Electronic Supplementary Information

A homoleptic, all-alkynyl-stabilized highly luminescent Au_8Ag_8 cluster with single crystal X-ray structure

Rui Zhang,‡[a] Chongyang Zhao,‡[b] Xiumin Li,[a] Zongyao Zhang,[a] Xicheng Ai,[a] Hui Chen*[b] and Rui Cao*[ac]

[a]*Department of Chemistry, Renmin University of China, Beijing 100872, China.*

[b]*Beijing National Laboratory for Molecular Sciences (BNLMS), Key Laboratory of Photochemistry, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.*

[c]*School of Chemistry and Chemical Engineering, Shaanxi Normal University, Xi'an 710119 China.*

‡These authors contributed equally to this work.

Correspondence E-mail: chenh@iccas.ac.cn; ruicao@ruc.edu.cn.

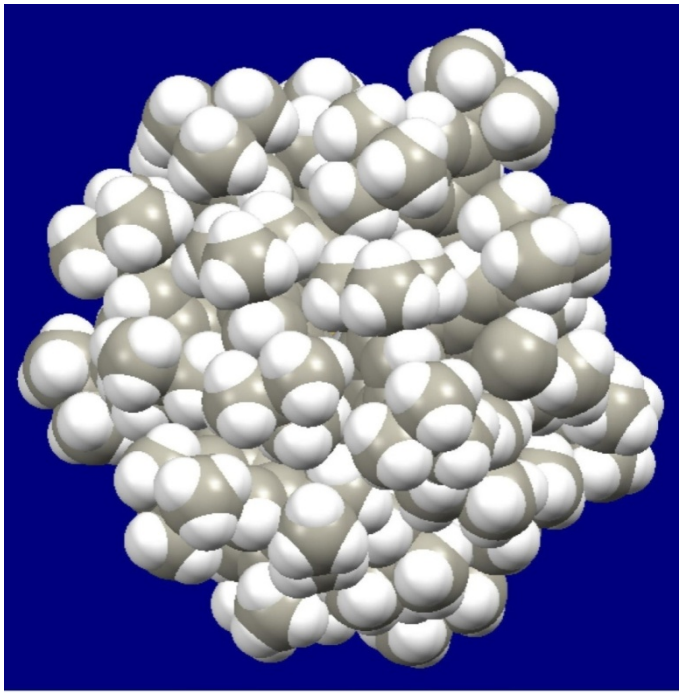

Figure S1. Space-filling diagram of complex **1**.

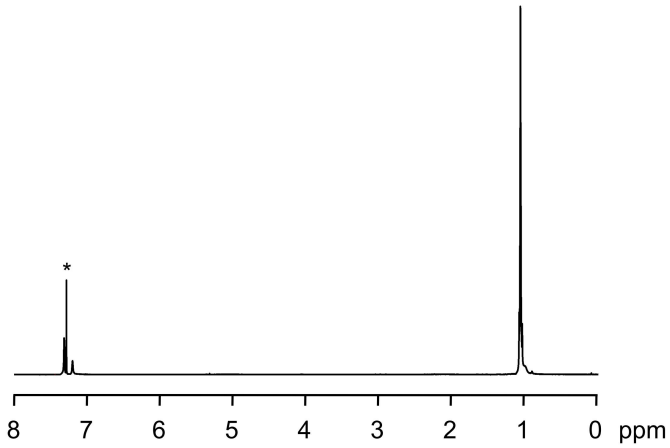

Figure S2. ^{1}H NMR spectrum of complex **1** in $CDCl_3$. The solvent residue peak of $CHCl_3$ is labeled (*).

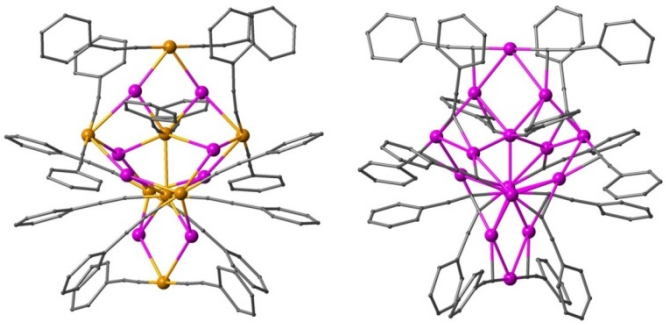

Figure S3. Crystal structure of $[Au_8Ag_8(ArC{\equiv}C)_{16}]$ (**1**, left) and its all-silver isostructural analogue $[Ag_{16}(ArC{\equiv}C)_{16}]$ (Ag_{16}, right). All hydrogen atoms and *tert*-butyl moieties are omitted for clarity. Color code: orange, gold; rose pink, silver; grey, carbon.

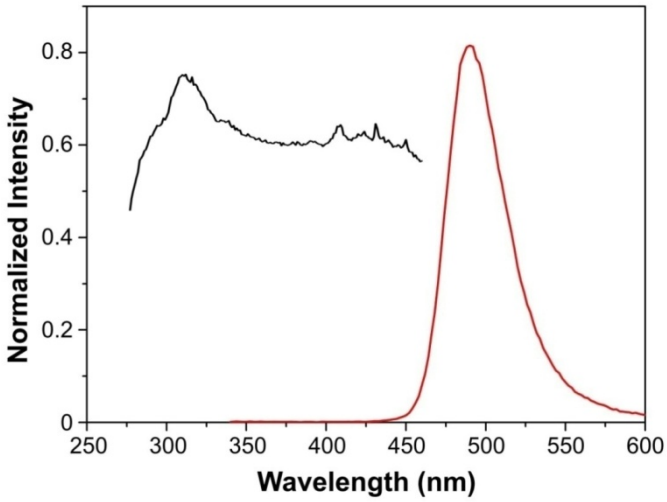

Figure S4. Excitation and emission spectra of **1** in the solid state.

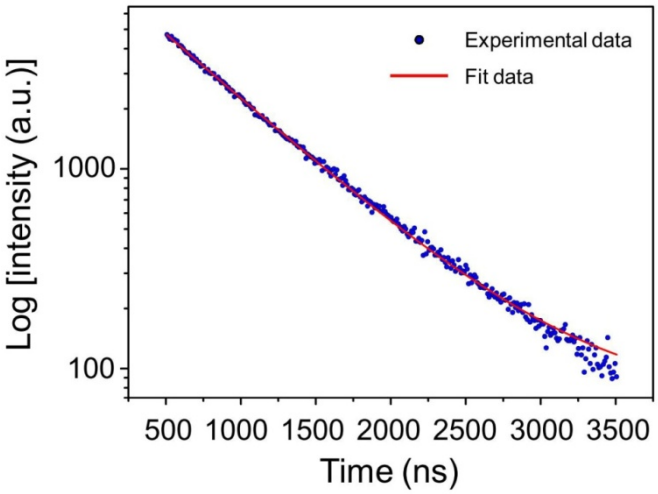

Figure S5. Lifetime of **1** at 273.2 nm in the solid state using picosecond pulsed diode laser (EPLED-270) as an excitation source, τ = 660 ns.

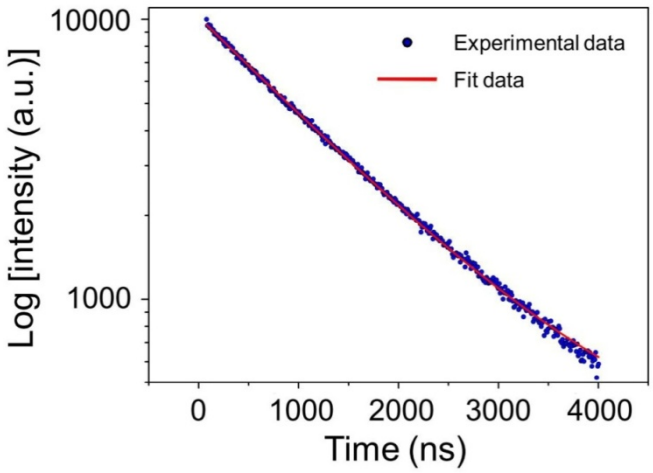

Figure S6. Lifetime of **1** at 273.2 nm in dichloromethane with a concentration of 1.0 × 10^{-5} M using picosecond pulsed diode laser (EPLED-270) as an excitation source, τ = 1243 ns.

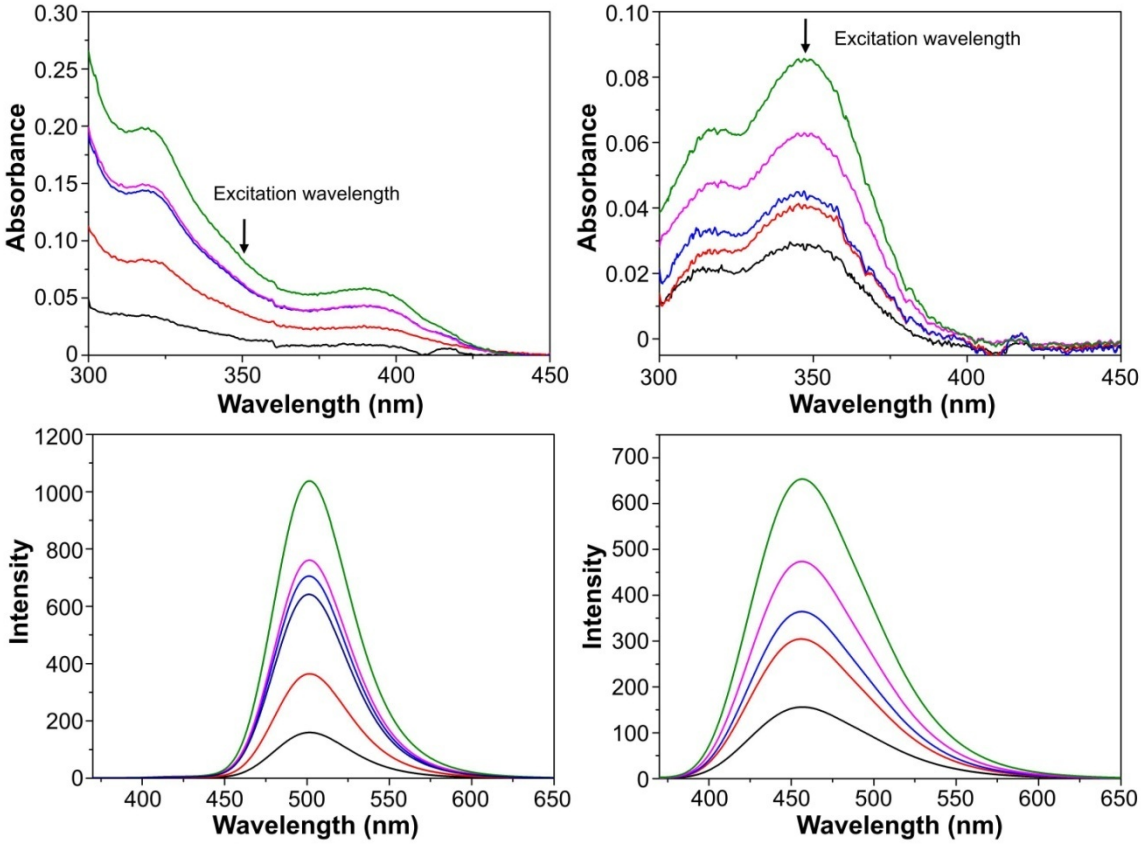

Figure S7. Absorption spectrum of **1** (top left) and quinine sulfate (top right) in dichloromethane. Emission spectrum of **1** (bottom left) and quinine sulfate (bottom right) in dichloromethane.

