

Supplementary Information

A density functional study on cationic $Au_nCu_m^+$ clusters and their monocarbonyls

by Yu Zhao, Zhenyu Li, and Jinlong Yang

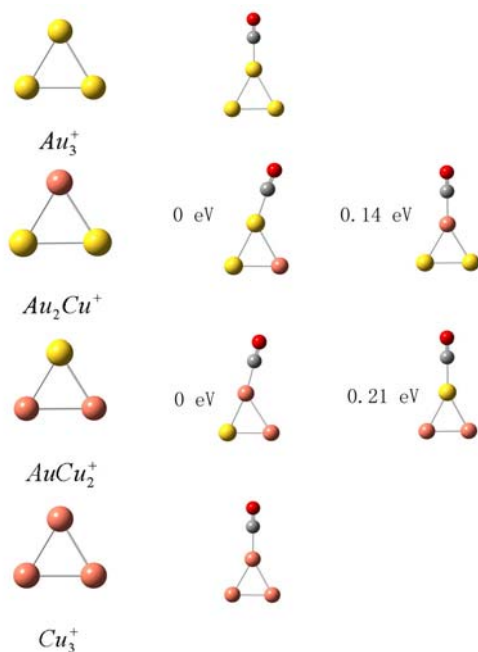


Figure S1. Isomers for $Au_nCu_m^+$ with $n+m=3$.

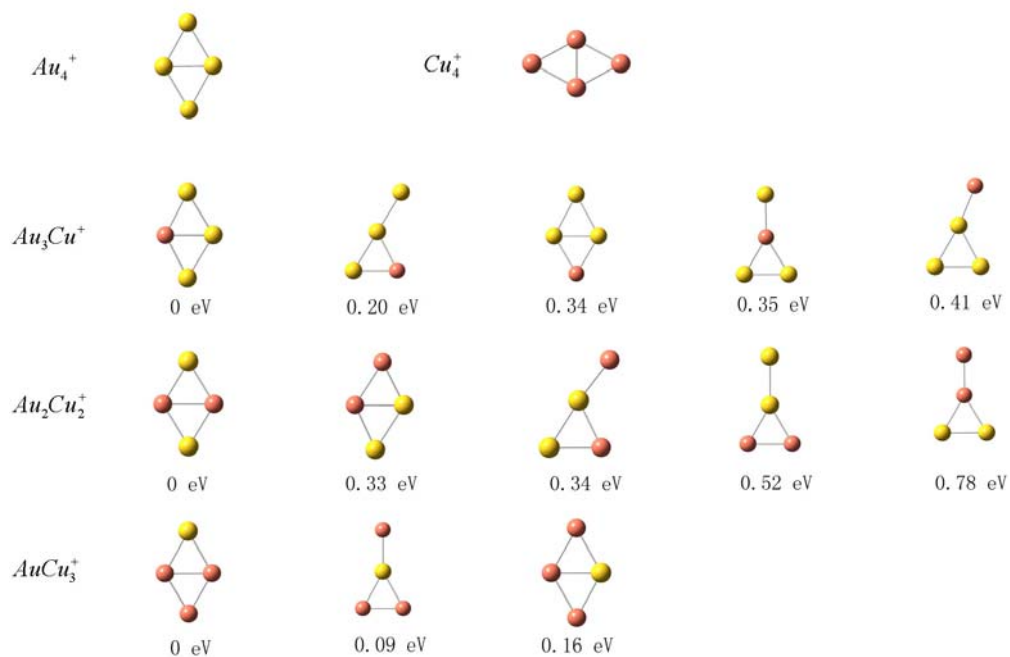


Figure S2. Isomers for $Au_nCu_m^+$ with $n+m=4$.

