

Observing the Real Time Formation of Phosphine-Ligated Gold Clusters by Electrospray Ionization Mass Spectrometry

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Supplemental Information

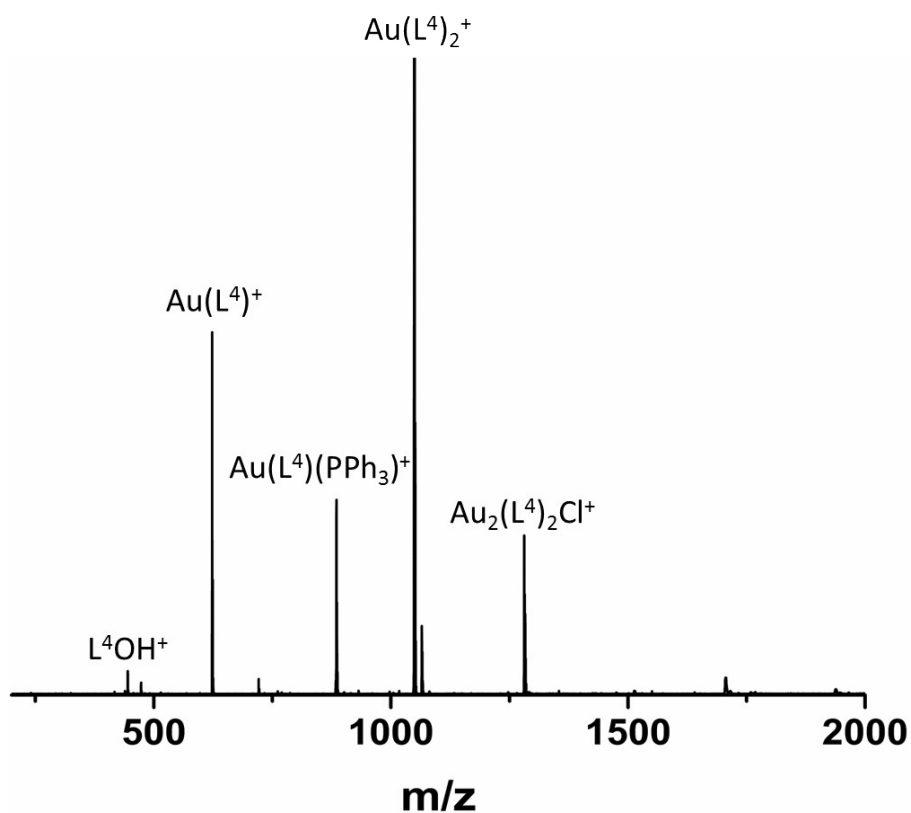


Figure S1: Mass spectrum of gold complexes prior to reduction using a ligand ratio of 2:1 $[\text{L}^4]/[\text{PPh}_3]$.

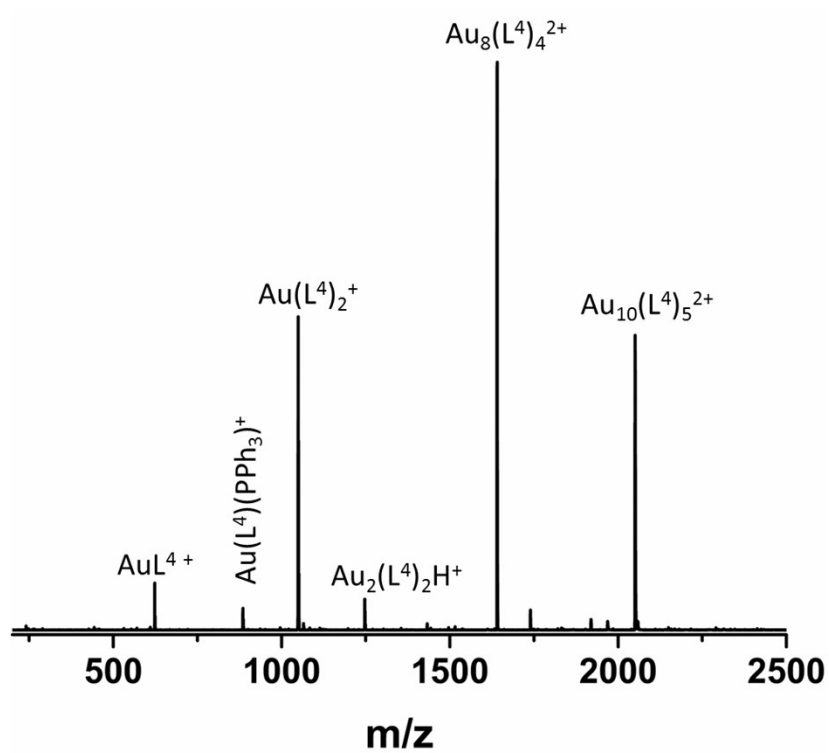


Figure S2: Mass spectrum showing products after 24 hours under non-oxidative conditions and 50:1 molar ratio of BTBA to $\text{Au}(\text{PPh}_3)\text{Cl}$