The Q.Y. of **1** was calculated using the following equation, by referencing to the standard quinine sulfate:

$$\varphi = \varphi_{ST}\left(\frac{Grad}{Grad_{ST}}\right)\left(\frac{\eta^2}{\eta_{ST}^2}\right)$$

In which, φ and φ_{ST} are the Q.Y. for **1** and quinine sulfate (0.1 M H_2SO_4), respectively, Grad is the gradient from the plot of integrated fluorescence *vs* absorbance, and η is the refractive index of the solvent (dichloromethane, 1.4244, and H_2O, 1.33).

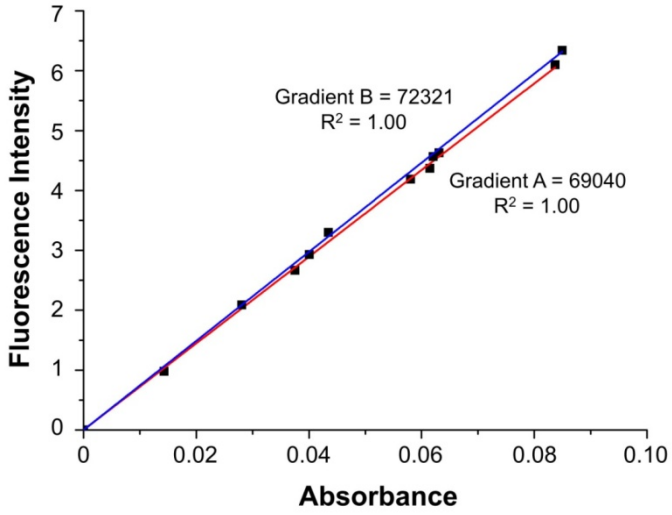

Figure S8. Linear plots for **1** and quinine sulfate. The gradient for each sample is proportional to the sample's fluorescence Q.Y. The calculated Q.Y. is 0.67.

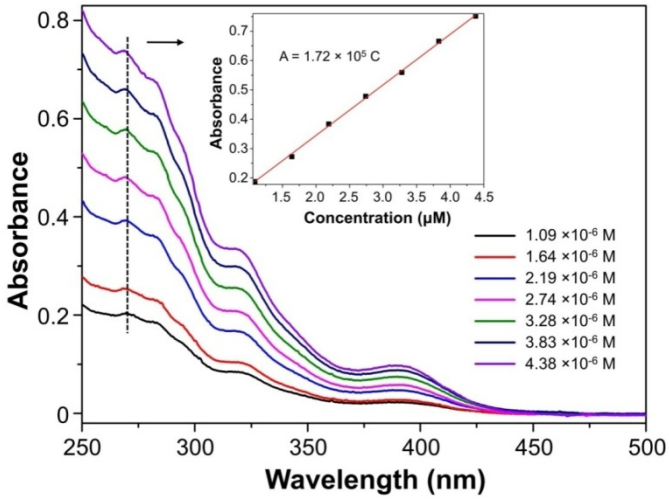

Figure S9. UV-vis absorption spectra of **1** as the concentration increases from 1.09 × 10^{-6} to 4.38 × 10^{-6} M. Inset: plot of absorbance at 276 nm as a function of concentration.

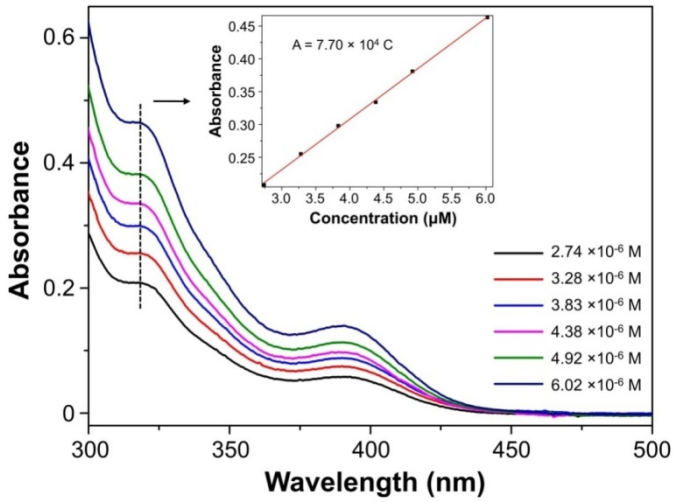

Figure S10. UV-vis absorption spectra of **1** as the concentration increases from 2.74 × 10^{-6} to 6.02 × 10^{-6} M. Inset: plot of absorbance at 319 nm as a function of concentration.

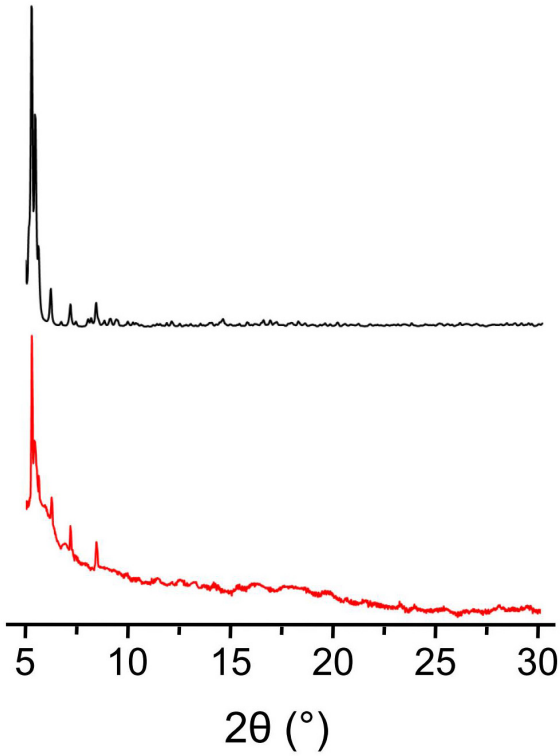

Figure S11. Powder X-ray diffraction data of complex **1**. Up: calculated. Bottom: collected.

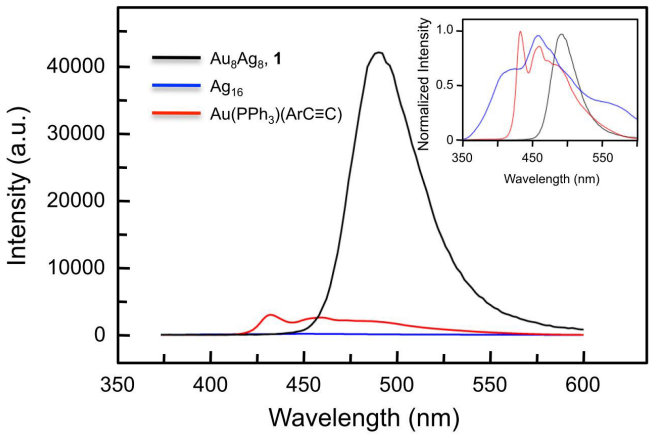

Figure S12. Emission spectra of **1**, Ag_{16} and $Au(PPh_3)(ArC{\equiv}C)$ in the solid state.

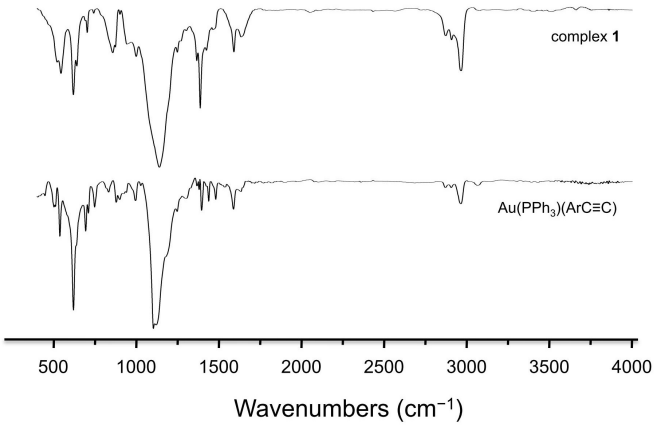

Figure S13. FTIR spectra of **1** (up) and $Au(PPh_3)(ArC{\equiv}C)$ (bottom) in 2% KBr pellet.

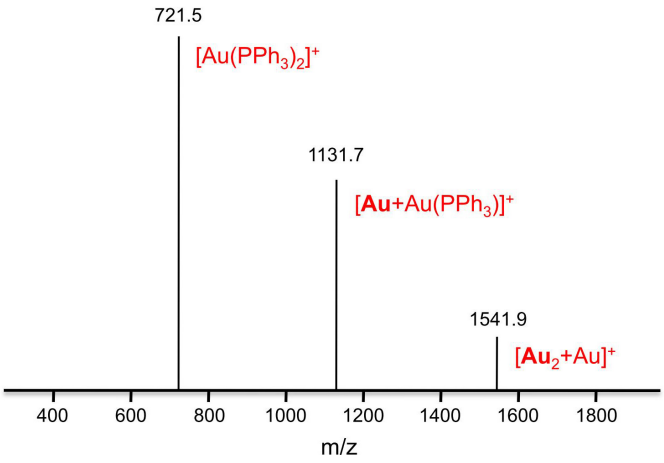

Figure S14. Mass spectrum of $Au(PPh_3)(ArC{\equiv}C)$. For simplicity, $Au(PPh_3)(ArC{\equiv}C)$ is denoted here as **Au**.

