^{1}H-NMR and MALDI investigation of thiol-exchange reaction in $Au_{25}(SR)_{18}$ cluster

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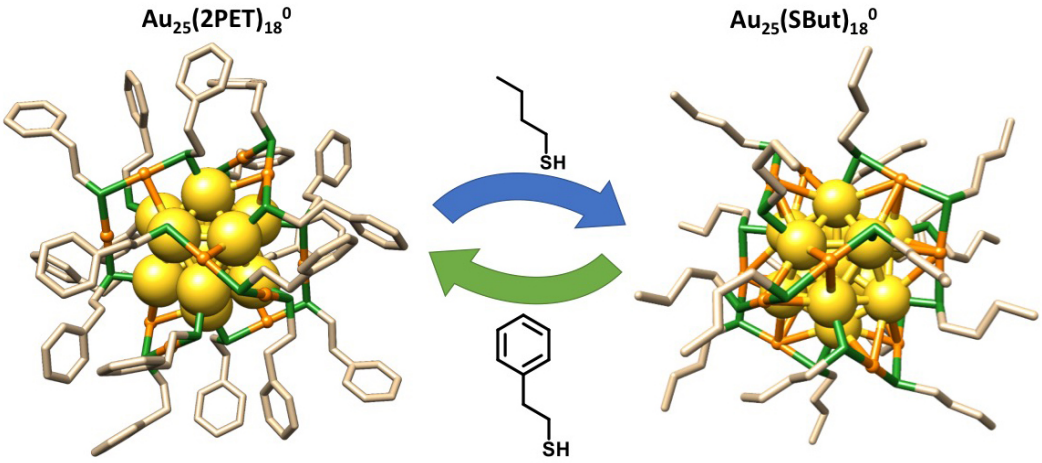
Small thiol protected gold nanoparticles (< 2nm), also known as gold cluster, are self-assembled systems formed by Au(0) core and a thiol protecting monolayer. The latter is fundamental not only for stabilization and solubility of the clusters themselves, but also is the principal responsible for their reactivity.[1] One of the most frequent reactions used to functionalized the monolayer are the thiol-exchange reactions.[2]. These reactions usually present difficulties in controlling the number of substitutions and the reaction time can vary from minutes to days. In this study we investigated the thiol-exchange reaction using nuclear magnetic resonance (NMR) spectroscopy and MALDI analysis.[3] Kinetic studies were performed on $Au_{25}(SC_2H_4Ph)_{18}$ exchange with butane thiol and vice versa ($Au_{25}(SButane)_{18}$ exchange with HSC_2H_4Ph, Figure 1). By these studies, were possible to understand: 1) the affinity of different thiol ligands towards the Au_{25} cluster, 2) calculating the number of thiols exchange, 3) the position of exchange and 4) obtaining the relative binding constants. From this information was possible to gain a clearer picture on the mechanism of this reaction that can help in fine-tuning the functionality of the monolayer.



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