

Supporting Information

Superior Oxygen Stability of *N*-Heterocyclic Carbene-coated Au Nanocrystals – Comparison with Dodecanethiol

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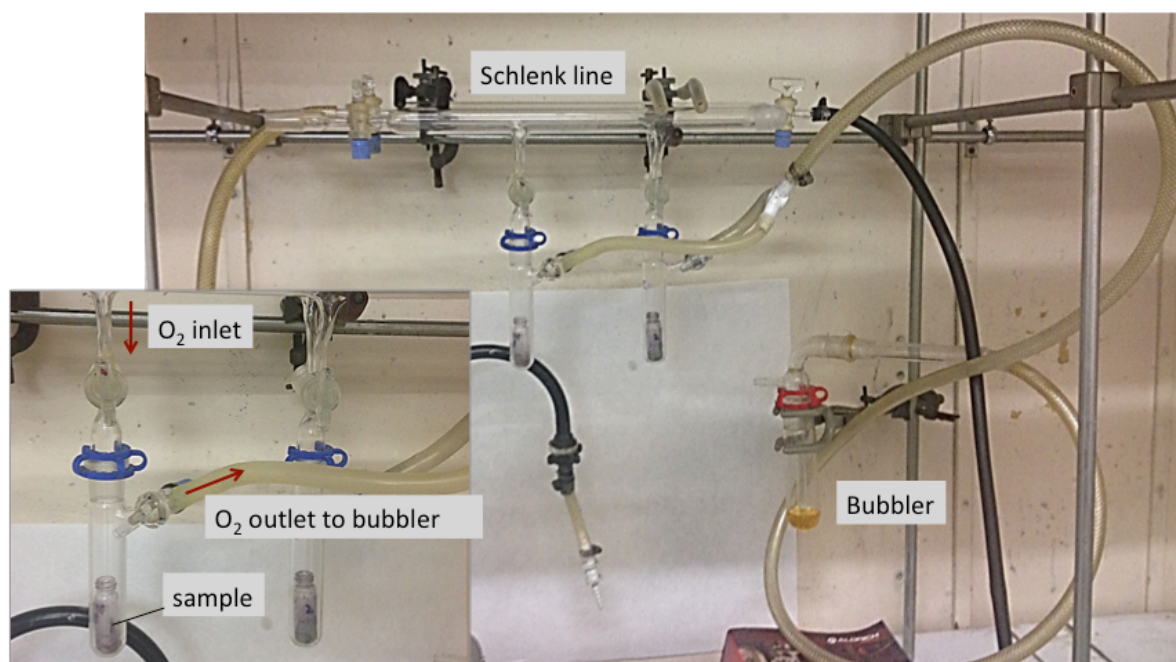


Figure S1. Set-up for one-week exposure of Au nanocrystals to molecular oxygen at a pressure of c.a. 1 atm. The vacuum/O₂ manifold (“Schlenk line”) was used to evaporate the solvent at the beginning of the experiment and introduce gaseous molecular oxygen. The gas outlet was equipped with a bubbler system. A slight flow of O₂ was maintained (c.a. one bubble every 5 s) so as the sample remains under oxygen for the time required.

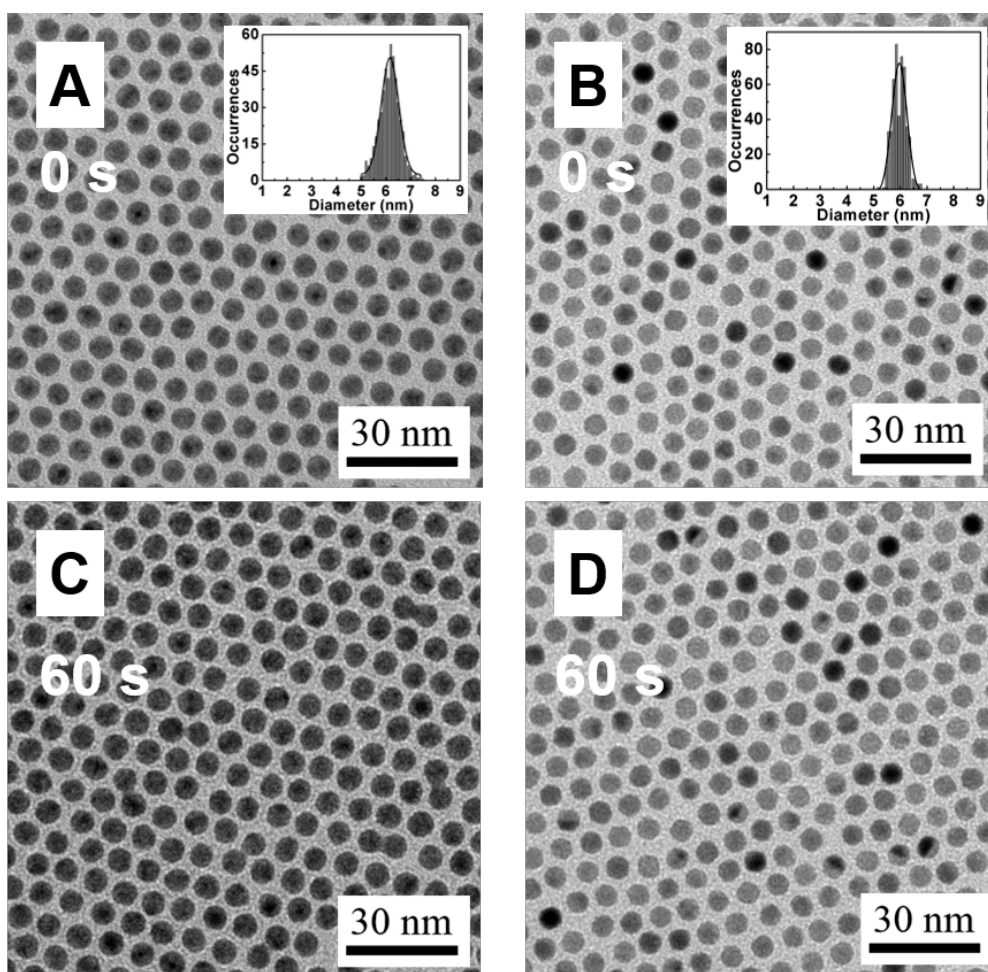


Figure S2. TEM images of $^{DDT}Au^1$ (A) and $^{DDT}Au^2$ (B), deposited on a TEM grid covered by amorphous carbon, before oxygen plasma exposure. Same areas after exposure to oxygen plasma for 60 s at 10 W : (C) $^{DDT}Au^1$ and (D) $^{DDT}Au^2$.

