Supplementary Information

Controlled Aggregation of Pt/PtH/Rh/RhH doped Silver Superatomic Nanoclusters into 16-electron Supermolecules

Tzu-Hao Chiu,[a] Michael N. Pillay,[a] Ying-Yann Wu,[a] Yoshiki Niihori,[b] Yuichi Negishi,[b] Jie-Ying Chen,[c] Yuan Jang Chen,[c] Samia Kahlal,[d] Jean-Yves Saillard,[d*] and C. W. Liu[a*]

a. Department of Chemistry, National Dong Hwa University, Hualien 97401, Taiwan (Republic of China).

b. Department of Applied Chemistry, Tokyo University of Science, 1-3 Kagurazaka, Shinjuku, Tokyo 162-8601, Japan.

c. Department of Chemistry, Fu Jen Catholic University, New Taipei City, 24205, Taiwan (Republic of China).

d. Univ Rennes, CNRS, ISCR-UMR 6226, F-35000 Rennes, France.* Correspondence: E-mail: chenwei@mail.ndhu.edu.tw; Tel: +886-3-890-3607; Fax : +886-3-890-0162; http://faculty.ndhu.edu.tw/~cwl/index.htm

Experimental Section

1.1 General remarks

All chemicals were purchased from commercial sources and used as received. Solvents were purified following standard protocols. All reactions were carried out under N_2 atmosphere by using standard Schlenk techniques. $[Ag(CH_3CN)_4]PF_6$ and $NH_4[S_2P(O^nPr)_2]$ were prepared by following the procedure reported in literature.[S1,S2] NMR spectra were recorded on a Bruker AVII-400 and AV-600 MHz NMR spectrometers. The chemical shift (δ) is reported in ppm and Hz, respectively. ESI-mass spectra recorded on a Bruker maXis Q-TOF mass spectrometer (Bruker Daltonik GmbH, Germany). UV–visible-NIR absorption spectra were measured on a Shimadzu UV3101PC spectrophotometer at 298 K, using quartz cells with a path length of 1 cm. Luminescence spectra and lifetime were recorded on an Edinburgh FLS920 fluorescence spectrometer. PLQY study was conducted on a HORIBA JOBIN YVON iHR 550 spectrometer, equipped with a HORIBA Symphony InGaAs-1700 (for the NIR) detector head mounted on the exit port. $[Ru(bpy)_2(en)]^{2+}$ (bpy = bpyridine; en = ethylenediamine) was the reference for the determination at 87 K.

1.2 Synthesis

1.2.1 Synthesis of $[(RhH)_2Ag_{33}\{S_2P(O^nPr)_2\}_{17}]$ (1)

In a Flame-dried Schlenk tube, $[Ag(CH_3CN)_4]PF_6$ (0.50 g, 0.86 mmol) and $NH_4[S_2P(O^nPr)_2]$ (0.14 g, 0.43 mmol) were dissolved in THF, and kept stirring at -20℃ for 5 minutes. $[Rh(COD)Cl]_2$ (0.02 g, 0.043 mmol) was added to the above solution. After 10 minutes, $NaBH_4$ (0.02 g, 0.86 mmol) was added, and kept stirring for 12 hours. The reaction mixture was dried under reduced pressure. The residue was washed with DCM/DI-Water. The DCM layer was dried under reduced pressure and subsequently purified by thin-layer chromatography, with MeOH as a mobile phase. Finally, a gray-black product can be obtained. The yield of **1** is 10% based on Ag.

$[(RhH)_2Ag_{33}\{S_2P(O^nPr)_2\}_{17}]$ **(1)**

$^{31}P\{^1H\}$ NMR (161.97 MHz, $CDCl_3$, δ, ppm, r.t.): 104.7 (br, 10 S_2P), 101.0 (s, 2 S_2P), 96.9 (br, 5 S_2P). ^1H NMR (400 MHz, $CDCl_3$, δ, ppm, r.t.): -12.1 (br, μ_4-H, 2H) 0.9-1.0 (m, CH_3, 102H), 1.67-1.89 (m, CH_2, 68H), 3.97 (q, OCH_2, 8H), 4.12 (q, OCH_2, 40H), 4.34 (q, OCH_2, 20H). ESI-MS (*m/z*): exp. 7392.983 (calc. for $[M + H]^+$: 7392.990). UV-vis [λ_{max} in nm, (ε in $M^{-1}cm^{-1}$)]: 380 (65500), 500 (35500), 708 (6000).

1.2.1 Synthesis of $[PtHPtAg_{32}\{S_2P(O^nPr)_2\}_{17}]$ (2) and $[Pt_2Ag_{33}\{S_2P(O^nPr)_2\}_{17}]$ (3)

In a Flame-dried Schlenk tube, $[Ag(CH_3CN)_4]PF_6$ (0.50 g, 0.86 mmol) and $NH_4[S_2P(O^nPr)_2]$ (0.14 g, 0.43 mmol) were dissolved in THF, and kept stirring at -20℃ for 5 minutes. $Pt[S_2P(O^nPr)_2]_2$ (0.02 g, 0.043 mmol) was added to the above solution. After 10 minutes, $NaBH_4$ (0.02 g, 0.86 mmol) was added, and kept stirring for 12 hours. The reaction mixture was dried under reduced pressure. The residue was washed with DCM/DI-Water. The DCM layer was dried under reduced pressure and further purified by thin-layer chromatography with MeOH as a mobile phase. The first brown band is $[PtAg_{20}\{S_2P(O^nPr)_2\}_{12}]$. The second purple band is $[PtHPtAg_{32}\{S_2P(O^nPr)_2\}_{17}]$ (**2**). The final purple band is $[Pt_2Ag_{33}\{S_2P(O^nPr)_2\}_{17}]$ (**3**) (Figure S22). The yields of **2**, and **3** are 2% and 11%, respectively, based on Ag.

$[PtHPtAg_{32}\{S_2P(O^nPr)_2\}_{17}]$ **(2)**

$^{31}P\{^1H\}$ NMR (161.97 MHz, $CDCl_3$, δ, ppm, r.t.): 106.0 (br, 5 S_2P), 104.8 (br, 5 S_2P), 101.0 (s, 2 S_2P), 96.2 (br, 5 S_2P). ^1H NMR (400 MHz, $CDCl_3$, δ, ppm, r.t.): -10.4 (br, $^1J_{1H\text{-}195Pt}$ = 512Hz at 293K) 0.9-1.0 (m, CH_3, 102H), 1.63-1.87 (m, CH_2, 68H), 3.99 (q, OCH_2, 8H), 4.12 (q, OCH_2, 40H), 4.31 (q, OCH_2, 20H). ESI-MS (*m/z*): exp. 3841.954 (calc. for $[M + 2Ag]^{2+}$: 3841.987). UV-vis [λ_{max} in nm, (ε in $M^{-1}cm^{-1}$)]: 490 (26000), 700 (4000).

1.3 X-ray crystallography

Single crystals suitable for X-ray diffraction analysis of **1**, **2**, and **3** was obtained by evaporating MeOH solution at 4°C within a week. The single crystals were mounted on the tip of glass fiber coated in paratone oil, then frozen. Data were collected on a Bruker APEX II CCD diffractometer using graphite monochromated Mo *K*α radiation (λ = 0.71073 Å) at 100 K. Absorption corrections for area detector were performed with SADABS[S3] and the integration of raw data frame was performed with SAINT.[S4] The structure was solved by direct methods and refined by least-squares against F^2 using the SHELXL-2018/3 package,[S5,S6] incorporated in SHELXTL/PC V6.14.[S7] All non-hydrogen atoms were refined anisotropically. CCDC 2342395 (**1**), 2342396 (**2**) and 2342397 (**3**) contains the supplementary crystallographic data for compounds **1-3** in this article. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

1.4 Computational Details

Geometry optimizations were performed by density functional theory (DFT) calculations with the Gaussian 16 package,[s8] using the BP86 functional[s9] and the all-electron Def2-TZVP set from EMSL Basis Set Exchange Library.[s10] All the optimized geometries were characterized as true minima by vibrational analysis. The NAO charges and Wiberg bond indices were computed with the NBO 6.0 program[s11] on single-point calculations performed with the BP86 functional and the Def2-SVP basis set for computational limitations.[s12] The UV-visible transitions were calculated by means of time-dependent DFT (TD-DFT) calculations, with the CAM-B3LYP functional[s13] and the Def2-TZVP basis set. Only singlet-singlet, *i.e.* spin-allowed, transitions have been computed. The UV-visible spectra were simulated from the computed TD-DFT transitions and their oscillator strengths by using the Multiwfn program,[s14] each transition is associated with a Gaussian function of half-height width equal to 2000 cm^{-1}. The compositions of the molecular orbitals were calculated using the AOMix program.[s15]

References

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S3. SADABS, version 2014-11.0, Bruker Area Detector Absorption Correxions (Bruker AXS Inc., Madison, WI, 2014).

S4. SAINT, included in G. Jogl, V4.043: Software for the CCD detector system (Bruker Analytical: Madison, WI, 1995).

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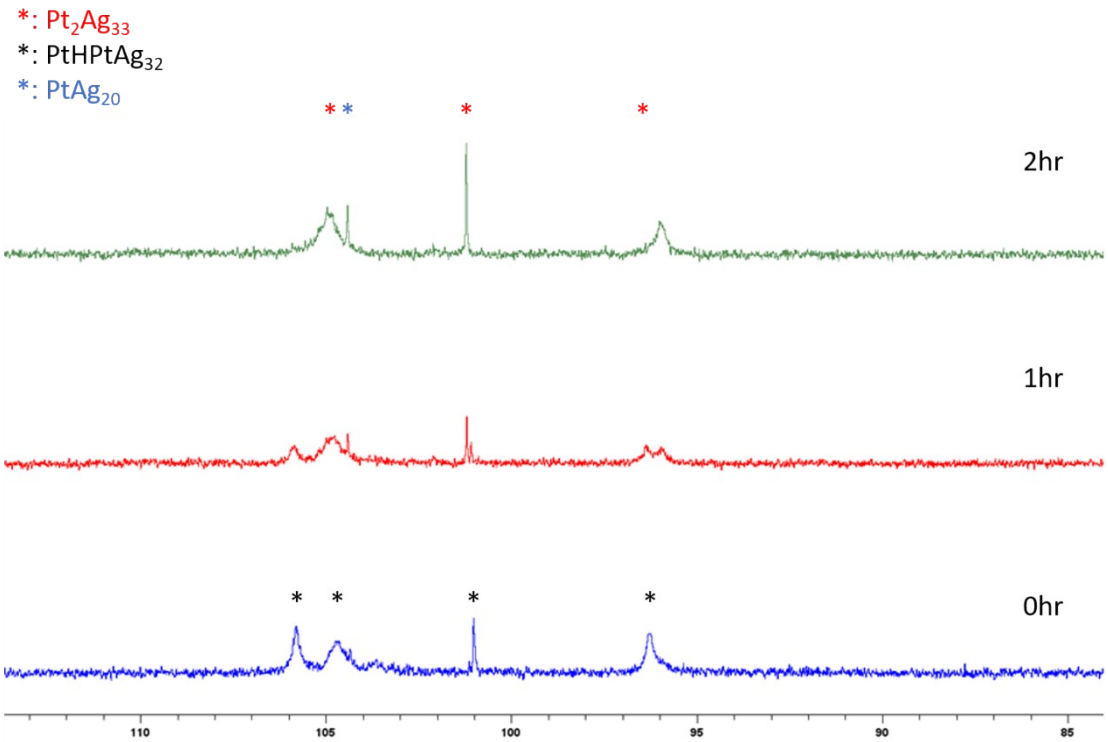

Figure S1. Time-dependent ^{31}P NMR spectra ($CDCl_3$) of **2** under 60°C.

