Supporting Information

Unexpected Reactivity of $Au_{25}(SCH_2CH_2Ph)_{18}$ Nanoclusters with Salts

Manzhou Zhu,[1]* Gerentt Chan,[2] Huifeng Qian[2] and Rongchao Jin[2]
[1]*Department of Chemistry, Anhui University, Hefei, Anhui 230026 P. R. China*
[2]*Department of Chemistry, Carnegie Mellon University, Pittsburgh, Pennsylvania, U. S. A.*

1. Supporting Figures and Table:

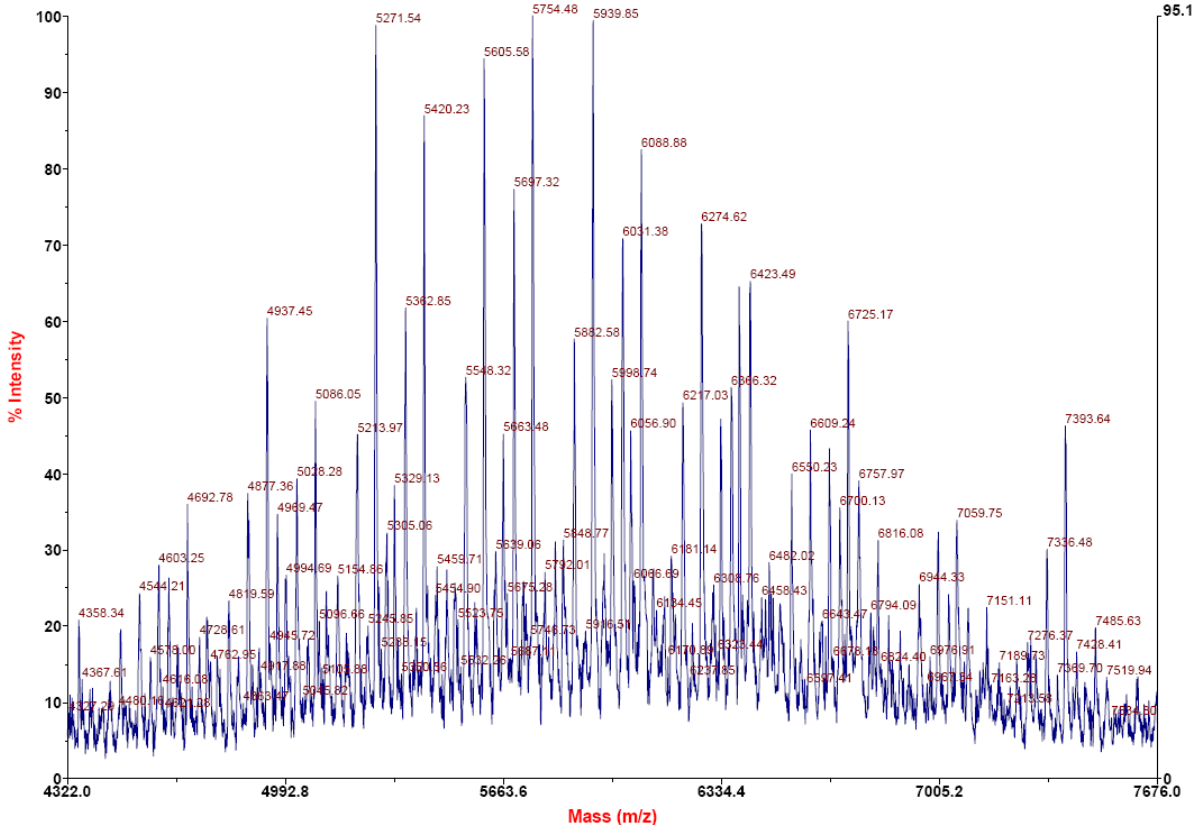

Figure S1. Zoomed-in mass spectrum of the 7 hr reaction product of Au_{25}^0 with NaBr in acetone.

Table S1. Assignment of mass peaks shown in Figure S1.

