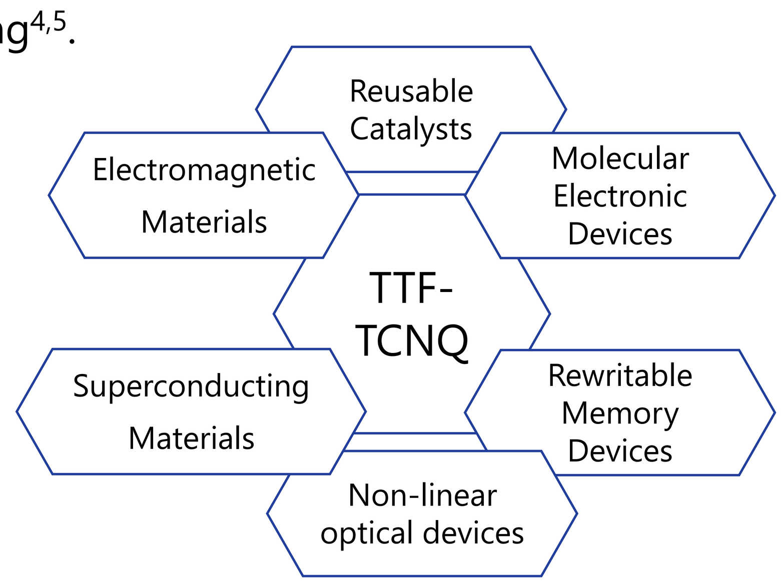
Funded by the European Union

Introduction

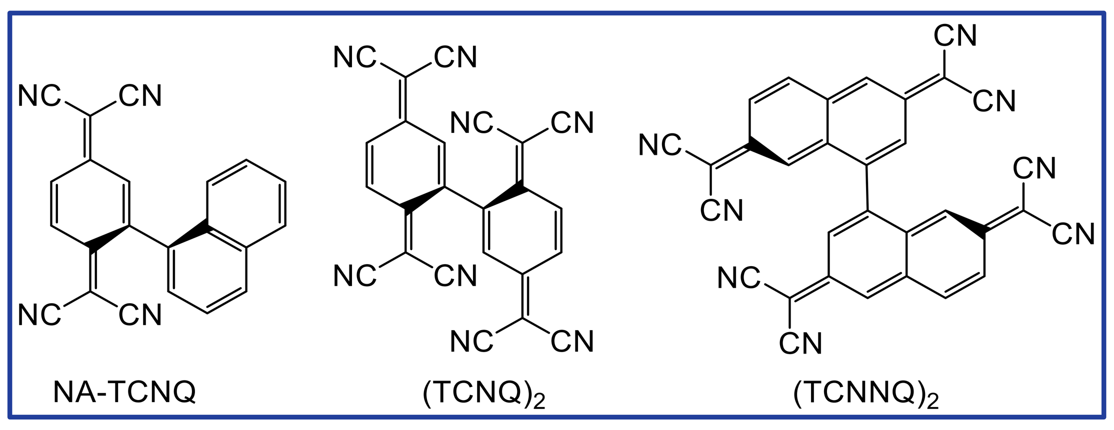
- Chirality can be introduced in molecular semiconductors to study the role of **Chiral Induced Spin Selectivity (CISS)**[1-3] effect. To date, the CISS effect has been exclusively measured on closed-shell structures. **We aim to design and synthesise chiral systems with unpaired localised electrons such as monoradical and diradical anions to increase the molecular diversity in understanding CISS.**
- The electron acceptor **Tetracyanoquinodimethane (TCNQ)** can give **radical anions** with electron donors such as **Tetrathiafulvalene (TTF)** and the resulting charge-transfer complexes (CT) are known to be highly conducting[4,5].



