

Supporting information

**Triphosphine-supported bimetallic Au^I-M^I (M = Ag, Cu) alkynyl
clusters**

Ilya S. Krytchankou,^a Dmitry V. Krupenya,^a Antti J. Karttunen,^b Sergey P. Tunik,^{*a} Tapani
A. Pakkanen,^c Pi-Tai Chou^d and Igor O. Koshevoy^{*c}

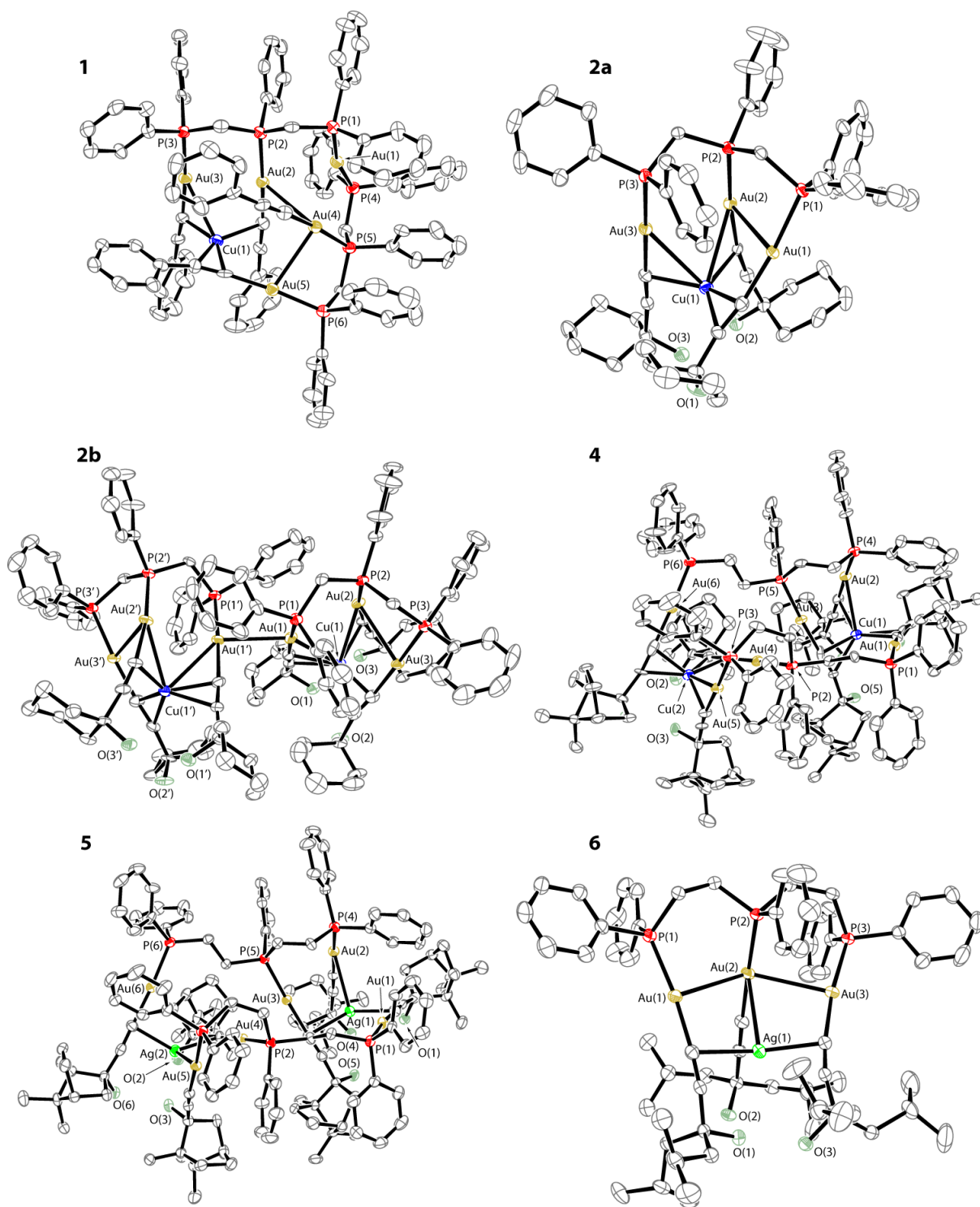


Figure S1. ORTEP views of the clusters 1, 2, 4–6.

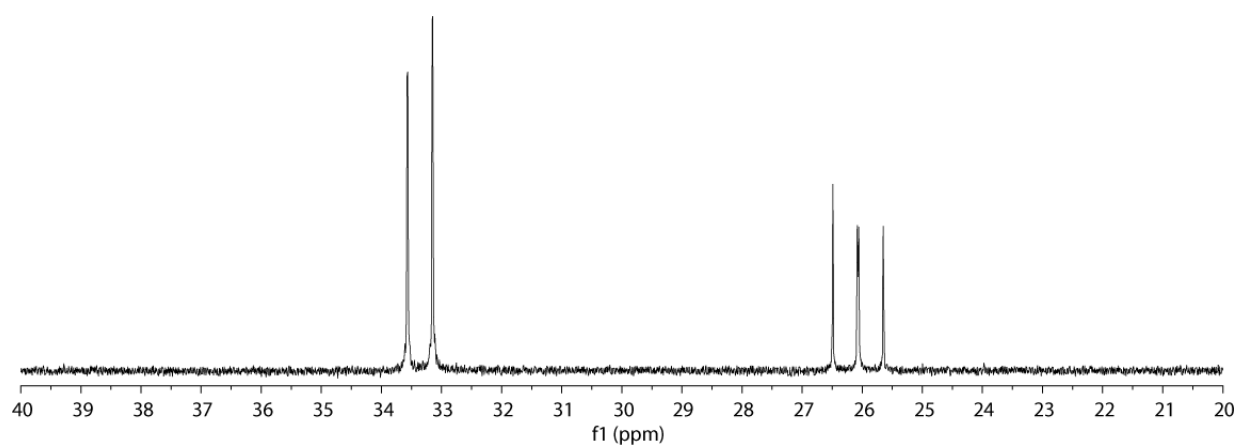


Figure S2. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **2** (CD_2Cl_2 , 298 K).

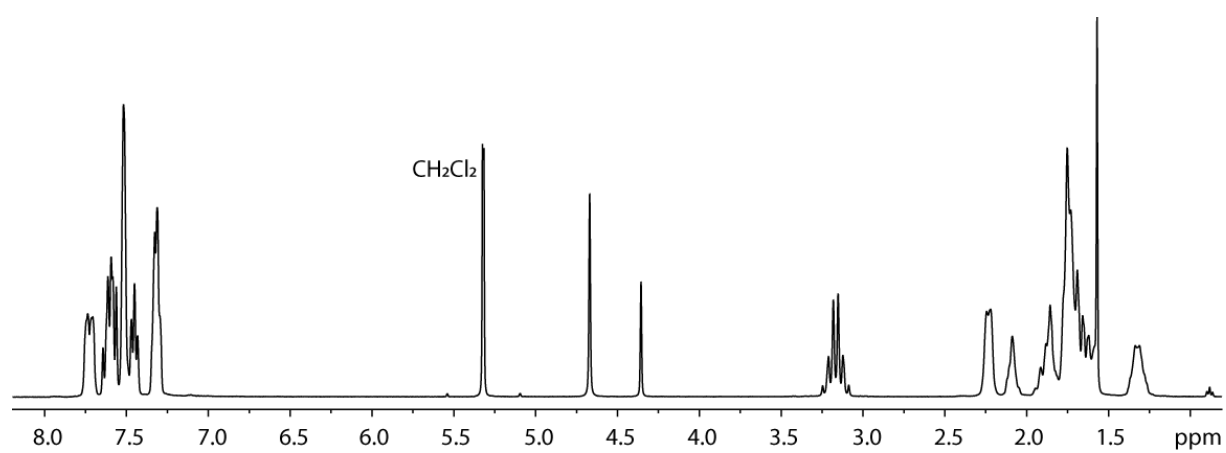


Figure S3. ^1H NMR spectrum of **2** (CD_2Cl_2 , 298 K).

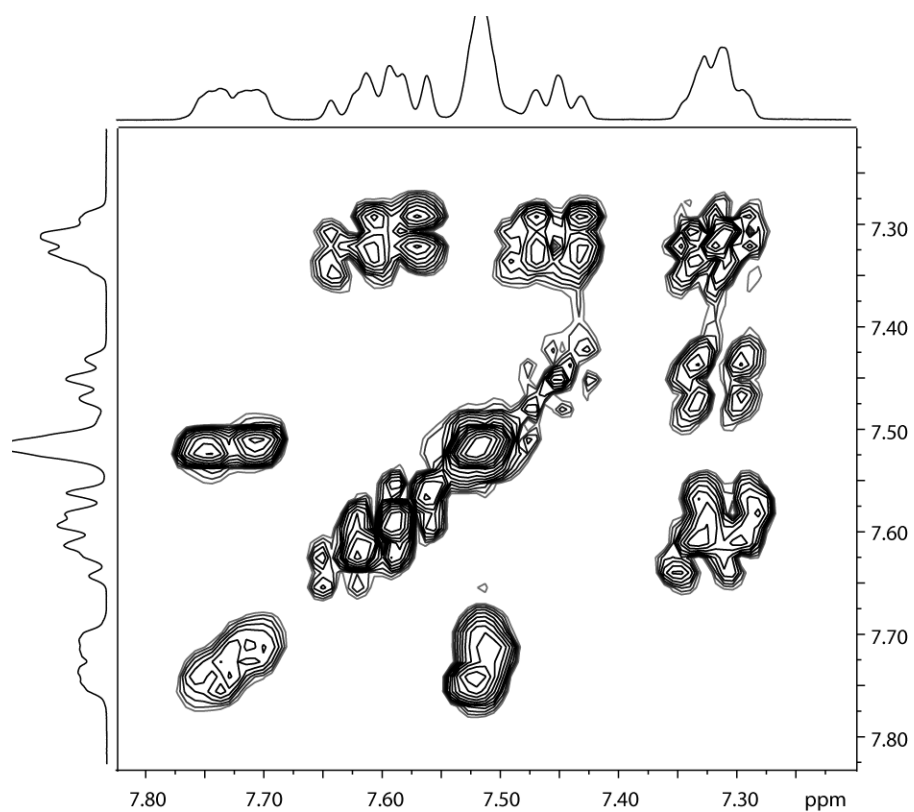


Figure S4. ^1H - ^1H COSY NMR spectrum of **2**, aromatic area, (CD_2Cl_2 , 298 K).

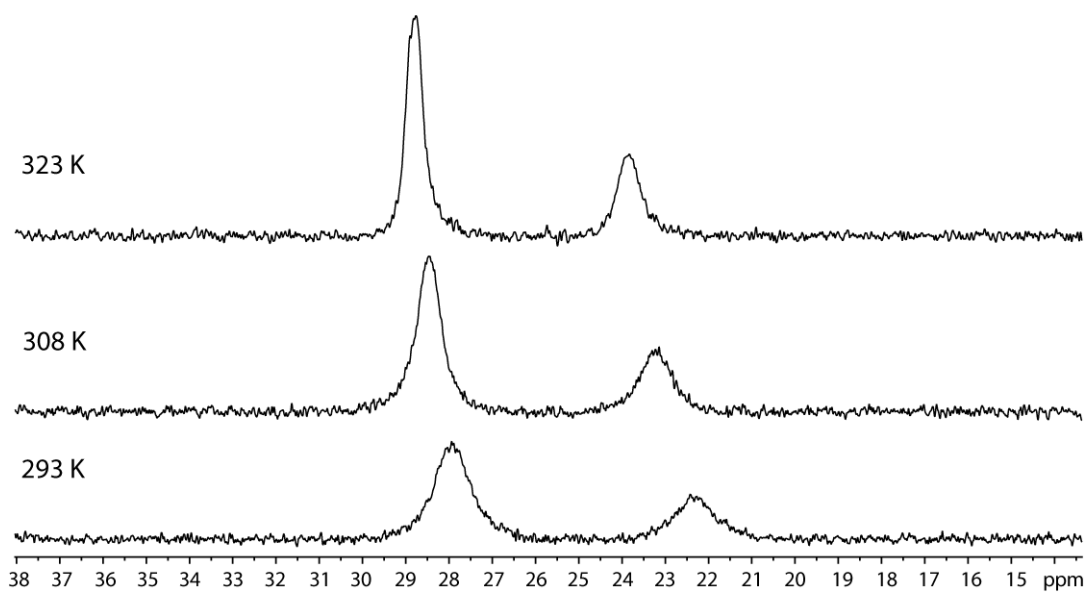


Figure S5. VT ^{31}P NMR spectra of **6** ($\text{acetone-}d_6$).