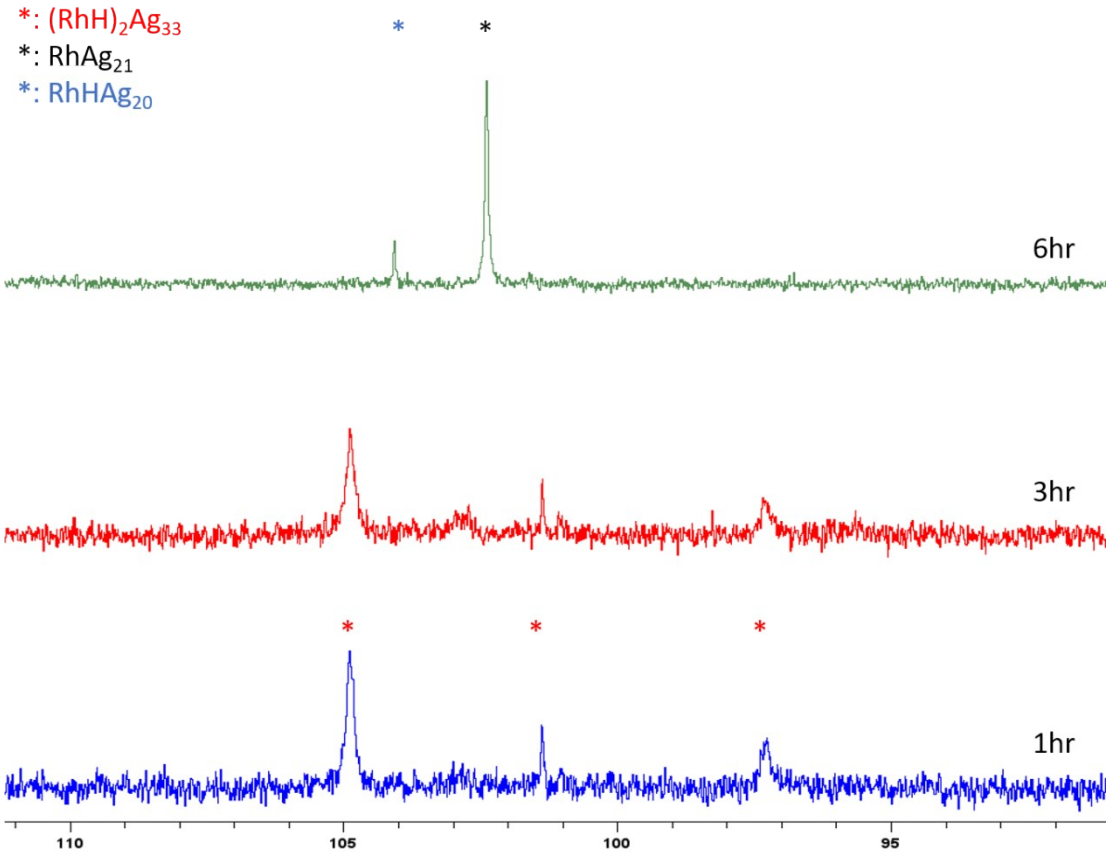

Figure S2. Time-dependent ^{31}P NMR spectra ($CDCl_3$) of **1** under 60°C.

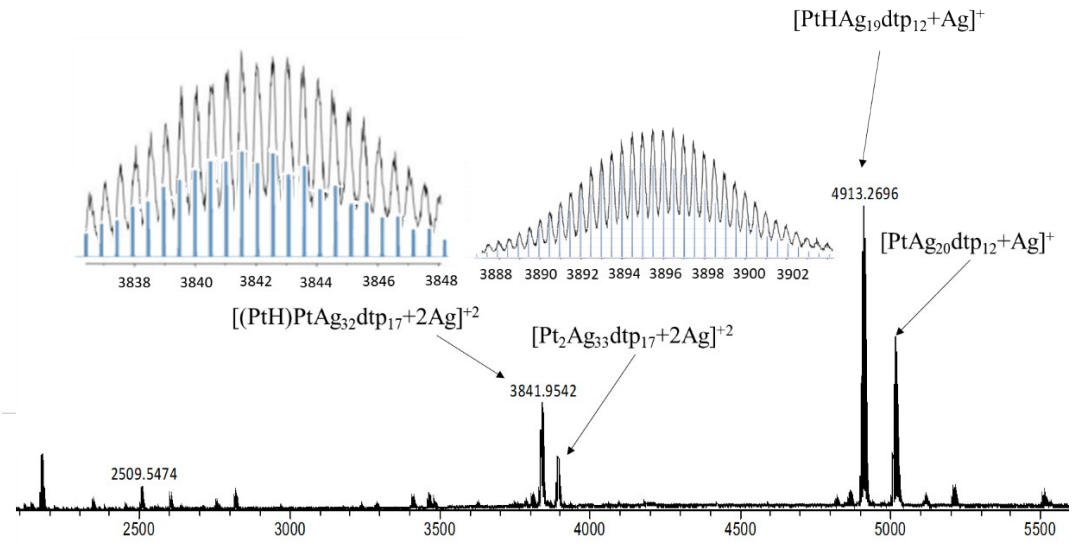

Figure S3. Positive-mode ESI mass spectrum of **2**. Insets: experimental (black) and simulated (blue).

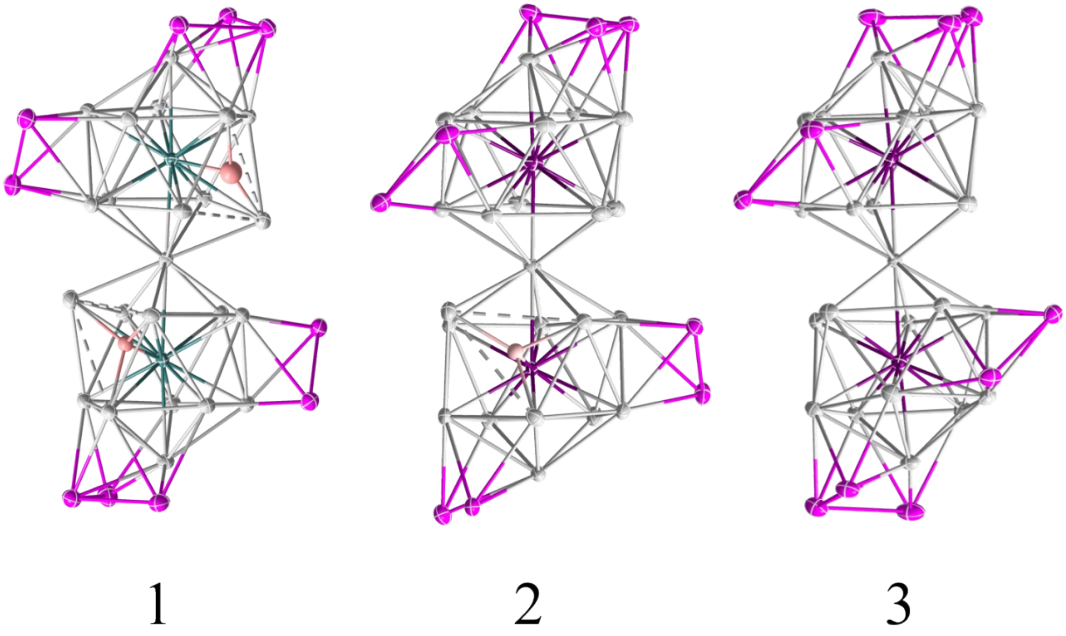

Figure S4. Metal framework of **1**-**3**.

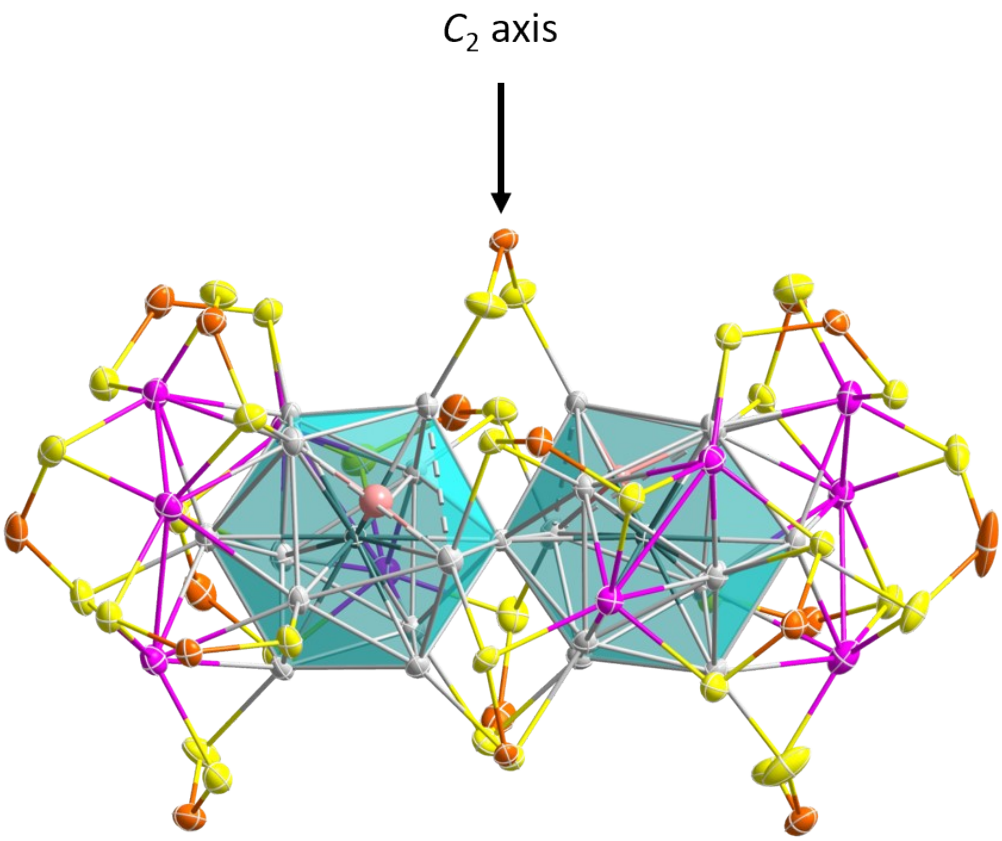

Figure S5. Side view of **1.**

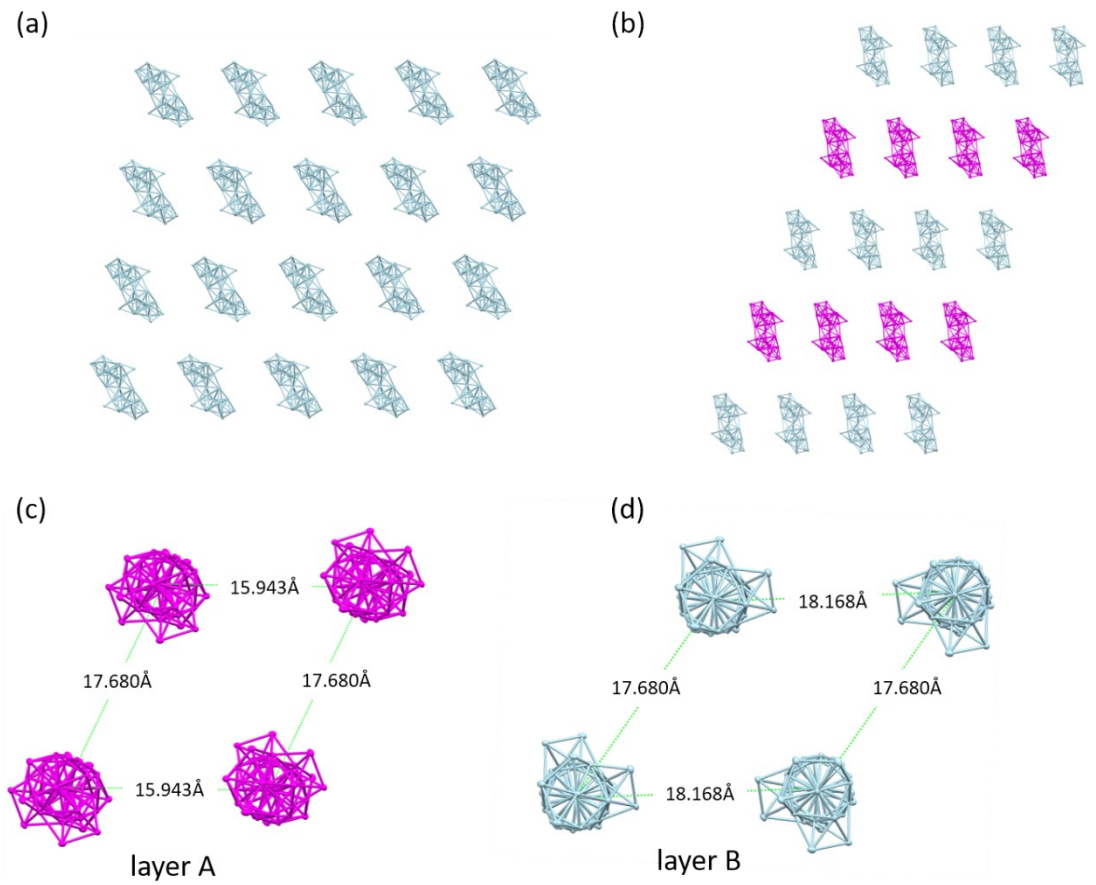

Figure S6. (a)Packing diagram of previously reported Pt_2Ag_{33}(b) packing diagram of **3** (c) layer A (d) layer B.

