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Supramolecular π-donor/acceptor arrays based on metal-organic cage inclusion complexes

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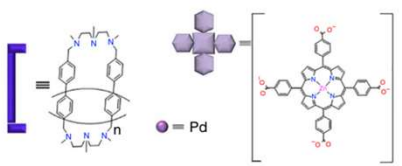
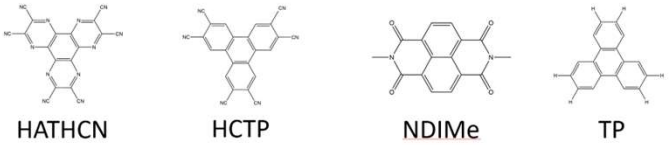
Background

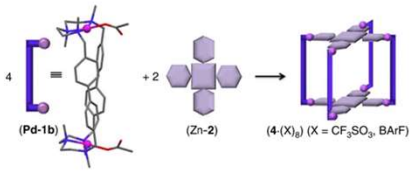
Tetragonal Prismatic Nanocage

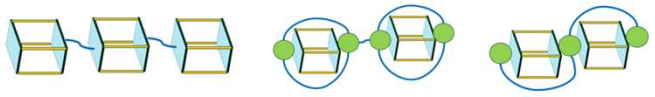


Guest Molecules (π-acceptors)



Establishing Structural Control

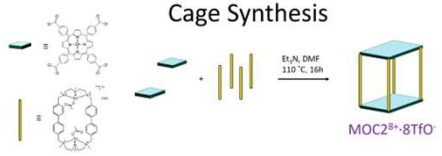


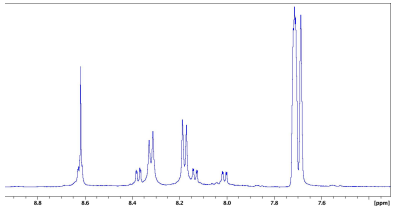


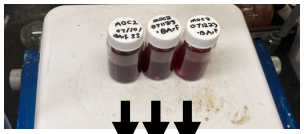
Ribas et al.
Nat. Comm. 5, 5557, (2014)

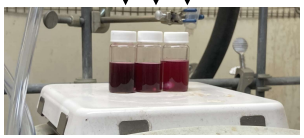
Analyze Conductive Properties

Synthesis

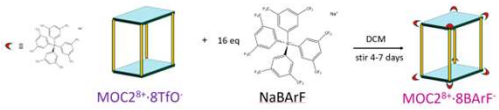








Ion Exchange

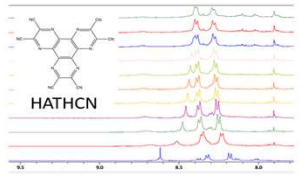


Ion Exchange Date	Equivalents of BArF	Duration (days)	Percent yield (%)	Percent Change
1/24/23*	10	1	20.80	0%
6/26/23	15	2	35.57	+71%
6/29/23	15	4	42.66	+105%
7/10/23	16	7	29.55	+42%
7/11/23	16	6	48.72	+134%
7/12/23	16	7	64.07	+208%

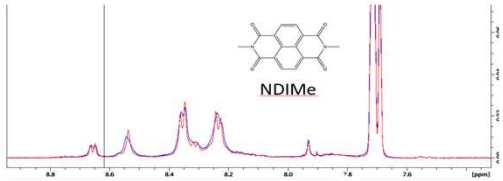
* This experiment was used as a reference and took place before the beginning of the REU program.

Characterization

NMR Titrations

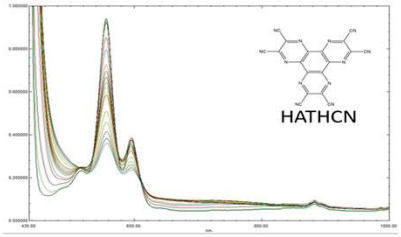


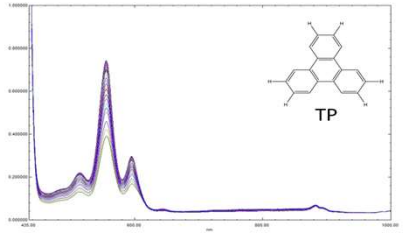
Pyrrole peak shift



Guests take time to equilibrate into cages

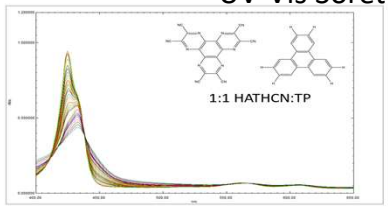
UV-Vis Q-Band Titrations

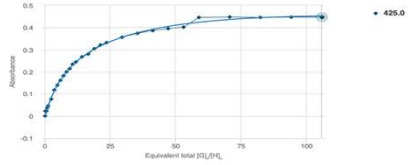




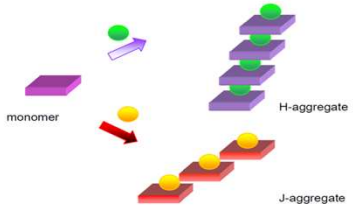
Charge band from 600-800 nm

UV-Vis Soret Band Titration





Soret band initially at 425 nm



Parameter (bounds)	Optimised	Error	Initial
K_{11} (0 → ∞)	101514.27 M^{-1}	± 6.3227 %	1000.00 M^{-1}
K_{12} (0 → ∞)	10256.14 M^{-1}	± 5.8663 %	100.00 M^{-1}

Rita Giovannetti (2012). The Use of Spectrophotometry UV-Vis for the Study of Porphyrins, Macro To Nano Spectroscopy, Dr. Jamal Uddin (Ed.), ISBN: 978-953-51-0664-7

Summary

- Optimized the ion exchange yield due to prolonged stirring and the addition of more BArF
- Synthesized substantial amounts of MOC2 to continue the project (~100 mg)
- Investigated guest equilibration in and guest stacking on cage inclusion complexes
- Further research would be focused on structural control mechanisms and their conductive properties

Acknowledgements

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