$[Ag_{25}Cu_4H_8Br_6(CCPh)_{12}(PPh_3)_{12}]^{3+}$: $Ag_{13}H_8$ silver hydride core protected by $[CuAg_3(CCPh)_3(PPh_3)_3]^+$ motifs

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Contents

24. **Table S6**. Gaussian cartesian coordinates for $[Ag_{25}Cu_4H_8Cl_6(CCH)_{12}(PH_3)_{12}]^{3+}$ (Model 2)

25. **Table S7**. Bond distances between Ag atoms of the core.

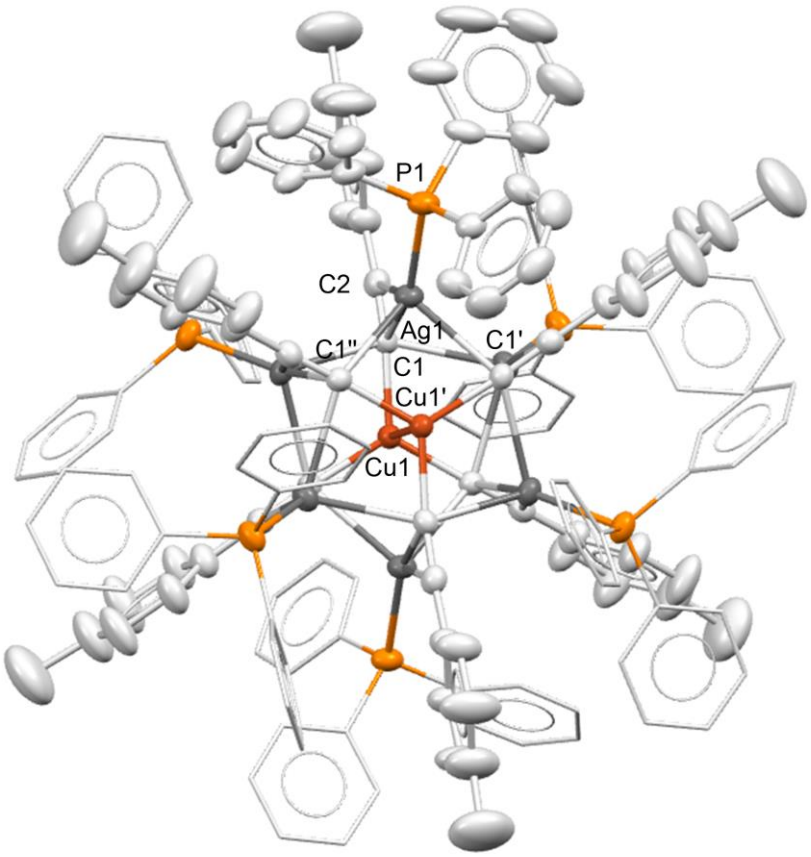


Figure S1. A crystal structure of $[CuAg_3(C{\equiv}CTol)_3(PPh_3)_3]_2(BF_4)_2$ **1**. Only one PPh_3 in an asymmetric unit is depicted as a thermal ellipsoid style for clarity. Hydrogens and anions are eliminated for clarity.

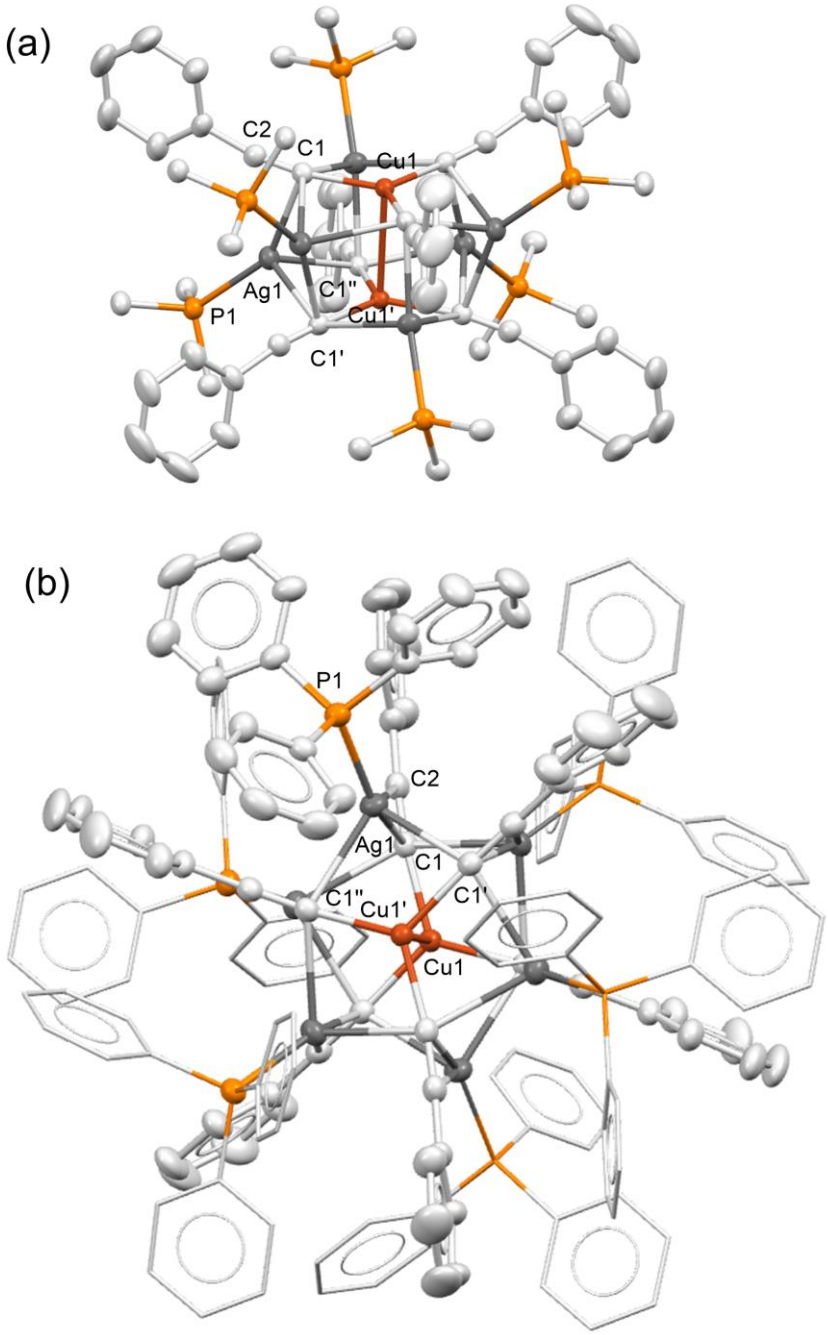


Figure S2. A crystal structure of $[CuAg_3(C{\equiv}CPh)_3(PPh_3)_3]_2(BF_4)_2$ **2**. (a) A side view of **2**. Only *ipso* carbons are depicted for PPh_3 ligands. (b) A top view of **2**. Only one PPh_3 in an asymmetric unit is depicted as a thermal ellipsoid style for clarity. Hydrogens and anions are eliminated for clarity.

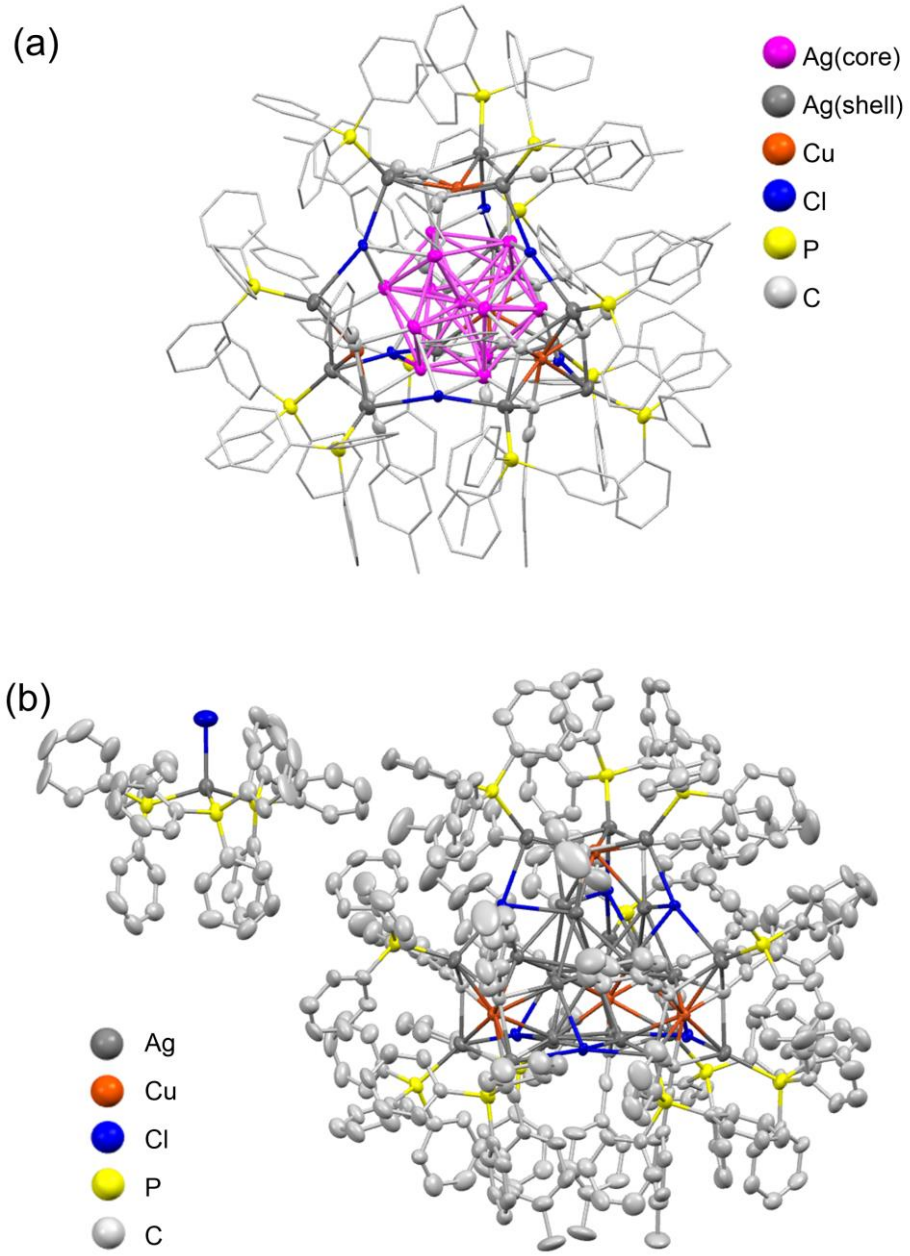


Figure S3. A crystal structure of **3**. (a) a drawing emphasizing core and shell structures of the cluster, (b) structures of the cluster and $[AgCl(PPh_3)_3]$, the latter of which co-crystalizes with the cluster. Counter anions and solvent molecules as well as hydrogen atoms were omitted for clarity.