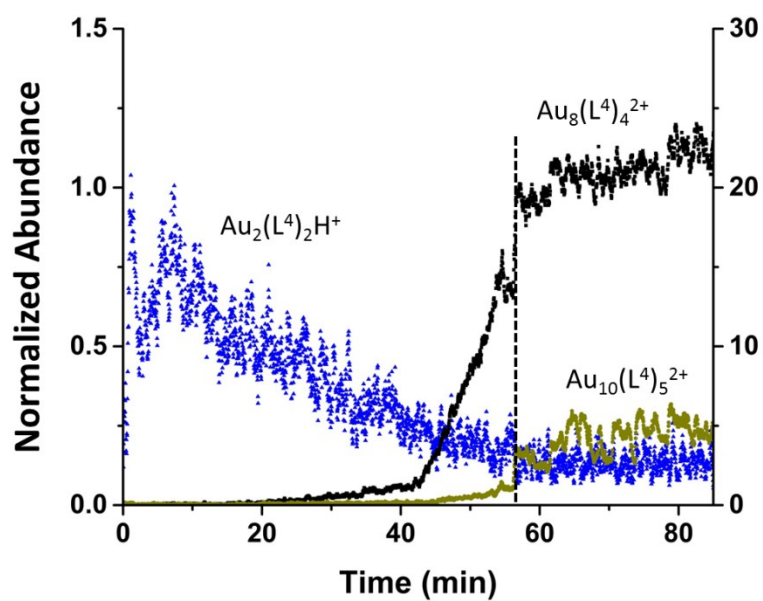


Figure S3: Selected ion chromatograms for; **Left Axis;** $\text{Au}_2(\text{L}^4)_2\text{H}^+$ (blue triangles), **Right Axis;** $\text{Au}_8(\text{L}^4)_4^{2+}$ (black squares) and $\text{Au}_{10}(\text{L}^4)_5^{2+}$ (dark yellow circles)

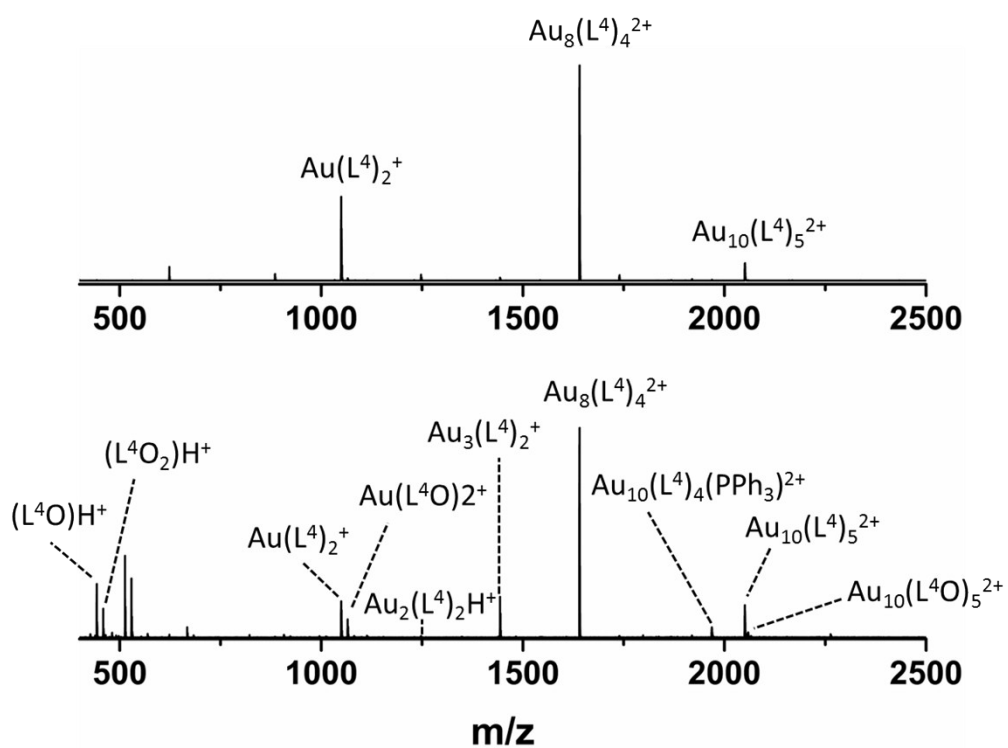


Figure S4: Top; Representative mass spectrum 30 minutes after the addition of air to preformed clusters. **Bottom;** Mass spectrum of same reaction mixture after 10 days

