

Supporting Information

Metallophilicity-assisted assembly of phosphine-based cage molecules

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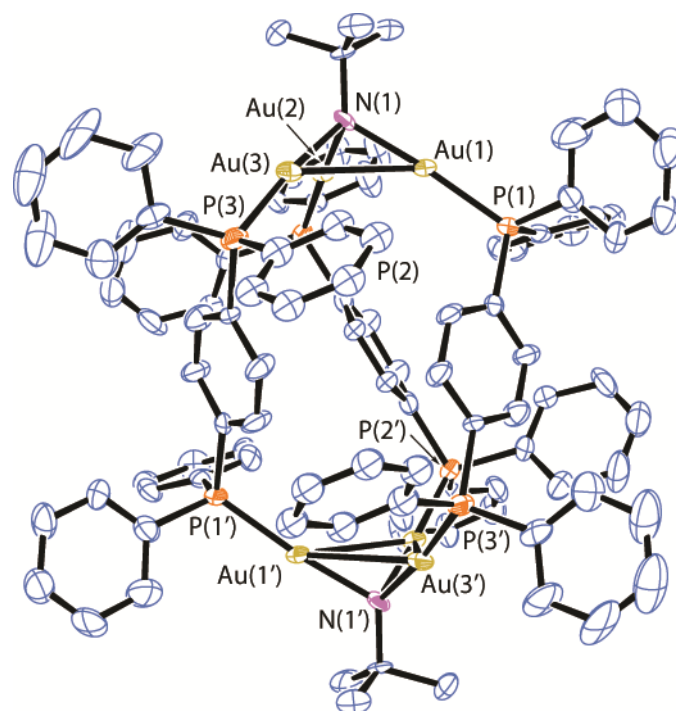


Figure S1. ORTEP view of the dication **1** (counterions and hydrogen atoms are omitted for clarity; ellipsoids are shown at 50% probability).