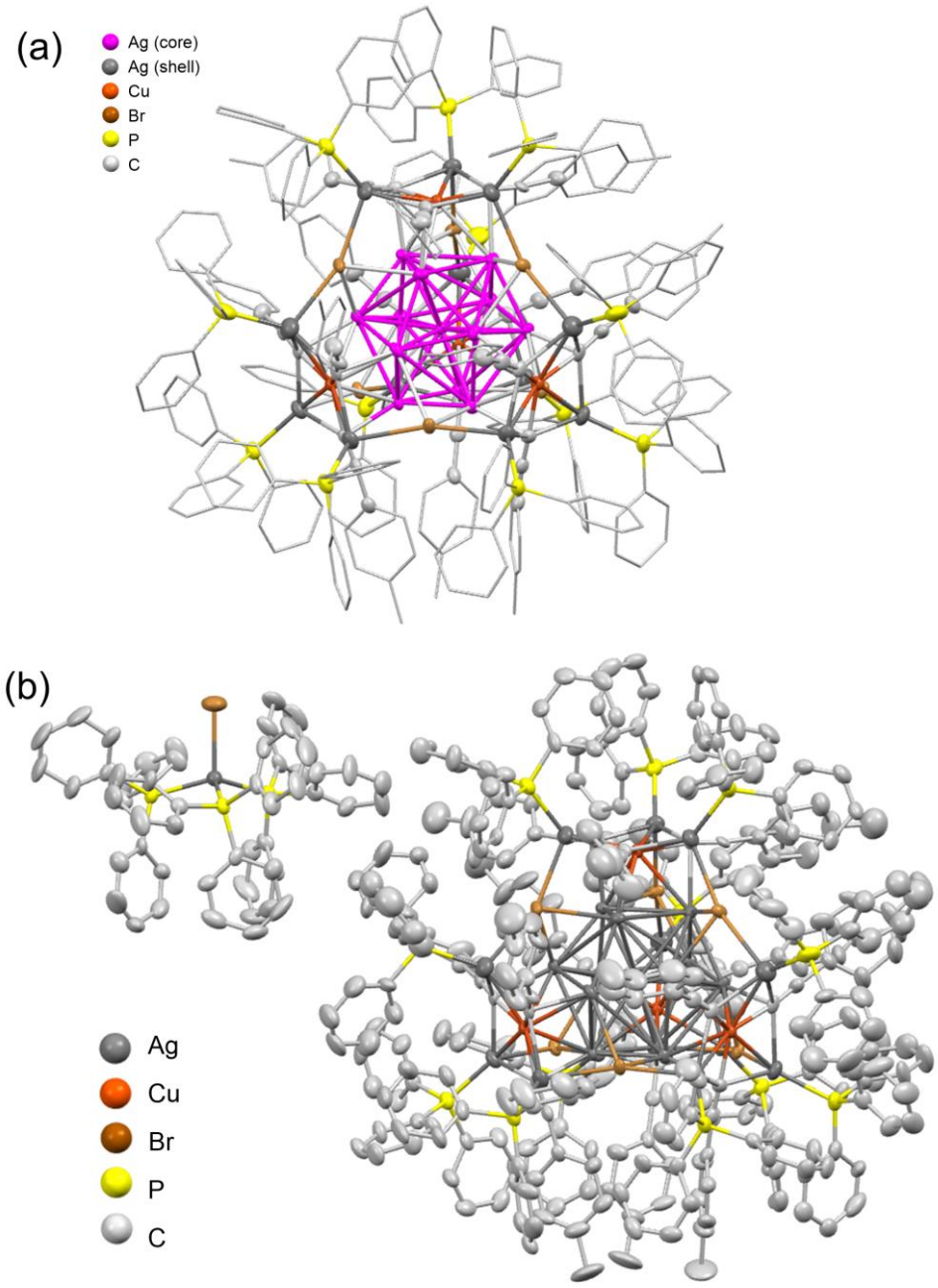


Figure S4. A crystal structure of **4**. (a) a drawing emphasizing core and shell structures of the cluster, (b) structures of the cluster and [$AgBr(PPh_3)_3$], the latter of which co-crystalizes with the cluster. Counter anions and solvent molecules as well as hydrogen atoms were omitted for clarity.

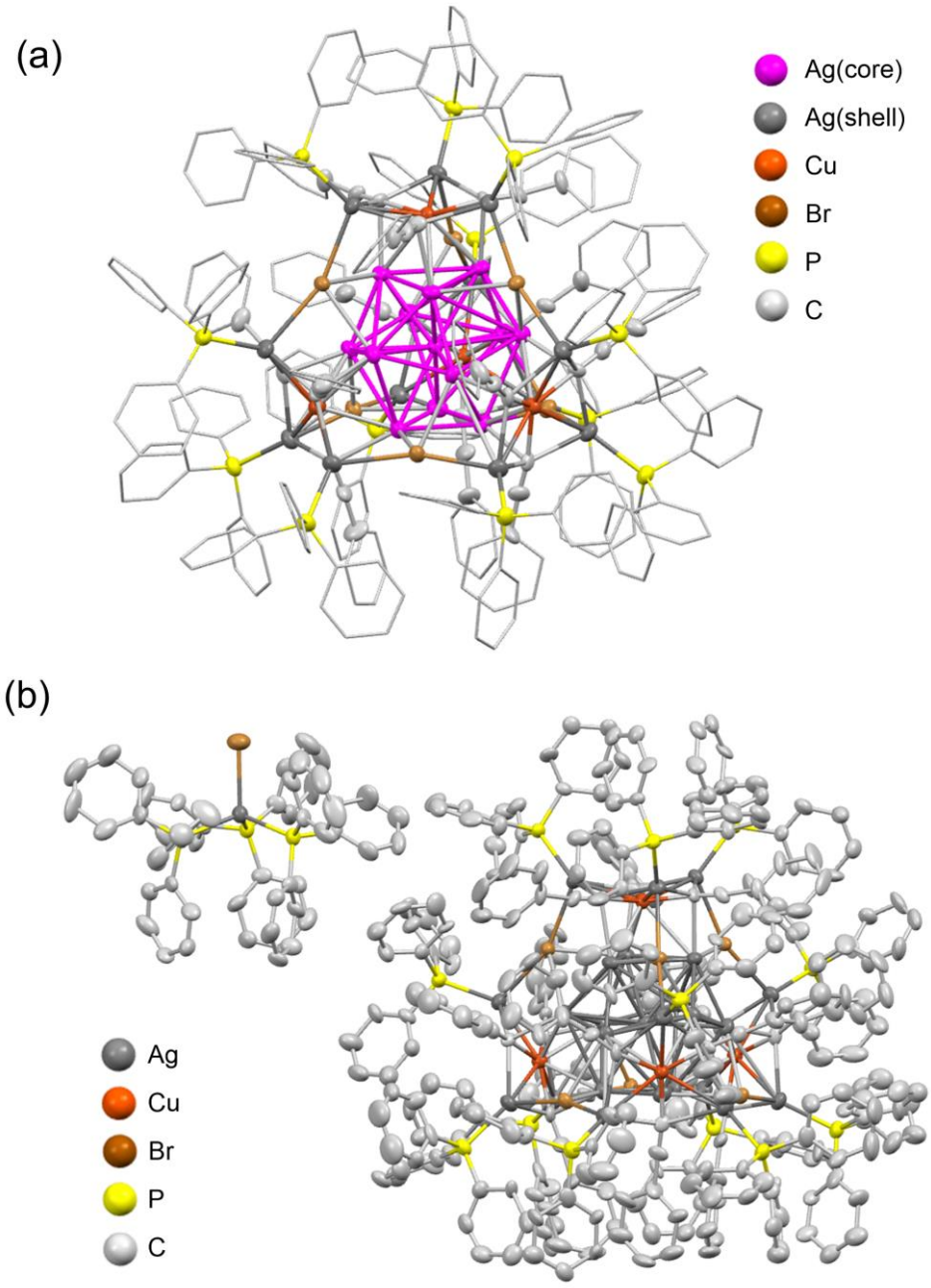


Figure S5. A crystal structure of **5**. (a) a drawing emphasizing core and shell structures of the cluster, (b) structures of the cluster and [$AgBr(PPh_3)_3$], the latter of which co-crystalizes with the cluster. Counter anions and solvent molecules as well as hydrogen atoms were omitted for clarity.

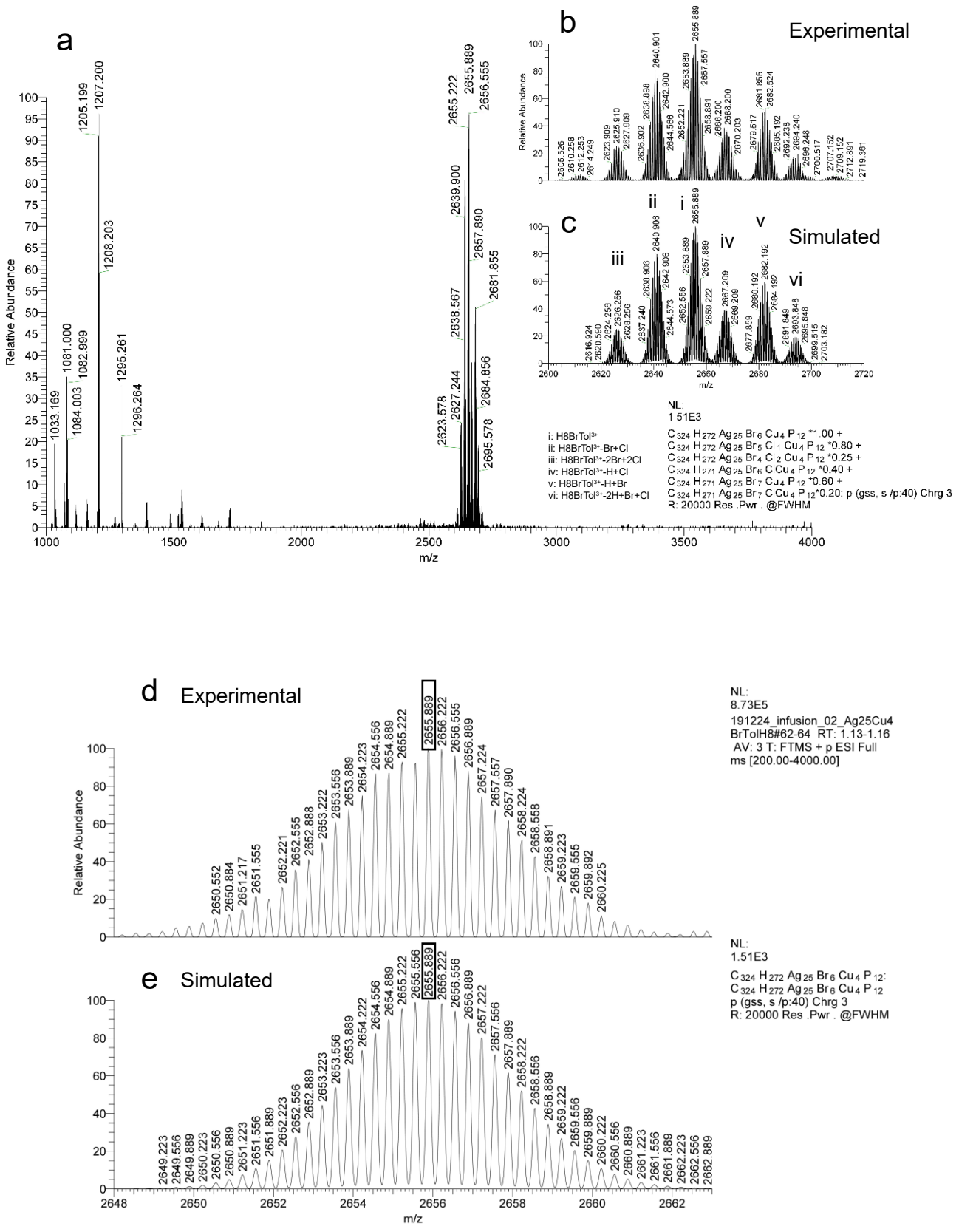


Figure S6. (a) ESI-MS spectra for **4**. (b) Main spectra. (c) Simulated ESI-MS spectra for $[Ag_{13}H_8Br_6\{CuAg_3(C{\equiv}CTol)_3(PPh_3)_3\}_4]^{3+}$ ($H8BrTol^{3+}$) and its derivatives formed by the exchange of the anions (Br^- and H^-) with Cl^-. These derivatives were formed after dissolving the sample into CH_2Cl_2. (d) and (e) Experimental and simulated ESI-MS spectra, respectively, for $H8BrTol^{3+}$.

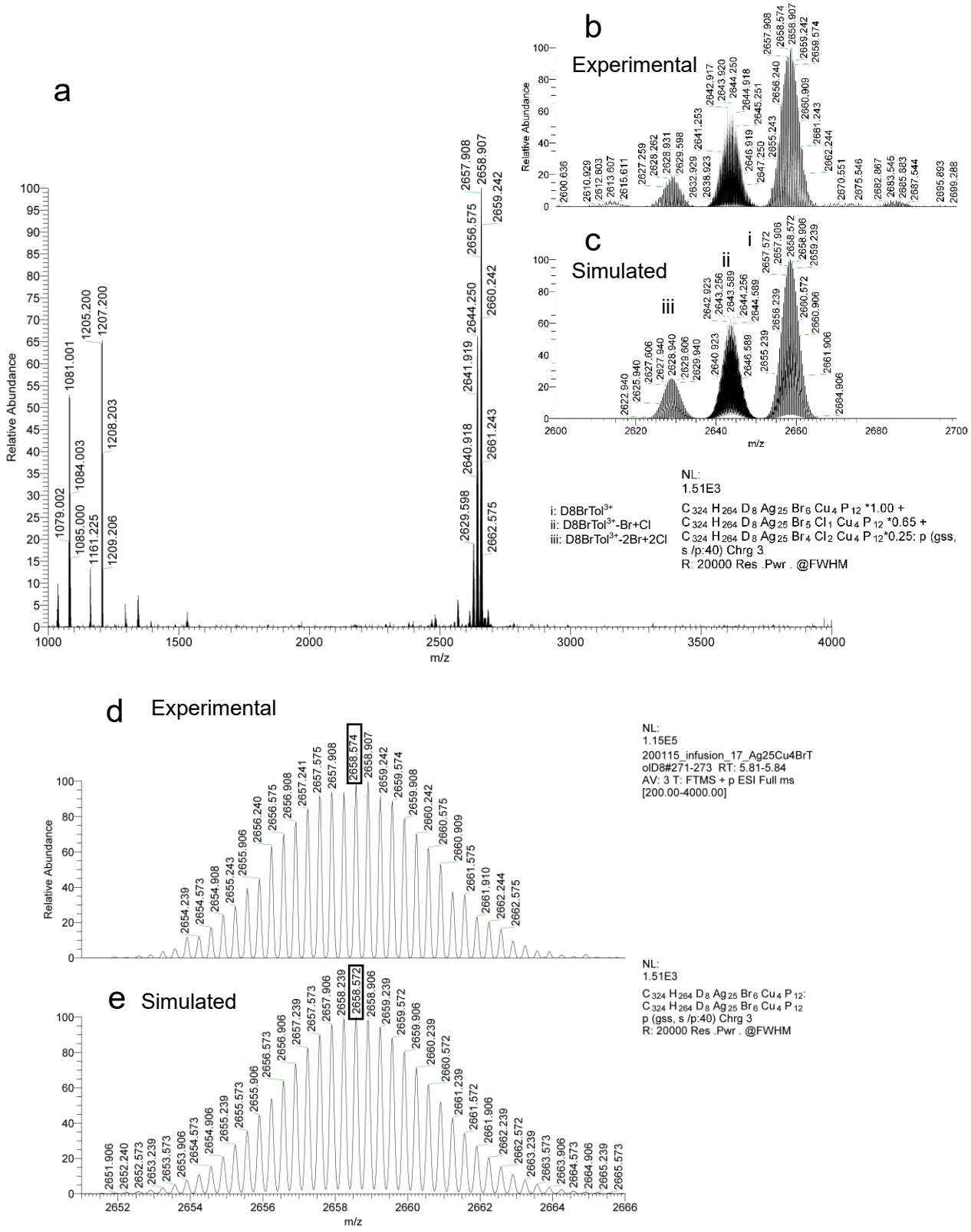


Figure S7. (a) ESI-MS spectra for deuterated **4**. (b) Main spectra. (c) Simulated ESI-MS spectra for $[Ag_{13}D_8Br_6\{CuAg_3(C{\equiv}CTol)_3(PPh_3)_3\}_4]^{3+}$ ($D8BrTol^{3+}$) and its derivatives formed by the exchange of Br^- with Cl^-. These derivatives were formed after dissolving the sample into CH_2Cl_2. (d) and (e) Experimental and simulated ESI-MS spectra, respectively, for $D8BrTol^{3+}$.