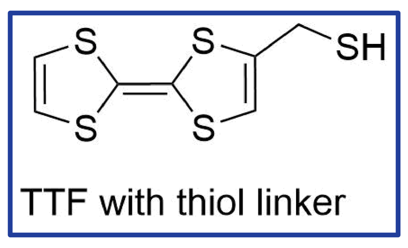


Targets

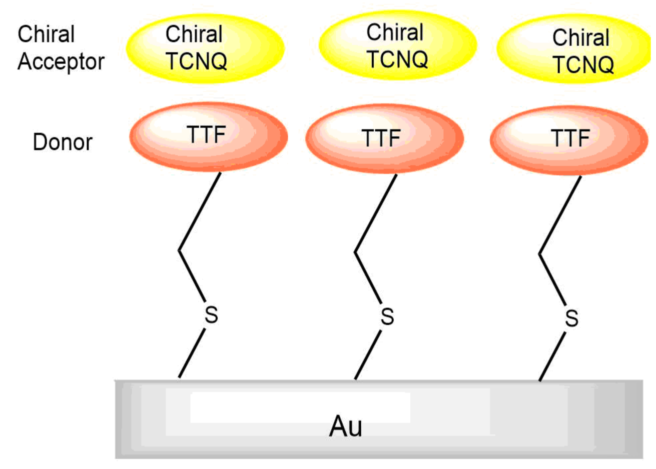
Chiral TCNQ electron acceptors



TTF Donor



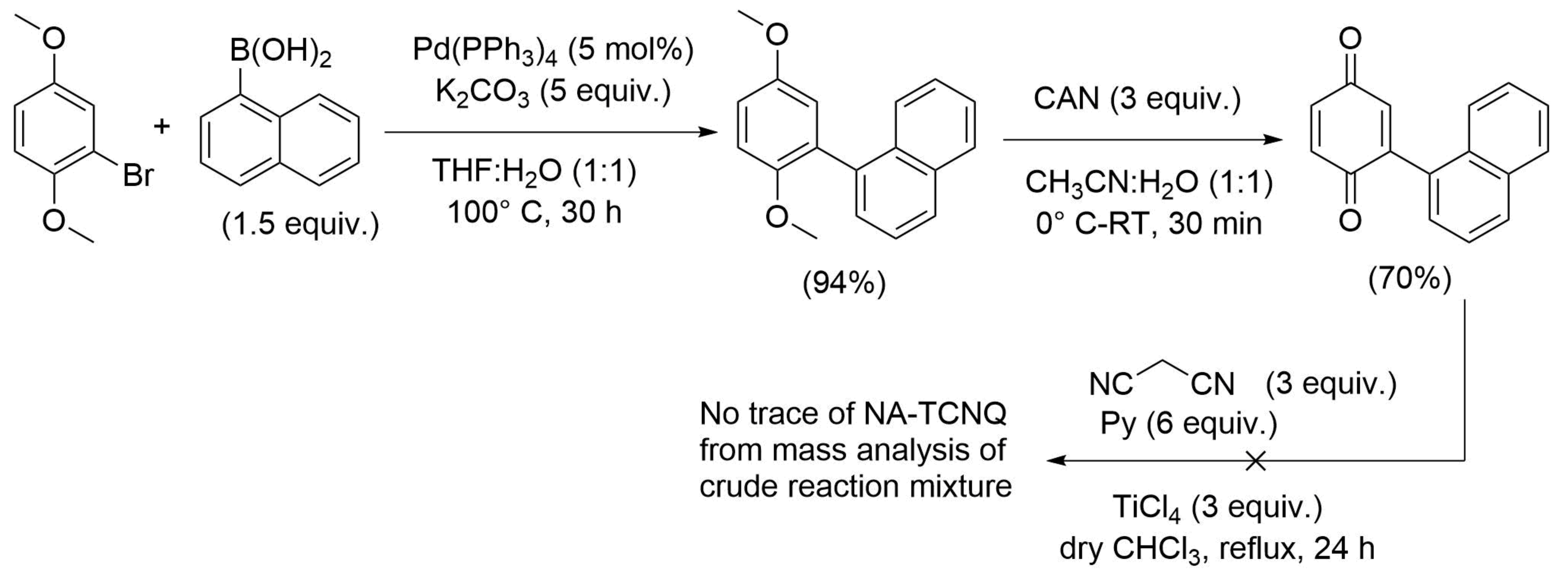
We have designed chiral TCNQs to make conducting CT complex with TTF based donor to study the CISS effect. These novel chiral TCNQs can behave as **redox active n-type semiconductor** that can contribute to the understanding of the CISS effect and can potentially open new avenues for the introduction of **organic materials in spintronic devices**.