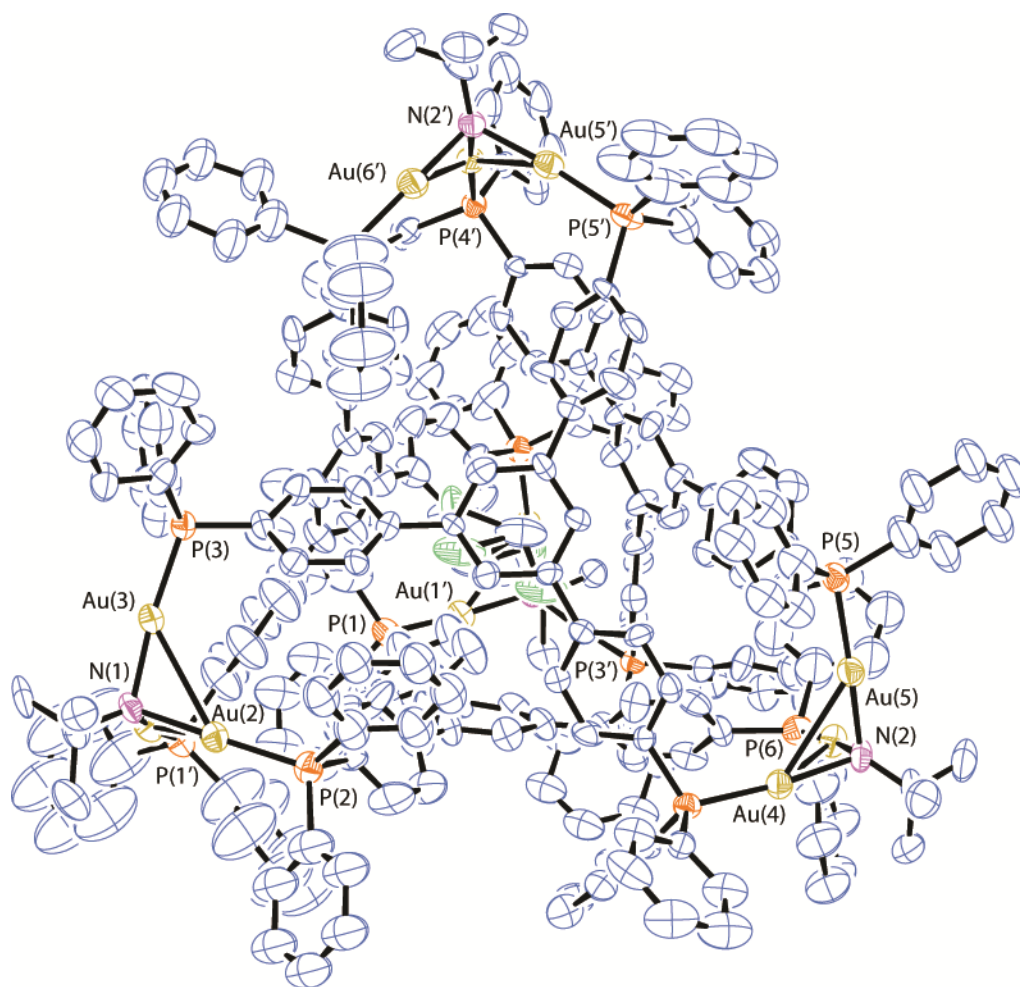


Figure S2. ORTEP view of the tetracation **4** (counterions and hydrogen atoms are omitted for clarity; ellipsoids are shown at 50% probability).

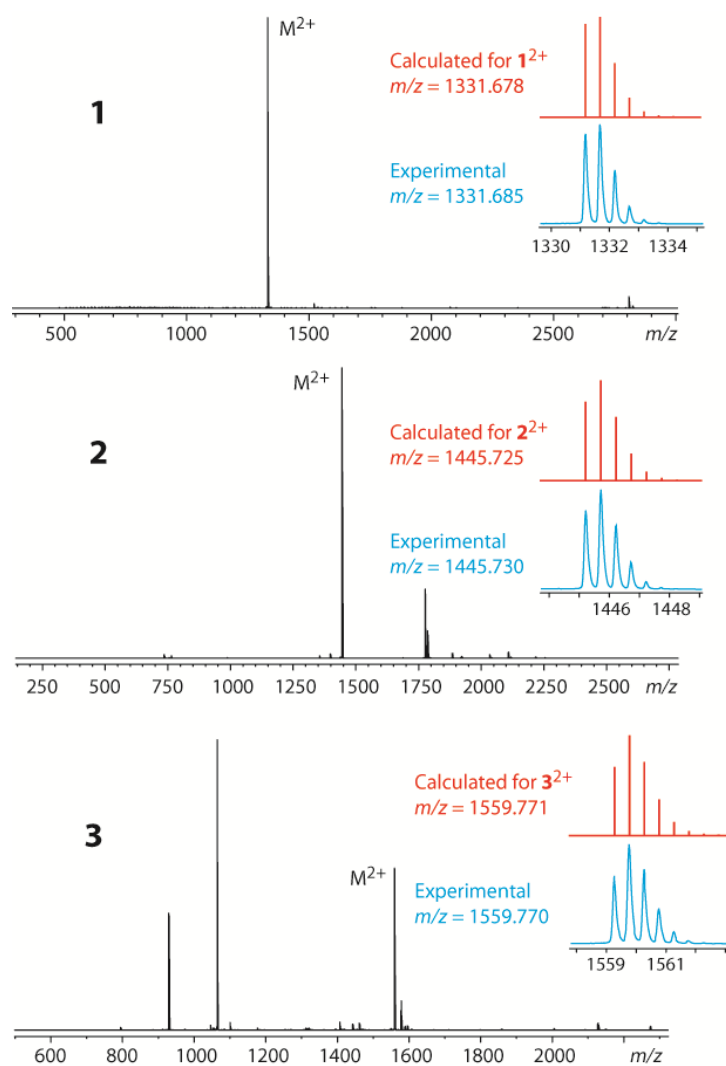


Figure S3. ESI-MS spectra of 1–3.

