SUPPLEMENTARY INFORMATION

Influence of Wing-tip Substituents and Reaction Conditions on the Structure, Properties and Cytotoxicity of Ag(I) and Au(I)-bis(NHC) complexes

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NMR SPECTRA

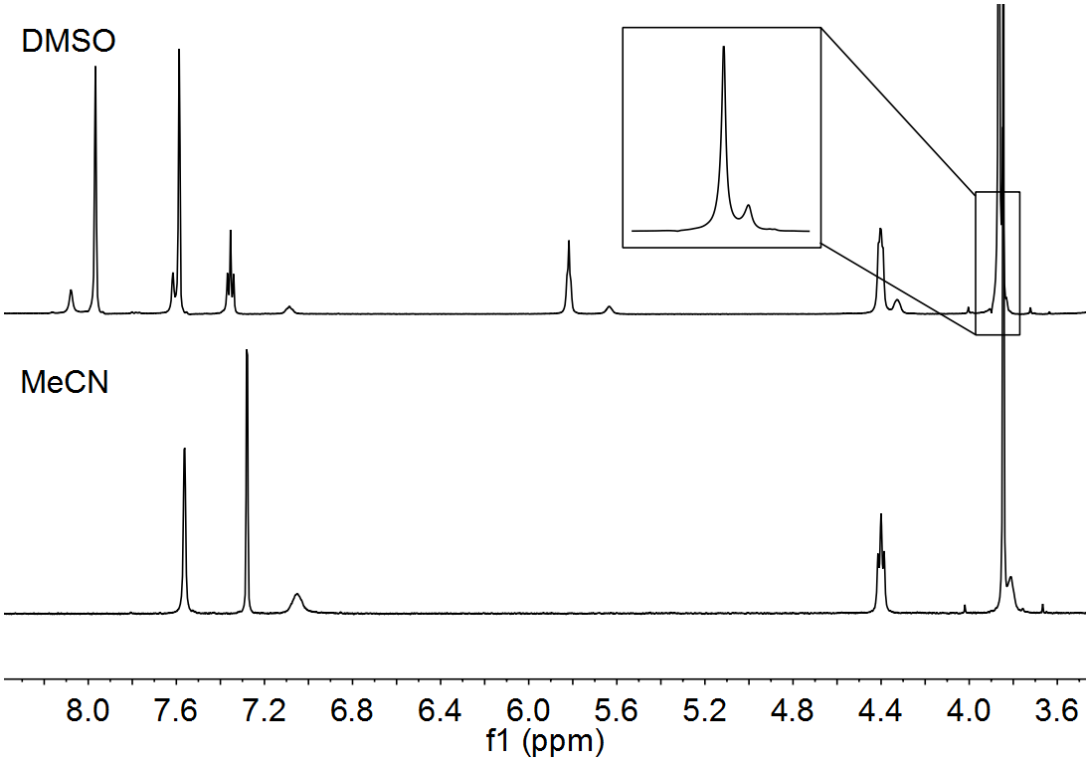


Figure S1. ^{1}H-NMR spectra of $\mathbf{Ag_2(L^{Me})_2(PF_6)_2}$ in acetonitrile-d_3 (bottom) and DMSO-d_6 (top) at room temperature.

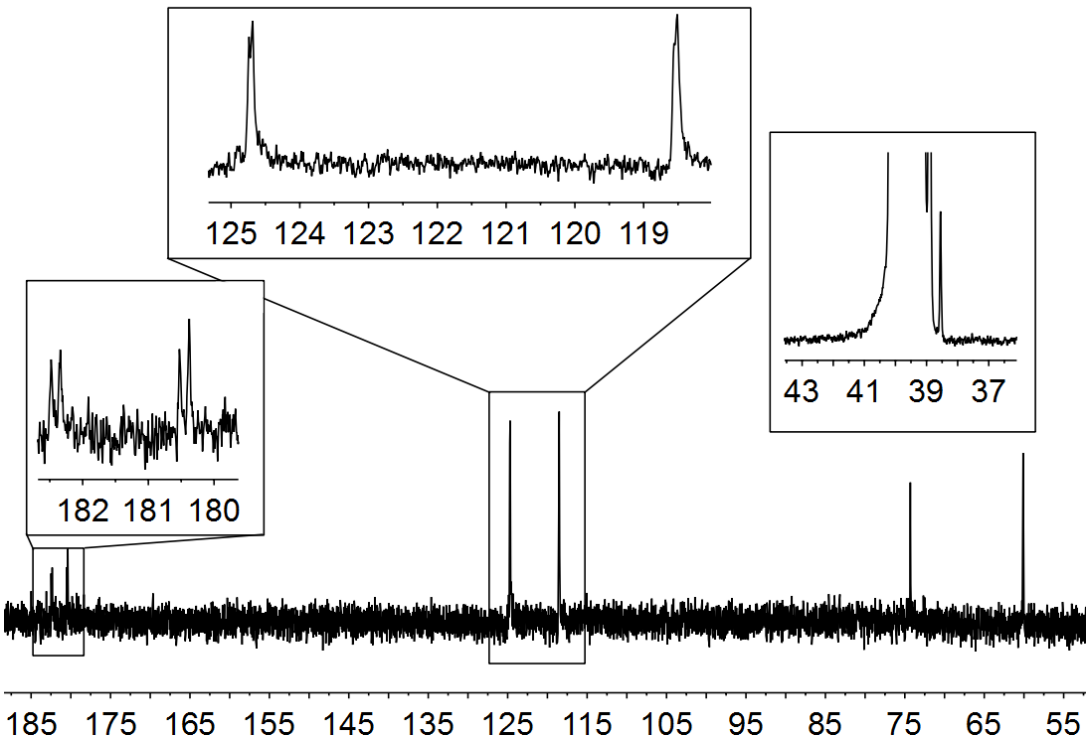


Figure S2. ^{13}C-NMR spectrum of $\mathbf{Ag_2(L^{Me})_2(PF_6)_2}$ in DMSO-d_6 at room temperature.

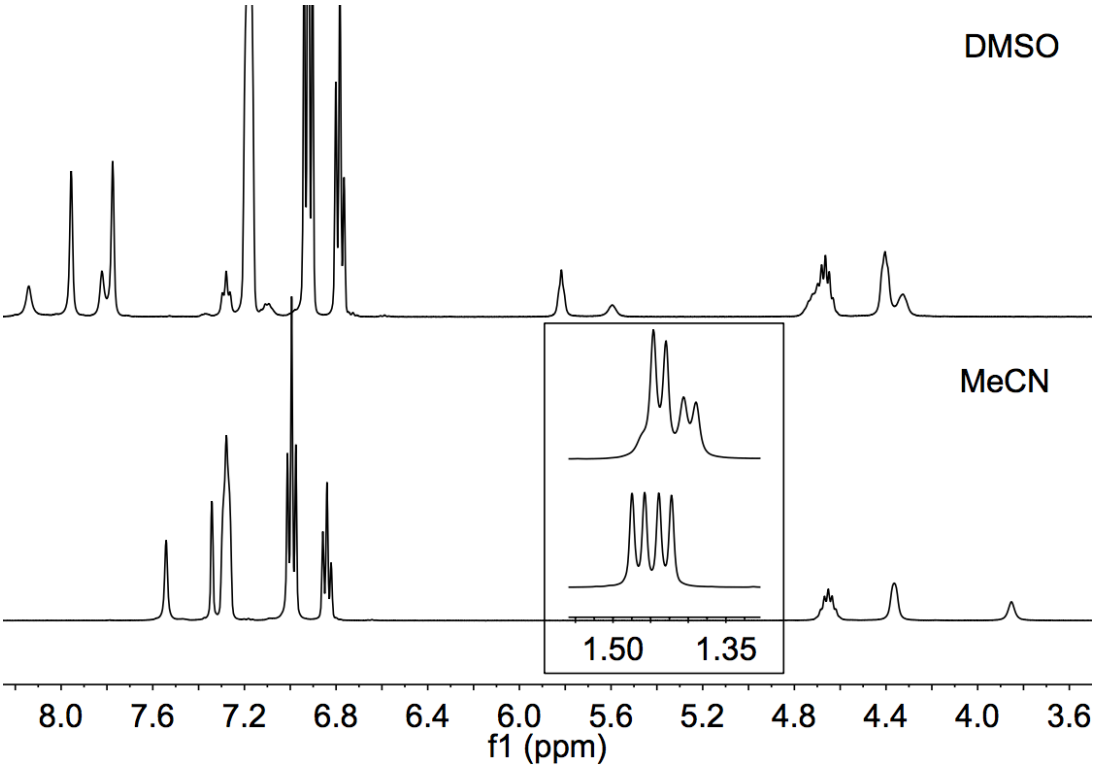


Figure S3. ^{1}H-NMR spectra of **$Ag_2(L^{IPr})_2(BPh_4)_2$** in acetonitrile-*d_3* (bottom) and DMSO-*d_6* (top) at room temperature.

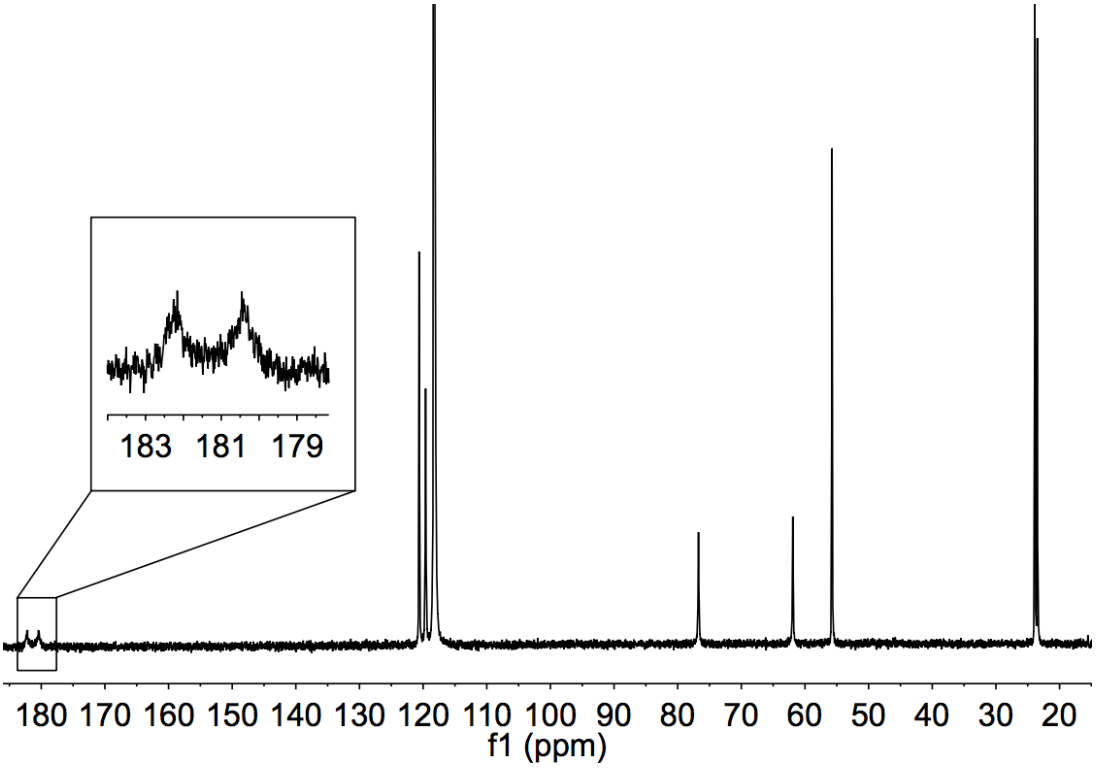


Figure S4. ^{13}C-NMR spectrum of **$Ag_2(L^{IPr})_2(PF_6)_2$** in acetonitrile-*d_3* at room temperature.

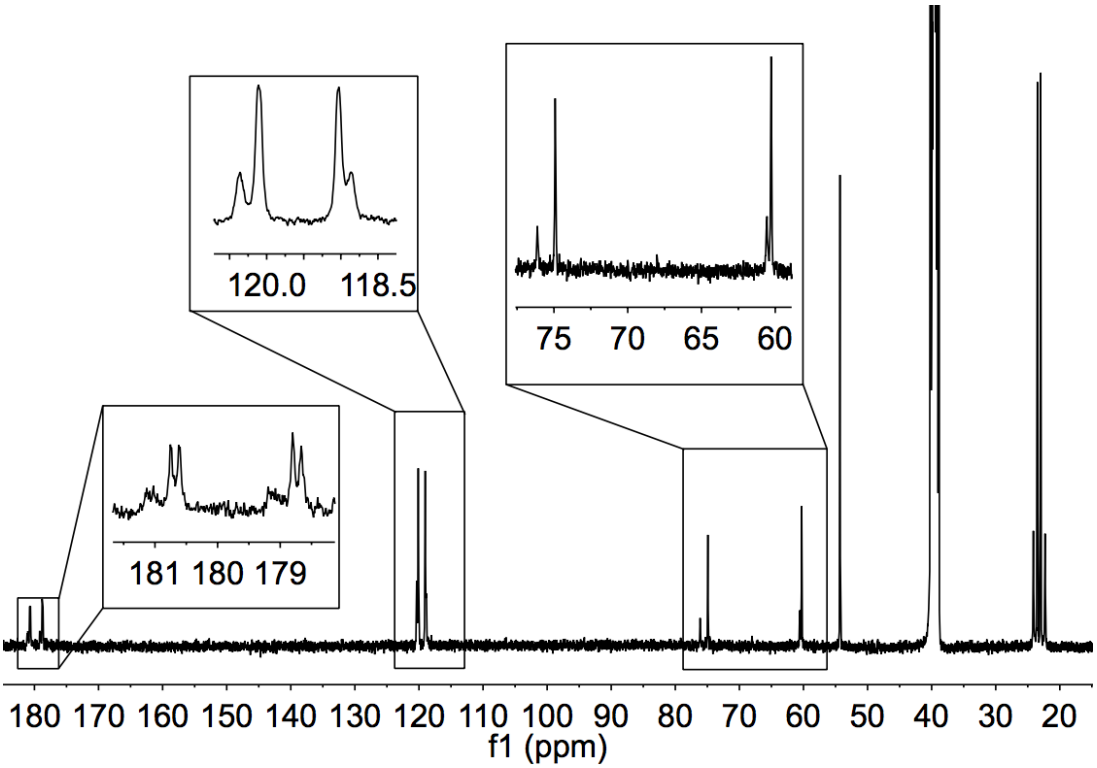


Figure S5. ^{13}C-NMR spectrum of **$Ag_2(L^{IPr})_2(PF_6)_2$** in DMSO-d_6 at room temperature.

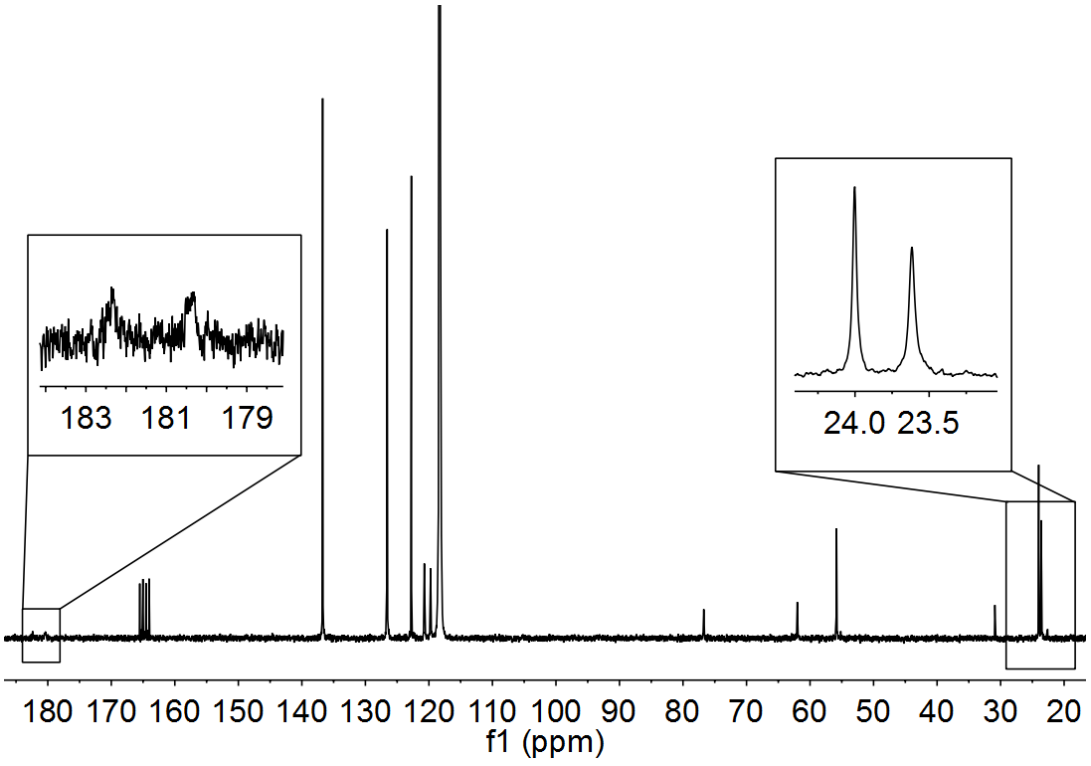


Figure S6. ^{13}C-NMR spectrum of **$Ag_2(L^{IPr})_2(BPh_4)_2$** in MECN-d_3 at room temperature.

