Electronic Supplementary Information

Using sodium acetate for the synthesis of [Au(NHC)X] complexes

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NMR spectra

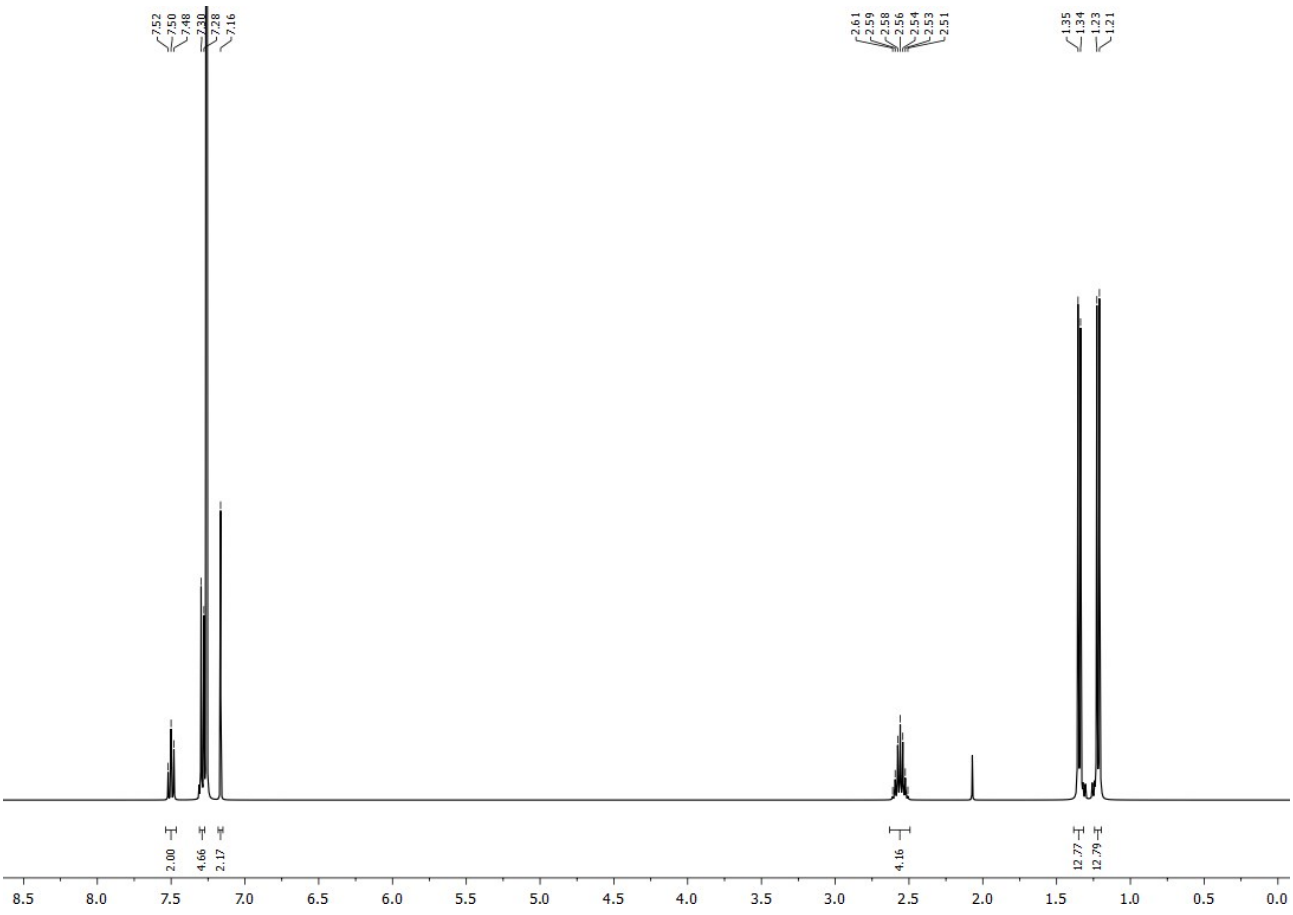

Figure S1: ^{1}H NMR spectrum of [Au(IPr)Cl] (**2a**) in $CDCl_3$ at 298 K

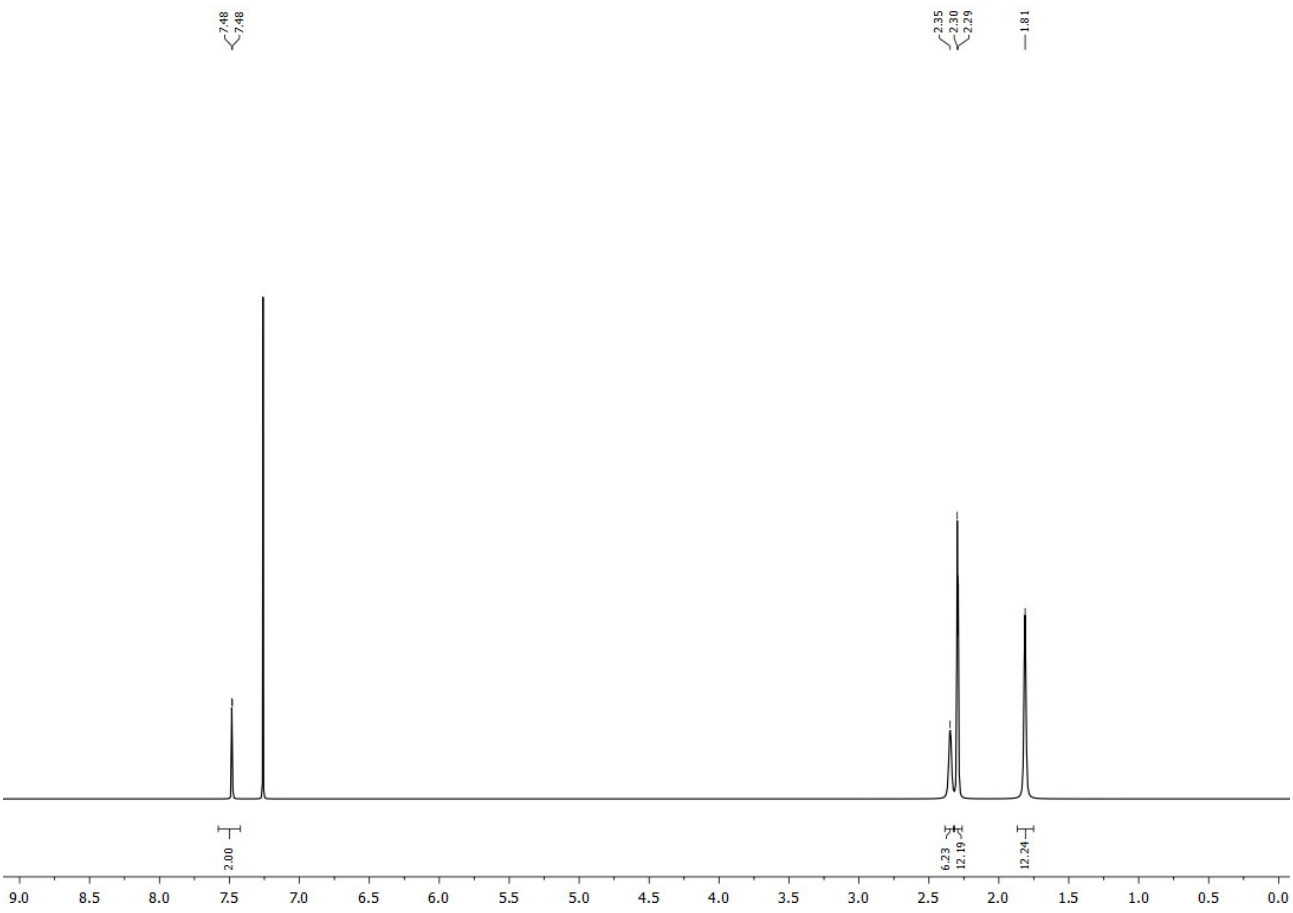

Figure S2: ^{1}H NMR spectrum of [Au(IAd)Cl] (**2b**) in $CDCl_3$ at 298 K

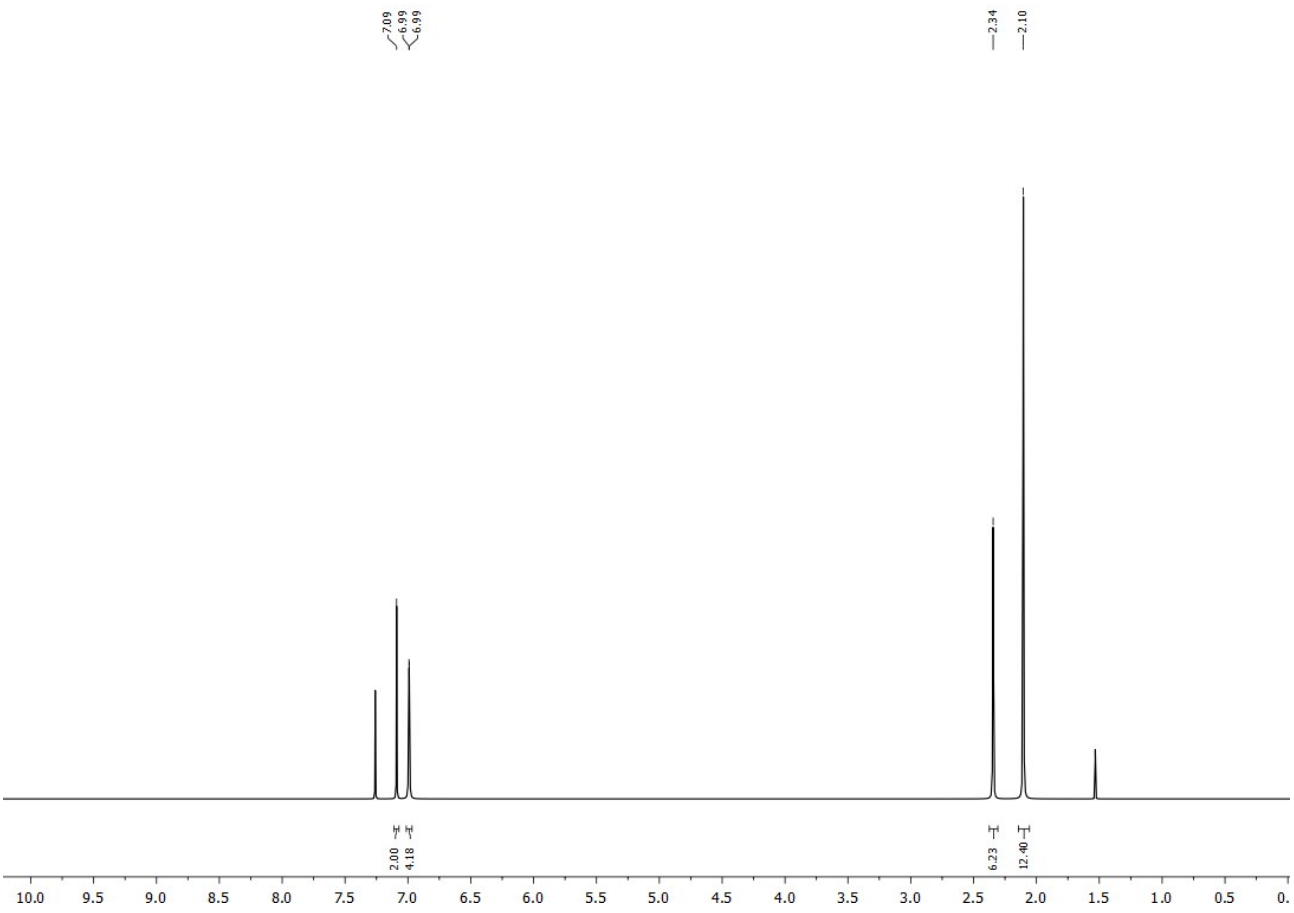