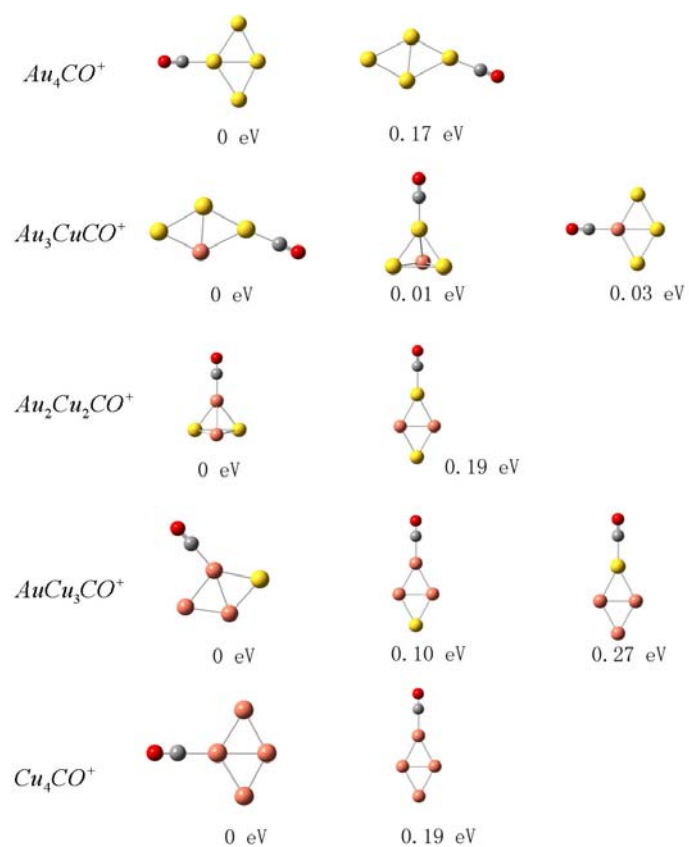


Figure S3. Isomers for $Au_nCu_mCO^+$ with $n+m=4$.