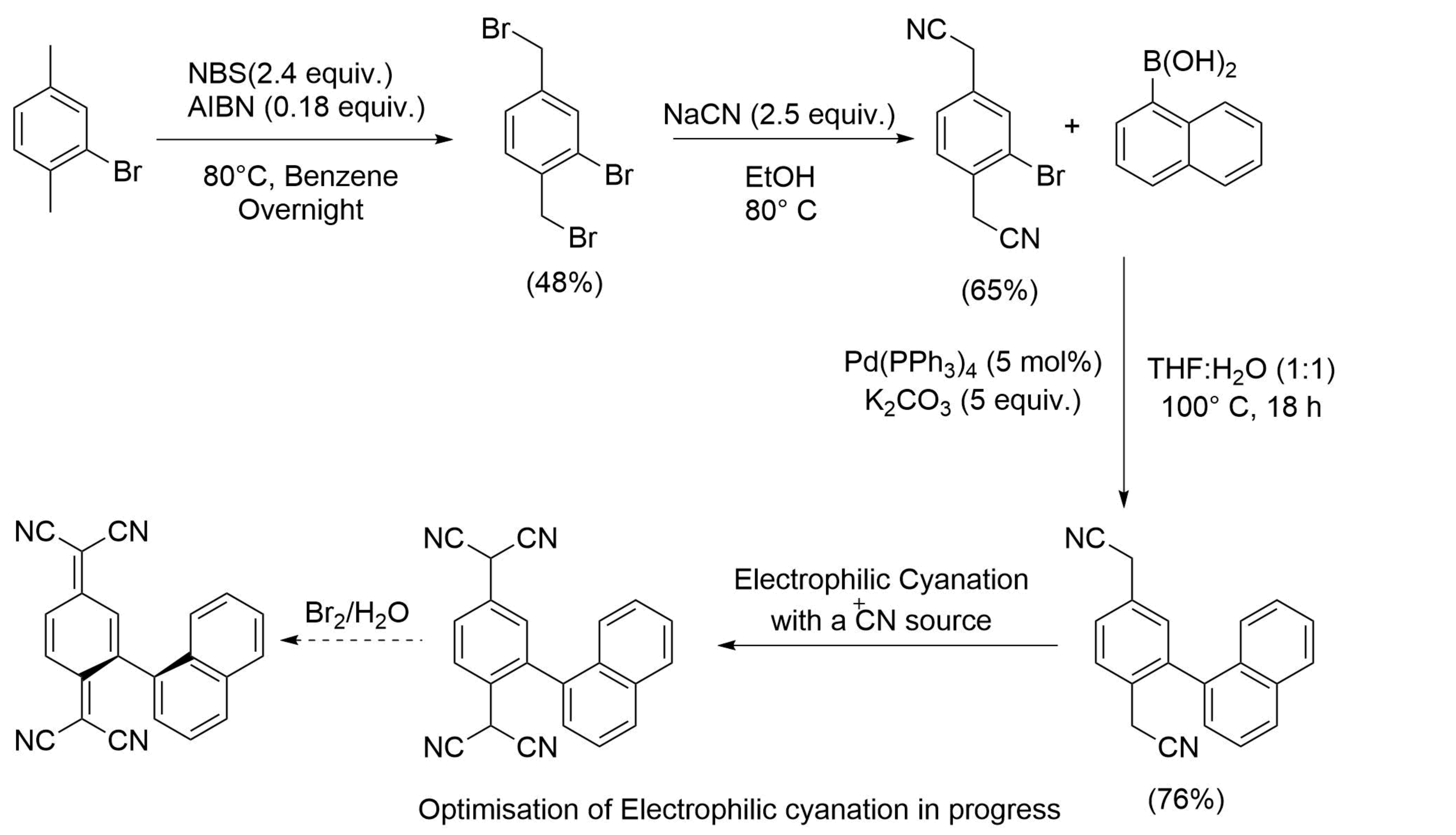
Synthesis

Synthetic attempts for NA-TCNQ

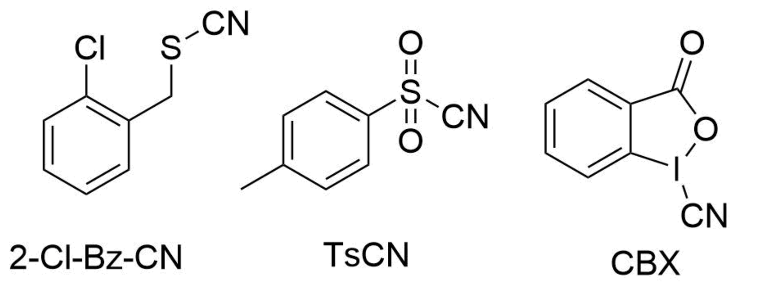