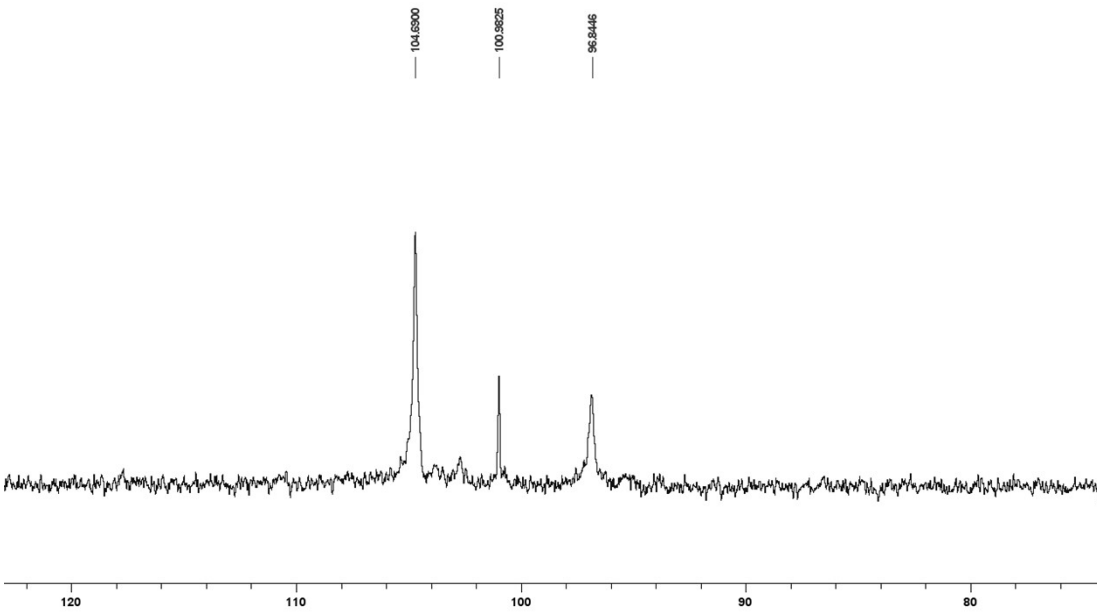

Figure S7. ^{31}P NMR spectrum ($CDCl_3$) of **1**.

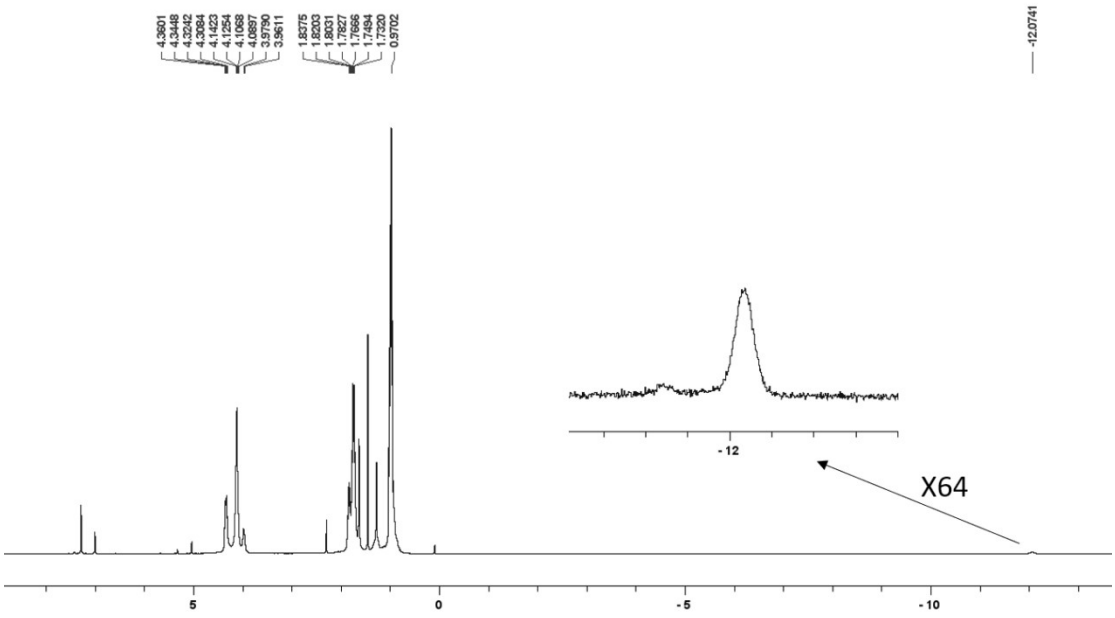

Figure S8. ^{1}H NMR spectrum ($CDCl_3$) of **1**.

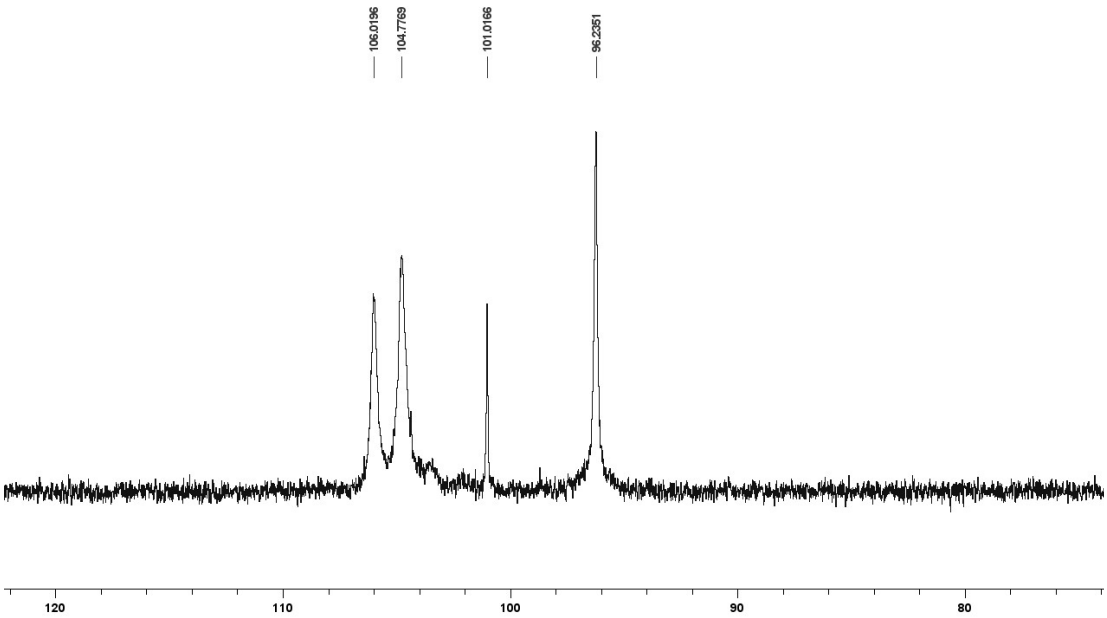

Figure S9. ^{31}P NMR spectrum ($CDCl_3$) of **2**.

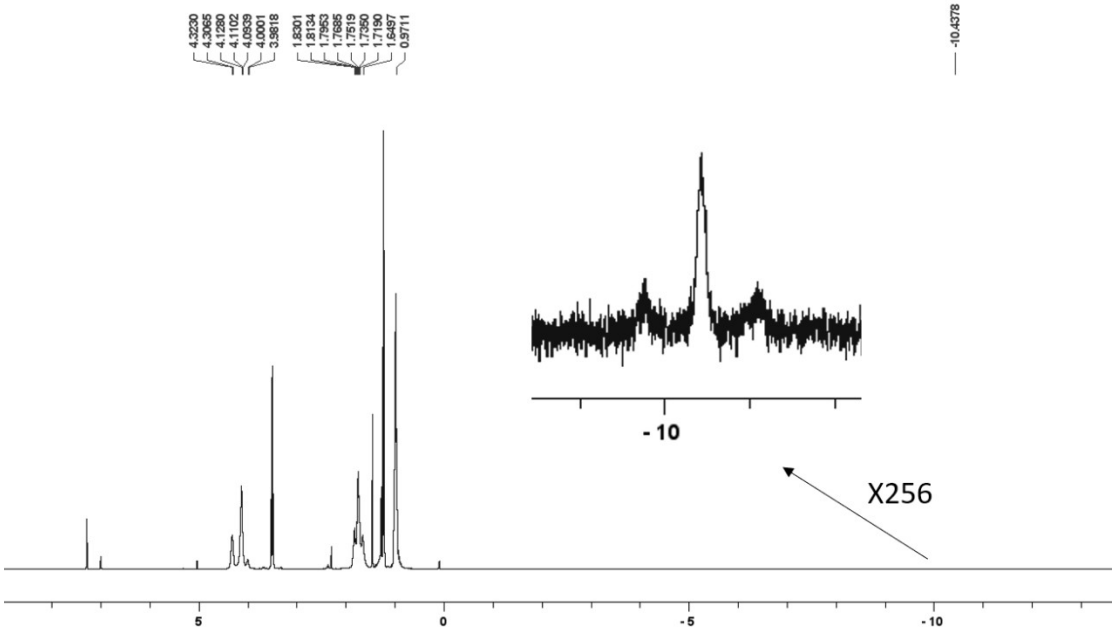

Figure S10. ^{1}H NMR spectrum ($CDCl_3$) of **2**.

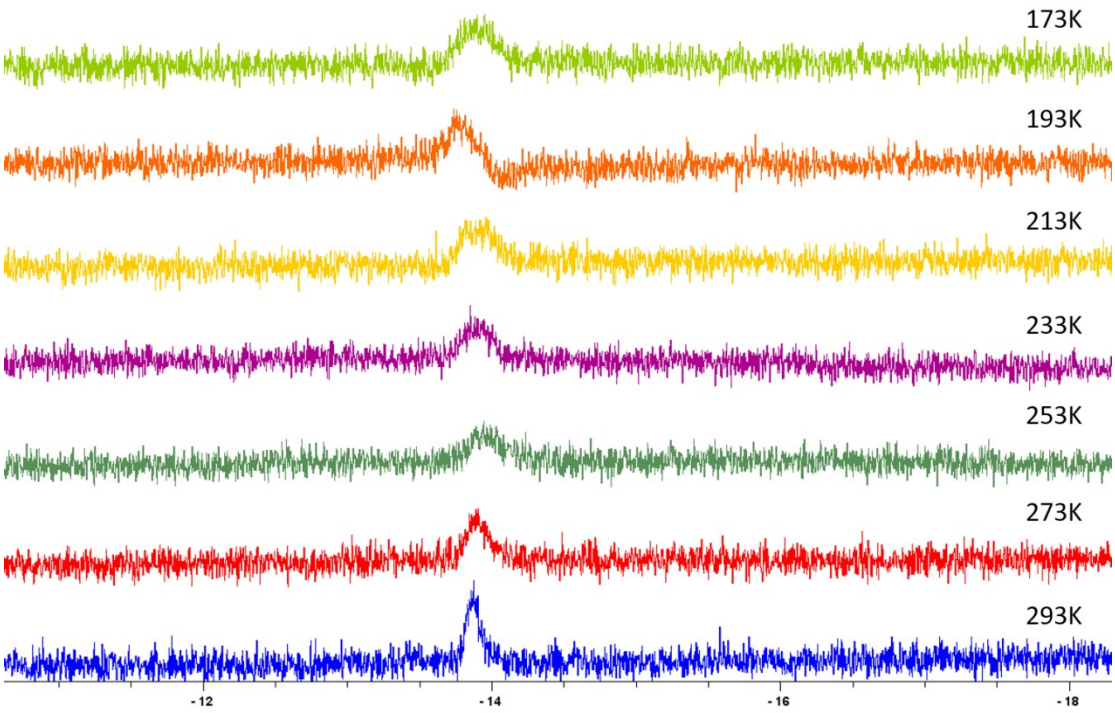

Figure S11. VT ^{1}H NMR spectrum (THF-d8) of **1**.