Figure S3: ^{1}H NMR spectrum of [Au(IMes)Cl] (**2c**) in $CDCl_3$ at 298 K

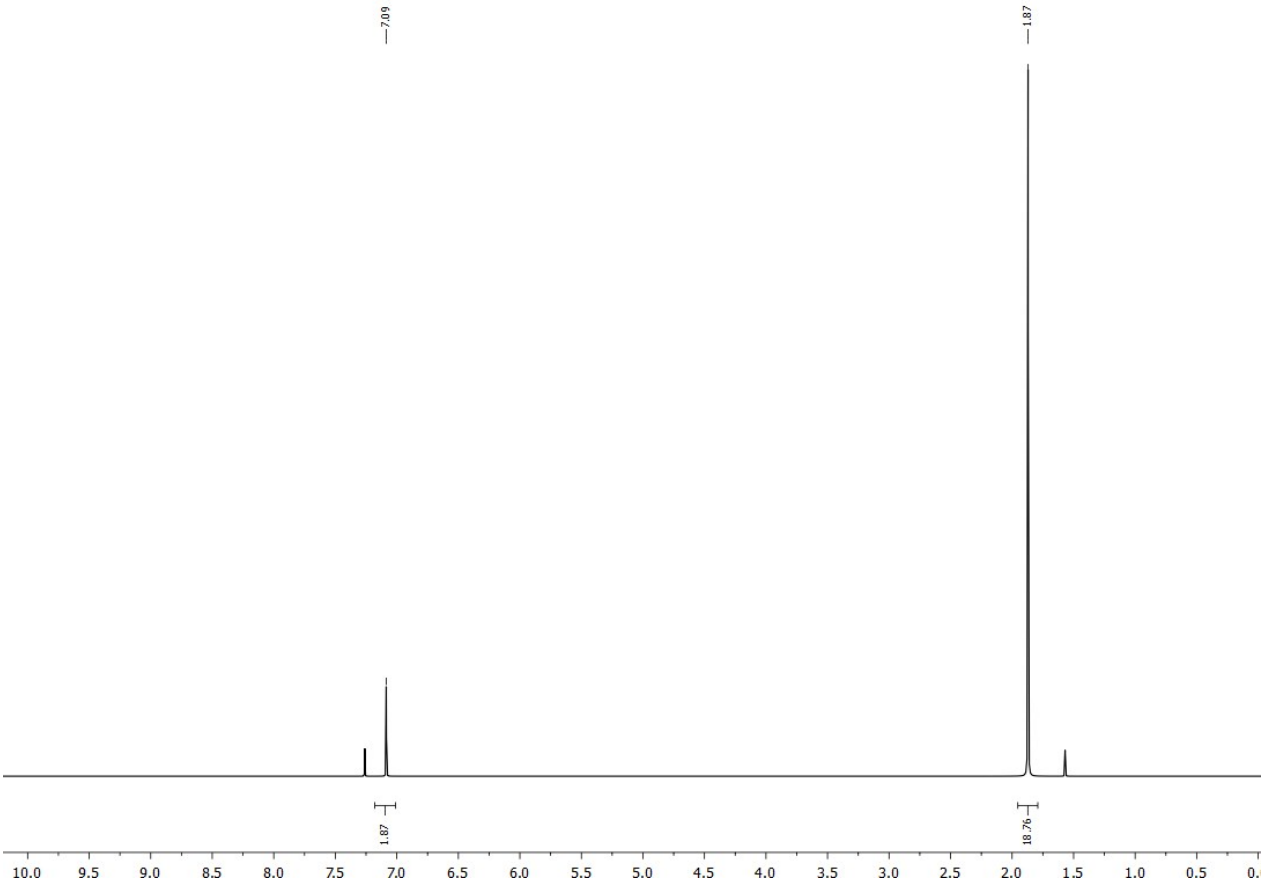

Figure S4: ^{1}H NMR spectrum of [Au(I^{t}Bu)Cl] (**2d**) in $CDCl_3$ at 298 K

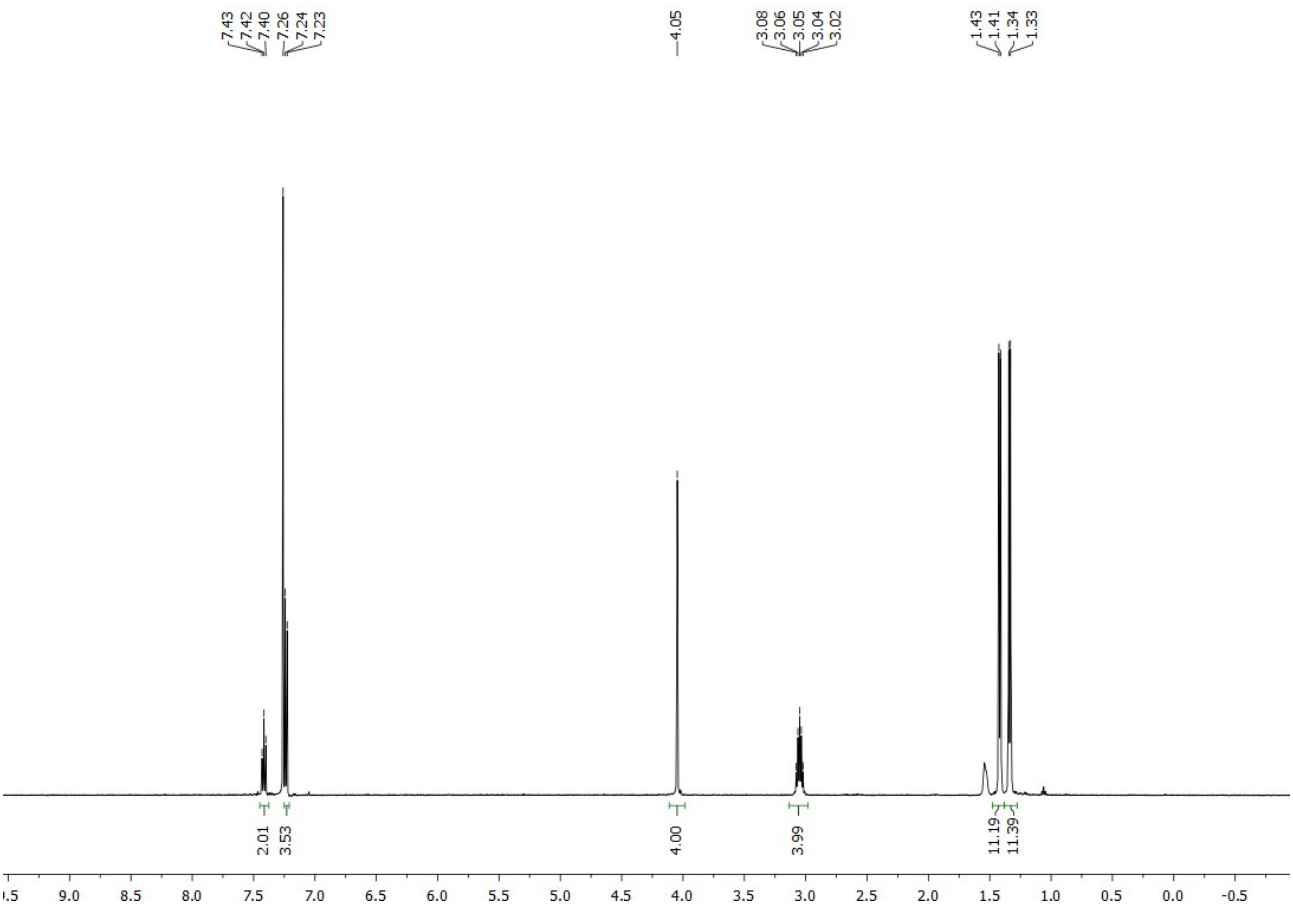

Figure S5: ^{1}H NMR spectrum of [Au(SIPr)Cl] (**2e**) in $CDCl_3$ at 298 K

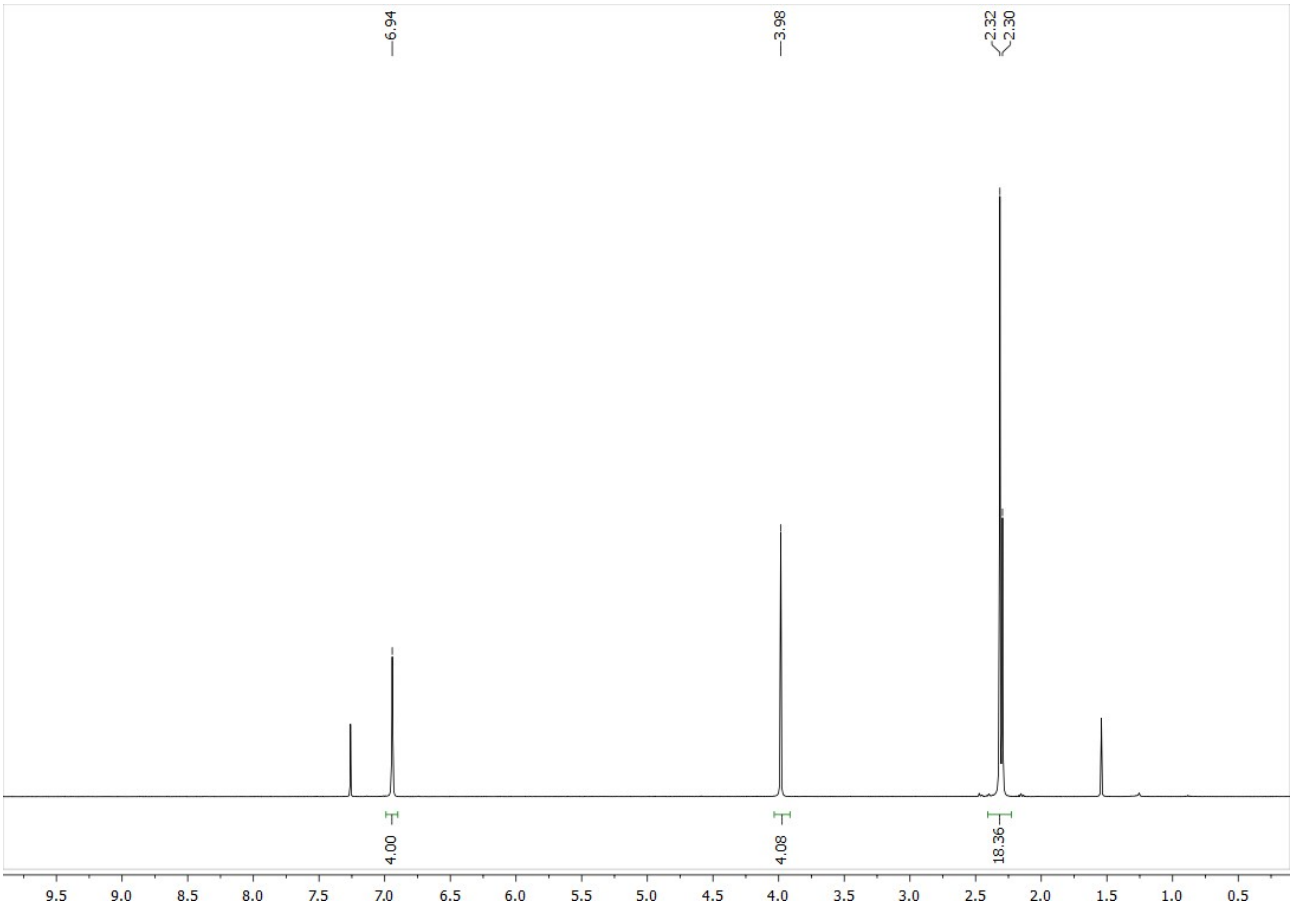

Figure S6: ^{1}H NMR spectrum of [Au(SIMes)Cl] (**2f**) in $CDCl_3$ at 298 K

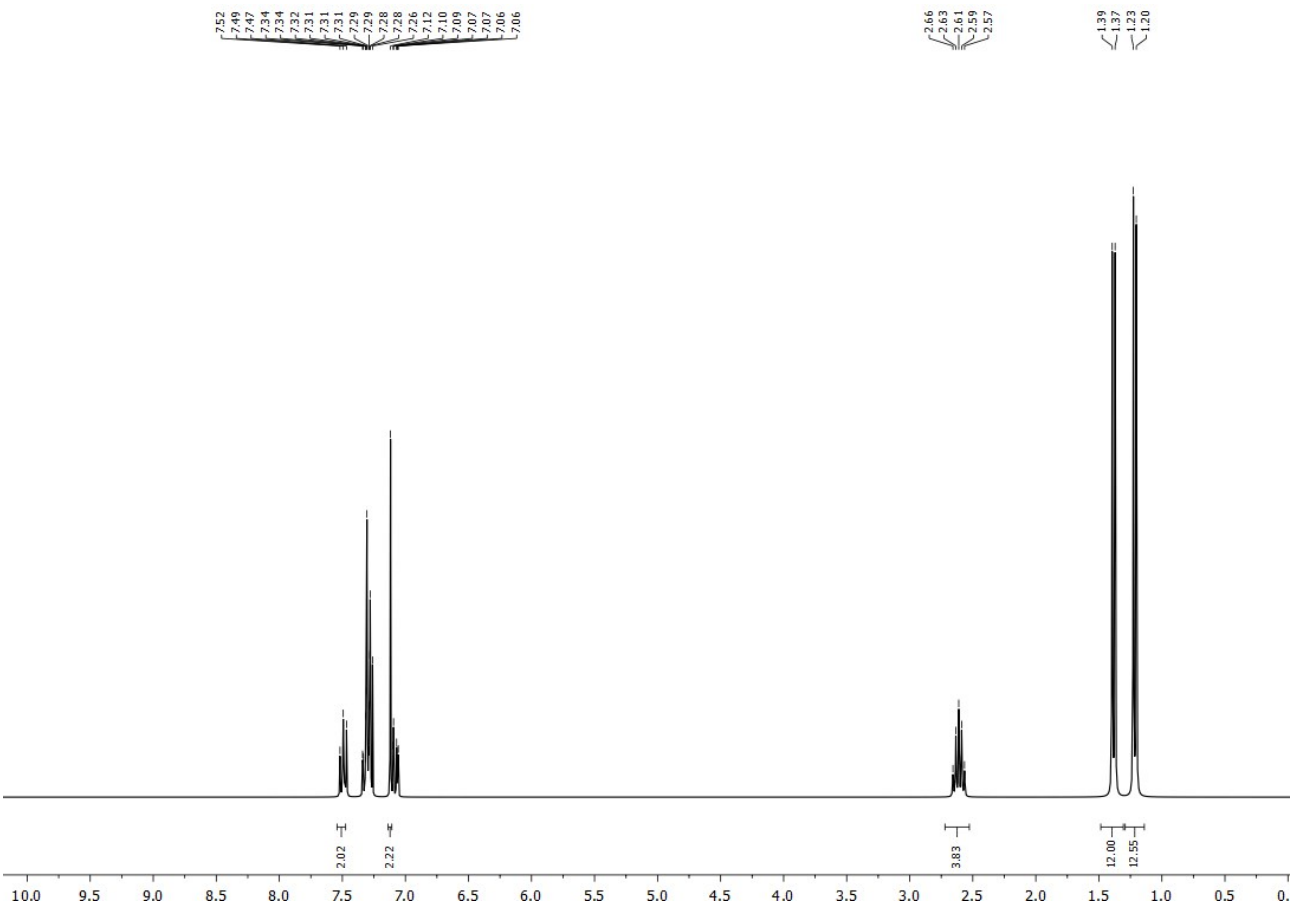