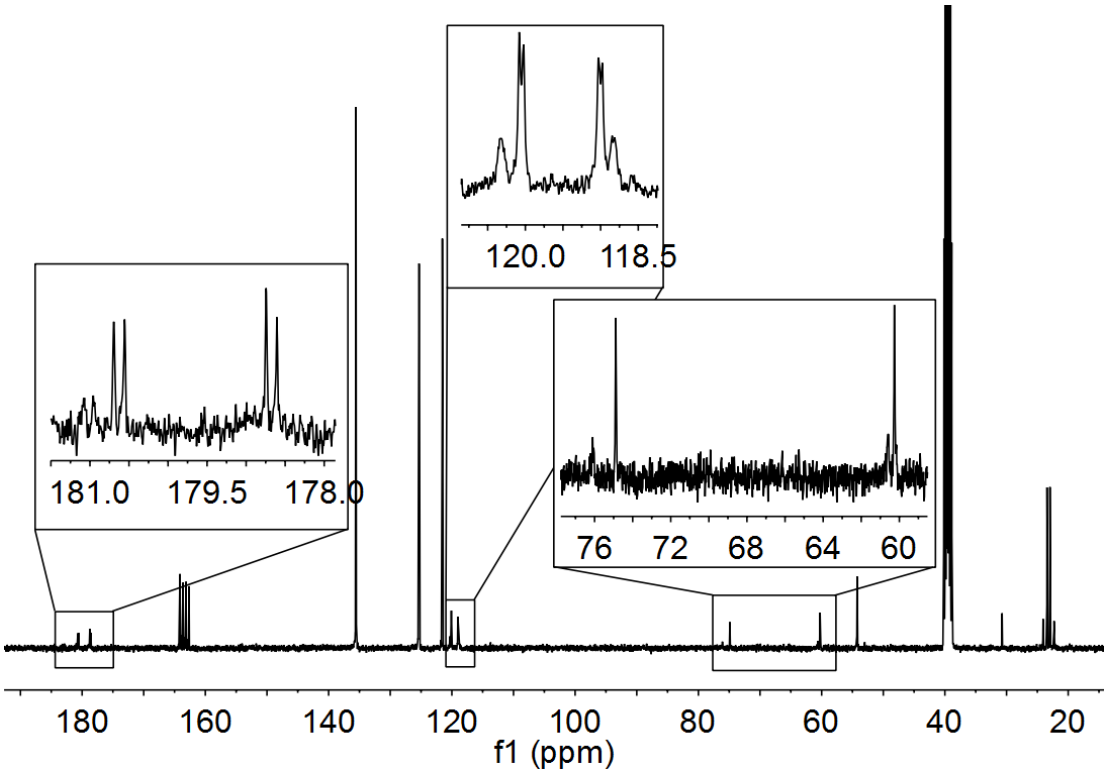


Figure S7. ^{13}C-NMR spectrum of $\mathbf{Ag_2(L^{iPr})_2(BPh_4)_2}$ in DMSO-d_6 at room temperature.

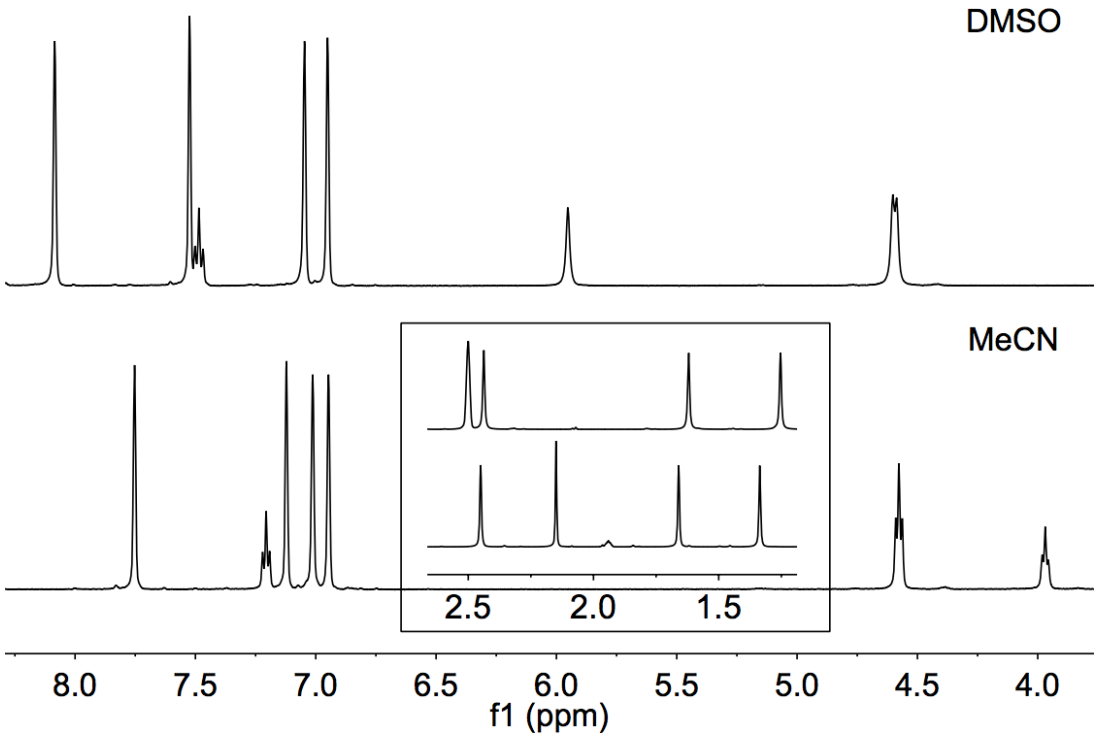


Figure S8. ^{1}H-NMR spectra of $\mathbf{Ag_2(L^{Mes})_2(PF_6)_2}$ in acetonitrile-d_3 (bottom) and DMSO-d_6 (top) at room temperature.

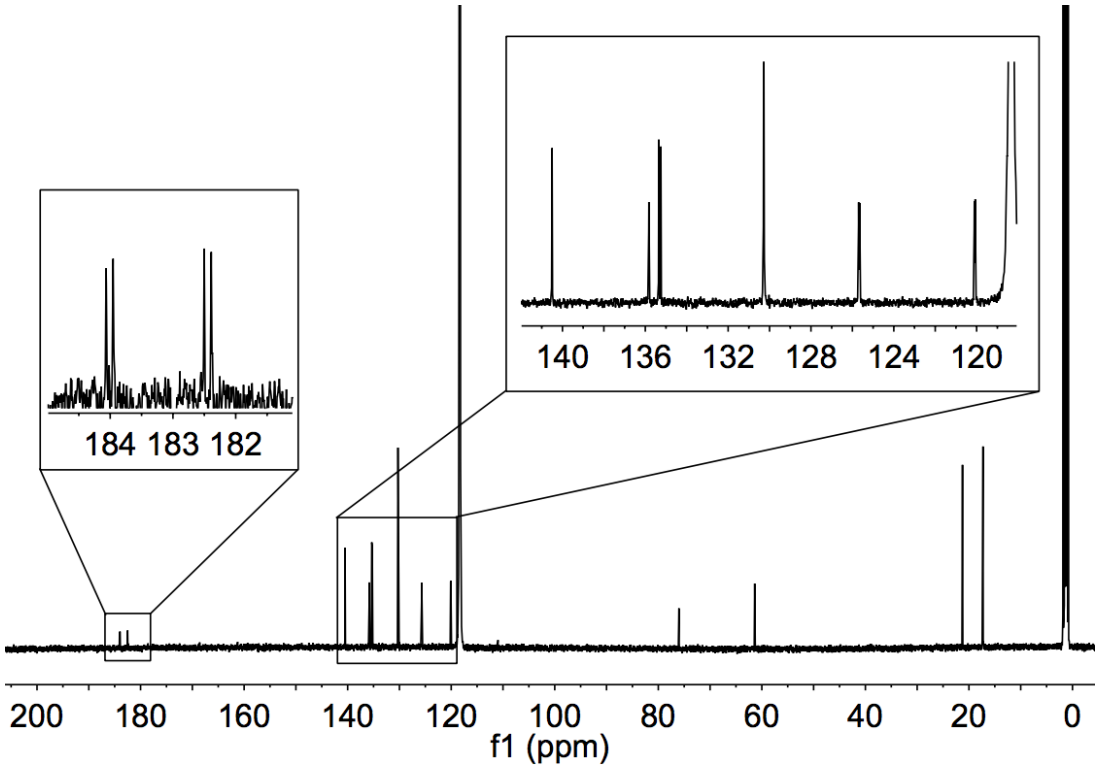
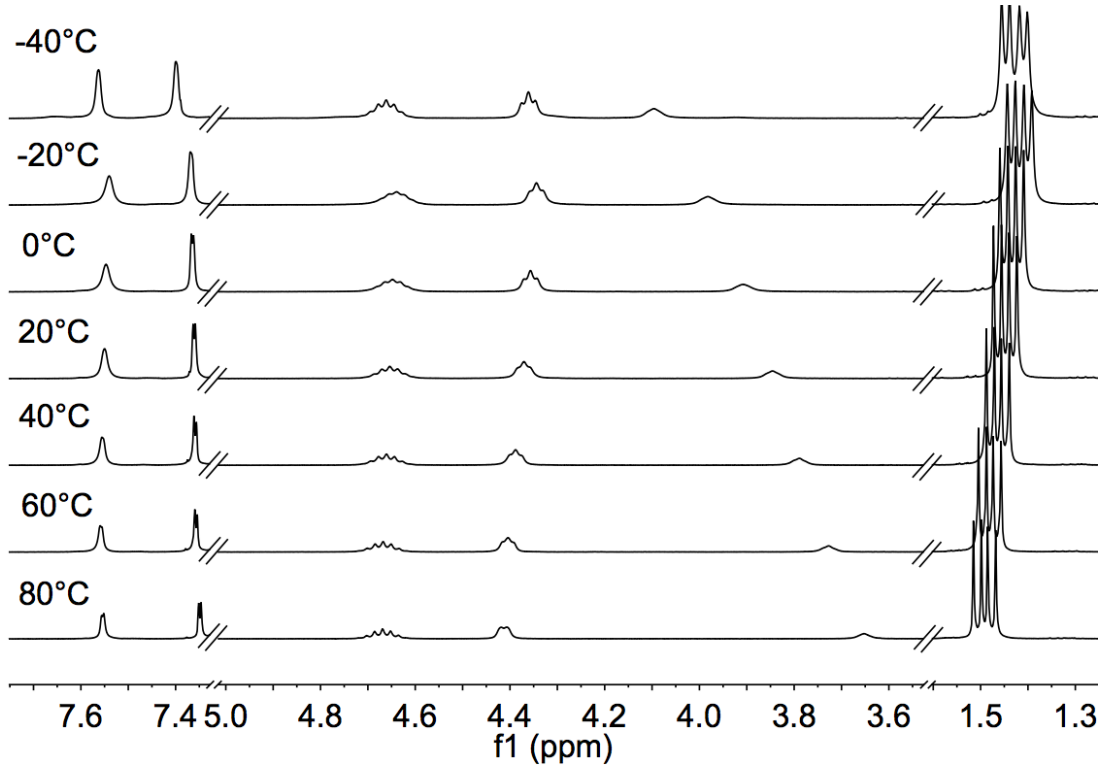


Figure S9. ^{13}C-NMR spectrum of **$Ag_2(L^{Mes})_2(PF_6)_2$** in MeCN-d_3 at room temperature.



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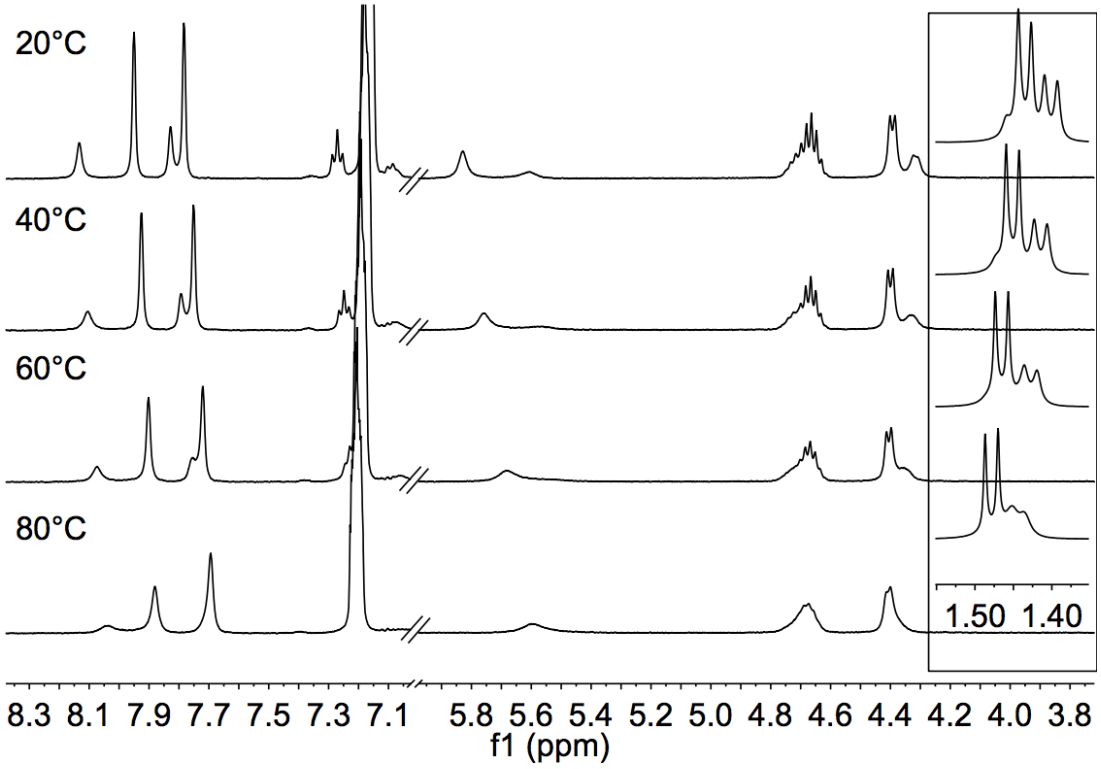

Figure S11. ^{1}H-VT-NMR spectra of **$Ag_2(L^{iPr})_2(BPh_4)_2$** in DMSO-d_6. The resonances for BPh_4 and solvent have been cut out for clarity.

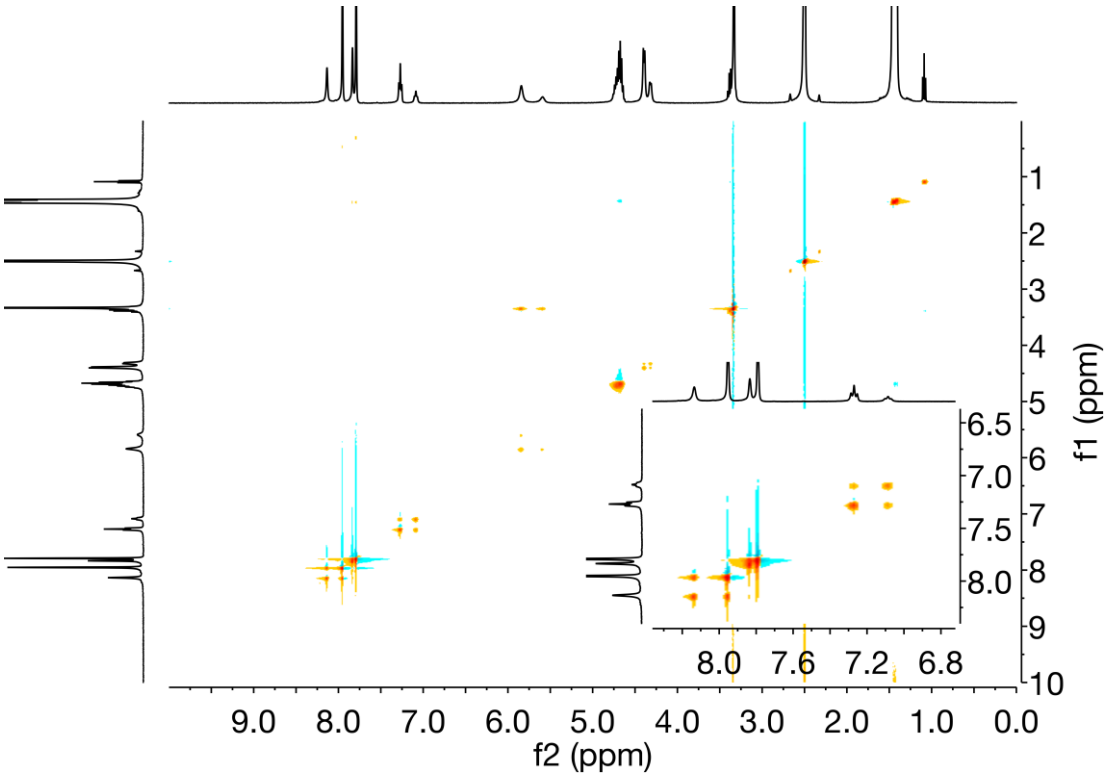

Figure S12. H,H-NOESY-NMR spectrum of **$Ag_2(L^{iPr})_2(PF_6)_2$** in DMSO-d_6 at RT.