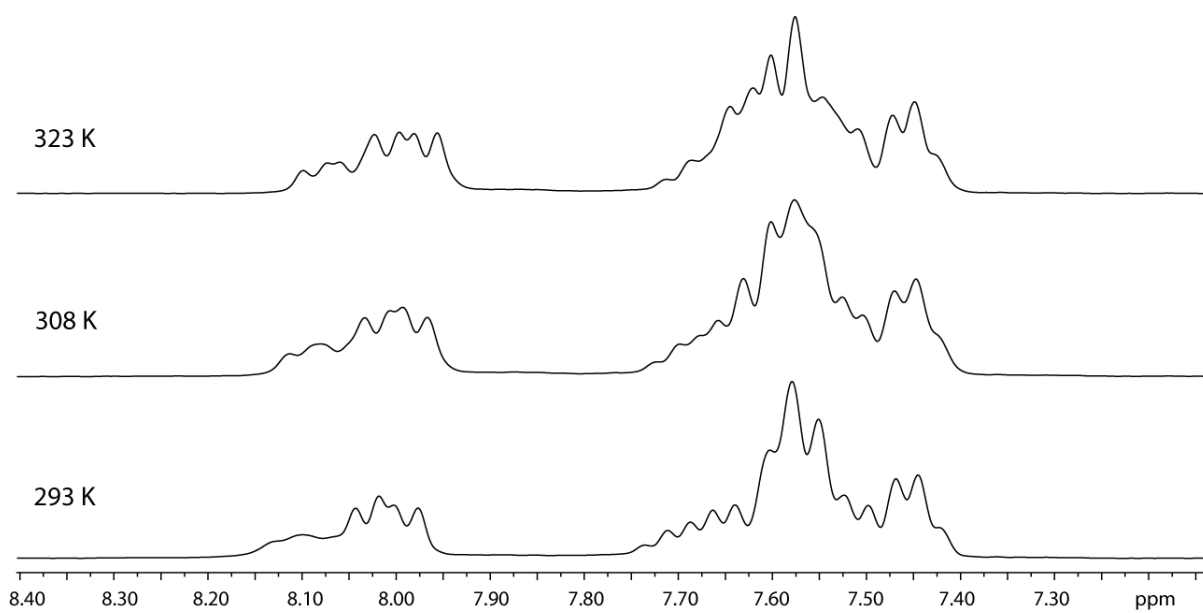


Figure S6. VT ^1H NMR spectra of **6**, aromatic region (acetone- d_6).

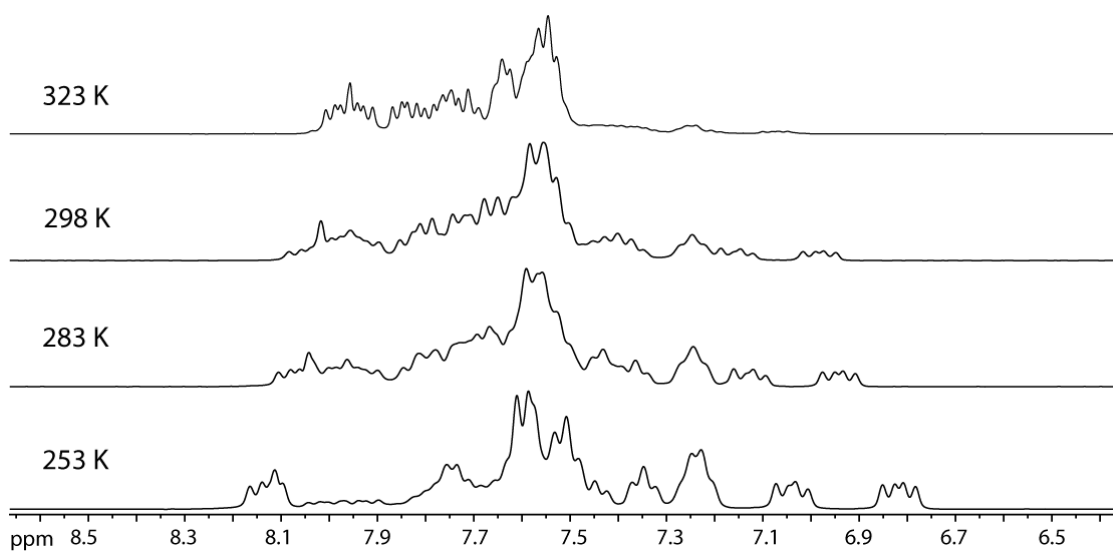


Figure S7. VT ^1H NMR spectra of **4** (acetone- d_6).

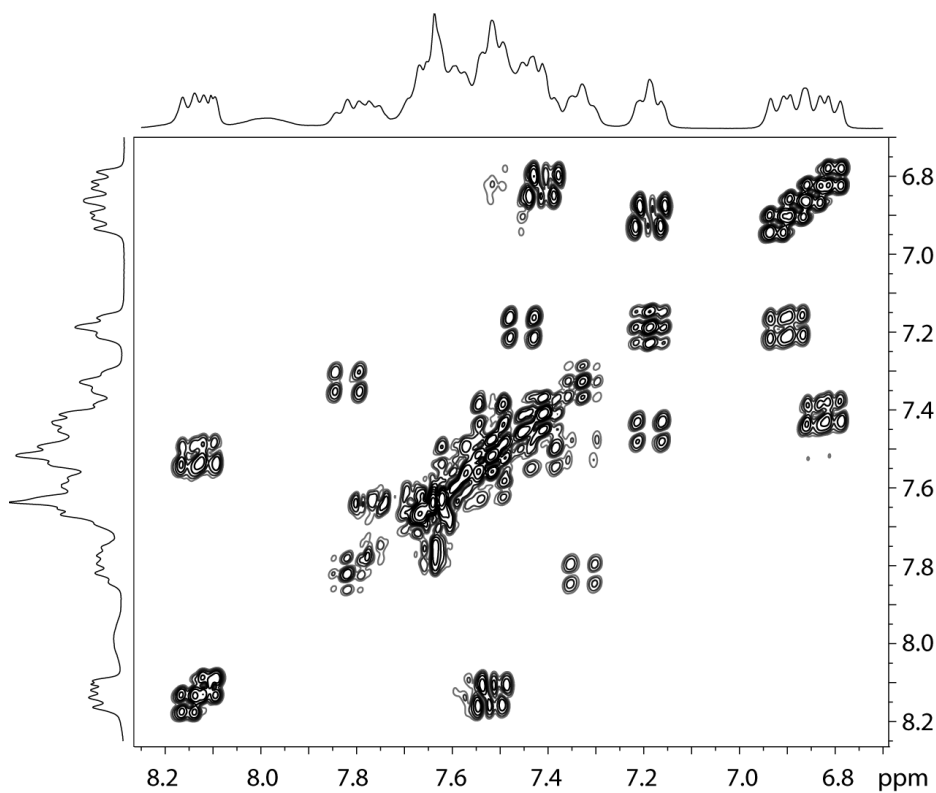


Figure S8. ^1H - ^1H COSY NMR spectrum of **4**, aromatic area, (CD_2Cl_2 , 253 K).

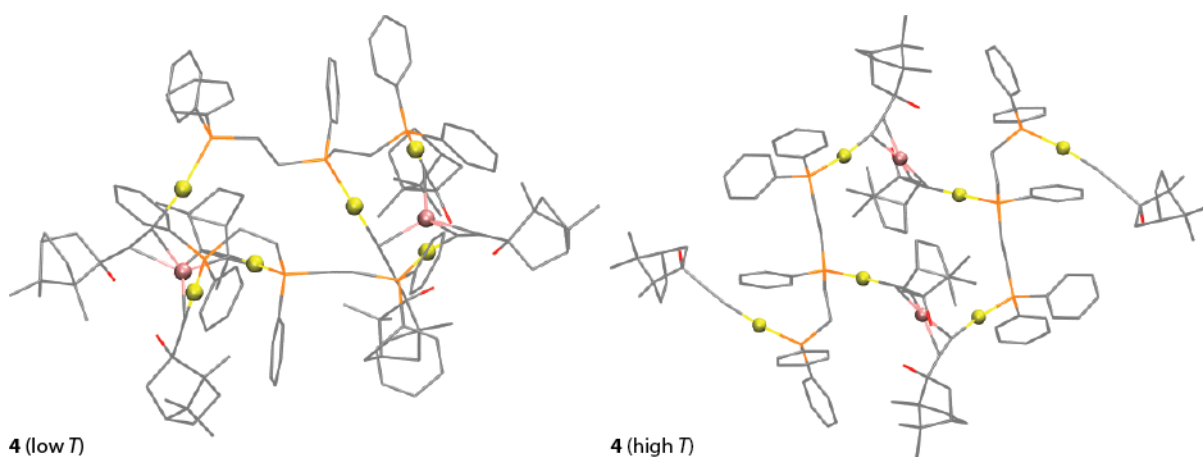


Figure S9. Optimized geometry of high-temperature isomeric forms of clusters **4** and **5**. The structural motifs of the two isomers are practically identical in the case of the Ag–Au complex **5**.

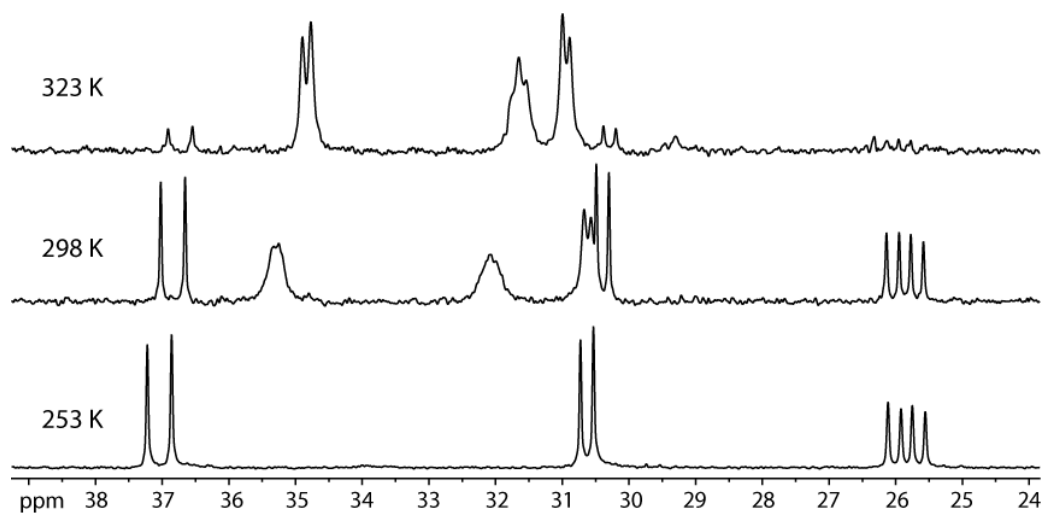


Figure S10. VT ^{31}P NMR spectra of **5** (acetone- d_6).