Figure S7: ^{1}H NMR spectrum of [Au(IPr)CCPh] (**3a**) in $CDCl_3$ at 298 K

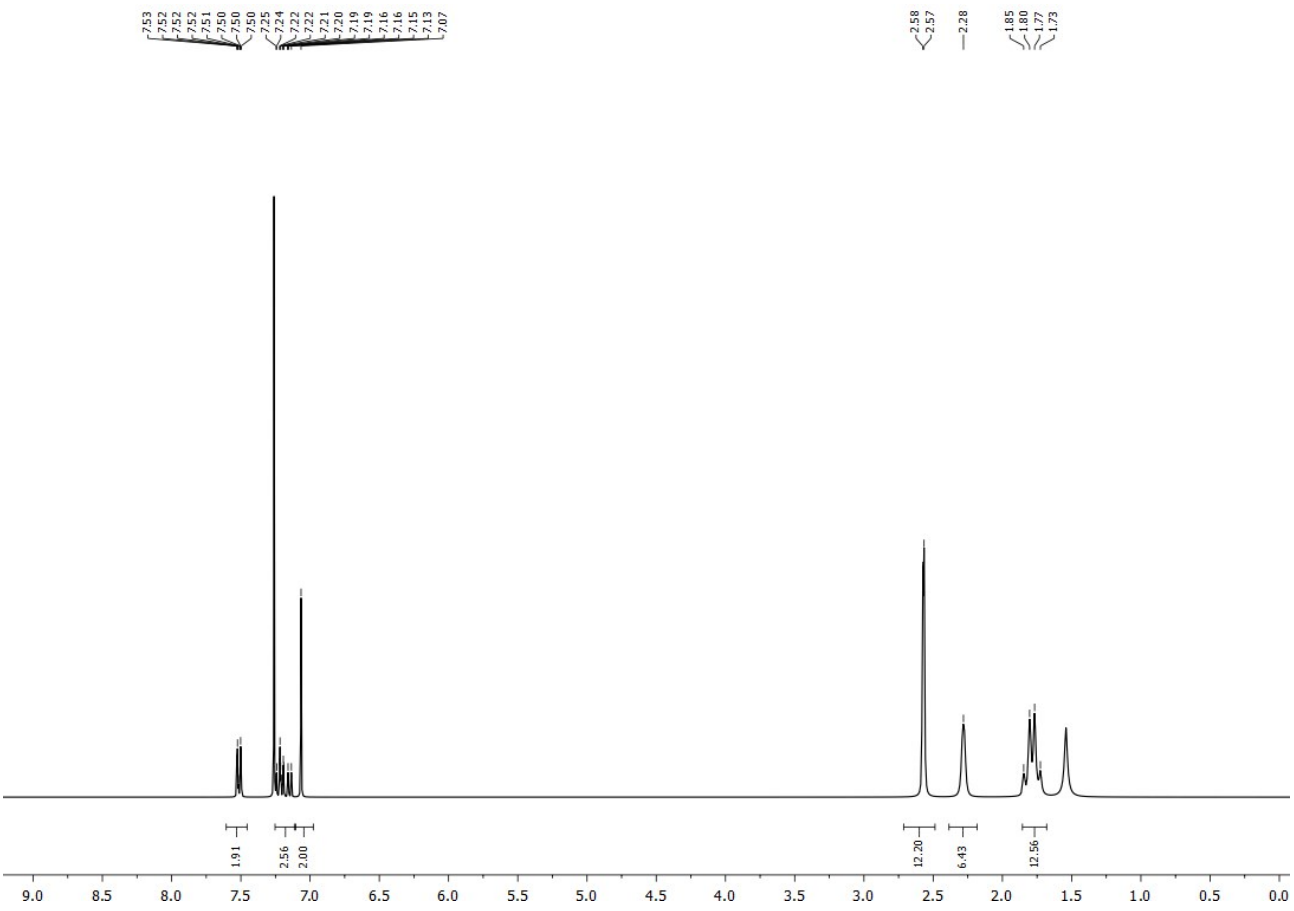

Figure S8: ^{1}H NMR spectrum of [Au(IAd)CCPh] (**3b**) in $CDCl_3$ at 298 K

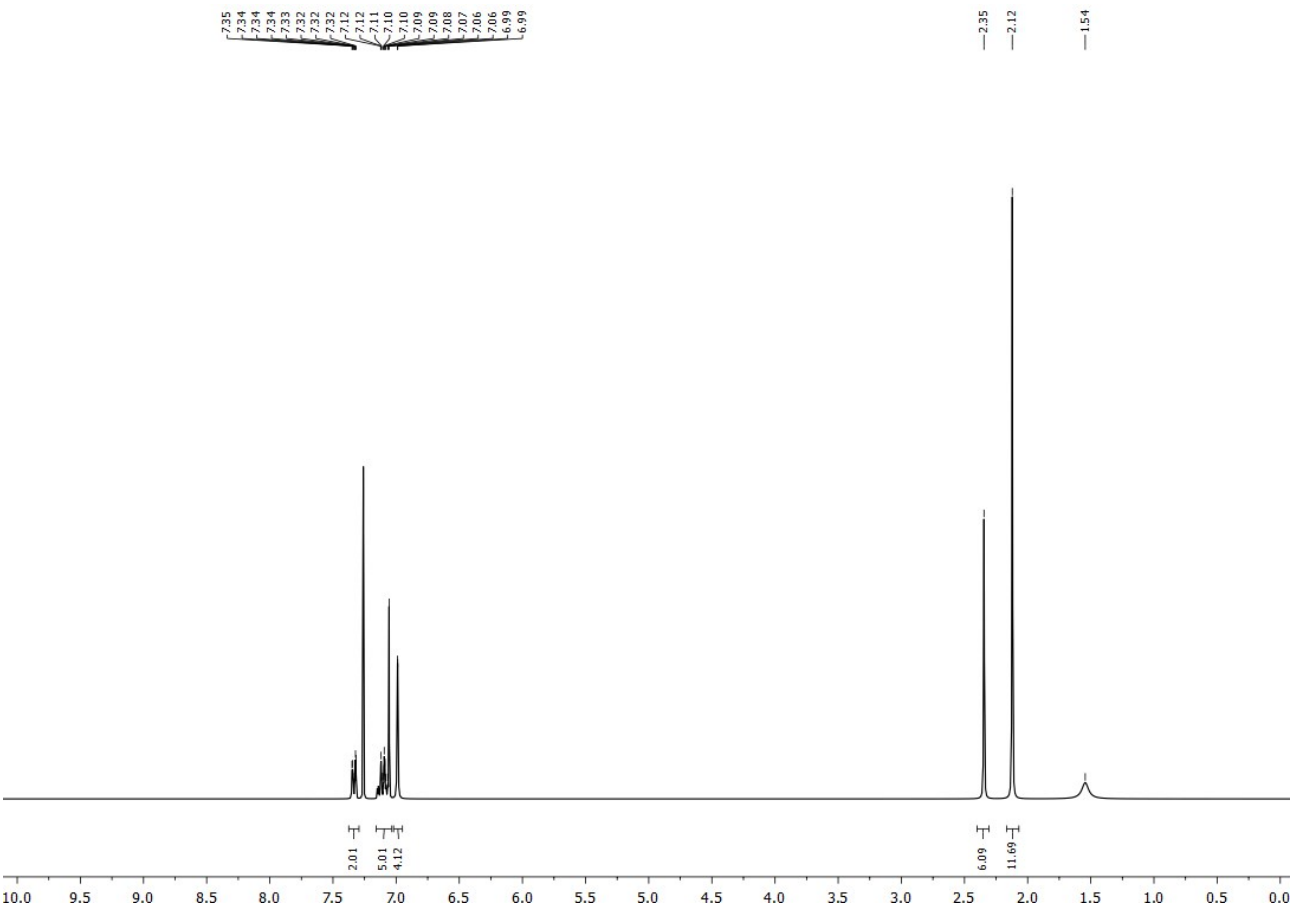

Figure S9: ^{1}H NMR spectrum of [Au(IMes)CCPh] (**3c**) in $CDCl_3$ at 298 K

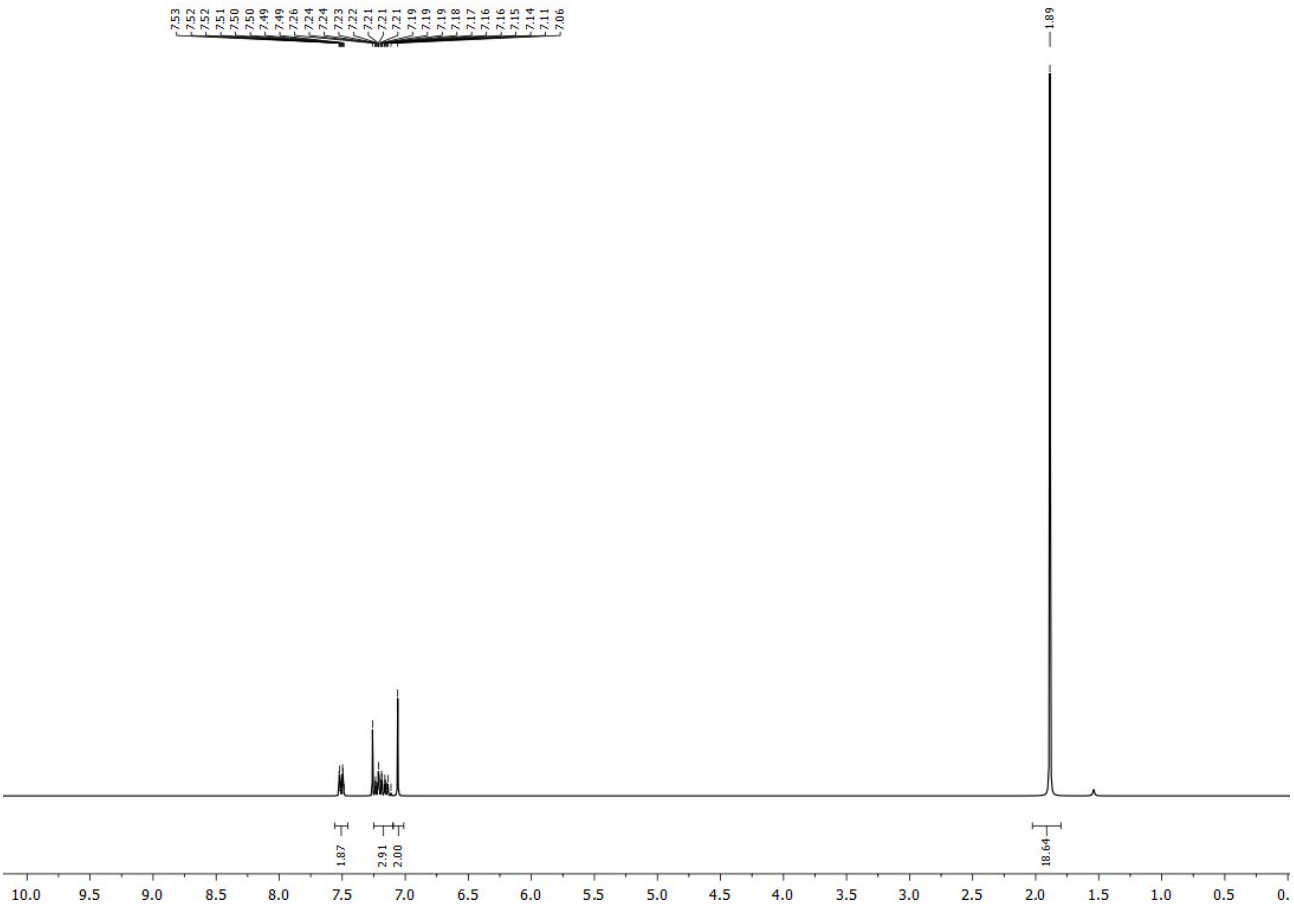

Figure S10: ^{1}H NMR spectrum of [Au(I^{t}Bu)CCPh] (**3d**) in $CDCl_3$ at 298 K

