Synthesis of sterically hindered Pentacenes

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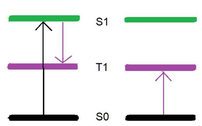
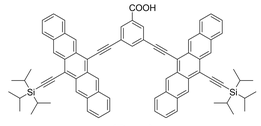
Introduction[1,3,4]

- Pentacenes dimers show good performance as electron donors in solar cells.
- Singlet fission (SF) is a spin-allowed process.
- SF converts one singlet excited state (S_1) into two triplet excited states (T_1).
- Several recent studies have demonstrated remarkably efficient solar cell devices based on SF.
- Requirement to have SF: The photoexcited chromophore in its S_1 state must share its energy with a neighboring S_0 chromophore, allowing both to arrive to the triplet state.
- Pentacene dimers undergoing singlet fission can surpass the Shockley-Queisser limit of 30% efficiency for photovoltaic devices.

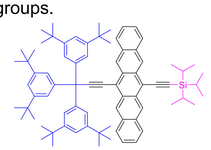




(Pnc_2)

Synthesis / purpose[2]

- Pentacenes can interact and react together if they are close enough together.
- Sterically hindered pentacenes such as **1** and **2** were synthesized to study intermolecular interactions between pentacenes toward the analysis of SF.
- We have synthesized **3** with triisopbutyl groups, which are slightly bigger than triisopropyl groups.



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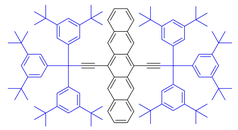

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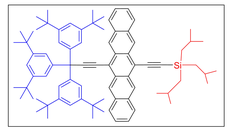

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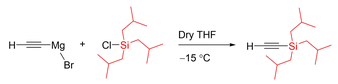
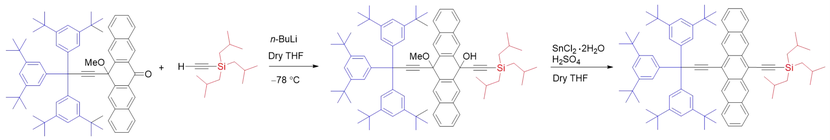
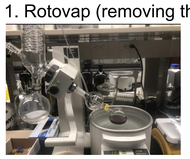




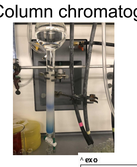
In collaboration with Professor Dirk M. Guldi and Bettina Basel, Department of Chemistry and Pharmacy, Interdisciplinary Center for Molecular Materials (ICMM), Friedrich-Alexander-Universitaet Erlangen-Nuernberg, Germany.