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

$[(\mu_3\text{-Bu}^t\text{NAu}_3)_2(\text{PPh}_2\text{C}_6\text{H}_4\text{PPh}_2)_3]^{2+}$ (1)

0.000000000000000	0.000000000000000	-9.82742676468305	n
0.19308093169600	-3.36802652485621	-7.86560404903517	au
-3.01333699699329	1.51680027059306	-7.86560404903517	au
2.82025606529735	1.85122625426318	-7.86560404903517	au
0.000000000000000	0.000000000000000	9.82742676468305	n
0.19308093169600	3.36802652485621	7.86560404903517	au
-3.01333699699329	-1.51680027059306	7.86560404903517	au
2.82025606529735	-1.85122625426318	7.86560404903517	au
-6.14367655317532	2.98028787061925	-5.32613418994343	p
5.65284328313454	3.83043603237504	-5.32613418994343	p
0.49083327004084	-6.81072390299423	-5.32613418994343	p
0.49083327004084	6.81072390299423	5.32613418994343	p
-6.14367655317532	-2.98028787061925	5.32613418994343	p
5.65284328313454	-3.83043603237505	5.32613418994343	p
4.20311935889617	4.51254144180280	-2.26189516573891	c
1.88959845448702	5.79850842792380	-2.29731634745683	c
5.27779577073043	3.84783912464568	0.05989463760073	c
0.69342854625355	6.49462477576150	-0.05989463760073	c
1.01168568582539	6.28293211988238	-4.10425927747298	h
4.07685637539668	4.53569447849944	2.29731634745683	c
7.05865162496228	2.80064109872152	0.14632160610880	h
1.80641584478323	5.89627886084364	2.26189516573891	c

-1.10389947410554	7.51329217304244	-0.14632160610880	h
4.93533598315872	4.01761156451099	4.10425927747298	h
1.80641584478323	-5.89627886084364	-2.26189516573891	c
4.07685637539668	-4.53569447849944	-2.29731634745683	c
0.69342854625355	-6.49462477576150	0.05989463760073	c
5.27779577073043	-3.84783912464568	-0.05989463760073	c
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7.05865162496228	-2.80064109872152	-0.14632160610880	h
1.01168568582539	-6.28293211988238	4.10425927747298	h
-6.00953520367938	1.38373741904082	-2.26189516573891	c
-5.96645482988369	-1.26281394942436	-2.29731634745683	c
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-5.97122431698399	-2.64678565111582	-0.05989463760073	c
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0.00000000000000	0.00000000000000	12.62782483207197	c
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-2.27046555178660	-3.43386882383815	-12.91425402002027	h
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2.46809005905835	-1.26613210037213	-15.69118382628462	h
4.10905041060052	-0.24934643434554	-12.91425402002027	h
2.54027529521032	-3.23753017464400	-12.94527299268291	h
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-2.33054759299840	1.50436263978632	15.69118382628462	h
-2.27046555178660	3.43386882383815	12.91425402002027	h
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7.97618148326349	-11.24447118373312	5.79955713231092	c
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11.06788078747547	3.78598288917259	5.59640637505861	h
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-4.80047041897141	-13.85109919971834	-2.06664924965841	h
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5.77644608616272	-13.03324812446975	-8.38767023266414	c
4.27664208366224	-12.01932924385129	-12.05218123982871	h
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6.67217981981591	6.91330477845090	-6.46959862144641	c
7.08387381058691	7.20164973014404	-9.06987226390424	c
7.11430993356824	8.94893711085047	-4.83556056757527	c
7.95166158344148	9.49765701993750	-10.02158288982422	c
6.71534662910647	5.62199501569594	-10.35649641752458	h
7.97618148326349	11.24447118373312	-5.79955713231092	c
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8.27072341979330	9.71334530927080	-12.05218123982871	h
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9.07327359414948	13.32337804738673	-9.13833419592855	h
8.54587096099602	2.08015179972128	-4.68323059802181	c
10.60156780717386	3.23290511752803	-3.47153830922189	c
8.73361692436104	-0.44403211172843	-5.45455693616905	c
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14.39563898678010	2.76822026691417	-2.06664924965841	h
11.06788078747547	-3.78598288917259	-5.59640637505861	h
14.69004422206325	-1.74088600424096	-3.38718937801215	h
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2.69487471016863	9.73563954224360	9.06987226390424	c
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1.51111718898891	8.62665828387230	10.35649641752458	h
5.74990695560324	12.52981138156782	5.79955713231092	c
4.19330361739582	10.23879104462266	2.80487672611179	h
5.77644608616272	13.03324812446975	8.38767023266414	c
4.27664208366224	12.01932924385129	12.05218123982871	h
6.95344959991617	13.62093489966694	4.52101543529682	h
7.00174705618605	14.51937445171338	9.13833419592855	h
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-4.75135155103343	7.34151806755416	5.45455693616905	c
-4.78947567739504	12.00706329377280	2.99981870802353	c
-0.72786903003405	11.70883563689808	2.91935152936490	h
-7.04085202938835	8.55560860215803	4.97300330163251	c
-4.72287614950409	5.54844345015595	6.48671955974092	h
-7.05979265080044	10.88457905928867	3.74124901061249	c
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-8.81269775405440	7.69207448342517	5.59640637505861	h
-8.85267361579706	11.85150847690313	3.38718937801215	h