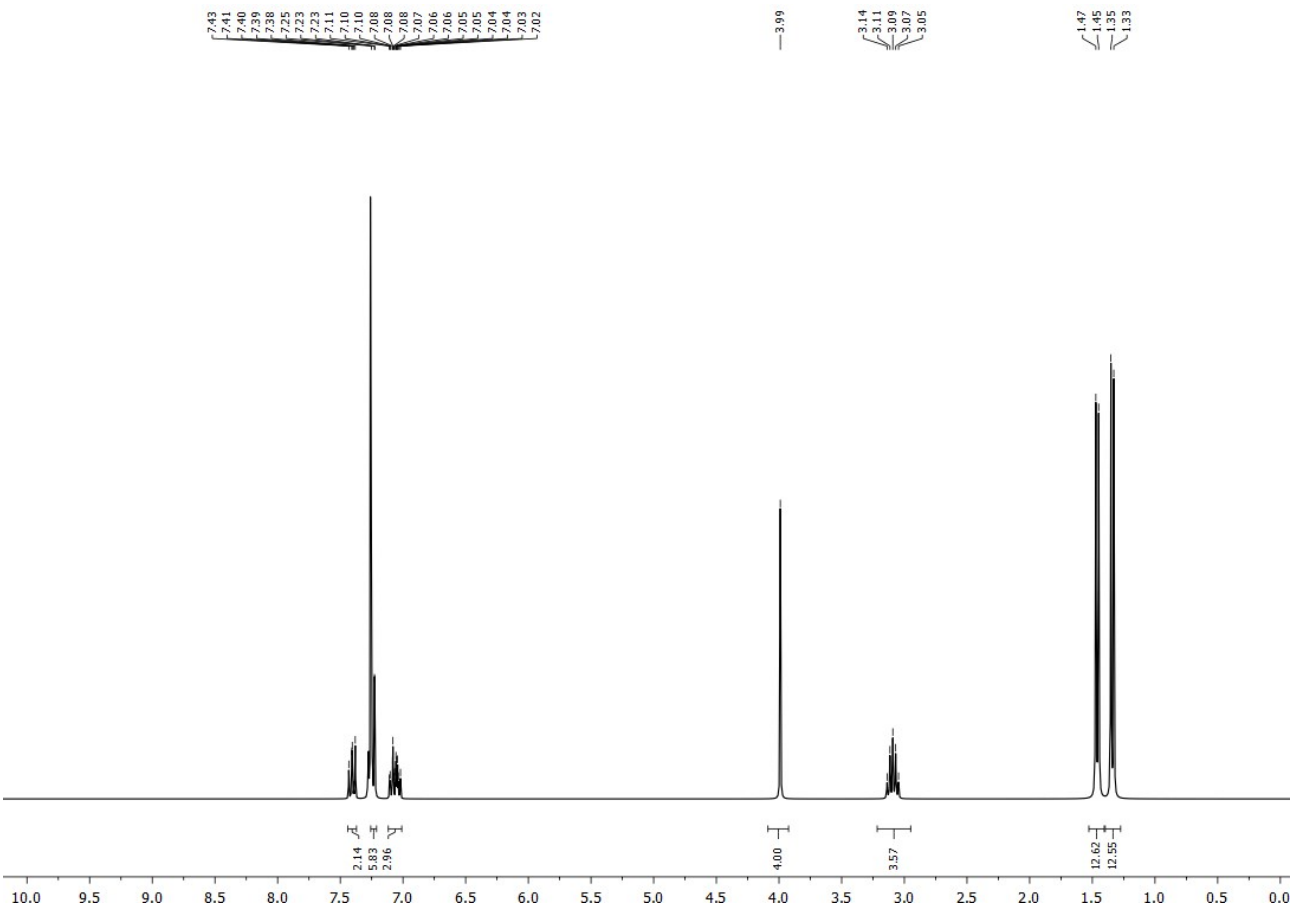

Figure S11: ^{1}H NMR spectrum of [Au(SIPr)CCPh] (**3e**) in $CDCl_3$ at 298 K

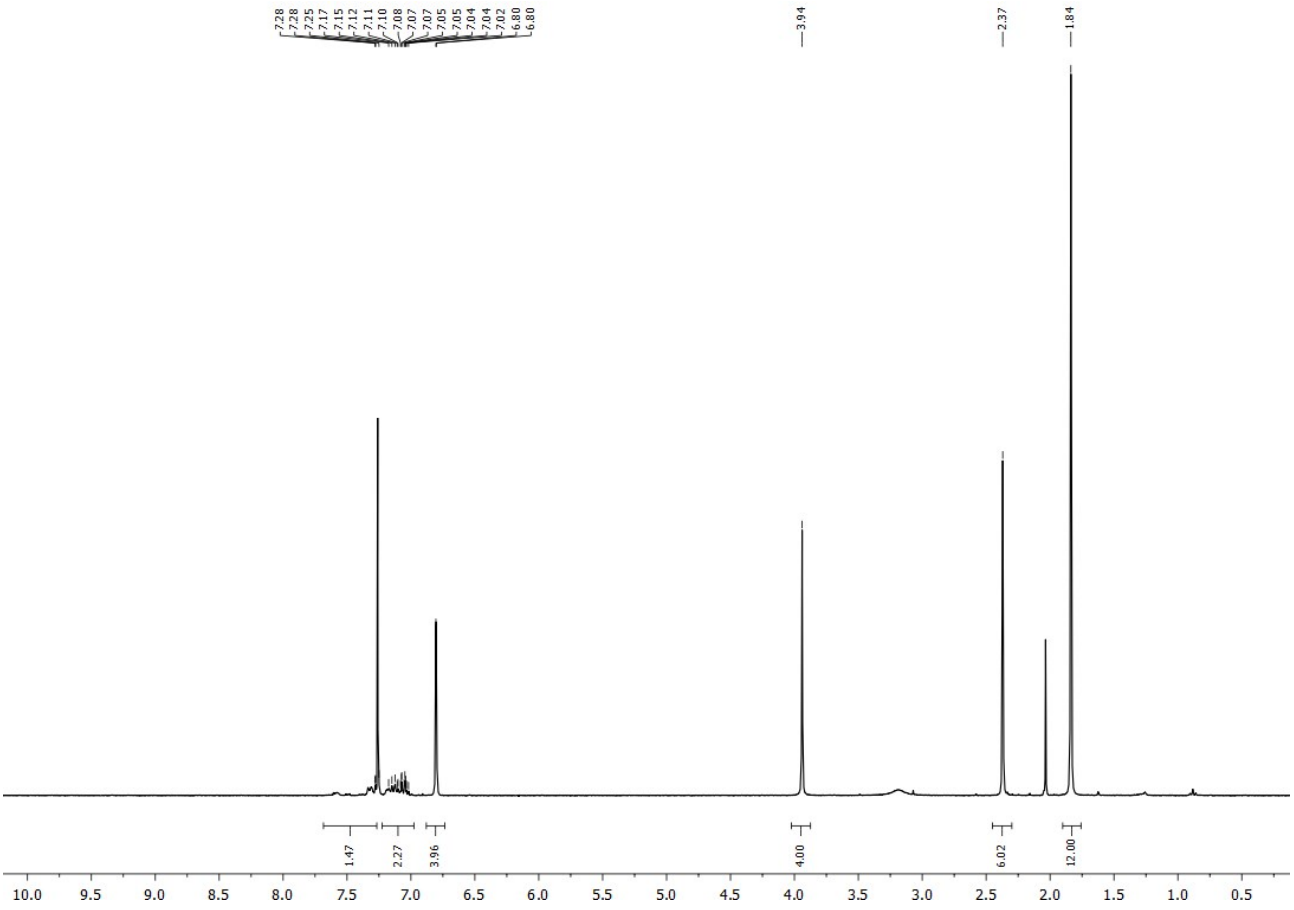

Figure S12: ^{1}H NMR spectrum of [Au(SIMes)CCPh] (**3f**) in $CDCl_3$ at 298 K

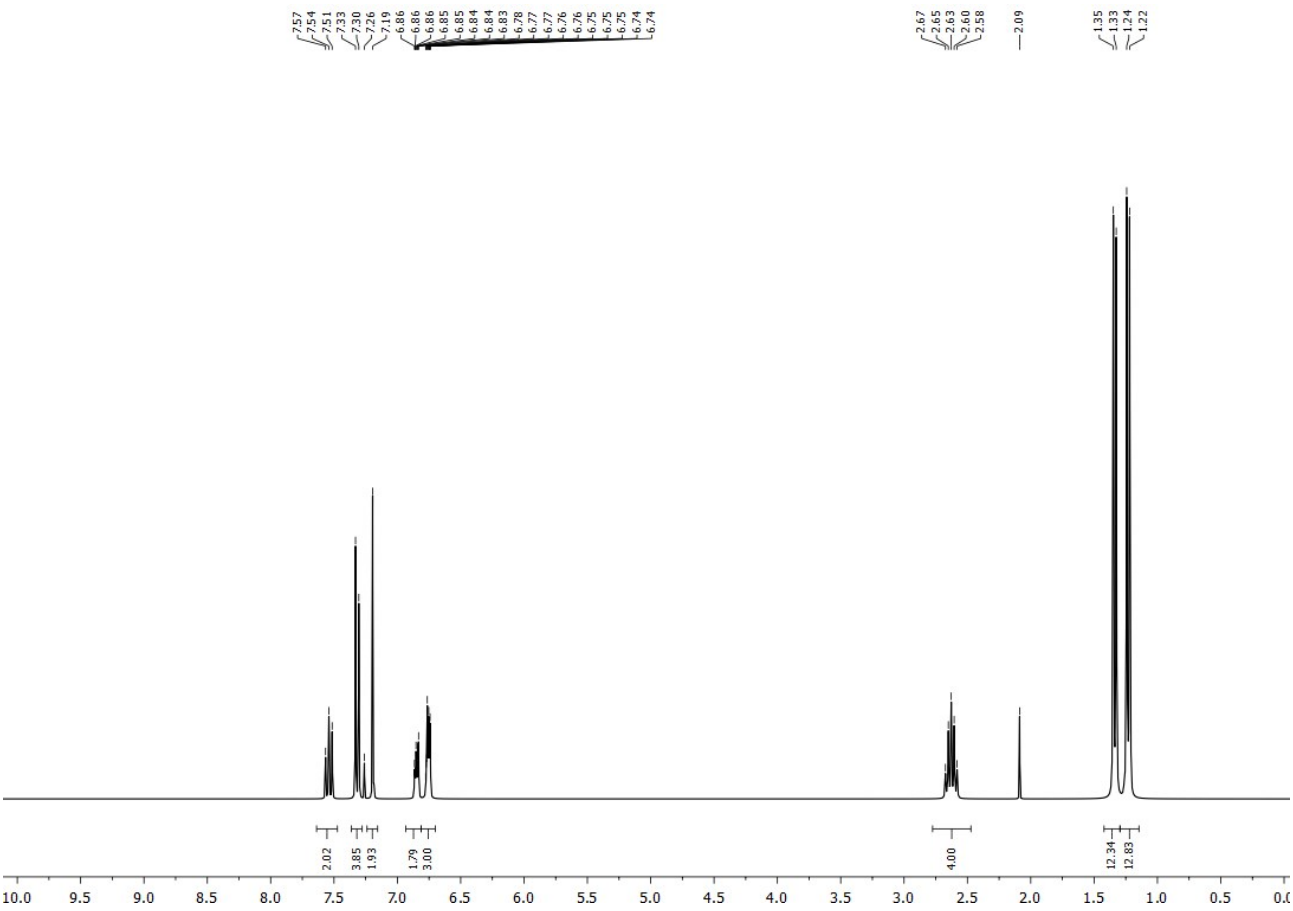

Figure S13: ^{1}H NMR spectrum of [Au(IPr)SPh] (**5a**) in $CDCl_3$ at 298 K

Computational details

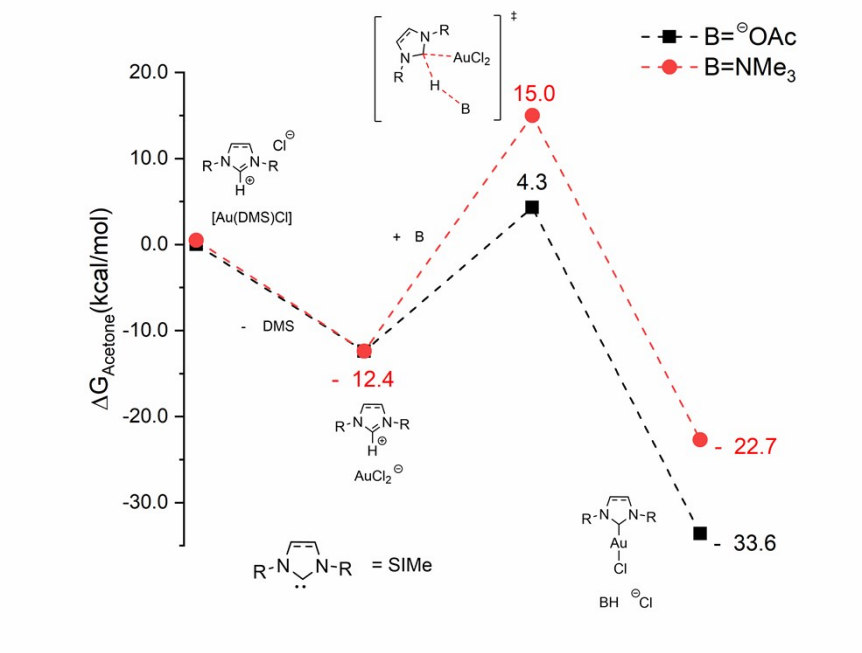