Peaks	Assigned Formula	Cal. Mass	Deviation
7393.64	**$Au_{25}(SC_2H_4Ph)_{18}$**	7393.72	-0.08
7059.75	$Au_{24}(SC_2H_4Ph)_{17}$	7059.52	0.23
6757.97	$Au_{23}(SC_2H_4Ph)_{16}S$	6757.37	0.6
6725.17	$Au_{23}(SC_2H_4Ph)_{16}$	6725.31	-0.14
6423.49	$Au_{22}(SC_2H_4Ph)_{15}S$	6423.15	0.34
6389.51	$Au_{22}(SC_2H_4Ph)_{15}$	6391.09	-1.58
6088.82	$Au_{21}(SC_2H_4Ph)_{14}S$	6088.94	-0.12
6056.9	$Au_{21}(SC_2H_4Ph)_{14}$	6056.9	0
5754.48	$Au_{20}(SC_2H_4Ph)_{13}S$	5754.77	-0.29
5420.23	$Au_{19}(SC_2H_4Ph)_{12}S$	5420.62	-0.39
5086.05	$Au_{18}(SC_2H_4Ph)_{11}S$	5086.42	-0.37
7336.52	**$Au_{25}(SC_2H_4Ph)_{17}Br$**	7336.53	-0.01
7276.37	$Au_{25}(SC_2H_4Ph)_{16}Br_2$	7279.26	-2.89
7001.80	$Au_{24}(SC_2H_4Ph)_{16}Br$	7002.36	-0.56
6944.33	$Au_{24}(SC_2H_4Ph)_{15}Br_2$	6945.07	-0.74
6667.04	$Au_{23}(SC_2H_4Ph)_{15}Br$	6668.18	-1.14
6609.24	$Au_{23}(SC_2H_4Ph)_{14}Br_2$	6610.9	-1.66
6550.23	$Au_{23}(SC_2H_4Ph)_{13}Br_3$	6553.77	-3.54
6366.32	$Au_{22}(SC_2H_4Ph)_{14}BrS$	6366.19	0.13
6332.88	$Au_{22}(SC_2H_4Ph)_{14}Br$	6334.15	-1.27
6274.62	$Au_{22}(SC_2H_4Ph)_{13}Br_2$	6276.72	-2.1
6217.03	$Au_{22}(SC_2H_4Ph)_{12}Br_3$	6219.42	-2.39
6031.38	$Au_{21}(SC_2H_4Ph)_{13}BrS$	6032.03	-0.65
5998.74	$Au_{21}(SC_2H_4Ph)_{13}Br$	5999.99	-1.25
5939.85	$Au_{21}(SC_2H_4Ph)_{12}Br_2$	5942.55	-2.7
5882.58	$Au_{21}(SC_2H_4Ph)_{11}Br_3$	5885.24	-2.66
5697.32	$Au_{20}(SC_2H_4Ph)_{12}BrS$	5697.80	-0.48
5605.58	$Au_{20}(SC_2H_4Ph)_{11}Br_2$	5608.39	-2.81
5548.32	$Au_{20}(SC_2H_4Ph)_{10}Br_3$	5551.20	-2.88
5362.85	$Au_{19}(SC_2H_4Ph)_{11}BrS$	5363.64	-0.79
5271.54	$Au_{19}(SC_2H_4Ph)_{10}Br_2$	5274.2	-2.66
4937.45	$Au_{18}(SC_2H_4Ph)_9Br_2$	4940.01	-2.56