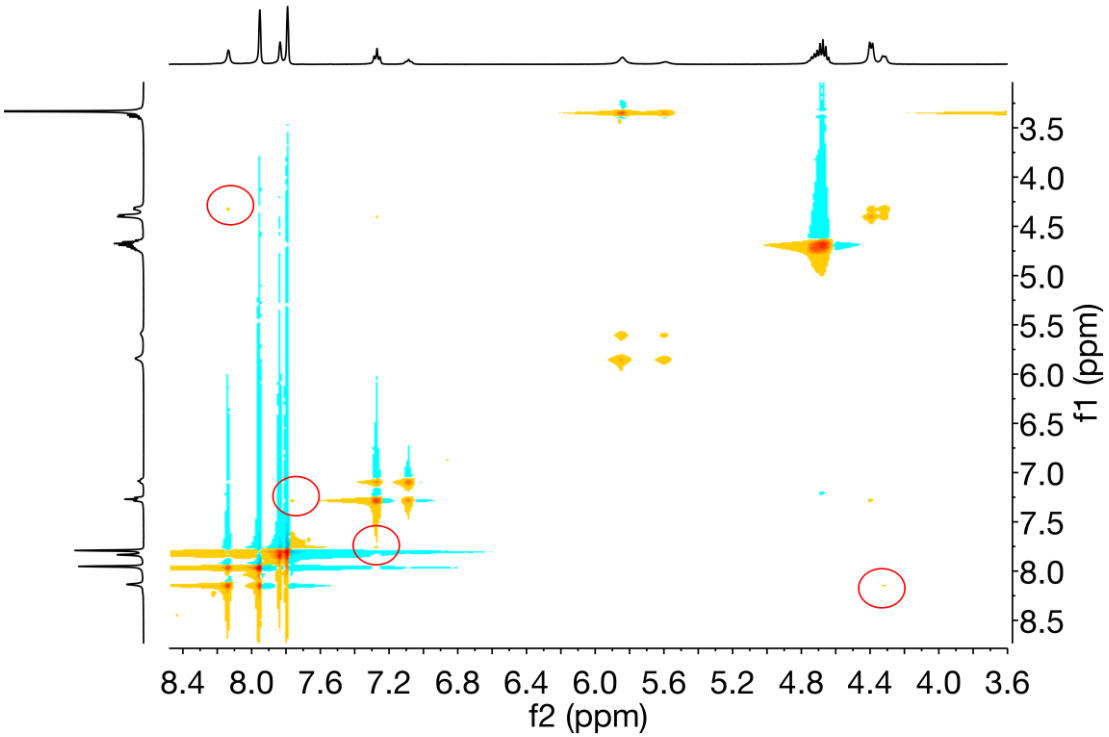

Figure S13. H,H-NOESY-NMR spectrum of $Ag_2(L^{IPr})_2(PF_6)_2$ in DMSO-d_6 at RT (Enlargement).

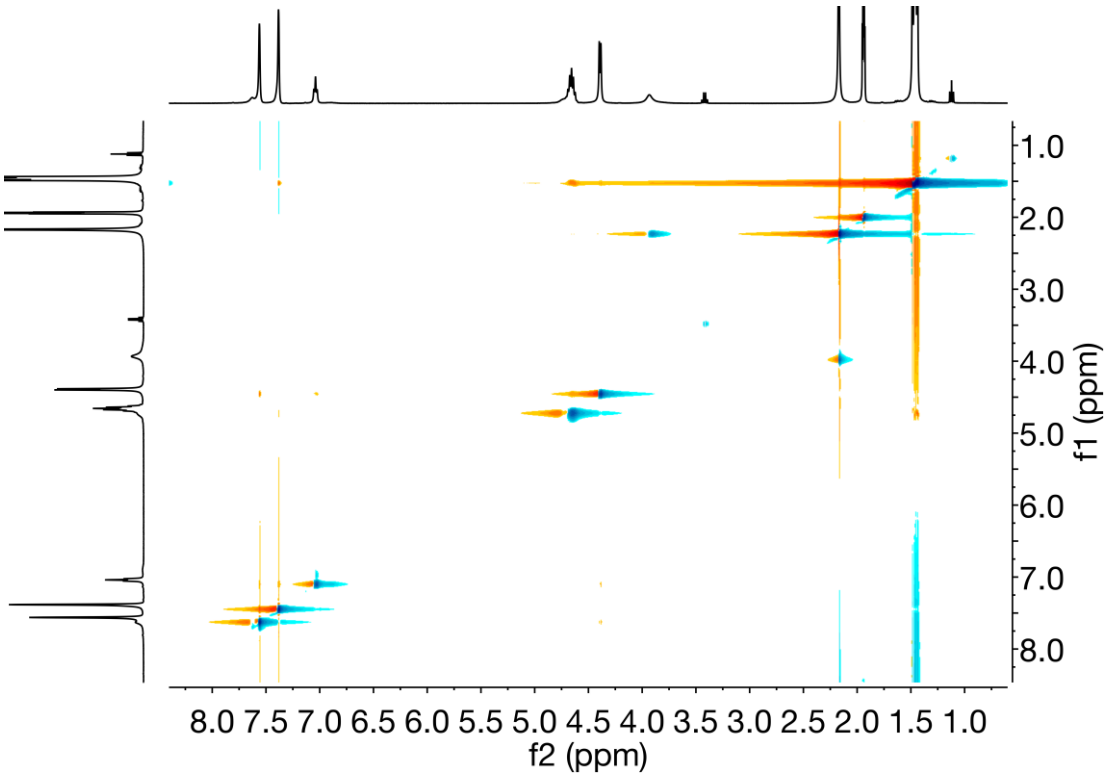

Figure S14. H,H-NOESY-NMR spectrum of $Ag_2(L^{IPr})_2(PF_6)_2$ in MeCN-d_3 at RT.

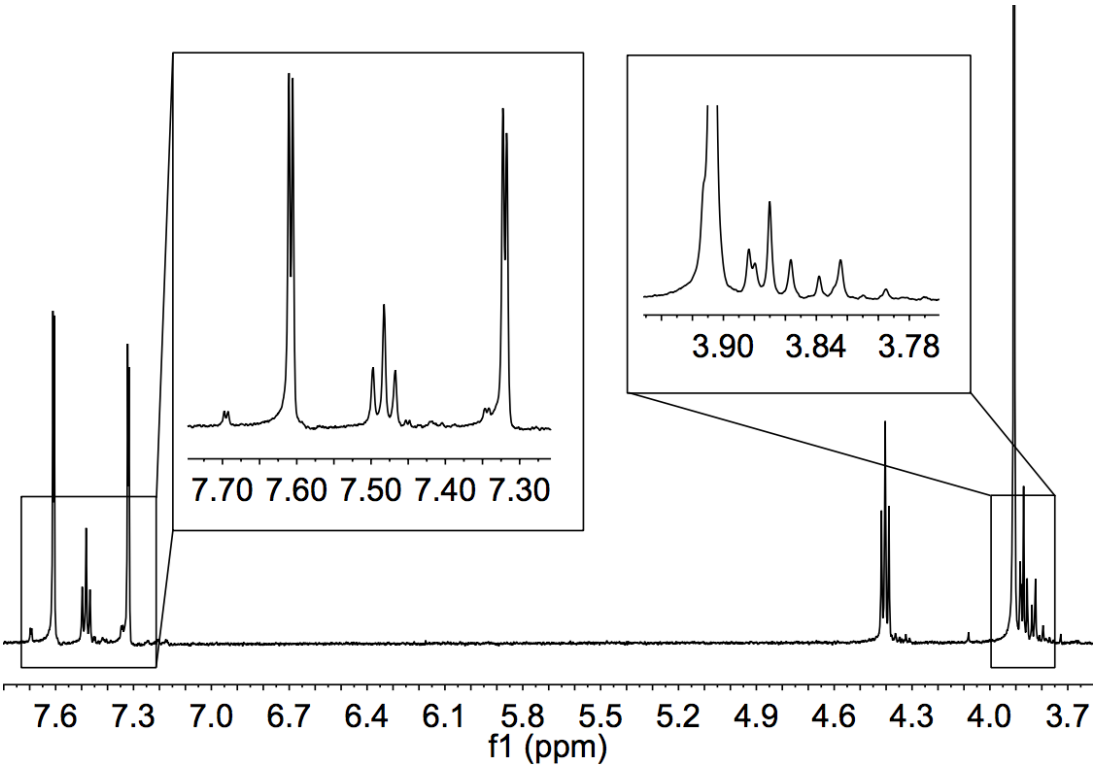

Figure S15. ^{1}H-NMR spectrum of **$Au_2(L^{Me})_2(PF_6)_2$** in MeCN-*d_3* at room temperature.

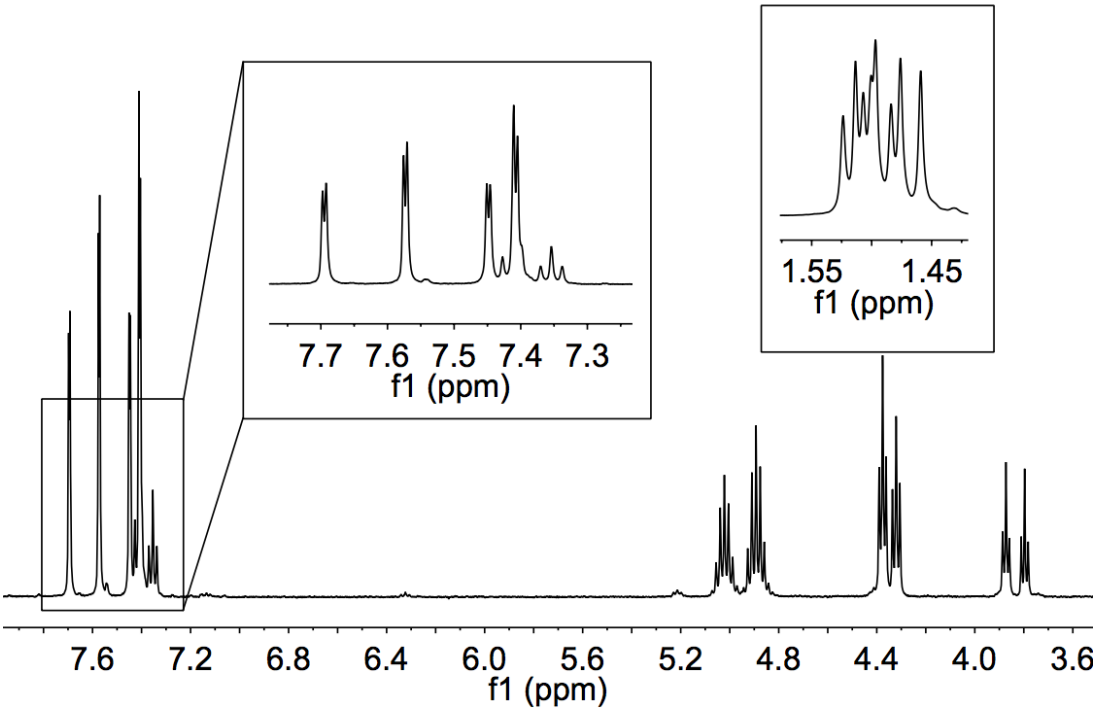

Figure S16. ^{1}H-NMR spectrum of **$Au_2(L^{IPr})_2(PF_6)_2$** in MeCN-*d_3* at room temperature.

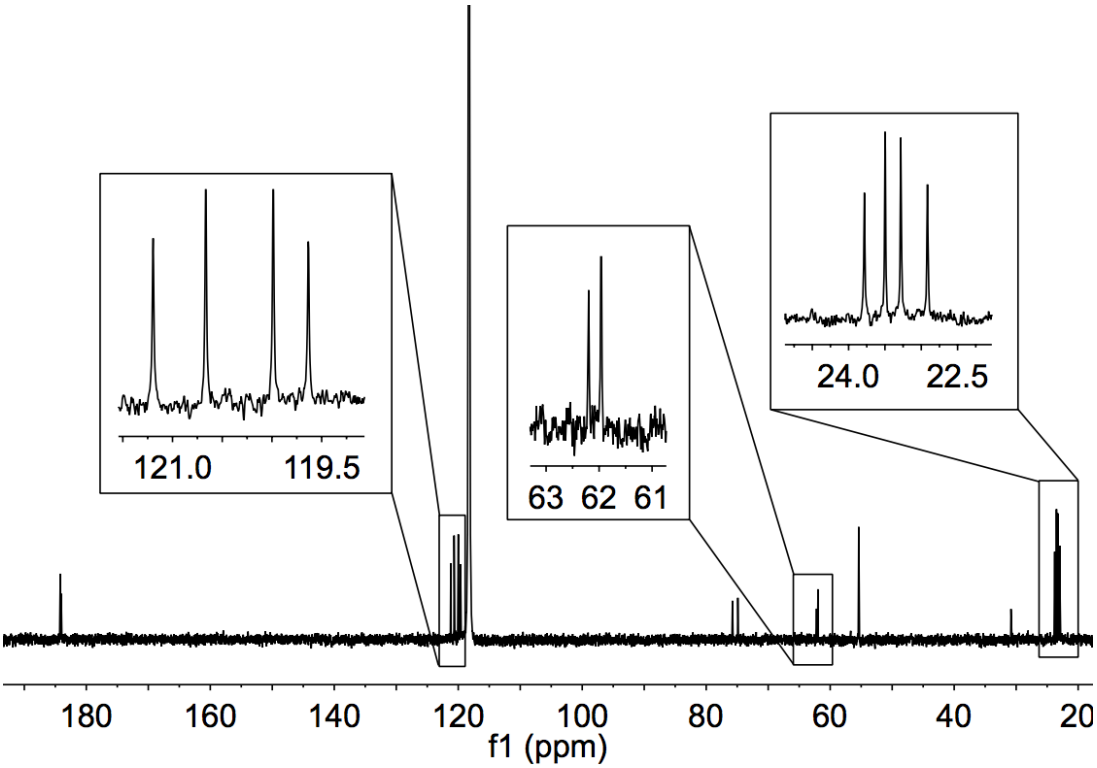

Figure S17. ^{13}C-NMR spectrum of **$Au_2(L^{IPr})_2(PF_6)_2$** in MeCN-d_3 at room temperature.

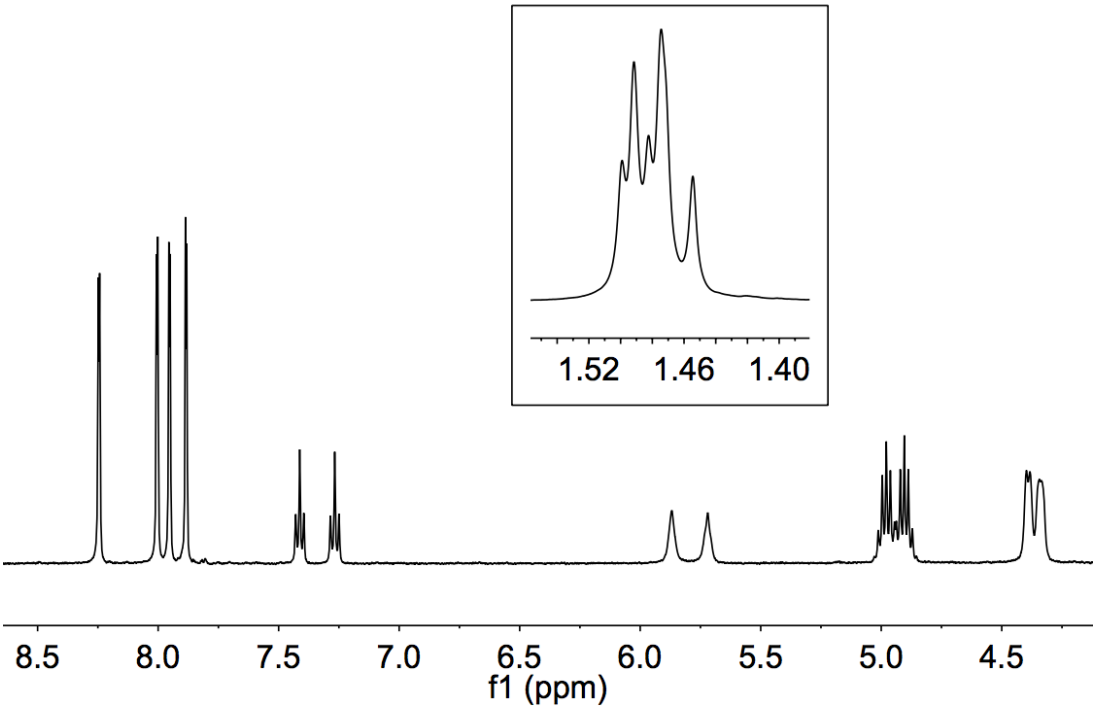

Figure S18. ^{1}H-NMR spectrum of **$Au_2(L^{IPr})_2(PF_6)_2$** in DMSO-d_6 at room temperature.

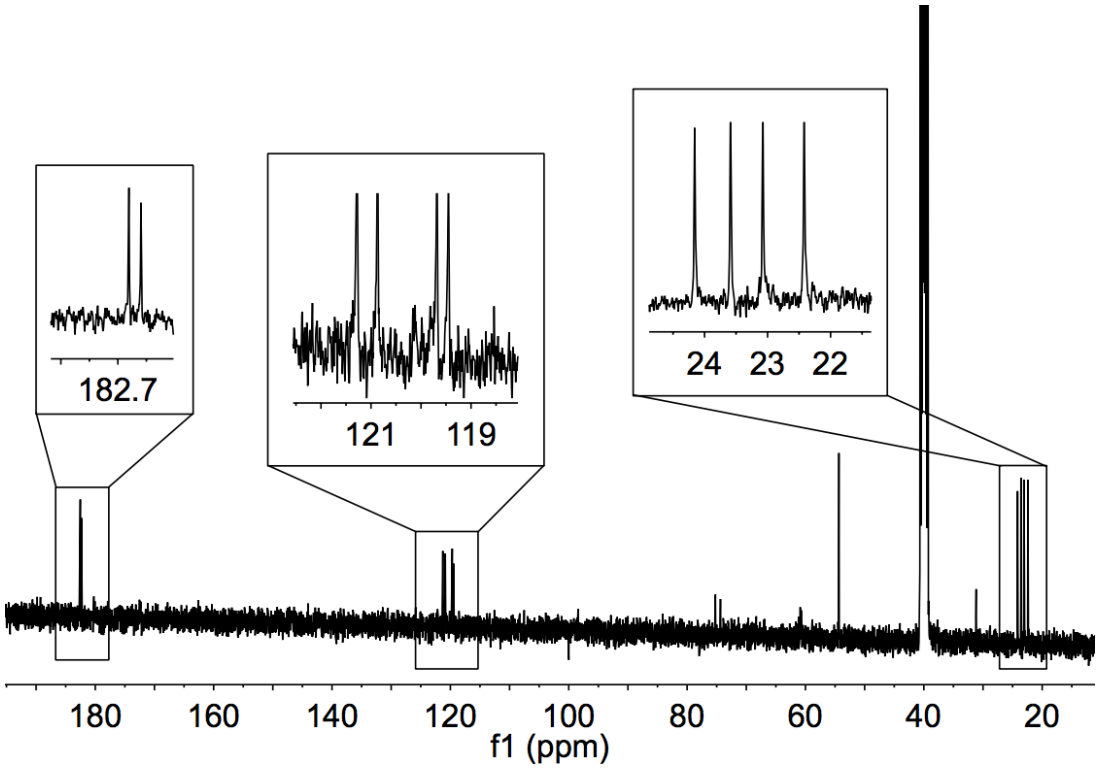

Figure S19. ^{13}C-NMR spectrum of **$Au_2(L^{IPr})_2(PF_6)_2$** in DMSO-d_6 at room temperature.