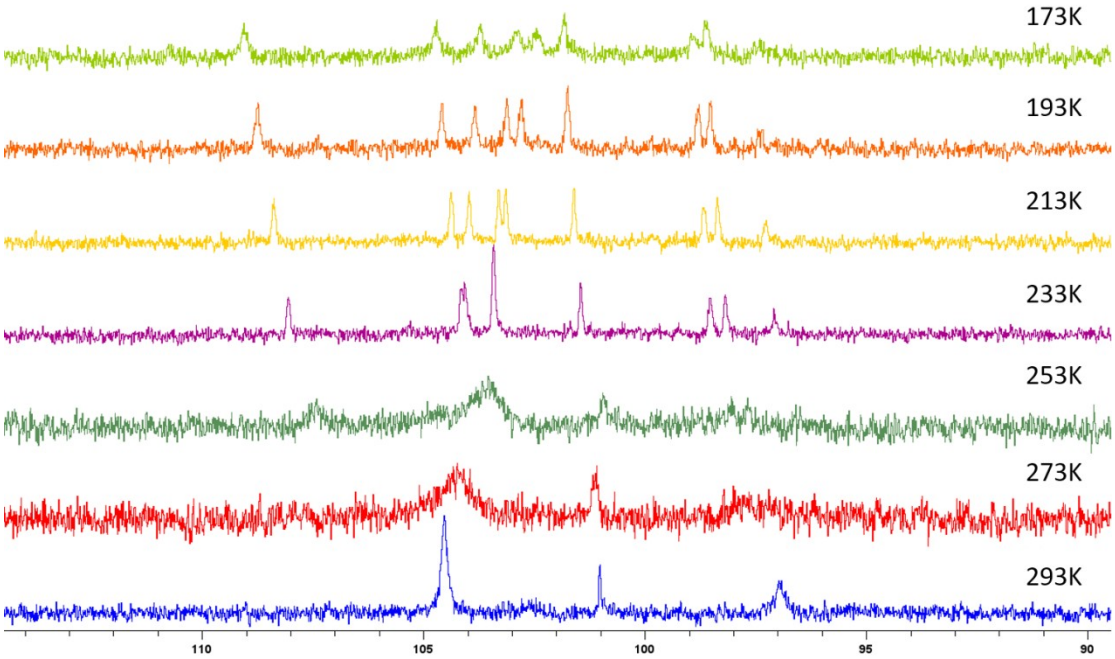

Figure S12. VT ^{31}P NMR spectrum (THF-d8) of **1**.

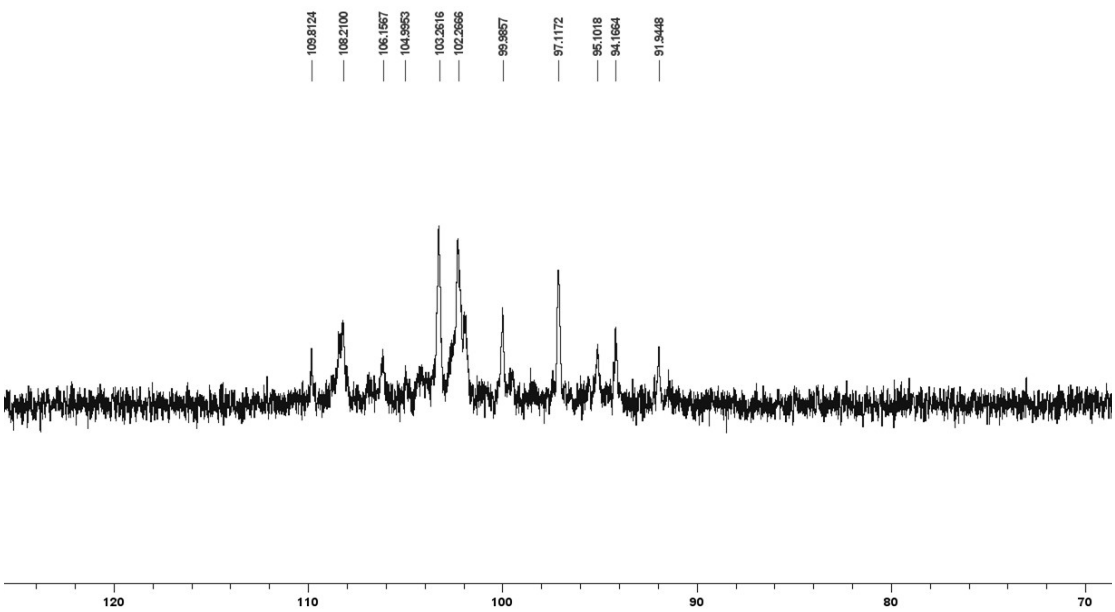

Figure S13. ^{31}P NMR spectrum (THF-d8) of **2** at 173K.

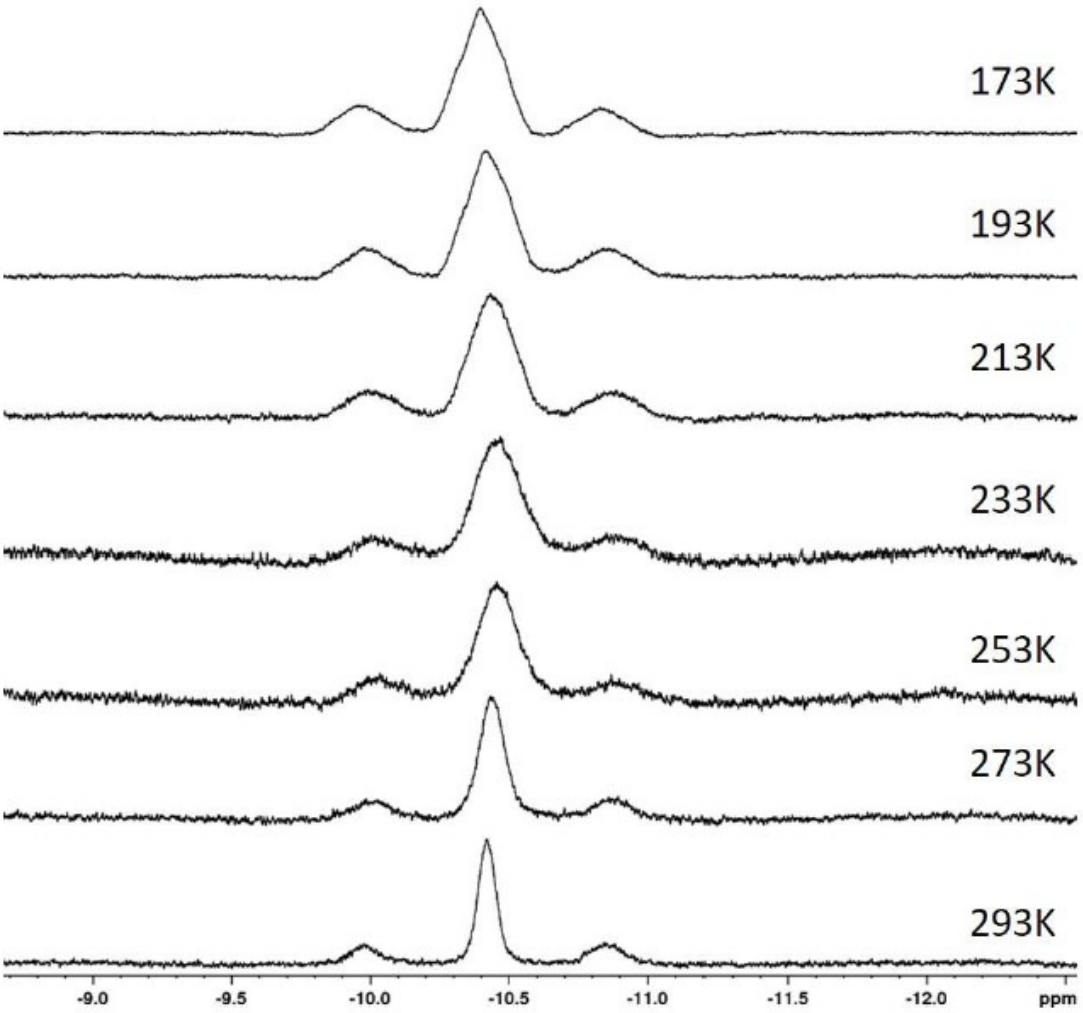

Figure S14. VT ^{1}H NMR spectrum (THF-d8) of **2**.

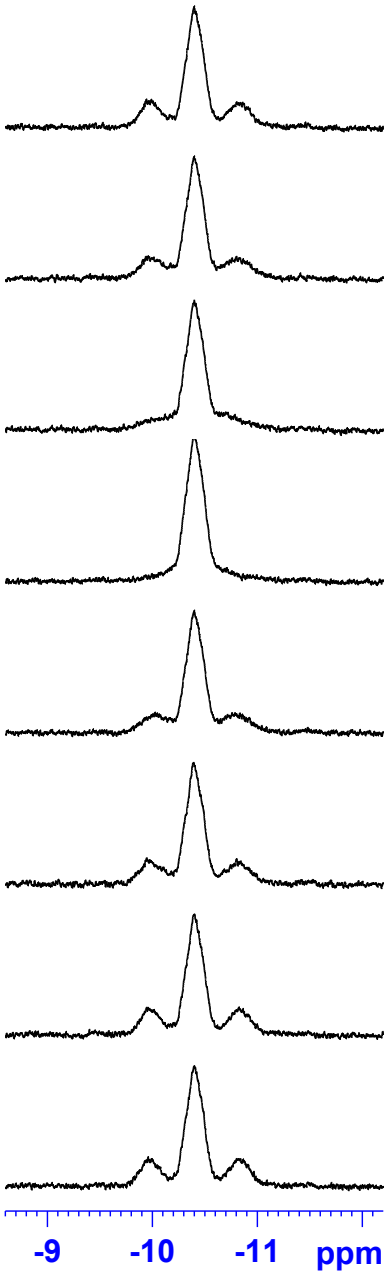

Figure S15. $^{1}H\{^{195}Pt\}$ NMR spectra of **2** at 173 K with various ^{195}Pt decoupling ranges.

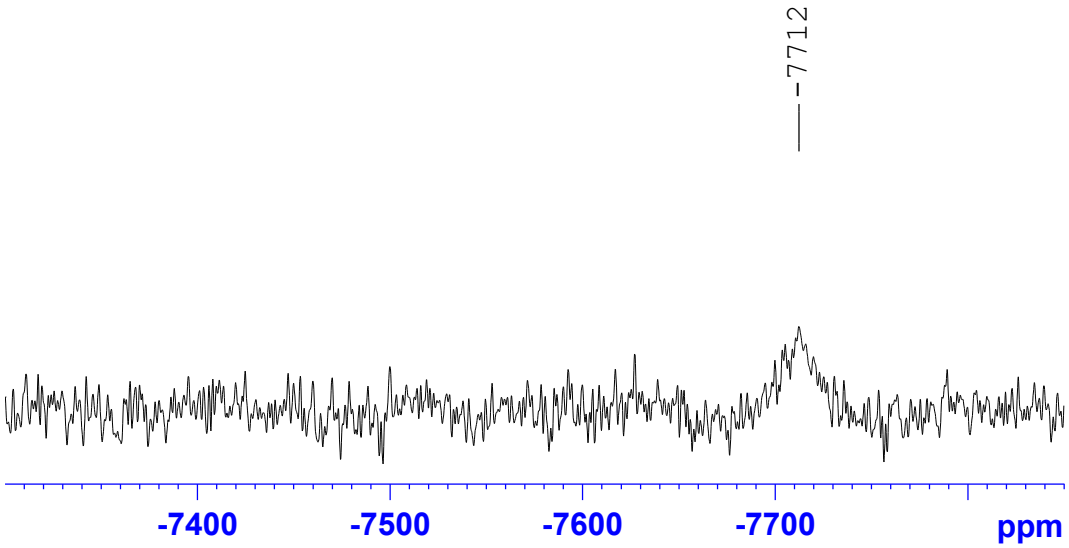

Figure S16. The $^{195}Pt\{^{1}H\}$ spectrum of **2** at 173K.