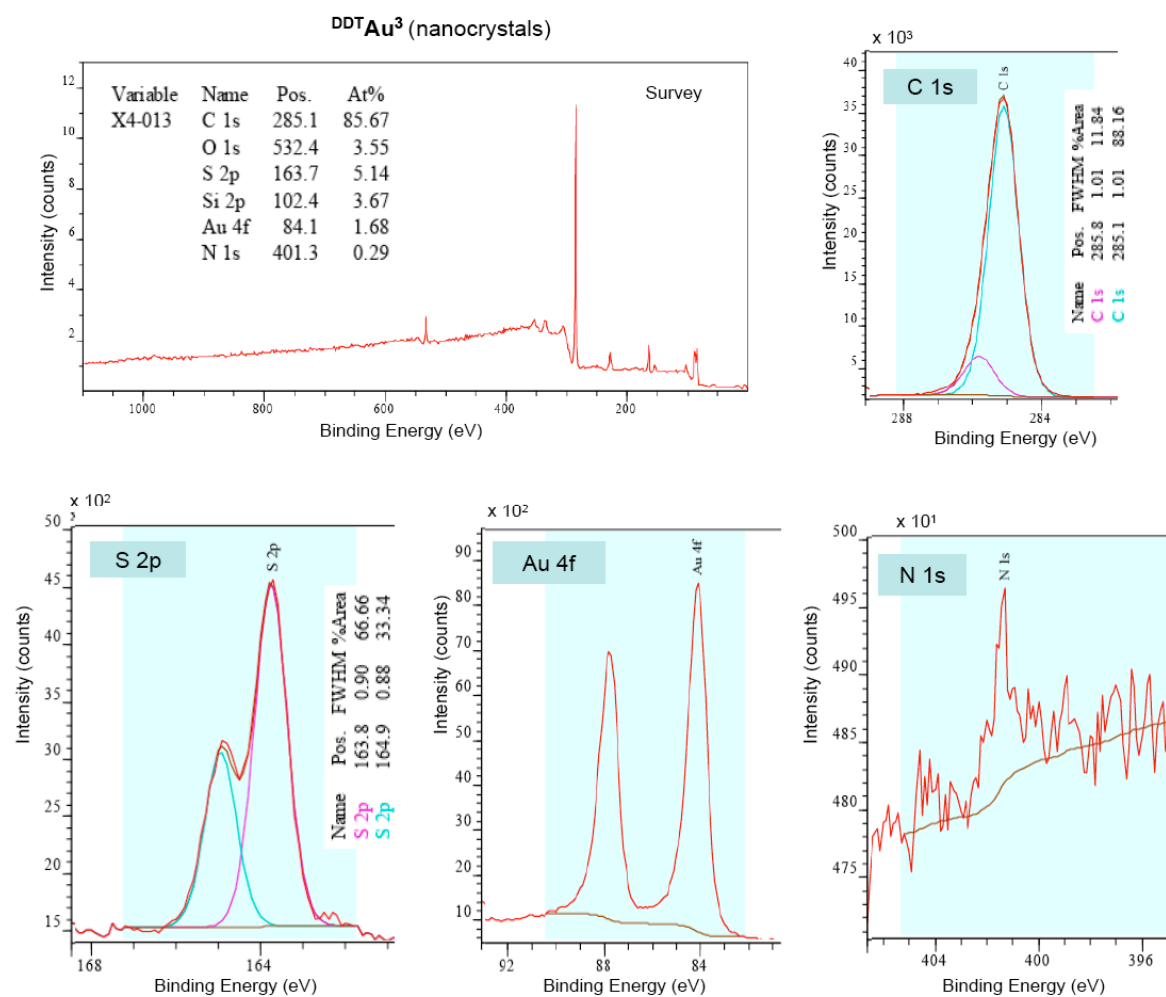


Figure S3. XPS spectra of **DDT⁺Au³⁺**. The following ratio are obtained from the data : S/Au = 3.1 ; N/Au = 0.17 ; S/N = 17.7. Under the assumption that the only nitrogen source is the NHC ligand, this leads to S/NHC = 35.4 and NHC/Au = 0.086.

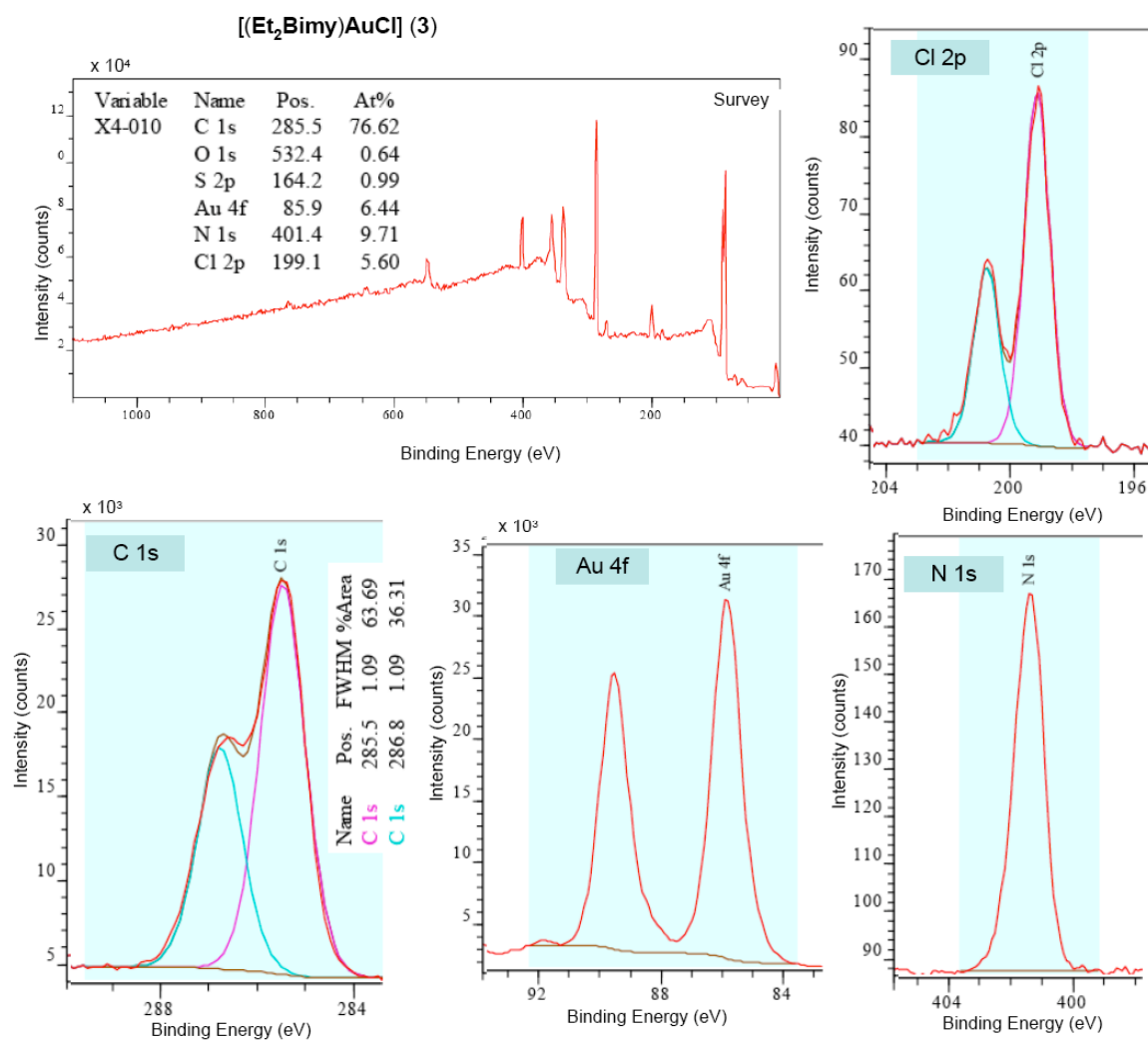


Figure S4. XPS spectra of the well-defined gold(I) complex [(Et₂Bimy)AuCl] (3).

