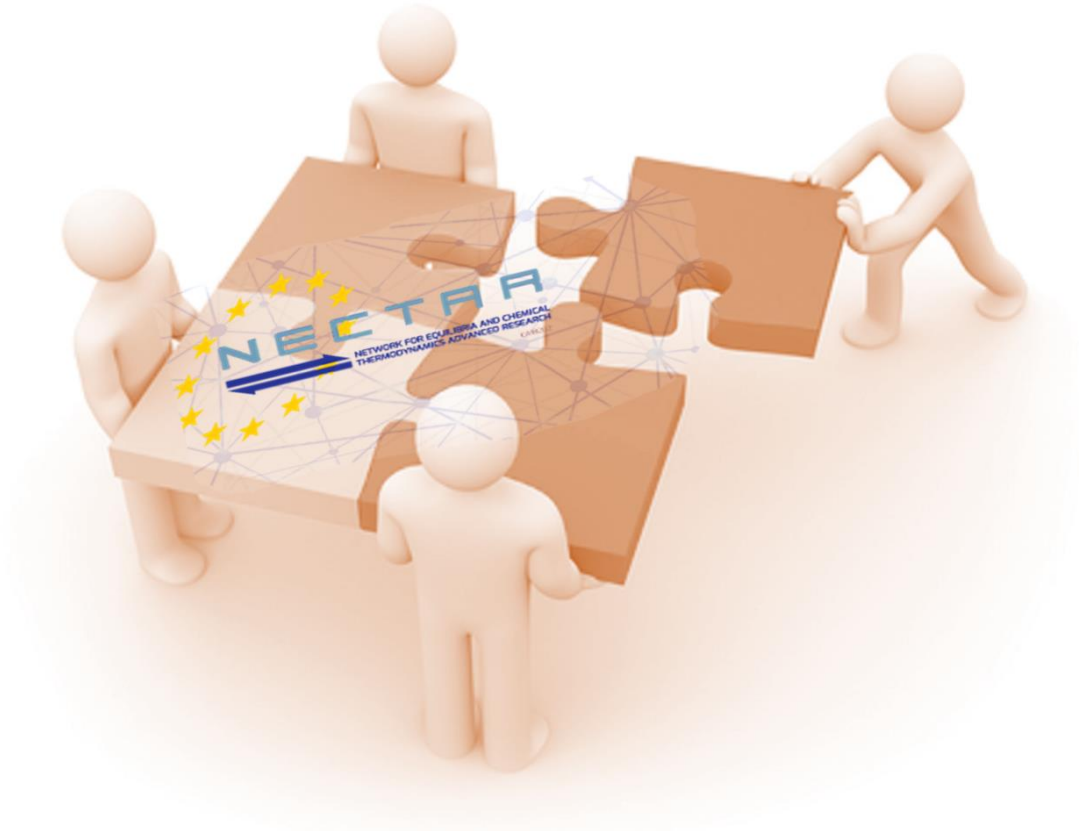
NECTAR's Spring Web-meeting

COST ACTION CA18202- NECTAR: Network for Equilibria and Chemical Thermodynamics Advanced Research



25th-26th March 2021

ONLINE

Strong complexes bearing labile ligands: challenges in catalysis with supported metal complexes

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The ideal prerequisites for a metal complex to be effectively used in catalysis surely include high thermodynamic stability and kinetic inertness towards demetallation. At the same time, ancillary/liable/fast exchangeable ligands, leaving thermodynamically and kinetically activated position(s) in the metal cation's first coordination sphere, are required for catalyst effectiveness and cycling abilities. This general picture results in the search of a perfect balance, where the complex is stable enough to remain unaltered under reaction conditions yet activated enough to display significant catalytic activity. Here we discuss some ongoing studies and past experiences (Figure 1), with CNTs-supported Pd(II) metal complexes catalysts for Sonogashira cross-coupling and oxygen reduction reaction, showing how different ligands' types (linear, tripodal, macrocyclic) come with their own pros and cons.

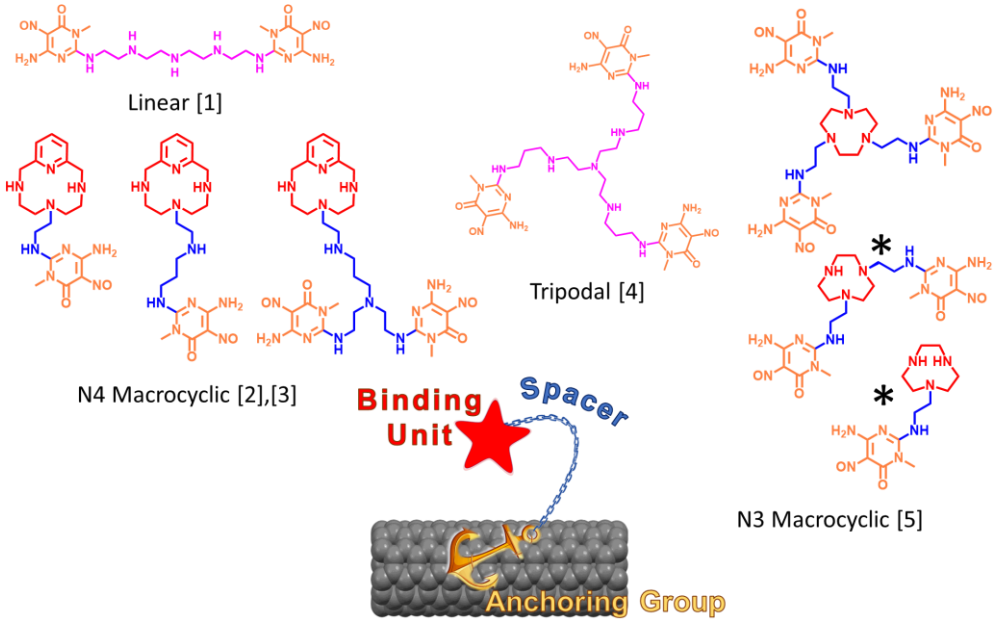

Figure 1. Some of our ligands and general scheme of CNT functionalization.

Cf. [1] *Inorg. Chim. Acta* **2020**, *511*, 11979; [2] *J. Catal*. **2017**, 533, 239 [3] *Inorg. Chem.* **2018**, 57, 14484; [4] *Inorg. Chim. Acta* **2021**, 518, 120250; [5] *Energies* **2020**, 13, 5539. * unpublished work.