$[(\mu_3\text{-Bu}^t\text{NAu}_3)_2(\text{PPh}_2(\text{C}_6\text{H}_4)_2\text{PPh}_2)_3]^{2+}$ (2)

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-3.14614889045816	-1.10200692893181	-11.96628265129037	au
0.00000000000000	0.00000000000000	14.00424503192364	n
0.61870844962764	-3.27564832769086	11.96628265129037	au
2.52744044083048	2.17364139875905	11.96628265129037	au
-3.14614889045816	1.10200692893181	11.96628265129037	au
5.12478816364012	-4.24547023876475	-9.25207127875773	p
-6.23907915960116	-2.31546161934372	-9.25207127875773	p
1.11429099596105	6.56093185810854	-9.25207127875773	p
1.11429099596105	-6.56093185810854	9.25207127875773	p
5.12478816364012	4.24547023876475	9.25207127875773	p
-6.23907915960116	2.31546161934372	9.25207127875773	p
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0.00000000000000	0.00000000000000	16.79867601676797	c
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4.08730239640692	-0.47051269011543	-17.10260908193423	h
2.64433565216842	0.86404520875574	-19.85479252454735	h
3.06453212882824	2.74622823810292	-17.07566986978152	h
-2.02008677421171	1.83327320560925	-17.76971841206574	c
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-3.91056948320143	1.28084855522737	-17.07566986978152	h
-1.63617525576050	3.77496405329514	-17.10260908193423	h
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-0.57761778102911	2.66608306712087	17.76971841206574	c
-0.57388272528348	2.72208445528861	19.85479252454735	h
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-1.63617525576050	-3.77496405329514	17.10260908193423	h
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2.64433565216842	-0.86404520875574	19.85479252454735	h
3.06453212882824	-2.74622823810292	17.07566986978152	h
4.08730239640692	0.47051269011543	17.10260908193423	h
4.44791365403750	-7.59526677513708	-8.84215341168389	c
6.35507873175417	-9.33790356174311	-8.26300843030573	c
1.93886818829705	-8.41686873737811	-9.05895150845194	c
5.74568826108490	-11.87156367938316	-7.87135099785272	c
8.32645040164440	-8.72114981647939	-8.14659323542920	h
1.33907560117792	-10.94828405659741	-8.65518180077720	c
0.45007482995433	-7.07762325968860	-9.58231970645425	h