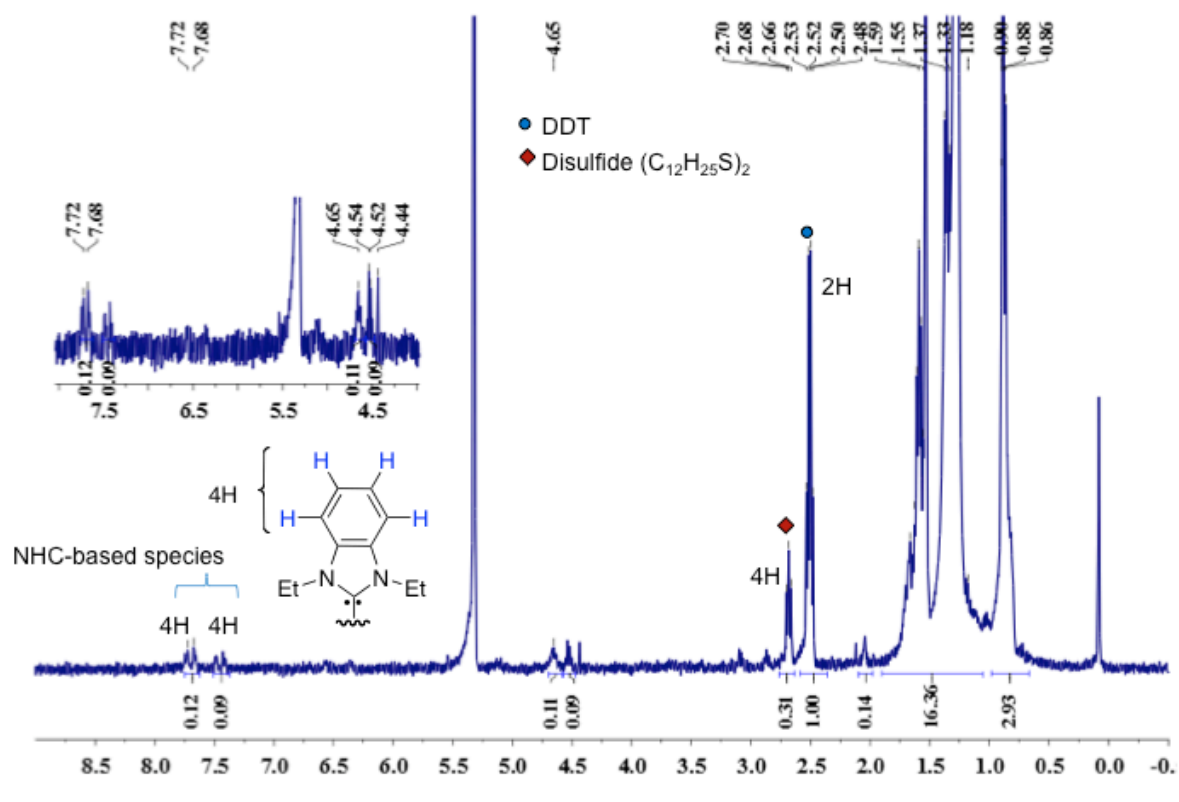


Figure S5. ^1H NMR spectrum of $^{\text{DDT}}\text{Au}^3$ in CD_2Cl_2 (400 MHz). DDT = dodecanethiol ($\text{C}_{12}\text{H}_{25}\text{SH}$).

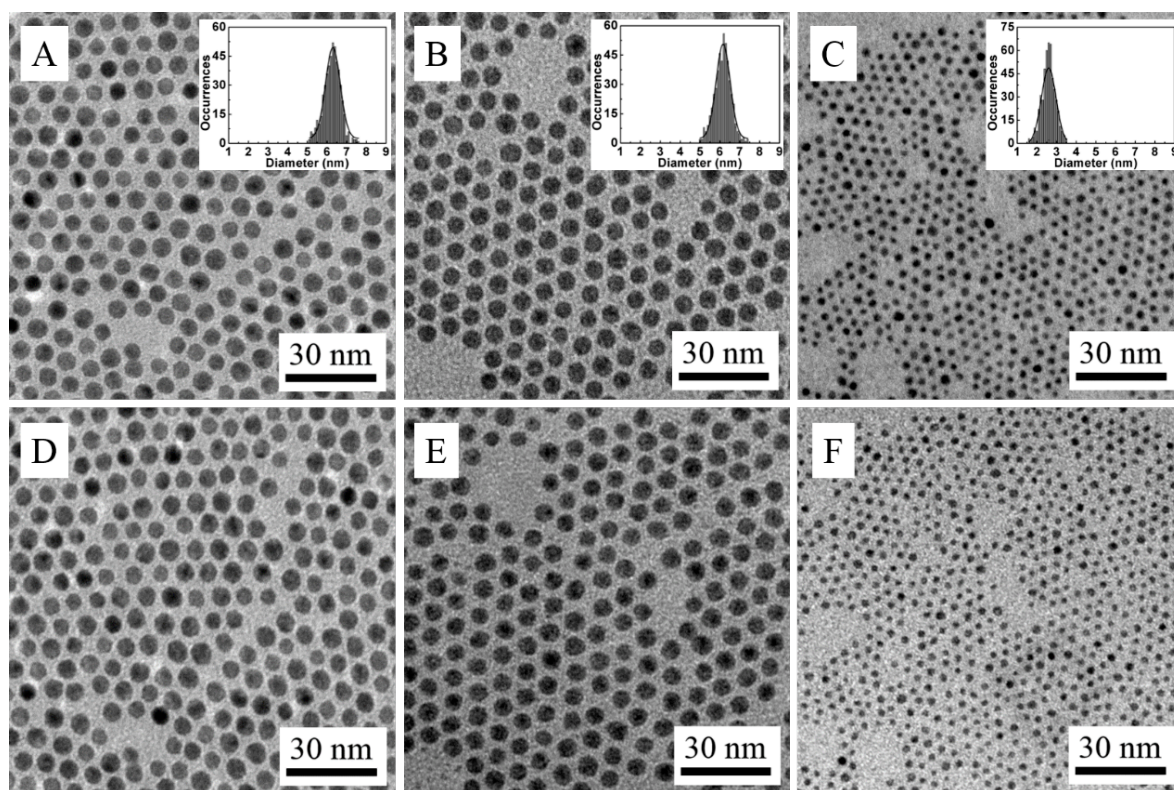


Figure S6. TEM images of $^{DDT}Au^3$ (A), $^{DDT}Au^4$ (B), and $^{DDT}Au^5$ (C), deposited on a TEM grid covered by amorphous carbon, before oxygen plasma exposure. Same areas after exposure to oxygen plasma for 60 s at 10 W : (D) $^{DDT}Au^3$, (E) $^{DDT}Au^4$, and (F) $^{DDT}Au^5$.