Figure S14: Calculated Gibbs energies (kcal mol^{-1}) for the formation of complex [Au(NHC)Cl] (NHC = SIMe) using NMe_3 and NaOAc as model bases.

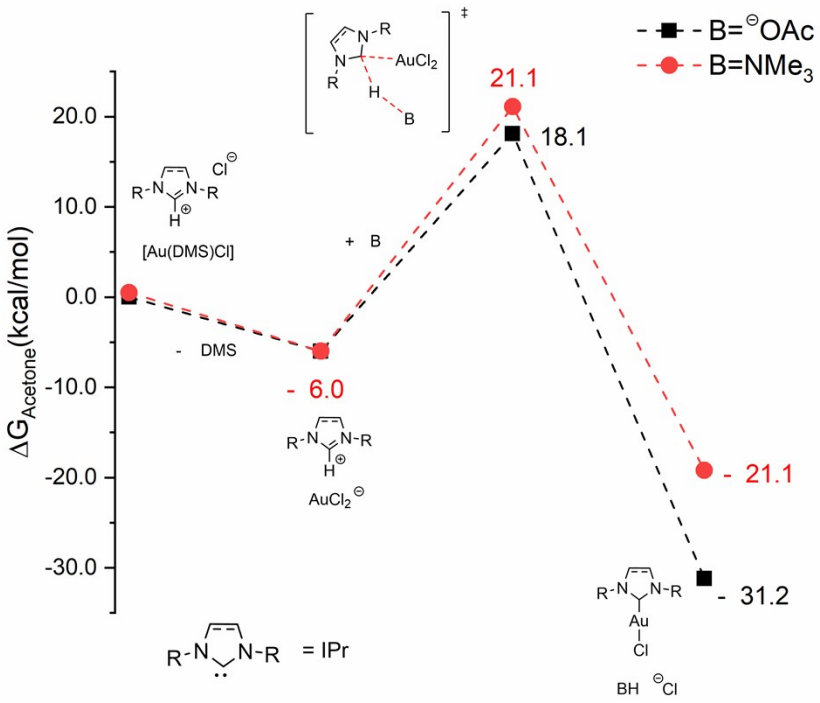

Figure S15: Calculated Gibbs energies (kcal mol^{-1}) for the formation of complex [Au(IPr)Cl] **2a** using NMe_3 and NaOAc as model bases.

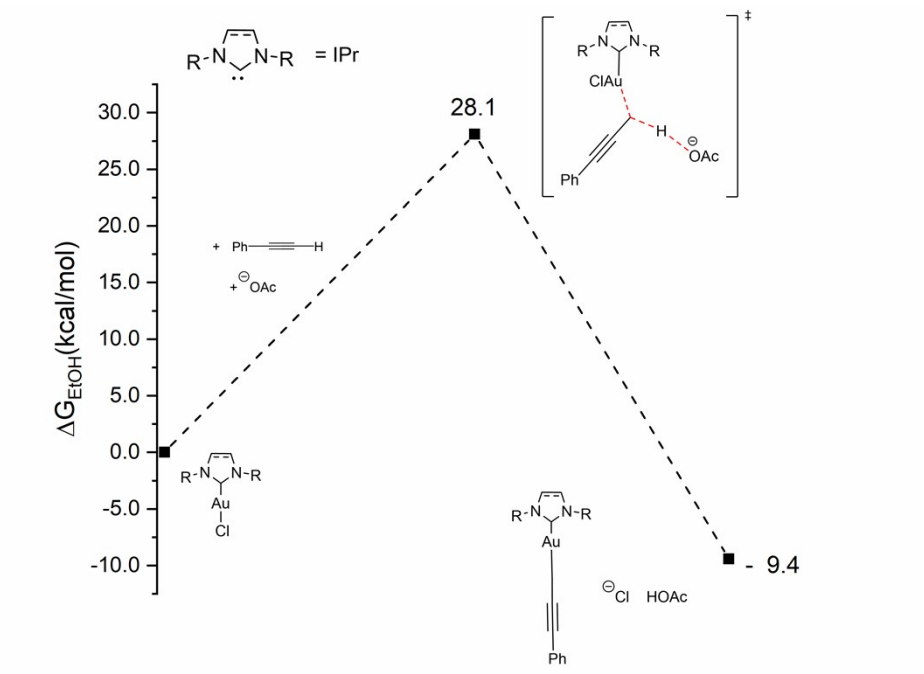

Figure S16: Calculated Gibbs energies (kcal mol^{-1}) for the formation of complex [Au(IPr)(C≡CPh)] **3a** in the presence of NaOAc as a weak base.