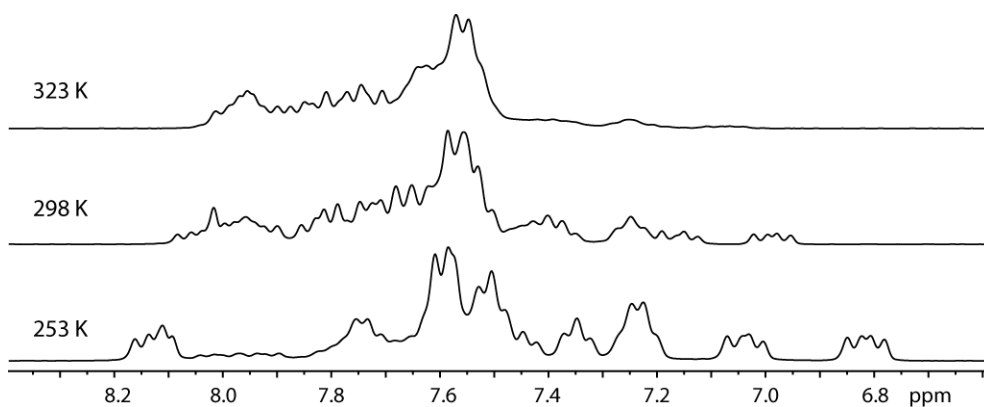


Figure S11. VT ^1P NMR spectra of **5** (acetone- d_6).

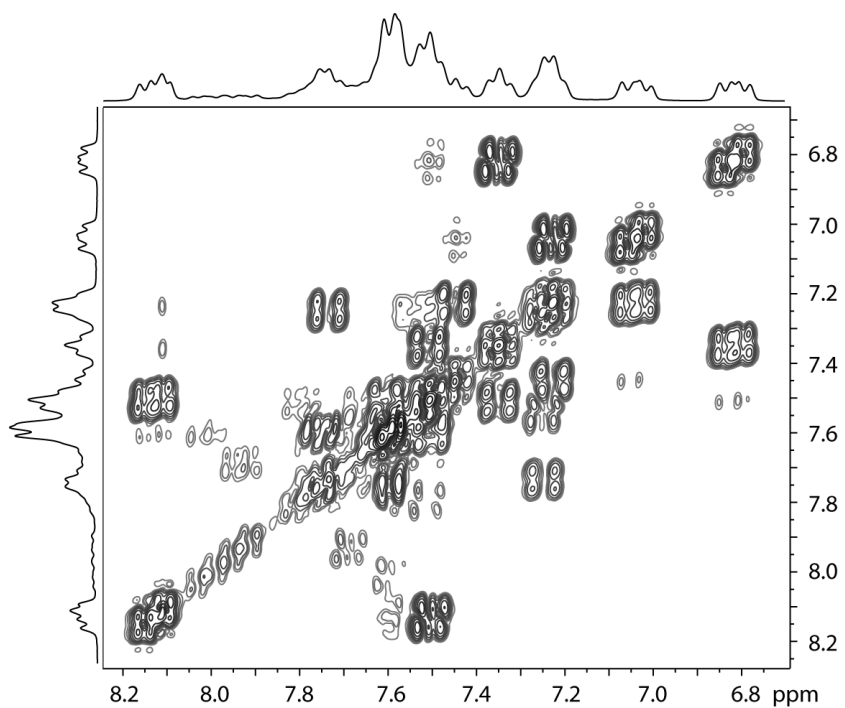


Figure S12. ^1H - ^1H COSY NMR spectrum of **5**, aromatic area, (acetone- d_6 , 253 K).

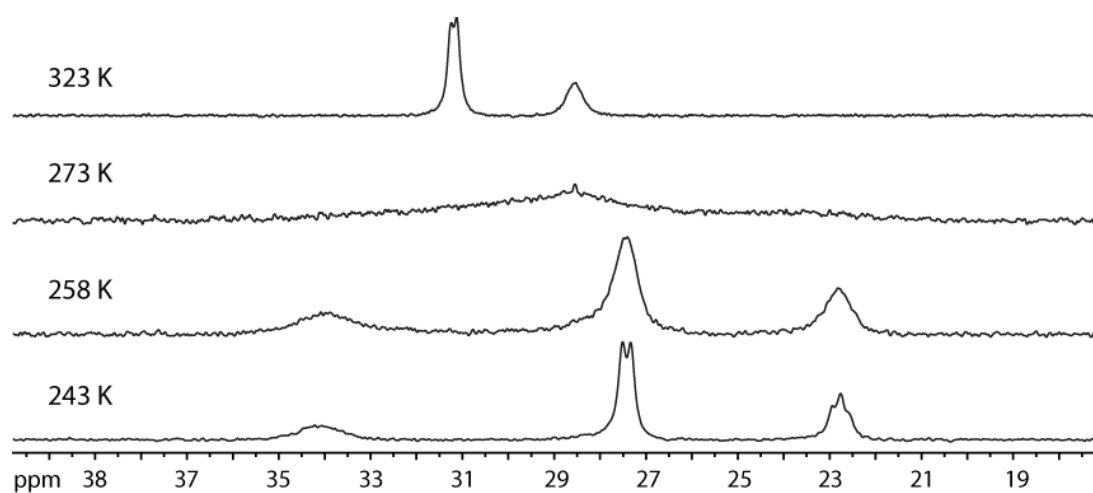


Figure S13. VT $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of **3** (acetone- d_6).

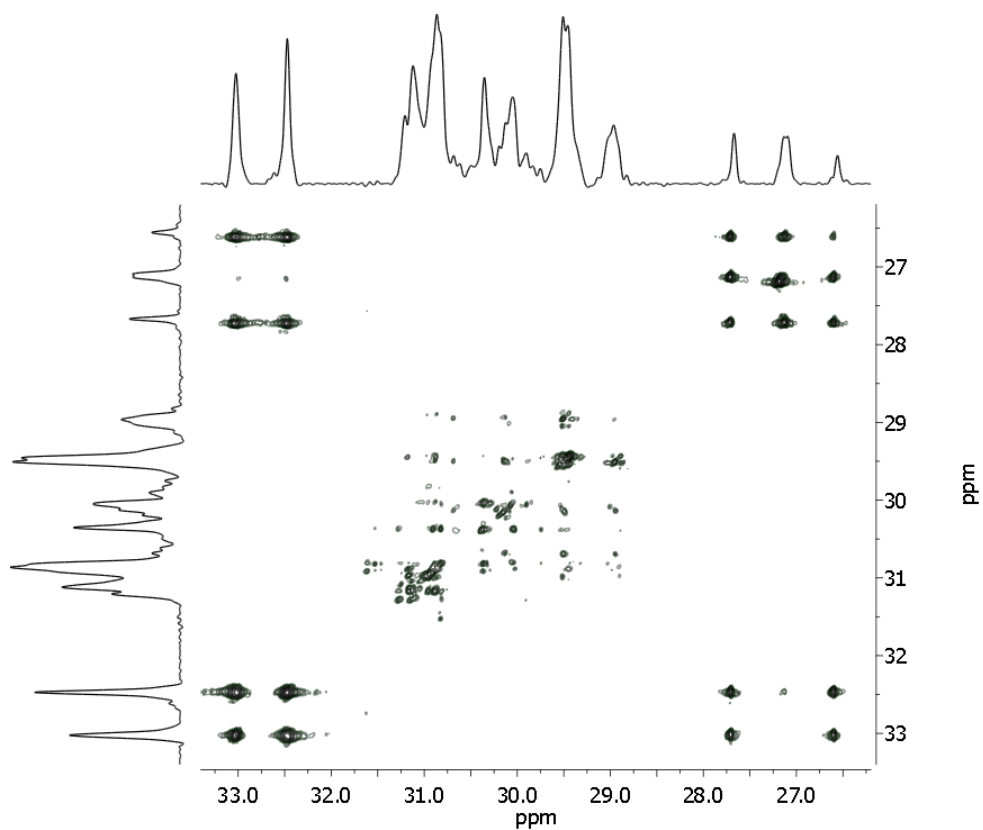


Figure S14. ^{31}P - ^{31}P COSY NMR spectrum of **1** (CD_2Cl_2 , 298 K).

Computational supporting information

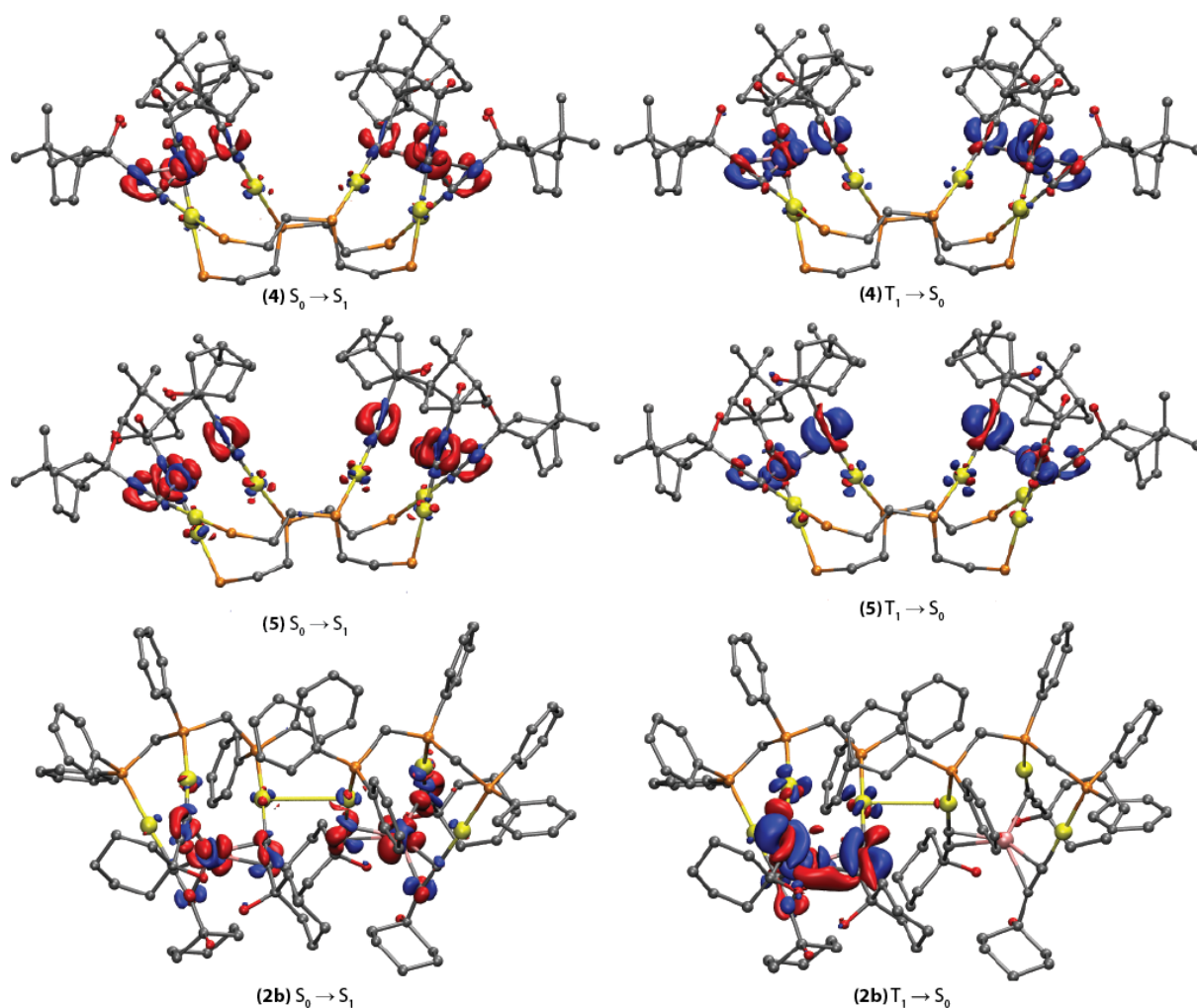


Figure S15. Electron density difference plots for the lowest energy singlet excitation ($S_0 \rightarrow S_1$) and the lowest energy triplet emission ($T_1 \rightarrow S_0$) of the Au^I-M^I complexes **4** and **5**, together with the dimeric structure **2b** (isovalue 0.002 a.u.). During the electronic transition, the electron density increases in the blue areas and decreases in the red areas. Hydrogen atoms and phosphine-based Ph rings omitted for clarity.