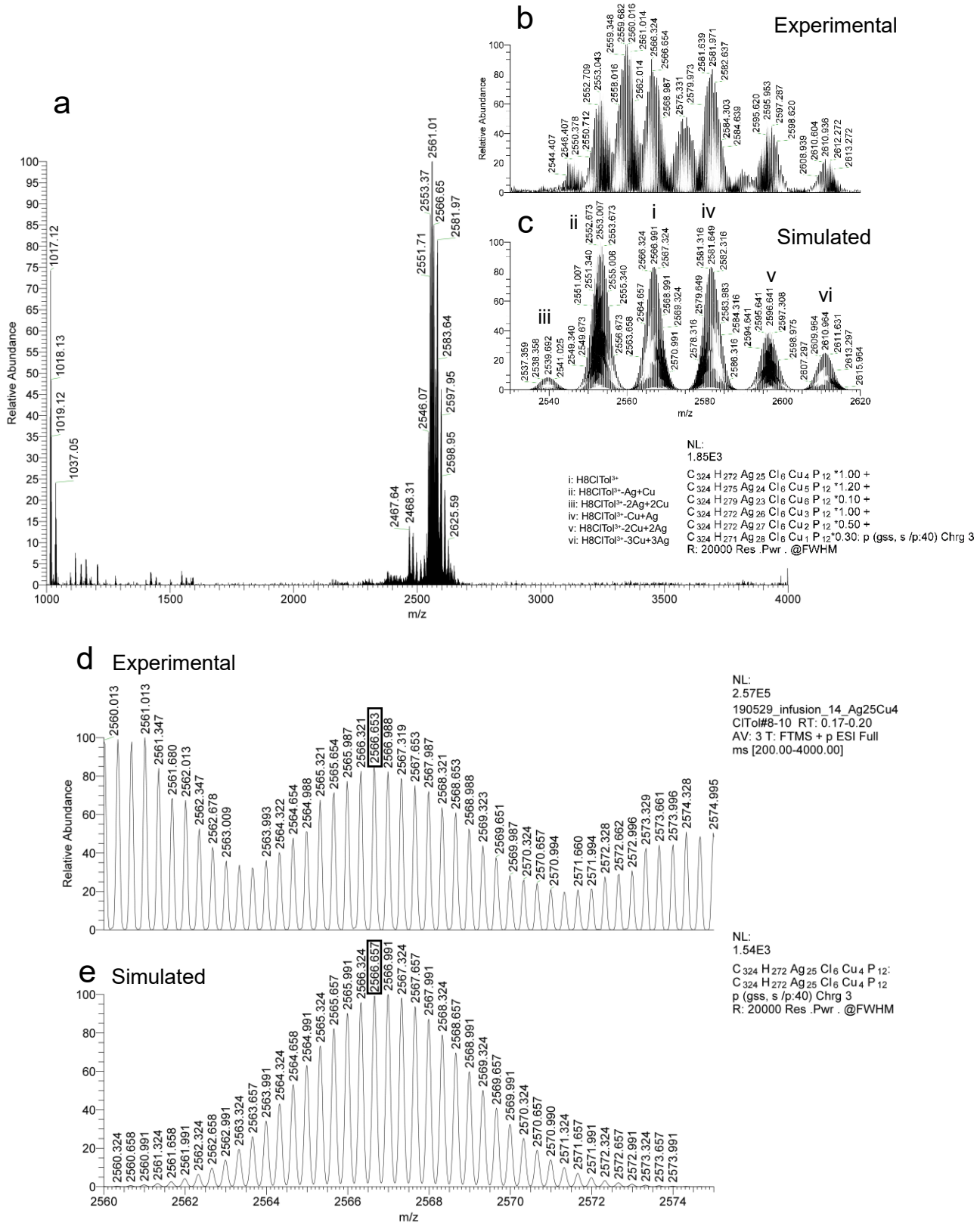


Figure S8. (a) ESI-MS spectra for **3**. (b) Main spectra. (c) Simulated ESI-MS spectra for $[Ag_{13}H_8Cl_6\{CuAg_3(C{\equiv}CTol)_3(PPh_3)_3\}_4]^{3+}$ ($H8ClTol^{3+}$) and its derivatives formed by the exchange between Ag with Cu. These derivatives were tentatively included for the simulation. (d) and (e) Experimental and simulated ESI-MS spectra for $H8ClTol^{3+}$.

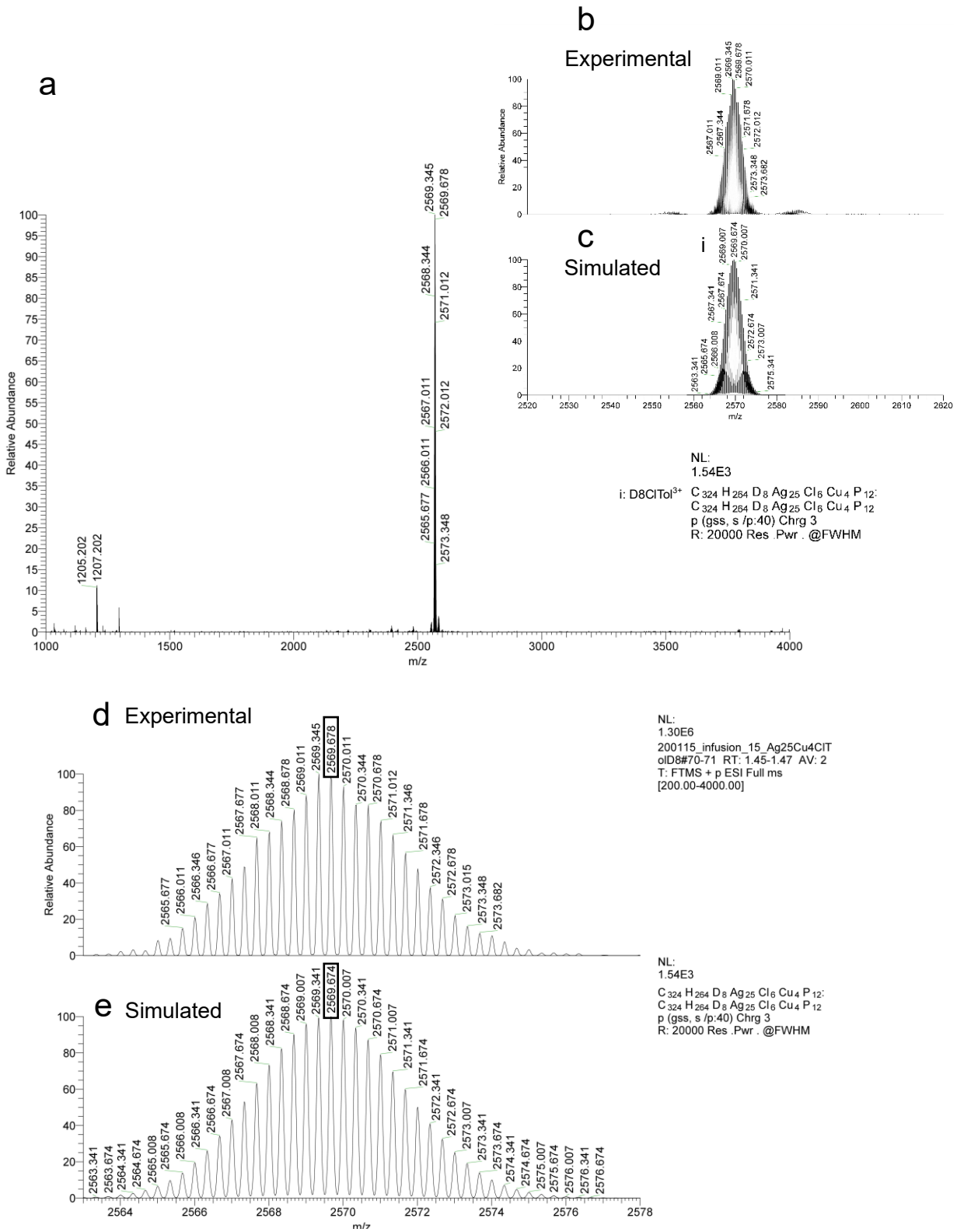


Figure S9. (a) ESI-MS spectra for deuterated **3**. (b) Main spectra. (c) Simulated ESI-MS spectra for $[Ag_{13}D_8Cl_6\{CuAg_3(C{\equiv}CTol)_3(PPh_3)_3\}_4]^{3+}$ ($D8ClTol^{3+}$). (d) and (e) Experimental and simulated ESI-MS spectra for $D8ClTol^{3+}$.

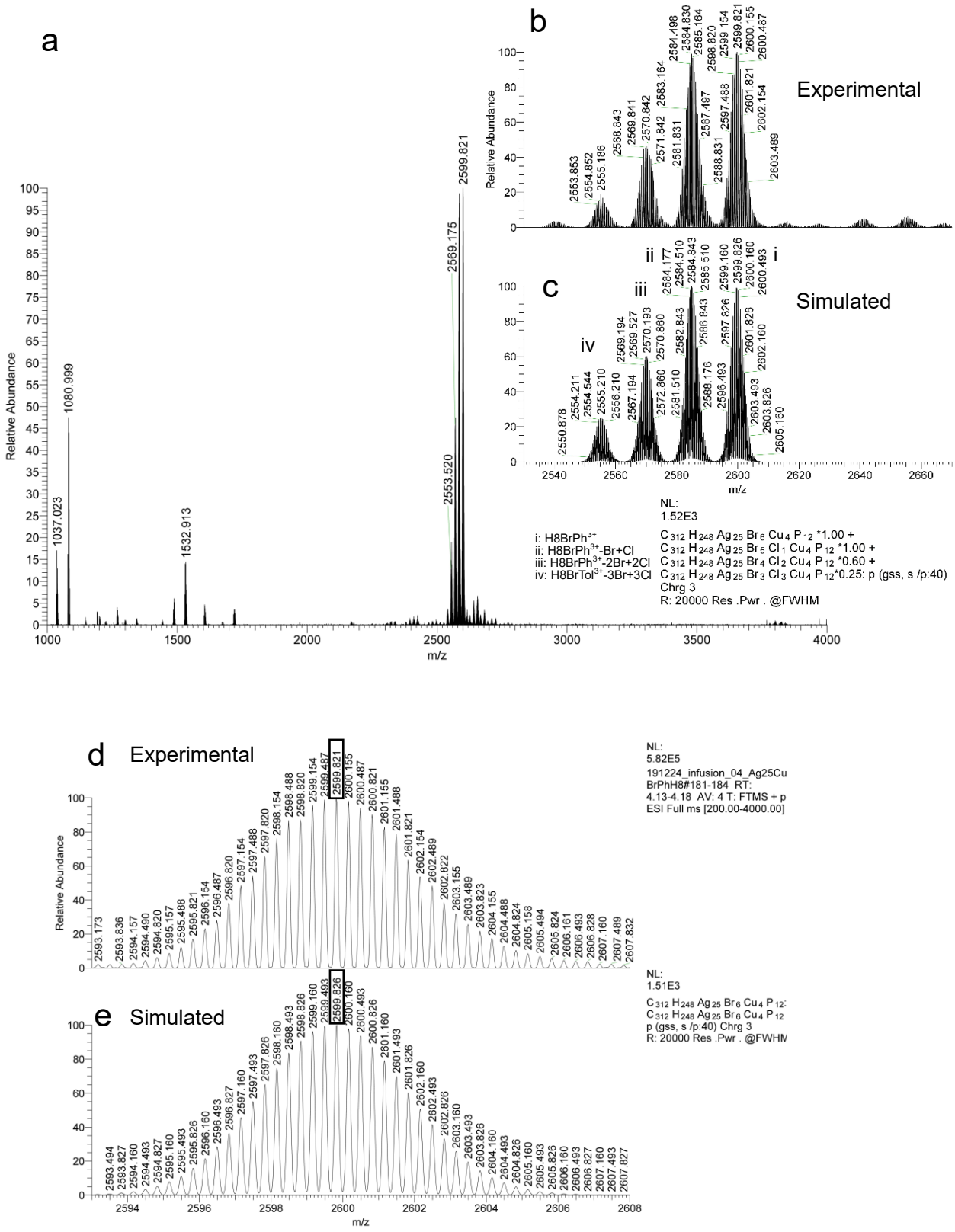


Figure S10. (a) ESI-MS spectra for **5**. (b) Main spectra. (c) Simulated ESI-MS spectra for $[Ag_{13}H_8Br_6\{CuAg_3(C{\equiv}CPh)_3(PPh_3)_3\}_4]^{3+}$ ($H8BrPh^{3+}$) and its derivatives formed by the exchange of Br with Cl. These derivatives were formed after dissolving the sample into CH_2Cl_2. (d) and (e) Experimental and simulated ESI-MS spectra for $H8BrPh^{3+}$.