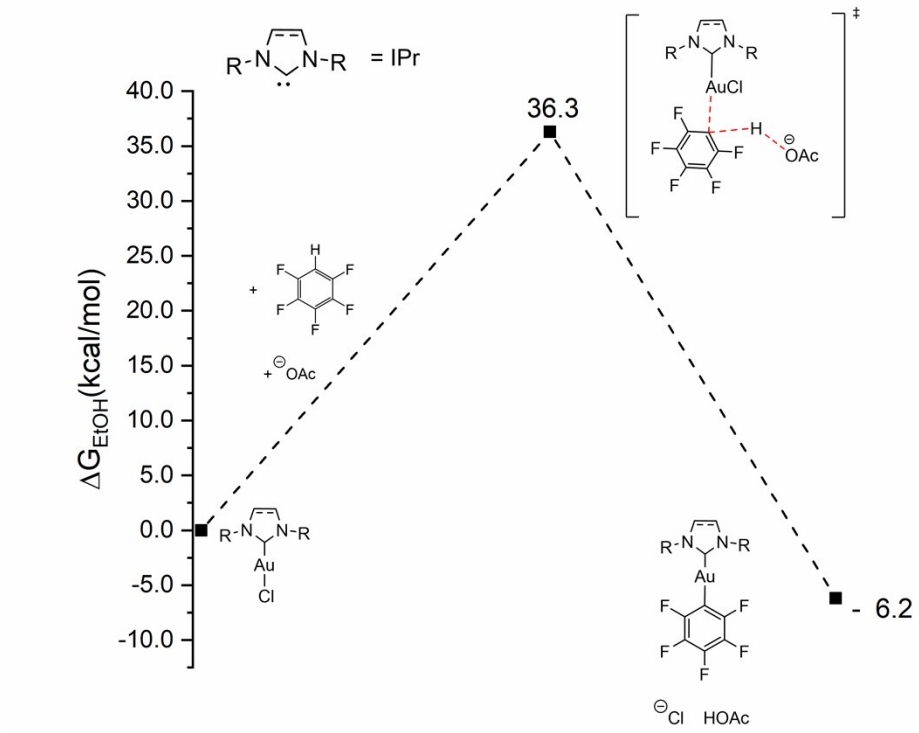

Figure S17: Calculated Gibbs energies (kcal mol^{-1}) for the C-H activation of pentafluorobenzene with complex [Au(IPr)Cl] **2a** in the presence of NaOAc.

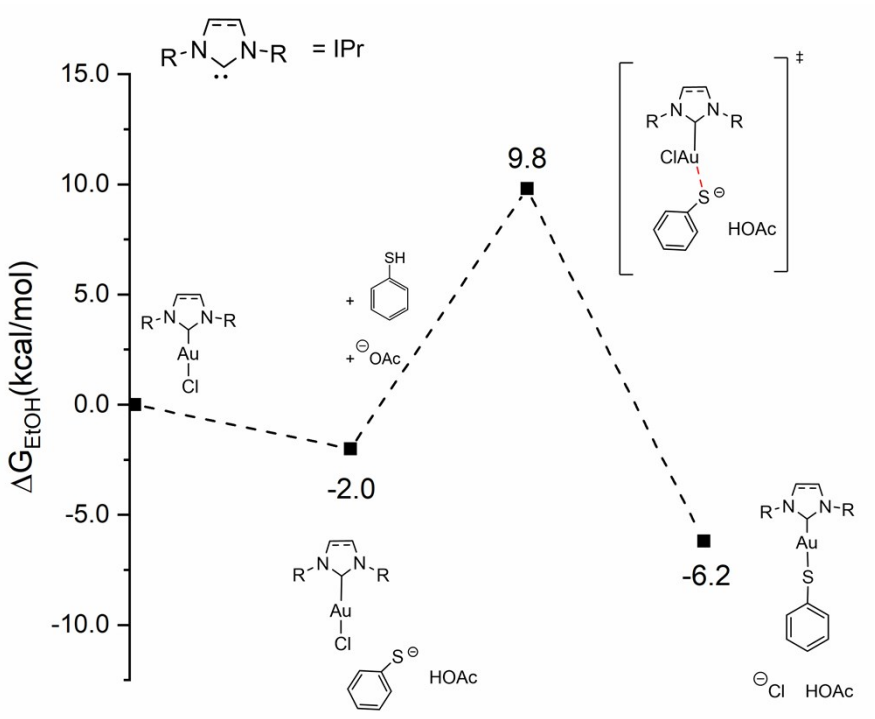

Figure S18: Calculated Gibbs energies (kcal mol^{-1}) for the formation of complex [Au(IPr)(SPh)] **5a** in the presence of NaOAc.

Cartesian Coordinates.

TS-SIMe-OAc

C	0.982378	-3.109073	-0.227167
N	0.812960	-1.819252	-0.877957
C	0.643315	-0.832203	0.024433
N	0.964503	-1.327240	1.229612
C	1.464544	-2.686287	1.155563
C	0.287810	-1.751007	-2.212475
Au	-1.180721	0.477651	-0.019026
Cl	-1.418590	2.836396	0.310096
C	1.142995	-0.530586	2.405962
Cl	-2.461201	-1.650201	-0.223039
O	2.245946	1.336143	-0.792139
C	3.418910	1.031750	-0.286491
O	3.641803	0.122431	0.484198
C	4.494791	1.970960	-0.779170
H	0.923610	-2.334362	-2.899386
H	-0.752407	-2.121330	-2.237063
H	0.278237	-0.700516	-2.532163
H	2.215816	-0.393994	2.629456
H	0.684676	0.451875	2.228830
H	0.641185	-0.997327	3.269811
H	1.700770	-3.748742	-0.764470
H	0.002503	-3.620595	-0.178035
H	2.569831	-2.680373	1.229402
H	1.059427	-3.313865	1.965507
H	4.263461	2.994767	-0.449193
H	5.471032	1.660894	-0.388641
H	4.507032	1.983330	-1.878842
H	1.515527	0.716033	-0.454092

TS-IPr-OAc

C	0.855399	-0.501323	2.762677
N	1.208140	-0.464964	1.423643
C	0.187577	-0.006416	0.637009
N	-0.799238	0.262550	1.541814
C	-0.414130	-0.035767	2.834969
Au	-0.852049	-0.681109	-1.326801
Cl	-1.387310	1.170538	-2.840091
Cl	-1.307522	-3.054241	-0.966543
O	1.896741	0.686667	-1.955572
C	1.873738	1.965287	-2.301259
O	1.738838	2.872632	-1.509893
C	2.001207	2.152686	-3.781312
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H	2.692953	1.421265	-4.220005
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H	1.538924	-0.842789	3.534085
H	-1.073852	0.112091	3.683593
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C	-2.159133	2.119768	0.716079
C	-3.228319	0.007084	1.415023
C	-3.427862	2.639066	0.457381
C	-4.474629	0.588621	1.159203
C	-4.576389	1.889958	0.688953
H	-3.514555	3.648407	0.054322
H	-5.378649	-0.005707	1.307882
H	-5.559275	2.319480	0.477922
C	2.561747	-0.635890	0.985887
C	2.931477	-1.814636	0.313926
C	3.476285	0.400151	1.252489
C	4.265090	-1.939469	-0.084322
C	4.800673	0.219362	0.841922
C	5.192423	-0.937227	0.179538
H	4.576070	-2.838649	-0.618707
H	5.531501	1.008391	1.034075
H	6.230090	-1.055285	-0.143990
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H	1.981297	1.701956	2.026317
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H	-0.152312	2.278344	0.065969
C	-3.156752	-1.437144	1.876520
H	-2.120156	-1.782521	1.741625

C	-4.026403	-2.353262	1.018034
H	-5.099288	-2.127537	1.134542
H	-3.742459	-2.273774	-0.039957
H	-3.869916	-3.401238	1.316141
C	-3.539029	-1.569079	3.352669
H	-4.585516	-1.261150	3.513163
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H	-2.912381	-0.946018	4.008298
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H	4.705027	1.645201	3.437461
H	3.259648	2.540383	3.970231
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H	0.564077	4.048401	1.637999
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TS-IPr-OAc-HCCPh

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C	-1.991784	-1.857507	1.594243
C	-1.295319	-0.674150	1.883413
C	-1.938904	0.558026	2.105598
C	-3.334725	0.555243	2.088859
N	0.135809	-0.720297	1.876888
C	0.871854	-0.439541	0.767073
N	2.149401	-0.720063	1.137304
C	2.205021	-1.193350	2.439638
C	0.930462	-1.193163	2.904821

Au	0.050049	0.123794	-0.959620
Cl	-0.426471	-1.378865	-2.967927
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C	3.960739	0.473178	0.011265
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C	5.396146	-0.768227	-1.505287
C	4.650714	-1.921672	-1.300418
C	3.551577	-1.919877	-0.435718
C	3.541821	1.761692	0.691489
C	4.024086	1.819274	2.142481
C	2.720873	-3.173874	-0.251927
C	3.524989	-4.263821	0.457250
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C	-1.935335	3.093594	1.978263
O	0.883167	3.782678	0.589583
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C	1.542661	5.678789	-0.710640
O	0.355585	3.872278	-1.595994
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H	-5.294349	-2.137400	-2.012177
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H	5.621701	1.323812	-1.064270

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H	6.247312	-0.784296	-2.191069
H	3.546602	3.891868	0.423260
H	5.081636	3.131879	-0.057007
H	3.639878	2.989004	-1.104787
H	3.653885	2.737842	2.623552
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H	-5.144538	-0.575395	1.799658
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H	-2.712618	-3.811912	-0.271871
H	-1.336481	-2.882529	-0.931194
H	-0.993962	-5.149596	2.058336
H	-1.267365	-3.898593	3.300670
H	-2.626706	-4.495765	2.323164
H	-1.252084	3.954017	1.993819
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H	-2.744948	3.278972	2.705132
H	0.067339	2.830950	3.797226
H	-1.344123	1.968962	4.472748
H	0.095154	1.062316	3.944556

IPr-Au-CCPh

C	5.944321	-0.698018	-0.860993
C	5.210764	0.166881	-0.026123
C	5.922955	1.053757	0.803968
C	7.313663	1.071720	0.797478
C	8.027542	0.209285	-0.035013
C	7.334858	-0.674232	-0.863277
C	3.784955	0.142213	-0.020923
C	2.556418	0.115417	-0.017110
Au	0.577777	0.042958	-0.005632
C	-1.445310	-0.048982	0.011391

N	-2.324721	0.980320	-0.004575
C	-3.629510	0.527907	0.019508
C	-3.564968	-0.829130	0.049779
N	-2.223181	-1.156537	0.045453
C	-1.934411	2.356433	-0.048579
C	-1.804464	2.972615	-1.303660
C	-1.414646	4.314009	-1.321601
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C	-1.287816	4.359152	1.088018
C	-1.674606	3.018229	1.161568
C	-2.003187	2.207319	-2.596840
C	-0.649667	1.894488	-3.238174
C	-1.759242	2.314927	2.501156
C	-0.370671	2.174811	3.126623
C	-1.703682	-2.489827	0.072458
C	-1.480930	-3.094300	1.320073
C	-0.962116	-4.391447	1.319763
C	-0.677717	-5.047621	0.126690
C	-0.899747	-4.417534	-1.092805
C	-1.416644	-3.120487	-1.148291
C	-1.721109	-2.356601	2.622194
C	-0.389839	-1.910971	3.230478
C	-1.604593	-2.423855	-2.481002
C	-0.251460	-2.132570	-3.131311
C	-2.550428	-3.173911	3.609946
C	-2.525774	-3.211346	-3.410928
C	-2.935670	2.930766	-3.565648
C	-2.741897	3.006720	3.444421
H	5.400232	-1.389444	-1.507516
H	5.362506	1.728159	1.454484
H	7.885386	-1.353882	-1.518946
H	7.847613	1.767419	1.449999
H	9.120093	0.225582	-0.038179
H	-4.342257	-1.587059	0.074349
H	-4.475149	1.209139	0.011728
H	-0.766329	-4.891768	2.270663
H	-2.295547	-1.446145	2.390488
H	-0.656256	-4.938172	-2.021835
H	-2.087407	-1.453926	-2.287148
H	-1.294347	4.825275	-2.279098
H	-2.476979	1.245109	-2.347606
H	-1.070338	4.905444	2.008750
H	-2.137587	1.296810	2.322528
H	-0.267935	-6.060137	0.148259