Optimized cartesian coordinates of the studied systems in atomic units (PBE0-DFT)

[Au₅Cu(C₂Ph)₄(PPh₂CH₂PPhCH₂PPh₂)₂]²⁺ (1)

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-2.77636834558382	3.42894887745562	6.62504226473708	p
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[Au₃Cu(C₂C₆H₁₁O)₃(Ph₂PCH₂PPhCH₂PPh₂)]²⁺ (2a)

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-0.34183527963763	4.34653006027645	3.82282484417227	c
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4.27099223856627	-6.29259064438526	-7.96346930085311	c
3.79250885402102	-7.09728181877918	-10.43726953544422	c
6.74594903978430	-5.66508294916667	-7.24906883395834	c
5.77739676545468	-7.31471825284580	-12.15963187016356	c
8.71863531864599	-5.89551957419688	-8.97432748829839	c
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-1.02875007066327	-7.48487904025720	-6.85805308673061	c
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-3.01423504438448	-11.34797263985460	-8.30510704680705	c
-5.47881871364064	-7.51956784741051	-7.92193337371152	c
-5.31666488046697	-10.07521224023725	-8.53232389818253	c
-1.02875007066327	-7.48487904025720	6.85805308673061	c
-0.87755230956466	-10.06362008428970	7.46774486908330	c
-3.34152439299558	-6.22069704611659	7.08588837547144	c
-3.01423504438448	-11.34797263985460	8.30510704680705	c
-5.47881871364064	-7.51956784741051	7.92193337371152	c
-5.31666488046697	-10.07521224023725	8.53232389818253	c

4.27099223856627	-6.29259064438526	7.96346930085311	c
6.74594903978430	-5.66508294916667	7.24906883395834	c
3.79250885402102	-7.09728181877918	10.43726953544422	c
8.71863531864599	-5.89551957419688	8.97432748829839	c
5.77739676545468	-7.31471825284580	12.15963187016356	c
8.23854891984927	-6.72561908244409	11.43211315619212	c
5.36233064260914	-3.89118991561915	0.00000000000000	c
5.39430626557967	-1.24616537612147	0.00000000000000	c
7.66527139035779	-5.21297293237669	0.00000000000000	c
7.69074405907715	0.05264180361715	0.00000000000000	c
9.95259258903464	-3.91083154030965	0.00000000000000	c
9.96577799711955	-1.27065824652912	0.00000000000000	c
-0.68868482322424	7.03001998711009	-4.52546703938225	c
1.81229984500933	8.48065130738333	-4.15012669737247	c
-1.47183764737475	7.14145383643104	-7.33587765216104	c
1.66493750997267	11.19347194690235	-5.13220255207033	c
-1.63834195542887	9.85839290103022	-8.29566539871385	c
0.83895370987126	11.28283947748902	-7.89554540328701	c
-0.68868482322424	7.03001998711009	4.52546703938225	c
-1.47183764737475	7.14145383643104	7.33587765216104	c
1.81229984500933	8.48065130738333	4.15012669737247	c
-1.63834195542887	9.85839290103022	8.29566539871385	c
1.66493750997267	11.19347194690235	5.13220255207033	c
0.83895370987126	11.28283947748902	7.89554540328701	c
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-8.73813541100496	3.26571195498807	-2.38608237866894	c
-8.73813541100496	3.26571195498807	2.38608237866894	c
-9.85247185646510	5.92835834515504	-2.38658242840219	c
-9.85247185646510	5.92835834515504	2.38658242840219	c
-11.3933313222356	6.43983937381171	0.00000000000000	c
-4.94236669834245	4.30095670025255	0.00000000000000	o
-5.20779130640554	6.11632818150807	0.00000000000000	h
1.86827571342739	-7.55423419294144	-11.03526819694966	h
7.14414389749867	-4.96527769045119	-5.34062800923473	h
5.38784095415146	-7.94938771236672	-14.08795103977045	h
10.64326261370290	-5.40678825978303	-8.39980936912557	h
9.78940647286736	-6.89998335056908	-12.78768352109320	h
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-3.48177297630382	-4.21809968983133	-6.58564038853335	h
-2.88492508450714	-13.35439075408147	-8.78561669189909	h
-7.28026820083858	-6.52049896544444	-8.08472034982740	h
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7.14414389749867	-4.96527769045119	5.34062800923473	h
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10.64326261370290	-5.40678825978303	8.39980936912557	h
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9.78940647286736	-6.89998335056908	12.78768352109320	h
3.62701719440563	-0.17551629675080	0.00000000000000	h
7.70064442710537	-7.28363364930557	0.00000000000000	h
7.68184516616005	2.11883422283935	0.00000000000000	h
11.73290442425847	-4.96181207111169	0.00000000000000	h
11.76213631760595	-0.24716000286509	0.00000000000000	h
3.31620354946289	7.45683738452143	-5.17176347044556	h
2.30620125414991	8.44031928063298	-2.12440085716670	h
-0.06773568527452	6.08099655801149	-8.45914160789067	h
-3.29833950512896	6.15946418808095	-7.53939520913495	h
3.51959899431427	12.11682429363107	-4.88770451434308	h
0.33803689615156	12.32011496396606	-3.96216216762798	h
-2.15855516256994	9.84931805685770	-10.31563371849812	h
-3.19752342705702	10.85659078415482	-7.31852743274164	h
0.65944867420098	13.25978195376145	-8.53729462917092	h
2.32784531859817	10.40905205742796	-9.07665259905970	h
-0.06773568527452	6.08099655801149	8.45914160789067	h
-3.29833950512896	6.15946418808095	7.53939520913495	h
3.31620354946289	7.45683738452143	5.17176347044556	h
2.30620125414991	8.44031928063298	2.12440085716670	h
-2.15855516256994	9.84931805685770	10.31563371849812	h
-3.19752342705702	10.85659078415482	7.31852743274164	h
3.51959899431427	12.11682429363107	4.88770451434308	h
0.33803689615156	12.32011496396606	3.96216216762798	h

0.65944867420098	13.25978195376145	8.53729462917092	h
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-2.58677210938229	9.90766461025171	3.24428178044495	h
4.62948775293063	-8.42740182329833	-3.10545324235539	h
1.38557398660935	-9.29137751469157	-2.67188310018775	h
4.62948775293063	-8.42740182329833	3.10545324235539	h
1.38557398660935	-9.29137751469157	2.67188310018775	h
-10.27481394584438	1.85316878232801	-2.46292218060620	h
-7.52711021985781	2.95883900435535	-4.05453122589816	h
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-7.52711021985781	2.95883900435535	4.05453122589816	h
-11.03529055067768	6.18758945102426	-4.08601700147827	h
-8.30428204074401	7.32653398212951	-2.55633387117595	h
-11.03529055067768	6.18758945102426	4.08601700147827	h
-8.30428204074401	7.32653398212951	2.55633387117595	h
-12.10581225960974	8.40150932022245	0.00000000000000	h
-13.07948534498535	5.20103992377348	0.00000000000000	h

[Au₃Cu(C₂C₆H₁₁O)₃(Ph₂PCH₂PPhCH₂PPh₂)]²⁺ (2b)

61.71085485730234	23.85551170666237	15.78166885521822	c
60.14354221472593	25.24873262657646	16.81014128208032	c
63.42815464063534	21.67987082951246	21.83637934660728	c
62.20990105059661	22.88294435202526	23.41576056714911	c
67.59064183788571	26.42014842150072	19.59166483889587	c
66.20230429382116	28.26993823030974	19.20244639461204	c
58.05768898931831	26.78380932767472	17.87809087053050	c
57.23518574487726	28.83563443351749	15.98551621217113	c
56.77924098164561	27.90512575649021	14.17169568011631	h
58.85120887290207	30.10279007537838	15.61532565026547	h
67.56671303037183	15.70711639528238	14.72785042486980	c
65.80328413821728	14.61452617393229	14.97251350969378	h
68.99469568382308	14.45557779787089	13.86088693977315	h
54.96415186817039	30.32932504730521	16.94899304386727	c
55.52068074204192	31.39463762147059	18.65503393156803	h
54.40888364002399	31.74329126372970	15.51694954775779	h
71.74109079433804	17.67945342205525	17.85472486230685	c
73.06823397861389	16.07091750501807	17.88956023087659	h
72.00350790824369	18.70135458439877	16.05519697916882	h
52.74802705933069	28.59624738793698	17.57954190963970	c
52.05604934989351	27.69771722595351	15.81834698411758	h
51.15647037684839	29.70800726517797	18.34369724641118	h
53.52752116207080	26.54591067920166	19.45067296874442	c
51.94598952267555	25.23015541132112	19.80017977756775	h
53.99238560918830	27.40866437799297	21.29190942584607	h
55.80564836579170	25.05107721112830	18.50393589035449	c
56.41587102300986	23.66288094487512	19.93388253937476	h
55.30262787365236	24.00535833150241	16.76628414755127	h
60.73677718925620	24.27139638397734	25.34516997220351	c
60.27763182470125	22.52856301738277	27.62439562524136	c
59.26776755929387	20.82702781383662	26.96796961767129	h
58.96598145968431	23.56666024072533	28.87490070343628	h
62.69632754967289	21.85165089991002	29.03509113179296	c
63.91151857156790	20.67646461263944	27.80015811504343	h
62.22558130049146	20.67883773096710	30.69567371765113	h
64.14347929384407	24.21061061171480	29.85453613732713	c
63.01973854759573	25.23963998353150	31.28705755127612	h
65.93423935553834	23.67976959009367	30.78791708094448	h
64.66112109220724	25.96280155156962	27.62063011617406	c
65.98999807203333	25.04391220564850	26.29019576412337	h
65.59260079112551	27.71282989318044	28.27299471041873	h
62.22639132830673	26.61887121035404	26.22451820329934	c
62.62561553291680	27.82343520255509	24.56415112459408	h
60.93509524489451	27.68949765294622	27.46905898822500	h
65.15053217527584	30.82828601835210	18.76825578631008	c
67.03051794830141	32.83066835835703	19.72348371937450	c
67.46684426745253	32.45910339782980	21.73277599755044	h
66.03249447592242	34.66434199701914	19.62470738734581	h
69.44675290181372	32.93866733609556	18.15863643863305	c
70.66782931042128	34.46656886086721	18.88198911675161	h
70.51228649778398	31.15757707289211	18.40563650808955	h
68.85279874904650	33.35342235567389	15.36701735269852	c
68.02166152218810	35.25616833613999	15.11503498820374	h