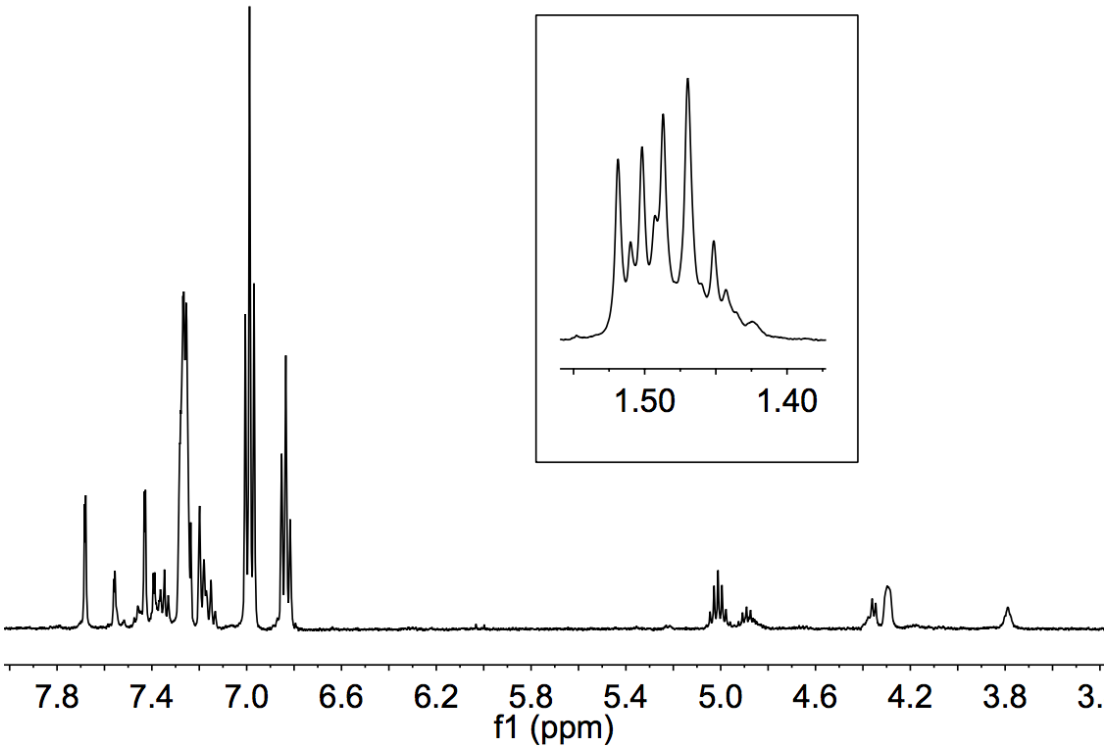

Figure S20. ^{1}H-NMR spectrum of **$Au_2(L^{IPr})_2(BPh_4)_2$** in MeCN-d_3 at room temperature.

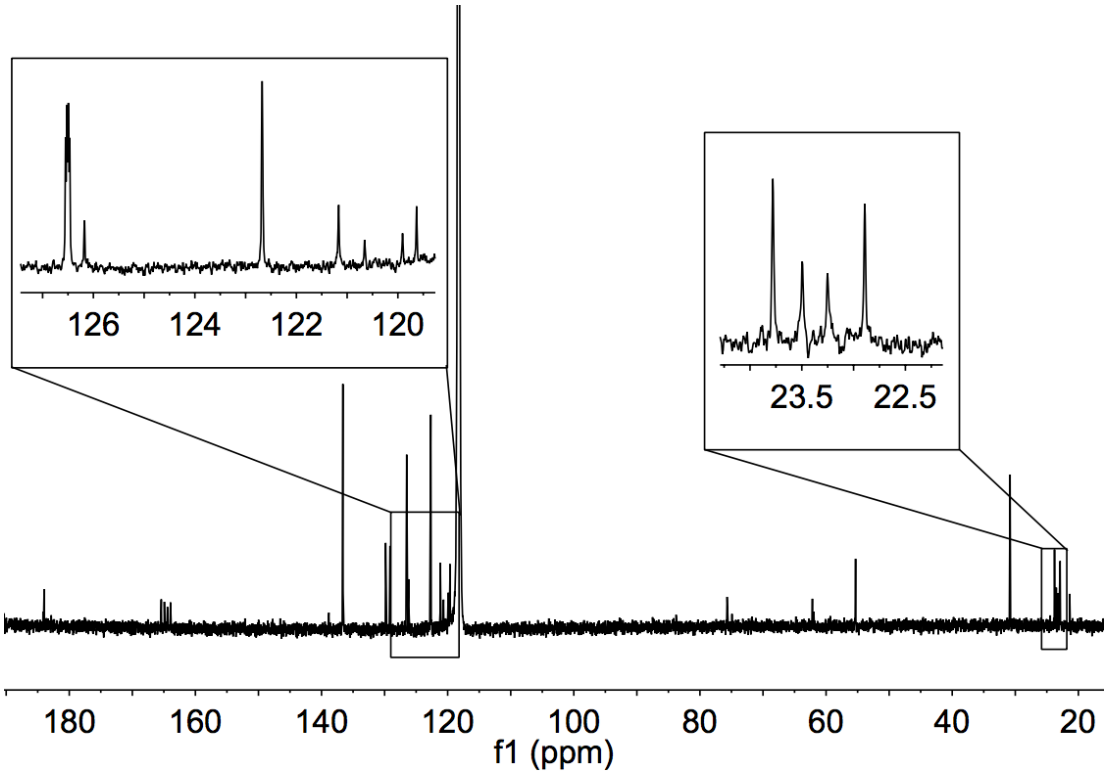

Figure S21. ^{13}C-NMR spectrum of $\mathbf{Au_2(L^{IPr})_2(BPh_4)_2}$ in MeCN-d_3 at room temperature.

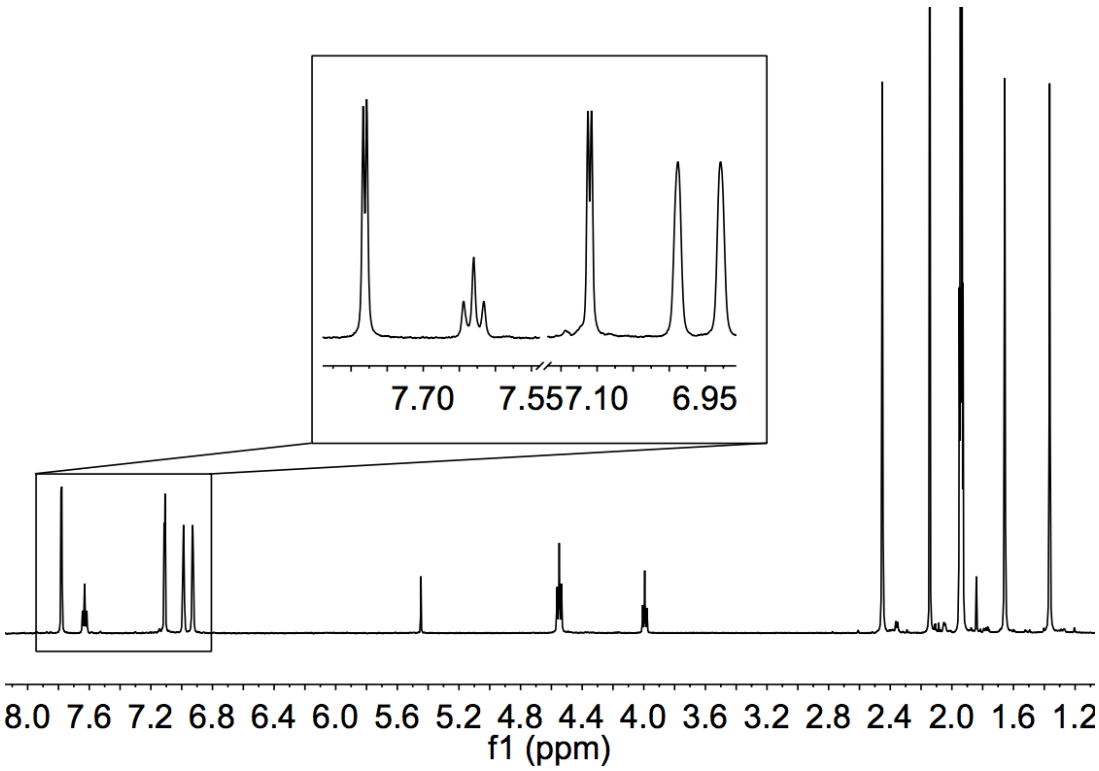

Figure S22. ^{1}H-NMR spectrum of $\mathbf{Au_2(L^{Mes})_2(PF_6)_2}$ in acetonitrile-d_3 at room temperature.

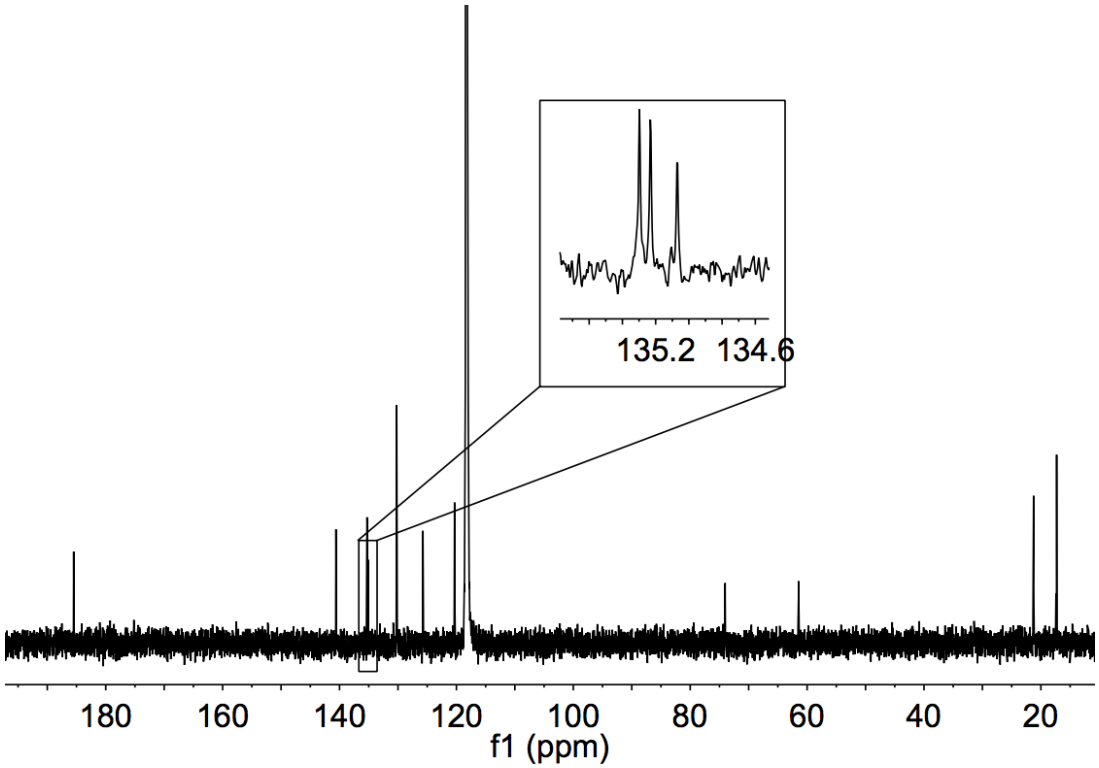

Figure S23. ^{13}C-NMR spectrum of **$Au_2(L^{Mes})_2(PF_6)_2$** in MeCN-d_3 at room temperature.

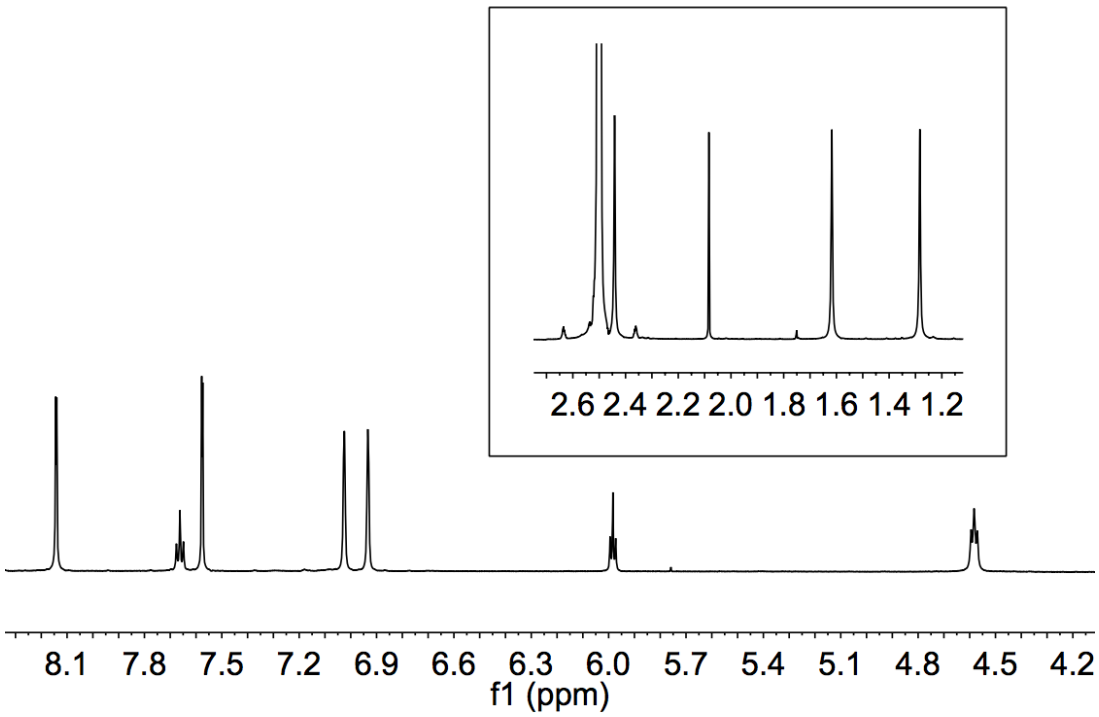

Figure S24. ^{1}H-NMR spectrum of **$Au_2(L^{Mes})_2(PF_6)_2$** in DMSO-d_6 at room temperature.

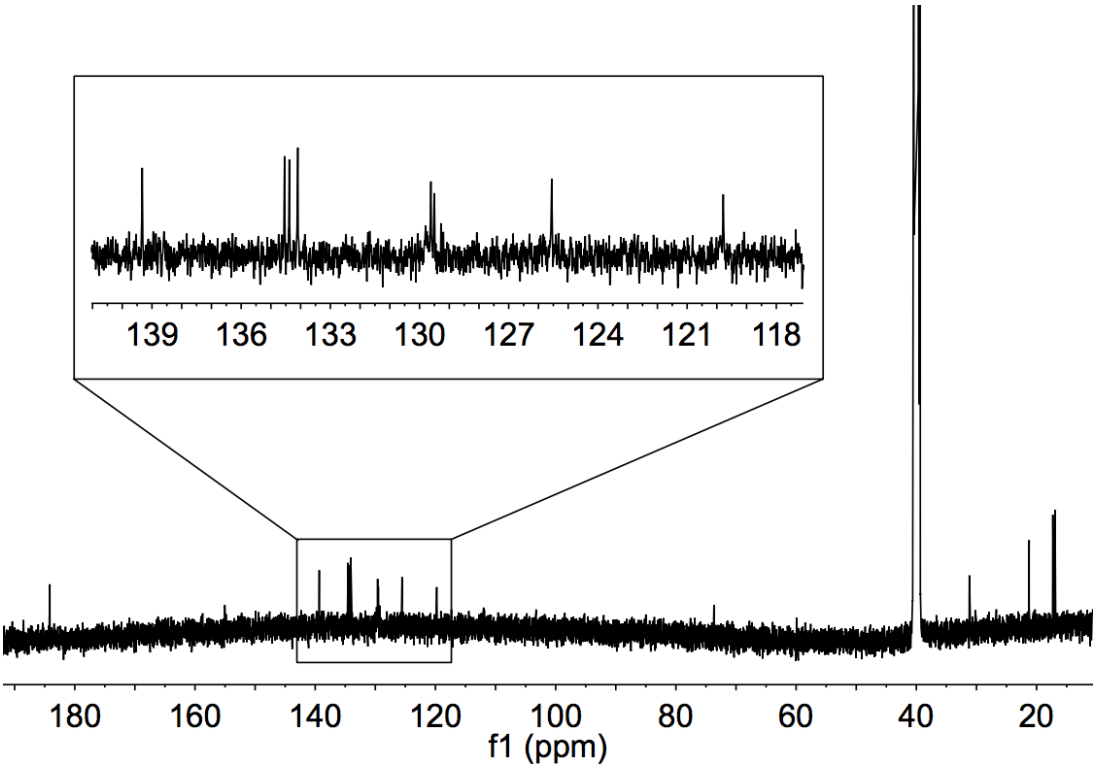

Figure S25. ^{13}C-NMR spectrum of $\mathbf{Au_2(L^{Mes})_2(PF_6)_2}$ in DMSO-d_6 at room temperature.