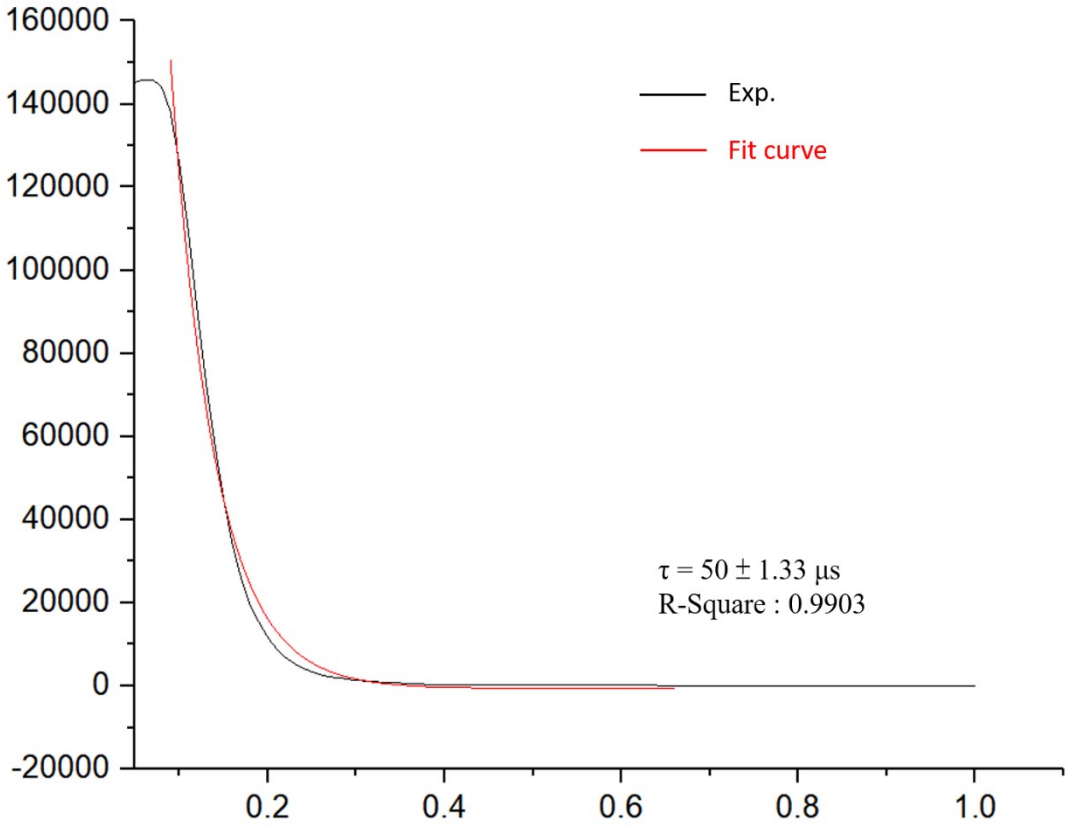

Figure S17. Time-resolved photoluminescence spectrum of **1**.

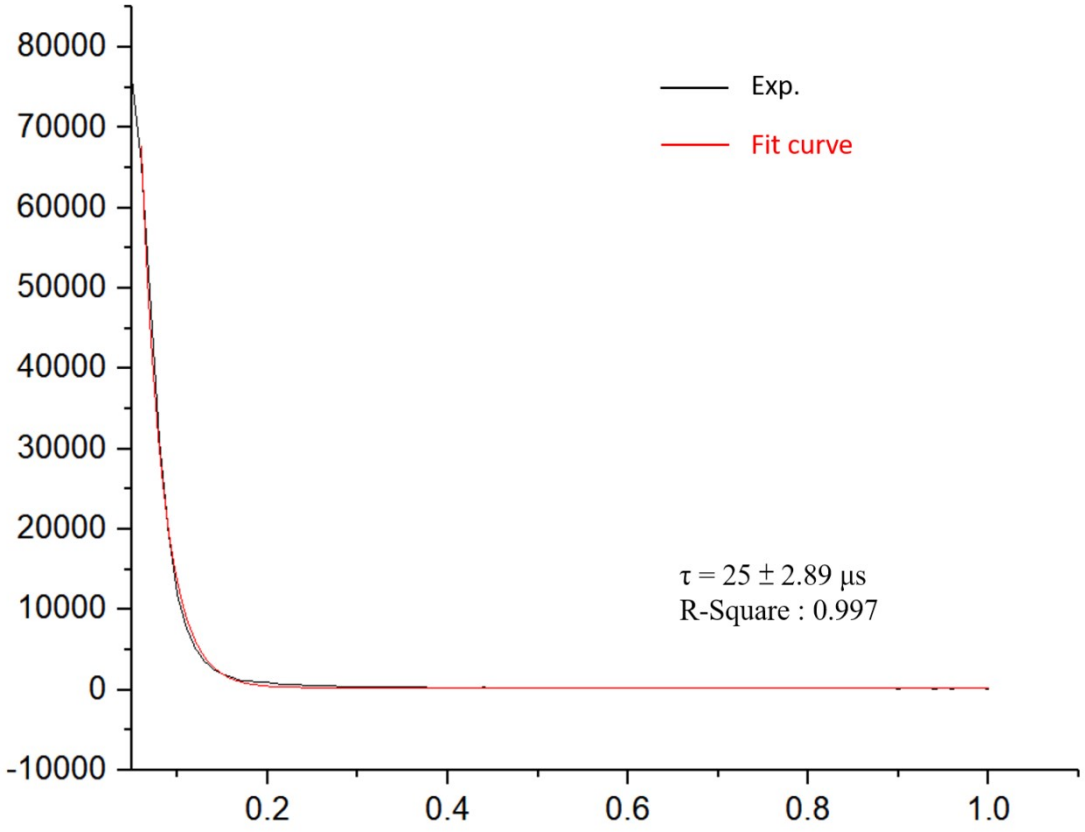

Figure S18. Time-resolved photoluminescence spectrum of **2**.

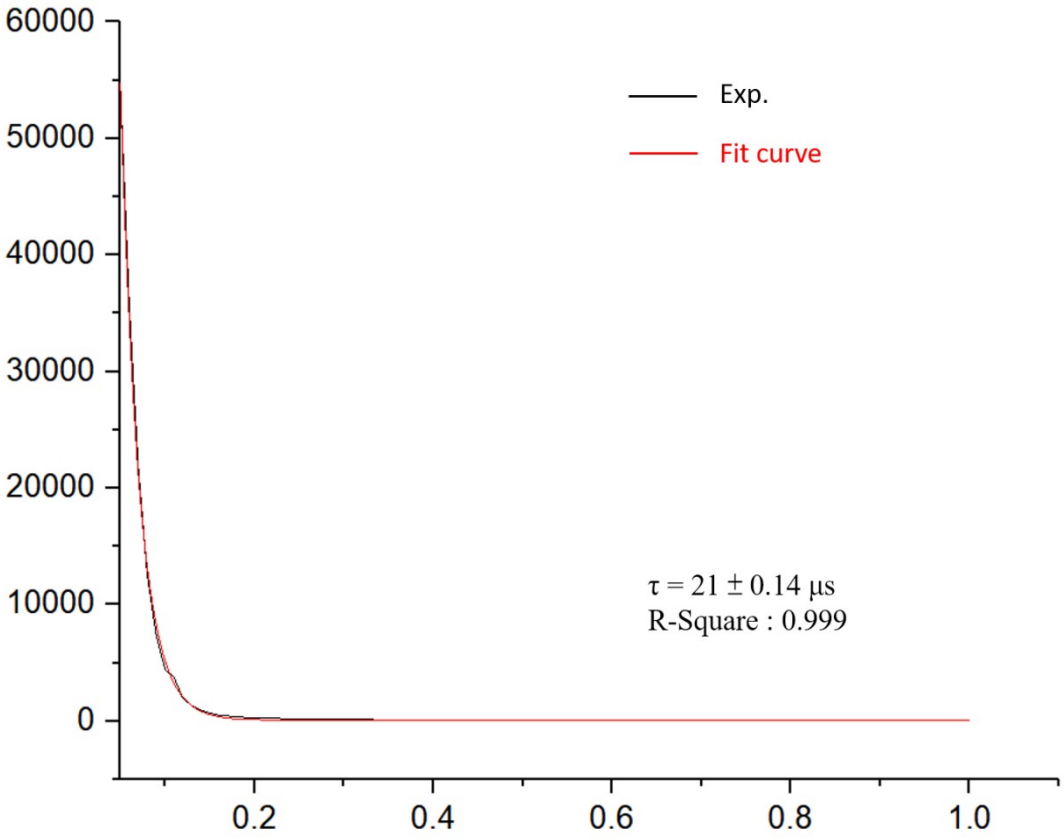

Figure S19. Time-resolved photoluminescence spectrum of **3**.

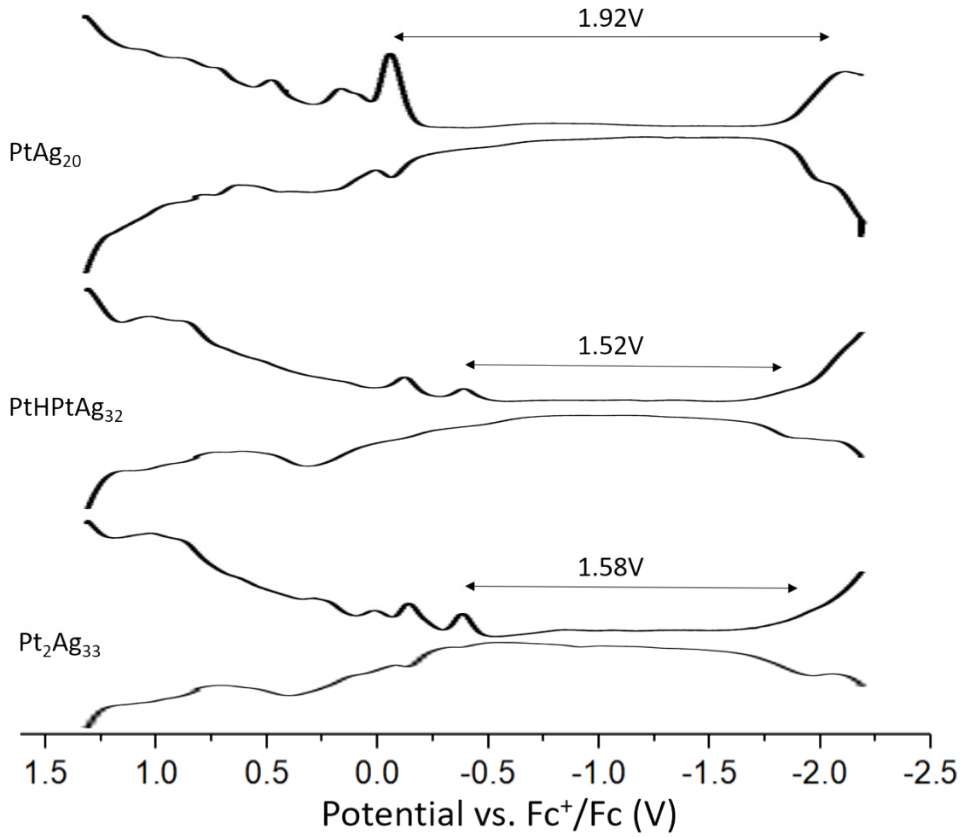

Figure S20. Differential pulse voltammograms of $PtAg_{20}[S_2P(OPr)_2]_{12}$, $PtHPtAg_{32}[S_2P(OPr)_2]_{17}$ and $Pt_2Ag_{33}[S_2P(OPr)_2]_{17}$.