70.61025162546811	33.32683275662924	14.24228515837968	h
67.00394613281688	31.37192874325421	14.37816968514518	c
67.91507243883301	29.48930231834795	14.38939288687081	h
66.49824591546043	31.77196463220440	12.39479910042462	h
64.59557818060480	31.26268521828344	15.95928999837917	c
63.32474766398218	29.76144800836246	15.26676581511590	h
63.56400382428955	33.07475388093809	15.83396144402259	h
69.83667994466664	19.70944804335100	11.67190433202993	c
70.39502448182576	22.20074258760430	12.37355826550036	c
69.00635867875991	23.31498936481043	13.43026493139798	h
72.71446920695151	23.27117835007470	11.71211823911837	c
73.13109818524123	25.22137735190122	12.25547134645422	h
74.47588549123621	21.86701511434781	10.34410810242991	c
76.28252621983846	22.71570362973036	9.80476034609657	h
73.92521550245165	19.38348569894506	9.63529139278231	c
75.29661242040945	18.28748984374948	8.54413089934258	h
71.61457039230504	18.30780807027369	10.29043337499777	c
71.18027883703337	16.37776439648935	9.68252087619122	h
65.76860697014315	16.67078840302251	9.69032540624767	c
65.67759482196583	18.06746172968918	7.43887439499977	c
66.24539626696870	20.05488772351313	7.40930612673337	h
64.85385616324436	16.94305084075581	5.20537152443695	c
64.78898013439847	18.06507618643610	3.47101907966383	h
64.10791522295841	14.41258069649373	5.19850825946726	c
63.47726595293144	13.52314408827846	3.44218933447285	h
64.18576917530605	13.01416479258370	7.43092014219438	c
63.62914760028382	11.02257782080176	7.43012046429385	h
65.00984159156411	14.13480713149178	9.67341163125566	c
65.06086429987238	12.99100370064093	11.39119133028629	h
68.60003890857158	13.47590279870714	19.54697676852015	c
67.11428787392568	13.02535825589670	21.68964406176251	c
65.90334765547728	14.52914157650699	22.43445363266733	h
67.20006748129087	10.67937827266083	22.88926526411266	c
66.04395075840698	10.34551242187914	24.56958482555198	h
68.76276671860440	8.77463490679141	21.95745729121376	c
68.82806077544579	6.93539253187920	22.89944287670507	h
70.25149601432800	9.21318354214833	19.82230836153873	c
71.48127907641609	7.72166832183876	19.09012117489736	h
70.17382113632937	11.55290332224589	18.62078764802763	c
71.35820621274938	11.86186980429599	16.95069254476872	h
72.05874220103735	18.15645972540288	23.33358828587372	c
70.42416238731494	19.07328269093894	25.20399677618485	c
69.41208349965778	20.85455156436182	24.91494110411702	h
70.07670028688591	17.71681086379762	27.43796934751354	c
68.80105396614138	18.45027070647217	28.88976925573036	h
71.35700720843117	15.44623633849323	27.81466612566820	c
71.09279086509359	14.39023134498847	29.57231712179269	h
72.98848340933522	14.52110992579791	25.95599714597418	c
73.99952634217132	12.74312545061298	26.25367727251203	h
73.34008539454869	15.86614828816605	23.72329895915697	c
74.64256675919796	15.13083464702256	22.29358488486646	h
75.85486769644761	20.52595762131381	20.07576046665188	c
77.52196429381503	20.29020368272101	22.11695102226176	c
76.83711593267144	19.65975738171398	23.96141137099460	h
80.07451727836226	20.87283106724486	21.80863110182741	c
81.36351798663489	20.68553719208094	23.41332880056731	h
80.97776818902976	21.69107874121532	19.47416001257593	c
82.98080249088432	22.14429533178115	19.23970014480886	h
79.31796003759456	21.94552930366864	17.43967165407969	c
80.01616468837055	22.60294700602548	15.60850257037570	h
76.76553131148344	21.38128390650051	17.73704569475574	c
75.48336771082867	21.62862995022182	16.13076363888640	h
58.82770939160144	27.91303485160785	20.18172430901173	o
60.22950855107982	29.11729554448049	19.89963766681302	h
62.80881898897085	31.12821845744195	20.08354947085630	o
63.16929653698114	31.33486154650614	21.87346806199367	h
58.35519810943111	24.95037494827868	24.40087046646899	o
58.57881364550892	26.11766886017583	22.96831916937623	h
66.79916062712294	18.32646965559275	12.54446032249190	p
68.43574272351954	16.54715094452391	18.00037531827537	p
72.47722762515124	19.94655284149264	20.43163592189358	p
63.97002522617220	24.68743814388780	19.09644374520544	cu
64.01875340757530	21.28019234020243	14.21021033641919	au
65.68952490536529	19.37202021791149	19.85868165615487	au
69.88355341750164	23.44759790879503	20.05275774330981	au
62.50759850730551	23.86229414822699	7.68297853125155	c
64.07364450483135	25.25943821686158	6.65792398251618	c

60.79448626133217	21.69315841804583	1.62530376910397	c
62.01295365556003	22.89903531287532	0.04825596168624	c
56.62451014390287	26.42437631334447	3.87669170068536	c
58.01038999152317	28.27523523421160	4.26948699020167	c
66.15822080338960	26.79877150802252	5.59359873558547	c
66.97680645048281	28.84880600567296	7.48979187118719	c
67.43223792959850	27.91621685135745	9.30266290344997	h
65.35902921602950	30.11359131384491	7.86039721953592	h
56.66385668396924	15.70390830699286	8.72399697874539	c
58.42905034906283	14.61464532255506	8.47733787104063	h
55.23808330283861	14.44845711115802	9.58892921102097	h
69.24687084297348	30.34656289744441	6.53033611731079	c
68.69049242128966	31.41365388422090	4.82536165993903	h
69.79929614235621	31.75912530813868	7.96486961619108	h
52.48646178302369	17.67489665836504	5.60001387743160	c
51.16161404175067	16.06453871304266	5.56248524155152	h
52.22235694156451	18.69362871744648	7.40109097260612	h
71.46558712583676	28.61700546255028	5.89921452403318	c
72.15698902622984	27.71678294511367	7.65975808402124	h
73.05655646688631	29.73167290003297	5.13805370088841	h
70.69013350441371	26.56835890915764	4.02454285575137	c
72.27345881119093	25.25483958391224	3.67473105774428	h
70.22601813207159	27.43312894640707	2.18405783050731	h
68.41282075900045	25.06963087283755	4.967067422291205	c
67.80549424206365	23.68286741947239	3.53449797959451	h
68.91544832022757	24.02189831634843	6.70360957474828	h
63.48716483058385	24.29073086971168	-1.87794332838834	c
63.95076915369441	22.55025512822153	-4.15807943599800	c
64.96081834159745	20.84882266316831	-3.50165882254437	h
65.26355016070575	23.59031793646141	-5.40576690370997	h
61.53461044790125	21.87301339554236	-5.57295465906841	c
60.31824351778536	20.69595258184538	-4.34096159391879	h
62.00863589763703	20.70197510856323	-7.23385997382118	h
60.08726800929971	24.23181953374668	-6.39240989345035	c
61.21278400687832	25.26311626338537	-7.82189871703235	h
58.29847164003488	23.70080024175909	-7.32943534501920	h
59.56465125773198	25.98119014559310	-4.15747037734263	c
58.23437309263298	25.05974939651007	-2.83019643356185	h
58.63281565876181	27.73119574216502	-4.80937268855049	h
61.99665964023095	26.63778663651457	-2.75687740599061	c
61.59388286489724	27.84012641764252	-1.09574473625967	h
63.28882775294610	27.71100826989441	-3.99827796117862	h
59.05961681988570	30.83390525807502	4.70773104595703	c
57.17760138048117	32.83598409910276	3.75587828187909	c
56.74182716080336	32.46761652634013	1.74588125963822	h
58.17375393440839	34.67048492572054	3.85802333050694	h
54.76110760434420	32.93865976904338	5.32069260944992	c
53.53862092881029	34.46675165825295	4.60013210194704	h
53.69734207589825	31.15701556453776	5.07012330082122	h
55.35419853607721	33.34859567078804	8.11321900862158	c
56.18295664469078	35.25185998898852	8.36912014865218	h
53.59659128205166	33.31761819577991	9.23759357720288	h
57.20538003928110	31.36750038443430	9.09849757486362	c
56.29663328103731	29.48375215720253	9.08360221510175	h
57.71031744287693	31.76441908144155	11.08269107757616	h
59.61402346405193	31.26422986905700	7.51741069112543	c
60.88675530451194	29.76343824512496	8.20738751518255	h
60.64321873280749	33.07742523984049	7.64594900069212	h
54.38742406968015	19.69653433131769	11.78767654411563	c
53.82447129784199	22.18845858964775	11.09194982538158	c
55.21096340645271	23.30771540234645	10.03768207394871	h
51.50318920709535	23.25314297356004	11.75630716412751	c
51.08294865934359	25.20387554682458	11.21766708009122	h
49.74434024602824	21.84243964317369	13.12089430114013	c
47.93618884611157	22.68652881805047	13.66239144070299	h
50.29968379169038	19.35831273757055	13.82395704877191	c
48.93032263870165	18.25717623750185	14.91250296126675	h
52.61225217395433	18.28845202264627	13.16612014541017	c
53.05015218992590	16.35779322591319	13.76946759840380	h
58.46175708249149	16.66181282605275	13.76258701608242	c
58.54993264768510	18.05397434914440	16.01697963612915	c
57.97752968123293	20.04002170212045	16.05089123102362	h
59.37698548464266	16.92683450531909	18.24789287273249	c
59.43946391880845	18.04528278062476	19.98463982593358	h
60.12942788377664	14.39826687538899	18.24916395642114	c
60.76293027569587	13.50672579318246	20.00338944500490	h
60.05416005703407	13.00431454587153	16.01387982683576	c

60.61564619827470	11.01409316047416	16.01032208954265	h
59.22667585725712	14.12765847746393	13.77400871006325	c
59.17797705047925	12.98735964989634	12.05384612952772	h
55.63386918405945	13.47868640784120	3.90139942636812	c
57.12144523551268	13.03336668277267	1.75890704167183	c
58.33087964242478	14.53985781313708	1.01713574382271	h
57.03918837807817	10.68920971892966	0.55548434293907	c
58.19677281652660	10.35937627723639	-1.12462125164429	h
55.47852119585441	8.78097378429846	1.48354486141133	c
55.41597697971381	6.94317422812768	0.53856150074751	h
53.98782780354369	9.21438602116621	3.61837151110880	c
52.75962302145631	7.72012789105098	4.34760814992885	h
54.06198841938440	11.55226341027184	4.82368606675215	c
52.87626175167063	11.85713376056787	6.49358495966868	h
52.169216427101409	18.15973094524016	0.12191680471576	c
53.80291279218995	19.08177962024562	-1.74669534254129	c
54.81212650832222	20.86420376604550	-1.45477921479256	h
54.15342298481288	17.72891674898154	-3.98237002612131	c
55.42844233515975	18.46643586630776	-5.43266922440061	h
52.87686766340073	15.45682864291232	-4.36265334682099	c
53.14355577614032	14.40354984870141	-6.12156558346460	h
51.24615961373992	14.52657102996112	-2.50586951598656	c
50.23799959730675	12.74742952512664	-2.80640465591422	h
50.89150127600443	15.86802845021327	-0.27149620536653	c
49.58972613610611	15.12864013125266	1.15675601238286	h
48.36898351732053	20.51872632498555	3.38294422254764	c
46.70212059745560	20.28286534909204	1.34158722711252	c
47.38784988323938	19.65589505124871	-0.50373355327476	h
44.14861940422244	20.86081103538216	1.65090032355962	c
42.85978975711558	20.67351188800086	0.04606592528559	h
43.24423431057517	21.67458068680931	3.98649566078539	c
41.24045295515732	22.12406797815327	4.22174411728060	h
44.90379549996114	21.92917574984333	6.02117201047703	c
44.20467670943792	22.58315930206494	7.85322064561662	h
47.45713549801451	21.36961404913192	5.72282585266101	c
48.73905741242697	21.61702018475584	7.32930087210140	h
65.38845241240652	27.93036086279359	3.29109530020856	o
63.98426996769710	29.13162522065940	3.57405268035462	h
61.40094881796987	31.13829767029549	3.39279442537668	o
61.04016811029072	31.34512095488731	1.60295065402618	h
65.86693983963590	24.97095168241791	-0.92995809792343	o
65.64059272053298	26.13675891127439	0.50339636491824	h
57.42726954816687	18.32083288033212	10.91177341418057	p
55.79344903585221	16.54772383351830	5.45284601176953	p
51.74749501932125	19.94489842634177	3.02643409950358	p
60.24666771422790	24.69508047759712	4.37021301565566	cu
60.20288768523949	21.28157111920376	9.25046304607041	au
58.53538053409473	19.37957854195882	3.59890460945847	au
54.33605417460868	23.44911193514575	3.41083815780856	au