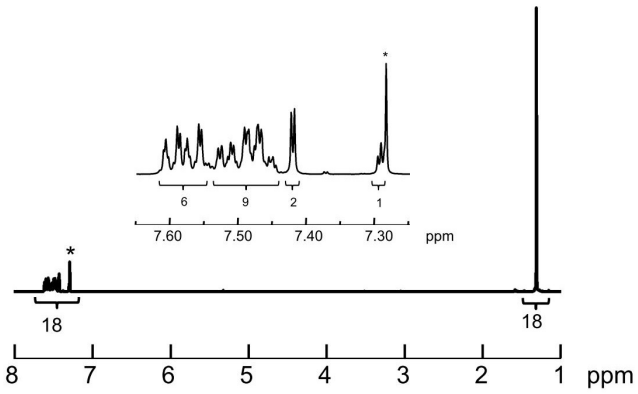

Figure S15. ^{1}H NMR spectrum of Au(PPh_3)(ArC≡C) in $CDCl_3$. The solvent residual peak of $CHCl_3$ is labeled (*).

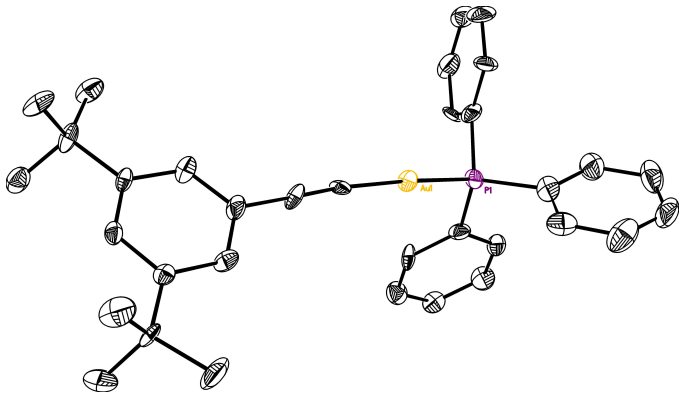

Figure S16. Thermal ellipsoid plot (50% probability) of $Au(PPh_3)(ArC{\equiv}C)$. All hydrogen atoms are omitted for clarity.

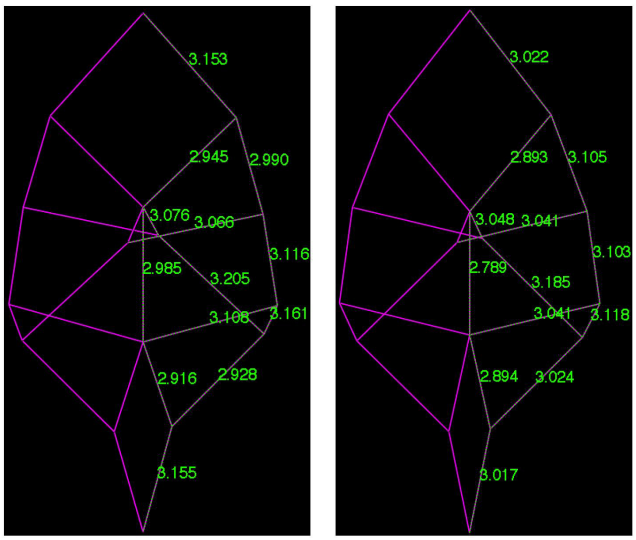

Figure S17. The d^{10}-d^{10} metal distances in the calculated ground state and triplet state of complex **1**. Due to the C_2 symmetry, only half of the metal distances are labeled.

Table S1. Crystal data and structure refinement parameters for complexes **1** and Au(ArC≡C)PPh_3.

molecular formula	$C_{257}H_{338}Ag_8Au_8Cl_2$	$C_{34}H_{36}AuP$
formula wt. (g mol^{-1})	5936.87	672.56
temperature (K)	173(2)	150(2)
radiation (λ, Å)	0.71073	0.71073
crystal system	Monoclinic	Triclinic
space group	$P2_1/n$ (#14)	$P\bar{1}$ (#2)
a (Å)	20.761(4)	9.2356(6)
b (Å)	39.030(8)	12.7366(8)
c (Å)	32.261(7)	28.0258(19)
α (°)	90	80.454(2)
β (°)	92.37(3)	83.007(2)
γ (°)	90	69.185(2)
Volume ($Å^3$)	26119(9)	3031.8(3)
Z	4	4
ρ_{calcd} (g cm^{-3})	1.510	1.473
μ (mm^{-1})	5.124	4.924
F(000)	11688	1336
crystal size (mm^3)	0.17 × 0.10 × 0.05	0.30 × 0.20 × 0.20
Theta range	0.82 to 27.49°	2.118 to 26.441°
reflections collected	198381	26988
independent reflections	59580 [R(int) = 0.0525]	12173 [R(int) = 0.0315]
Completeness	99.4%	97.8%
goodness-of-fit on F^2	1.104	1.063
final R indices	$R1^a$ = 0.0659	$R1^a$ = 0.0567
[R > 2σ (I)]	wR_2^b = 0.1763	wR_2^b = 0.1518
R indices (all data)	$R1^a$ = 0.0786	$R1^a$ = 0.0692
	wR_2^b = 0.1889	wR_2^b = 0.1609
largest diff. peak and hole (e $Å^{-3}$)	3.924 and −3.603	5.115 and −1.877

$^aR_1 = \Sigma||F_o| - |F_c|| / |F_o|$, $^bwR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{0.5}$

Table S2. Bond distances of Ag^{I}–C, Au^{I}–C, Au^{I}–Ag^{I} and Au^{I}–Au^{I} of **1**.

bond distance	Ag^{I}–C	Au^{I}–C	Au^{I}-Ag^{I}	Au-Au
(shortest) Å	2.211(13)	1.993(9)	2.749(3)	2.9592(9)
(longest) Å	2.707(9)	2.024(8)	3.1752(10)	
(average) Å	2.463(10)	2.007(9)	2.9352(7)	

Table S3. Luminescence data of complex **1**.

dichloromethane solution					solid state	
λ_{abs}/nm ($10^{-5}\varepsilon$/cm^{-1} M^{-1})	λ_{ex}/nm	λ_{em}/nm	Q.Y.	τ_{obs}/ns	λ_{em}/nm	τ_{obs}/ns
276 (1.72), 319 (0.77)	272, 320	489	0.67	1243	491	660

DFT-optimized Cartesian coordinates

Au_8Ag_8 cluster (singlet ground state)

Ag	0.338701	2.133858	-3.286503
Ag	0.955681	2.842482	0.881294
Ag	-0.955681	-2.842482	0.881294
Ag	-2.807798	1.038628	-0.577174
Ag	2.807798	-1.038628	-0.577174
Au	0.000000	0.000000	-5.582604
Au	-1.233616	3.593398	-1.204489
Au	0.000000	0.000000	-1.285414
Au	1.233616	-3.593398	-1.204489
Au	3.558619	1.196447	1.593466
Au	0.000000	0.000000	1.699420
Au	-3.558619	-1.196447	1.593466
Au	0.000000	0.000000	5.899699
C	0.076173	2.004794	-5.554486
C	0.133134	3.242481	-5.486179
C	0.171075	4.666954	-5.633730
C	-0.480178	5.508471	-4.705265
H	-0.970561	5.043140	-3.847517
C	-0.496858	6.894859	-4.888134
C	0.155036	7.426423	-6.021771
H	0.134083	8.506820	-6.171315
C	0.819430	6.618624	-6.957248
C	0.822993	5.229624	-6.743737
H	1.318453	4.555996	-7.446155
C	1.516112	7.184367	-8.204491
C	3.011512	6.795728	-8.178727
H	3.522924	7.178746	-9.081937
H	3.147593	5.699483	-8.150092
H	3.509385	7.221167	-7.289016
C	1.416303	8.717790	-8.280364
H	0.365426	9.055318	-8.338750
H	1.935616	9.079232	-9.186822
H	1.891200	9.199866	-7.406234
C	0.849081	6.587473	-9.465819
H	-0.227614	6.837439	-9.493824
H	0.940904	5.486844	-9.491334
H	1.325816	6.990817	-10.379321
C	-1.235555	7.835650	-3.925078
C	-2.455544	8.434681	-4.662840
H	-2.147732	9.004023	-5.558963
H	-3.011504	9.118424	-3.993153
H	-3.143547	7.632113	-4.988282
C	-0.298587	8.973532	-3.462711
H	0.068614	9.583271	-4.307508
H	0.577191	8.560030	-2.931524
H	-0.836902	9.647594	-2.769975
C	-1.728849	7.098583	-2.671386
H	-2.236151	7.812774	-2.000303
H	-0.893045	6.644084	-2.110033
H	-2.453587	6.300650	-2.909794
C	-0.076173	-2.004794	-5.554486
C	-0.133134	-3.242481	-5.486179
C	-0.171075	-4.666954	-5.633730
C	0.480178	-5.508471	-4.705265
H	0.970561	-5.043140	-3.847517
C	0.496858	-6.894859	-4.888134
C	-0.155036	-7.426423	-6.021771
H	-0.134083	-8.506820	-6.171315
C	-0.819430	-6.618624	-6.957248
C	-0.822993	-5.229624	-6.743737
H	-1.318453	-4.555996	-7.446155
C	-1.516112	-7.184367	-8.204491
C	-3.011512	-6.795728	-8.178727
H	-3.522924	-7.178746	-9.081937
H	-3.147593	-5.699483	-8.150092
H	-3.509385	-7.221167	-7.289016
C	-1.416303	-8.717790	-8.280364
H	-0.365426	-9.055318	-8.338750
H	-1.935616	-9.079232	-9.186822
H	-1.891200	-9.199866	-7.406234
C	-0.849081	-6.587473	-9.465819
H	0.227614	-6.837439	-9.493824
H	-0.940904	-5.486844	-9.491334
H	-1.325816	-6.990817	-10.379321
C	1.235555	-7.835650	-3.925078
C	2.455544	-8.434681	-4.662840
H	2.147732	-9.004023	-5.558963
H	3.011504	-9.118424	-3.993153
H	3.143547	-7.632113	-4.988282
C	0.298587	-8.973532	-3.462711
H	-0.068614	-9.583271	-4.307508
H	-0.577191	-8.560030	-2.931524
H	0.836902	-9.647594	-2.769975

