

# Statistical Self-Assembly of Catalytically Active Heteroleptic Metallosupramolecular Cages

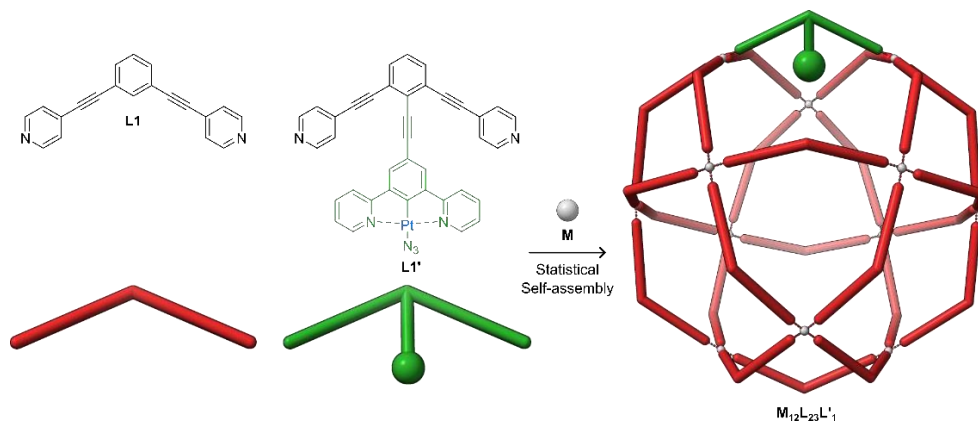
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The concept of catalytically active metallosupramolecular cages is inspired by nature's enzymes and mimics their confined microenvironments that allow selective chemical transformations.<sup>[1]</sup> The envisioned discrete heteroleptic  $M_2L_4$  or  $M_{12}L_{24}$  cages consist of concave bis(pyridyl) ligands and Pd(II) or Pt(II) cations. In a statistical approach, NCN-Pt-azide *endo*-functionalized analogues of the ligands will be incorporated into the cages. Post-assembly, the catalytically active species is obtained *via* photochemically induced  $N_2$  loss and the formed metallonitrene can undergo C–H insertion reactions with aldehydes to give amides *via* nitrogen atom transfer.<sup>[2]</sup>



**Figure 1:** Example of a statistically self-assembled heteroleptic  $M_{12}L_{24-x}L'_x$  cage.

A library of ligands containing different chromophores will be synthesized and studied, to obtain light-harvesting cages that facilitate the light induced nitrene formation.

## References:

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- [2] a) T. Schmidt-Räntsch, H. Verplancke, J. N. Lienert, S. Demeshko, M. Otte, G. P. van Trieste, K. A. Reid, J. H. Reibenspies, D. C. Powers, M. C. Holthausen, S. Schneider, *Angew. Chem. Int. Ed.* **2022**, 61, e202115626