[Au₃Cu(C₂C₆H₁₁O)₃(Ph₂P(CH₂)₂PPh(CH₂)₂PPh₂)]₂²⁺ (3)

4.32331079320317	8.98166797854273	1.43163168795719	au
-4.96920066634335	8.332405187998714	2.35565914301103	au
-2.39910720734744	3.45757072780666	-0.26904985825766	au
2.39910720734744	-3.45757072780666	-0.26904985825766	au
4.96920066634335	-8.332405187998714	2.35565914301103	au
-4.32331079320317	-8.98166797854273	1.43163168795719	au
1.27984768748427	-9.08017044910219	-1.86632280566399	cu
-1.27984768748427	9.08017044910219	-1.86632280566399	cu
-7.68658253153848	-6.63539562700529	2.92527701045490	p
-5.07330843157163	1.52464475904673	2.59236878782270	p
-4.36601530480346	7.21277011081610	6.53516918109684	p
4.36601530480346	-7.21277011081610	6.53516918109684	p
5.07330843157163	-1.52464475904673	2.59236878782270	p
7.68658253153848	6.63539562700529	2.92527701045490	p
1.66531136878516	11.18376164882255	-0.11957326518278	c
0.40417368976701	12.80851144399717	-1.25313511160803	c
0.27292786398903	-5.16827906052879	-2.88678746598364	c
-0.82971570652555	-6.35084734183494	-4.57384302959201	c
5.35127133836779	-9.22055878415888	-1.30802295279487	c
5.61097322473017	-9.52099052586750	-3.6055745888231	c
-5.35127133836779	9.22055878415888	-1.30802295279487	c
-5.61097322473017	9.52099052586750	-3.6055745888231	c

-0.27292786398903	5.16827906052879	-2.88678746598364	c
0.82971570652555	6.35084734183494	-4.57384302959201	c
-1.66531136878516	-11.18376164882255	-0.11957326518278	c
-0.40417368976701	-12.80851144399717	-1.25313511160803	c
6.86797828545960	3.40177197677980	3.97161561417361	c
5.35131417466570	1.91732776637797	2.02449670321348	c
4.08062425920775	-1.73895091569939	5.94340797104239	c
2.70668053632719	-4.13541933490729	6.79828707321498	c
-2.70668053632719	4.13541933490729	6.79828707321498	c
-4.08062425920775	1.73895091569939	5.94340797104239	c
-5.35131417466570	-1.91732776637797	2.02449670321348	c
-6.86797828545960	-3.40177197677980	3.97161561417361	c
0.50038067953416	-15.03954706981556	-2.68343770064280	c
2.97773153099817	-16.10484560101881	-1.62100711290964	c
-1.57815711113255	-17.08499187769450	-2.61717896707838	c
3.79373050794448	-18.50098096040767	-3.00585271187643	c
-0.75414341091273	-19.47350197807873	-4.00699951096768	c
1.72436477856611	-20.50913791231282	-2.95813270562489	c
-0.50038067953416	15.03954706981556	-2.68343770064280	c
-2.97773153099817	16.10484560101881	-1.62100711290964	c
1.57815711113255	17.08499187769450	-2.61717896707838	c
-3.79373050794448	18.50098096040767	-3.00585271187643	c
0.75414341091273	19.47350197807873	-4.00699951096768	c
-1.72436477856611	20.50913791231282	-2.95813270562489	c
6.11691267537224	-9.91123004185868	-6.32580972754256	c
6.67910455221897	-7.37174388374007	-7.61970084107106	c
8.37663753913194	-11.72319023379667	-6.65030945723300	c
7.37800149927001	-7.71818565521201	-10.39635187965645	c
9.07238789027114	-12.06061971533550	-9.42835206626350	c
9.60136529176684	-9.52958426220745	-10.70553797158278	c
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-7.37800149927001	7.71818565521201	-10.39635187965645	c
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2.13153339111804	7.54258211675913	-6.74968199517998	c
4.92857052321640	8.02077679644897	-6.14040967030159	c
1.89648610298344	5.79417972884314	-9.07175054692634	c
6.35895663476393	9.06157084706031	-8.41817539119189	c
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6.10137771096259	7.33156844260360	-10.71133088415582	c
-2.13153339111804	-7.54258211675913	-6.74968199517998	c
-4.92857052321640	-8.02077679644897	-6.14040967030159	c
-1.89648610298344	-5.79417972884314	-9.07175054692634	c
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-9.24058758085643	-7.95430209555195	5.70610774855819	c
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7.74499802611596	9.13677471521368	7.54601623674039	c
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1.09648903008798	12.65362872761561	10.65165946818400	c
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-15.37507719026738	4.56963735727834	1.37535419371907	h
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4.44710878606732	-14.62963267767666	-1.72786739218259	h
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5.54360010031280	-19.23323037206997	-2.13670723998691	h
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2.01031383315465	17.51700940900389	-0.61971778600845	h
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-5.03121715761927	-9.33405937391042	-4.52278862895149	h
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-8.36969144328523	-9.30961075684817	-7.91335956229924	h
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-5.78785512411970	-3.65997478739298	5.73806303288930	h
-8.64532178668593	-2.44065860885527	4.49062029452060	h
-3.41736178046607	-2.68087598957212	1.81726518368811	h
-6.20843521794315	-2.05248262856880	0.12423596428962	h
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-15.39060661372321	-5.86653585765840	-4.60865929416168	h
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-5.70468731229627	-9.34382970724383	7.25509302170333	h
-15.00140074718047	-8.60238197399053	8.51962548015567	h
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-3.46496770017901	8.31845658370232	11.98658393105780	h
-0.67723922280094	10.87784843067577	4.72505299842960	h
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2.27243547801333	13.77203715227662	6.89458395181630	h
2.37567381427091	13.96568377177591	11.61025303053246	h
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-13.02667932291134	9.68377717262250	8.89213862974374	h
-13.29725191903435	6.77514360629922	12.58890722651347	h
3.46496770017901	-8.31845658370232	11.98658393105780	h
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7.84201909095089	-3.64646310001149	-1.56706745321405	h
13.90987171354010	-3.07503178591466	5.59628958719499	h
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15.37507719026738	-4.56963735727834	1.37535419371907	h
-9.48416235485030	1.85878763619601	6.25788640907384	h
-7.84201909095089	3.64646310001149	-1.56706745321405	h
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-12.31199120483830	4.84914668384665	-2.20131042722787	h

[Au₃Cu(C₂C₁₀H₁₇O)₃(Ph₂P(CH₂)₂PPh(CH₂)₂PPh₂)]₂²⁺ (4)

4.31272651990157	8.34596345693934	3.03497965826509	au
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1.63512721050299	-4.07457837366749	0.61484308578610	au
4.21290645392600	-9.21143295664339	2.95880057906916	au
-4.31272651990157	-8.34596345693934	3.03497965826509	au
0.39632899325900	-9.26630040190665	-1.05225043221164	cu
-0.39632899325900	9.26630040190665	-1.05225043221164	cu
-7.12961546890883	-5.61766777563980	4.93923651399849	p
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3.74683945394333	-8.36993211985233	7.21918709657956	p
4.37525281008453	-2.42617487965702	3.60570551378226	p
7.12961546890883	5.61766777563980	4.93923651399849	p
2.47015903356610	11.01993112929984	1.07372868685454	c
1.99622333562324	12.81080382581693	-0.36559867458105	c
-0.66030815196759	-5.44077426516036	-2.08583816761100	c
-1.99157123433391	-6.19209785885533	-3.85080986773414	c
4.39156367690009	-9.91551897689168	-0.76409085176649	c
4.56487801571500	-10.29801601475232	-3.05905638020400	c
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1.99157123433391	6.19209785885533	-3.85080986773414	c
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4.73224694261510	1.05608088873429	3.34736131042842	c
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-2.04778141095782	5.33838392776109	7.66787917863518	c
-3.37726361594208	2.87829828849191	6.93390372011031	c
-4.73224694261510	-1.05608088873429	3.34736131042842	c
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13.01017987024956	5.82733661326356	12.25808334440110	h
6.17204875336004	10.20262698833822	13.03655904565181	h
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-12.79668069020157	8.17599450686065	13.10799180271139	h
2.94341249049678	-9.64238699677465	12.64151542535358	h
0.14559277515908	-12.10598204164066	5.35279905834485	h
0.09235688800513	-12.67786009906119	14.74780411316723	h
-2.69508114437680	-15.13703046504005	7.48450184802851	h
-2.73726908780677	-15.44623250877010	12.19242617198265	h
5.24307304469255	-5.44906014624855	11.85714018034523	h
8.53871375435131	-10.89611541009423	6.71904646778564	h
9.17803665404604	-5.43703531124835	14.35783104379026	h
12.45625627846912	-10.91960154943632	9.29276074098341	h
12.79668069020157	-8.17599450686065	13.10799180271139	h
8.75966125610537	-3.16238324088721	7.25059251870457	h
7.15080288283539	-4.14569685175424	-0.72145574870441	h
13.18803261926540	-4.30087499972050	6.48861981745186	h
11.62718778415701	-5.26445038345827	-1.45830560776718	h
14.67559703086544	-5.34851409684367	2.14154984856392	h
-8.75966125610537	3.16238324088721	7.25059251870457	h
-7.15080288283539	4.14569685175424	-0.72145574870441	h
-13.18803261926540	4.30087499972050	6.48861981745186	h
-11.62718778415701	5.26445038345827	-1.45830560776718	h
-2.06521494270018	-14.96504660810237	-2.16178453682031	c
-0.30265471240154	-17.25283739393210	-1.45988428967328	c
-4.74146405909413	-16.22203454397654	-2.10517115707422	c
-1.71566202207549	-19.55934318076450	-2.67935823367482	c
-0.75188435478327	-17.75459277260739	1.38099150647301	c
-4.22478528567560	-18.95322636671324	-1.30402697569600	c
-6.04532791513176	-15.24485370971155	-0.81145244000535	h
-5.53683097494785	-16.09481695660455	-4.02194115127892	h
0.68323326597533	-19.08680542502563	2.08903127961512	h
-0.54913079104475	-16.01211975496200	2.50360258181148	h
-3.44423710834731	-18.89375951166177	1.49380217851552	c
-5.80525790987641	-20.24331702641375	-1.72340850258844	h
-3.44479855170160	-20.79915842970364	2.33325752064915	h
-4.76043616039930	-17.73639668760948	2.62486550403494	h
2.06521494270018	14.96504660810237	-2.16178453682031	c
0.30265471240154	17.25283739393210	-1.45988428967328	c
4.74146405909413	16.22203454397654	-2.10517115707422	c
1.71566202207549	19.55934318076450	-2.67935823367482	c
0.75188435478327	17.75459277260739	1.38099150647301	c
4.22478528567560	18.95322636671324	-1.30402697569600	c
6.04532791513176	15.24485370971155	-0.81145244000535	h
5.53683097494785	16.09481695660455	-4.02194115127892	h
-0.68323326597533	19.08680542502563	2.08903127961512	h
0.54913079104475	16.01211975496200	2.50360258181148	h
3.44423710834731	18.89375951166177	1.49380217851552	c
5.80525790987641	20.24331702641375	-1.72340850258844	h
3.44479855170160	20.79915842970364	2.33325752064915	h
4.76043616039930	17.73639668760948	2.62486550403494	h
4.86092402596950	-10.92055041337862	-5.76555016196989	c
6.22947469693845	-8.78235021300919	-7.31177008925456	c
6.65490022212791	-13.22131886654712	-6.20617346038192	c
7.37800739965019	-10.27373688189818	-9.60197521179190	c
8.64135577807775	-8.12730985483038	-5.79569069435971	c
8.78284127332536	-12.16499629920343	-7.86401990825208	c
5.56330644152431	-14.70195636314208	-7.17475871323793	h
9.48248640501797	-6.37863072824327	-6.55565747963585	h
8.19835350803560	-7.76721782287180	-3.79356142314540	h
10.39383575332779	-10.43654432283530	-6.17916902523535	c
9.86336181639421	-13.64706153809484	-8.84992623284360	h
12.18233996828549	-9.90977864118488	-7.10655509277451	h
10.89507151755329	-11.37083157961254	-4.38446641495538	h
-4.86092402596950	10.92055041337862	-5.76555016196989	c
-6.22947469693845	8.78235021300919	-7.31177008925456	c
-6.65490022212791	13.22131886654712	-6.20617346038192	c
-7.37800739965019	10.27373688189818	-9.60197521179190	c
-8.64135577807775	8.12730985483038	-5.79569069435971	c
-8.78284127332536	12.16499629920343	-7.86401990825208	c
-5.56330644152431	14.70195636314208	-7.17475871323793	h
-9.48248640501797	6.37863072824327	-6.55565747963585	h
-8.19835350803560	7.76721782287180	-3.79356142314540	h