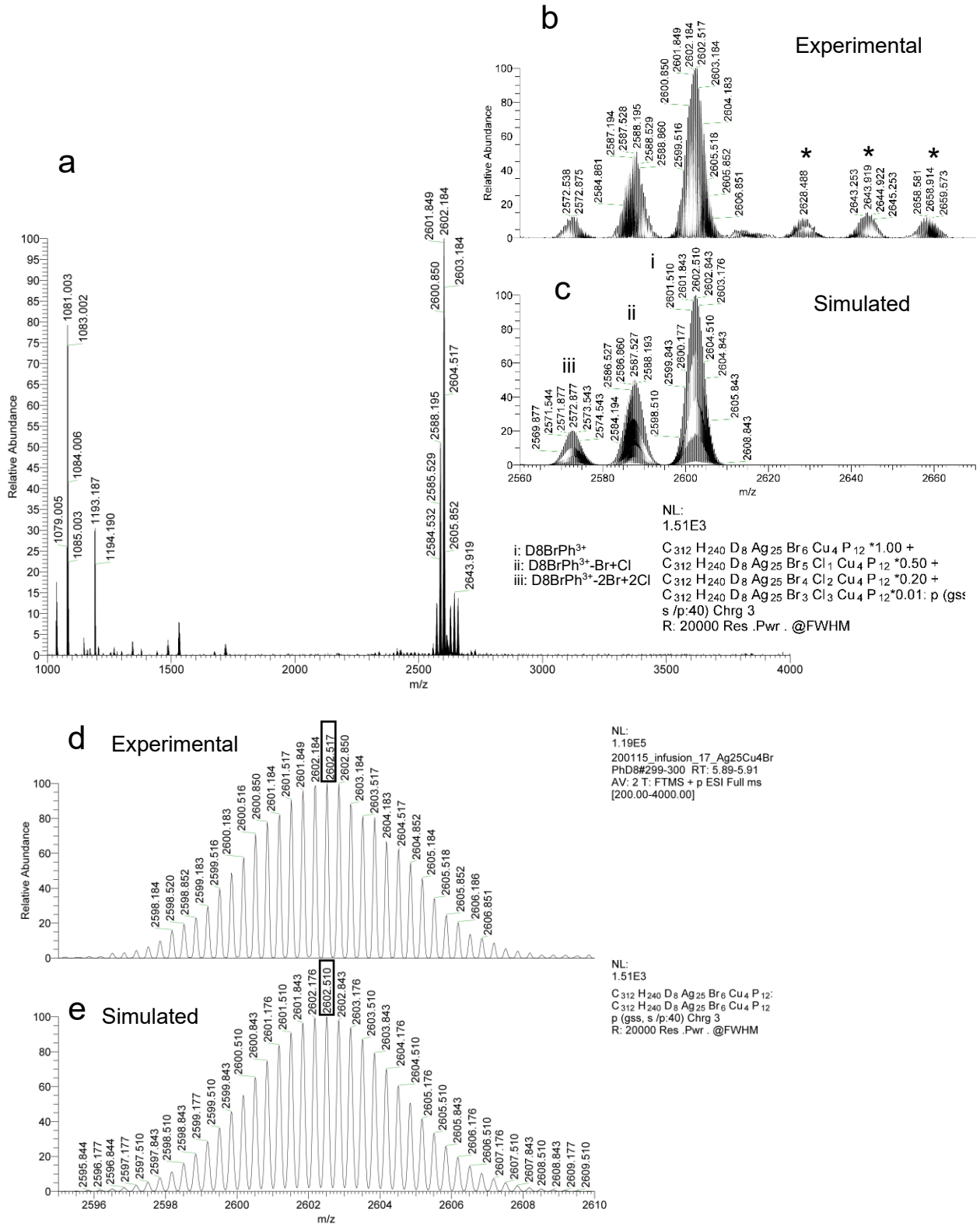


Figure S11. (a) ESI-MS spectra for deuterated **5**. (b) Main spectra. The spectra marked with * are the contamination from the previously measured deuterated **4** (see Figure S7). (c) Simulated ESI-MS spectra for $[Ag_{13}D_8Br_6\{CuAg_3(C{\equiv}CPh)_3(PPh_3)_3\}_4]^{3+}$ ($D8BrPh^{3+}$) and its derivatives formed by the exchange of Br^- with Cl^-. These derivatives were formed after dissolving the sample into CH_2Cl_2. (d) and (e) Experimental and simulated ESI-MS spectra for $D8BrPh^{3+}$.

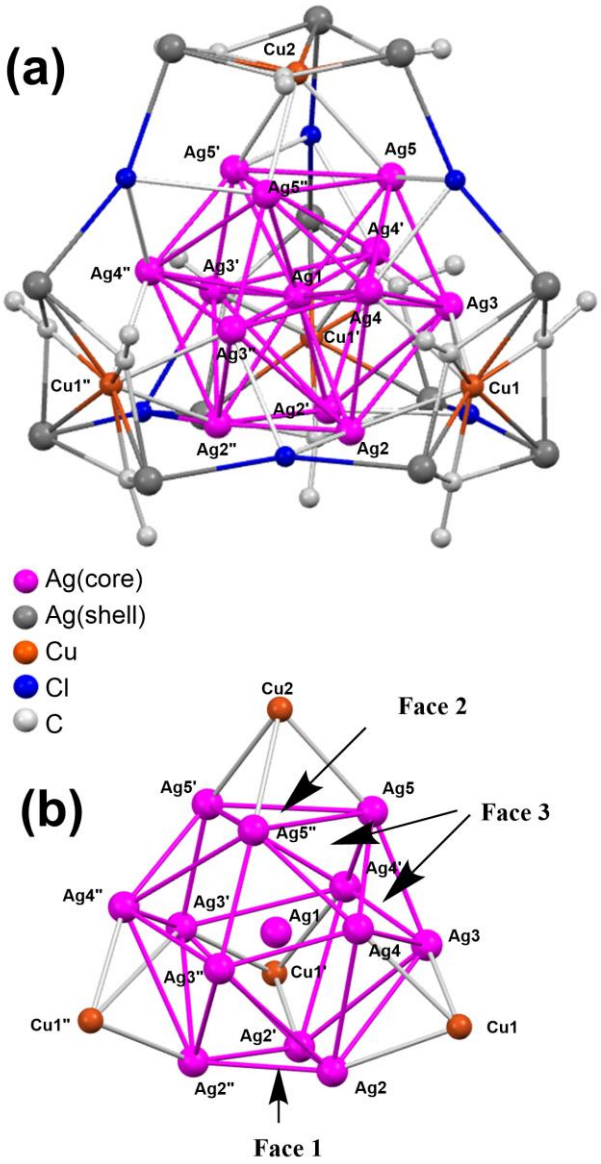


Figure S12. (a) The core and shell structure of ClH_8Tol, in which PPh_3 and Tol groups are omitted for clarity. (b) The $Ag_{13}Cu_4$ structure extracted from the crystal structure.

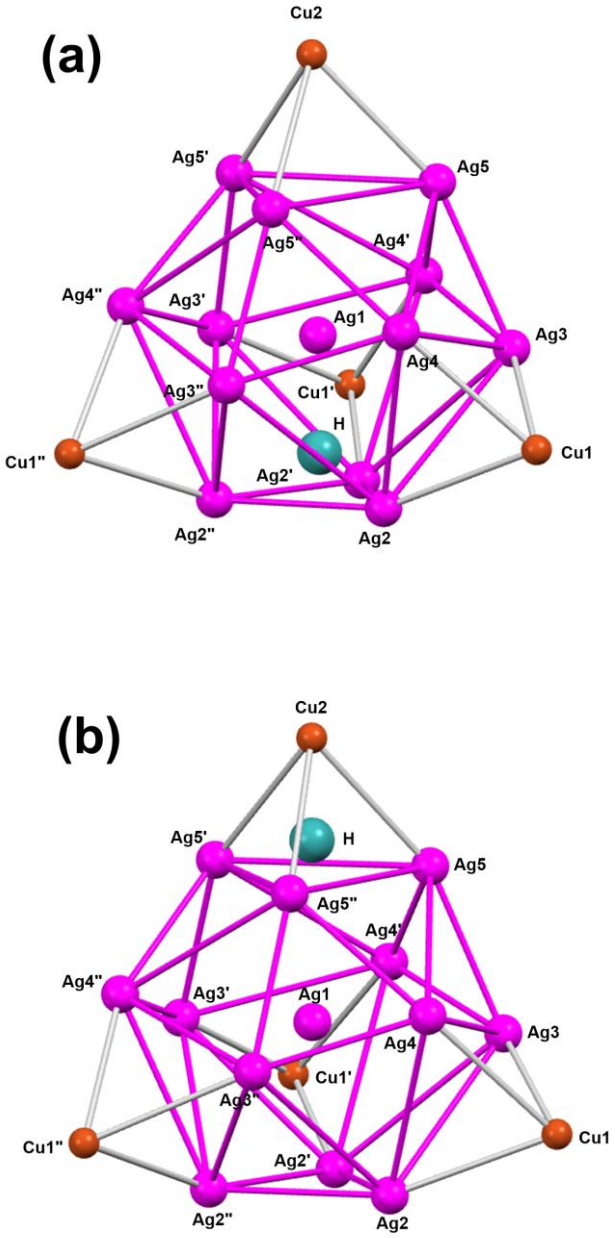


Figure S13. The optimized hydrogen positions and $Ag_{13}Cu_4$. (a) Face 1, (b) Face 2.