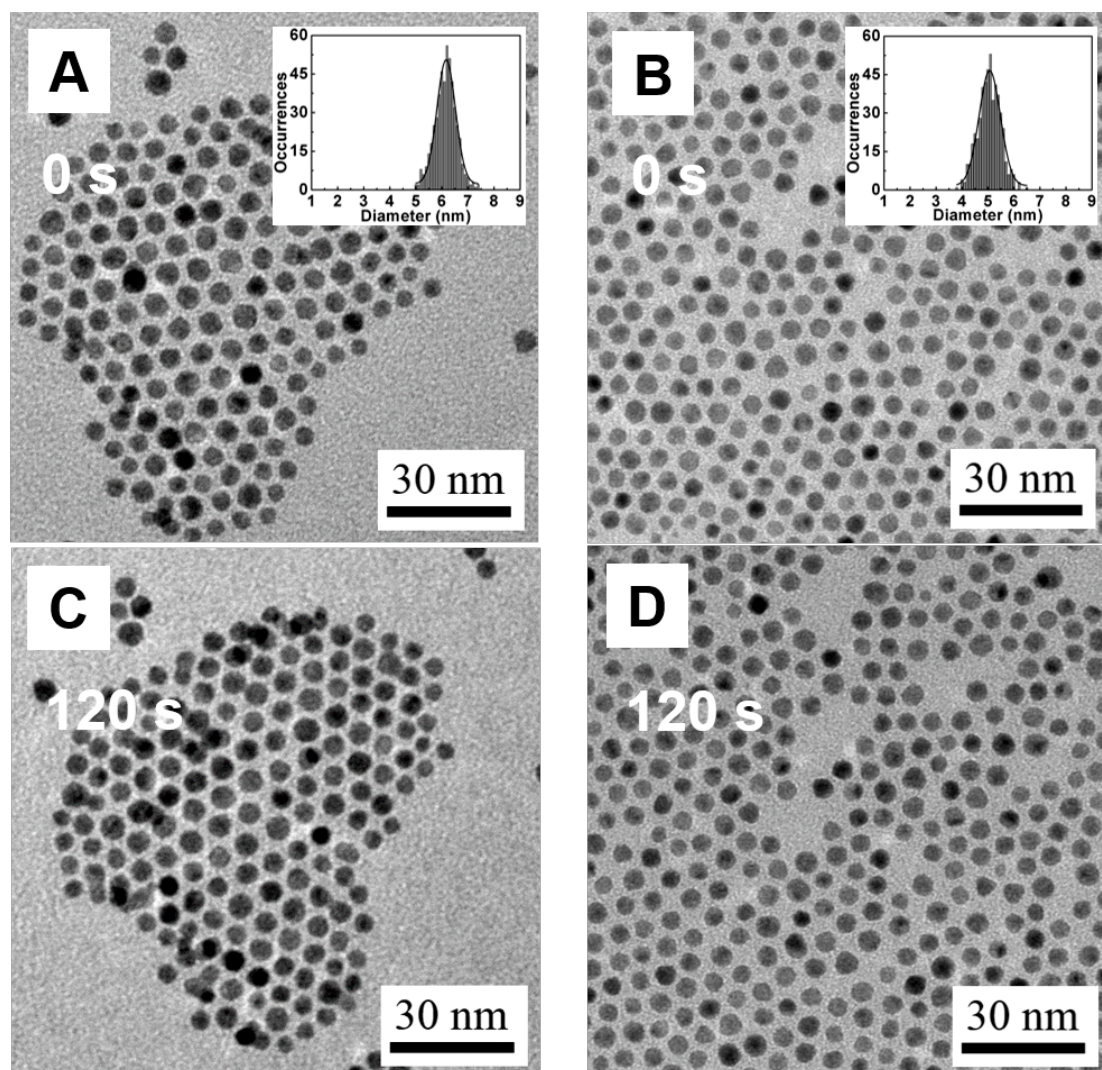


Figure S7. TEM images of ${}^{\text{NHC}}\text{Au}^7$ (A) and ${}^{\text{NHC}}\text{Au}^9$ (B) deposited on a TEM grid covered by amorphous carbon before oxygen plasma exposure. Same areas after exposure to oxygen plasma for 120 s at 10 W : (C) ${}^{\text{NHC}}\text{Au}^7$ and (D) ${}^{\text{NHC}}\text{Au}^9$.