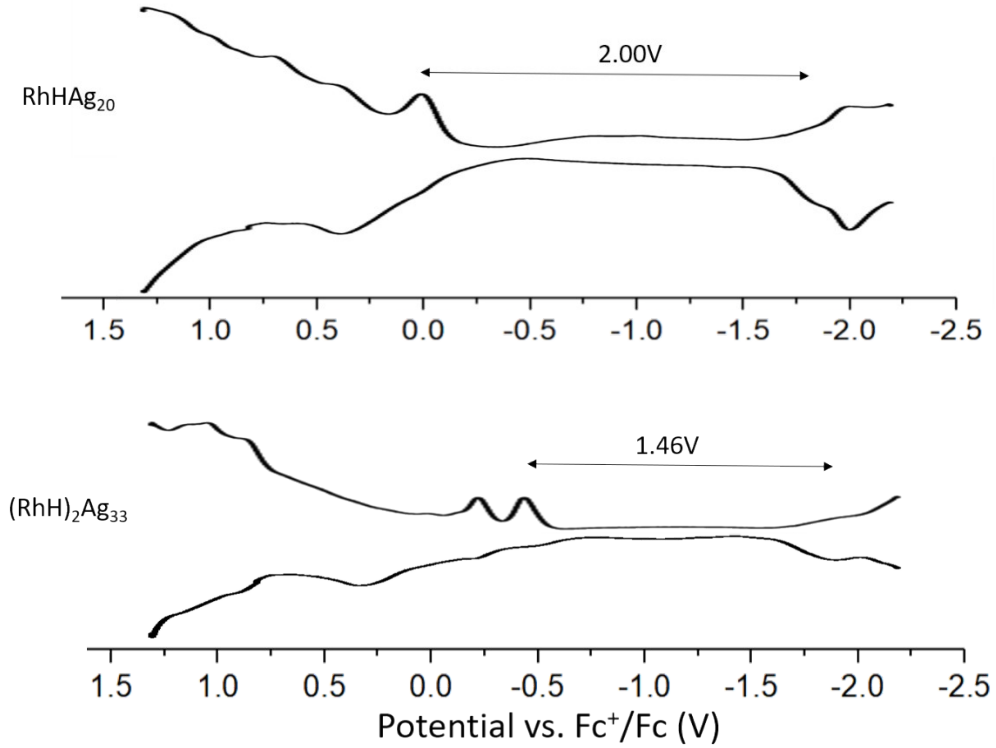

Figure S21. Differential pulse voltammograms of $RhHAg_{20}[S_2P(OPr)_2]_{12}$ and $(RhH)_2Ag_{33}[S_2P(OPr)_2]_{17}$.

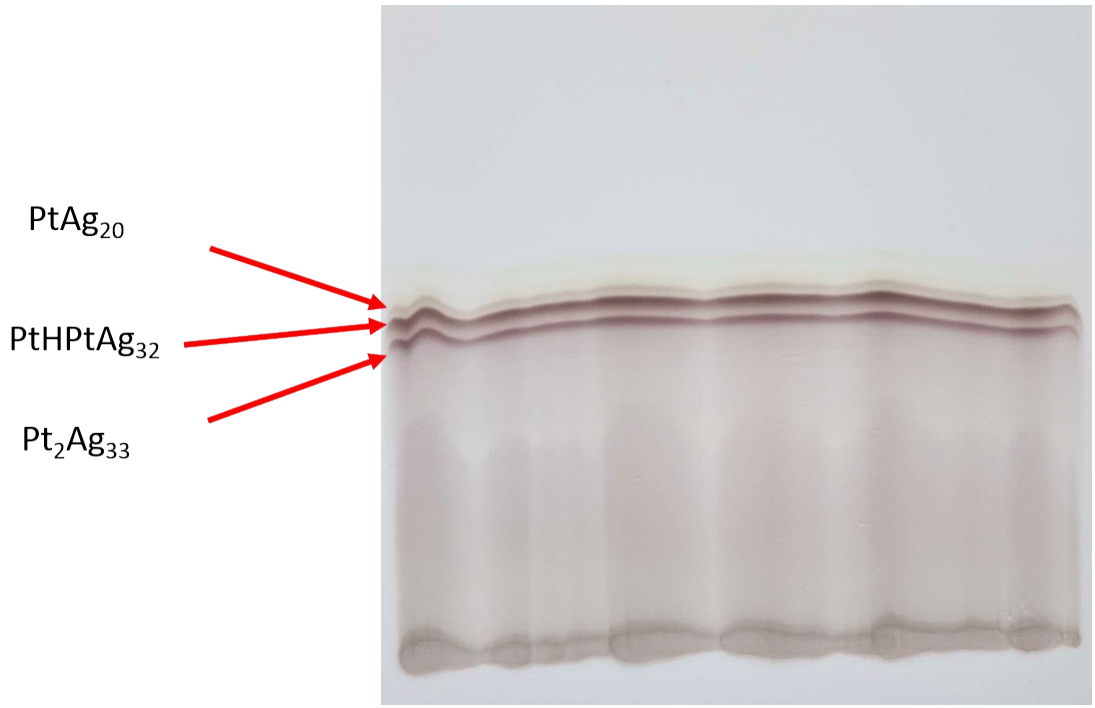

Figure S22. Photo of TLC under eluent combination: ether: hexane = 1:4.

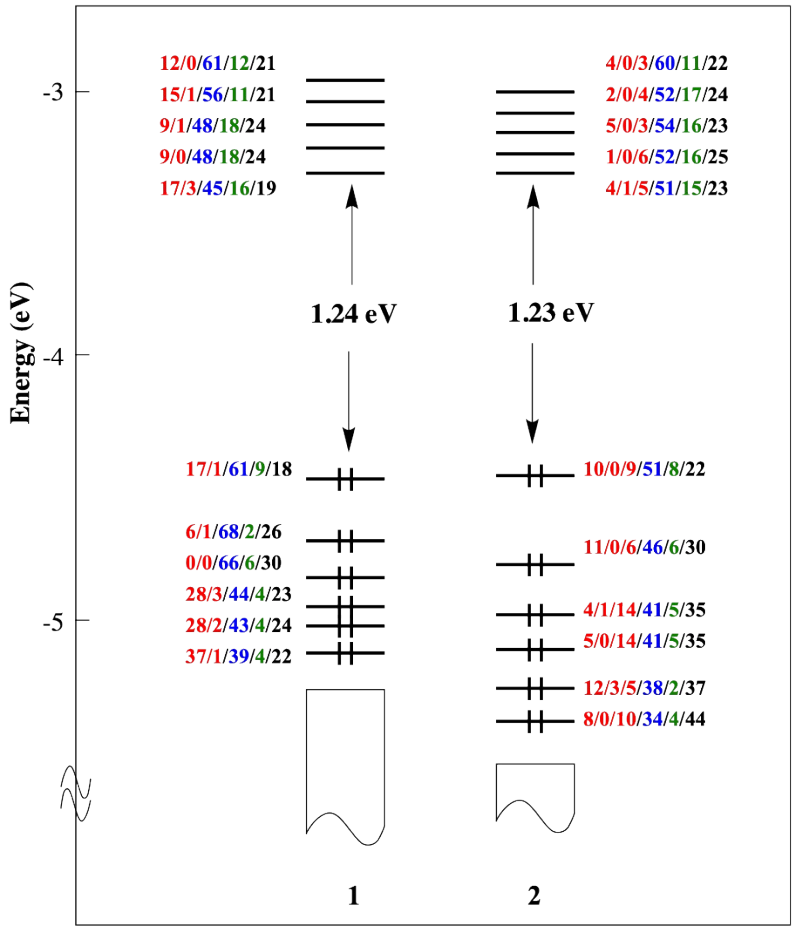

Figure S23. The Kohn-Sham frontier MO diagram of compounds **1** and **2** with orbital compositions as follows. **1**: **Rh_2/H_2/Ag_{23}(ico)/Ag_{10}(cap)/ligands**; **2**: **Pt/H/Pt/Ag_{23}(ico)/Ag_9(cap)/ligands**. The hydride of **2** lies in the left-side icosahedron.

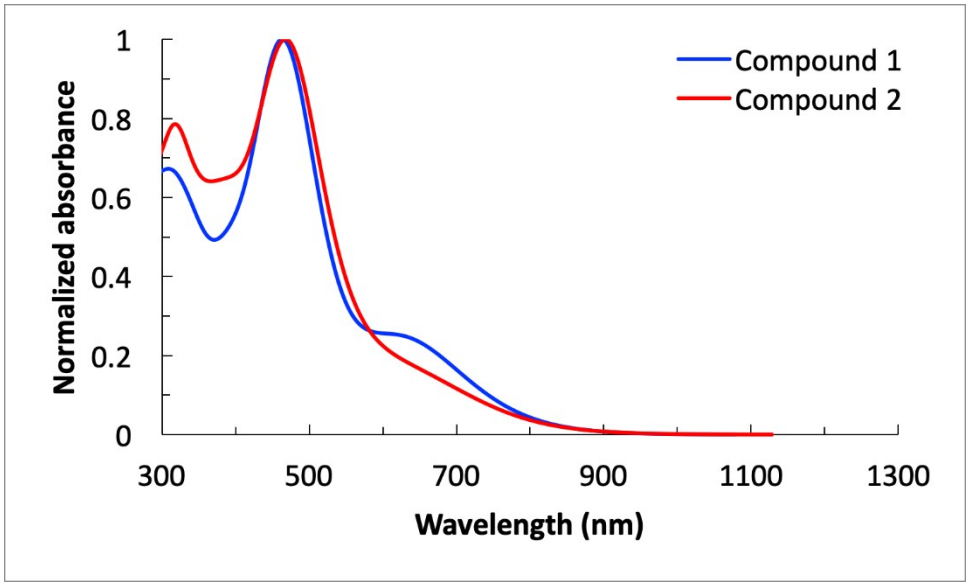

Figure S24. The TD-DFT-simulated UV-vis spectra of **1** and **2**.

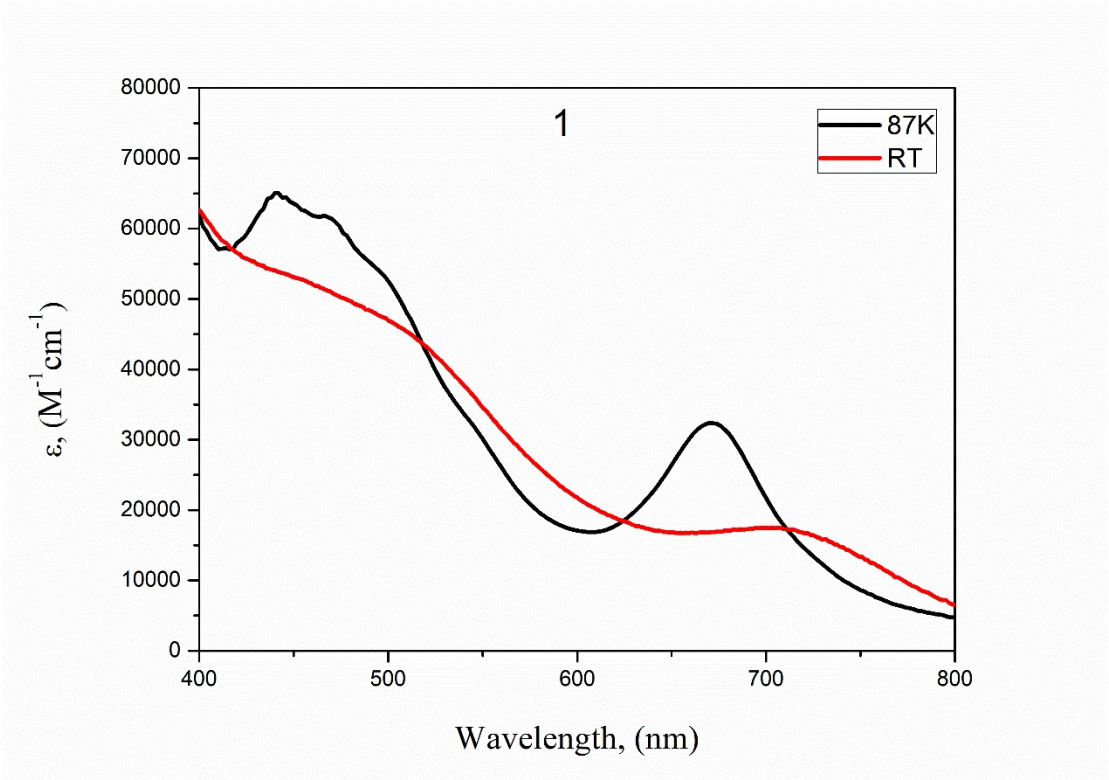

Figure S25. Low-temperature excitation spectra of Compound **1**.