C	1.728849	-7.098583	-2.671386
H	2.236151	-7.812774	-2.000303
H	0.893045	-6.644084	-2.110033
H	2.453587	-6.300650	-2.909794
C	-2.386520	2.412928	-2.358240
C	-2.847062	1.892778	-3.381654
C	-3.297765	1.448548	-4.656767
C	-3.540554	0.087610	-4.942643
H	-3.427429	-0.640962	-4.137683
C	-3.889668	-0.306295	-6.239504
C	-3.991674	0.688218	-7.236735
H	-4.259417	0.377198	-8.247657
C	-3.747214	2.046374	-6.983402
C	-3.405229	2.413039	-5.673929
H	-3.179904	3.452924	-5.426282
C	-4.150448	-1.772353	-6.617277
C	-3.208570	-2.181165	-7.773475
H	-2.152904	-2.070101	-7.465426
H	-3.372482	-1.569506	-8.678685
H	-3.386929	-3.239722	-8.044964
C	-5.621473	-1.926423	-7.066328
H	-5.827041	-2.978004	-7.343627
H	-5.851321	-1.289795	-7.940250
H	-6.307973	-1.643126	-6.246785
C	-3.899064	-2.722265	-5.437443
H	-4.062249	-3.765798	-5.759485
H	-4.582462	-2.527299	-4.592882
H	-2.859376	-2.646485	-5.074009
C	-3.799286	3.129610	-8.071602
C	-2.395859	3.764556	-8.212708
H	-1.644195	2.997749	-8.475652
H	-2.065437	4.241215	-7.273361
H	-2.401618	4.539332	-9.003449
C	-4.817356	4.219956	-7.665387
H	-4.856859	5.011985	-8.437240
H	-4.544324	4.695905	-6.706193
H	-5.830113	3.789698	-7.554986
C	-4.217068	2.557824	-9.437184
H	-4.247940	3.370515	-10.186096
H	-5.221747	2.098099	-9.396284
H	-3.498078	1.798970	-9.796250
C	2.386520	-2.412928	-2.358240
C	2.847062	-1.892778	-3.381654
C	3.297765	-1.448548	-4.656767
C	3.540554	-0.087610	-4.942643
H	3.427429	0.640962	-4.137683
C	3.889668	0.306295	-6.239504
C	3.991674	-0.688218	-7.236735
H	4.259417	-0.377198	-8.247657
C	3.747214	-2.046374	-6.983402
C	3.405229	-2.413039	-5.673929
H	3.179904	-3.452924	-5.426282
C	4.150448	1.772353	-6.617277
C	3.208570	2.181165	-7.773475
H	2.152904	2.070101	-7.465426
H	3.372482	1.569506	-8.678685
H	3.386929	3.239722	-8.044964
C	5.621473	1.926423	-7.066328
H	5.827041	2.978004	-7.343627
H	5.851321	1.289795	-7.940250
H	6.307973	1.643126	-6.246785
C	3.899064	2.722265	-5.437443
H	4.062249	3.765798	-5.759485
H	4.582462	2.527299	-4.592882
H	2.859376	2.646485	-5.074009
C	3.799286	-3.129610	-8.071602
C	2.395859	-3.764556	-8.212708
H	1.644195	-2.997749	-8.475652
H	2.065437	-4.241215	-7.273361
H	2.401618	-4.539332	-9.003449
C	4.817356	-4.219956	-7.665387
H	4.856859	-5.011985	-8.437240
H	4.544324	-4.695905	-6.706193
H	5.830113	-3.789698	-7.554986
C	4.217068	-2.557824	-9.437184
H	4.247940	-3.370515	-10.186096
H	5.221747	-2.098099	-9.396284
H	3.498078	-1.798970	-9.796250
C	1.503512	1.342851	-1.403527
C	2.425158	2.141472	-1.633988
C	3.555625	2.965572	-1.916615
C	3.383362	4.292522	-2.367762
H	2.368283	4.687753	-2.433688
C	4.491521	5.059985	-2.736524
C	5.772690	4.472914	-2.635076
H	6.636657	5.067011	-2.937102
C	5.973816	3.160048	-2.181733
C	4.842889	2.412190	-1.815733

H	4.941542	1.383133	-1.462609
C	4.357497	6.493742	-3.271082
C	4.912078	6.557669	-4.711954
H	5.971693	6.247340	-4.759896
H	4.842004	7.592209	-5.097918
H	4.330499	5.901376	-5.382792
C	5.162332	7.455077	-2.369294
H	6.235327	7.192493	-2.343338
H	4.778773	7.433781	-1.333936
H	5.077564	8.489823	-2.751749
C	2.892934	6.961036	-3.297345
H	2.842547	7.996109	-3.681038
H	2.448902	6.955525	-2.285268
H	2.267971	6.335290	-3.960584
C	7.358785	2.502662	-2.092803
C	7.355762	1.192100	-2.914349
H	7.092539	1.390175	-3.970022
H	6.635018	0.456379	-2.515162
H	8.356214	0.721802	-2.885366
C	7.666411	2.177658	-0.614263
H	8.649095	1.674853	-0.531616
H	6.902421	1.509349	-0.178667
H	7.695754	3.100115	-0.006612
C	8.468436	3.418626	-2.635932
H	8.545329	4.355312	-2.053386
H	8.298801	3.677013	-3.697515
H	9.442767	2.901086	-2.566802
C	-1.503512	-1.342851	-1.403527
C	-2.425158	-2.141472	-1.633988
C	-3.555625	-2.965572	-1.916615
C	-3.383362	-4.292522	-2.367762
H	-2.368283	-4.687753	-2.433688
C	-4.491521	-5.059985	-2.736524
C	-5.772690	-4.472914	-2.635076
H	-6.636657	-5.067011	-2.937102
C	-5.973816	-3.160048	-2.181733
C	-4.842889	-2.412190	-1.815733
H	-4.941542	-1.383133	-1.462609
C	-4.357497	-6.493742	-3.271082
C	-4.912078	-6.557669	-4.711954
H	-5.971693	-6.247340	-4.759896
H	-4.842004	-7.592209	-5.097918
H	-4.330499	-5.901376	-5.382792
C	-5.162332	-7.455077	-2.369294
H	-6.235327	-7.192493	-2.343338
H	-4.778773	-7.433781	-1.333936
H	-5.077564	-8.489823	-2.751749
C	-2.892934	-6.961036	-3.297345
H	-2.842547	-7.996109	-3.681038
H	-2.448902	-6.955525	-2.285268
H	-2.267971	-6.335290	-3.960584
C	-7.358785	-2.502662	-2.092803
C	-7.355762	-1.192100	-2.914349
H	-7.092539	-1.390175	-3.970022
H	-6.635018	-0.456379	-2.515162
H	-8.356214	-0.721802	-2.885366
C	-7.666411	-2.177658	-0.614263
H	-8.649095	-1.674853	-0.531616
H	-6.902421	-1.509349	-0.178667
H	-7.695754	-3.100115	-0.006612
C	-8.468436	-3.418626	-2.635932
H	-8.545329	-4.355312	-2.053386
H	-8.298801	-3.677013	-3.697515
H	-9.442767	-2.901086	-2.566802
C	-4.653204	0.154692	0.597617
C	-5.323716	1.031075	0.037175
C	-6.215508	2.007646	-0.508247
C	-7.606976	1.809300	-0.413931
H	-7.968270	0.890621	0.053743
C	-8.505761	2.773424	-0.889273
C	-7.980745	3.935411	-1.487663
H	-8.668141	4.691617	-1.862184
C	-6.595745	4.159800	-1.602147
C	-5.723757	3.184409	-1.101274
H	-4.642584	3.322169	-1.166171
C	-10.014304	2.533849	-0.715678
C	-10.419672	1.245460	-1.466906
H	-11.505276	1.061873	-1.356966
H	-9.883481	0.362902	-1.074302
H	-10.187301	1.331042	-2.544300
C	-10.854231	3.701105	-1.262561
H	-11.928690	3.487700	-1.113915
H	-10.688160	3.850547	-2.344997
H	-10.624009	4.647089	-0.739149
C	-10.329636	2.371745	0.790244
H	-10.029869	3.277241	1.349014
H	-9.793702	1.511308	1.230765
H	-11.414038	2.209976	0.939821

C	-6.000496	5.425732	-2.236415
C	-7.088696	6.421160	-2.672999
H	-6.615475	7.317924	-3.113511
H	-7.704401	6.751900	-1.816119
H	-7.757023	5.985638	-3.438288
C	-5.169867	5.023569	-3.477844
H	-4.744339	5.924123	-3.960941
H	-5.797921	4.496010	-4.219087
H	-4.334740	4.353294	-3.205734
C	-5.082222	6.127120	-1.208359
H	-4.669001	7.056416	-1.642421
H	-4.229359	5.489583	-0.911958
H	-5.640242	6.385358	-0.289757
C	-1.295211	1.550727	1.802846
C	-2.060777	2.515808	1.952213
C	-2.903365	3.649748	2.152844
C	-4.273239	3.467288	2.446069
H	-4.665761	2.449548	2.470400
C	-5.085255	4.569402	2.723213
C	-4.505661	5.856229	2.665106
H	-5.142248	6.717041	2.875664
C	-3.151115	6.068167	2.368272
C	-2.350499	4.940909	2.118738
H	-1.286211	5.048257	1.900970
C	-6.563023	4.425908	3.114964
C	-6.990370	2.951597	3.200569
H	-6.409762	2.395398	3.958771
H	-6.876719	2.444679	2.226647
H	-8.056062	2.886605	3.488644
C	-7.441438	5.134664	2.060206
H	-8.509319	5.059859	2.341195
H	-7.311332	4.668561	1.067252
H	-7.187876	6.207197	1.972314
C	-6.782851	5.077778	4.498641
H	-6.524129	6.151906	4.494723
H	-6.162573	4.578242	5.265264
H	-7.844627	4.986964	4.794172
C	-2.520847	7.467005	2.299605
C	-2.117393	7.748196	0.835556
H	-1.631183	8.740144	0.753078
H	-3.008492	7.739304	0.182533
H	-1.414045	6.984860	0.457793
C	-3.496785	8.563572	2.760672
H	-3.831108	8.396412	3.801604
H	-4.388689	8.620103	2.109708
H	-2.993373	9.547012	2.720826
C	-1.266926	7.525721	3.198274
H	-0.817078	8.535419	3.148768
H	-0.491678	6.801059	2.890811
H	-1.522518	7.308190	4.251198
C	0.124934	4.745570	-0.293207
C	1.060573	5.425149	0.141062
C	2.138017	6.263698	0.560030
C	2.029433	7.662170	0.479228
H	1.088997	8.089893	0.123033
C	3.110822	8.490454	0.825610
C	4.295108	7.878592	1.269067
H	5.147273	8.503488	1.540507
C	4.434666	6.475898	1.363790
C	3.344424	5.681316	1.004223
H	3.400649	4.593872	1.049554
C	2.967650	10.012398	0.657654
C	2.789793	10.327586	-0.846492
H	3.660115	9.969883	-1.425556
H	2.689305	11.418669	-1.000909
H	1.887620	9.839177	-1.257446
C	1.730190	10.520661	1.431241
H	1.604264	11.608120	1.271721
H	1.843148	10.339481	2.514374
H	0.802611	10.021113	1.097824
C	4.203129	10.769492	1.174621
H	4.384054	10.561950	2.245436
H	4.047187	11.858079	1.062223
H	5.113180	10.502838	0.606973
C	5.766409	5.855342	1.811922
C	6.858942	6.203231	0.775048
H	6.985410	7.295771	0.664702
H	6.595113	5.785928	-0.213945
H	7.830516	5.774259	1.086925
C	6.163275	6.413874	3.196037
H	7.116470	5.962581	3.530294
H	5.388859	6.175208	3.948448
H	6.294995	7.510872	3.177945
C	5.674034	4.322887	1.918031
H	6.646874	3.913949	2.242385
H	5.426552	3.855980	0.947543
H	4.911568	4.006191	2.652777
C	4.653204	-0.154692	0.597617