H	-0.559315	-1.319127	4.143639
H	0.231627	-2.779874	3.498591
H	0.185578	-1.295638	2.521222
H	-2.769344	-2.578087	4.509307
H	-3.507330	-3.492394	3.169010
H	-2.016080	-4.077830	3.941307
H	-0.386059	-1.564485	-4.064898
H	0.392252	-1.543756	-2.459373
H	0.281032	-3.064825	-3.377232
H	-2.689648	-2.657329	-4.348102
H	-2.093669	-4.188374	-3.678300
H	-3.506580	-3.395682	-2.946492
H	-0.853313	6.048634	-0.174717
H	-0.781886	1.279649	-4.142205
H	-0.128373	2.819903	-3.529688
H	0.004646	1.348194	-2.540958
H	-3.112467	2.312274	-4.458923
H	-3.909871	3.149718	-3.102488
H	-2.506552	3.884426	-3.910365
H	-0.426974	1.603035	4.065989
H	0.319512	1.651759	2.446459
H	0.064852	3.159871	3.357340
H	-2.828922	2.445852	4.387779
H	-2.411345	4.026379	3.697123
H	-3.744943	3.082235	2.997423

TS-IPr-OAc-HC$_6$F$_5$

C	-4.055543	-0.242090	2.352726
C	-3.632545	-1.492948	1.918778
C	-2.272901	-1.771506	1.762391
C	-1.365105	-0.735782	2.047133
C	-1.760681	0.548522	2.462779
C	-3.133464	0.763641	2.616262
N	0.031237	-1.033535	1.944651
C	0.845052	-0.666867	0.922123
N	2.055395	-1.185563	1.265079
C	2.000741	-1.860250	2.468789
C	0.717841	-1.765898	2.898973
Au	0.604903	0.413309	-0.739275
Cl	1.736196	1.466501	-2.611326
C	3.237344	-1.050786	0.471607
C	4.005693	0.117253	0.596193
C	5.191016	0.185789	-0.139322
C	5.574881	-0.852750	-0.980113
C	4.763111	-1.972034	-1.126538

C	3.570284	-2.091210	-0.409540
C	3.557785	1.284779	1.450857
C	4.375008	1.378769	2.738862
C	2.623002	-3.244285	-0.672335
C	3.308431	-4.605236	-0.582455
C	-1.786245	-3.126156	1.275274
C	-2.750231	-4.263945	1.592941
C	-0.748002	1.656495	2.700153
C	0.098668	1.417587	3.953653
C	-1.900165	0.824149	-1.437231
C	-2.993086	1.292619	-0.730075
C	-4.246896	0.685304	-0.707896
C	-4.425733	-0.494427	-1.419693
C	-3.367210	-1.004994	-2.163799
C	-2.147057	-0.331064	-2.159889
C	3.571316	2.589788	0.656773
C	1.928411	-3.040521	-2.021056
C	-1.451166	-3.103496	-0.217281
C	-1.369062	3.045206	2.760409
O	0.317835	3.354766	0.122642
C	0.096718	3.844030	-0.968685
C	0.841152	5.052078	-1.473947
O	-0.754104	3.384919	-1.850863
H	1.648769	4.663352	-2.114801
H	0.196166	5.692252	-2.090924
H	1.276155	5.613460	-0.637991
H	-1.041749	2.431900	-1.638904
H	2.874255	-2.337212	2.902622
H	0.230155	-2.135036	3.796257
H	5.808382	1.083998	-0.070131
H	2.510478	1.104040	1.731814
H	5.046474	-2.758143	-1.830425
H	1.841415	-3.220587	0.102099
H	-4.373425	-2.258294	1.683450
H	-0.847751	-3.343678	1.811285
H	-3.489167	1.749999	2.912199
H	-0.084535	1.663492	1.818462
H	6.501143	-0.773525	-1.554850
H	3.064720	3.383430	1.225517
H	4.600264	2.922940	0.441012
H	3.030370	2.466381	-0.294046
H	4.013159	2.209897	3.365074
H	4.306316	0.452074	3.330775
H	5.440898	1.559348	2.521522

H	1.181452	-3.830431	-2.198031
H	1.416717	-2.066502	-2.061673
H	2.658464	-3.065969	-2.845740
H	2.573071	-5.413858	-0.718450
H	4.075474	-4.728066	-1.363736
H	3.798645	-4.748051	0.393477
H	-5.123048	-0.035224	2.449589
H	-0.964474	-4.046643	-0.513637
H	-2.357958	-2.987173	-0.826972
H	-0.777769	-2.274018	-0.475469
H	-2.290408	-5.229496	1.331251
H	-3.021472	-4.289520	2.659929
H	-3.679057	-4.181997	1.007007
H	-0.566404	3.795935	2.765314
H	-1.987691	3.237270	1.876167
H	-1.977147	3.185783	3.671010
H	0.826066	2.236136	4.072423
H	-0.535365	1.396141	4.856132
H	0.667543	0.478773	3.917493
F	-5.593779	-1.140414	-1.376052
F	-5.268985	1.186409	-0.002832
F	-2.904484	2.434235	-0.008789
F	-3.537410	-2.160831	-2.821960
F	-1.172710	-0.918006	-2.887485

IPr-Au-C_6F_5

C	1.688184	-3.048088	1.234142
C	1.929649	-2.424664	-0.000255
C	1.687780	-3.047886	-1.234677
C	1.200890	-4.357058	-1.206794
C	0.962555	-5.006098	-0.000308
C	1.201272	-4.357249	1.206206
N	2.400515	-1.072417	-0.000197
C	1.575084	-0.001107	-0.000008
N	2.402408	1.068745	0.000056
C	3.726941	0.676791	-0.000027
C	3.725736	-0.682810	-0.000196
C	1.933888	2.421809	0.000200
C	1.693601	3.045788	-1.234154
C	1.208849	4.355747	-1.206114
C	0.971062	5.004843	0.000454
C	1.208269	4.355295	1.206888
C	1.693013	3.045325	1.234668
C	1.881530	2.322118	-2.552429
C	2.777137	3.099643	-3.514553

C	1.880503	2.321283	2.552800
C	0.522679	1.995288	3.177302
Au	-0.449480	0.000458	0.000054
C	-2.489146	0.001841	0.000053
C	1.876311	-2.324208	-2.552857
C	2.771268	-3.102439	-3.515019
C	1.877168	-2.324601	2.552369
C	2.772180	-3.103121	3.514243
C	0.518912	-1.996184	-3.177239
C	0.519980	-1.996341	3.177081
C	2.776713	3.098116	3.514936
C	0.523842	1.995372	-3.176868
H	4.538081	-1.403503	-0.000306
H	4.540554	1.396052	0.000033
H	0.990597	-4.871647	-2.147081
H	0.573953	-6.027061	-0.000327
H	0.991271	-4.871988	2.146476
H	0.998795	4.870141	2.147216
H	0.584124	6.026437	0.000552
H	0.999830	4.870956	-2.146343
H	2.378587	-1.367435	-2.342079
H	2.379624	-1.367923	2.341578
H	2.381339	1.363771	2.341939
H	2.383015	1.364899	-2.341757
H	0.648257	-1.412579	-4.101979
H	-0.033566	-2.914830	-3.429578
H	-0.104167	-1.411012	-2.482906
H	2.938044	-2.523474	-4.436367
H	3.752084	-3.321735	-3.066243
H	2.315926	-4.060910	-3.809024
H	0.649656	-1.412900	4.101878
H	-0.103112	-1.410922	2.482971
H	-0.032661	-2.914895	3.429402
H	2.939233	-2.524311	4.435637
H	2.316749	-4.061561	3.808208
H	3.752871	-3.322508	3.065237
H	2.942647	2.518867	4.436257
H	3.757839	3.315920	3.066110
H	2.322858	4.057275	3.808992
H	0.651240	1.411461	4.102009
H	-0.028385	2.914760	3.429733
H	-0.101367	1.411082	2.483025
H	0.652668	1.411776	-4.101686
H	-0.099820	1.410696	-2.482643

H	-0.027774	2.914576	-3.429073
H	2.943499	2.520512	-4.435870
H	2.322548	4.058442	-3.808646
H	3.758104	3.318198	-3.065746
C	-3.224802	-1.177888	0.000243
C	-4.617874	-1.202135	0.000190
C	-5.315733	0.003689	-0.000062
C	-4.616288	1.208599	-0.000251
C	-3.223255	1.182531	-0.000201
F	-2.599466	-2.360894	0.000467
F	-5.288229	-2.348520	0.000366
F	-6.641024	0.004571	-0.000116
F	-5.285161	2.355854	-0.000488
F	-2.596352	2.364729	-0.000395

IPr-Au-Cl SPh HOAc

C	-0.958095	-2.891602	1.169706
C	0.291806	-2.254673	1.279956
C	1.504802	-2.968598	1.300502
C	1.443272	-4.360795	1.202272
C	0.223131	-5.016305	1.092493
C	-0.959356	-4.287443	1.077817
N	0.349344	-0.827482	1.408319
C	0.745196	0.021526	0.425743
N	0.777203	1.241766	1.016948
C	0.414573	1.157439	2.346576
C	0.149501	-0.147327	2.594131
C	1.279655	2.431599	0.396445
C	0.383097	3.338160	-0.192763
C	0.922175	4.497344	-0.760545
C	2.290281	4.739104	-0.747359
C	3.155273	3.821245	-0.161390
C	2.668839	2.650375	0.424061
C	-1.109467	3.101212	-0.215051
C	-1.831070	4.000293	0.788610
C	3.632443	1.666944	1.056814
C	4.367629	2.291542	2.241963
Au	1.346127	-0.432029	-1.409737
Cl	2.161228	-0.975230	-3.508439
C	2.851769	-2.292441	1.462908
C	3.425956	-2.559457	2.854698
C	-2.268904	-2.132653	1.181572
C	-2.865809	-2.103793	2.590883
C	-1.705863	3.253509	-1.611977
C	4.599695	1.089502	0.024861

C	3.826709	-2.684371	0.355535
C	-3.292052	-2.687838	0.194897
O	-2.576615	1.057305	1.885242
C	-3.009981	1.331933	3.094390
O	-2.277951	1.285927	4.063224
C	-4.464775	1.726889	3.196881
S	-4.661276	1.185552	-0.202665
C	-4.018574	0.188347	-1.493638
H	-4.595613	2.734118	2.770415
H	-5.095486	1.055617	2.594089
H	-4.770661	1.733056	4.249761
H	0.302493	2.029334	2.981426
H	-0.227405	-0.626769	3.489961
H	0.247515	5.216951	-1.229311
H	-1.289355	2.068922	0.111777
H	4.231246	4.012592	-0.161279
H	3.041876	0.828328	1.451281
H	2.370883	-4.937976	1.211323
H	2.695702	-1.208691	1.378547
H	-1.913986	-4.807455	0.981515
H	-2.061216	-1.093052	0.893241
H	2.688284	5.649153	-1.203670
H	-2.761501	2.940539	-1.583697
H	-1.662578	4.298243	-1.962758
H	-1.180579	2.621657	-2.343099
H	-2.905103	3.759943	0.773835
H	-1.457378	3.847702	1.812624
H	-1.706200	5.065972	0.532865
H	5.262992	0.345901	0.494295
H	4.052932	0.594476	-0.792434
H	5.235015	1.874120	-0.416151
H	5.017369	1.546651	2.728527
H	5.004375	3.133130	1.924549
H	3.660283	2.671650	2.994760
H	0.193667	-6.106032	1.012217
H	4.773188	-2.133117	0.466709
H	4.064498	-3.759680	0.380755
H	3.409333	-2.446348	-0.634873
H	4.378218	-2.021739	2.990878
H	2.731433	-2.228197	3.641845
H	3.619906	-3.633421	3.008946
H	-4.148472	-2.000188	0.142978
H	-2.878445	-2.771967	-0.819948
H	-3.669812	-3.675550	0.508184