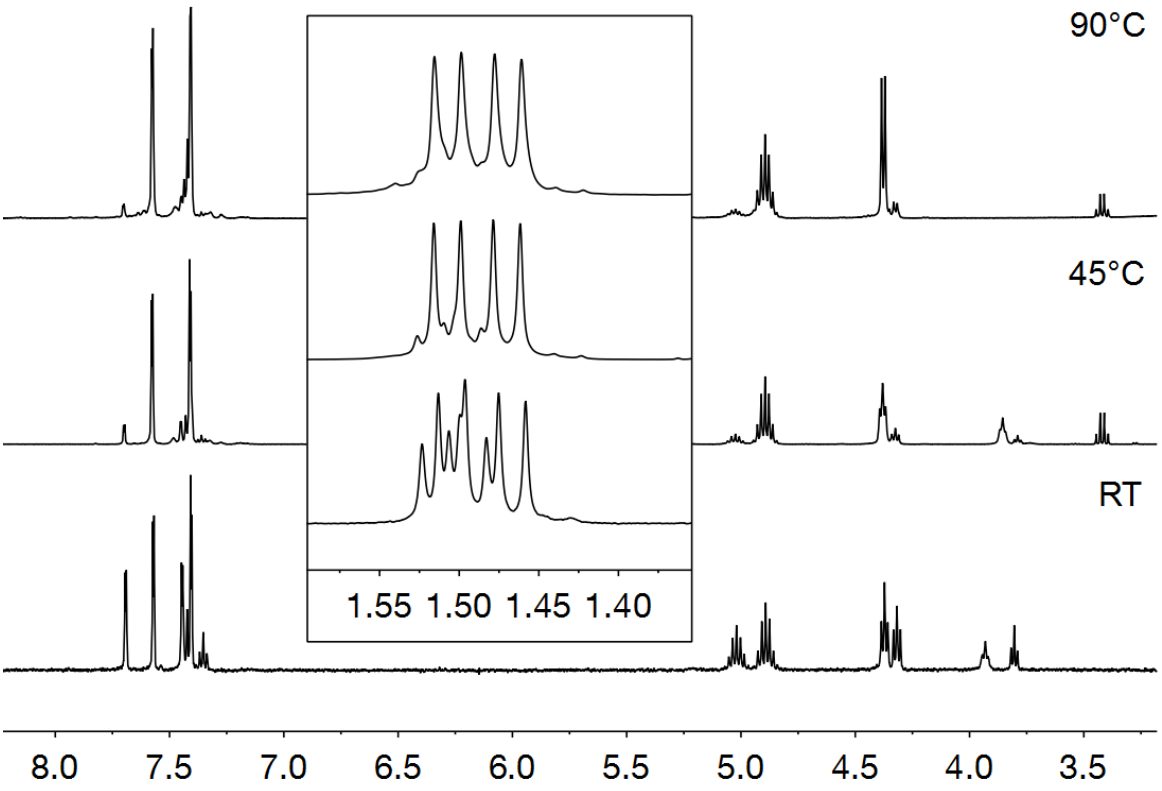

Figure S26. Formation of anti/syn isomers of $\mathbf{Au_2(L^{IPr})_2(PF_6)_2}$ in MeCN-d_3 at different temperatures.

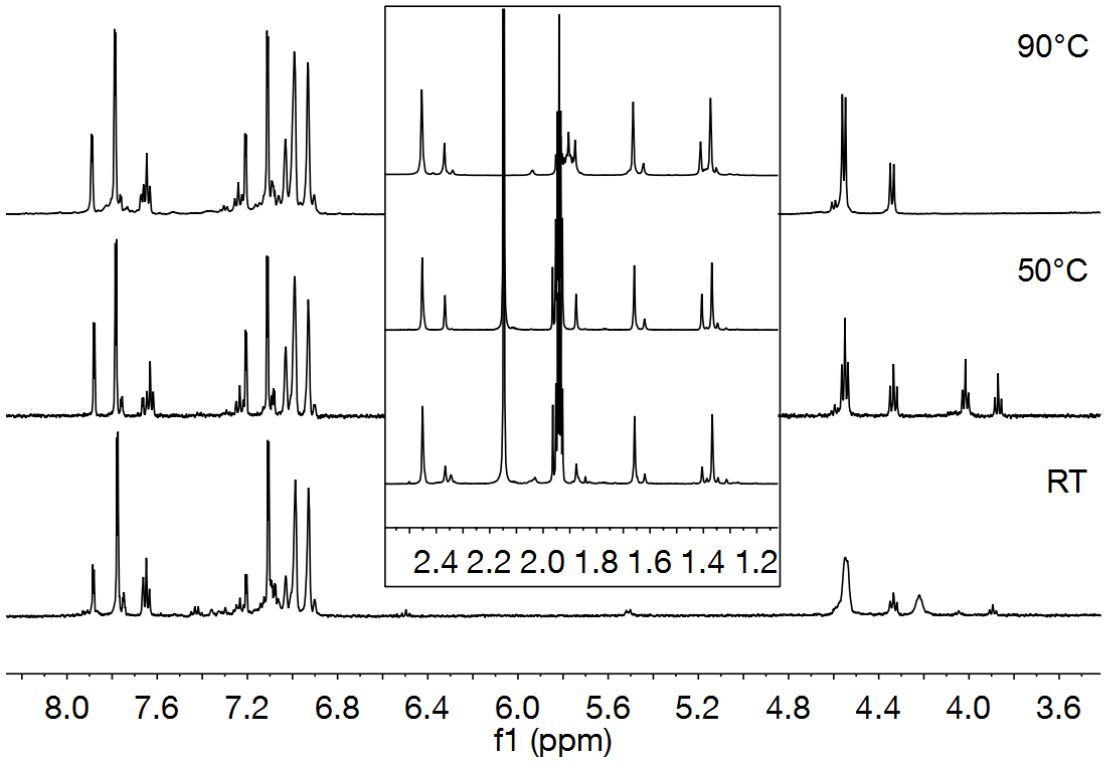

Figure S27. Formation of anti/syn isomers of $\mathbf{Au_2(L^{Mes})_2(PF_6)_2}$ in MeCN-d_3 at different temperatures.

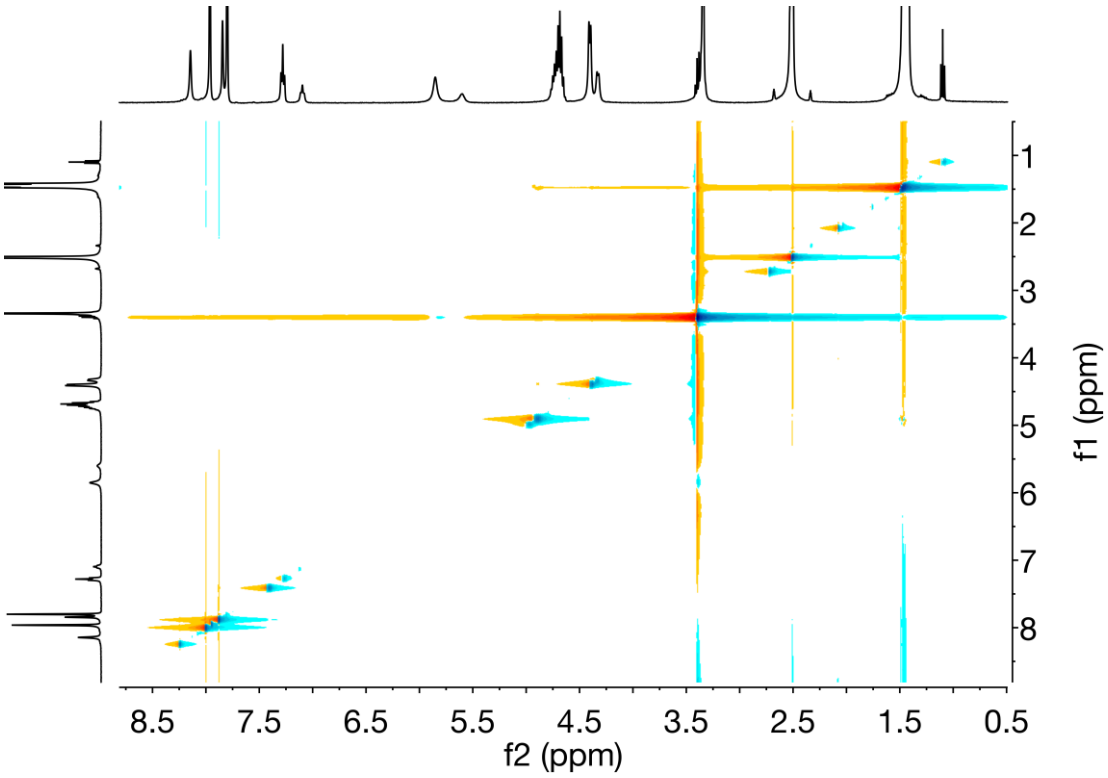

Figure S28. H,H-NOESY NMR spectrum of $\mathbf{Au_2(L^{IPr})_2(PF_6)_2}$ in DMSO-d_6 at RT.

UV-VIS SPECTRA

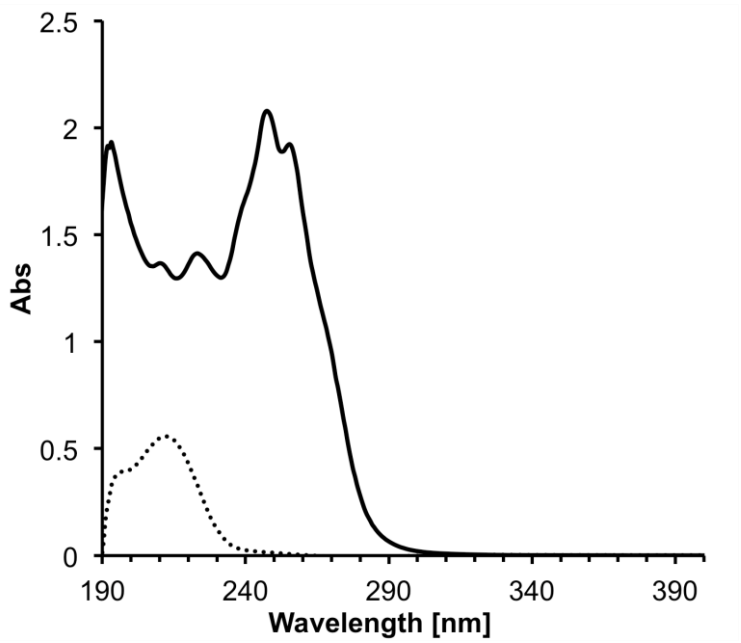

Figure S29. UV-VIS spectra of $\mathbf{Au_2(L^{Me})_2(PF_6)_2}$ (solid line) and $\mathbf{H_2L^{Me}(PF_6)_2}$ (dashed line) in acetonitrile ($6.5x10^{-5}$ mol/L).

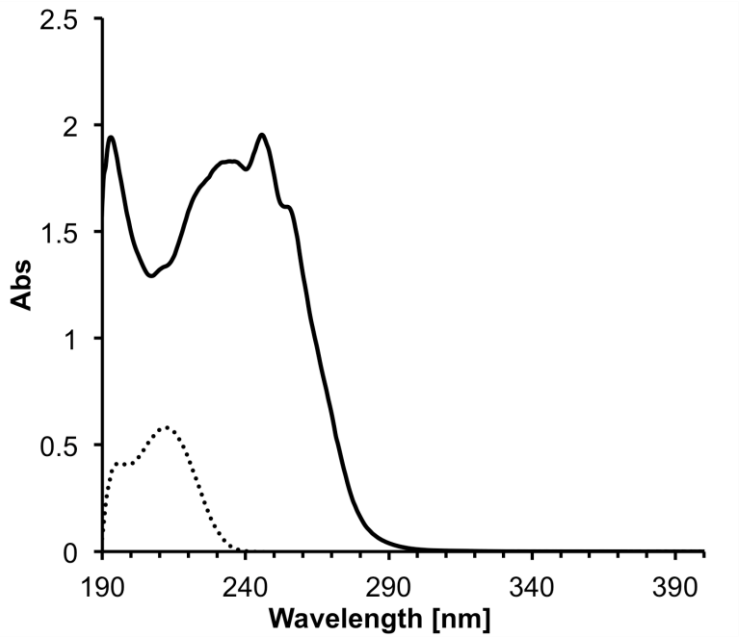

Figure S30. UV-VIS spectra of $\mathbf{Au_2(L^{IPr})_2(PF_6)_2}$ (solid line) and $\mathbf{H_2L^{IPr}(PF_6)_2}$ (dashed line) in acetonitrile ($6.5x10^{-5}$ mol/L).

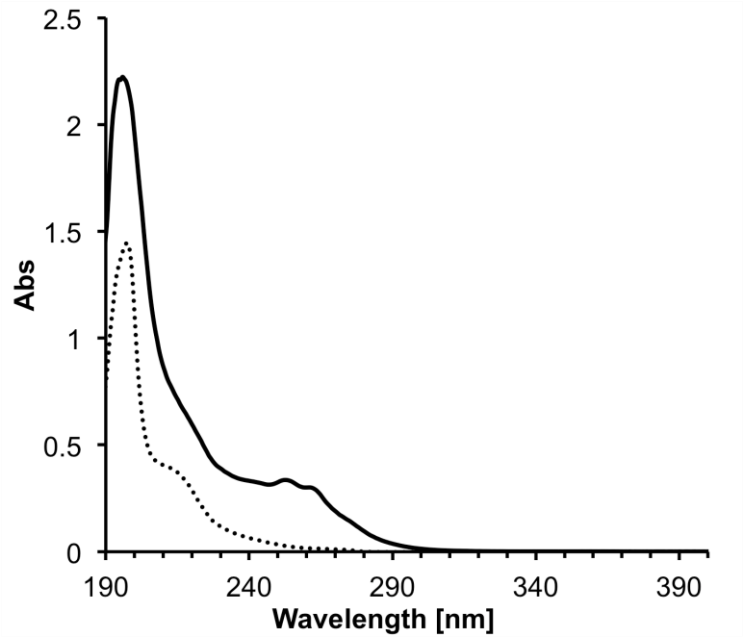

Figure S31. UV-VIS spectra of $\mathbf{Au_2(L^{Mes})_2(PF_6)_2}$ (solid line) and $\mathbf{H_2L^{Mes}(PF_6)_2}$ (dashed line) in acetonitrile ($1.3x10^{-5}$ mol/L).

ADDITIONAL CRYSTALLOGRAPHIC INFORMATION

$H_2L^{IPr}(BPh_4)_2$

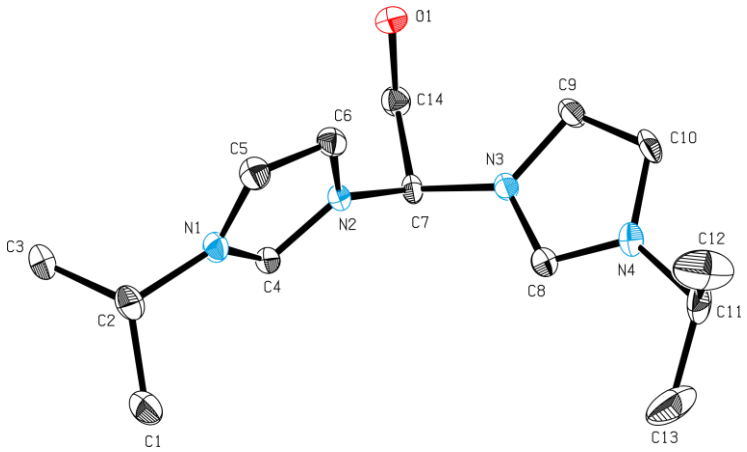

Figure S32. ORTEP style representation of the cation of $\mathbf{H_2L^{IPr}(BPh_4)_2}$ with ellipsoids at 50% probability. Hydrogen atoms, BPh_4^- and co-crystallized acetone molecules are omitted for clarity. Selected bond lengths [Å] and bond angles [deg]: C4–N1 1.330(2), C4–N2 1.334(2), C8–N3 1.339(2), C8–N4 1.321(2), C5–C6 1.344(3), C9–C10 1.350(3), C7–N2 1.467(2), N3-C7 1.473(2); N1–C4–N2 108.35(15), N3–C8–N4 108.71(14), N2–C7–N3 107.76(14).

$Ag_2(L^{IPr})_2(BPh_4)_2$

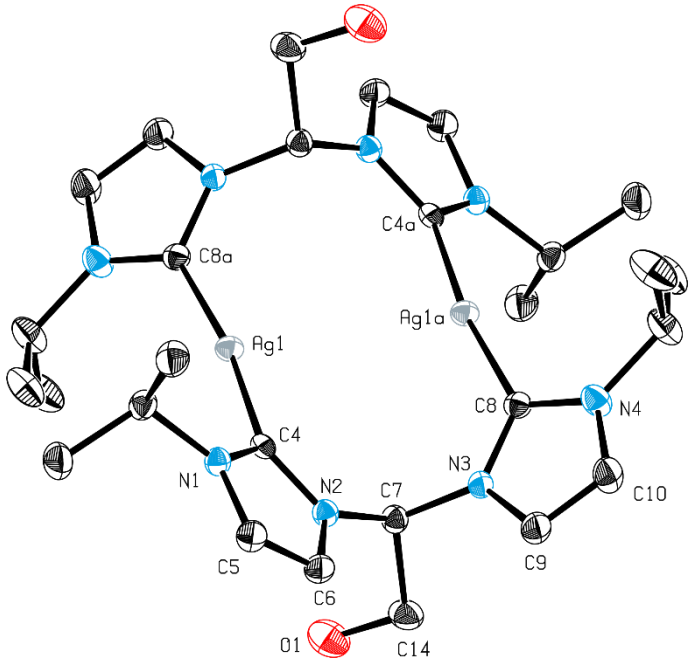

Figure S33. ORTEP style representation of the cation of **$Ag_2(L^{IPr})_2(BPh_4)_2$** with ellipsoids at 50% probability. Hydrogen atoms and BPh_4^- are omitted for clarity.