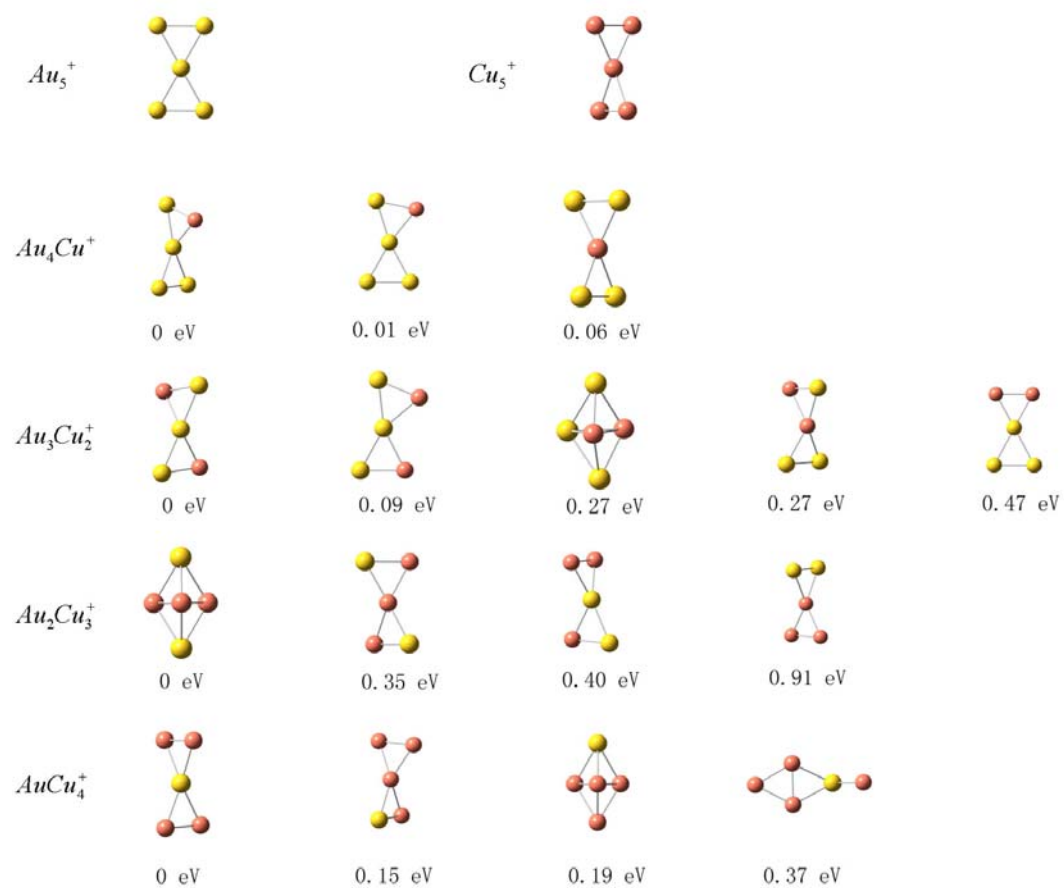


Figure S4. Isomers for $Au_nCu_m^+$ with $n+m=5$.

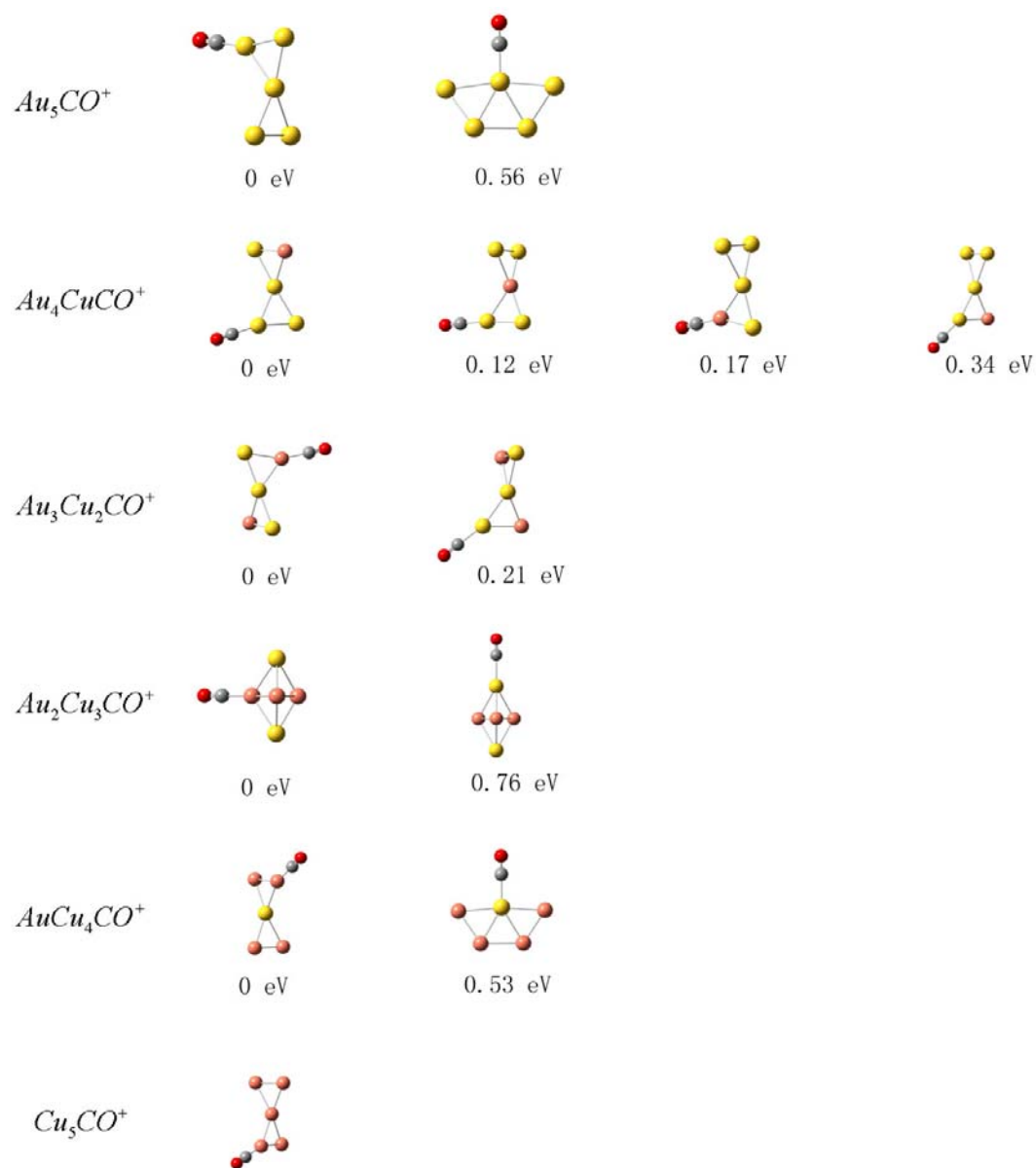
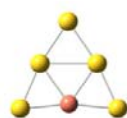
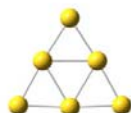
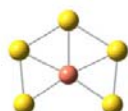