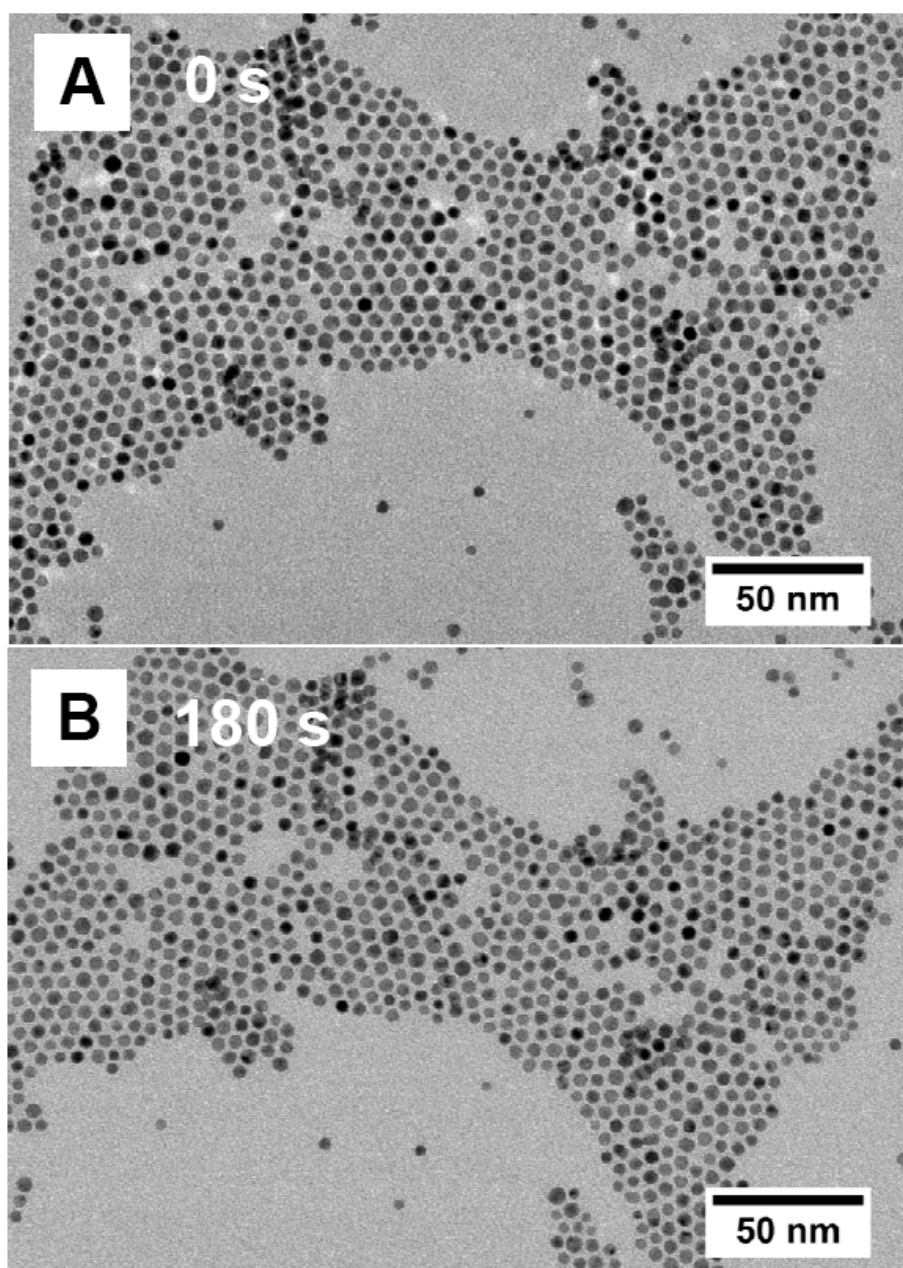


Figure S8. TEM images of $^{\text{NHC}}\text{Au}^{10}$ deposited on a TEM grid covered by amorphous carbon before (A) and after (B) oxygen plasma exposure for 180 s at 10 W.

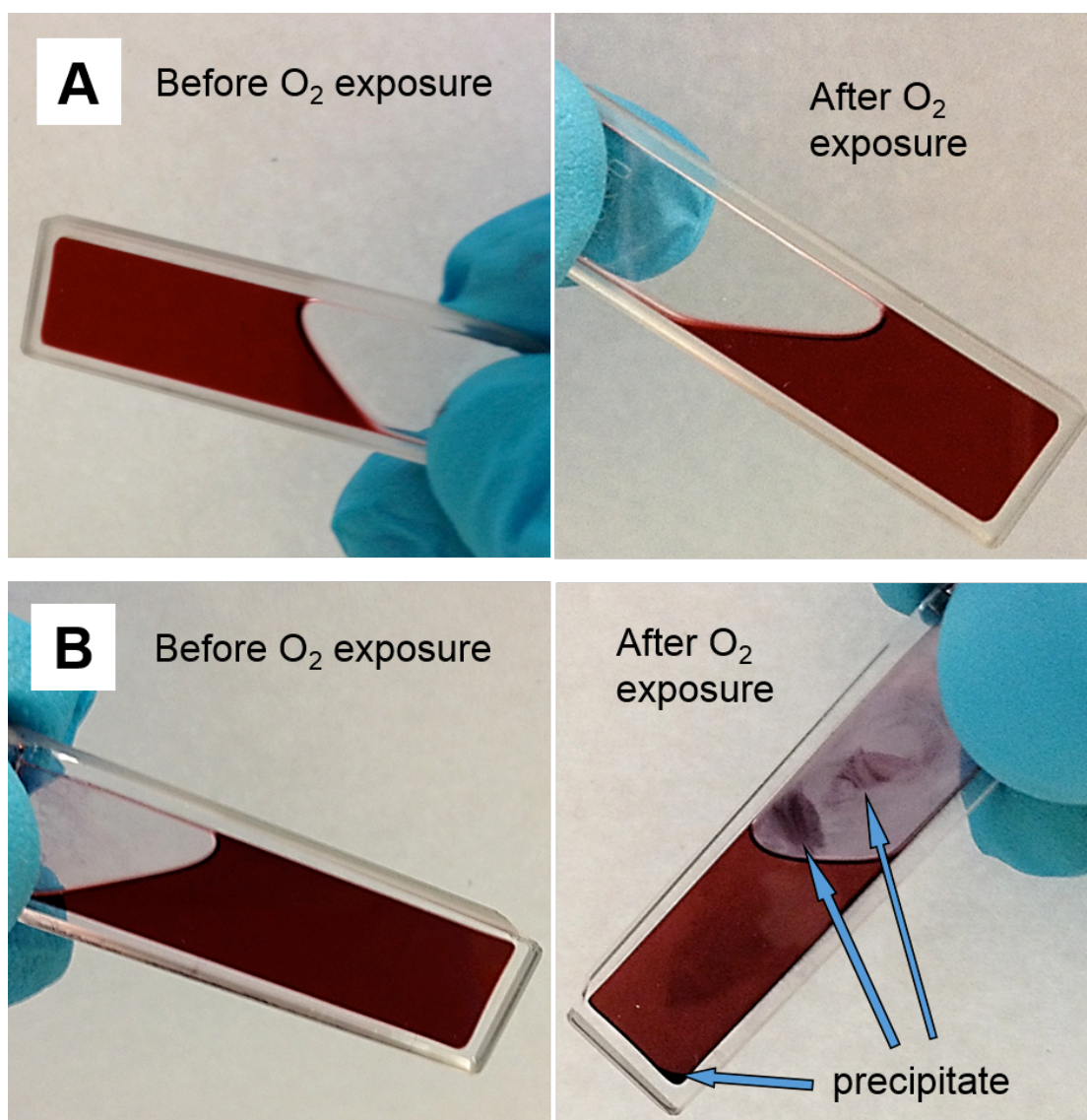


Figure S9. Photographs of dispersions in toluene of NHC-Au^{10} (A) and DDT-Au^2 (B), before (left) and after (right) one-week exposure to molecular oxygen at c.a. 1 atm. The dry NC samples were taken off with 0.6 mL of toluene, transferred into the vial and diluted 10 times (DDT-Au^2) or 12 times (NHC-Au^{10}) with toluene to increase the transparency of the solution.