$Ag_2(L^{IPr})_2(BPh_4)_2$·DMSO

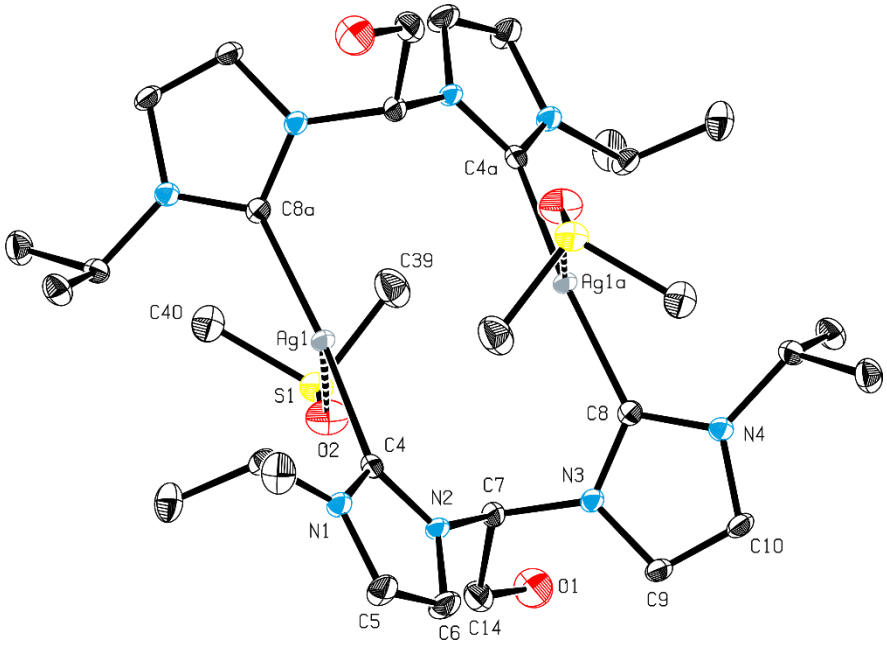

Figure S34. ORTEP style representation of the cation of **$Ag_2(L^{IPr})_2(BPh_4)_2$·DMSO** with ellipsoids at 50% probability. Hydrogen atoms, BPh_4^- and co-crystallized DMSO molecules are omitted for clarity.

$Au_2(L^{IPr})_2(BPh_4)_2$

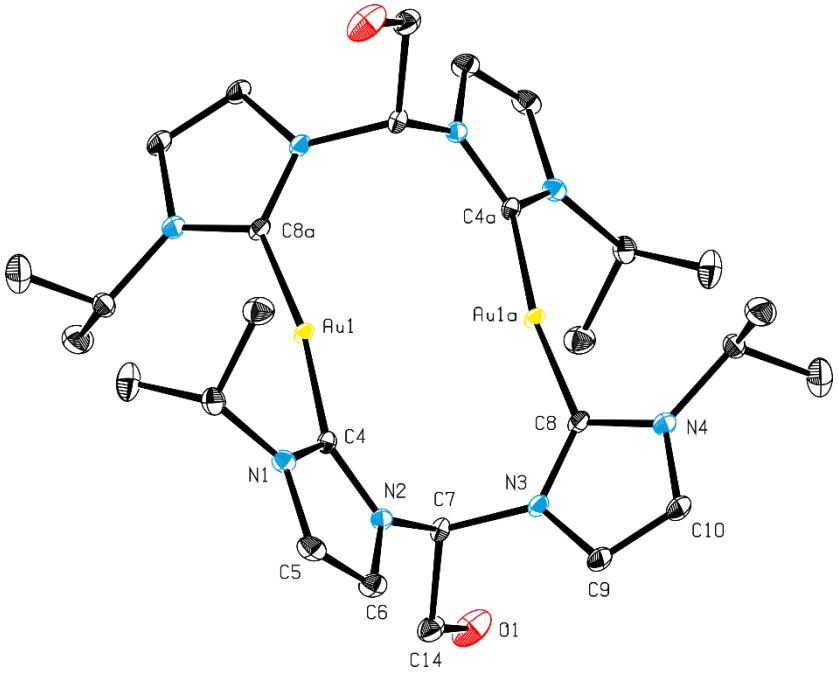

Figure S35. ORTEP style representation of the cation of $Au_2(L^{IPr})_2(BPh_4)_2$ with ellipsoids at 50 % probability. Hydrogen atoms and $BPh4^-$ are omitted for clarity.

Table S1. Crystallographic details for Ag(I) complexes.

	$Ag_2(L^{IPr})_2(PF_6)_2$ (CCDC 1511530)	$Ag_2(L^{IPr})_2(BPh_4)_2$ (CCDC 1511531)	$Ag_2(L^{IPr})_2(BPh_4)_2$ ·DMSO (CCDC 1511527)	$Ag_2(L^{Mes})_2(PF_6)_2$ (CCDC 1511526)
formula	$C_{28}H_{44}Ag_2F_{12}N_8O_2P_2$· $2(C_2H_{10}O)$	$C_{76}H_{84}Ag_2B_2N_8O_2$	$C_{76}H_{84}Ag_2B_2N_8O_2$·$4(C_2H_6OS)$	$C_{52}H_{60}Ag_2F_{12}N_8O_2P_2$ ·C_2H_3N·H_2O
fw	1178.63	1378.87	1691.38	1378.02
color/habit	colorless/shard	colorless/ fragment	colorless/ fragment	colorless/fragment
cryst dimens [mm³]	0.27×0.26×0.14	0.23×0.16×0.13	0.22×0.21×0.17	0.42×0.30×0.19
cryst syst	monoclinic	monoclinic	triclinic	monoclinic
space group	$P2_1/c$	$P2_1/n$	$P\bar{1}$	$P2_1/c$
a, [Å]	8.2134(11)	9.9899(7)	10.980(2)	12.4267(9)
b, [Å]	23.932(3)	14.7429(9)	14.280(3))	15.8703(11)
c, [Å]	12.3064(14)	22.6289(14)	14.447(3)	30.676(2)
α, [deg]	90	90	102.950(11)	90
β, [deg]	90.035(7)	100.939(3)	98.253(11)	100.465(5)

γ, [deg]	90	90	109.318(11)	90
V, [Å^3]	2419.0(5)	3272.2 (4)	2024.1(7)	5949.2(7)
Z	2	2	1	4
T, [K]	123(2)	123(2)	100(2)	100(2)
D_{calcd}, [g cm^{-3}]	1.618	1.400	1.388	1.538
μ, [mm^{-1}]	0.97	0.65	0.65	0.80
F(000)	1200	1432	893	2796
ϑ range, deg	3.01 to 27.88	1.66 to 25.35	1.83 to 26.02	1.67 to 30.50
index ranges (h, k, l)	±10, ±31, ±16	±12, ±17, ±27	±13, ±17, ±17	−17≤ h ≤+16, −22≤ k ≤+21, −37≤ l ≤+43
no. of reflns collected	82069	77780	62925	41345
no. of indep reflns/R_{int}	5754/0.056	5996/0.0528	7946/0.0690	16957/0.0502
no. of obsd reflns (I>2σ(I))	4961	5489	7186	12874
no. of data/restraints/ params	5754/181/344	5996/0/411	7946/0/488	16957/1/757
$R1/wR2$ ($I > 2\sigma(I)$)[a]	0.0244/0.0531	0.0286/0.0711	0.0267/0.0659	0.0451/0.0931
$R1/wR2$ (all data)[a]	0.0311/0.0559	0.0319/0.0735	0.0311/0.0682	0.0656/0.1015
GOF (on F^2)[a]	1.043	1.033	1.040	1.020
largest diff peak and hole [e Å^{-3}]	+0.701/−0.554	+1.362/−0.555	+0.428/−0.473	+751/−0.615

[a] $R1 = \Sigma(\|F_o| - |F_c\|)/\Sigma|F_o|$; $wR2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; GOF = $\{\Sigma[w(F_o^2 - F_c^2)^2]/(n - p)\}^{1/2}$

Table S2. Crystallographic details for Au(I) complexes and **$H_2L^{IPr}(BPh_4)_2$**.

	$Au_2(L^{IPr})_2(PF_6)_2$ (CCDC 1511529)	**$Au_2(L^{IPr})_2(BPh_4)_2$** (CCDC 1511528)	**$Au_2(L^{Mes})_2(PF_6)_2$** (CCDC 1511533)	**$H_2L^{IPr}(BPh_4)_2$** (CCDC 1511532)
formula	$C_{28}H_{44}Au_2F_{12}N_8O_2P_2$ ·$C_4H_{10}O$	$C_{76}H_{84}Au_2B_2N_8O_2$	$C_{52}H_{60}Au_2F_{12}N_8O_2P_2$ ·3(C_4H_8O)	$C_{62}H_{64}B_2N_4O$ ·2(C_2H_6O)
fw	1356.83	1557.07	1729.28	1019.00
color/habit	colorless/fragment	colorless/fragment	colorless/fragment	colorless/fragment

cryst dimens [mm^3]	0.55×0.20×0.11	0.23×0.17×0.15	0.52×0.20×0.18	0.55×0.41×0.36
cryst syst	monoclinic	monoclinic	monoclinic	triclinic
space group	$P2_1/c$	$P2_1/n$	$P2_1$	$P\bar{1}$
a, [Å]	8.1974(3)	10.0106(4)	12.7112(7)	11.9017 (4)
b, [Å]	23.8226(9)	14.8180(7)	22.4182(11)	15.3089 (5)
c, [Å]	12.3123(4)	22.5591(10)	13.1902(7)	17.2755 (5)
α, [deg]	90	90	90	102.960 (1)
β, [deg]	90.292(1)	101.129(2)	106.3979(16)	105.720 (1)
γ, [deg]	90	90	90	98.213 (1)
V, [Å^3]	2404.36(15)	3283.4(3)	3605.8(3)	2882.32 (16)
Z	2	2	2	2
T, [K]	100(2)	123(2)	100(2)	100(2)
D_{calcd}, [g cm^{-3}]	1.874	1.575	1.593	1.174
μ, [mm^{-1}]	6.25	4.52	4.19	0.07
F(000)	1328	1560	1720	1092
ϑ range, deg	2.38 to 28.36	2.25 to 27.88	2.23 to 26.37	1.82 to 25.35
index ranges (h, k, l)	±10, ±31, ±16	±13, ±19, ±29	±15, ±28, ±16	±14, ±18, ±20
no. of reflns collected	116889	74721	149399	107091
no. of indep reflns/R_{int}	6009/0.0400	7833/0.0587	14749/0.0385	10538/0.0402
no. of obsd reflns (I>2σ(I))	5552	6372	14222	8559
no. of data/restraints/ params	6009/153/344	7833/113/461	14749/550/964	10538/0/703
$R1/wR2$ ($I > 2\sigma(I)$)[a]	0.0180/0.0346	0.0259/0.0453	0.0186/0.0365	0.0446/0.0932
$R1/wR2$ (all data)[a]	0.0216/0.0353	0.0394/0.0494	0.0205/0.0369	0.0608/0.1008
GOF (on F^2)[a]	1.131	1.025	1.111	1.068
largest diff peak and hole [e Å^{-3}]	+0.617/−1.321	+1.412/−1.856	+0.877/−1.414	+0.322/−0.301

[a] $R1 = \Sigma(\|F_o| - |F_c\|)/\Sigma|F_o|$; $wR2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; $GOF = \{\Sigma[w(F_o^2 - F_c^2)^2]/(n - p)\}^{1/2}$.

CYTOTOXICITY STUDIES

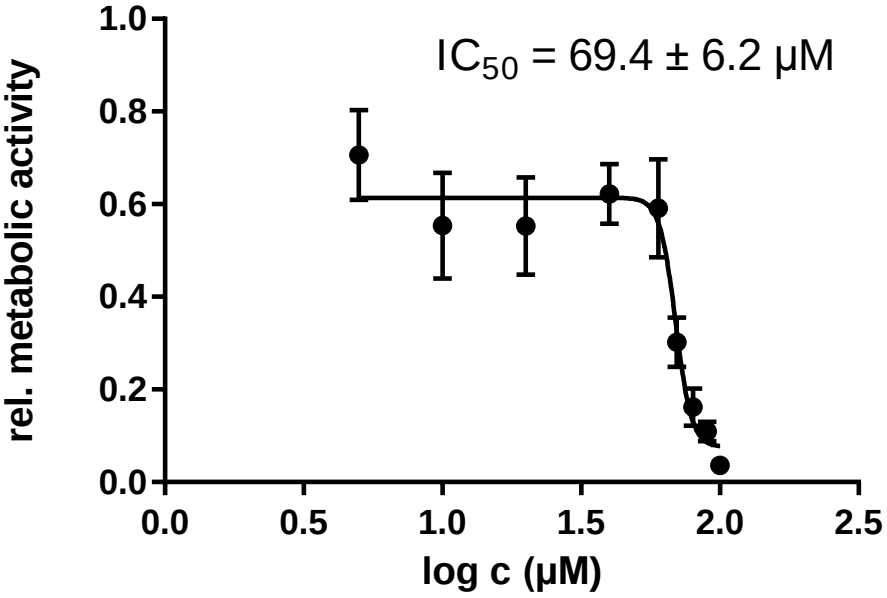

Figure S36.The metabolic activity of $Au_2(L^{Me})_2(PF_6)_2$ in human liver cancer cell lines HepG2.

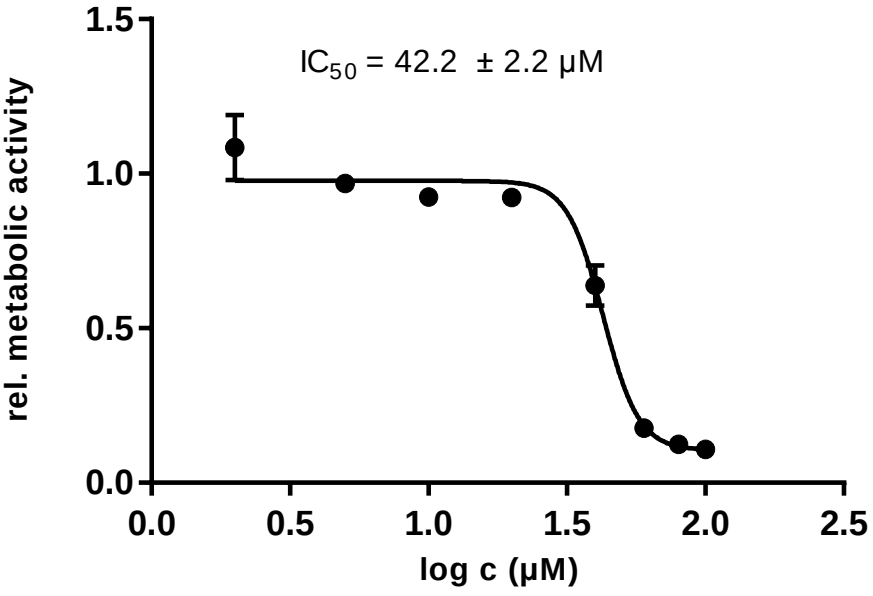

Figure S37. The metabolic activity of $Au_2(L^{Mes})_2(PF_6)_2$ in human lung cancer cell lines A549.

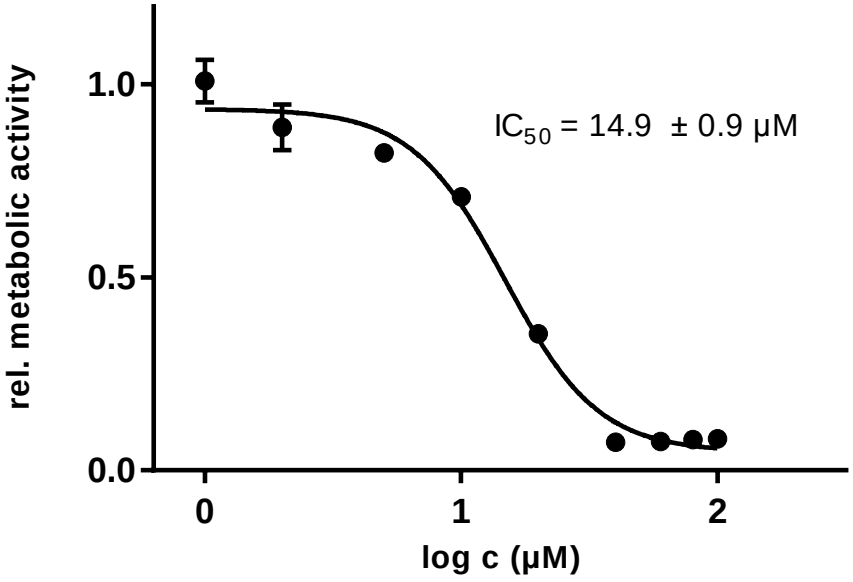

Figure S38. The metabolic activity of $Au_2(L^{Mes})_2(PF_6)_2$ in human liver cancer cell lines HepG2.

DFT CALCULATIONS

Table S3. Mean bonding lengths of $[Ag_2(L^{IPr})_2]^{2+}$ determined by SC-XRD experiments compared to calculations (ωB97x-D, 6-31+g(d), LANL2DZ)

	mean d_{C-C} [Å]	mean d_{C-N} [Å]	mean d_{C-O} [Å]	mean d_{C-Ag} [Å]
SC-XRD	1.468	1.401	1.406	2.088
Calculations	1.488	1.401	1.408	2.138
Δ = (Calc.-Exp.)	0.020 (1.3%)	---	0.002 (0.14%)	0.050 (2.3%)

Table S4. Atomic coordinates for the anti, exo isomer of $[Ag_2(L^{IPr})_2]^{2+}$ in acetonitrile and the corresponding free enthalpy.

