

**MS18-2-2 NMR, Kinetic-Mechanistic and SC-XRD Study of Carbon Dioxide Capturing Model Molecular Materials
#MS18-2-2**

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Abstract

The effects of climate change, also brought upon by environmental pollution, has been gaining significant international awareness over the past decade and motivated many governments to upscale their efforts to achieve greenhouse gas (GHG) neutrality. A pollutant at the forefront of the GHGs is carbon dioxide (CO₂), which is considered the leading contributor (74.4%) to global warming. Global emissions of CO₂ from fossil fuels were at record levels in 2019 (36.6 GtCO₂ – down to 34 GtCO₂ in 2020), with China and the USA emitting 10.37 and 4.71 GtCO₂ respectively, in 2020. [1,2].

In this study, Platinum Group Metal (PGM) complexes and other nucleophiles were identified which displayed activities as entities which exhibit potential as CO₂ capturing/conversion catalysts to further drive the process. It firstly focused on the synthesis of a range of PGM complexes [Rh, Pt, Pd] which incorporates 1,5-cyclooctadiene (COD) as a ligand (a known π -accepting modality) in the system to offer a different probe for evaluating structural changes induced at the metal centres. The essence of this is focused primarily on utilizing accurate single-crystal X-ray diffraction (SC-XRD) to evaluate the COD conformation in the complexes and scrutinise distortions therein, as for example, described by the so-called Venus fly-trap parameters, the jaw, twist and bite dihedral angles (ψ , τ , χ). [3,4] Special focus was given to the influence the ligands have on the coordinated COD, “mimicking” the Venus fly-trap plant, see below.

The SC-XRD was then supplemented by evaluating the organometallic PGM complexes and associated nucleophiles for catalytic potential in the cycloaddition of CO₂ to an epoxide (epichlorohydrin, EPI) under ambient conditions as initially introduced by Arayachukiat et al. and Yingcharoen et al., [5,6] but focusing on detailed mechanistic and possible kinetic pathways involved. Several carefully studied parameters will be discussed in this presentation, which include the effects of (i) a range of acids based on their Bronsted acidity (pKa values) and number of acidic protons, (ii) [(Bu₄N)I], (iii) [EPI], (iv) [CO₂] under atmospheric pressure, and (v) [Metal complex].

References

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Venus fly-trap leaf mimicking COD ligand