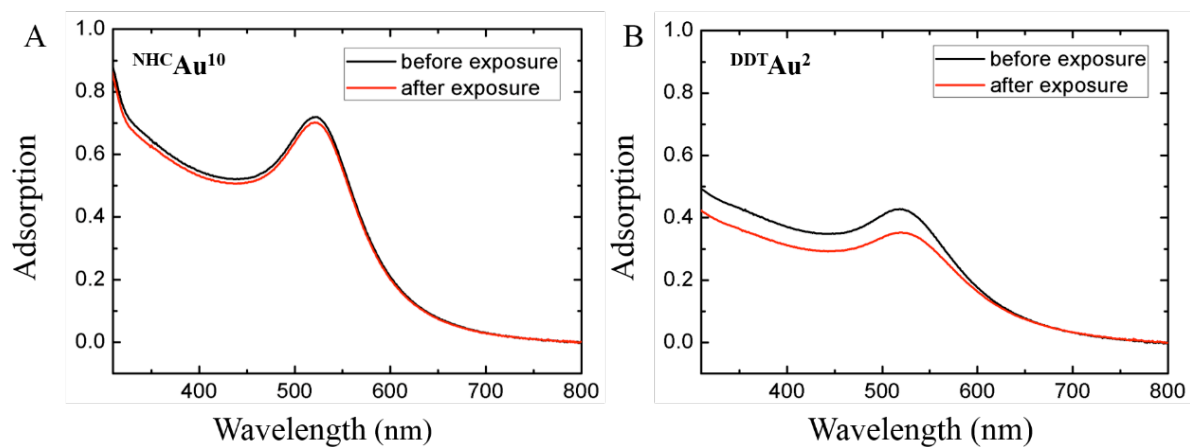


Figure S10. UV-Vis spectra of NHC-Au^{10} (A) and DDT-Au^2 (B) in toluene before and after one-week exposure to O_2 (1 Atm). A suspension of 1 mg of Au NCs in toluene (1 mL) was initially prepared, then diluted 20 times with toluene for the analysis.

Display Report

Analysis Info

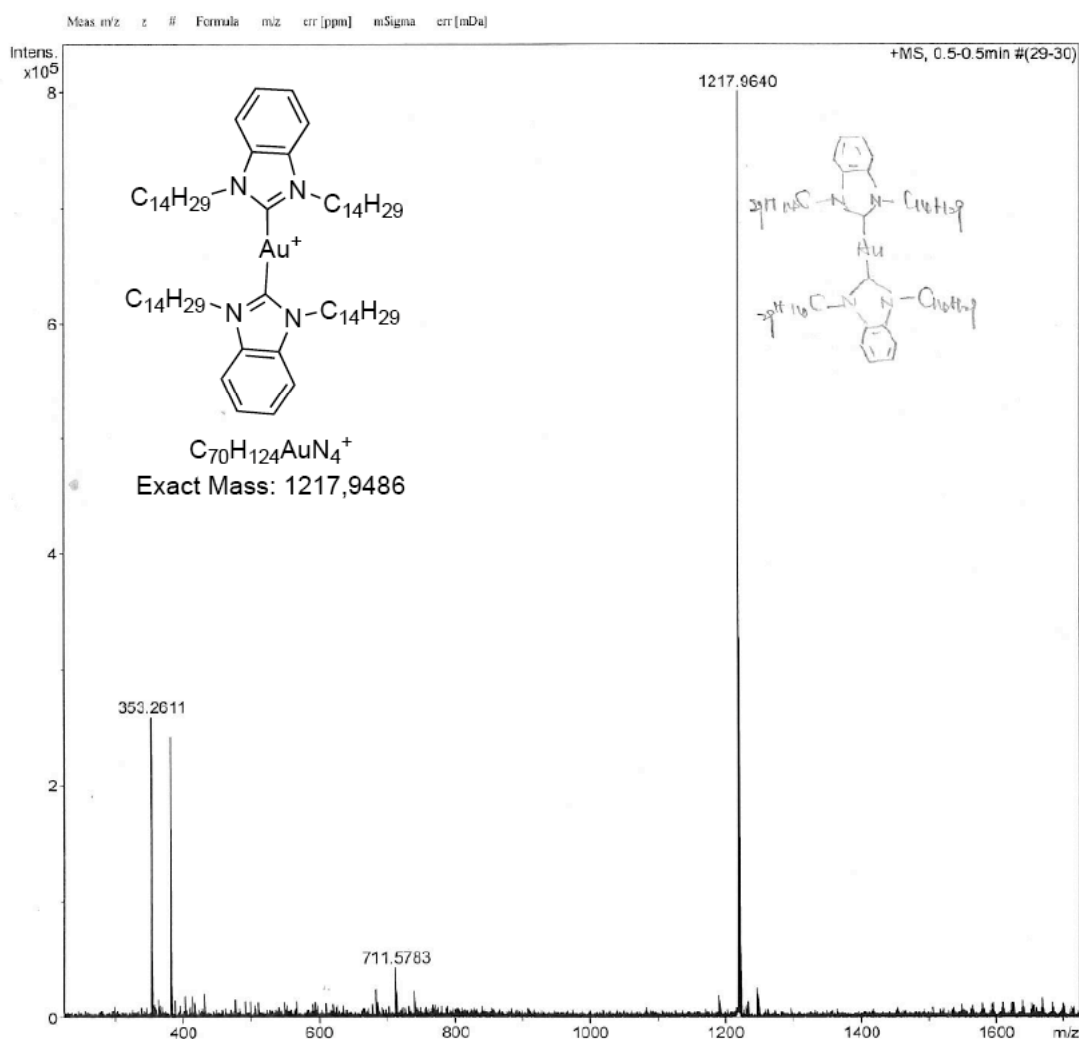
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 Sample Name Xiang NHC-5
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Acquisition Date 6/8/2015 11:16:23 AM

Operator BDAL@DE
 Instrument / Ser# micrOTOF 235

Acquisition Parameter

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Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



Bruker Compass DataAnalysis 4.0

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Figure S11. O₂ treatment of ^{NHC}Au¹⁰ for one week : Mass spectrum of the supernatant after dispersion of the NCs in toluene, precipitation with methanol and centrifugation.

