Contribution ID: **117** Type: **Poster**

Anion receptor design for the development of $[PtCl_6]^{2-}$ selective reagents

The word document has the full version of the Abstract, and is attached under the attachments section.

The ever-increasing demand for Platinum Group Metals (PGM's), coupled with their low natural abundance and complex processes required for their extraction has rendered this rare group of metals as the most sought after in the advent of the 21st century. Consequently, there is an increasing need to engineer new reagents with molecular functionalities that offer high selectivity and loading capacities. This will enable more efficient recovery of PGM chlorido species from feed solutions derived from mineral ores, and also secondary sources such as spent catalytic converters. The innovation of the aforesaid reagents undoubtedly requires a design strategy that considers both the electronic and stereochemical requirements of the target anion. Herein, a two-fold anion receptor design method for developing highly selective reagents for $[PtCl_6]^{2-}$ in HCl medium is reported (Figure 1).

Through a combination of theory, molecular modelling techniques and crystallography (see below), we were able to prove that derivatization of the protonated form of triethylenetetramine, ([TETAH4]4+), by R groups offers greater complementarity to $[PtCl_6]^{2-}$ (lower ΔU_{reorg}) and hence higher binding energies to the anion in silico.

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Session Classification: SIG Poster

Track Classification: SIG Seminar: Chemistry, Material Science and Health Science