Exo-BODIPY, *Endo*-Alkoxy Functionalized Pd_2L_4 Cages

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Self-assembled coordination cages (SCCs) show favorable properties for an array of applications like drug delivery, host-guest chemistry, and catalysis. Modification of the SCCs interiors by installation of *endo* facing functionalities on the constituent ligands gives control over properties like guest binding, catalytic activity, or inducement of self-sorting effects.[1] Additionally, SCCs have received increasing attention for light harvesting applications, as their reliable self-assembly is predestined to arrange multiple chromophoric units in a fixed spatial arrangement, thus facilitating control over the rates of energy transfer. [2]

In this study we present the synthesis of a series of *endo*-alkoxy, *exo*-BODIPY functionalized 1,3-bis(3-pyridyl) ligands and their self-assembly into Pd_2L_4 coordination cages (Figure 1). All these cages show intense fluorescence which may be harnessed for light harvesting applications. Additionally, these complexes show distinct changes in their ^{1}H-NMR spectra, dependent on the length of the *endo* facing alkoxy groups, thus highlighting the impact such modifications may have on the self-assembly of SCCs.

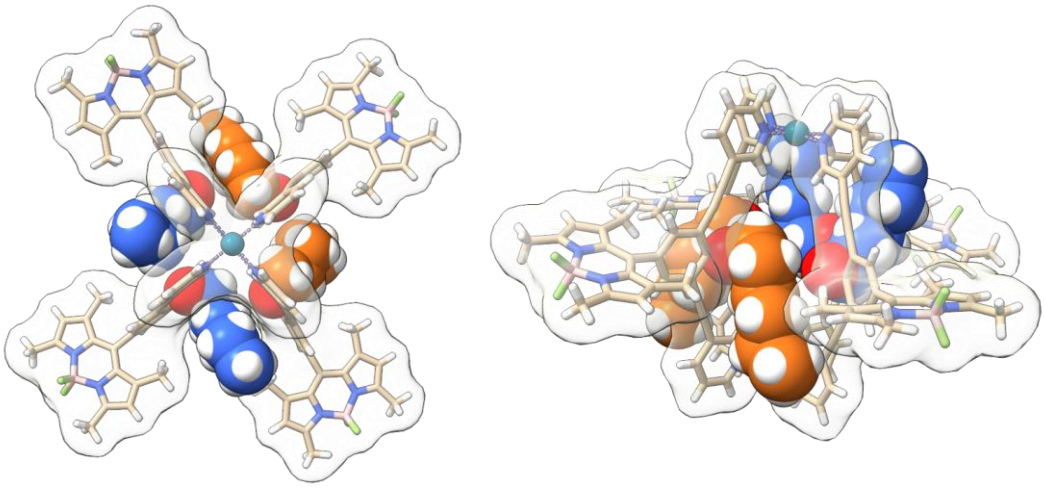

Figure 1: Crystal Structure of a self-assembled Pd_2L_4 cage. The *endo* directed hexadecyloxy-chains are closely packed between the backbones of two neighboring ligands and point either up or down (marked in blue and orange, respectively).

References:

[1] P.M. Bogie, T.F. Miller, R.J. Hooley, *Isr. J. Chem.* **2019**, 59, 130-139.
[2] P. Jia, et. al., *J. Am. Soc.* **2021**, 143, 1 399-408.