Display Report

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Sample Name	Kiang-au10-before o2-supernatant		
Comment			

Acquisition Parameter					
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Focus	Not active			Set Dry Heater	180 °C
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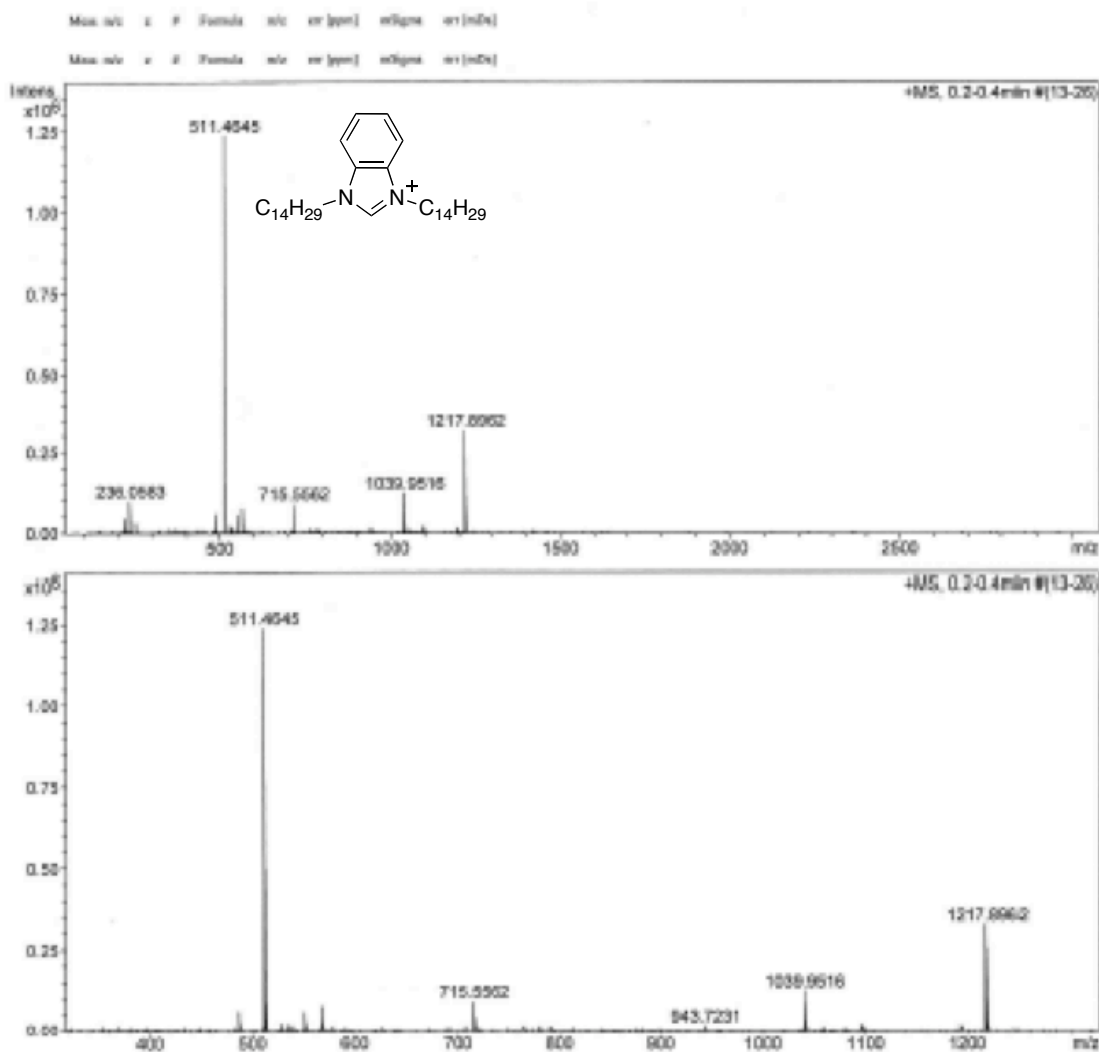


Figure S12. Mass spectrum of the supernatant from NHC-Au^{10} without O_2 treatment, after dispersion of the NCs in toluene, precipitation with methanol and centrifugation.

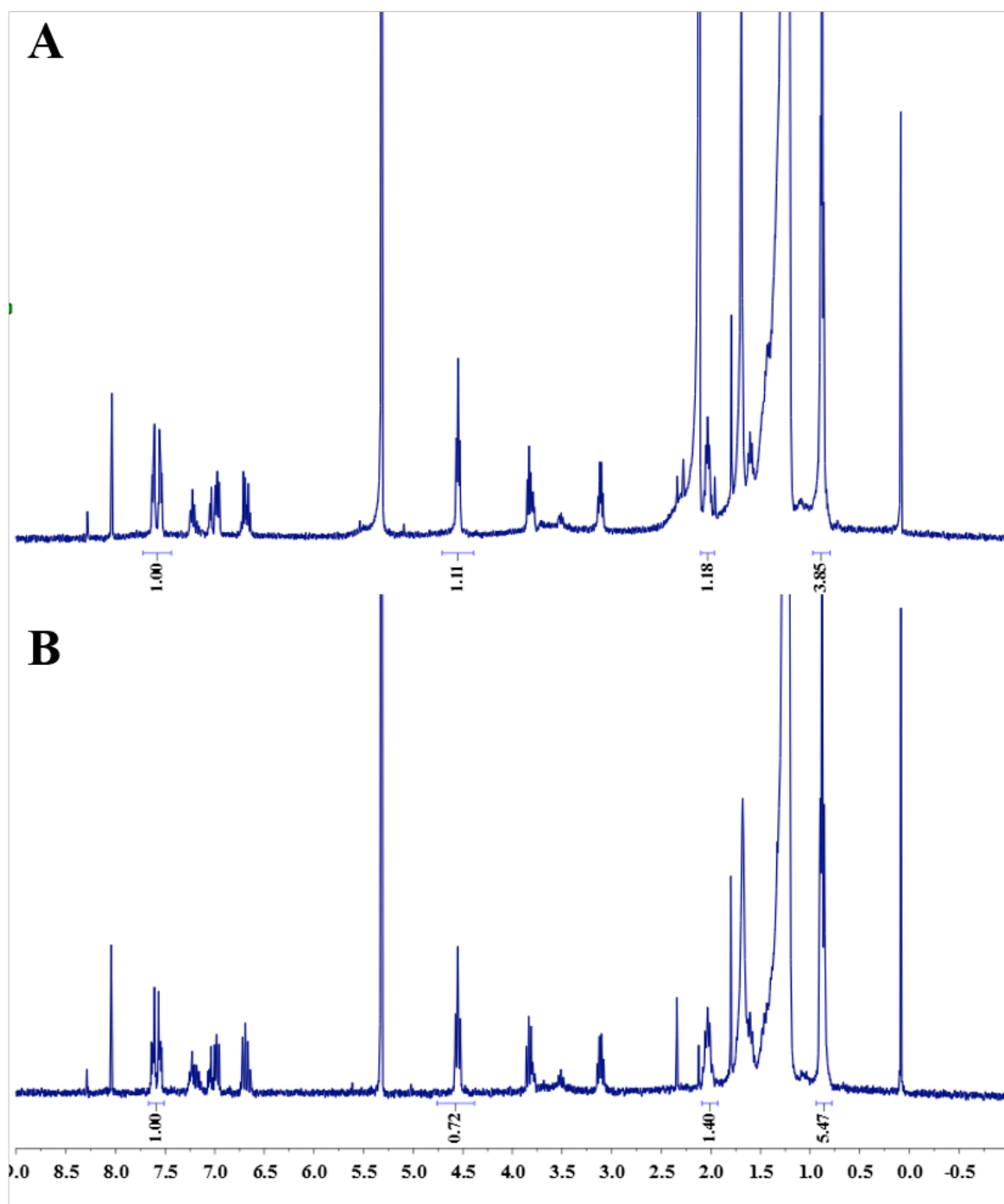


Figure S13. ^1H NMR spectra (400 MHz) of $^{\text{NHC}}\text{Au}^{10}$ in CD_2Cl_2 before (A), and after (B) one-week exposure to nitrogen (N_2). A sample of $^{\text{NHC}}\text{Au}^{10}$ before size selection (see experimental) was analyzed to have the maximum amount of matter for the experiment.