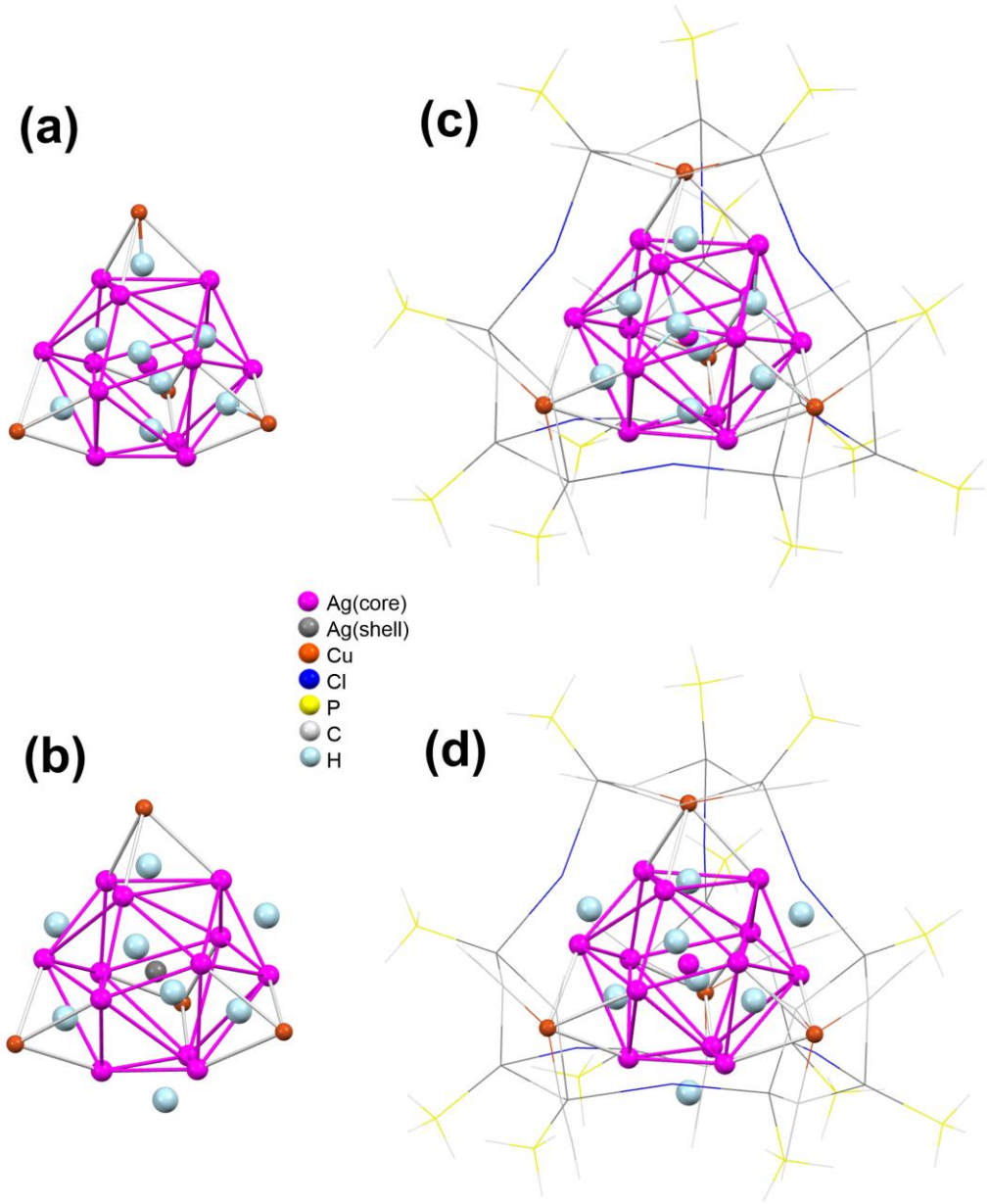
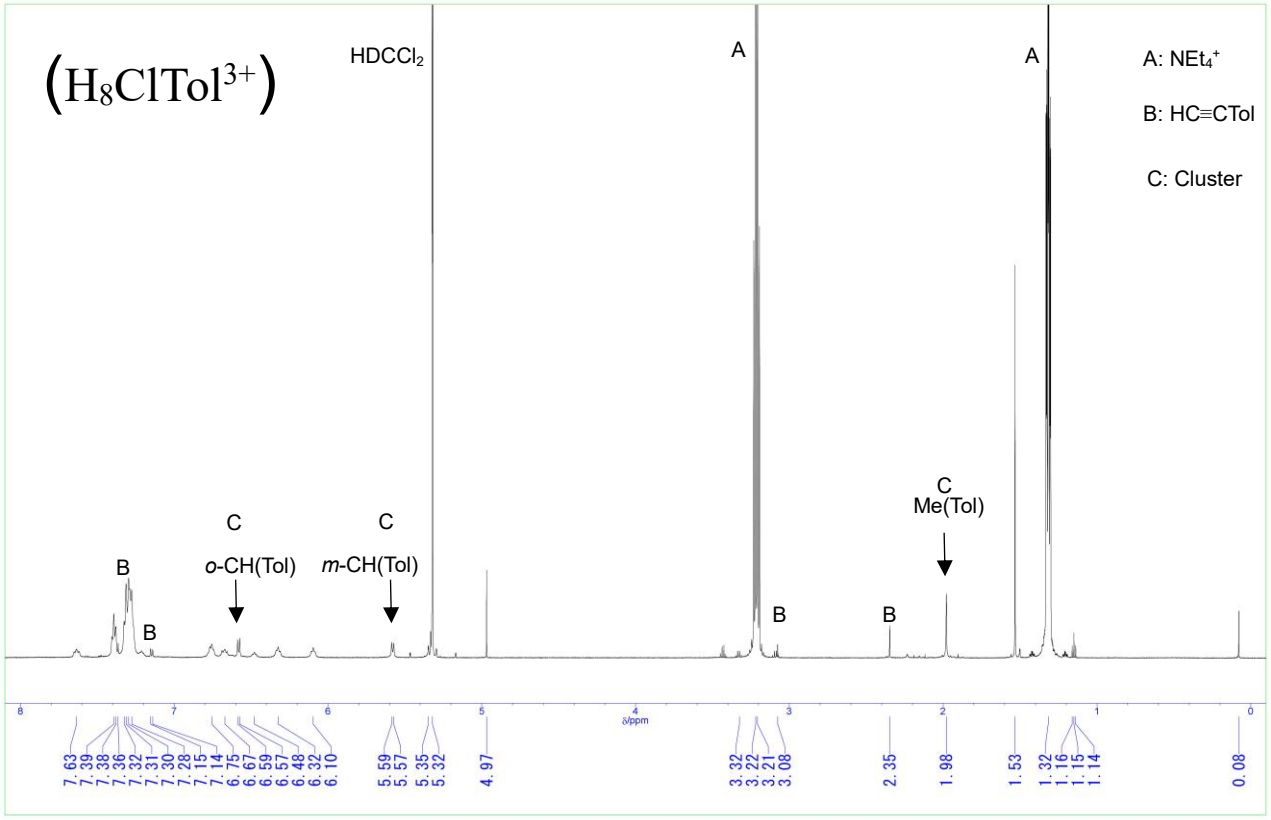


Figure S14. The structures of eight hydrogens and $Ag_{13}Cu_4$. (a) Model 1, (b) Model 2. The structures of eight hydrogens and the cluster, including simplified ligands whose aromatic group/s were replaced with hydrogen; the C≡CAr and PPh_3 were exchanged with C≡CH and PH_3, respectively. (c) Model 1, (d) Model 2.



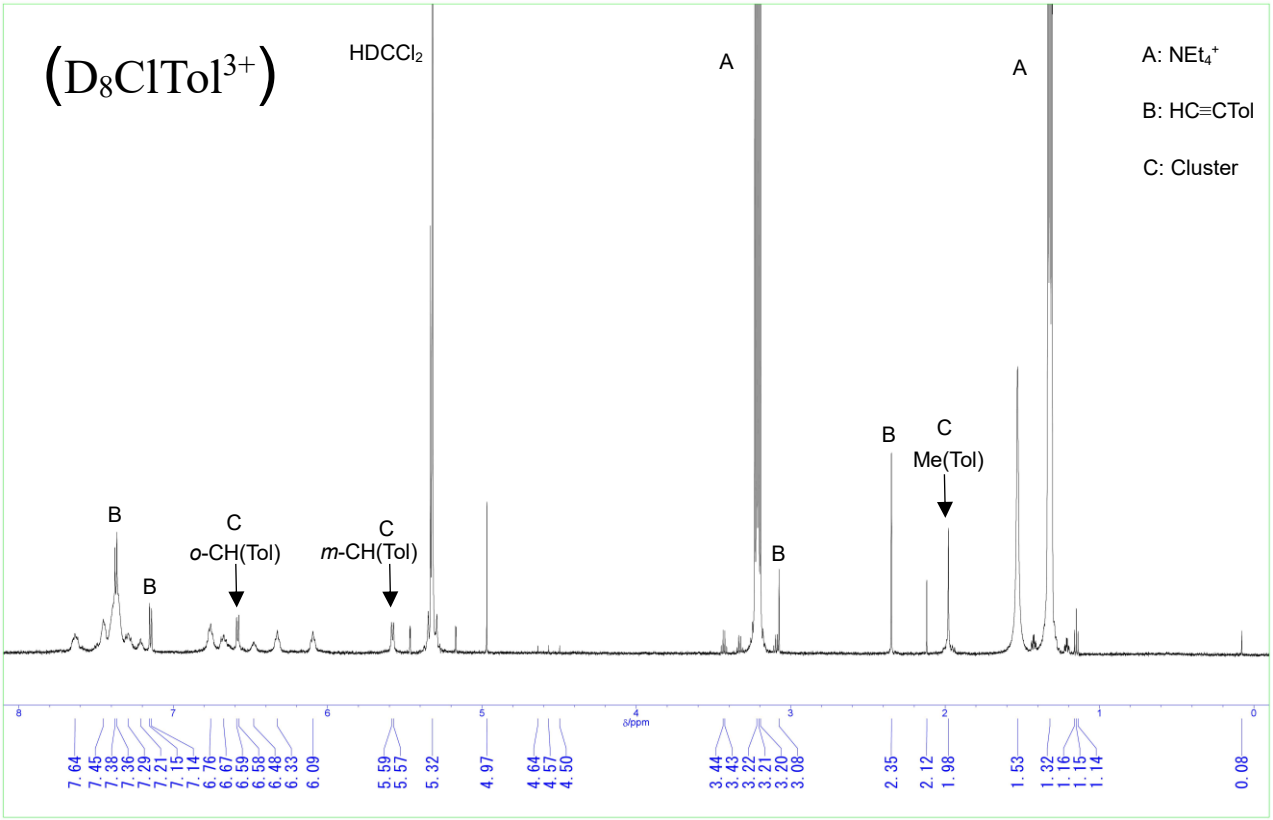
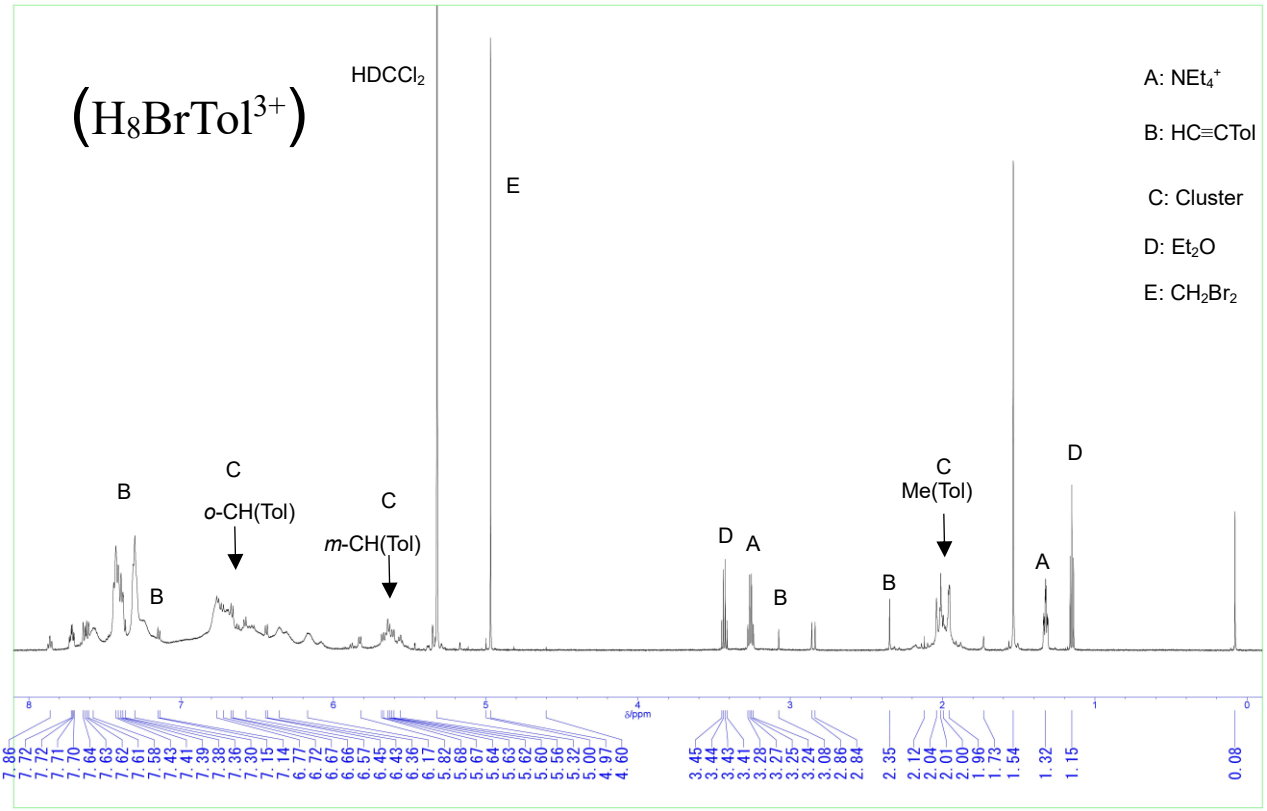


Figure S15. ^{1}H NMR of crude product containing $[Ag_{13}H_8Cl_6\{CuAg_3(C{\equiv}CTol)_3(PPh_3)_3\}_4]^{3+}$ (H_8ClTol^{3+}) (upper) and $[Ag_{13}D_8Cl_6\{CuAg_3(C{\equiv}CTol)_3(PPh_3)_3\}_4]^{3+}$ (D_8ClTol^{3+}) (lower).