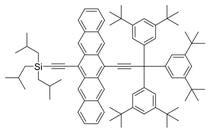
Methods for Compound 3

1. Rotovap (removing the solvent)



2. Column chromatography

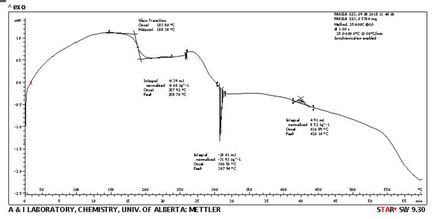




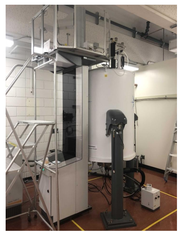
3. Concentration

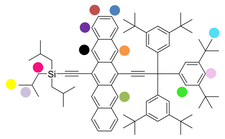
4. TLC

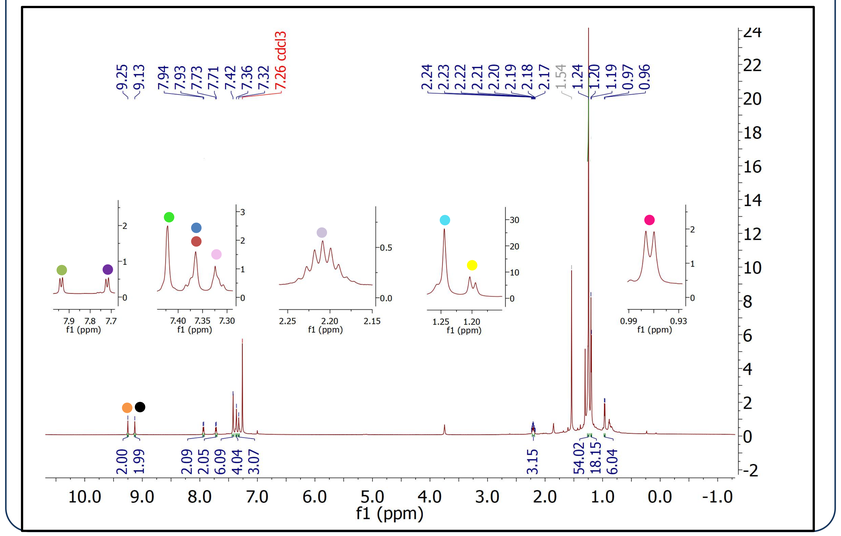
5. DSC



Nuclear Magnetic Resonance Data







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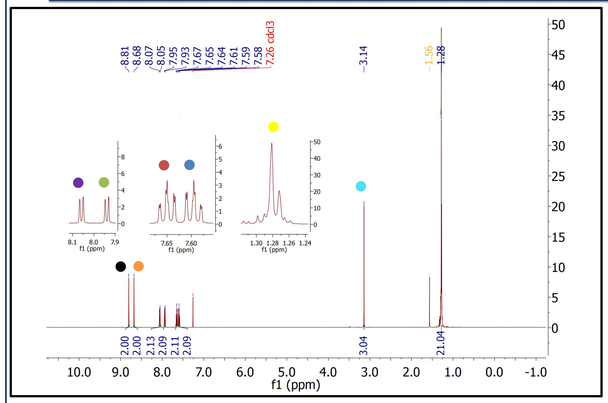
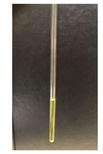
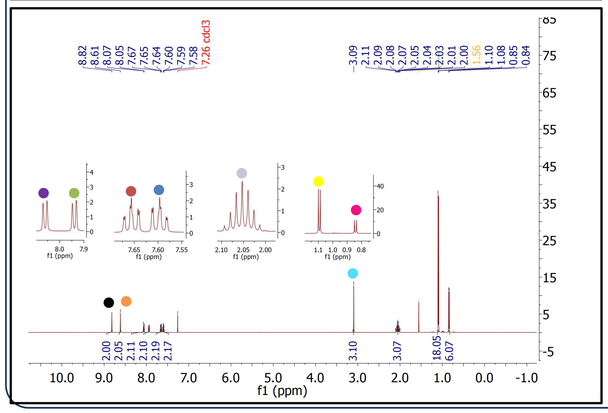
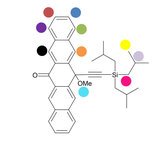
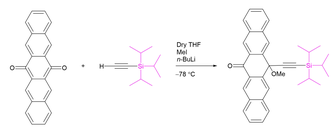






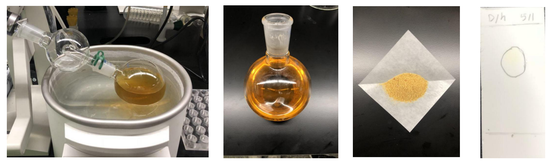


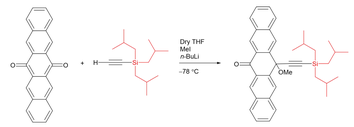
Synthesis of the precursor



4

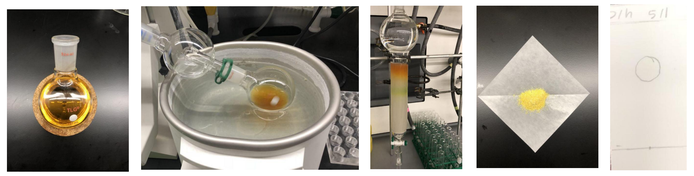
- Purification of **4** by recrystallization CH_2Cl_2/MeOH)





5

- Purification of **5** by column chromatography (CH_2Cl_2/hexanes b5:1)



Conclusion

- Compound **3** is synthesized in 16% as a dark blue solid.
- By having sterically hindered pentacenes such as molecule **3**, pentacenes cannot approach each other anymore, so aggregation and reactivity is reduced.
- Compound **4** is synthesized in 40% as a pale orange solid.
- Compound **5** is synthesized in 50% as a bright yellow solid.
- Compound **4** and **5** can be used as precursors for synthesizing pentacene dimers for SF.

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References

[1] J. E. Anthony, *Chem. Rev.* 2006, *106*, 5028-5048.
[2] J. L. Marshall, D. Lehnherr, B. D. Lindner, R. R. Tykwinski, *ChemPlusChem* 2017, *82*, 967-1001.
[3] P. Sullivan, T. Jones, *Organic Electronics* 2008, *9*, 656-660.
[4] Zirzlmeier, J., Lehnherr, D., Coto, P. B., Chernick, E. T., Casillas, R., Basel, B. S., Guldi, D. M. *Proc. Natl. Acad. Sci.* 2015, 112(17), 5325-5330.