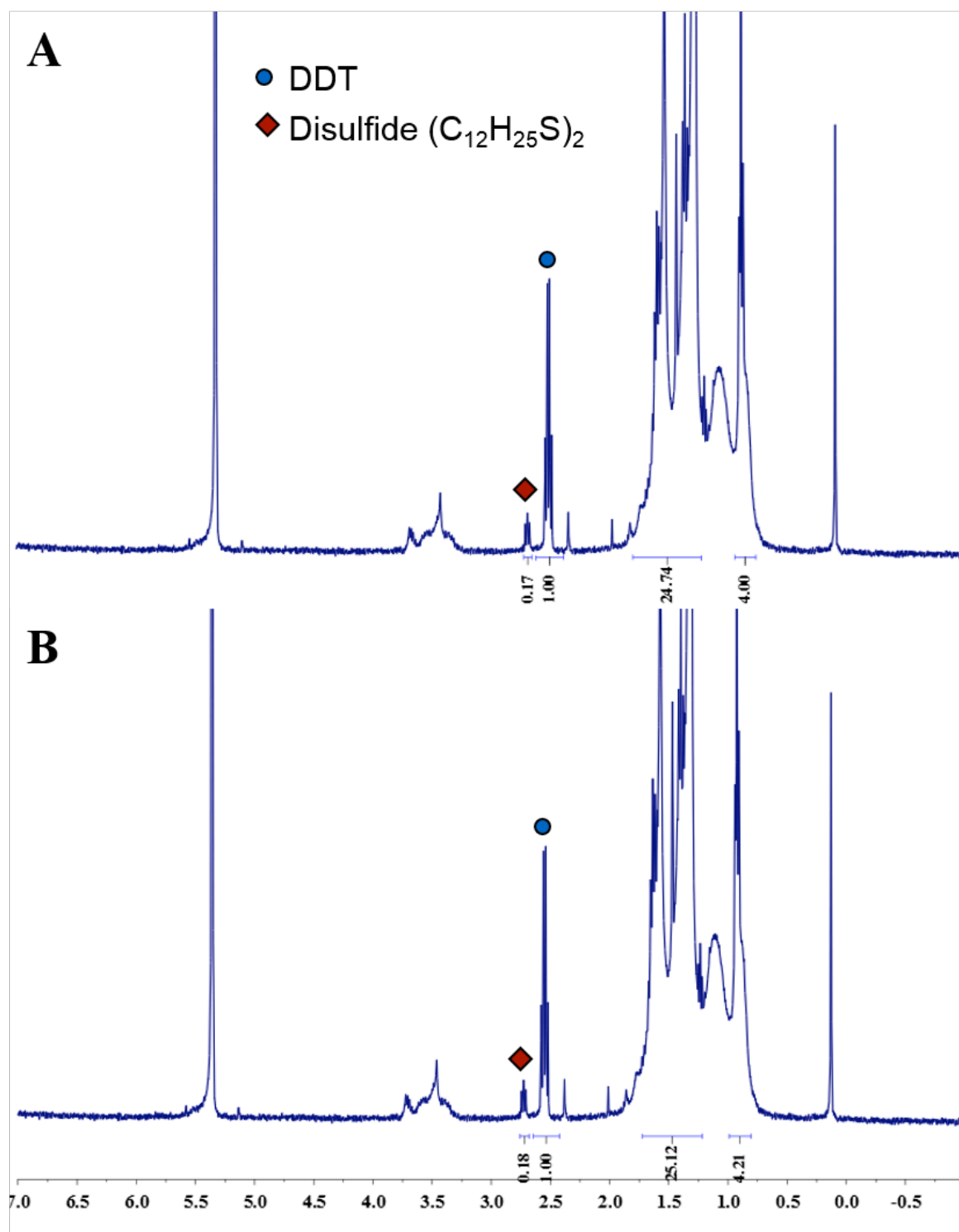


Figure S14. ^1H NMR spectra of $^{\text{DDT}}\text{Au}^2$ before (A), and after (B) one-week exposure to nitrogen (N_2).

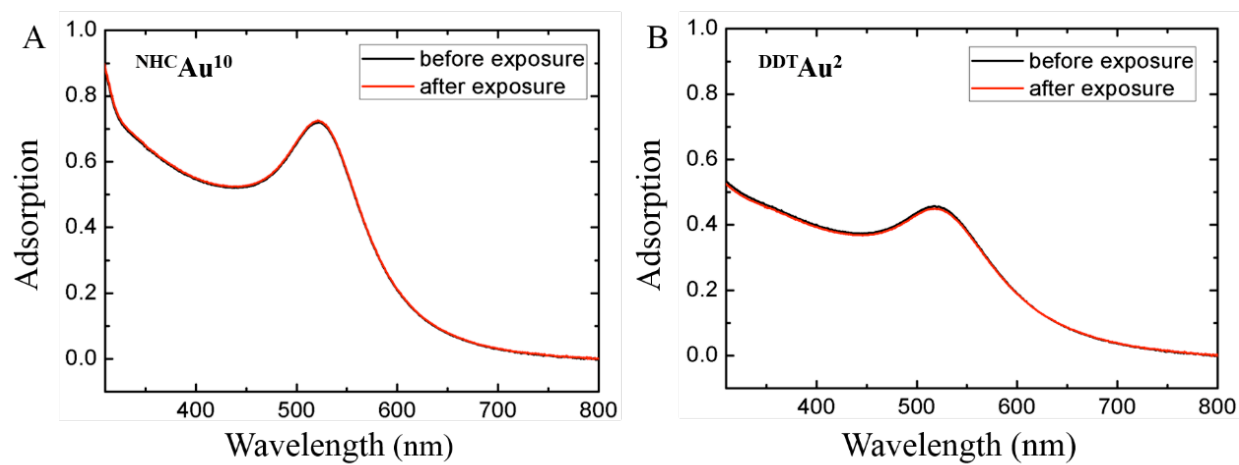


Figure S15. UV-Vis spectra of ^{NHC}Au¹⁰ (A) and ^{DDT}Au² (B) in toluene before and after one-week exposure to N₂. A suspension of 1 mg of Au NCs in toluene (1 mL) was initially prepared, then diluted 20 times with toluene for the analysis.