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Effect of cyclodextrin on the size distribution of the Au nanoparticles stabilized by rutin

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Abstract

The effect of α- and β-cyclodextrin on the formation of nanoparticles in $HAuCl_4$ rutin system was studied. The range of cyclodextrin concentration from $2.5 \cdot 10^{-4}$ M to $5 \cdot 10^{-3}$ M and influence of the sequence of initial components mixing were investigated. It is found that in the presence of α- and β-cyclodextrin the hydrodynamic radius of small gold nanoparticles decreases from 2.5 nm to 1 nm. It is concluded that the stabilized gold nanoparticles have interactions with with cyclodextrin, and rutin as well . In the systems studied cyclodextrin molecule evokes the association of larger gold nanoparticles perhaps due to hydrogen bonds between sugar residues of the rutin in the ligand shell of nanoparticles and cyclodextrin. The formation of aggregated nanoparticles hinders to diagnose the particle size by dynamic light scattering. Therefore, to clarify polymodal particle size distributions in the initial solutions it was used centrifugation. With the help of calculations by PBE density functional method the structure of supramolecular neutral and positively charged adducts of Au_{13} cluster with β-cyclodextrin modeling partially oxidized $Au_{13}L$ cluster due to the presence of ligand shell L. The quantum-chemical study carried out shows that under stabilization of Au_{13} cluster by β-cyclodextrin molecule about half of the gold atoms can coordinate additional ligands from a solution. Rutin ligands having several chelating units can not provide full coverage of all atoms of the outer part of the cluster upon binding to the surface atoms Au_{13} cluster due to steric hindrance. Free surface atoms of gold are good candidates for activation of substrates, including light alkanes. However, routin degradation products formed during its deep oxidation under the influence of $HAuCl_4$ can block the active sites available on the surface of the Au nanoclusters stabilized. It is considered variation of methods of synthesis of gold nanoclusters stabilized with cyclodextrin in order to form catalytic sites capable to activate C-H bonds of light alkanes under mild conditions.

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