C	5.323716	-1.031075	0.037175
C	6.215508	-2.007646	-0.508247
C	7.606976	-1.809300	-0.413931
H	7.968270	-0.890621	0.053743
C	8.505761	-2.773424	-0.889273
C	7.980745	-3.935411	-1.487663
H	8.668141	-4.691617	-1.862184
C	6.595745	-4.159800	-1.602147
C	5.723757	-3.184409	-1.101274
H	4.642584	-3.322169	-1.166171
C	10.014304	-2.533849	-0.715678
C	10.419672	-1.245460	-1.466906
H	11.505276	-1.061873	-1.356966
H	9.883481	-0.362902	-1.074302
H	10.187301	-1.331042	-2.544300
C	10.854231	-3.701105	-1.262561
H	11.928690	-3.487700	-1.113915
H	10.688160	-3.850547	-2.344997
H	10.624009	-4.647089	-0.739149
C	10.329636	-2.371745	0.790244
H	10.029869	-3.277241	1.349014
H	9.793702	-1.511308	1.230765
H	11.414038	-2.209976	0.939821
C	6.000496	-5.425732	-2.236415
C	7.088696	-6.421160	-2.672999
H	6.615475	-7.317924	-3.113511
H	7.704401	-6.751900	-1.816119
H	7.757023	-5.985638	-3.438288
C	5.169867	-5.023569	-3.477844
H	4.744339	-5.924123	-3.960941
H	5.797921	-4.496010	-4.219087
H	4.334740	-4.353294	-3.205734
C	5.082222	-6.127120	-1.208359
H	4.669001	-7.056416	-1.642421
H	4.229359	-5.489583	-0.911958
H	5.640242	-6.385358	-0.289757
C	2.010312	-0.064827	5.881013
C	3.248033	-0.134595	5.811197
C	4.672308	-0.277025	5.920855
C	5.201006	-1.141073	6.905232
H	4.496864	-1.665654	7.550735
C	6.582388	-1.308892	7.045351
C	7.428419	-0.597009	6.169267
H	8.506322	-0.722668	6.273906
C	6.937042	0.262806	5.174246
C	5.544113	0.416676	5.063219
H	5.110754	1.081529	4.310033
C	7.187847	-2.191295	8.148605
C	7.761964	-1.267106	9.248892
H	6.965326	-0.633254	9.680897
H	8.543045	-0.600011	8.838522
H	8.210955	-1.868100	10.062697
C	6.134389	-3.121280	8.781398
H	6.616586	-3.774449	9.531461
H	5.659643	-3.768159	8.018895
H	5.339038	-2.555187	9.299345
C	8.322357	-3.072256	7.580092
H	9.165731	-2.469768	7.197672
H	7.950721	-3.705040	6.754517
H	8.720898	-3.731932	8.373321
C	7.866707	1.057569	4.243714
C	9.328602	0.585573	4.344171
H	9.419698	-0.488603	4.096477
H	9.751056	0.751645	5.351673
H	9.949927	1.152977	3.626996
C	7.796018	2.549984	4.644167
H	8.440720	3.158659	3.981257
H	8.135206	2.691333	5.686947
H	6.763396	2.934349	4.565758
C	7.417387	0.895998	2.776610
H	8.103292	1.448869	2.108593
H	6.399511	1.283340	2.598901
H	7.419692	-0.167160	2.476911
C	-2.425016	-2.454258	2.671217
C	-1.792275	-3.192806	3.435589
C	-1.188568	-4.118636	4.341528
C	0.029506	-3.836834	4.992287
H	0.514738	-2.878122	4.790886
C	0.590549	-4.758459	5.890686
C	-0.103769	-5.960706	6.124895
H	0.321133	-6.681283	6.821182
C	-1.319884	-6.272307	5.490660
C	-1.848302	-5.339045	4.590388
H	-2.784192	-5.533848	4.060838
C	1.901829	-4.425801	6.621924
C	2.953779	-3.909552	5.620055
H	2.631518	-2.981786	5.118774
H	3.161351	-4.664756	4.842432

H	3.900302	-3.680780	6.143473
C	2.497057	-5.657194	7.330362
H	3.465988	-5.383797	7.787925
H	2.679613	-6.482266	6.616289
H	1.843511	-6.028848	8.140198
C	1.609498	-3.338294	7.680921
H	1.226003	-2.415517	7.210314
H	2.535144	-3.079639	8.230613
H	0.858459	-3.693002	8.410572
C	-2.086071	-7.575901	5.761799
C	-2.392112	-8.280408	4.423180
H	-1.456962	-8.498372	3.878199
H	-3.025009	-7.667237	3.758691
H	-2.923934	-9.234062	4.604278
C	-3.411544	-7.235073	6.480771
H	-3.992866	-8.157008	6.673616
H	-4.034791	-6.558135	5.869119
H	-3.216390	-6.735412	7.447292
C	-1.283464	-8.547595	6.644676
H	-1.857448	-9.482090	6.784333
H	-1.085699	-8.126055	7.646931
H	-0.316433	-8.810563	6.177530
C	1.295211	-1.550727	1.802846
C	2.060777	-2.515808	1.952213
C	2.903365	-3.649748	2.152844
C	4.273239	-3.467288	2.446069
H	4.665761	-2.449548	2.470400
C	5.085255	-4.569402	2.723213
C	4.505661	-5.856229	2.665106
H	5.142248	-6.717041	2.875664
C	3.151115	-6.068167	2.368272
C	2.350499	-4.940909	2.118738
H	1.286211	-5.048257	1.900970
C	6.563023	-4.425908	3.114964
C	6.990370	-2.951597	3.200569
H	6.409762	-2.395398	3.958771
H	6.876719	-2.444679	2.226647
H	8.056062	-2.886605	3.488644
C	7.441438	-5.134664	2.060206
H	8.509319	-5.059859	2.341195
H	7.311332	-4.668561	1.067252
H	7.187876	-6.207197	1.972314
C	6.782851	-5.077778	4.498641
H	6.524129	-6.151906	4.494723
H	6.162573	-4.578242	5.265264
H	7.844627	-4.986964	4.794172
C	2.520847	-7.467005	2.299605
C	2.117393	-7.748196	0.835556
H	1.631183	-8.740144	0.753078
H	3.008492	-7.739304	0.182533
H	1.414045	-6.984860	0.457793
C	3.496785	-8.563572	2.760672
H	3.831108	-8.396412	3.801604
H	4.388689	-8.620103	2.109708
H	2.993373	-9.547012	2.720826
C	1.266926	-7.525721	3.198274
H	0.817078	-8.535419	3.148768
H	0.491678	-6.801059	2.890811
H	1.522518	-7.308190	4.251198
C	-2.010312	0.064827	5.881013
C	-3.248033	0.134595	5.811197
C	-4.672308	0.277025	5.920855
C	-5.201006	1.141073	6.905232
H	-4.496864	1.665654	7.550735
C	-6.582388	1.308892	7.045351
C	-7.428419	0.597009	6.169267
H	-8.506322	0.722668	6.273906
C	-6.937042	-0.262806	5.174246
C	-5.544113	-0.416676	5.063219
H	-5.110754	-1.081529	4.310033
C	-7.187847	2.191295	8.148605
C	-7.761964	1.267106	9.248892
H	-6.965326	0.633254	9.680897
H	-8.543045	0.600011	8.838522
H	-8.210955	1.868100	10.062697
C	-6.134389	3.121280	8.781398
H	-6.616586	3.774449	9.531461
H	-5.659643	3.768159	8.018895
H	-5.339038	2.555187	9.299345
C	-8.322357	3.072256	7.580092
H	-9.165731	2.469768	7.197672
H	-7.950721	3.705040	6.754517
H	-8.720898	3.731932	8.373321
C	-7.866707	-1.057569	4.243714
C	-9.328602	-0.585573	4.344171
H	-9.419698	0.488603	4.096477
H	-9.751056	-0.751645	5.351673
H	-9.949927	-1.152977	3.626996