3.24095609815811	-12.67572136077849	-8.05776240540589	c
7.24165402519032	-13.23037172623859	-7.43642950340714	h
-0.62124141347181	-11.57822986013467	-8.84097668585786	h
2.77323389130438	-14.66824480667165	-7.76524187553543	h
8.44632513245812	-4.05654272618397	-10.12969386343261	c
9.10688770486276	-4.87157571528576	-12.56435567872547	c
10.30710940490814	-3.09910513841326	-8.51417976212852	c
11.61168666907889	-4.75728651602495	-13.35842930313820	c
7.65094543062416	-5.59595780524955	-13.84632045871680	h
12.81335619133804	-2.97469056671937	-9.32756752067471	c
9.80842201581265	-2.44299716619223	-6.61862248187175	h
13.46786845175679	-3.80636234581692	-11.74014674053885	c
12.11835381391582	-5.40197540635976	-15.25566605460274	h
14.26517623627223	-2.22540115184910	-8.06073843550840	h
15.43435933511189	-3.70846282849283	-12.37005885999200	h
4.44791365403750	7.59526677513708	8.84215341168389	c
6.35507873175417	9.33790356174311	8.26300843030573	c
1.93886818829705	8.41686873737811	9.05895150845194	c
5.74568826108490	11.87156367938316	7.87135099785272	c
8.32645040164440	8.72114981647939	8.14659323542920	h
1.33907560117792	10.94828405659741	8.65518180077720	c
0.45007482995433	7.07762325968860	9.58231970645425	h
3.24095609815811	12.67572136077849	8.05776240540589	c
7.24165402519032	13.23037172623859	7.43642950340714	h
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8.44632513245812	4.05654272618397	10.12969386343261	c
9.10688770486276	4.87157571528576	12.56435567872547	c
10.30710940490814	3.09910513841326	8.51417976212852	c
11.61168666907889	4.75728651602495	13.35842930313820	c
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13.46786845175679	3.80636234581692	11.74014674053885	c
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14.26517623627223	2.22540115184910	8.06073843550840	h
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-7.73623161864136	5.28646077023965	10.12969386343261	c
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-7.83745848131880	7.37666601502929	8.51417976212852	c
-9.92577431049821	7.67737237819492	13.35842930313820	c
-8.67171433316402	3.82793420326428	13.84632045871680	h
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-7.01990861520220	7.27284405363625	6.61862248187175	h
-10.03034071336439	9.76033504113996	11.74014674053885	c
-10.73742483948415	7.79381455171931	15.25566605460274	h
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-10.92880268602105	11.51231586109802	12.37005885999200	h
-8.80165080280740	0.05437283066758	8.84215341168389	c
-11.26440106843585	0.83470784387771	8.26300843030573	c
-8.25865624103698	-2.52932526303432	9.05895150845194	c
-13.15391985935288	-0.95986984336609	7.87135099785272	c
-11.71596249210341	2.85034266293548	8.14659323542920	h
-10.15102992145043	-4.31446854009072	8.65518180077720	c
-6.35443895628308	-3.14903539349989	9.58231970645425	h
-12.59797475880634	-3.531111036683426	8.05776240540589	c
-15.07866502902915	-0.34372951188666	7.43642950340714	h
-9.71642048299620	-6.32712577601686	8.84097668585786	h
-14.08968957715902	-4.93243140283029	7.76524187553543	h
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4.90932233668172	10.17261140562087	-8.26300843030573	c
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10.33766189646806	5.25110408411777	-8.84097668585786	h
11.31645568585463	9.73581340384138	-7.76524187553543	h
-0.71009351381676	9.34300349642367	-10.12969386343261	c
-0.33453552653464	10.32258395946617	-12.56435567872547	c
-2.46965092358931	10.47577115344260	-8.51417976212852	c
-1.68591235858067	12.43465889421984	-13.35842930313820	c
1.02076890253979	9.42389200851380	-13.84632045871680	h
-3.83052049649214	12.58403725279694	-9.32756752067471	c
-2.78851340061039	9.71584121982844	-6.61862248187175	h

