Porphyrin stacks organized by multivalent interactions

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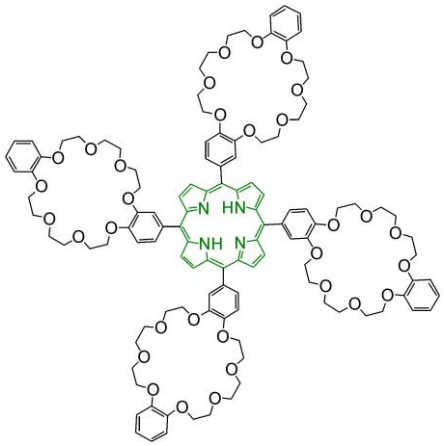

Abstract:

In order to investigate multivalent binding in synthetic pseudorotaxanes, the synthesis of tetravalent porphyrins substituted with crown ethers (host) and secondary ammonium ions (guest) is required for an extension of previous studies on di- and trivalent pseudorotaxanes.
The project comprises the following steps:

a) Design of suitable hosts and guests by molecular modelling. In particular, the spacer structure must carefully be considered to avoid unfavourable strain in the final complexes.
b) Synthesis of the host and guest compounds. The synthesis should preferably be modular so that small structural variations are easy to achieve.
c) Binding studies by MS, NMR (binding motifs and structure determination of the complex) and ITC (thermochemical data). In these studies, a double mutant cycle analysis must be performed in order to obtain insight into the allosteric and chelate cooperativity of host-guest binding.
d) Investigation of other properties, for example the optical properties of the porphyrins, potential energy transfer processes between the two porphyrins and the like.
e) Preparation of supramolecular polymers based on the tetravalent compounds and their characterization.

The project is based on previous work in our groups; expertise in the synthesis of such compounds, the thermodynamic analysis and the assessment of cooperativity exists.

Publication/s:

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W. Jiang, K. Nowosinski, N. L. Löw, E. V. Dzyuba, F. Klautzsch, A. Schäfer, J. Huuskonen, K. Rissanen, C. A. Schalley: J. Am. Chem. Soc. 2012, 134*,* 1860-1868