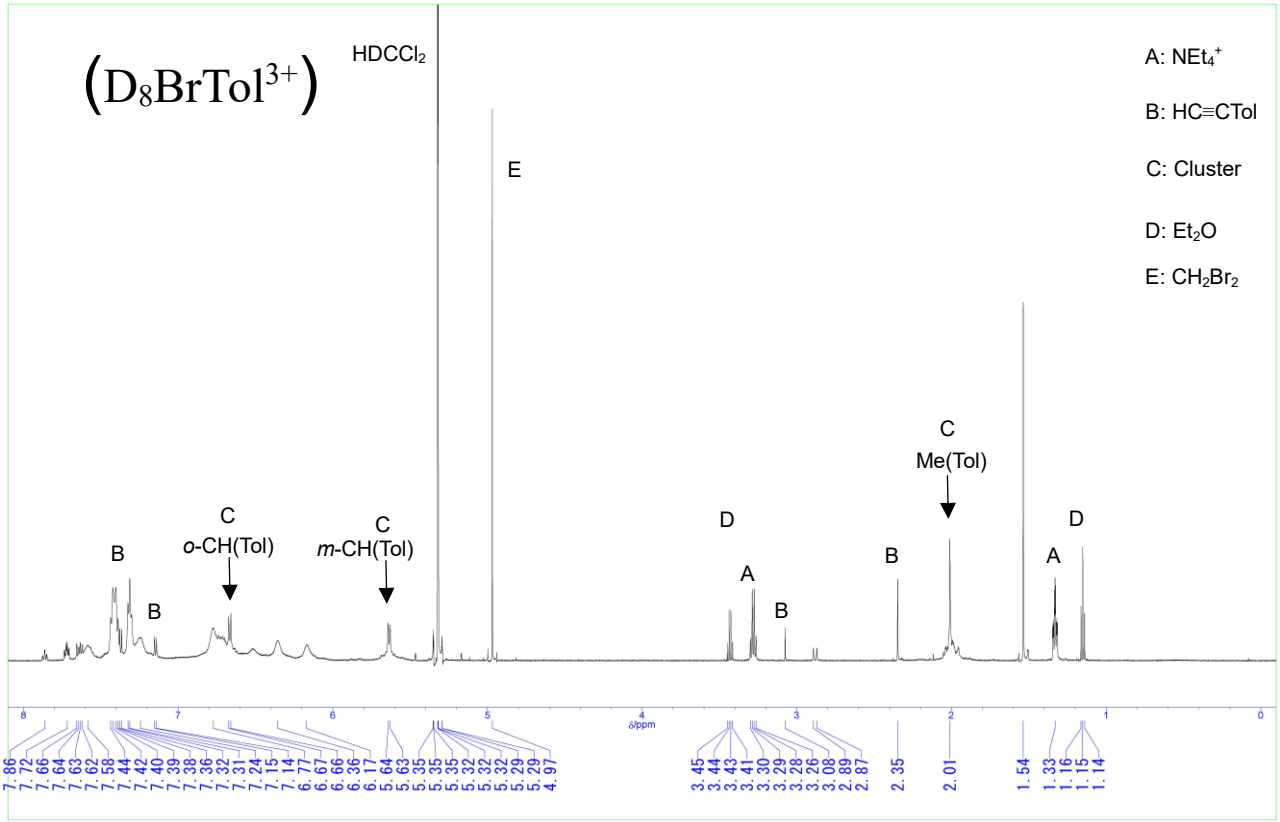
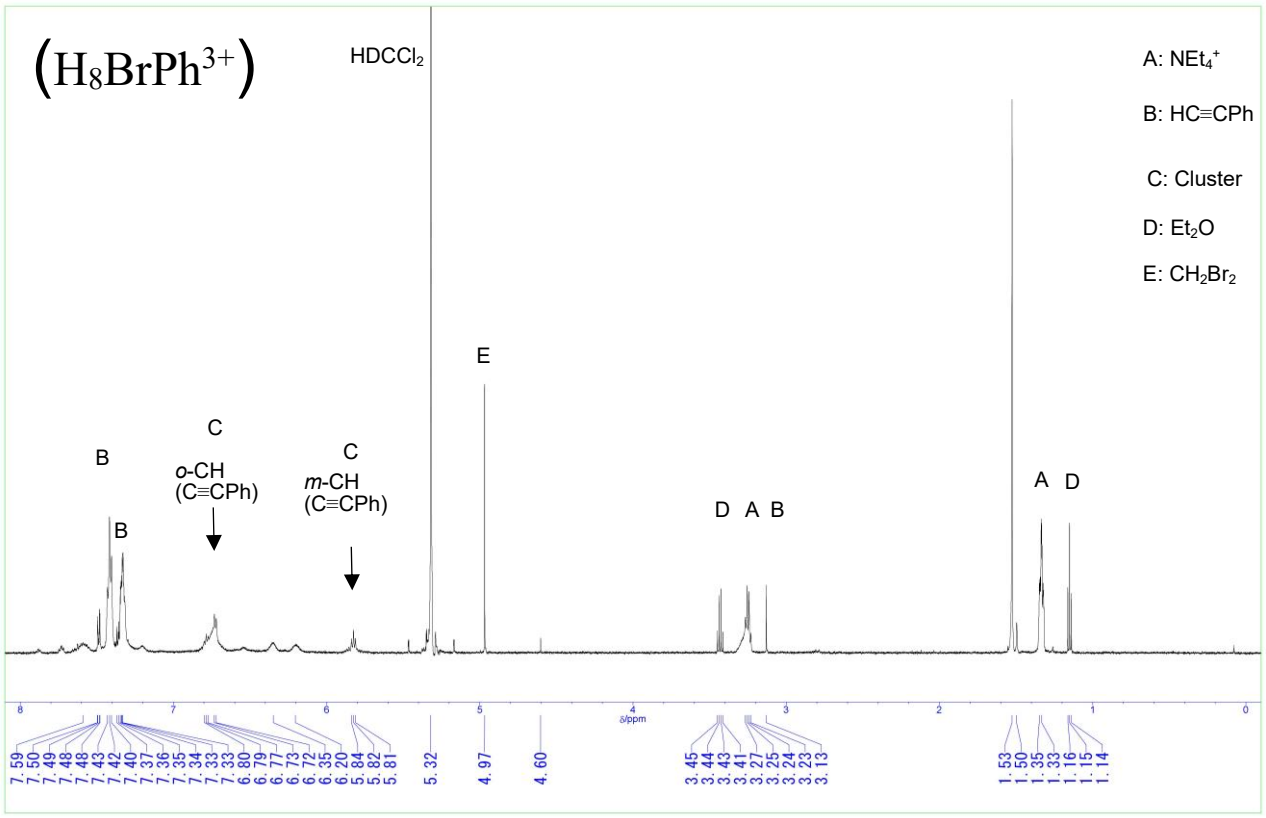


Figure S16. ^{1}H NMR of crude product containing $[Ag_{13}H_8Br_6\{CuAg_3(C{\equiv}CTol)_3(PPh_3)_3\}_4]^{3+}$ (H_8BrTol^{3+}) (upper) and $[Ag_{13}D_8Br_6\{CuAg_3(C{\equiv}CTol)_3(PPh_3)_3\}_4]^{3+}$ (D_8BrTol^{3+}) (lower).



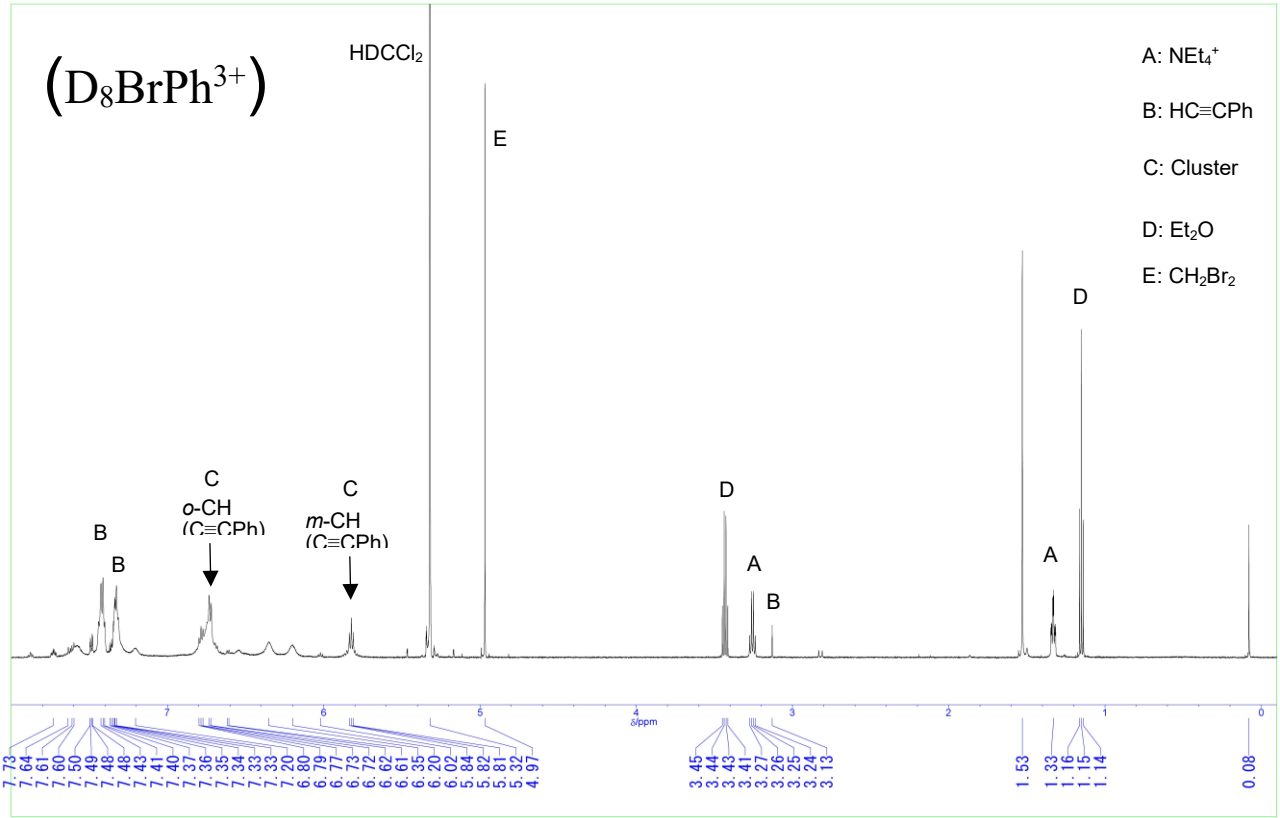
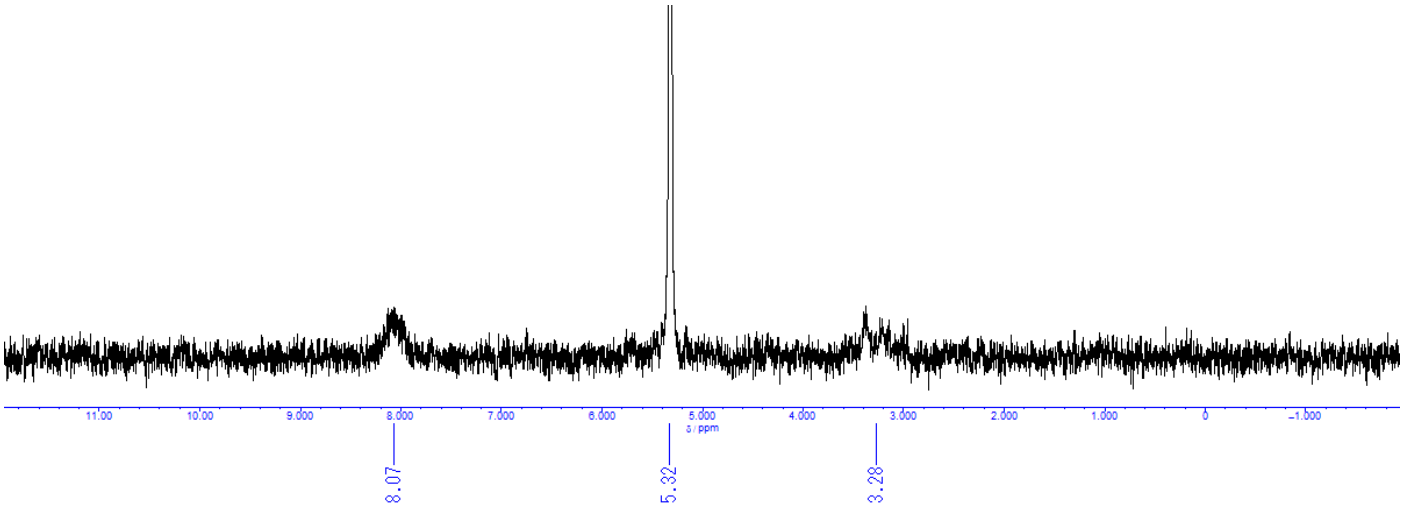
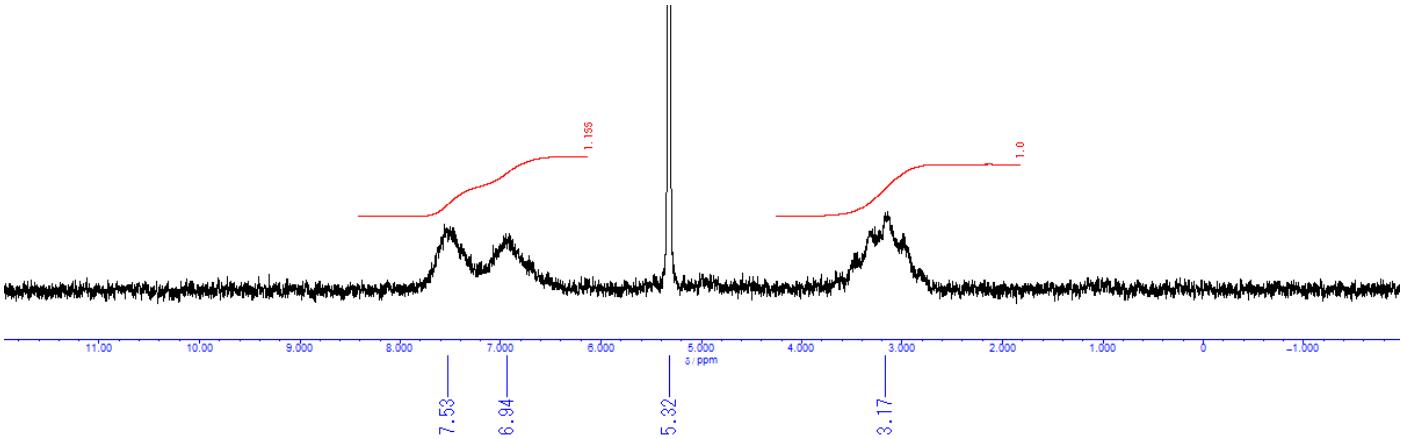


