

Functionalization of 1,3,6,8-Tetraazapyrene for fused Donor-Acceptor EnsemblesI. Kolly¹, P. Zhou¹, R. Häner^{1*}, S. X. Liu^{1*}¹Department of Chemistry, Biochemistry, and Pharmaceutical Sciences, University of Bern, Freiestrasse 3, 3012 Bern, Switzerland

Controllable charge-transfer pathways in molecular ensembles are key characteristics for the successful fabrication of organic electronics. To approach this goal, multiple strategies can be followed. For instance, oxidation or reduction can be used to control charge transfer in a chemical way. With this purpose, efficient synthetic approaches to tetrathiafulvalene (TTF)-based electron donor-acceptor (D-A) ensembles were developed.^[1] To achieve TTF-annulated D-A systems, tetraazapyrene (TAP) was introduced as a p-conjugated electron acceptor.^[2] This work focusses on the synthesis of the TAP building blocks (Figure 1) which are the core compounds of the conjugated ensembles. The construction of the TAP core contains a multi-step reaction starting with nitration of 1,5-dinitronaphthalene followed by reduction to obtain a tin salt.^[3] The electronic properties of the resulting D-A ensembles are described in detail.

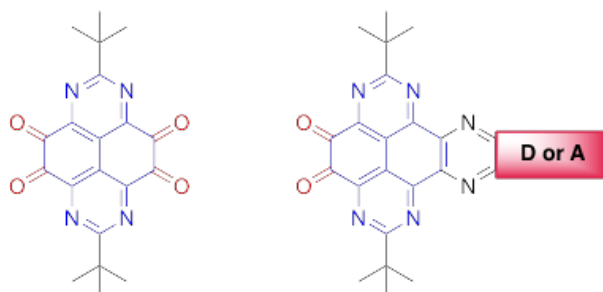


Figure 1: TAP building blocks for Schiff-base reactions

[1] Ping Zhou, Ulrich Aschauer, Silvio Decurtins, Thomas Feurer, Robert Häner, Shi-Xia Liu, *Chem. Commun.*, **2020**, 56, 13421.

[2] Ping Zhou, Ulrich Aschauer, Silvio Decurtins, Thomas Feurer, Robert Häner, Shi-Xia Liu, *Chem. Commun.*, **2021**, 57, 12972.

[3] Sonja Geib, Susanne C. Martens, Ute Zschieschang, Florian Lombeck, Hubert Wadepohl, Hagen Klauk, Lutz H. Gade, *J. Org. Chem.*, **2012**, 77, 6107.