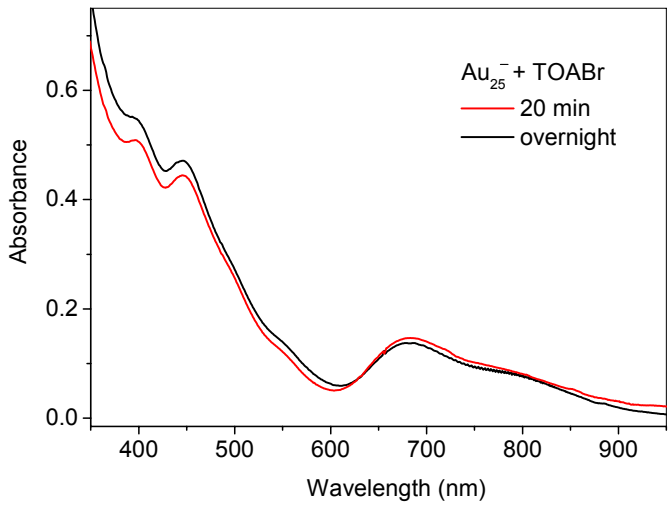

Figure S2. Stability of Au_{25}^- (0.5 mg/2 mL CH_2Cl_2) in the presence of excess TOABr (10 eqs). Au_{25}^- shows no changes after ~12 hr.

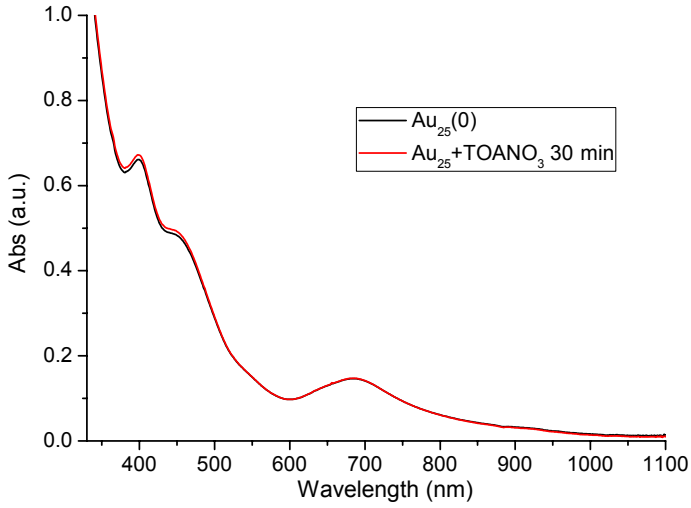

Figure S3. Stability of Au_{25}^0 (0.5mg/2ml CH_2Cl_2) in the presence of excess $TOANO_3$. No changes was observed within 12 h (longer time not tested). In the figure, only the 30 min spectrum was shown.

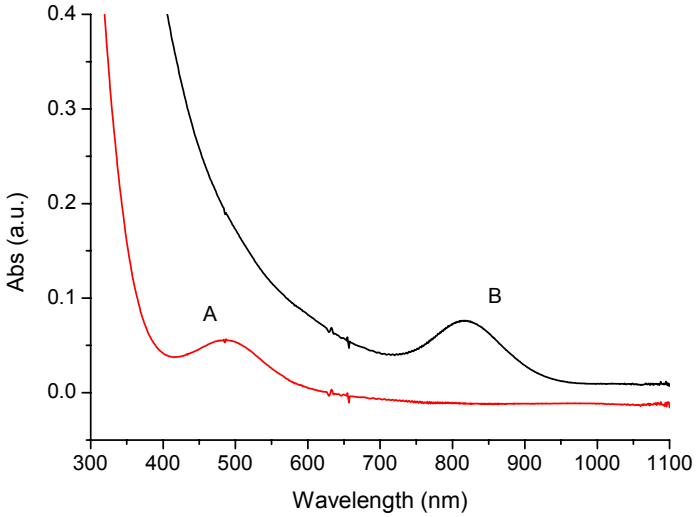

Figure S4. Reaction of Au_{25}^{0} with *excess* NaI. Adding NaI at a ratio of Au_{25}^{0}/NaI=8/7 leads to immediate conversion of Au_{25}^{0} to Au_{25}^{-}. Adding excess NaI (> 5 equivalents) leads to cluster decomposition after overnight. HPLC shows species B (see figure for its absorption spectrum), presumably a Au(I) complex. It is initially soluble in toluene, but after being dry under nitrogen, the majority can no longer be dissolved in toluene, perhaps due to aggregation or polymerization of Au(I), only a little amount can be dissolved in toluene, which shows spectrum A (see figure). This product seems quite labile and has not been identified.