C	-7.796018	-2.549984	4.644167
H	-8.440720	-3.158659	3.981257
H	-8.135206	-2.691333	5.686947
H	-6.763396	-2.934349	4.565758
C	-7.417387	-0.895998	2.776610
H	-8.103292	-1.448869	2.108593
H	-6.399511	-1.283340	2.598901
H	-7.419692	0.167160	2.476911
C	2.425016	2.454258	2.671217
C	1.792275	3.192806	3.435589
C	1.188568	4.118636	4.341528
C	-0.029506	3.836834	4.992287
H	-0.514738	2.878122	4.790886
C	-0.590549	4.758459	5.890686
C	0.103769	5.960706	6.124895
H	-0.321133	6.681283	6.821182
C	1.319884	6.272307	5.490660
C	1.848302	5.339045	4.590388
H	2.784192	5.533848	4.060838
C	-1.901829	4.425801	6.621924
C	-2.953779	3.909552	5.620055
H	-2.631518	2.981786	5.118774
H	-3.161351	4.664756	4.842432
H	-3.900302	3.680780	6.143473
C	-2.497057	5.657194	7.330362
H	-3.465988	5.383797	7.787925
H	-2.679613	6.482266	6.616289
H	-1.843511	6.028848	8.140198
C	-1.609498	3.338294	7.680921
H	-1.226003	2.415517	7.210314
H	-2.535144	3.079639	8.230613
H	-0.858459	3.693002	8.410572
C	2.086071	7.575901	5.761799
C	2.392112	8.280408	4.423180
H	1.456962	8.498372	3.878199
H	3.025009	7.667237	3.758691
H	2.923934	9.234062	4.604278
C	3.411544	7.235073	6.480771
H	3.992866	8.157008	6.673616
H	4.034791	6.558135	5.869119
H	3.216390	6.735412	7.447292
C	1.283464	8.547595	6.644676
H	1.857448	9.482090	6.784333
H	1.085699	8.126055	7.646931
H	0.316433	8.810563	6.177530
C	-0.124934	-4.745570	-0.293207
C	-1.060573	-5.425149	0.141062
C	-2.138017	-6.263698	0.560030
C	-2.029433	-7.662170	0.479228
H	-1.088997	-8.089893	0.123033
C	-3.110822	-8.490454	0.825610
C	-4.295108	-7.878592	1.269067
H	-5.147273	-8.503488	1.540507
C	-4.434666	-6.475898	1.363790
C	-3.344424	-5.681316	1.004223
H	-3.400649	-4.593872	1.049554
C	-2.967650	-10.012398	0.657654
C	-2.789793	-10.327586	-0.846492
H	-3.660115	-9.969883	-1.425556
H	-2.689305	-11.418669	-1.000909
H	-1.887620	-9.839177	-1.257446
C	-1.730190	-10.520661	1.431241
H	-1.604264	-11.608120	1.271721
H	-1.843148	-10.339481	2.514374
H	-0.802611	-10.021113	1.097824
C	-4.203129	-10.769492	1.174621
H	-4.384054	-10.561950	2.245436
H	-4.047187	-11.858079	1.062223
H	-5.113180	-10.502838	0.606973
C	-5.766409	-5.855342	1.811922
C	-6.858942	-6.203231	0.775048
H	-6.985410	-7.295771	0.664702
H	-6.595113	-5.785928	-0.213945
H	-7.830516	-5.774259	1.086925
C	-6.163275	-6.413874	3.196037
H	-7.116470	-5.962581	3.530294
H	-5.388859	-6.175208	3.948448
H	-6.294995	-7.510872	3.177945
C	-5.674034	-4.322887	1.918031
H	-6.646874	-3.913949	2.242385
H	-5.426552	-3.855980	0.947543
H	-4.911568	-4.006191	2.652777
Ag	-0.338701	-2.133858	-3.286503
Ag	2.155384	-0.374888	3.626730
Ag	-2.155384	0.374888	3.626730

Au_8Ag_8 cluster (lowest triplet state)

Ag	1.881228	-0.214079	-3.405545
Ag	2.859681	-0.747960	0.857606
Ag	-2.859681	0.747960	0.857606
Ag	0.791416	2.869753	-0.561671
Ag	-0.791416	-2.869753	-0.561671
Au	0.000000	0.000000	-5.761014
Au	3.389449	1.453272	-1.264570
Au	0.000000	0.000000	-1.217892
Au	-3.389449	-1.453272	-1.264570
Au	1.424704	-3.395471	1.664737
Au	0.000000	0.000000	1.570816
Au	-1.424704	3.395471	1.664737
Au	0.000000	0.000000	6.032572
C	2.005927	0.032257	-5.680722
C	3.239586	0.036537	-5.556670
C	4.668629	0.083306	-5.628399
C	5.412810	0.837608	-4.693619
H	4.868643	1.333345	-3.887000
C	6.801886	0.948040	-4.812164
C	7.436200	0.279348	-5.881452
H	8.519753	0.367291	-5.974546
C	6.727505	-0.479091	-6.825219
C	5.332730	-0.573767	-6.678988
H	4.732491	-1.143412	-7.391624
C	7.405712	-1.164244	-8.021977
C	7.104055	-2.678564	-7.998444
H	7.557698	-3.172351	-8.878385
H	6.017912	-2.880184	-8.018257
H	7.518040	-3.143794	-7.086677
C	8.933298	-0.979377	-8.007599
H	9.217994	0.086548	-8.073754
H	9.378466	-1.498657	-8.876033
H	9.384443	-1.406672	-7.093158
C	6.849028	-0.547958	-9.326975
H	7.039814	0.540632	-9.357158
H	5.758563	-0.702952	-9.414870
H	7.332234	-1.012627	-10.207448
C	7.643539	1.793179	-3.846182
C	8.357632	2.909214	-4.643341
H	9.035904	2.497620	-5.412346
H	8.958499	3.539046	-3.960207
H	7.618118	3.555949	-5.151378
C	8.692283	0.901158	-3.144135
H	9.366598	0.406850	-3.866961
H	8.193108	0.115006	-2.550477
H	9.312602	1.510693	-2.459635
C	6.778966	2.452043	-2.763058
H	7.417931	3.063110	-2.103627
H	6.270517	1.702202	-2.132197
H	6.011252	3.117974	-3.193621
C	-2.005927	-0.032257	-5.680722
C	-3.239586	-0.036537	-5.556670
C	-4.668629	-0.083306	-5.628399
C	-5.412810	-0.837608	-4.693619
H	-4.868643	-1.333345	-3.887000
C	-6.801886	-0.948040	-4.812164
C	-7.436200	-0.279348	-5.881452
H	-8.519753	-0.367291	-5.974546
C	-6.727505	0.479091	-6.825219
C	-5.332730	0.573767	-6.678988
H	-4.732491	1.143412	-7.391624
C	-7.405712	1.164244	-8.021977
C	-7.104055	2.678564	-7.998444
H	-7.557698	3.172351	-8.878385
H	-6.017912	2.880184	-8.018257
H	-7.518040	3.143794	-7.086677
C	-8.933298	0.979377	-8.007599
H	-9.217994	-0.086548	-8.073754
H	-9.378466	1.498657	-8.876033
H	-9.384443	1.406672	-7.093158
C	-6.849028	0.547958	-9.326975
H	-7.039814	-0.540632	-9.357158
H	-5.758563	0.702952	-9.414870
H	-7.332234	1.012627	-10.207448
C	-7.643539	-1.793179	-3.846182
C	-8.357632	-2.909214	-4.643341
H	-9.035904	-2.497620	-5.412346
H	-8.958499	-3.539046	-3.960207
H	-7.618118	-3.555949	-5.151378
C	-8.692283	-0.901158	-3.144135
H	-9.366598	-0.406850	-3.866961
H	-8.193108	-0.115006	-2.550477
H	-9.312602	-1.510693	-2.459635
C	-6.778966	-2.452043	-2.763058
H	-7.417931	-3.063110	-2.103627
H	-6.270517	-1.702202	-2.132197
H	-6.011252	-3.117974	-3.193621

C	2.111503	2.515889	-2.401076
C	1.570085	2.929360	-3.434686
C	1.098053	3.340184	-4.710941
C	-0.274256	3.539531	-4.978667
H	-0.986094	3.418198	-4.160237
C	-0.696993	3.862010	-6.272629
C	0.279774	3.983917	-7.285341
H	-0.053237	4.234657	-8.293431
C	1.648492	3.780972	-7.051397
C	2.044634	3.461485	-5.745192
H	3.094218	3.269928	-5.510939
C	-2.175039	4.081358	-6.627065
C	-2.566798	3.159939	-7.805016
H	-2.410337	2.100562	-7.531405
H	-1.978514	3.373946	-8.715066
H	-3.635212	3.306811	-8.054779
C	-2.381554	5.558903	-7.032009
H	-3.441843	5.738257	-7.294160
H	-1.760398	5.833325	-7.904311
H	-2.112798	6.230438	-6.195314
C	-3.101028	3.764785	-5.443667
H	-4.153444	3.889824	-5.753005
H	-2.928737	4.438802	-4.586500
H	-2.976054	2.722023	-5.101541
C	2.711590	3.857547	-8.157918
C	3.383004	2.472057	-8.304897
H	2.633238	1.697465	-8.549179
H	3.886266	2.160119	-7.373234
H	4.141955	2.497315	-9.110347
C	3.779601	4.907551	-7.774572
H	4.555182	4.967260	-8.561606
H	4.281705	4.651092	-6.824247
H	3.323027	5.907969	-7.658348
C	2.105499	4.253192	-9.515364
H	2.904488	4.303722	-10.277789
H	1.618207	5.244613	-9.471218
H	1.362021	3.511200	-9.859404
C	-2.111503	-2.515889	-2.401076
C	-1.570085	-2.929360	-3.434686
C	-1.098053	-3.340184	-4.710941
C	0.274256	-3.539531	-4.978667
H	0.986094	-3.418198	-4.160237
C	0.696993	-3.862010	-6.272629
C	-0.279774	-3.983917	-7.285341
H	0.053237	-4.234657	-8.293431
C	-1.648492	-3.780972	-7.051397
C	-2.044634	-3.461485	-5.745192
H	-3.094218	-3.269928	-5.510939
C	2.175039	-4.081358	-6.627065
C	2.566798	-3.159939	-7.805016
H	2.410337	-2.100562	-7.531405
H	1.978514	-3.373946	-8.715066
H	3.635212	-3.306811	-8.054779
C	2.381554	-5.558903	-7.032009
H	3.441843	-5.738257	-7.294160
H	1.760398	-5.833325	-7.904311
H	2.112798	-6.230438	-6.195314
C	3.101028	-3.764785	-5.443667
H	4.153444	-3.889824	-5.753005
H	2.928737	-4.438802	-4.586500
H	2.976054	-2.722023	-5.101541
C	-2.711590	-3.857547	-8.157918
C	-3.383004	-2.472057	-8.304897
H	-2.633238	-1.697465	-8.549179
H	-3.886266	-2.160119	-7.373234
H	-4.141955	-2.497315	-9.110347
C	-3.779601	-4.907551	-7.774572
H	-4.555182	-4.967260	-8.561606
H	-4.281705	-4.651092	-6.824247
H	-3.323027	-5.907969	-7.658348
C	-2.105499	-4.253192	-9.515364
H	-2.904488	-4.303722	-10.277789
H	-1.618207	-5.244613	-9.471218
H	-1.362021	-3.511200	-9.859404
C	1.433284	-1.403866	-1.469860
C	2.298169	-2.282304	-1.649183
C	3.198947	-3.349647	-1.902964
C	4.522594	-3.094584	-2.336008
H	4.844177	-2.055428	-2.419684
C	5.372232	-4.152689	-2.665695
C	4.876807	-5.471664	-2.547808
H	5.536907	-6.297229	-2.818188
C	3.571063	-5.755667	-2.118090
C	2.737740	-4.675947	-1.789263
H	1.713816	-4.843024	-1.448064
C	6.803622	-3.932323	-3.178077
C	6.936936	-4.526640	-4.597427
H	6.710066	-5.608041	-4.614052