Figure S17. ^{1}H NMR of crude product containing $[Ag_{13}H_8Br_6\{CuAg_3(C{\equiv}CPh)_3(PPh_3)_3\}_4]^{3+}$ (H_8BrPh^{3+}) (upper) and $[Ag_{13}D_8Br_6\{CuAg_3(C{\equiv}CPh)_3(PPh_3)_3\}_4]^{3+}$ (D_8BrPh^{3+}) (lower).

D_8ClTol^{3+}



D_8BrTol^{3+}



D_8BrPh^{3+}

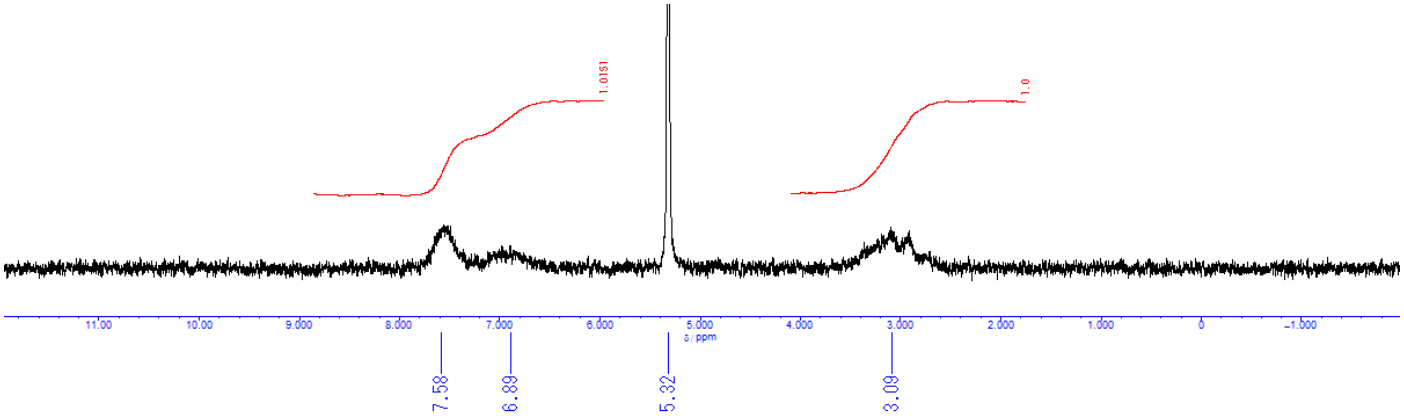
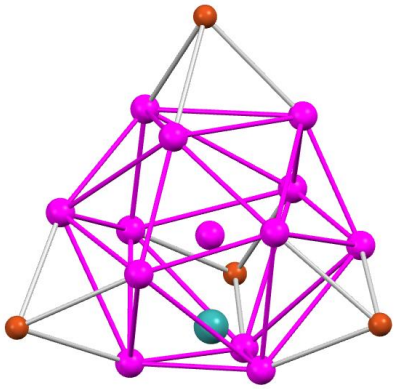


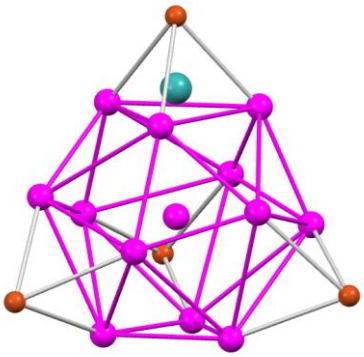
Figure S18. ^2H NMR of D_8ClTol^{3+}, D_8BrTol^{3+}, and D_8BrPh^{3+}. For D_8BrTol^{3+} and D_8BrPh^{3+}, two broad resonances are observed at 6.9 and 7.5 ppm, owing to one of the six Br ion is replaced with Cl ion after dissolving the cluster in CD_2Cl_2. Such substitution products are also observed on ESI-MS spectra as shown in Figures S7 and S11.

Table S1. Gaussian cartesian coordinates for $Ag13Cu4H^{16+}$ (Face 1).



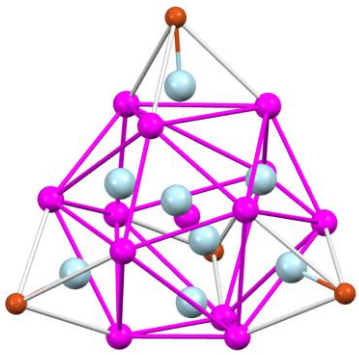
Ag	0.012013	0.001988	-0.000042
Ag	2.588059	1.483714	0.453511
Ag	0.351247	2.337329	-1.882890
Ag	-0.402315	2.650691	1.329572
Ag	-2.296751	0.597512	1.832228
Ag	2.496931	-1.258354	1.128686
Ag	0.290130	0.450844	2.972359
Ag	-0.572132	-2.447942	1.615976
Ag	-2.376232	-1.764693	-0.466024
Ag	2.522163	-0.471641	-1.584864
Ag	0.179957	-2.808417	-1.089820
Ag	-0.497076	-0.146539	-2.945136
Ag	-2.270965	1.405673	-1.363682
Cu	1.622132	4.104015	-0.075886
Cu	-4.469055	0.151288	0.001568
Cu	1.418139	-2.057398	3.634031
Cu	1.411198	-2.187774	-3.559763
H	-0.666386	-1.711503	0.007464

Table S2. Gaussian cartesian coordinates for $Ag13Cu4H^{16+}$ (Face 2).



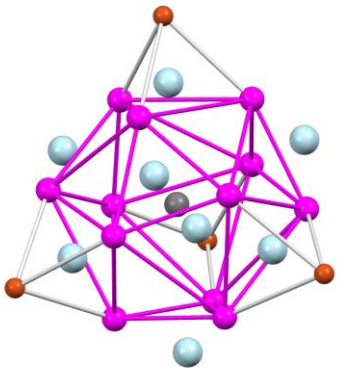
Ag	-0.009205	0.004605	0.000922
Ag	-2.662297	-1.323071	0.483530
Ag	-0.480484	-2.344658	-1.837430
Ag	0.259159	-2.636030	1.380365
Ag	2.265864	-0.681893	1.841579
Ag	-2.418608	1.421944	1.106313
Ag	-0.306092	-0.372662	2.979780
Ag	0.712487	2.448918	1.568158
Ag	2.472136	1.626835	-0.501965
Ag	-2.492493	0.585939	-1.591492
Ag	-0.023610	2.798522	-1.143612
Ag	0.501652	0.068178	-2.947714
Ag	2.189815	-1.549525	-1.338232
Cu	-1.844426	-4.002345	0.004038
Cu	4.456713	-0.393134	0.001106
Cu	-1.292948	2.207757	3.594621
Cu	-1.292056	2.199730	-3.600144
H	-1.182381	-2.561975	0.001480

Table S3. Gaussian cartesian coordinates for $Ag_{13}Cu_4H_8^{9+}$ (Model 1).



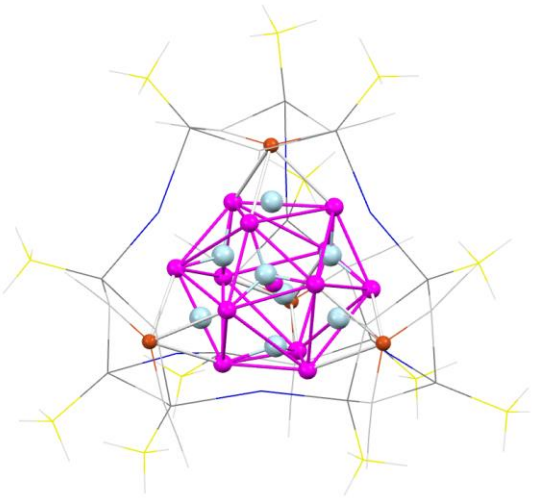
Ag	0.011141	-0.000022	-0.000026
Ag	2.536688	1.630027	-0.042221
Ag	0.272769	1.664854	-2.504769
Ag	-0.490676	2.912511	0.469521
Ag	-2.316025	1.049288	1.589128
Ag	2.536480	-0.780184	1.432197
Ag	0.274319	1.336566	2.694089
Ag	-0.491440	-1.862546	2.287656
Ag	-2.317317	-1.899258	0.114632
Ag	2.535570	-0.851903	-1.392297
Ag	0.272191	-3.001711	-0.189645
Ag	-0.492808	-1.049543	-2.756705
Ag	-2.317120	0.851926	-1.701558
Cu	1.484464	3.935041	-1.330214
Cu	-4.472411	0.001234	0.001390
Cu	1.484839	-0.816533	4.072607
Cu	1.482040	-3.119746	-2.743791
H	-0.635012	-1.703199	0.552133
H	1.903729	-0.000540	-0.000555
H	-0.633810	1.329915	1.199260
H	-0.635045	0.373663	-1.751016
H	0.971050	2.584380	-0.861999
H	-2.948014	0.000868	0.001028
H	0.969504	-2.038938	-1.807626
H	0.971188	-0.546263	2.668927

Table S4. Gaussian cartesian coordinates for $Ag_{13}Cu_4H_8^{9+}$ (Model 2).



Ag	0.011160	-0.000023	-0.000026
Ag	2.536655	1.629661	-0.053253
Ag	0.272572	1.648045	-2.515813
Ag	-0.490682	2.915537	0.450151
Ag	-2.315853	1.059838	1.582165
Ag	2.536573	-0.770521	1.437172
Ag	0.274411	1.354544	2.685034
Ag	-0.491276	-1.847272	2.300004
Ag	-2.317182	-1.898443	0.127458
Ag	2.535516	-0.861100	-1.386643
Ag	0.272191	-3.002865	-0.169572
Ag	-0.492936	-1.067865	-2.749615
Ag	-2.317121	0.840479	-1.707063
Cu	1.484342	3.926074	-1.356537
Cu	-4.472411	0.001181	0.001627
Cu	1.485088	-0.789294	4.077864
Cu	1.481945	-3.137954	-2.722964
H	-1.165860	-3.080003	1.043657
H	3.482193	-0.000977	-0.001251
H	-1.163978	2.443990	2.146237
H	-1.166511	0.636787	-3.188569
H	0.956350	2.537949	-0.865090
H	-2.902661	0.000687	0.001243
H	0.954531	-2.018779	-1.766556
H	0.956724	-0.520603	2.630697

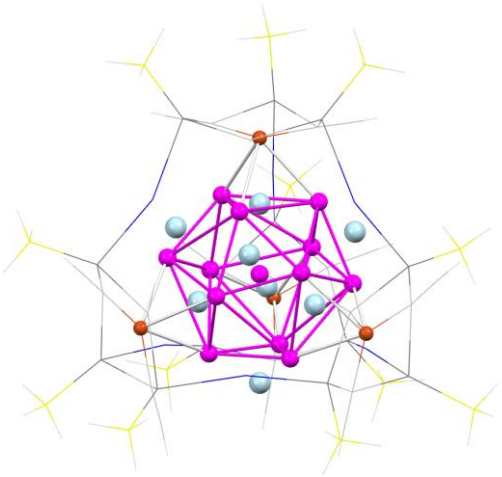
Table S5. Gaussian cartesian coordinates for $[Ag_{25}Cu_4H_8Cl_6(CCH)_{12}(PH_3)_{12}]^{3+}$ (Model 1)