-10.39383575332779	10.43654432283530	-6.17916902523535	c
-9.86336181639421	13.64706153809484	-8.84992623284360	h
-12.18233996828549	9.90977864118488	-7.10655509277451	h
-10.89507151755329	11.37083157961254	-4.38446641495538	h
3.49014740107134	7.02942049072935	-6.05916706880820	c
6.38180762328151	7.38209832849810	-5.46183151603067	c
3.54113943149680	4.98851181540117	-8.30404149000375	c
7.50853647874200	7.16938823477487	-8.12632953962871	c
7.35438163379840	4.91809389232312	-4.23147564791094	c
6.42272980761494	4.54871769081934	-8.65968205381753	c
9.59472694651351	7.20789690847213	-8.09836332215542	h
6.83413490598105	8.66459857004861	-9.40561714187205	h
9.21590952741627	5.27112841559478	-3.35974207394612	h
6.08492167612677	4.27078896262706	-2.70778300772545	h
7.54614310411009	3.03511328903047	-6.45887527975529	c
6.84425744039346	3.73834956301560	-10.53120628229476	h
9.53650416312757	2.57683053602875	-6.87806964451411	h
6.57390971116222	1.22771480609650	-6.11264594774967	h
-3.49014740107134	-7.02942049072935	-6.05916706880820	c
-6.38180762328151	-7.38209832849810	-5.46183151603067	c
-3.54113943149680	-4.98851181540117	-8.30404149000375	c
-7.50853647874200	-7.16938823477487	-8.12632953962871	c
-7.35438163379840	-4.91809389232312	-4.23147564791094	c
-6.42272980761494	-4.54871769081934	-8.65968205381753	c
-9.59472694651351	-7.20789690847213	-8.09836332215542	h
-6.83413490598105	-8.66459857004861	-9.40561714187205	h
-9.21590952741627	-5.27112841559478	-3.35974207394612	h
-6.08492167612677	-4.27078896262706	-2.70778300772545	h
-7.54614310411009	-3.03511328903047	-6.45887527975529	c
-6.84425744039346	-3.73834956301560	-10.53120628229476	h
-9.53650416312757	-2.57683053602875	-6.87806964451411	h
-6.57390971116222	-1.22771480609650	-6.11264594774967	h
1.65986521161425	13.97675938694320	-4.61988774862091	o
-0.13247906554643	13.59080039521669	-4.94797200160865	h
2.38385815499951	9.28590562503658	-6.98456864335139	o
2.73425081298584	10.73014822719297	-5.86479459607120	h
-1.65986521161425	-13.97675938694320	-4.61988774862091	o
0.13247906554643	-13.59080039521669	-4.94797200160865	h
-2.38385815499951	-9.28590562503658	-6.98456864335139	o
-2.73425081298584	-10.73014822719297	-5.86479459607120	h
-7.36154236310161	14.02313453407191	-4.42134392702270	h
7.36154236310161	-14.02313453407191	-4.42134392702270	h
-2.43500446568035	11.57610853926610	-6.71217501834773	o
-1.30871909099003	10.10999116878947	-6.88662571884639	h
2.43500446568035	-11.57610853926610	-6.71217501834773	o
1.30871909099003	-10.10999116878947	-6.88662571884639	h
-2.44876592114241	16.89273247451771	-2.14835178999537	c
-2.71858672313810	16.68006041742564	-4.20484985238535	h
-3.25563363914684	15.21036815939505	-1.21205715261477	h
-3.56781950835654	18.54808653811970	-1.54927111028242	h
7.04959062604843	9.74862982961958	-4.00109477811429	c
6.48176239360911	11.48272769218562	-5.01011796468768	h
6.15603914196185	9.77245969361731	-2.11761814034315	h
9.11709884304880	9.84452600910362	-3.73429428391388	h
2.44876592114241	-16.89273247451771	-2.14835178999537	c
2.71858672313810	-16.68006041742564	-4.20484985238535	h
3.25563363914684	-15.21036815939505	-1.21205715261477	h
3.56781950835654	-18.54808653811970	-1.54927111028242	h
4.58200403544017	-6.51529861847098	-7.87364757606927	c
3.79898230934259	-5.69400762194263	-6.11812856619405	h
5.67975536700706	-5.02677365989865	-8.83908060271006	h
2.98589029913892	-7.00611268012881	-9.11924336308403	h
-7.04959062604843	-9.74862982961958	-4.00109477811429	c
-6.48176239360911	-11.48272769218562	-5.01011796468768	h
-6.15603914196185	-9.77245969361731	-2.11761814034315	h
-9.11709884304880	-9.84452600910362	-3.73429428391388	h
-4.58200403544017	6.51529861847098	-7.87364757606927	c
-3.79898230934259	5.69400762194263	-6.11812856619405	h
-5.67975536700706	5.02677365989865	-8.83908060271006	h
-2.98589029913892	7.00611268012881	-9.11924336308403	h
1.90602316401491	19.54239801743196	-5.56775326565171	c
0.02555103967957	19.85948142605928	-6.41721516263398	h
3.12972101927541	21.11211914390198	-6.19772579101603	h
2.64196419602072	17.77161744949484	-6.35844061770053	h
0.58499701390700	22.12598509939811	-1.95722423375394	c
1.81945714401550	23.65547877940000	-2.65783503465847	h
-1.27831400893936	22.38599560408434	-2.85970597557131	h

0.33750109980510	22.41987192342842	0.08679169481052	h
-0.58499701390700	-22.12598509939811	-1.95722423375394	c
-1.81945714401550	-23.65547877940000	-2.65783503465847	h
1.27831400893936	-22.38599560408434	-2.85970597557131	h
-0.33750109980510	-22.41987192342842	0.08679169481052	h
-1.90602316401491	-19.54239801743196	-5.56775326565171	c
-2.64196419602072	-17.77161744949484	-6.35844061770053	h
-0.02555103967957	-19.85948142605928	-6.41721516263398	h
-3.12972101927541	-21.11211914390198	-6.19772579101603	h
2.08932885297553	2.56808016514369	-7.70927153770622	c
2.59170717498784	1.72723737887668	-5.87303783121482	h
0.03715495200151	2.92648567488614	-7.66867753049770	h
2.45753019701468	1.14797643490504	-9.19357046325743	h
2.45859631830702	6.08335673471066	-10.75693784000506	c
2.58076052234534	4.62817174863749	-12.24762941413131	h
0.45855985939829	6.61071642540662	-10.54630524755928	h
3.47471423893539	7.77282150497496	-11.41242660259691	h
-2.45859631830702	-6.08335673471066	-10.75693784000506	c
-0.45855985939829	-6.61071642540662	-10.54630524755928	h
-3.47471423893539	-7.77282150497496	-11.41242660259691	h
-2.58076052234534	-4.62817174863749	-12.24762941413131	h
-2.08932885297553	-2.56808016514369	-7.70927153770622	c
-2.59170717498784	-1.72723737887668	-5.87303783121482	h
-0.03715495200151	-2.92648567488614	-7.66867753049770	h
-2.45753019701468	-1.14797643490504	-9.19357046325743	h
5.48222083215414	-11.50687726896848	-11.40865147694921	c
4.40880776885244	-10.04687176206501	-12.44545970967081	h
6.51172001418650	-12.63106366916206	-12.83463818113729	h
4.09675002144654	-12.73600956182669	-10.47611801307521	h
9.13735384306969	-8.66935709714468	-11.25147123874848	c
10.10984025607248	-9.89080584789577	-12.63567105063129	h
8.03784104440347	-7.26915339834863	-12.34025719190959	h
10.60523478498981	-7.63462509338671	-10.20225770772379	h
-9.13735384306969	8.66935709714468	-11.25147123874848	c
-10.10984025607248	9.89080584789577	-12.63567105063129	h
-8.03784104440347	7.26915339834863	-12.34025719190959	h
-10.60523478498981	7.63462509338671	-10.20225770772379	h
-5.48222083215414	11.50687726896848	-11.40865147694921	c
-4.09675002144654	12.73600956182669	-10.47611801307521	h
-4.40880776885244	10.04687176206501	-12.44545970967081	h
-6.51172001418650	12.63106366916206	-12.83463818113729	h

[Au₃Cu(C₂C₁₀H₁₇O)₃(Ph₂P(CH₂)₂PPh(CH₂)₂PPh₂)]₂²⁺ (4 high temperature isomer)

-3.92020115175969	-7.74367800952755	3.81499310270926	au
15.44446155314793	-2.96513576989723	2.66150698239963	au
4.75122101473017	-4.36642460919295	-2.58081269227954	au
-4.75122101473017	4.36642460919295	2.58081269227954	au
-15.44446155314793	2.96513576989723	-2.66150698239963	au
3.92020115175969	7.74367800952755	-3.81499310270926	au
0.44140646560871	-8.71099452282094	-0.87441886397851	cu
-0.44140646560871	8.71099452282094	0.87441886397851	cu
-7.16156332506546	-5.53738168859105	5.77540979199912	p
-8.14041216471382	1.80837793411862	1.51255558494529	p
-12.18896292294406	5.83348478722734	-3.15197233008292	p
12.18896292294406	-5.83348478722734	3.15197233008292	p
8.14041216471382	-1.80837793411862	-1.51255558494529	p
7.16156332506546	5.53738168859105	-5.77540979199912	p
1.32088773786629	10.02121677027500	-2.25265780633817	c
1.99967265713271	-6.70724346216927	-3.73741415430573	c
17.94197054829274	-0.26671194046551	1.91488470025752	c
-17.94197054829274	0.26671194046551	-1.91488470025752	c
-1.99967265713271	6.70724346216927	3.73741415430573	c
-1.32088773786629	-10.02121677027500	2.25265780633817	c
7.33428333740904	2.13421696183462	-5.00271747553852	c
7.62311625603319	1.58787112138721	-2.19115897168143	c
8.87490831719682	-1.66484153198497	1.89432026284901	c
9.12907891416297	-4.11897663111385	3.39882610877600	c
-9.12907891416297	4.11897663111385	-3.39882610877600	c
-8.87490831719682	1.66484153198497	-1.89432026284901	c
-7.62311625603319	-1.58787112138721	2.19115897168143	c
-7.33428333740904	-2.13421696183462	5.00271747553852	c
-6.89585810979348	-5.54255606368752	9.21097964373915	c
-9.03879011438636	-5.62110144193536	10.76229251383062	c