Figure S5. Isomers for $Au_nCu_mCO^+$ with $n+m=5$.

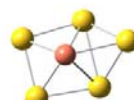
Au_6^+



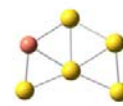
0 eV



0.003 eV

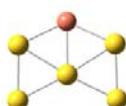


0.01 eV

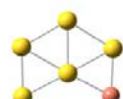


0.06 eV

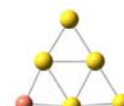
Au_5Cu^+



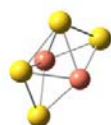
0.06 eV



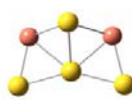
0.13 eV



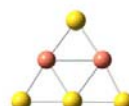
0.25 eV



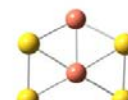
0 eV



0.28 eV



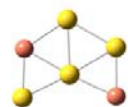
0.30 eV



0.34 eV



0.35 eV



0.36 eV



0.37 eV

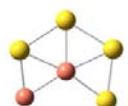


0.41 eV

$Au_4Cu_2^+$



0.43 eV



0.46 eV



0.53 eV



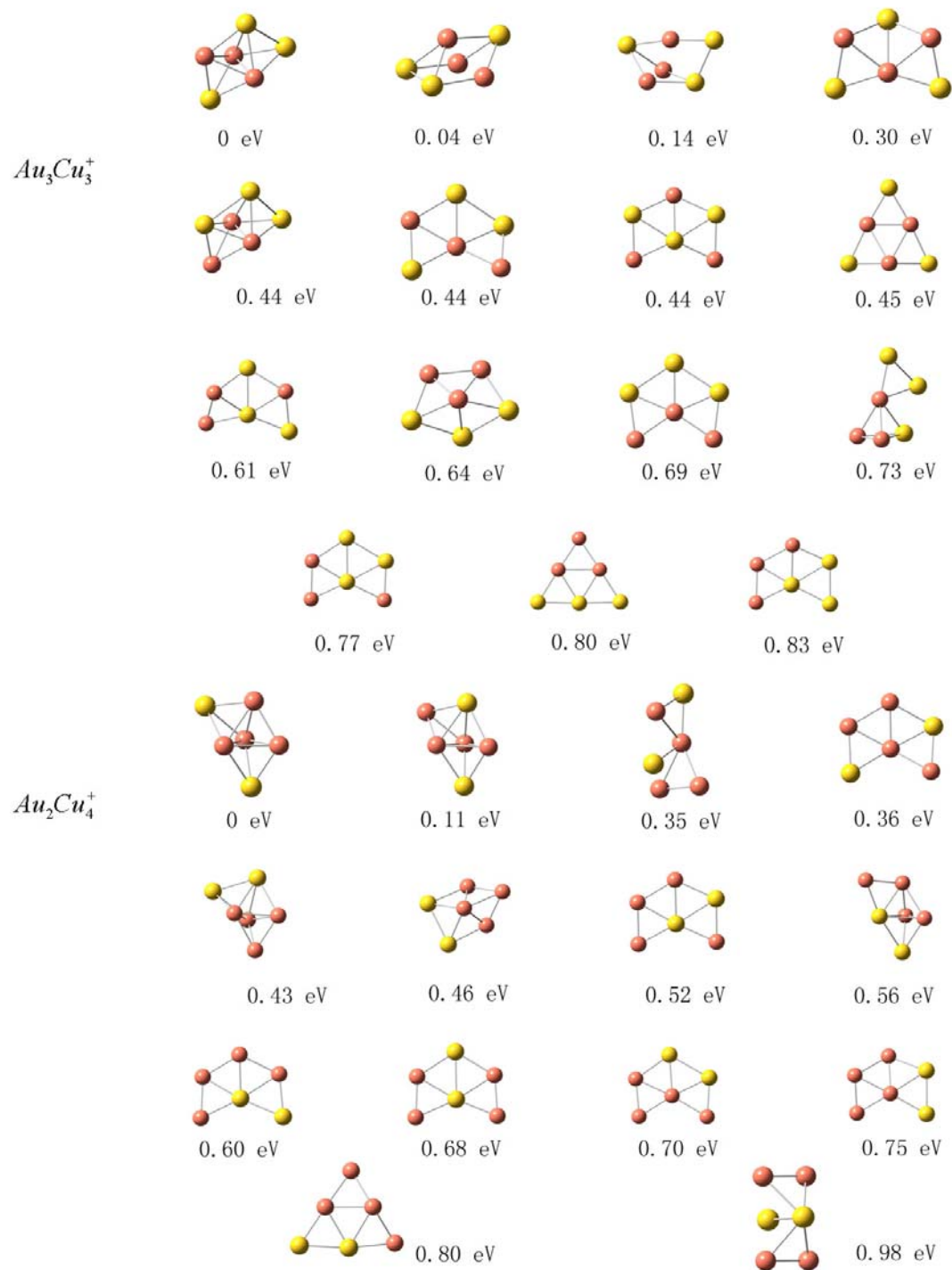
0.55 eV



0.59 eV



0.72 eV



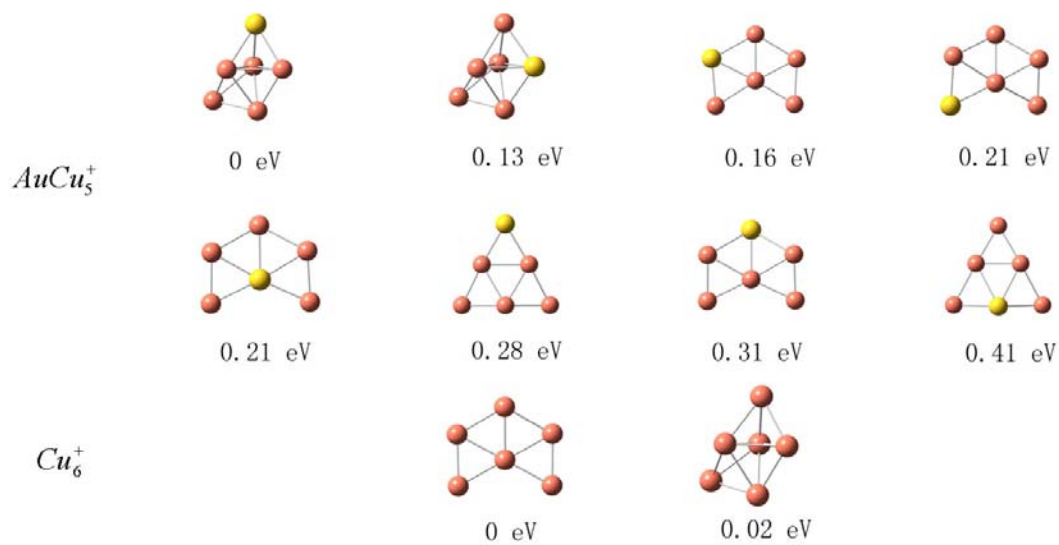
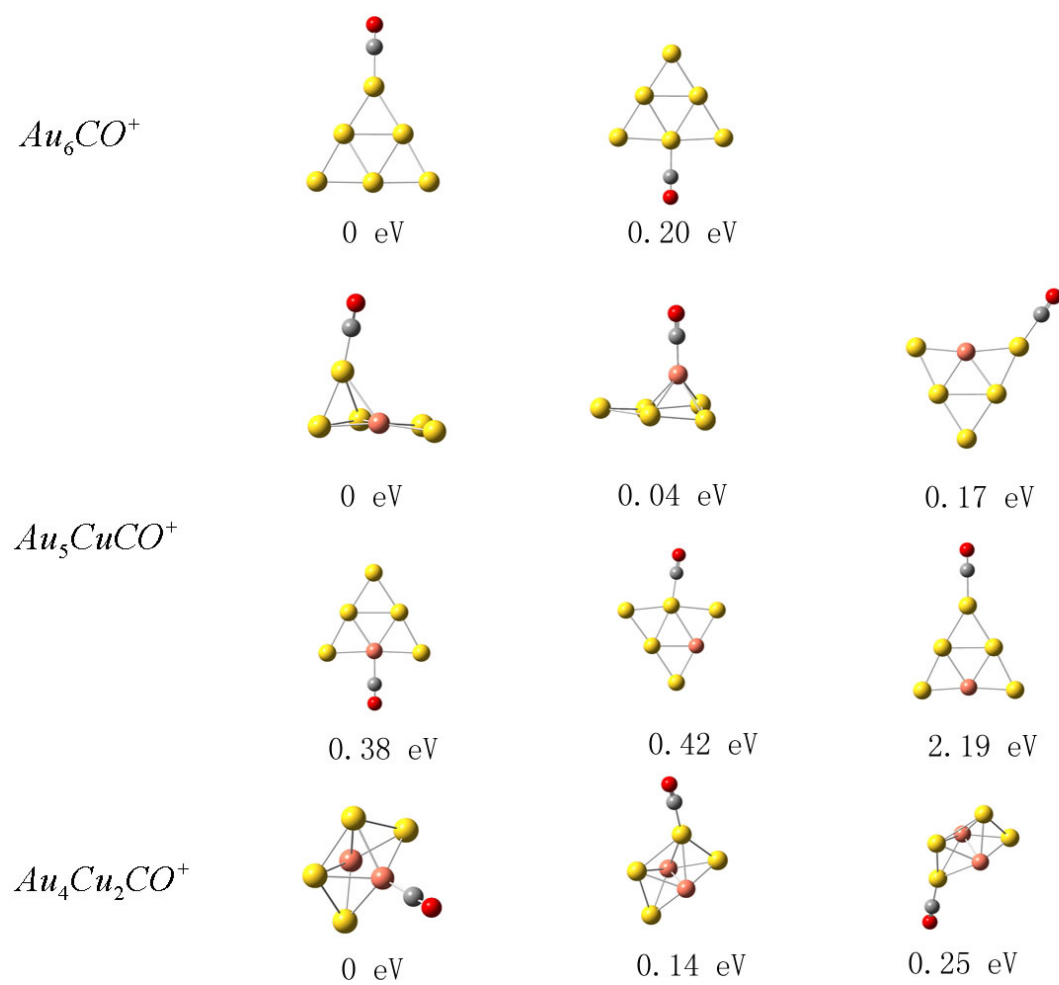


Figure S6. Isomers for $Au_nCu_m^+$ with $n+m=6$.



