

## FUNCTIONALIZED SILICA GEL WITH THIOURONIUM GROUPS FOR RECOVERY PRECIOUS METALS: EXPERIMENTAL AND THEORETICAL STUDIES.

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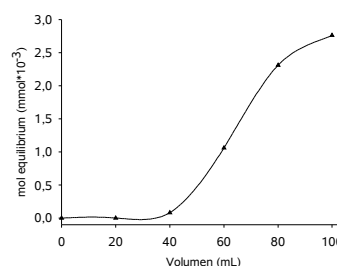
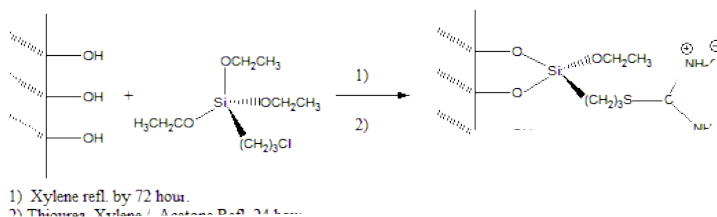
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**Abstract** – The silylant agent 3-cloropropyltriethoxisilyl was immobilized on silica gel in anhydrous conditions and after reagent with thiourea to obtain thiuronium salt functionalized silica gel. The product was characterized by  $S_{BET}$ , Termo gravimetry TG, infrared spectroscopy, silicon and carbon NMR in solid state. The signal assignment ( FTIR and NMR ) and the coordinate form or ionic exchange mechanism for the chemisorb palladium complexes was studied by a computational approach using the Amsterdam Density Functional (ADF) software. This work was done to use the modified inorganic support to recover precious metals.

The modification of inorganic supports such as silica gel has been employed in heterogeneous catalysis, ionic chromatography, chemisorptions of interesting metals and industrial applications, because its high stability in front of extreme conditions of pH and temperature<sup>1,2</sup>. The modified inorganic support with thiuronium groups were synthesized in anhydrous conditions, figure 1, and were characterized using  $S_{BET}$ , FT-IR, TGM, <sup>29</sup>Si-NMR and <sup>13</sup>C-NMR solid state<sup>3</sup>. The modification of the matrix produce a decrease in the area in relation to the unmodified matrix, that can be seen in the 463, 6 m<sup>2</sup> g<sup>-1</sup> silica gel area changed to 388, 0 m<sup>2</sup> g<sup>-1</sup> for the Thiuronium group. This fact can be due to the difficulty of the gaseous nitrogen to reach the pores of the functionalized matrix<sup>4</sup>. Although it is difficult to assign all the FTIR characteristic absorption bands of the organic moiety due to the high intensity of the silica gel matrix, masking some of the C-H stretching, the observed frequency bands are comparable with those obtained by theoretical calculations.

The organofunctionalization grade for modified matrix was 0, 5974 mmol g<sup>-1</sup> for nitrogen and 0, 9758 mmol g<sup>-1</sup> for sulfur. To explore the adsorption capacities of the 0,2 g of the modified silica gel, we analyzed the concentration Palladium (II) in the eluted solution when 100 mL of 0,7894 mol/L of solution passed through the column; the graph of adsorption has a form of distorted S, figure 2, it is observed an inflection point when around 60 ml of solution were passed through the column, corresponding to 0, 0727 mmol of palladium (II) retained in the column<sup>4</sup>.

DFT calculations were employed to study the electronic properties of this compound<sup>5</sup>. The geometry optimization using LDA and GGA (PW91) functionals and the conformations energies were calculated for some model systems of coordination of thiuronium to Pd(II).



**Figure 1.** Reactions of functionalized silica gel with sililant agents and his modified. **Figure 2:** Absorption Tetrachlorine palladium (II) on the modified silica gel.

### References

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