m/z	Relative Intensity	Calculated m/z	Δ Mass error	Au	L ₄	PPH ₃	H	O	Cl	Na	Charge
443.16759	18.47	443.1692758	0.001686		1		1	1			1
459.16238	100	459.1641908	0.001811		1		1	2			1
465.14929	5.02	465.1512458	0.001956		1			1		1	1
481.14436	31.78	481.1461608	0.001801		1			2		1	1
623.13143	1.24	623.1331208	0.001691	1	1						1
721.14701	1.05	721.14877	0.00176	1		2					1
821.10547	1.52	821.1074808	0.002011	2	1		1				1
901.21718	0.43	901.2191678	0.001988	1	1	1		1			1
907.31071	1.42	907.3127756	0.002066		2			2		1	1
919.12126	0.05	919.12313	0.00187	2		2	1				1
923.30588	0.94	923.3076906	0.001811		2			3		1	1
939.30026	6.31	939.3026056	0.002346		2			4		1	1
955.29586	0.18	955.2975206	0.001661		2			5		1	1
1017.06403	0.23	1017.066241	0.002211	3	1						1
1019.07967	1.39	1019.081841	0.002171	3	1		2				1
1065.29229	0.12	1065.294651	0.002361	1	2			1			1
1081.28716	0.93	1081.289566	0.002406	1	2			2			1
1099.19125	0.09	1099.193528	0.002278	2	1	1	1	1			1
1230.1468	0.43	1230.149548	0.002748	6	3						2
1247.26998	<0.05	1247.274096	0.00412	2	2		1				1
1263.26605	0.2	1263.269011	0.002961	2	2		1	1			1
1279.15434	0.61	1279.157373	0.003033	3	1	1					1
1329.13357	0.44	1329.136728	0.003158	7	3		1				2
1427.11271	1.78	1427.116108	0.003398	8	3						2
1435.10934	0.05	1435.113566	0.004226	8	3			1			2
1443.22954	0.72	1443.232856	0.003316	3	2						1
1459.22445	1	1459.227771	0.003321	3	2			1			1
1476.12026	0.21	1476.123933	0.003673	8	2	2					2
1477.12685	0.3	1477.131733	0.004883	4	1	1	1				1
1558.15777	2.11	1558.161674	0.003904	8	3	1					2
1566.15498	0.39	1566.159132	0.004152	8	3	1		1			2
1607.16542	0.12	1607.169499	0.004079	8	2	3					2
1640.19523	0.97	1640.199416	0.004186	8	4						2
1641.20185	3.17	1641.207216	0.005366	4	2		1				1
1648.19255	2.28	1648.196873	0.004323	8	4			1			2
1656.1899	0.22	1656.194331	0.004431	8	4			2			2
1657.19561	0.31	1657.202131	0.006521	4	2		1	1			1
1697.2002	0.25	1697.204698	0.004498	8	3	2		1			2
1755.12354	0.06	1755.128234	0.004694	10	3	1					2
1787.23517	0.13	1787.239897	0.004727	8	4	1		2			2
1804.13096	0.26	1804.136059	0.005099	10	2	3					2
1837.16065	2.83	1837.165976	0.005326	10	4						2
1845.15754	0.09	1845.163433	0.005893	10	4			1			2
1853.1378	0.21	1853.143883	0.006083	10	1	5					2
1877.26958	0.14	1877.275096	0.005516	8	5			3			2
1886.16808	0.14	1886.1738	0.00572	10	3	2					2
1894.16504	0.19	1894.171258	0.006218	10	3	2		1			2
1935.17533	0.29	1935.181625	0.006295	10	2	4					2
1943.17269	0.21	1943.179082	0.006392	10	2	4		1			2
1976.20259	0.22	1976.208999	0.006409	10	4	1		1			2
1984.18745	0.09	1984.189449	0.001999	10	1	6					2
2025.21017	0.16	2025.216824	0.006654	10	3	3		1			2
2033.20715	0.08	2033.214281	0.007131	10	3	3		2			2
2034.12654	0.05	2034.132536	0.005996	12	4						2
2050.24228	0.18	2050.249283	0.007003	10	5						2
2058.2395	0.25	2058.246741	0.007241	10	5			1			2
2066.23701	0.12	2066.244198	0.007188	10	5			2			2
2115.24398	0.09	2115.252023	0.008043	10	4	2		2			2
2157.22557	0.26	2157.233921	0.00835	11	5		1	1			2
2165.21865	<0.05	2165.231378	0.012728	11	5		1	2			2
2174.20698	0.06	2174.214447	0.007467	11	5			1	1		2

Table S1: Experimental and calculated mass to charge ratios of gold clusters formed in uncontrolled oxidative conditions