H	7.970447	-4.389977	-4.967844
H	6.250326	-4.020017	-5.297170
C	7.802598	-4.639209	-2.236599
H	7.615957	-5.726779	-2.182483
H	7.736500	-4.228703	-1.213929
H	8.835114	-4.492352	-2.605916
C	7.161900	-2.439523	-3.239846
H	8.200227	-2.318138	-3.598636
H	7.095976	-1.971941	-2.241286
H	6.506541	-1.882953	-3.934525
C	3.016249	-7.183131	-2.008644
C	1.711493	-7.290195	-2.831956
H	1.893703	-7.032955	-3.892220
H	0.924491	-6.617290	-2.447317
H	1.313202	-8.320703	-2.784778
C	2.713861	-7.486520	-0.524793
H	2.290644	-8.503698	-0.421650
H	1.987947	-6.767447	-0.105382
H	3.635128	-7.431217	0.082756
C	4.012516	-8.232256	-2.530544
H	4.948489	-8.233663	-1.941760
H	4.265136	-8.059483	-3.592995
H	3.565374	-9.239972	-2.449179
C	-1.433284	1.403866	-1.469860
C	-2.298169	2.282304	-1.649183
C	-3.198947	3.349647	-1.902964
C	-4.522594	3.094584	-2.336008
H	-4.844177	2.055428	-2.419684
C	-5.372232	4.152689	-2.665695
C	-4.876807	5.471664	-2.547808
H	-5.536907	6.297229	-2.818188
C	-3.571063	5.755667	-2.118090
C	-2.737740	4.675947	-1.789263
H	-1.713816	4.843024	-1.448064
C	-6.803622	3.932323	-3.178077
C	-6.936936	4.526640	-4.597427
H	-6.710066	5.608041	-4.614052
H	-7.970447	4.389977	-4.967844
H	-6.250326	4.020017	-5.297170
C	-7.802598	4.639209	-2.236599
H	-7.615957	5.726779	-2.182483
H	-7.736500	4.228703	-1.213929
H	-8.835114	4.492352	-2.605916
C	-7.161900	2.439523	-3.239846
H	-8.200227	2.318138	-3.598636
H	-7.095976	1.971941	-2.241286
H	-6.506541	1.882953	-3.934525
C	-3.016249	7.183131	-2.008644
C	-1.711493	7.290195	-2.831956
H	-1.893703	7.032955	-3.892220
H	-0.924491	6.617290	-2.447317
H	-1.313202	8.320703	-2.784778
C	-2.713861	7.486520	-0.524793
H	-2.290644	8.503698	-0.421650
H	-1.987947	6.767447	-0.105382
H	-3.635128	7.431217	0.082756
C	-4.012516	8.232256	-2.530544
H	-4.948489	8.233663	-1.941760
H	-4.265136	8.059483	-3.592995
H	-3.565374	9.239972	-2.449179
C	-0.186472	4.618691	0.666450
C	0.601329	5.369854	0.076159
C	1.468107	6.352983	-0.498957
C	1.167150	7.721062	-0.344773
H	0.257249	7.993489	0.194166
C	2.019695	8.708695	-0.855820
C	3.172627	8.296624	-1.551651
H	3.841544	9.053866	-1.956194
C	3.499401	6.938675	-1.725719
C	2.635784	5.975358	-1.187319
H	2.855236	4.910654	-1.294286
C	1.677800	10.188643	-0.617259
C	0.325031	10.518759	-1.287403
H	0.064970	11.581903	-1.124759
H	-0.491539	9.900859	-0.873490
H	0.371947	10.333344	-2.376222
C	2.748355	11.131706	-1.193228
H	2.467188	12.181336	-0.989943
H	2.845880	11.017010	-2.288179
H	3.737214	10.952817	-0.732730
C	1.572700	10.446066	0.904578
H	2.527474	10.204928	1.406653
H	0.782168	9.830678	1.371225
H	1.333847	11.509217	1.097179
C	4.774103	6.471898	-2.444578
C	5.595447	7.651707	-2.991963
H	6.495608	7.267796	-3.505862
H	5.933116	8.325635	-2.183335

H	5.017304	8.244270	-3.724534
C	4.390110	5.552255	-3.626772
H	5.298659	5.229512	-4.169951
H	3.731397	6.080212	-4.339838
H	3.858935	4.646892	-3.284024
C	5.651571	5.688124	-1.439753
H	6.594560	5.371827	-1.922373
H	5.140405	4.780323	-1.070892
H	5.897929	6.314353	-0.563300
C	1.430457	1.408670	1.836427
C	2.361451	2.232782	1.928455
C	3.441142	3.134905	2.103852
C	3.187314	4.500455	2.380622
H	2.149559	4.834179	2.415973
C	4.244479	5.374335	2.636938
C	5.562699	4.867929	2.568231
H	6.389567	5.553347	2.758287
C	5.847089	3.520944	2.289469
C	4.766193	2.655016	2.067102
H	4.931558	1.596192	1.862599
C	4.020788	6.844434	3.019507
C	2.528699	7.160705	3.216207
H	2.075625	6.540041	4.010992
H	1.960301	7.007686	2.282715
H	2.405842	8.219489	3.510879
C	4.577807	7.749603	1.899097
H	4.452884	8.815407	2.170130
H	4.043074	7.568267	0.950026
H	5.654321	7.564457	1.727997
C	4.759639	7.141345	4.343699
H	5.853728	7.022560	4.243690
H	4.412452	6.458929	5.141280
H	4.561822	8.181988	4.661645
C	7.281518	2.978337	2.199452
C	7.591800	2.688709	0.714417
H	8.616419	2.282062	0.604120
H	7.516413	3.615241	0.116656
H	6.879232	1.955585	0.296158
C	8.313572	3.986520	2.734982
H	8.103503	4.257416	3.786431
H	8.337341	4.912382	2.131808
H	9.323648	3.539098	2.693821
C	7.414707	1.673811	3.012918
H	8.459598	1.312762	2.971518
H	6.773344	0.864233	2.622219
H	7.139612	1.832454	4.070974
C	4.672896	0.206388	-0.364680
C	5.432574	-0.653413	0.093232
C	6.352760	-1.646950	0.546807
C	7.738668	-1.423817	0.483591
H	8.091506	-0.462612	0.102398
C	8.648303	-2.419593	0.878639
C	8.128572	-3.637687	1.348527
H	8.816183	-4.426440	1.657898
C	6.741158	-3.892413	1.423753
C	5.864921	-2.884506	1.017315
H	4.785349	-3.030793	1.046663
C	10.156523	-2.159336	0.727864
C	10.495230	-2.097760	-0.780773
H	10.235392	-3.049358	-1.278566
H	11.576270	-1.909617	-0.924444
H	9.934669	-1.289199	-1.285250
C	10.541706	-0.815004	1.385876
H	11.625271	-0.631026	1.260661
H	10.314468	-0.827011	2.466506
H	10.003121	0.036897	0.933045
C	10.999829	-3.269771	1.379090
H	10.767406	-3.369887	2.455696
H	12.073928	-3.026615	1.284005
H	10.836533	-4.248562	0.892344
C	6.225225	-5.255784	1.908154
C	6.706945	-6.354462	0.933514
H	7.809764	-6.388849	0.866450
H	6.305855	-6.168547	-0.079479
H	6.352505	-7.346414	1.273200
C	6.763855	-5.542824	3.326970
H	6.402853	-6.527086	3.680687
H	6.411873	-4.774496	4.040087
H	7.868407	-5.554956	3.356279
C	4.687810	-5.298352	1.957279
H	4.354706	-6.293237	2.300322
H	4.237306	-5.124138	0.963583
H	4.277921	-4.545572	2.654804
C	0.186472	-4.618691	0.666450
C	-0.601329	-5.369854	0.076159
C	-1.468107	-6.352983	-0.498957
C	-1.167150	-7.721062	-0.344773
H	-0.257249	-7.993489	0.194166