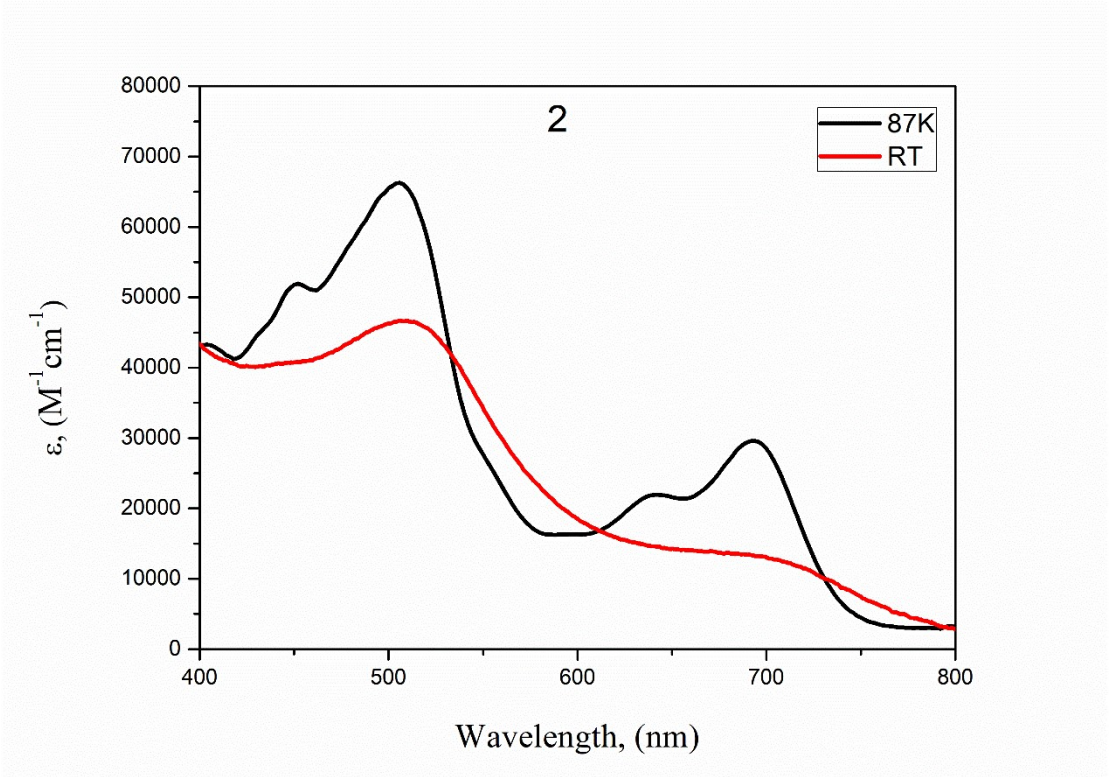

Figure S26. Low-temperature excitation spectra of Compound **2**.

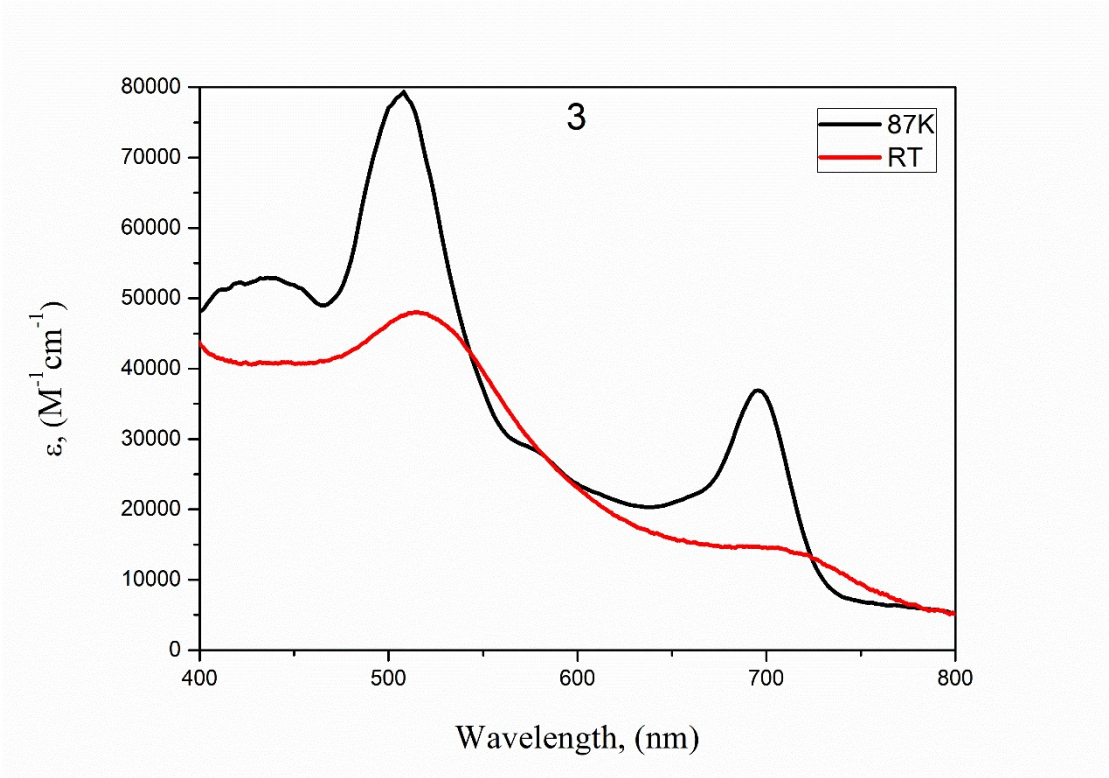

Figure S27. Low-temperature excitation spectra of Compound **3**.

Table S1. Selected X-ray crystallographic data of **1**,**2** and **3**.

Compound	**1**	**2**	**3**
CCDC no.	2342395	2342396	2342397
Chemical formula	$C_{204}H_{480}Ag_{66}O_{68}P_{34}Rh_4S_{68}$	$C_{102}H_{239}Ag_{32}O_{34}P_{17}Pt_2S_{34}$	$C_{102}H_{238}Ag_{33}O_{34}P_{17}Pt_2S_{34}$
Formula weight	14785.97	7468.47	7575.33
Wavelength, Å	0.71073	0.71073	0.71073
Crystal System	Triclinic	Triclinic	Monoclinic
Space group	$P\bar{1}$	$P\bar{1}$	$C2/c$
a, Å	16.193(2)	19.4846(11)	44.382(7)
b, Å	34.224(5)	20.7482(12)	17.680(3)
c, Å	38.997(5)	30.0519(17)	28.939(4)
α, deg.	72.855(4)	98.0114(14)	90
β, deg.	84.982(3)	102.1599(14)	111.569(5)
γ, deg.	83.671(2)	116.0390(13)	90
V, Å^3	20491(5)	10292.5(10)	21118(6)
Z	2	2	4
Temperature, K	100(2)	100(2)	100(2)
ρ_{calcd}, g/cm^3	2.396	2.410	2.383
μ, mm^{-1}	3.759	4.846	4.814
θ_{max}, deg.	25.000	25.000	25.000
Completeness, %	99.7	98.8	100
Reflection collected / unique	233268 / 71948 [R(int) = 0.0907]	67817 / 35841 [R(int) = 0.0445]	91475 / 18602 [R(int) = 0.0280]
Restraints / parameters	1470 / 4132	861 / 2070	359 / 1063
[a] $R1$, [b] $wR2$ [I > 2σ(I)]	0.0666, 0.1254	0.0555, 0.1333	0.0364, 0.0733
[a] $R1$, [b] $wR2$ (all data)	0.1174, 0.1519	0.0802, 0.1511	0.0448, 0.0811
GOF	1.103	1.032	1.113
Largest diff. peak and hole, e/Å^3	2.570 and -1.806	3.721 and -1.917	2.805 and -1.366

[a] $R1 = \Sigma \mid \Box F_o \Box - \Box Fc \Box \mid / \Sigma \Box F_o \Box$. [b] $wR2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$.

Table S2. Cartesian coordinates of the DFT-optimised structures of **1**, **2**, and **3**.

1

Ag	-0.010295	0.015327	-0.039281
Rh	-2.842274	0.027720	0.052654
Ag	-5.689982	0.194844	0.284859
Ag	-4.010817	2.572892	0.575700
Ag	-4.013423	0.465799	2.673238
Ag	-4.078994	-2.176638	1.257358
Ag	-4.417730	-1.575933	-1.718860
Ag	-4.154450	1.311926	-2.123495
Ag	-1.327861	-2.688926	-0.047693
Ag	-1.538361	-1.035542	2.335123
Ag	-1.482807	1.826784	1.821179
Ag	-1.553212	2.263943	-1.164577
Ag	-1.668868	-0.335833	-2.568506
Rh	2.836773	0.015214	0.041589
Ag	5.687163	-0.194789	0.280958
Ag	1.533660	-2.277573	-1.062943
Ag	1.471184	-1.694010	1.889255
Ag	1.539992	1.176119	2.287547
Ag	1.310114	2.733768	-0.154717
Ag	1.641169	0.284879	-2.550908
Ag	4.097565	2.248884	1.134677
Ag	4.448383	1.554531	-1.736236
Ag	4.119698	-1.345919	-2.094327
Ag	3.988100	-2.527912	0.654214
Ag	3.999159	-0.346455	2.674585
Ag	-6.776625	-1.372123	2.610093
Ag	-6.819600	-2.620878	-0.338460
Ag	-6.935332	0.081712	-2.428473
Ag	-3.848695	4.363803	-1.808892
Ag	-1.762101	4.667631	0.741574
Ag	1.768342	-4.605633	0.909236
Ag	6.918986	-0.160045	-2.418878
Ag	6.911692	2.590875	-0.424118
Ag	3.849083	-4.388103	-1.691910
Ag	6.775563	1.396327	2.570021
S	-8.016643	0.720349	1.583220

S	-8.934328	-1.242409	-1.255872
S	-7.822888	-3.700547	1.832873
S	-4.435624	-4.682471	1.771329
S	-5.550128	-1.757717	4.828476
S	-5.060799	1.711929	4.658157
S	-7.577560	2.597297	-2.513102
S	-4.435130	3.138013	-4.036115
S	-6.012502	-1.216385	-4.496272
S	-5.588091	-3.914279	-2.305926
S	-5.748141	4.573807	0.034379
S	-3.463813	5.073691	2.648012
S	0.059708	2.693058	3.840583
S	0.812964	4.972918	1.226143
S	-2.035372	6.204420	-1.437035
S	0.212775	3.676692	-2.548645
S	-0.053021	-2.487255	3.942995
S	-0.795622	-4.860290	1.409374
S	-1.731950	-1.155900	-4.958388
S	1.201083	0.784660	-4.965524
S	-0.220063	-3.736408	-2.418007
S	2.050508	-6.211914	-1.221825
S	5.758275	-4.522449	0.147466
S	3.503807	-4.962577	2.791413
S	4.371835	-3.225749	-3.955820
S	7.540413	-2.691116	-2.505355
S	7.998045	-0.732512	1.601843
S	8.973189	1.137728	-1.280864
S	4.491235	4.745949	1.640012
S	7.862652	3.692761	1.761767
S	5.664903	3.834092	-2.416129
S	6.083740	1.088000	-4.552324
S	5.072147	-1.653225	4.628099
S	5.541838	1.804893	4.779035
P	-9.403739	-0.054971	0.322011
P	-6.273273	-4.805956	2.573112
P	-5.658807	0.079608	5.673726
P	-6.481129	3.209924	-4.069515
P	-6.421878	-3.114800	-3.987062

P	-4.984341	5.744304	1.518950
P	0.900375	4.421947	3.188979
P	-0.334917	5.615205	-2.389692
P	-0.878755	-4.249309	3.347550
P	0.182570	-0.868387	-5.514988
P	0.351184	-5.664279	-2.200614
P	5.003712	-5.668552	1.654108
P	6.416299	-3.295021	-4.043439
P	9.410032	-0.004942	0.342071
P	6.316763	4.826728	2.473868
P	6.518711	2.986368	-4.062258
P	5.652595	-0.025144	5.644158
H	-10.383803	-0.749696	1.081145
H	-10.160504	1.033567	-0.178750
H	-6.677101	-6.170513	2.526079
H	-6.234014	-4.582981	3.975336
H	-6.979209	0.281736	6.167021
H	-4.954976	-0.040901	6.904635
H	-6.861695	4.542459	-4.376203
H	-6.853893	2.540885	-5.265172
H	-7.823749	-3.349304	-3.948282
H	-6.043006	-3.955683	-5.067743
H	-4.684898	7.023132	0.980501
H	-6.067117	6.062454	2.382309
H	2.266414	4.444536	3.576285
H	0.334508	5.473249	3.955772
H	-0.379048	6.146734	-3.702503
H	0.723294	6.367557	-1.816547
H	-2.245924	-4.291745	3.726787
H	-0.310046	-5.289731	4.128759
H	0.947785	-2.019811	-5.186041
H	0.225110	-0.922299	-6.933610
H	0.403143	-6.239425	-3.498374
H	-0.706426	-6.405702	-1.612704
H	4.695277	-6.959519	1.139790
H	6.092307	-5.979561	2.509658
H	6.748193	-2.610550	-5.243667
H	6.782642	-4.625082	-4.379765