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-1.38092897443158	13.19578995807901	-15.25566605460274	h
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-9.92577431049821	-7.67737237819492	-13.35842930313820	c
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-10.73742483948415	-7.79381455171931	-15.25566605460274	h
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-10.92880268602105	-11.51231586109802	-12.37005885999200	h
-8.80165080280740	-0.05437283066758	-8.84215341168389	c
-11.26440106843585	-0.83470784387771	-8.26300843030573	c
-8.25865624103698	2.52932526303432	-9.05895150845194	c
-13.15391985953288	0.95986984336609	-7.87135099785272	c
-11.71596249210341	-2.85034266293548	-8.14659323542920	h
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-6.35443895628308	3.14903539349989	-9.58231970645425	h
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-15.07866502902915	0.34372951188666	-7.43642950340714	h
-9.71642048299620	6.32712577601686	-8.84097668585786	h
-14.08968957715902	4.93243140283029	-7.76524187553543	h
-0.71009351381676	-9.34300349642367	10.12969386343261	c
-0.33453552653464	-10.32258395946617	12.56435567872547	c
-2.46965092358931	-10.47577115344260	8.51417976212852	c
-1.68591235858067	-12.43465889421984	13.35842930313820	c
1.02076890253979	-9.42389200851380	13.84632045871680	h
-3.83052049649214	-12.58403725279694	9.32756752067471	c
-2.78851340061039	-9.71584121982844	6.61862248187175	h
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11.31645568585463	-9.73581340384138	7.76524187553543	h
-2.92531022422775	-3.84875257353115	-1.25756940717152	c
-1.38551804291897	-3.85148584721897	-3.41132735327805	c
-5.50101759494847	-3.27462281839448	-1.54967900928221	c
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-6.51468508624798	-2.77439227333007	-3.92519587596790	c
-6.74138204467913	-3.26914028941577	0.10418033052502	h
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-0.08539775106759	6.40133239308780	-1.54967900928221	c
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-3.96387418344550	1.54843556994718	-3.23040999244166	h
0.85464835435690	7.02907891901141	-3.92519587596790	c
0.53953248317034	7.47277825201633	0.10418033052502	h
0.04009428012325	5.71463941216744	-6.07704482954958	c
-2.29122475818402	2.63394231720788	-7.42933691308309	h
2.23269168883966	8.56104591633595	-4.10191449738041	h
4.79577261367261	-0.60901668136596	-1.25756940717152	c
4.02824360746736	0.72584910103992	-3.41132735327805	c
5.58641534601611	-3.12670957469327	-1.54967900928221	c
4.08450632669325	-0.40163129612479	-5.78434328453293	c
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5.66003673189114	-4.25468664568134	-3.92519587596790	c
6.20184956150888	-4.20363796260050	0.10418033052502	h
4.92897576434314	-2.89204237121692	-6.07704482954958	h
3.42667333789686	0.66728768776330	-7.42933691308309	h

6.29773740209201	-6.21409067952143	-4.10191449738041	h
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5.58641534601611	3.12670957469327	1.54967900928221	c
4.02824360746736	-0.72584910103992	3.41132735327805	c
5.66003673189114	4.25468664568134	3.92519587596790	c
6.20184956150888	4.20363796260050	-0.10418033052502	h
4.084564832669325	0.40163129612479	5.78434328453293	c
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4.92897576434314	2.89204237121692	6.07704482954958	c
6.29773740209201	6.21409067952143	4.10191449738041	h
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-0.08539775106759	-6.40133239308780	1.54967900928221	c
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-3.96387418344550	-1.54843556994718	3.23040999244166	h
0.04009428012325	-5.71463941216744	6.07704482954958	c
2.23269168883967	-8.56104591633595	4.10191449738041	h
-2.29122475818402	-2.63394231720788	7.42933691308309	h
-2.92531022422775	3.84875257353115	1.25756940717152	c
-5.501017159494847	3.27462281839448	1.54967900928221	c
-1.38551804291897	3.85148584721897	3.41132735327805	c
-6.51468508624798	2.77439227333007	3.92519587596790	c
-6.74138204467913	3.26914028941577	-0.10418033052502	h
-2.39007606874560	3.33647059277212	5.78434328453293	c
0.64095255202509	4.20703352524274	3.23040999244166	h
-4.96907004446641	2.82259704095045	6.07704482954958	c
-8.53042909093178	2.34695523681441	4.10191449738041	h
-1.13544857971287	3.30123000497118	7.42933691308309	h

$[(\mu_3\text{-Bu}^t\text{Au}_3)_2(\text{PPh}_2(\text{C}_6\text{H}_4)_3\text{PPh}_2)_3]^{2+}$ (3)