C	-2.019695	-8.708695	-0.855820
C	-3.172627	-8.296624	-1.551651
H	-3.841544	-9.053866	-1.956194
C	-3.499401	-6.938675	-1.725719
C	-2.635784	-5.975358	-1.187319
H	-2.855236	-4.910654	-1.294286
C	-1.677800	-10.188643	-0.617259
C	-0.325031	-10.518759	-1.287403
H	-0.064970	-11.581903	-1.124759
H	0.491539	-9.900859	-0.873490
H	-0.371947	-10.333344	-2.376222
C	-2.748355	-11.131706	-1.193228
H	-2.467188	-12.181336	-0.989943
H	-2.845880	-11.017010	-2.288179
H	-3.737214	-10.952817	-0.732730
C	-1.572700	-10.446066	0.904578
H	-2.527474	-10.204928	1.406653
H	-0.782168	-9.830678	1.371225
H	-1.333847	-11.509217	1.097179
C	-4.774103	-6.471898	-2.444578
C	-5.595447	-7.651707	-2.991963
H	-6.495608	-7.267796	-3.505862
H	-5.933116	-8.325635	-2.183335
H	-5.017304	-8.244270	-3.724534
C	-4.390110	-5.552255	-3.626772
H	-5.298659	-5.229512	-4.169951
H	-3.731397	-6.080212	-4.339838
H	-3.858935	-4.646892	-3.284024
C	-5.651571	-5.688124	-1.439753
H	-6.594560	-5.371827	-1.922373
H	-5.140405	-4.780323	-1.070892
H	-5.897929	-6.314353	-0.563300
C	0.068884	-2.009471	5.978547
C	0.074314	-3.245081	5.870678
C	0.023789	-4.675175	5.955882
C	-0.805164	-5.267918	6.936089
H	-1.374446	-4.604062	7.585873
C	-0.880100	-6.656879	7.067690
C	-0.104890	-7.448115	6.193148
H	-0.158197	-8.533028	6.293229
C	0.730529	-6.893934	5.211929
C	0.781621	-5.492433	5.100380
H	1.420092	-5.011567	4.353160
C	-1.745843	-7.336797	8.140291
C	-0.822025	-8.093500	9.122781
H	-0.113635	-7.397519	9.609208
H	-0.232468	-8.870992	8.603293
H	-1.421909	-8.588453	9.910169
C	-2.579411	-6.317480	8.936699
H	-3.204375	-6.846146	9.679572
H	-3.253544	-5.742654	8.274595
H	-1.938649	-5.603645	9.484863
C	-2.717055	-8.336471	7.474715
H	-2.180996	-9.118216	6.907777
H	-3.392625	-7.814255	6.775352
H	-3.332353	-8.839445	8.244625
C	1.611213	-7.758381	4.296985
C	1.320356	-9.261031	4.457522
H	0.265617	-9.495242	4.221408
H	1.540047	-9.617866	5.480068
H	1.957160	-9.836589	3.760685
C	3.092016	-7.501520	4.661315
H	3.757981	-8.100942	4.011366
H	3.288899	-7.778585	5.713117
H	3.357730	-6.437352	4.533721
C	1.367258	-7.381301	2.821619
H	1.999926	-8.002717	2.161530
H	1.601986	-6.324254	2.610537
H	0.309766	-7.543098	2.546876
C	-2.607712	2.157655	2.714824
C	-3.311644	1.474553	3.468808
C	-4.200213	0.805794	4.365915
C	-3.841902	-0.398272	5.004806
H	-2.852558	-0.817508	4.804983
C	-4.730540	-1.032217	5.887530
C	-5.976733	-0.421949	6.123313
H	-6.672009	-0.903623	6.808213
C	-6.364103	0.780174	5.504307
C	-5.463249	1.380698	4.616182
H	-5.716851	2.308186	4.097363
C	-4.318262	-2.329652	6.602166
C	-3.704969	-3.322043	5.594055
H	-2.789260	-2.927638	5.122254
H	-4.425092	-3.565049	4.793696
H	-3.425034	-4.261866	6.104698
C	-5.518461	-3.026887	7.270185
H	-5.185986	-3.982596	7.716424
H	-6.311783	-3.253437	6.533125

H	-5.954421	-2.418602	8.083063
C	-3.279679	-1.975685	7.691336
H	-2.374926	-1.521806	7.248789
H	-2.970771	-2.886825	8.239021
H	-3.704625	-1.260665	8.419692
C	-7.715525	1.453704	5.788505
C	-8.401427	1.825406	4.457308
H	-8.529744	0.930221	3.823606
H	-7.819940	2.559584	3.873834
H	-9.398036	2.266891	4.649297
C	-7.464715	2.737644	6.613462
H	-8.420385	3.256688	6.819748
H	-6.804025	3.436411	6.067968
H	-6.981593	2.496693	7.578478
C	-8.665703	0.533814	6.576951
H	-9.640141	1.037595	6.714377
H	-8.271990	0.295087	7.581800
H	-8.845517	-0.414121	6.035885
C	-1.430457	-1.408670	1.836427
C	-2.361451	-2.232782	1.928455
C	-3.441142	-3.134905	2.103852
C	-3.187314	-4.500455	2.380622
H	-2.149559	-4.834179	2.415973
C	-4.244479	-5.374335	2.636938
C	-5.562699	-4.867929	2.568231
H	-6.389567	-5.553347	2.758287
C	-5.847089	-3.520944	2.289469
C	-4.766193	-2.655016	2.067102
H	-4.931558	-1.596192	1.862599
C	-4.020788	-6.844434	3.019507
C	-2.528699	-7.160705	3.216207
H	-2.075625	-6.540041	4.010992
H	-1.960301	-7.007686	2.282715
H	-2.405842	-8.219489	3.510879
C	-4.577807	-7.749603	1.899097
H	-4.452884	-8.815407	2.170130
H	-4.043074	-7.568267	0.950026
H	-5.654321	-7.564457	1.727997
C	-4.759639	-7.141345	4.343699
H	-5.853728	-7.022560	4.243690
H	-4.412452	-6.458929	5.141280
H	-4.561822	-8.181988	4.661645
C	-7.281518	-2.978337	2.199452
C	-7.591800	-2.688709	0.714417
H	-8.616419	-2.282062	0.604120
H	-7.516413	-3.615241	0.116656
H	-6.879232	-1.955585	0.296158
C	-8.313572	-3.986520	2.734982
H	-8.103503	-4.257416	3.786431
H	-8.337341	-4.912382	2.131808
H	-9.323648	-3.539098	2.693821
C	-7.414707	-1.673811	3.012918
H	-8.459598	-1.312762	2.971518
H	-6.773344	-0.864233	2.622219
H	-7.139612	-1.832454	4.070974
C	-0.068884	2.009471	5.978547
C	-0.074314	3.245081	5.870678
C	-0.023789	4.675175	5.955882
C	0.805164	5.267918	6.936089
H	1.374446	4.604062	7.585873
C	0.880100	6.656879	7.067690
C	0.104890	7.448115	6.193148
H	0.158197	8.533028	6.293229
C	-0.730529	6.893934	5.211929
C	-0.781621	5.492433	5.100380
H	-1.420092	5.011567	4.353160
C	1.745843	7.336797	8.140291
C	0.822025	8.093500	9.122781
H	0.113635	7.397519	9.609208
H	0.232468	8.870992	8.603293
H	1.421909	8.588453	9.910169
C	2.579411	6.317480	8.936699
H	3.204375	6.846146	9.679572
H	3.253544	5.742654	8.274595
H	1.938649	5.603645	9.484863
C	2.717055	8.336471	7.474715
H	2.180996	9.118216	6.907777
H	3.392625	7.814255	6.775352
H	3.332353	8.839445	8.244625
C	-1.611213	7.758381	4.296985
C	-1.320356	9.261031	4.457522
H	-0.265617	9.495242	4.221408
H	-1.540047	9.617866	5.480068
H	-1.957160	9.836589	3.760685
C	-3.092016	7.501520	4.661315
H	-3.757981	8.100942	4.011366
H	-3.288899	7.778585	5.713117
H	-3.357730	6.437352	4.533721

C	-1.367258	7.381301	2.821619
H	-1.999926	8.002717	2.161530
H	-1.601986	6.324254	2.610537
H	-0.309766	7.543098	2.546876
C	2.607712	-2.157655	2.714824
C	3.311644	-1.474553	3.468808
C	4.200213	-0.805794	4.365915
C	3.841902	0.398272	5.004806
H	2.852558	0.817508	4.804983
C	4.730540	1.032217	5.887530
C	5.976733	0.421949	6.123313
H	6.672009	0.903623	6.808213
C	6.364103	-0.780174	5.504307
C	5.463249	-1.380698	4.616182
H	5.716851	-2.308186	4.097363
C	4.318262	2.329652	6.602166
C	3.704969	3.322043	5.594055
H	2.789260	2.927638	5.122254
H	4.425092	3.565049	4.793696
H	3.425034	4.261866	6.104698
C	5.518461	3.026887	7.270185
H	5.185986	3.982596	7.716424
H	6.311783	3.253437	6.533125
H	5.954421	2.418602	8.083063
C	3.279679	1.975685	7.691336
H	2.374926	1.521806	7.248789
H	2.970771	2.886825	8.239021
H	3.704625	1.260665	8.419692
C	7.715525	-1.453704	5.788505
C	8.401427	-1.825406	4.457308
H	8.529744	-0.930221	3.823606
H	7.819940	-2.559584	3.873834
H	9.398036	-2.266891	4.649297
C	7.464715	-2.737644	6.613462
H	8.420385	-3.256688	6.819748
H	6.804025	-3.436411	6.067968
H	6.981593	-2.496693	7.578478
C	8.665703	-0.533814	6.576951
H	9.640141	-1.037595	6.714377
H	8.271990	-0.295087	7.581800
H	8.845517	0.414121	6.035885
C	-4.672896	-0.206388	-0.364680
C	-5.432574	0.653413	0.093232
C	-6.352760	1.646950	0.546807
C	-7.738668	1.423817	0.483591
H	-8.091506	0.462612	0.102398
C	-8.648303	2.419593	0.878639
C	-8.128572	3.637687	1.348527
H	-8.816183	4.426440	1.657898
C	-6.741158	3.892413	1.423753
C	-5.864921	2.884506	1.017315
H	-4.785349	3.030793	1.046663
C	-10.156523	2.159336	0.727864
C	-10.495230	2.097760	-0.780773
H	-10.235392	3.049358	-1.278566
H	-11.576270	1.909617	-0.924444
H	-9.934669	1.289199	-1.285250
C	-10.541706	0.815004	1.385876
H	-11.625271	0.631026	1.260661
H	-10.314468	0.827011	2.466506
H	-10.003121	-0.036897	0.933045
C	-10.999829	3.269771	1.379090
H	-10.767406	3.369887	2.455696
H	-12.073928	3.026615	1.284005
H	-10.836533	4.248562	0.892344
C	-6.225225	5.255784	1.908154
C	-6.706945	6.354462	0.933514
H	-7.809764	6.388849	0.866450
H	-6.305855	6.168547	-0.079479
H	-6.352505	7.346414	1.273200
C	-6.763855	5.542824	3.326970
H	-6.402853	6.527086	3.680687
H	-6.411873	4.774496	4.040087
H	-7.868407	5.554956	3.356279
C	-4.687810	5.298352	1.957279
H	-4.354706	6.293237	2.300322
H	-4.237306	5.124138	0.963583
H	-4.277921	4.545572	2.654804
Ag	-1.881228	0.214079	-3.405545
Ag	-0.234736	-1.923430	3.719742
Ag	0.234736	1.923430	3.719742