Prolate-Shaped NHC-Protected Gold Nanoclusters and their Applications

NHCs have emerged as valuable protecting ligands in the synthesis of gold nanoclusters. In this work, we use a single, simple NHC to synthesize three distinct prolate-shaped clusters and demonstrate their viability as electrocatalysts and bioimaging tools. First, we optimize a molecular precursor to prepare an unprecedented N-heterocyclic carbene-stabilized hydrido gold nanocluster, $[Au_{24}(NHC)_{14}Cl_2H_3]^{3+}$. This cluster comprises a dimer of two Au_{12} kernels, each adopting an icosahedral shape with one missing vertex. The two kernels are joined through triangular faces, which are capped with three hydrides. The reactivity of this $Au_{24}H_3$ cluster in the electrocatalytic reduction reaction of CO_2 is demonstrated and benchmarked against related catalysts. Using the same NHC and the addition of thiol ligands, we expanded the scope of available clusters to larger Au_{25} and Au_{37} clusters stabilized by a combination of NHCs and thiols. The bi- and tri-icosahedral clusters are characterized by ESI-MS, NMR, UV-Vis, SCXRD and DFT studies. The clusters displayed unusually long emission wavelengths. NIR-II imaging demonstrates the clusters' emission in aqueous media and their potential in bioimaging applications.