Ag	-0.000027	0.000013	0.011998	Ag	3.562466	-4.628872	0.666838
Ag	1.068605	1.231406	-2.511366	Ag	1.360807	-2.287316	5.151947
Ag	-0.725685	2.917712	-0.250551	Cu	2.457160	-3.350041	-1.460612
Ag	2.309524	1.833032	0.514377	Cl	2.222804	-3.068279	2.654527
Ag	1.879307	-0.297096	2.339298	Cl	3.745686	0.387085	-2.635775
Ag	-0.221665	4.927760	-3.089217	C	2.122611	-3.069636	-3.414331
Ag	3.964001	3.187985	-2.795652	C	2.015552	-2.719613	-4.578155
Ag	2.227438	5.399664	0.666838	C	1.442132	-4.811719	-0.526522
Ag	1.300555	2.322104	5.151947	C	0.643305	-5.613746	-0.119533
Cu	1.672667	3.802984	-1.460612	C	4.193566	-2.762145	-0.694257
Cu	-0.000028	0.000003	4.495749	C	5.200420	-2.493674	-0.037984
Cl	1.545786	3.459136	2.654529	C	-0.914894	-1.745392	4.717507
Cl	-2.208131	3.050288	-2.635782	C	-1.314794	-2.913653	4.755769
C	1.597048	3.373044	-3.414333	Ag	-1.600787	0.309711	-2.511384
C	1.347460	3.105297	-4.578156	Ag	-2.164054	-2.087325	-0.250549
C	3.445999	3.654795	-0.526522	Ag	-2.742252	1.083663	0.514405
C	4.539968	3.364034	-0.119533	Ag	-0.682325	1.776037	2.339308
C	0.295322	5.012769	-0.694262	Ag	-4.156729	-2.655846	-3.089216
C	-0.440618	5.750601	-0.037987	Ag	-4.742826	1.838921	-2.795655
C	1.968955	0.080344	4.717508	Ag	-5.789999	-0.770778	0.666838
C	3.180706	0.318226	4.755769	Ag	-2.661254	-0.034779	5.151948
Ag	0.532162	-1.541190	-2.511380	Cu	-4.129821	-0.452927	-1.460613
Ag	2.889764	-0.830402	-0.250553	Cl	-3.768588	-0.390843	2.654535
Ag	0.432729	-2.916669	0.514378	Cl	-1.537547	-3.437367	-2.635782
Ag	-1.196982	-1.478940	2.339291	C	-3.719649	-0.303497	-3.414337
Ag	4.378404	-2.271907	-3.089214	C	-3.363006	-0.385676	-4.578156
Ag	0.778833	-5.026895	-2.795654	C	-4.888228	1.156931	-0.526523

C	-5.183268	2.249721	-0.119530
C	-4.488776	-2.250622	-0.694251
C	-4.759896	-3.256815	-0.037982
C	-1.054162	1.665064	4.717507
C	-1.866010	2.595436	4.755768
P	5.574089	3.960415	-4.383987
H	6.817869	3.724207	-3.915163
H	5.402236	3.307433	-5.552958
H	5.411693	5.286107	-4.580924
P	6.455637	-2.709486	-4.187083
H	6.326897	-2.463789	-5.508293
H	7.413970	-1.910272	-3.671998
H	6.799403	-4.001705	-4.001099
P	-0.881293	6.945512	-4.187066
H	-1.289910	6.662111	-5.442149
H	-1.893659	7.519718	-3.503056
H	0.167209	7.794537	-4.236124
P	-6.216882	2.847050	-4.383946
H	-6.730741	3.981955	-3.863819
H	-5.533225	3.137839	-5.511094
H	-7.219507	1.990764	-4.673982
P	-8.058279	-0.648110	1.409367
H	-8.397873	-1.807539	2.011838
H	-8.190470	0.370068	2.285864
H	-8.867856	-0.437692	0.349696
P	-4.147168	-0.462476	6.974313
H	-5.055523	0.532780	7.057430
H	-4.782732	-1.635988	6.770844
H	-3.442530	-0.525766	8.124123
P	1.673095	3.822749	6.974351
H	3.000490	3.981419	7.162516
H	1.112133	5.018388	6.694647
H	1.117108	3.316023	8.095372
P	2.474096	-3.360340	6.974332
H	2.090989	-2.788007	8.135475
H	2.150640	-4.670936	6.990432
H	3.809448	-3.228161	6.826557
P	4.590432	-6.654575	1.409346
H	5.383566	-7.141409	0.431304
H	5.333164	-6.405583	2.508828
H	3.635382	-7.560996	1.707186
P	-5.574298	-4.236013	-4.187058
H	-5.239200	-4.310185	-5.492715
H	-5.424184	-5.449217	-3.614293
H	-6.860364	-3.841152	-4.074295
P	0.642837	-6.807491	-4.383995
H	1.870127	-7.054364	-4.889357
H	0.174880	-7.918236	-3.775820
H	-0.193182	-6.455800	-5.383894
P	3.467877	7.302689	1.409343
H	4.116289	7.853984	0.361379
H	2.622994	8.210069	1.943581
H	4.364968	6.919104	2.342347
H	-3.090643	-0.445087	-5.611205
H	1.930779	-2.454018	-5.611197
H	1.159868	2.899112	-5.611209
H	-1.066979	6.435542	0.494379
H	-2.530754	3.431385	4.820490
H	-5.476988	3.213798	0.239815
H	6.106793	-2.293697	0.494348
H	5.521722	3.136307	0.239831
H	4.237024	0.475997	4.820490
H	-5.039866	-4.141761	0.494341
H	-0.044778	-6.350121	0.239825
H	-1.706287	-3.907349	4.820489
H	-0.000125	-0.000025	-1.967260
H	-1.093036	1.526086	0.689089
H	-0.775157	-1.709794	0.688849
H	1.868008	0.183571	0.688802
H	1.442628	-1.987125	-0.856371
H	-0.000060	-0.000030	2.672601
H	-2.442475	-0.255757	-0.855964
H	0.999260	2.243312	-0.855871

Table S6. Gaussian cartesian coordinates for $[Ag_{25}Cu_4H_8Cl_6(CCH)_{12}(PH_3)_{12}]^{3+}$ (Model 2)



Ag	-0.000039	0.000012	0.011578	Ag	0.955535	-4.996342	-2.796018
Ag	1.023435	1.268904	-2.507197	Ag	3.723323	-4.500609	0.667059
Ag	-0.824489	2.888315	-0.251517	Ag	1.441102	-2.237922	5.152076
Ag	2.240128	1.913356	0.511483	Cu	2.575791	-3.263840	-1.461629
Ag	1.883849	-0.230002	2.338786	Cl	2.330198	-2.988855	2.655384
Ag	-0.395686	4.917085	-3.089104	Cl	3.730845	0.519160	-2.636555
Ag	3.849186	3.325739	-2.796025	C	2.229715	-2.992305	-3.414837
Ag	2.035927	5.474841	0.667059	C	2.110137	-2.646764	-4.578277
Ag	1.217632	2.366947	5.152081	C	1.610291	-4.758127	-0.526619
Cu	1.538685	3.862625	-1.461640	C	0.840715	-5.587562	-0.119423
Cu	-0.000031	0.000007	4.499997	C	4.288631	-2.612445	-0.693446
Cl	1.423306	3.512433	2.655385	C	5.285151	-2.308520	-0.037845
Cl	-2.315099	2.971397	-2.636557	C	-0.852486	-1.777258	4.717435
C	1.476516	3.427132	-3.414841	C	-1.211223	-2.958367	4.755636
C	1.237083	3.150781	-4.578277	Ag	-1.610655	0.251867	-2.507197
C	3.315512	3.773620	-0.526625	Ag	-2.089171	-2.158187	-0.251543
C	4.418586	3.521905	-0.119421	Ag	-2.777146	0.983407	0.511508
C	0.118140	5.020253	-0.693444	Ag	-0.742668	1.746419	2.338706
C	-0.643334	5.731405	-0.037849	Ag	-4.060471	-2.801208	-3.089102
C	1.965350	0.150328	4.717439	Ag	-4.804715	1.670615	-2.796026
C	3.167642	0.430280	4.755634	Ag	-5.759343	-0.974220	0.667058
Ag	0.587211	-1.520836	-2.507231	Ag	-2.658628	-0.129011	5.152077
Ag	2.913671	-0.730122	-0.251526	Cu	-4.114476	-0.598785	-1.461638
Ag	0.537004	-2.896752	0.511472	Cl	-3.753496	-0.523565	2.655384
Ag	-1.141159	-1.516429	2.338759	Cl	-1.415740	-3.490548	-2.636552
Ag	4.456166	-2.115864	-3.089099	C	-3.706231	-0.434921	-3.414842

C	-3.347213	-0.504008	-4.578277
C	-4.925890	0.984512	-0.526622
C	-5.259296	2.065671	-0.119424
C	-4.406657	-2.407796	-0.693450
C	-4.641915	-3.422775	-0.037844
C	-1.112951	1.626943	4.717441
C	-1.956517	2.528095	4.755639
P	5.430845	4.154561	-4.383940
H	6.682270	3.962418	-3.915109
H	5.282217	3.495933	-5.552884
H	5.221891	5.473699	-4.580884
P	6.547069	-2.480151	-4.187049
H	6.409841	-2.239168	-5.508287
H	7.476691	-1.647602	-3.672003
H	6.936313	-3.759395	-4.001078
P	-1.125618	6.910030	-4.187032
H	-1.524016	6.612478	-5.442150
H	-2.157675	7.448218	-3.503059
H	-0.107811	7.795590	-4.236098
P	-6.313393	2.625923	-4.383899
H	-6.867046	3.742049	-3.863770
H	-5.640469	2.940714	-5.511020
H	-7.285242	1.734895	-4.673938
P	-8.030309	-0.931928	1.409298
H	-8.328925	-2.102655	2.011787
H	-8.198409	0.080900	2.285852
H	-8.846904	-0.750217	0.349701
P	-4.128186	-0.608458	6.974270
H	-5.071119	0.354174	7.057473
H	-4.722027	-1.803611	6.770845
H	-3.421831	-0.646848	8.124121
P	1.537180	3.879301	6.974308
H	2.858198	4.084712	7.162559
H	0.934469	5.054443	6.694649
H	0.999464	3.353344	8.095367
P	2.591029	-3.270910	6.974287
H	2.188010	-2.712514	8.135473
H	2.313990	-4.592153	6.990474
H	3.920882	-3.091792	6.826557
P	4.822241	-6.488441	1.409275
H	5.632113	-6.947093	0.431300
H	5.555838	-6.213476	2.508785
H	3.899834	-7.428029	1.707175
P	-5.421404	-4.429862	-4.187024
H	-5.083962	-4.492241	-5.492711
H	-5.228602	-5.637098	-3.614297
H	-6.720617	-4.080731	-4.074273
P	0.882593	-6.780506	-4.383948
H	2.117776	-6.984028	-4.889307
H	0.454104	-7.907161	-3.775779
H	0.034655	-6.458605	-5.383820
P	3.208099	7.420377	1.409272
H	3.836693	7.994296	0.361385
H	2.331769	8.297521	1.943529
H	4.118155	7.068766	2.342334
H	-3.073052	-0.553828	-5.611142
H	2.016156	-2.384413	-5.611136
H	1.056902	2.938251	-5.611147
H	-1.293250	6.393914	0.494358
H	-2.650181	3.339957	4.820518
H	-5.586948	3.018574	0.239805
H	6.183878	-2.076926	0.494326
H	5.407634	3.329146	0.239819
H	4.217558	0.625137	4.820518
H	-4.890683	-4.316904	0.494321
H	0.179272	-6.347738	0.239814
H	-1.567394	-3.965061	4.820517
H	0.000095	-0.000014	-3.518115
H	-2.034634	2.613362	1.208245
H	-1.246227	-3.068438	1.208067
H	3.280779	0.455334	1.207951
H	1.322644	-1.687321	-0.746623
H	0.000108	0.000323	2.341014
H	-2.122917	-0.301978	-0.746964
H	0.799741	1.988788	-0.746973

Table S7. Bond distances between Ag atoms of the core.

This work			icosahedron		
cluster	Ag–Ag/Å		CSD refcode	Ag–Ag/Å	Ag–Ag/Å
	center	surface		center	surface
		small	UYACED	2.802	2.950
H8ClTol	3.006	2.832	NOXNAS	2.772	2.915
H8BrTol	3.027	2.835	NOXNEW	2.770	2.913
H8BrPh	3.014	2.829	TORRAW	2.791	2.935
		large	TORREA	2.788	2.931
H8ClTol		3.321	YUBMAM	2.784	2.927
H8BrTol		3.301	GETMAW	2.806	2.926
H8BrPh		3.293	MOYMIY	2.779	2.922
		others	NAVSOV	2.791	2.934
H8ClTol		3.540	NAVSUB	2.777	2.921
H8BrTol		3.730			
H8BrPh		3.679			
average	3.016		average	2.786	2.927