H	10.165180	-1.118946	-0.107783
H	10.380209	0.699442	1.102225
H	6.750529	6.177062	2.428719
H	6.184929	3.822611	-5.159511
H	7.922555	3.195107	-3.984529
H	4.938901	0.070347	6.871700
H	6.967853	-0.242400	6.142447
H	6.253926	4.603042	3.879042
H	-2.483475	-1.292254	-0.890630
H	2.480709	1.311215	-0.944645

2

Pt	-2.998563	0.120179	0.036290
H	-3.056190	-0.891558	-1.319538
Pt	2.654767	-0.145138	0.181625
Ag	-5.868154	0.342218	0.272754
Ag	-4.200564	-0.343116	2.608030
Ag	-4.305601	-2.330997	0.338381
Ag	-4.745649	-0.470670	-2.309168
Ag	-4.157516	2.303904	-1.469858
Ag	-4.151726	2.398742	1.479268
Ag	-1.530715	-2.295554	-1.042008
Ag	-1.685135	-1.789839	1.936751
Ag	-1.683766	1.103599	2.401019
Ag	-1.537624	2.624783	-0.053769
Ag	-1.734154	0.746429	-2.411001
Ag	-0.166345	0.008244	0.081520
Ag	1.354354	-1.572962	-1.914894
Ag	1.243959	-2.505017	0.952927
Ag	1.243611	-0.102626	2.721899
Ag	1.439575	2.322645	0.899378
Ag	1.460335	1.460107	-1.896296
Ag	3.825305	-2.645710	-0.479134
Ag	3.766469	-1.657993	2.337700
Ag	3.838196	1.324246	2.292610
Ag	4.049214	2.164695	-0.599423
Ag	3.936678	-0.223377	-2.327978
Ag	5.501132	-0.330989	0.328303

Ag	-6.649062	-2.190254	2.283355
Ag	-7.205829	-2.023675	-1.055941
Ag	-3.426105	5.022777	-0.192412
Ag	-1.732605	3.806968	-2.814814
Ag	1.559639	-4.579777	-1.265785
Ag	3.710000	-3.129462	-3.426704
Ag	6.639584	1.090241	-2.005627
Ag	6.517200	2.520924	0.988457
Ag	6.578242	0.123535	3.120250
S	-7.951213	-0.061656	2.868207
S	-8.392653	0.287556	-0.599651
S	-8.026051	-3.821835	0.695509
S	-4.795697	-4.761837	-0.376472
S	-4.738606	-3.570825	3.394084
S	-4.685094	-0.546563	5.141203
S	-6.288861	3.456876	2.558326
S	-3.314734	5.240454	2.353826
S	-5.641199	4.628269	-1.500385
S	-3.837178	3.621227	-4.311144
S	-6.256520	-2.816258	-3.307456
S	-5.957774	0.447261	-4.426647
S	-1.051964	-4.888561	-1.039799
S	-0.336658	-4.108169	2.334561
S	-0.239700	-1.426546	4.530218
S	-0.416565	2.034584	4.416770
S	0.034750	4.476477	1.191404
S	-1.392766	6.117808	-1.548759
S	0.729613	3.203162	-3.672136
S	-1.525633	0.862953	-4.982825
S	-0.255878	-2.256652	-3.853827
S	1.982128	-5.028292	-3.874877
S	3.306864	-5.764069	0.238890
S	5.601885	-4.135885	-1.855704
S	4.931582	-3.616620	3.512105
S	5.204076	-0.547645	5.173793
S	4.073619	3.397191	3.784453
S	7.492445	2.596946	3.422959
S	5.814677	3.130821	-3.406314

S	5.217547	4.518302	-0.226927
S	4.180247	-1.001648	-4.850472
S	7.314808	-1.115382	-3.246694
S	7.847495	-1.275720	1.295274
S	8.677733	1.758995	-0.410019
P	-9.169888	0.042430	1.272798
P	-6.554301	-5.215596	0.485466
P	-4.417641	-2.538304	5.116024
P	-5.276436	5.154907	2.890798
P	-5.111568	4.918333	-3.444959
P	-6.828842	-1.351865	-4.601895
P	-1.199011	-5.305691	0.948129
P	-0.701375	0.321349	5.449657
P	0.240665	5.687626	-0.420694
P	0.174241	1.894617	-5.151360
P	0.274416	-4.098927	-4.486590
P	4.803385	-5.856338	-1.103363
P	5.355081	-2.569775	5.171829
P	5.914483	3.244388	4.554619
P	6.112247	4.588342	-2.063083
P	6.229581	-0.941151	-4.913982
P	9.192497	0.012157	0.488324
H	-10.068879	-1.058199	1.235347
H	-10.071906	1.119570	1.474494
H	-7.108756	-6.309637	-0.229505
H	-6.359307	-5.795592	1.767423
H	-5.193955	-3.113609	6.159912
H	-3.106671	-2.882813	5.542866
H	-5.317008	5.502105	4.269501
H	-5.971848	6.266976	2.338529
H	-4.681713	6.263402	-3.611214
H	-6.312181	4.929216	-4.201995
H	-8.246524	-1.231083	-4.592778
H	-6.638714	-1.876187	-5.910802
H	-2.582530	-5.443767	1.238389
H	-0.699480	-6.620094	1.133002
H	-2.037712	0.239114	5.930746
H	0.043045	0.408456	6.656943

H	0.779838	6.917574	0.035856
H	1.277811	5.216074	-1.268019
H	0.153817	2.640364	-6.359848
H	1.296993	1.051700	-5.371630
H	4.463061	-6.712196	-2.186484
H	5.875240	-6.580188	-0.518479
H	4.549708	-3.009030	6.258005
H	6.640636	-2.955367	5.644100
H	6.287912	4.513349	5.070953
H	5.917680	2.455888	5.736494
H	5.719949	5.821845	-2.647401
H	7.498765	4.823802	-1.857402
H	6.650697	-1.932743	-5.839228
H	6.536835	0.247475	-5.627972
H	9.961434	-0.736015	-0.439925
H	10.167896	0.323730	1.471171
H	-0.784582	-5.014537	-4.248634
H	0.295722	-4.070174	-5.905799

3

Ag	0.169517	5.656046	0.245258
Ag	-0.324210	3.970428	-2.292903
Ag	-2.380053	4.060431	-0.158337
Ag	1.909938	4.080698	2.051863
Ag	2.394318	4.021548	-0.883805
Ag	1.173175	1.469155	-2.020143
Ag	-1.896685	1.493158	-1.513627
Ag	-2.133470	1.503997	1.479205
Ag	-1.046084	4.035063	2.544713
Ag	2.597457	1.507509	0.651702
Ag	0.000000	0.000000	0.241603
Ag	0.556102	1.524399	2.772101
Ag	-1.702387	6.619882	-1.849623
Ag	2.386053	3.762268	-3.837060
Ag	4.234801	1.767572	-1.878404
Ag	-2.581699	6.569406	1.371091
Ag	0.139561	6.859198	3.028257
Pt	0.089336	2.816711	0.250543

Ag	-0.169517	-5.656046	0.245258
Ag	0.324210	-3.970428	-2.292903
Ag	2.380053	-4.060431	-0.158337
Ag	-1.909938	-4.080698	2.051863
Ag	-2.394318	-4.021548	-0.883805
Ag	-1.173175	-1.469155	-2.020143
Ag	1.896685	-1.493158	-1.513627
Ag	2.133470	-1.503997	1.479205
Ag	1.046084	-4.035063	2.544713
Ag	-2.597457	-1.507509	0.651702
Ag	-0.556102	-1.524399	2.772101
Ag	1.702387	-6.619882	-1.849623
Ag	-2.386053	-3.762268	-3.837060
Ag	-4.234801	-1.767572	-1.878404
Ag	2.581699	-6.569406	1.371091
Ag	-0.139561	-6.859198	3.028257
Pt	-0.089336	-2.816711	0.250543
S	-2.827864	4.237875	4.386399
S	-2.299239	7.666752	3.733207
S	-4.699750	5.136107	0.548053
S	-3.906537	5.651691	-2.849127
S	-2.218316	8.689905	-0.230817
S	1.114108	8.091274	0.924461
S	0.316156	7.348893	-3.344548
S	0.056703	4.204250	-4.915454
S	1.188512	5.651152	5.023014
S	3.952872	5.372007	2.883523
S	5.668668	3.577010	-0.691011
S	3.616820	5.751345	-2.537455
S	-1.663167	0.209046	-4.019166
S	-4.291371	-2.112851	-4.552215
S	-4.604351	0.830875	-1.608892
S	-4.320571	0.132027	1.851130
S	1.704913	0.380028	4.756679
S	-1.704913	-0.380028	4.756679
S	2.827864	-4.237875	4.386399
S	2.299239	-7.666752	3.733207
S	4.699750	-5.136107	0.548053

S	3.906537	-5.651691	-2.849127
S	2.218316	-8.689905	-0.230817
S	-1.114108	-8.091274	0.924461
S	-0.316156	-7.348893	-3.344548
S	-0.056703	-4.204250	-4.915454
S	-1.188512	-5.651152	5.023014
S	-3.952872	-5.372007	2.883523
S	-5.668668	-3.577010	-0.691011
S	-3.616820	-5.751345	-2.537455
S	1.663167	-0.209046	-4.019166
S	4.291371	2.112851	-4.552215
S	4.604351	-0.830875	-1.608892
S	4.320571	-0.132027	1.851130
P	-2.637438	6.122188	5.033202
P	-5.123183	5.942550	-1.284646
P	-0.367209	9.331252	0.301863
P	0.000000	6.249432	-4.984635
P	3.179103	5.816226	4.682719
P	5.464735	5.015140	-2.081740
P	-3.384767	-0.334196	-4.931299
P	-5.337032	0.924079	0.277550
P	0.000000	0.000000	5.768749
P	2.637438	-6.122188	5.033202
P	5.123183	-5.942550	-1.284646
P	0.367209	-9.331252	0.301863
P	0.000000	-6.249432	-4.984635
P	-3.179103	-5.816226	4.682719
P	-5.464735	-5.015140	-2.081740
P	3.384767	0.334196	-4.931299
P	5.337032	-0.924079	0.277550
H	-3.806865	6.465112	5.762322
H	3.806865	-6.465112	5.762322
H	-1.644485	6.224068	6.044416
H	1.644485	-6.224068	6.044416
H	-5.384287	7.325096	-1.084217
H	5.384287	-7.325096	-1.084217
H	-6.419526	5.476502	-1.629496
H	6.419526	-5.476502	-1.629496

H	-0.544212	10.348729	1.275490
H	0.544212	-10.348729	1.275490
H	0.157889	10.074523	-0.786467
H	-0.157889	-10.074523	-0.786467
H	-1.244942	6.559547	-5.594382
H	1.244942	-6.559547	-5.594382
H	0.907200	6.673751	-5.991560
H	-0.907200	-6.673751	-5.991560
H	3.624053	7.114826	5.057191
H	-3.624053	-7.114826	5.057191
H	3.799872	5.038252	5.697797
H	-3.799872	-5.038252	5.697797
H	6.256730	6.124766	-1.685707
H	-6.256730	-6.124766	-1.685707
H	6.112916	4.644671	-3.292032
H	-6.112916	-4.644671	-3.292032
H	-4.366549	0.675975	-4.752318
H	4.366549	-0.675975	-4.752318
H	-3.157907	-0.251474	-6.330418
H	3.157907	0.251474	-6.330418
H	-5.612997	2.287696	0.564780
H	5.612997	-2.287696	0.564780
H	-6.630524	0.341911	0.277520
H	6.630524	-0.341911	0.277520
H	-0.270444	1.058362	6.678270
H	0.270444	-1.058362	6.678270