Ag-anti-exo (MeCN)							
Ag	-1.8407960	-0.2936430	-0.0188540	H	0.4177240	5.2533760	1.5038230
Ag	1.5323530	0.2348830	0.0111300	C	-3.4707380	1.9484710	-3.6515110
N	-2.0327890	-3.1440430	1.2996380	H	-2.4021320	1.7698010	-3.8075180
N	1.5719960	-2.7875670	-1.0755110	H	-4.0306060	1.3259300	-4.3560030
N	3.4227870	-2.2315740	-0.1580380	H	-3.6873850	2.9965910	-3.8859820
N	-0.6694630	-3.1860680	-0.3487570	C	-5.3622150	1.8280890	-1.9514900
N	-3.0614220	2.3408520	-1.2540810	H	-5.6072130	1.5855140	-0.9124820
N	0.5619810	3.1415580	0.9910540	H	-5.6487250	2.8681980	-2.1430960
N	2.5031830	3.1885360	0.0935250	H	-5.9634970	1.1895800	-2.6060230
N	-1.7171880	2.8113880	0.3423030	C	4.1702430	3.6950390	-1.6605460
C	-1.4846300	-2.3586510	0.3520480	H	3.3544390	3.8053330	-2.3817240
C	-0.7053670	-4.4722630	0.1607860	H	4.4595750	4.6879000	-1.2996320
C	0.1694020	-2.7413230	-1.4527620	H	5.0338250	3.2719790	-2.1823060
C	2.1832830	-1.7687690	-0.4162580	C	4.8568270	2.6358340	0.5470690
C	-3.0018070	-2.6834200	2.3099040	H	4.5559830	1.9283130	1.3263940
C	4.4760160	-1.4540970	0.5216970	H	5.7852580	2.2774530	0.0920870
C	-2.2375800	1.7701140	-0.3542840	H	5.0630580	3.6027530	1.0196140
C	-3.0565290	3.7186150	-1.1315540	C	5.0984190	-2.2620520	1.6549190
C	-2.2072990	4.0190380	-0.1226020	H	4.3297430	-2.6443990	2.3337990
C	-0.7387030	2.6483970	1.4071030	H	5.6891830	-3.1058490	1.2827710
C	1.4886760	2.3509900	0.3898970	H	5.7702160	-1.6170670	2.2291430
C	2.2254240	4.4797240	0.5026570	C	5.5018320	-0.9566690	-0.4910980
C	-3.8799650	1.5944420	-2.2257980	H	5.0242720	-0.3528020	-1.2694120

C	3.7753840	2.7634570	-0.5207540	H	6.2523390	-0.3418150	0.0148590
H	-0.0820410	-1.6941290	-1.6236780	H	6.0208500	-1.7923760	-0.9739950
H	-3.1228890	-1.6145620	2.1146390	C	-4.3446420	-3.3788130	2.1131150
H	3.9526330	-0.5969070	0.9540320	H	-5.0763100	-2.9684870	2.8160170
H	-3.6496300	4.3657320	-1.7584480	H	-4.7192760	-3.2246190	1.0963100
H	-1.9229100	4.9741030	0.2901840	H	-4.2708960	-4.4562550	2.2980940
H	-0.6356550	1.5736690	1.5615480	C	-2.4302390	-2.8689970	3.7117380
H	2.9125910	5.2999600	0.3688370	H	-2.2948120	-3.9287670	3.9549120
H	-3.6448420	0.5428710	-2.0390630	H	-1.4648530	-2.3625510	3.8103130
H	3.5646840	1.7753370	-0.9387860	H	-3.1197990	-2.4433460	4.4471690
C	3.5940430	-3.5125940	-0.6495280	C	-1.1996760	3.2770630	2.7178510
C	2.4240220	-3.8714640	-1.2235120	H	-0.3954650	3.1576900	3.4539510
C	-1.5682300	-4.4427930	1.2016370	H	-1.4048980	4.3484330	2.5996920
H	4.5197400	-4.0585080	-0.5588780	C	-0.1096520	-3.5152150	-2.7371360
H	2.1481010	-4.7862240	-1.7240050	H	0.5970760	-3.1745020	-3.5033710
H	-1.8828060	-5.2294910	1.8692620	H	0.0283720	-4.5941170	-2.5936670
H	-0.1276270	-5.2889520	-0.2422470	O	-2.3648840	2.5804800	3.0968140
C	0.9957690	4.4562440	1.0639050	O	-1.4428910	-3.2218850	-3.0877730
H	-2.7153090	2.9738290	3.9058110	H	-1.6770950	-3.7276210	-3.8761420

G[Hartree] = -1972.161345

Table S5. Atomic coordinates for the anti, exo isomer of $[Ag_2(L^{IPr})_2]^{2+}$ in DMSO and the corresponding free enthalpy.

Ag-anti-exo (DMSO)							
Ag	1.8412160	0.3020090	-0.0197670	H	-0.3980290	-5.2572200	1.4977460
Ag	-1.5255270	-0.2419340	0.0062280	C	3.4905290	-1.9319600	-3.6540690
N	2.0157890	3.1508880	1.3039200	H	2.4219460	-1.7587990	-3.8164610

N	-1.5793670	2.7811550	-1.0808090	H	4.0510020	-1.3075550	-4.3564760
N	-3.4268360	2.2134250	-0.1644360	H	3.7137020	-2.9791530	-3.8866510
N	0.6565850	3.1892800	-0.3473540	C	5.3714610	-1.7980570	-1.9441290
N	3.0715590	-2.3254780	-1.2591550	H	5.6088760	-1.5543320	-0.9035940
N	-0.5473450	-3.1456990	0.9849730	H	5.6660220	-2.8362490	-2.1340520
N	-2.4898260	-3.1969480	0.0908920	H	5.9731740	-1.1557390	-2.5945590
N	1.7299670	-2.8047840	0.3364480	C	-4.1711950	-3.7153760	-1.6460560
C	1.4785210	2.3659780	0.3500910	H	-3.3590590	-3.8428150	-2.3685610
C	0.6759970	4.4718270	0.1717270	H	-4.4697640	-4.7008290	-1.2726500
C	-0.1759160	2.7443650	-1.4560050	H	-5.0321200	-3.2905850	-2.1708350
C	-2.1846100	1.7585010	-0.4223650	C	-4.8381070	-2.6338400	0.5546820
C	2.9814900	2.6930350	2.3181040	H	-4.5329440	-1.9181960	1.3247840
C	-4.4747170	1.4302750	0.5165220	H	-5.7705120	-2.2818200	0.1028140
C	2.2468670	-1.7598350	-0.3571510	H	-5.0401740	-3.5957620	1.0392680
C	3.0704840	-3.7034500	-1.1413000	C	-5.0965930	2.2336550	1.6528440
C	2.2225590	-4.0094610	-0.1330290	H	-4.3273880	2.6178250	2.3301550
C	0.7514920	-2.6488370	1.4021790	H	-5.6918470	3.0759580	1.2843840
C	-1.4766850	-2.3573470	0.3855160	H	-5.7638770	1.5854590	2.2287850
C	-2.2088770	-4.4872680	0.5000790	C	-5.5015300	0.9315080	-0.4941120
C	3.8896940	-1.5740300	-2.2268460	H	-5.0248900	0.3291810	-1.2742370
C	-3.7645280	-2.7736720	-0.5191570	H	-6.2505010	0.3154450	0.0126470
H	0.0827090	1.6996800	-1.6315850	H	-6.0232480	1.7664690	-0.9755450
H	3.1461640	1.6360140	2.0922520	C	4.3006890	3.4428940	2.1710130
H	-3.9466870	0.5742710	0.9455480	H	5.0331100	3.0376630	2.8760520
H	3.6649070	-4.3471000	-1.7705010	H	4.7018520	3.3343840	1.1583070
H	1.9409480	-4.9667930	0.2763600	H	4.1851250	4.5108460	2.3871880
H	0.6446230	-1.5751200	1.5606130	C	2.3763800	2.8150360	3.7124790
H	-2.8944240	-5.3091730	0.3682710	H	2.1908480	3.8611100	3.9804920
H	3.6466440	-0.5239420	-2.0420870	H	1.4314190	2.2664270	3.7781000
H	-3.5539850	-1.7904480	-0.9487440	H	3.0686740	2.3985110	4.4506550
C	-3.6058130	3.4934790	-0.6550120	C	1.2140590	-3.2816950	2.7100290
C	-2.4379190	3.8598550	-1.2284560	H	0.4087510	-3.1685120	3.4459650
C	1.5362030	4.4446380	1.2146780	H	1.4222820	-4.3519990	2.5874620
H	-4.5346860	4.0338810	-0.5639600	C	0.1007110	3.5277860	-2.7349970
H	-2.1679520	4.7769630	-1.7278880	H	-0.6032980	3.1884110	-3.5043320
H	1.8398200	5.2300740	1.8888480	H	-0.0435920	4.6049250	-2.5848960
H	0.0902380	5.2848460	-0.2271790	O	2.3769780	-2.5845280	3.0948040
C	-0.9782030	-4.4611370	1.0588080	O	1.4358650	3.2455660	-3.0878460
H	2.7234810	-2.9812300	3.9038340	H	1.6641920	3.7591180	-3.8728250

G[Hartree] = -1972.156319

Table S6. Atomic coordinates for the syn, meso isomer of $[Ag_2(L^{IPr})_2]^{2+}$ in acetonitrile and the corresponding free enthalpy.

Ag-syn-meso (MeCN)							
O	-1.9821290	-3.9714400	-2.7453360	H	-4.2837320	-3.3774390	-1.2774590
N	-0.1685580	-2.1983550	2.4155130	H	-6.0142260	-1.2525520	-1.3583680
N	-2.8259210	-1.7851400	-1.0114370	Ag	-1.2965680	0.9174050	-0.4635180
N	-4.1791910	-0.1276510	-1.0888010	Ag	1.4400670	-0.9012800	0.0594740
N	-1.2239540	-2.5377980	0.5863010	C	-5.1162960	1.5800860	0.4107970
C	-0.0803010	-2.0046980	1.0836460	H	-5.9458330	0.9431520	0.7383020
C	-1.5832800	-2.5225140	-0.8244710	H	-4.2772130	1.4386660	1.0998520
C	-2.8758740	-0.4301460	-0.9466820	H	-5.4405130	2.6236420	0.4746670
C	0.8440130	-1.6990670	3.3700360	C	-5.8277340	1.4598750	-2.0287490
C	-1.6345940	-3.9489930	-1.3831690	H	-6.0806470	2.5236310	-2.0628400
H	-1.2303170	-3.6744340	-3.2756220	H	-5.5234990	1.1498510	-3.0334650
H	-0.7943490	-1.9683420	-1.3358380	H	-6.7378540	0.9166820	-1.7522290
H	1.8034710	-1.8245220	2.8598060	C	0.8610930	-2.5308900	4.6460100
H	-2.3770150	-4.5531730	-0.8548330	H	0.9559900	-3.5996080	4.4297360
N	4.3213490	-0.2823790	-0.9292210	H	1.7230020	-2.2319420	5.2496510
N	1.3774870	2.7069220	-0.4053340	H	-0.0349370	-2.3686890	5.2544590
N	0.1612870	2.9602600	1.3390430	C	0.6093580	-0.2154290	3.6434730
N	3.0912200	1.3833710	-1.4566260	H	0.6630280	0.3629910	2.7149190
C	3.0507670	0.1634190	-0.8612210	H	-0.3717000	-0.0531550	4.1042160
C	5.1458660	0.6312450	-1.5591070	H	1.3779450	0.1613400	4.3259490
C	4.3687970	1.6854530	-1.8938250	C	5.2959140	-2.4615180	-1.5298560
C	1.9535340	2.2766030	-1.6723370	H	6.2001730	-2.0473110	-1.9894670
C	0.2171770	2.2914540	0.1675140	H	5.5447470	-3.4514360	-1.1356070
C	1.2597010	3.7846330	1.5000410	H	4.5339860	-2.5810360	-2.3067690
C	2.0313260	3.6234210	0.4033990	C	5.8158930	-1.3576730	0.7041250
C	4.7846650	-1.5766340	-0.3978820	H	6.0723380	-2.3177880	1.1621490
H	6.1992930	0.4609530	-1.7147770	H	6.7386780	-0.9165710	0.3111140
H	4.6053120	2.6096030	-2.3981200	H	5.4199710	-0.6986790	1.4835580
H	1.4035500	4.4102110	2.3658380	C	-2.0954550	3.8252620	1.8140540
H	2.9752460	4.0700090	0.1313890	H	-2.9480900	3.7512620	2.4964640
H	3.8921480	-2.0357230	0.0363690	H	-1.7442600	4.8634990	1.8147140
C	-4.7042740	1.2506970	-1.0209880	H	-2.4401100	3.5766910	0.8052790
H	-3.8587320	1.8836160	-1.3053470	C	-0.5529310	3.1559080	3.7055950
C	-0.9856780	2.8815520	2.2701010	H	-0.3470280	4.2183860	3.8756310
H	-1.3382040	1.8474960	2.2039870	H	-1.3662180	2.8705290	4.3789600
C	-1.3542580	-2.8263410	2.7512480	H	0.3337410	2.5780660	3.9831170
C	-2.0219010	-3.0472120	1.5957080	H	-0.6542470	-4.4032980	-1.1990450
H	-1.6250250	-3.0707060	3.7654870	H	2.3733790	3.1724810	-2.1352200

H	-2.9804110	-3.5080760	1.4144780	C	0.9488280	1.6820910	-2.6689630
C	-4.9444740	-1.2720790	-1.2249950	H	0.6069490	0.6984790	-2.3397920
C	-4.0919640	-2.3216610	-1.1778220	H	0.0840000	2.3496520	-2.7497030
H	1.6272570	2.3209430	-4.3901870	O	1.5761220	1.4813280	-3.9140990

G[Hartree] = -1972.161716

Table S7. Atomic coordinates for the syn, meso isomer of **$[Ag_2(L^{IPr})_2]^{2+}$** in DMSO and the corresponding free enthalpy.

Ag-syn-meso (DMSO)							
O	-1.9788940	-3.9656090	-2.7752870	H	-4.2884690	-3.3724600	-1.2786540
N	-0.1838170	-2.1980800	2.3972130	H	-6.0197820	-1.2471380	-1.3187770
N	-2.8256250	-1.7814430	-1.0333990	Ag	-1.2916120	0.9202190	-0.4957250
N	-4.1798750	-0.1237930	-1.0776850	Ag	1.4412520	-0.8990830	0.0570650
N	-1.2269990	-2.5400160	0.5616890	C	-5.1006480	1.5616680	0.4560850
C	-0.0875580	-2.0047300	1.0659000	H	-5.9262210	0.9194130	0.7834190
C	-1.5831510	-2.5196840	-0.8500930	H	-4.2545500	1.4111090	1.1346950
C	-2.8742400	-0.4270110	-0.9627400	H	-5.4255830	2.6036620	0.5387620
C	0.8202690	-1.6948270	3.3583360	C	-5.8375540	1.4761320	-1.9772260
C	-1.6348880	-3.9444630	-1.4123210	H	-6.0913430	2.5401790	-1.9939040
H	-1.2261730	-3.6629610	-3.3010270	H	-5.5437030	1.1806580	-2.9894390
H	-0.7935900	-1.9634910	-1.3582690	H	-6.7448770	0.9288870	-1.6993930
H	1.7842200	-1.8197100	2.8564800	C	0.8282170	-2.5233230	4.6361940
H	-2.3783480	-4.5493680	-0.8862990	H	0.9281390	-3.5923800	4.4236340
N	4.3382180	-0.2815020	-0.8874020	H	1.6840660	-2.2211380	5.2468130
N	1.3898300	2.7038460	-0.3911250	H	-0.0732290	-2.3624500	5.2369770
N	0.1423260	2.9470510	1.3319940	C	0.5801480	-0.2112890	3.6268460
N	3.1179640	1.3876210	-1.4257070	H	0.6452280	0.3666330	2.6987040
C	3.0672810	0.1653200	-0.8364040	H	-0.4067620	-0.0500280	4.0752960
C	5.1728590	0.6337230	-1.5012010	H	1.3396850	0.1672700	4.3184460
C	4.4019980	1.6903070	-1.8423950	C	5.3054730	-2.4642130	-1.4849950
C	1.9848720	2.2836090	-1.6524650	H	6.2121770	-2.0526030	-1.9421870
C	0.2172090	2.2893460	0.1555330	H	5.5503630	-3.4549480	-1.0902410
C	1.2413830	3.7640650	1.5218670	H	4.5459470	-2.5820960	-2.2645570
C	2.0330380	3.6090030	0.4385150	C	5.8190080	-1.3649700	0.7521550
C	4.7926270	-1.5782610	-0.3550470	H	6.0652640	-2.3259970	1.2138160
H	6.2283140	0.4634430	-1.6425500	H	6.7479580	-0.9317550	0.3648960
H	4.6471250	2.6164880	-2.3387850	H	5.4235610	-0.7016780	1.5282230

H	1.3721710	4.3807950	2.3960710	C	-2.1271600	3.8021160	1.7578520
H	2.9840570	4.0533410	0.1886120	H	-3.0043430	3.7074800	2.4057280
H	3.8963000	-2.0339380	0.0747870	H	-1.7874130	4.8437250	1.7881060
C	-4.7040060	1.2530460	-0.9845870	H	-2.4310380	3.5681290	0.7325500
H	-3.8615150	1.8901880	-1.2682950	C	-0.6237400	3.1367820	3.6820330
C	-1.0241340	2.8624900	2.2377290	H	-0.4230440	4.1994400	3.8569340
H	-1.3704460	1.8268600	2.1624370	H	-1.4508790	2.8503660	4.3379200
C	-1.3701810	-2.8281070	2.7258020	H	0.2576170	2.5603920	3.9790860
C	-2.0302240	-3.0503000	1.5663820	H	-0.6554070	-4.4001920	-1.2268410
H	-1.6473070	-3.0722900	3.7383530	H	2.4125250	3.1825680	-2.1020950
H	-2.9872860	-3.5122280	1.3804110	C	0.9927120	1.6972940	-2.6661170
C	-4.9477530	-1.2673230	-1.2050520	H	0.6405540	0.7143820	-2.3456760
C	-4.0946150	-2.3170960	-1.1782610	H	0.1324090	2.3694570	-2.7569510
H	1.7081720	2.3421960	-4.3684000	O	1.6344880	1.4977060	-3.9040590

G[Hartree] = -1972.156273

Table S8. Atomic coordinates for the anti, exo isomer of **$[Au_2(L^{IPr})_2]^{2+}$** in acetonitrile and the corresponding free enthalpy.