Attempt-1: The Lehnert's condensation approach



Attempt-2: The Double Cyanation Approach

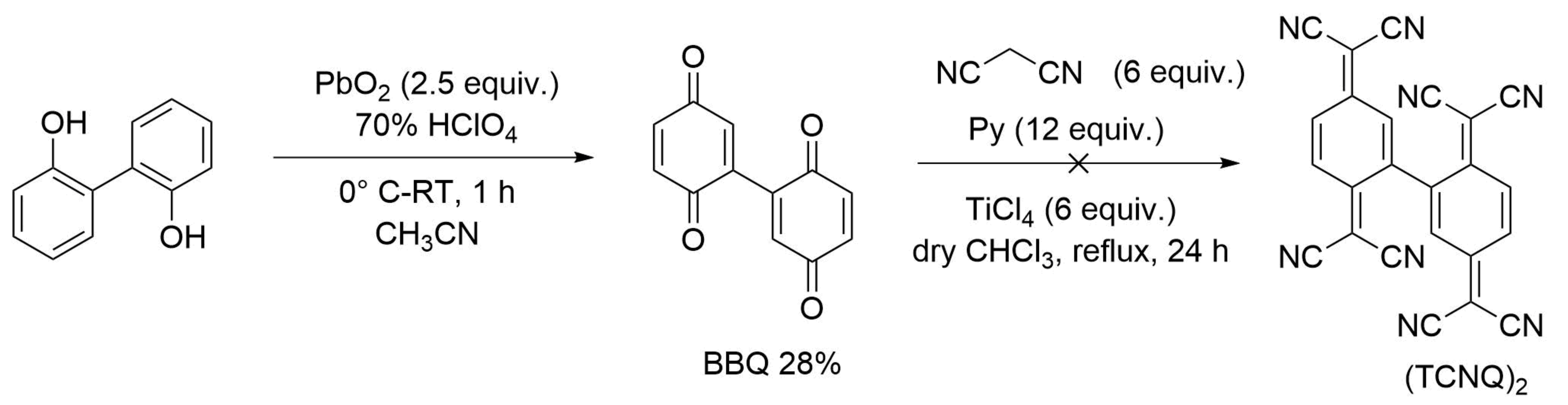


Source of Electrophilic Cyanide:

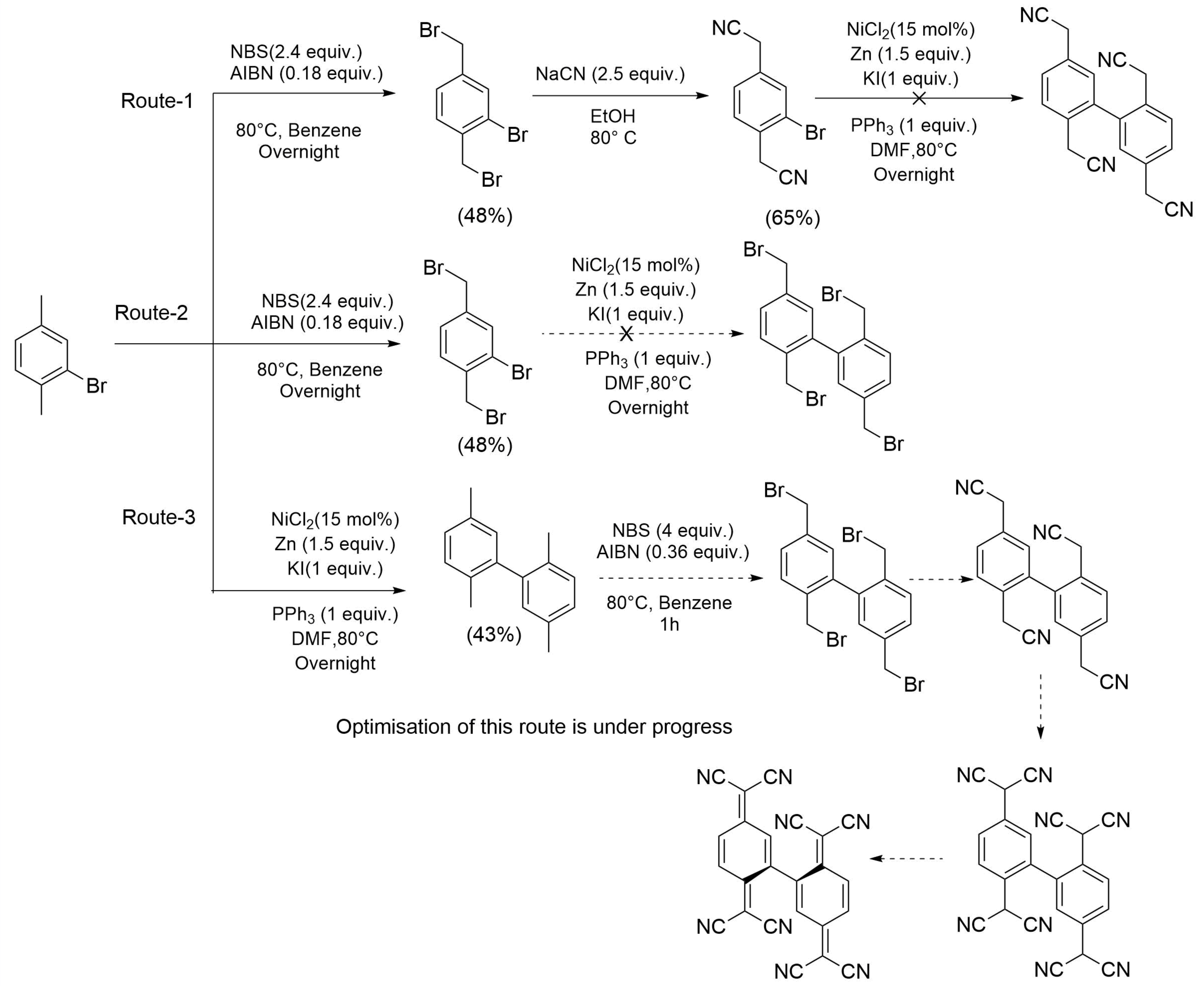


Synthetic attempts for $(TCNQ)_2$

Attempt-1: The Lehnert's condensation approach



Attempt-2 : The Double Cyanation Approach



Conclusion

- The synthesis of the chiral TCNQs utilising a double cyanation approach is currently under progress
- After optimising the synthetic routes, chiral TCNQ-TTF charge-transfer complexes will be fabricated into highly ordered thin films on Au surface.
- Further the magnetic properties of these chiral CT complexes in presence and absence of external electric field will be quantified.
- Quantification of CISS effect by various complementary methods, including spin polarized AFM, SQUID, Hall effect, and photoelectron spectroscopy with a Mott polarimeter will also be achieved.

References

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Acknowledgement

"Funded by the European Union, in the frame of the Marie Skłodowska-Curie Actions (MSCA), Doctoral Network (DN) CISSE project n° 101071886. Views and opinions expressed are, however, those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Executive Agency (REA). Neither the European Union nor the granting authority can be held responsible for them"