H	-3.826369	-1.567353	2.571895
H	-3.050962	-3.127036	2.958256
H	-2.218330	-1.590143	3.314817
H	-3.314971	1.106693	1.141108
C	-2.638997	-0.009886	-1.708646
C	-2.167469	-0.814809	-2.742183
C	-3.056753	-1.459656	-3.603221
C	-4.427734	-1.275295	-3.410467
C	-4.899477	-0.467390	-2.380212
H	-1.919923	0.472832	-1.045043
H	-1.087673	-0.939479	-2.871667
H	-2.683610	-2.092322	-4.412220
H	-5.144211	-1.771031	-4.073480
H	-5.973725	-0.331301	-2.230524

TS-IPr-OAc-HSPh

C	-0.930241	-2.604616	1.934913
C	-1.764423	-1.516472	1.626120
C	-3.066295	-1.666047	1.121816
C	-3.556008	-2.966213	0.973765
C	-2.768950	-4.062067	1.305488
C	-1.470198	-3.881722	1.769153
N	-1.276024	-0.183742	1.817860
C	-0.695101	0.564766	0.843592
N	-0.533012	1.787958	1.413954
C	-1.032355	1.811770	2.703391
C	-1.505605	0.566345	2.956977
Au	-0.596843	0.101468	-1.080783
Cl	-0.560297	-0.429416	-3.364481
C	0.048398	2.915945	0.755186
C	1.373641	3.255742	1.076689
C	1.931785	4.351424	0.414699
C	1.196501	5.070469	-0.522150
C	-0.116437	4.716866	-0.809242
C	-0.724646	3.630898	-0.173361
C	2.183008	2.411779	2.040568
C	2.847053	1.259764	1.288578
C	-2.178968	3.295868	-0.440821
C	-2.517341	3.253880	-1.927380
C	-3.924940	-0.478129	0.734752
C	-4.362688	-0.548581	-0.727114
C	0.502762	-2.398934	2.390651
C	1.383357	-3.621224	2.164969
C	3.203963	3.215206	2.838891
C	-3.087768	4.256695	0.328578

C	-5.113656	-0.325148	1.683274
C	0.586274	-1.968328	3.857883
O	0.520856	-2.965287	-0.764084
C	0.401741	-3.154952	-1.963179
C	-0.747664	-3.940547	-2.538389
O	1.200662	-2.683764	-2.879622
S	2.623901	-0.155227	-2.139514
C	3.867632	-0.709629	-1.052355
C	3.667844	-1.794363	-0.165953
C	4.664996	-2.198266	0.716665
C	5.897705	-1.540107	0.767293
C	6.114773	-0.469813	-0.103684
C	5.126506	-0.067567	-0.997088
H	-1.466340	-3.198313	-2.922863
H	-0.420466	-4.560146	-3.384800
H	-1.225925	-4.547374	-1.759587
H	1.748763	-1.874802	-2.535447
H	-1.986246	0.145200	3.834426
H	-0.995733	2.707643	3.315784
H	-0.849271	-4.753304	1.976387
H	0.912889	-1.589502	1.763635
H	-4.563320	-3.118195	0.578448
H	-3.306333	0.425408	0.834030
H	-0.682877	5.289916	-1.546352
H	-2.361819	2.282926	-0.054787
H	2.964779	4.635485	0.622104
H	1.480631	1.973934	2.768430
H	-3.162339	-5.073727	1.175759
H	2.430312	-3.358056	2.373257
H	1.111701	-4.450761	2.839755
H	1.313499	-3.956057	1.121955
H	1.638824	-1.818772	4.145472
H	0.055582	-1.027738	4.057215
H	0.162277	-2.745591	4.515221
H	-4.924014	0.359745	-0.999135
H	-3.491977	-0.619664	-1.397561
H	-5.019151	-1.413911	-0.913306
H	-5.703792	0.568802	1.425028
H	-5.785012	-1.197554	1.627626
H	-4.783538	-0.225923	2.729216
H	1.657223	5.915218	-1.040439
H	-3.567745	2.951893	-2.062625
H	-2.391511	4.236578	-2.410067
H	-1.893244	2.514687	-2.452162

H	-4.146527	3.985704	0.187658
H	-2.871666	4.236332	1.408433
H	-2.953837	5.294237	-0.018980
H	3.362979	0.575901	1.980268
H	2.128490	0.680245	0.691437
H	3.592689	1.637441	0.574269
H	3.673768	2.570282	3.597048
H	4.016084	3.592283	2.197710
H	2.746072	4.075598	3.353019
H	7.073370	0.059858	-0.088944
H	6.675127	-1.859561	1.466765
H	4.476210	-3.047407	1.382109
H	2.698215	-2.299533	-0.185325
H	5.303454	0.769269	-1.678375

IPr-Au-SPh

C	3.830096	2.487858	0.927672
C	2.982202	3.069106	-0.009216
C	1.605814	2.830747	0.022463
C	1.120518	1.987252	1.035532
C	1.953547	1.365128	1.979118
C	3.321948	1.639768	1.905115
N	-0.285572	1.722556	1.081023
C	-0.867669	0.679800	0.443461
N	-2.185049	0.797143	0.725961
C	-2.428042	1.897669	1.526368
C	-1.222720	2.482444	1.754316
Au	0.084581	-0.728535	-0.618705
C	-3.178952	-0.115659	0.251237
C	-3.502660	-1.224244	1.049700
C	-4.466941	-2.107610	0.557574
C	-5.072039	-1.891589	-0.676033
C	-4.719646	-0.790726	-1.449332
C	-3.760153	0.122533	-1.004101
C	-2.798815	-1.501538	2.363215
C	-3.783139	-1.729118	3.508545
C	-3.340006	1.286508	-1.878940
C	-4.527611	2.159984	-2.279303
C	0.698385	3.409558	-1.044786
C	0.879937	4.916836	-1.208069
C	1.422877	0.390595	3.010980
C	1.766024	0.827562	4.433961
C	2.922634	-2.133858	-1.351201
C	3.805858	-3.206416	-1.562350
C	5.160146	-3.088790	-1.263796

C	5.671335	-1.900241	-0.742400
C	4.803822	-0.829178	-0.530533
C	3.449145	-0.937641	-0.833737
C	-1.823769	-2.670513	2.210146
C	-2.564417	0.787654	-3.099005
C	0.898477	2.666727	-2.367445
C	1.913663	-1.027379	2.714187
H	-3.429020	2.157637	1.857622
H	-0.945830	3.362806	2.326634
H	-4.740228	-2.986580	1.145631
H	-2.201901	-0.612265	2.618141
H	-5.190290	-0.643121	-2.424028
H	-2.653573	1.916190	-1.292215
H	3.397800	3.712493	-0.787642
H	-0.342614	3.239292	-0.728900
H	4.002513	1.165367	2.615368
H	0.325197	0.378365	2.928158
H	-5.820867	-2.596769	-1.044261
H	-1.267561	-2.834548	3.146337
H	-2.357188	-3.602512	1.965310
H	-1.095068	-2.479290	1.407067
H	-3.241775	-1.858172	4.458280
H	-4.475150	-0.880638	3.621753
H	-4.387696	-2.635986	3.351632
H	-2.205127	1.635863	-3.702187
H	-1.692005	0.187825	-2.796854
H	-3.198958	0.159626	-3.744058
H	-4.184972	3.030061	-2.860170
H	-5.243995	1.607931	-2.907491
H	-5.072138	2.530455	-1.397397
H	4.903582	2.686648	0.884796
H	0.203115	3.044063	-3.133440
H	1.924640	2.799648	-2.744774
H	0.724392	1.586064	-2.246941
H	0.153998	5.312108	-1.935029
H	0.733861	5.447721	-0.255035
H	1.884532	5.168781	-1.581851
H	1.474502	-1.742978	3.426507
H	1.633869	-1.340996	1.696401
H	3.009549	-1.099483	2.792472
H	1.322461	0.134670	5.165436
H	2.853856	0.833559	4.604853
H	1.388445	1.839274	4.647579
H	5.181983	0.113355	-0.126624

H	6.734008	-1.809804	-0.505373
H	5.823102	-3.940861	-1.437101
H	3.411417	-4.144253	-1.961249
H	2.787543	-0.083511	-0.667334
S	1.224059	-2.372566	-1.781953

OAc

C	0.000000	0.219922	0.000000
O	1.104351	0.795974	0.000000
O	-1.151122	0.699825	0.000000
C	0.046384	-1.347167	0.000000
H	1.078602	-1.733660	0.000000
H	-0.491369	-1.734635	0.883263
H	-0.491369	-1.734635	-0.883263

OAcH Cl

C	-1.185605	0.275150	0.000000
O	0.000000	0.805489	0.000000
O	-1.469556	-0.905165	0.000000
Cl	2.309272	-0.817952	0.000000
C	-2.272038	1.346794	0.000000
H	0.828421	0.104350	0.000000
H	-3.265498	0.879719	0.000000
H	-2.159121	1.993429	0.883964
H	-2.159121	1.993429	-0.883964

HCCPh

C	0.000000	-0.592013	0.000000
C	1.211306	0.121328	0.000000
C	1.206222	1.511797	0.000000
C	-0.001088	2.210697	0.000000
C	-1.207384	1.510931	0.000000
C	-1.211409	0.119871	0.000000
H	2.152921	-0.431004	0.000000
H	2.153511	2.056087	0.000000
H	-0.001286	3.303167	0.000000
H	-2.155464	2.053786	0.000000
H	-2.153201	-0.432165	0.000000
C	0.000788	-2.021389	0.000000
C	0.001742	-3.234717	0.000000
H	0.002464	-4.308893	0.000000

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C	-1.196943	0.967314	0.000000
C	0.000087	1.670608	0.000000
C	1.196944	0.967262	0.000000
C	1.210695	-0.426621	0.000000
C	0.000000	-1.118430	0.000000

C	-1.210780	-0.426414	0.000000
H	-0.000009	2.760678	0.000000
F	2.351551	1.612953	0.000000
F	2.351002	-1.092520	0.000000
F	-0.000325	-2.436988	0.000000
F	-2.350805	-1.092607	0.000000
F	-2.351425	1.613274	0.000000

HSPh

C	0.000000	-0.514274	0.000000
C	-1.206236	0.198316	0.000000
C	-1.196112	1.590036	0.000000
C	0.009261	2.290682	0.000000
C	1.209318	1.581977	0.000000
C	1.210454	0.189364	0.000000
H	-2.156693	-0.341211	0.000000
H	-2.145325	2.131403	0.000000
H	0.013549	3.382657	0.000000
H	2.162240	2.116874	0.000000
H	2.159449	-0.352662	0.000000
S	-0.089595	-2.278191	0.000000
H	1.240186	-2.502625	0.000000