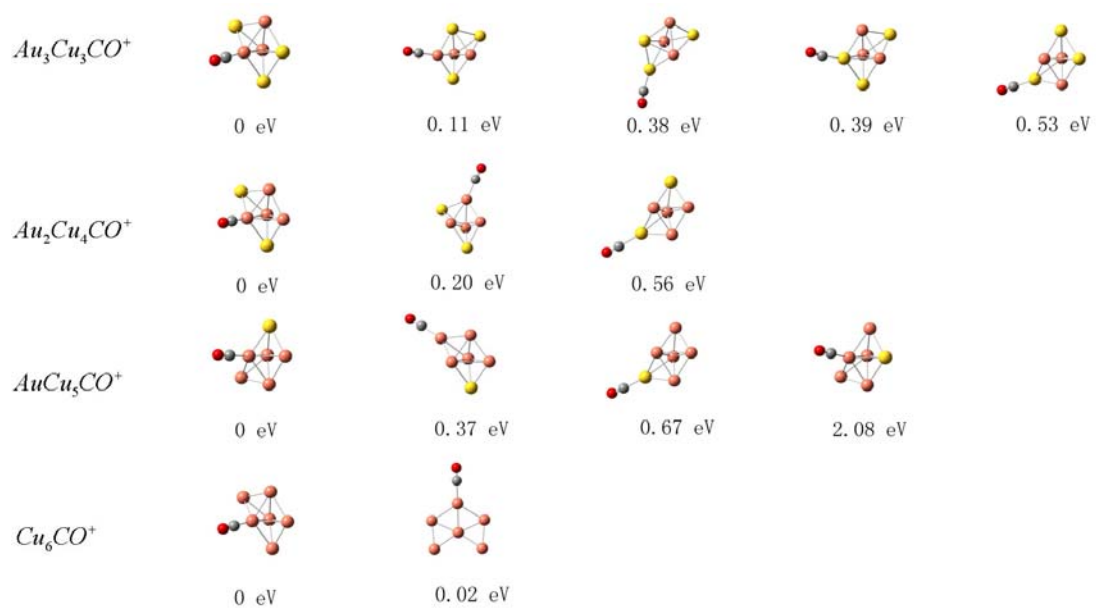


Figure S7. Isomers for $Au_nCu_mCO^+$ with $n+m=6$.

TABLE I: NBO charge on atoms of Au_nCu_m^+ and $\text{Au}_n\text{Cu}_m\text{CO}^+$ ($n+m=2$)

No.	1	2	3 (C atom)	4 (O atom)
Au_2^+	0.500	0.500		
Au_2CO^+	0.416	0.427	0.463	-0.306
AuCu^+	(Au) 0.271	(Cu) 0.729		
AuCuCO^+	(Au) 0.293	(Cu) 0.615	0.407	-0.315
Cu_2^+	0.500	0.500		
Cu_2^+	0.437	0.486	0.399	-0.322

TABLE II: NBO charge on atoms of Au_nCu_m^+ and $\text{Au}_n\text{Cu}_m\text{CO}^+$ ($n+m=3$)

No.	1	2	3	4 (C atom)	5 (O atom)
Au_3^+	0.333	0.333	0.333		
Au_3CO^+	0.262	0.262	0.347	0.448	-0.319
Au_2Cu^+	0.205	0.205	(Cu) 0.590		
Au_2CuCO^+	0.285	0.002	(Cu) 0.587	0.449	-0.322
AuCu_2^+	(Au) -0.016	0.508	0.508		
AuCu_2CO^+	(Au) -0.116	(0.539	0.485	0.422	-0.330
Cu_3^+	0.333	0.333	0.333		
Cu_3^+	0.283	0.283	0.353	0.418	-0.337

TABLE III: NBO charge on atoms of Au_nCu_m^+ and $\text{Au}_n\text{Cu}_m\text{CO}^+$ ($n+m=4$)

No.	1	2	3	4	5 (C atom)	6 (O atom)
Au_4^+	0.291	0.209	0.291	0.209		
Au_4CO^+	0.346	0.220	0.109	0.220	0.434	-0.329
Au_3Cu^+	0.203	0.137	0.137	(Cu) 0.524		
Au_3CuCO^+	0.050	0.042	0.260	(Cu) 0.526	0.450	-0.328
Au_2Cu_2^+	0.062	(Cu) 0.438	0.062	(Cu) 0.438		
$\text{Au}_2\text{Cu}_2\text{CO}^+$	-0.093	(Cu) 0.591	-0.093	(Cu) 0.519	0.413	-0.338
AuCu_3^+	(Au) -0.020	0.355	0.355	0.311		
AuCu_3CO^+	(Au) -0.075	0.404	0.274	0.338	0.401	-0.343
Cu_4^+	0.249	0.251	0.249	0.251		
Cu_4^+	0.120	0.267	0.294	0.267	0.393	-0.340