Au-anti-exo (MeCN)							
N	-2.8828840	2.7744400	-0.7376200	H	-3.4062150	-3.1848090	3.3339980
N	1.2274000	2.9518970	0.6907780	H	-5.0175490	-2.4495440	3.3688740
N	3.0487440	2.7754080	-0.4324170	H	-4.7750030	-3.9677550	2.5053830
N	-1.1669530	2.9553950	0.5402700	C	-5.2150380	-2.0111080	0.5853950
N	-2.8836590	-2.7739050	0.7375910	H	-4.9664350	-1.3862070	-0.2789520
N	1.2265690	-2.9521620	-0.6904840	H	-5.5763880	-2.9798770	0.2224000
N	3.0480700	-2.7758910	0.4324810	H	-6.0278920	-1.5264450	1.1354200
N	-1.1678320	-2.9552400	-0.5403810	C	4.6687180	-3.0772220	2.2791330
C	-1.9497160	2.0483530	-0.0935340	H	3.8325910	-3.3202310	2.9421160
C	-1.6178140	4.2410940	0.2989430	H	5.1312070	-4.0085470	1.9356010
C	-0.0151720	2.5989020	1.3563120	H	5.4201880	-2.5378440	2.8629320
C	2.0307940	2.0505550	0.0712490	C	5.3305140	-1.9286680	0.1076470
C	-4.0046900	2.1849190	-1.4988380	H	4.9795340	-1.2627900	-0.6876270
C	4.2217170	2.1938060	-1.1210800	H	6.1813530	-1.4525890	0.6048290
C	-1.9502800	-2.0480310	0.0935720	H	5.6801160	-2.8620920	-0.3478550
C	-2.7006120	-4.1229380	0.5038480	C	4.6698630	3.0771220	-2.2785980
C	-1.6190950	-4.2408350	-0.2992060	H	3.8339870	3.3210970	-2.9415420
C	-0.0158500	-2.5989800	-1.3562250	H	5.1328510	4.0079290	-1.9343310

C	2.0302870	-2.0508780	-0.0712890	H	5.4211030	2.5377130	-2.8626610
C	2.8937390	-4.1145280	0.1301810	C	5.3306740	1.9266750	-0.1078490
C	-4.0053270	-2.1841200	1.4988220	H	4.9792140	1.2604780	0.6869420
C	4.2212690	-2.1944750	1.1209060	H	6.1812990	1.4504250	-0.6052310
H	-0.0269630	1.5121210	1.4465640	H	5.6807440	2.8595930	0.3483220
H	-3.6451300	1.2001280	-1.8092330	C	-5.2145780	2.0125800	-0.5855290
H	3.8668650	1.2429980	-1.5270270	H	-6.0275680	1.5281510	-1.1355600
H	-3.3436580	-4.8823180	0.9182540	H	-4.9663350	1.3877290	0.2789590
H	-1.1530380	-5.1219870	-0.7094610	H	-5.5755760	2.9815660	-0.2227790
H	-0.0274340	-1.5122000	-1.4464860	C	-4.3100320	3.0056990	-2.7454810
H	3.5996410	-4.8701810	0.4338270	H	-4.7735050	3.9686680	-2.5057410
H	-3.6453860	-1.1995490	1.8094910	H	-3.4049130	3.1850760	-3.3340620
H	3.8669000	-1.2431830	1.5261460	H	-5.0165460	2.4504490	-3.3691150
C	2.8948810	4.1139910	-0.1296470	C	-0.0911190	-3.1960590	-2.7576700
C	1.7468440	4.2305920	0.5739060	H	0.8132120	-2.8885590	-3.2967250
C	-2.6994170	4.1234430	-0.5040470	H	-0.1184200	-4.2927450	-2.7303420
H	3.6009770	4.8695270	-0.4331380	C	-0.0906030	3.1959880	2.7577310
H	1.2760910	5.1059140	0.9910160	H	0.8135640	2.8883560	3.2969850
H	-3.3422080	4.8830010	-0.9185320	H	-0.1177390	4.2926770	2.7303680
H	-1.1514880	5.1221560	0.7090970	O	-1.2592870	-2.6742700	-3.3464330
C	1.7456150	-4.2309860	-0.5732520	O	-1.2589810	2.6744050	3.3462570
H	1.2745530	-5.1062810	-0.9900700	H	-1.3570960	3.0482650	4.2310760
C	-4.3111640	-3.0050040	2.7452790	H	-1.3574910	-3.0483870	-4.2311320
Au	1.9030260	-0.0001500	-0.0001010	Au	-1.8725520	0.0001520	0.0000350

G[Hartree] = -1951.591571

Table S9. Atomic coordinates for the anti, exo isomer of **$[Au_2(L^{IPr})_2]^{2+}$** in DMSO and the corresponding free enthalpy.

Au-anti-exo (DMSO)							
N	-2.8995610	2.7718590	-0.6876110	H	-3.5196060	-3.2274860	3.2554940
N	1.2385920	2.9560660	0.6648240	H	-5.1169280	-2.4609000	3.2496720
N	3.0380180	2.7732750	-0.4915810	H	-4.8739240	-3.9664850	2.3644090
N	-1.1581840	2.9581110	0.5544370	C	-5.2106680	-1.9704090	0.4697640
N	-2.8991570	-2.7721650	0.6876530	H	-4.9207410	-1.3382010	-0.3761150
N	1.2389980	-2.9559060	-0.6649260	H	-5.5755770	-2.9273830	0.0797120
N	3.0384200	-2.7729930	0.4914700	H	-6.0342290	-1.4797730	0.9983050
N	-1.1577750	-2.9582070	-0.5544180	C	4.6090790	-3.0541070	2.3823010

C	-1.9463490	2.0490090	-0.0691010	H	3.7534190	-3.2910460	3.0223630
C	-1.6233410	4.2417370	0.3300620	H	5.0825000	-3.9885970	2.0630070
C	0.0073000	2.6047140	1.3518090	H	5.3416090	-2.5062380	2.9821180
C	2.0325180	2.0513020	0.0389390	C	5.3304670	-1.9313690	0.2169140
C	-4.0374740	2.1784430	-1.4217280	H	5.0013910	-1.2795230	-0.5990400
C	4.1938310	2.1852540	-1.2024680	H	6.1648640	-1.4436850	0.7307560
C	-1.9460540	-2.0491990	0.0691080	H	5.6963050	-2.8706510	-0.2132420
C	-2.7207070	-4.1208020	0.4496830	C	4.6085980	3.0543840	-2.3824750
C	-1.6227560	-4.2418920	-0.3300150	H	3.7528890	3.2911240	-3.0225440
C	0.0076340	-2.6046590	-1.3518330	H	5.0818940	3.9889800	-2.0633050
C	2.0328200	-2.0511000	-0.0389690	H	5.3411920	2.5065450	-2.9822420
C	2.8877300	-4.1138700	0.1980210	C	5.3301880	1.9320160	-0.2169610
C	-4.0371480	-2.1788900	1.4217630	H	5.0012110	1.2802320	0.5990840
C	4.1941620	-2.1848920	1.2024090	H	6.1646420	1.4443750	-0.7307530
H	-0.0018320	1.5182910	1.4451980	H	5.6959080	2.8714020	0.2130660
H	-3.6740050	1.2060250	-1.7647390	C	-5.2109520	1.9697650	-0.4697230
H	3.8291490	1.2288530	-1.5865060	H	-6.0344490	1.4790280	-0.9982700
H	-3.3775630	-4.8782570	0.8454480	H	-4.9209260	1.3375710	0.3761330
H	-1.1537170	-5.1247050	-0.7330740	H	-5.5759920	2.9266740	-0.0796360
H	-0.0016240	-1.5182330	-1.4451790	C	-4.4005110	3.0177510	-2.6397000
H	3.5871030	-4.8676200	0.5211460	H	-4.8745220	3.9659450	-2.3643110
H	-3.6738170	-1.2064090	1.7647410	H	-3.5201040	3.2271720	-3.2554330
H	3.8293530	-1.2285910	1.5865740	H	-5.1173150	2.4603510	-3.2496180
C	2.8871490	4.1141630	-0.1982760	C	-0.0459670	-3.2067400	-2.7520400
C	1.7526020	4.2346530	0.5266000	H	0.8701510	-2.9079580	-3.2757840
C	-2.7212980	4.1205150	-0.4496070	H	-0.0804860	-4.3030770	-2.7208680
H	3.5864140	4.8679750	-0.5214910	C	-0.0462980	3.2068440	2.7519950
H	1.2885060	5.1123620	0.9462380	H	0.8698690	2.9081660	3.2757130
H	-3.3782690	4.8778880	-0.8453380	H	-0.0809200	4.3031760	2.7207830
H	-1.1544140	5.1246060	0.7331300	O	-1.1997650	-2.6804480	-3.3650380
C	1.7531840	-4.2344390	-0.5268440	O	-1.2000240	2.6804690	3.3650590
H	1.2891980	-5.1121660	-0.9465650	H	-1.2861600	3.0637430	4.2469750
C	-4.4000490	-3.0182130	2.6397630	H	-1.2859770	-3.0637980	-4.2469120
Au	1.9106630	0.0000910	0.0001080	Au	-1.8577240	-0.0000900	-0.0000390

G[Hartree] = -1951.584257

Table S10. Atomic coordinates for the syn, meso isomer of $[Au_2(L^{IPr})_2]^{2+}$ in acetonitrile and the corresponding free enthalpy.

Au-syn-meso (MeCN)							
O	-1.4325120	-3.9242590	-2.7345570	H	-5.8091100	-1.9121890	-1.3132820
N	0.1908300	-2.1491660	2.4293640	C	-5.3554320	0.9125620	0.5973870
N	-2.5807130	-2.0189430	-0.9448260	H	-6.0757180	0.1354440	0.8763010
N	-4.1552390	-0.5579560	-0.9626290	H	-4.5149050	0.8778100	1.2985940
N	-0.8621270	-2.5782520	0.6114660	H	-5.8453730	1.8859950	0.6999990
C	0.2320930	-1.9427320	1.0991500	C	-6.0011830	0.8224980	-1.8611080
C	-1.2476120	-2.5924170	-0.7926090	H	-6.4043940	1.8391840	-1.8479130
C	-2.8254580	-0.6896170	-0.8163430	H	-5.6384980	0.6125820	-2.8720810
C	1.1481580	-1.5462860	3.3808110	H	-6.8278450	0.1409950	-1.6328240
C	-1.1276690	-4.0002850	-1.3619000	C	1.3540130	-2.4380960	4.5979560
H	-1.3330220	-4.8013040	-3.1267630	H	1.5872400	-3.4672880	4.3077380
H	-0.5468130	-1.9443040	-1.3192220	H	2.1970760	-2.0499440	5.1765580
H	2.0923940	-1.4808330	2.8334940	H	0.4813040	-2.4448140	5.2599530
H	-1.7886850	-4.7004040	-0.8334570	C	0.6832120	-0.1395810	3.7479770
N	4.2796040	0.1487330	-0.9661860	H	0.6196530	0.4888470	2.8534880
N	0.9574540	2.7469490	-0.4761730	H	-0.2992650	-0.1650410	4.2324910
N	-0.2253980	2.9746500	1.3029330	H	1.3978000	0.3179120	4.4393090
N	2.8053380	1.6061630	-1.5155610	C	5.5555520	-1.8814160	-1.5179980
C	2.9621620	0.4173700	-0.8764300	H	6.3768640	-1.3561240	-2.0178380
C	4.9442580	1.1445220	-1.6550220	H	5.9593840	-2.8074460	-1.0974430
C	4.0165970	2.0632080	-2.0022630	H	4.8011670	-2.1430420	-2.2665180
C	1.5544290	2.3341020	-1.7408450	C	5.9496680	-0.6282640	0.6657340
C	-0.1504090	2.2726150	0.1530600	H	6.3560130	-1.5218840	1.1491190
C	0.8117680	3.8824720	1.3961980	H	6.7894080	-0.0700920	0.2375930
C	1.5585510	3.7392890	0.2812150	H	5.4723250	-0.0095210	1.4322190
C	4.9433610	-1.0431680	-0.4018700	C	-2.5301620	3.6494180	1.8716470
H	6.0064060	1.1201820	-1.8389430	H	-3.3406420	3.5046400	2.5929240
H	4.1071070	2.9895030	-2.5477520	H	-2.2844180	4.7166850	1.8402100
H	0.9338050	4.5499080	2.2332380	H	-2.8946110	3.3465470	0.8847600
H	2.4560200	4.2456600	-0.0384480	C	-0.8395050	3.1776170	3.6963780
H	4.1406580	-1.6143450	0.0714160	H	-0.6993310	4.2563620	3.8249670
C	-4.8758480	0.7263740	-0.8384370	H	-1.6008010	2.8604730	4.4145620
H	-4.1288460	1.4904260	-1.0686590	H	0.0952350	2.6692330	3.9506440
C	-1.3176150	2.8242470	2.2931880	H	-0.0940940	-4.3229260	-1.1901940
H	-1.5774660	1.7618670	2.2709170	H	1.8482870	3.2537960	-2.2502770
C	-0.9231460	-2.8897760	2.7771700	C	0.6317060	1.5944940	-2.7043070
C	-1.5871660	-3.1660830	1.6319320	H	0.4227150	0.5781480	-2.3559100
H	-1.1500000	-3.1619610	3.7950110	H	-0.3098490	2.1485140	-2.7941160

H	-2.5014210	-3.7127580	1.4613710	O	1.3345480	1.5706450	-3.9297160
C	-4.7486080	-1.7895760	-1.1661280	H	0.8578900	1.0012730	-4.5468600
C	-3.7598740	-2.7122580	-1.1567520	Au	1.5825400	-0.7693950	0.0813000
H	-3.8024170	-3.7779950	-1.3083330	Au	-1.4806520	0.7907690	-0.3685320

G[Hartree] = -1951.591156

Table S11. Atomic coordinates for the syn, meso isomer of **$[Au_2(L^{IPr})_2]^{2+}$** in DMSO and the corresponding free enthalpy.

Au-syn-meso (DMSO)							
O	-1.5233190	-3.8420670	-2.8403330	H	-5.8646650	-1.8243760	-1.2214960
N	0.1640740	-2.2033370	2.3551800	C	-5.1376860	1.0128920	0.7856400
N	-2.6262590	-1.9724640	-0.9837590	H	-5.8306110	0.2583860	1.1750620
N	-4.1833840	-0.4945390	-0.9036830	H	-4.2065810	0.9581090	1.3593030
N	-0.8989020	-2.5935950	0.5343420	H	-5.5818460	2.0005650	0.9443690
C	0.2013340	-1.9742140	1.0286690	C	-6.1454820	0.8760330	-1.5400090
C	-1.2994490	-2.5680920	-0.8655600	H	-6.5410930	1.8941990	-1.4822310
C	-2.8498600	-0.6440140	-0.8178140	H	-5.9474640	0.6487890	-2.5921610
C	1.1283070	-1.6217550	3.3129130	H	-6.9272810	0.2034310	-1.1714830
C	-1.2091570	-3.9618570	-1.4727890	C	1.3218670	-2.5284790	4.5205970
H	-1.4456410	-4.7109950	-3.2546840	H	1.5412960	-3.5578550	4.2204300
H	-0.5959260	-1.9165660	-1.3842550	H	2.1704150	-2.1585480	5.1031970
H	2.0739630	-1.5625100	2.7671880	H	0.4496740	-2.5301650	5.1833650
H	-1.8786550	-4.6651160	-0.9593090	C	0.6796600	-0.2135420	3.6947470
N	4.2953690	0.1314850	-0.9083720	H	0.6325860	0.4284040	2.8087740
N	0.9901180	2.7477620	-0.4907410	H	-0.3071370	-0.2318370	4.1707640
N	-0.1913870	2.9623420	1.2902040	H	1.3946320	0.2248130	4.3981010
N	2.8404090	1.5925470	-1.4980790	C	5.8155310	-1.7636780	-1.3313510
C	2.9737200	0.3925240	-0.8758710	H	6.6920080	-1.1674080	-1.6079950
C	4.9869500	1.1476710	-1.5377450	H	6.1792160	-2.7021900	-0.9022610
C	4.0712880	2.0678380	-1.9120770	H	5.2507620	-1.9982330	-2.2390030
C	1.5982250	2.3267660	-1.7476080	C	5.6883050	-0.6542280	0.9575640
C	-0.1191540	2.2718450	0.1333470	H	6.1079360	-1.5463080	1.4327980
C	0.8478460	3.8664250	1.3919760	H	6.5139620	0.0308840	0.7352090
C	1.5943370	3.7312140	0.2757510	H	5.0155400	-0.1694110	1.6723430
C	4.9373860	-1.0544530	-0.3074600	C	-2.4905160	3.6380960	1.8728070
H	6.0568960	1.1342770	-1.6693750	H	-3.3041990	3.4828850	2.5881930
H	4.1834510	3.0050210	-2.4346330	H	-2.2408230	4.7049930	1.8642430

H	0.9716820	4.5258790	2.2351070	H	-2.8514760	3.3586070	0.8776870
H	2.4936690	4.2378840	-0.0382970	C	-0.7988200	3.1284870	3.6874030
H	4.1106810	-1.7156340	-0.0355400	H	-0.6523530	4.2041170	3.8339350
C	-4.8764320	0.7968440	-0.7023150	H	-1.5598320	2.8036880	4.4025230
H	-4.1731500	1.5536860	-1.0602760	H	0.1339400	2.6111300	3.9312390
C	-1.2817170	2.8009590	2.2800840	H	-0.1809380	-4.3093560	-1.3187000
H	-1.5449660	1.7397690	2.2412600	H	1.9054150	3.2415910	-2.2575970
C	-0.9523960	-2.9437150	2.6943790	C	0.6809220	1.5892200	-2.7170200
C	-1.6226810	-3.1955290	1.5473690	H	0.4594180	0.5762580	-2.3666830
H	-1.1769560	-3.2332830	3.7079110	H	-0.2554630	2.1499490	-2.8182450
H	-2.5399030	-3.7356850	1.3721470	O	1.3942320	1.5533520	-3.9363940
C	-4.7982860	-1.7146600	-1.1117170	H	0.9153650	0.9857060	-4.5533800
C	-3.8207740	-2.6477730	-1.1629280	Au	1.5686460	-0.8023520	0.0333700
H	-3.8818530	-3.7090470	-1.3375740	Au	-1.4699230	0.8103880	-0.3923280

G[Hartree] = -1951.584299