-4.48739497726864	-5.40984680932553	10.30627863381875	c
-8.76839343247545	-5.54824890045268	13.38176319142433	c
-4.22947287792538	-5.32536051928195	12.92510190524980	c
-6.36958189678886	-5.39524439160196	14.46367121834885	c
-10.23072502129181	-6.87987659568516	4.995394542215763	c
-10.37520780892657	-9.49002627511476	4.55292290242972	c
-12.43807766413950	-5.41826112046398	4.85759229721816	c
-12.68868945539526	-10.61398519288869	3.99309961006766	c
-14.74657386298242	-6.53865875824811	4.25018097497502	c
-14.86737497050257	-9.13881599632941	3.82745198419636	c
6.89585810979348	5.54255606368752	-9.21097964373915	c
9.03879011438636	5.62110144193536	-10.76229251383062	c
4.48739497726864	5.40984680932553	-10.30627863381875	c
8.76839343247545	5.54824890045268	-13.38176319142433	c
4.22947287792538	5.32536051928195	-12.92510190524980	c
6.36958189678886	5.39524439160196	-14.46367121834885	c
10.23072502129181	6.87987659568516	-4.995394542215763	c
10.37520780892657	9.49002627511476	-4.55292290242972	c
12.43807766413950	5.41826112046398	-4.85759229721816	c
12.68868945539526	10.61398519288869	-3.99309961006766	c
14.74657386298242	6.53865875824811	-4.25018097497502	c
14.86737497050257	9.13881599632941	-3.82745198419636	c
11.88064636973520	-8.10447681162884	0.57718379116493	c
14.08630262801135	-8.84298970154585	-0.69143763195989	c
9.57376196209126	-9.22207935547755	-0.09212211660371	c
13.98357277542678	-10.67526045235565	-2.58068516809179	c
9.47055688034704	-11.04886431127992	-1.98999182729575	c
11.67910390006419	-11.77841474846484	-3.23266410189214	c
12.21838984083488	-7.70279022489084	6.05745981358555	c
11.19050734569592	-10.13683319345203	6.20397022390753	c
13.31073765455890	-6.61625827347531	8.21396914241858	c
11.23075741351644	-11.45010068918764	8.48801067162296	c
13.33626890424450	-7.93250626856365	10.49460275276562	c
12.29519179255380	-10.35067497470372	10.63405782790855	c
-11.88064636973520	8.10447681162884	-0.57718379116493	c
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3.74857163813329	14.82961622533447	11.41146337401679	h
2.74779647128511	6.45490387354006	12.54689737510868	h
-0.15333826636280	6.04506696305114	10.93571181725857	h

[Au₃Ag(C₂C₁₀H₁₇O)₃(Ph₂P(CH₂)₂PPh(CH₂)₂PPh₂)]₂²⁺ (5)

4.95826578927249	8.57838405953169	2.51974973283300	au
-4.52870773286003	9.28267682367692	3.70553904927018	au
-2.30894930155352	4.17139567034724	0.33928805336450	au
2.30894930155352	-4.17139567034724	0.33928805336450	au

4.52870773286003	-9.28267682367692	3.70553904927018	au
-4.95826578927249	-8.57838405953169	2.51974973283300	au
-7.80470881432903	-5.65256366942274	4.06717292872423	p
-4.70113666575400	2.33715531931881	3.50278627489271	p
-3.48790720178632	7.83236332089223	7.68780364023570	p
3.48790720178632	-7.83236332089223	7.68780364023570	p
4.70113666575400	-2.33715531931881	3.50278627489271	p
7.80470881432903	5.65256366942274	4.06717292872423	p
2.98746105813440	11.37763017165791	0.90121641792720	c
2.40501112701080	13.24713001483644	-0.38416468466151	c
0.48762191062120	-5.71336533022569	-2.59661563627533	c
-0.39947186691494	-6.58138241766242	-4.57125106756220	c
5.18749799159352	-10.64639959693105	0.23871172786823	c
5.68304185473908	-11.51506381383135	-1.86504351947336	c
-5.18749799159352	10.64639959693105	0.23871172786823	c
-5.68304185473908	11.51506381383135	-1.86504351947336	c
-0.48762191062120	5.71336533022569	-2.59661563627533	c
0.39947186691494	6.58138241766242	-4.57125106756220	c
-2.98746105813440	-11.37763017165791	0.90121641792720	c
-2.40501112701080	-13.24713001483644	-0.38416468466151	c
6.58699026411838	2.50997248323508	5.00586306008819	c
5.17555600630421	1.09228859787226	2.93346187979113	c
3.36452335452804	-2.41844309949043	6.73922111600984	c
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-1.84364391845763	4.74077465086155	7.54377325057560	c
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-5.17555600630421	-1.09228859787226	2.93346187979113	c
-6.58699026411838	-2.50997248323508	5.00586306008819	c
-10.30382251113607	-5.02466420065702	1.77926322433425	c
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-14.21781427967461	-4.33735101604131	-1.72177223899367	c
-9.36138174627901	-6.69243056676934	6.96695622739415	c
-11.85354433752459	-6.00182723242189	7.53363617728887	c
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-9.08543125078440	-8.90416686236988	10.96518178367605	c
-11.56454433491193	-8.20541527725917	11.52596397319749	c
10.30382251113607	5.02466420065702	1.77926322433425	c
11.57450183943475	2.70327894234943	1.63019578947468	c
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13.51699204834878	2.36684048611342	-0.11890420472721	c
12.96318103615813	6.65160331501865	-1.58405453076422	c
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0.89825069097323	11.51935971342881	12.97179918582733	c
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-8.18050278743569	9.02572910771347	9.68676079276470	c
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-10.06930059617421	7.12347089797161	13.38370092053410	c
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-2.46564221142416	-13.00757848380015	11.45889867664266	c
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9.44195335303020	-3.44327058190548	5.82132351336239	c
8.98529342256818	-4.46554962726705	1.38900105285475	c
11.95978238570475	-4.21867888612906	5.73177520478850	c
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-12.99645533082078	5.10314677545615	3.47568955848093	c
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-5.35943103898662	-2.87212714583847	6.65364805032563	h
-8.22445309501363	-1.42685125782002	5.71258767813978	h
-3.30232525851891	-1.94078171837752	2.55946036256584	h
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-12.96402816836063	-4.89768131085996	6.18269104833353	h
-6.05639184450822	-8.76363520505796	8.24049549349726	h
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1.05902406045079	11.60241504535359	15.03108747073962	h
3.42480219548817	14.10661741682392	7.63320640972080	h
3.85724400139437	14.26281091462804	12.33299712936312	h
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-8.27696460652090	10.38090637771800	8.12578596125480	h
-7.89150906932713	4.17567212025373	15.19051724678707	h
-11.80027012933753	10.11782705675848	11.20680533840364	h
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1.90706076621747	20.01859310593374	-2.56228538502899	c
2.16244417557113	18.24008179057528	1.61939933770036	c
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6.47809236701981	2.89582608976666	-9.92048908956886	h
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-4.35149199635919	-7.63550239221892	-7.07974516481598	c
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-3.65579101305004	-1.67461079701992	-8.61192665277799	h
0.92714625537684	14.49844193590415	-4.35443397047998	o
-0.92733511433624	14.47266562423412	-4.22527157644439	h
0.36463079707712	10.08656750591669	-7.27008449338678	o
1.19333899420330	11.31045887396946	-6.14537278746748	h
-0.92714625537684	-14.49844193590415	-4.35443397047998	o
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-3.89100854732597	13.00786732905122	-5.60981736301909	o
-3.12669937915304	11.42548338941415	-6.20182029012887	h
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3.12669937915304	-11.42548338941415	-6.20182029012887	h
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-2.96606976520516	17.45036684236354	-2.56076449466854	h
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-2.80803567368340	19.26557580541748	0.25447149279297	h
5.60741029693986	9.65395076348402	-5.48769734890260	c
5.05879346269169	11.57938105857105	-6.07034684637577	h
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7.68052397793542	9.52305747759394	-5.69092372800854	h
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2.96606976520516	-17.45036684236354	-2.56076449466854	h
2.58028590126579	-15.90708584810670	0.41397149299063	h
2.80803567368340	-19.26557580541748	0.25447149279297	h
7.07173895854176	-8.61739957898347	-7.04465808269834	c
6.20276930469457	-7.42187443343366	-5.56584503869564	h
8.54614845395258	-7.48742920919879	-7.99298564903531	h
5.61103436389481	-9.03772853779326	-8.46946103113174	h
-5.60741029693986	-9.65395076348402	-5.48769734890260	c
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-7.07173895854176	8.61739957898347	-7.04465808269834	c
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-5.61103436389481	9.03772853779326	-8.46946103113174	h
1.20095258320811	20.01213719780962	-5.36959624862635	c
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1.61059595600199	18.22670632963156	-6.34280310169273	h
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2.26006844280499	24.10270226471648	-2.59605563268119	h
-0.83062123564030	23.01884016633737	-1.87142851640142	h
1.57783036542488	22.92156800739526	0.46970189554771	h
-1.19686263389001	-22.63962411507914	-1.55525463688353	c
-2.26006844280499	-24.10270226471648	-2.59605563268119	h
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-0.86659629033880	7.52495898117684	-11.32164296611444	c
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-2.68585554765320	8.15575711576074	-10.53848035981136	h
0.14629265822034	9.21638021399083	-11.97699865225968	h
0.86659629033880	-7.52495898117684	-11.32164296611444	c
2.68585554765320	-8.15575711576074	-10.53848035981136	h
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1.08718079054269	-2.42314837818802	-10.46874685570262	h
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5.82502719613172	-14.98089548601672	-8.86330127146100	h
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12.50939740866325	-13.54531635869021	-10.33888449209936	h
10.94970818352192	-10.60057751898368	-10.72336679324996	h
13.07564619198247	-11.05806544354635	-8.16012393099158	h
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-12.50939740866325	13.54531635869021	-10.33888449209936	h
-10.94970818352192	10.60057751898368	-10.72336679324996	h
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-7.54398975344781	14.17722154521272	-9.69970908676456	c
-5.82502719613172	14.98089548601672	-8.86330127146100	h
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-8.53372839284219	15.68120793426169	-10.75629602422855	h
0.82688580775150	-9.81796421405805	-0.64731593756950	ag
-0.82688580775150	9.81796421405805	-0.64731593756950	ag

[Au₃Ag(C₂C₉H₁₉O)₃(Ph₂P(CH₂)₂PPh(CH₂)₂PPh₂)]⁺ (6)

2.01018167743851	1.00346557552693	-5.07130129540581	au
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2.01018167743851	1.00346557552693	5.07130129540581	au
-2.38316448874610	0.68201046970757	0.00000000000000	ag
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6.80758396522994	3.33256981631718	0.00000000000000	p
6.03223161737116	1.40467891432075	-6.72994742015966	p
7.91145616102954	3.99105250632043	5.28571122082729	c
9.04491198165291	3.45629545141677	2.68709886008858	c
9.04491198165291	3.45629545141677	-2.68709886008858	c
7.91145616102954	3.99105250632043	-5.28571122082729	c
-1.69038170187903	1.10798735373743	-4.21839643840693	c
2.51436496633377	-3.57087144605087	0.00000000000000	c
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-4.01609120699586	1.35808926834601	4.30330253767419	c
-4.01609120699586	1.35808926834601	-4.30330253767419	c
1.43685061108761	-5.62214083405076	0.00000000000000	c
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5.82838861961482	0.46040799851975	-11.93287615342801	c
5.54060039974832	4.86553280800056	-10.74454941951828	c
5.54539591515204	1.13105656147801	-14.46357853014605	c
5.26167297298614	5.52583095411904	-13.27940227525658	c
5.26673973846478	3.66260605531000	-15.14273649035358	c
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-6.73145876203487	1.80535157779946	4.80672758139630	c
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2.92465831966677	11.16319395786601	0.00000000000000	c
-0.58898616761930	9.07825931158544	0.00000000000000	h
6.70284528155852	12.72752685640858	0.00000000000000	h
2.00186609982919	13.01303114543611	0.00000000000000	h