TABLE IV: NBO charge on atoms of Au_nCu_m^+ and $\text{Au}_n\text{Cu}_m\text{CO}^+$ ($n+m=5$)

No.	1	2	3	4	5	6(C atom)	7(O atom)
Au_5^+	0.247	0.247	0.247	0.247	0.013		
Au_5CO^+	0.232	0.234	0.049	0.357	0.024	0.446	-0.341
Au_4Cu^+	0.027	-0.051	0.227	0.229	(Cu) 0.568		
Au_4CuCO^+	-0.004	-0.044	0.355	0.018	(Cu) 0.568	0.449	-0.341
Au_3Cu_2^+	-0.012	(Cu) 0.569	-0.114	(Cu) 0.569	-0.012		
$\text{Au}_3\text{Cu}_4\text{CO}^+$	-0.068	(Cu) 0.545	-0.092	(Cu) 0.567	-0.026	0.419	-0.345
Au_2Cu_3^+	(Au) -0.329	0.553	0.552	0.552	(Au) -0.329		
$\text{Au}_2\text{Cu}_3\text{CO}^+$	(Au) -0.316	0.539	0.539	0.494	(Au) -0.316	0.407	-0.347
AuCu_4^+	(Au) -0.310	0.328	0.328	0.328	0.328		
AuCu_4CO^+	(Au) -0.328	0.300	0.301	0.257	0.416	0.390	-0.336
Cu_5^+	0.265	0.265	0.264	0.265	-0.059		
Cu_5CO^+	0.349	0.140	0.250	0.250	-0.051	0.417	-0.355

No.	1	2	3	4	5	6	7(C atom)	8(O atom)
Au_6^+	0.225	0.05	0.225	0.223	0.223	0.054		
Au_6CO^+	0.325	0.068	0.086	0.065	0.240	0.091	0.456-0.330	
Au_5Cu^+	0.065	(Cu)0.500	0.066	0.057	0.057	0.255		
Au_5CuCO^+	-0.036	(Cu) 0.417	0.280	0.154	-0.074	0.139	0.452	-0.331
Au_4Cu_2^+	0.050	0.048	-0.070	(Cu) 0.522 (Cu)	0.523	-0.071		
$\text{Au}_4\text{Cu}_4\text{CO}^+$	0.053	0.054	-0.050	(Cu) 0.476 (Cu)	0.485	-0.058	0.395	-0.347
Au_3Cu_3^+	(Au) -0.107	0.417	(Au) -0.080	0.506	0.501	(Au) -0.237		
$\text{Au}_3\text{Cu}_3\text{CO}^+$	(Au) -0.095	0.423	(Au) -0.066	0.446	0.469	(Au) -0.223	0.400	-0.353
Au_2Cu_4^+	0.245	0.245	(Au) -0.221	0.477	0.477	(Au) -0.222		
$\text{Au}_2\text{Cu}_4\text{CO}^+$	0.255	0.261	(Au) -0.207	0.445	0.413	(Au) -0.207	0.396	-0.356
AuCu_5^+	(Au) -0.259	0.100	0.244	0.113	0.401	0.401		
AuCu_5CO^+	(Au) -0.230	0.109	0.261	0.139	0.381	0.315	0.388	-0.336
Cu_6^+	0.137	0.230	0.274	-0.052	0.137	0.274		
Cu_6CO^+	0.117	0.115	0.112	0.212	0.324	0.112	0.372	-0.365

TABLE V: NBO charge on atoms of Au_nCu_m^+ and $\text{Au}_n\text{Cu}_m\text{CO}^+$ ($n+m=6$)