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-3.09896932241540	-1.24788478716931	-16.17945411029167	au
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5.36089152691554	-4.17578363180435	-13.65409691342012	p
-6.29678046930759	-2.55477643333946	-13.65409691342012	p
0.93588894239193	6.73056006514380	-13.65409691342012	p
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-4.74626641194374	-3.12784294402850	-0.57793026967154	c
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0.22917892980451	-6.02270117637084	-3.41541542083665	h
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-6.49090136114293	-2.10362966794477	-0.98802376451937	h
-1.84242186961186	-4.78691287499765	2.57149567345196	c
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-5.33040168304184	-2.81287581296254	3.41541542083665	h
-1.84242186961186	4.78691287499765	-2.57149567345196	c
-4.07329005775683	3.50633049973718	-1.92941445932249	c
-0.33565824260467	5.67430875788630	-0.57793026967154	c
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-0.99992625795813	5.28073791686863	1.92941445932249	c
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-3.22437722064478	3.98904058107072	2.57149567345196	c
-6.49090136114293	2.10362966794477	0.98802376451937	h
0.22917892980451	6.02270117637084	3.41541542083665	h
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5.07321631571504	1.77440741713147	-1.92941445932249	c
5.08192465454843	-2.54646581385787	-0.57793026967154	c
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5.10122275323734	3.20982536340827	-3.41541542083665	h
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5.06724741316625	-4.56947063823641	-0.98802376451937	h
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5.10122275323734	-3.20982536340827	3.41541542083665	h
0.00000000000000	0.00000000000000	-20.98496869800709	c
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4.10721056058328	-0.24542122923266	-21.29070097588863	h
2.59114696632727	1.00245707848540	-24.04518944466628	h
2.91078470677854	2.90944419531193	-21.26900336447432	h
-2.11616234327699	1.72033926204036	-21.95981963674189	c
-2.16372677933552	1.74277055853566	-24.04518944466628	h
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1.06426023064408	-3.97553559867342	-21.26900336447432	h
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-1.84106426114821	-3.67965929877321	21.29070097588863	h
-2.16372677933552	-1.74277055853565	24.04518944466628	h
-3.97504493742261	-1.06609140336149	21.26900336447432	h
2.54793867569317	-0.97248071678966	21.95981963674189	c
2.59114696632727	-1.00245707848540	24.04518944466628	h
2.91078470677854	-2.90944419531193	21.26900336447432	h
4.10721056058328	0.24542122923266	21.29070097588863	h
4.86495943921002	-7.58364509139150	-13.63152244608190	c
6.87567679946794	-9.29662128768671	-13.47739402346138	c
2.37414444387170	-8.48232035517420	-13.72807265120073	c
6.39162967555875	-11.88649986070039	-13.39859883381835	c
8.82690951112887	-8.61045403757623	-13.44410370823315	h
1.90186972237747	-11.06962472149860	-13.63767223816742	c
0.79711341155151	-7.15090021521834	-13.90224234202278	h
3.91006350578230	-12.77295386785371	-13.47248127827735	c
7.96718978188473	-13.22058766109268	-13.29269820973388	h
-0.04506468704098	-11.75967137500662	-13.72461716928368	h
3.53934402774356	-14.80633199829416	-13.42356420498361	h
8.64866974113340	-3.70290058900072	-14.56096574975641	c
9.29829331589603	-4.21347342629019	-17.08050894038123	c
10.48876539823883	-2.80589794849202	-12.88857269768702	c
11.77106712922610	-3.86077827269052	-17.90380826854436	c
7.85690326979605	-4.88751586194881	-18.40576856440853	h
12.96216882567638	-2.43966026678053	-13.72961956077582	c
9.99997535426089	-2.38369448260867	-10.92524761835256	h
13.60643675502539	-2.97090451583443	-16.22797341056878	c
12.26804335746478	-4.26999853463675	-19.86794652119249	h
14.39572274303805	-1.73765012311878	-12.41580577080600	h
15.54752357016844	-2.68521879019051	-16.87942382432729	h
4.86495943921002	7.58364509139150	13.63152244608190	c
6.87567679946794	9.29662128768675	13.47739402346138	c
2.37414444387170	8.48232035517420	13.72807265120073	c
6.39162967555875	11.88649986070039	13.39859883381835	c
8.82690951112887	8.61045403757623	13.44410370823315	h
1.90186972237747	11.06962472149857	13.63767223816742	c
0.79711341155151	7.15090021521834	13.90224234202278	h
3.91006350578230	12.77295386785371	13.47248127827735	c
7.96718978188473	13.22058766109268	13.29269820973388	h
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9.29829331589603	4.21347342629019	17.08050894038123	c
10.48876539823883	2.80589794849202	12.88857269768702	c
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9.99997535426089	2.38369448260867	10.92524761835256	h
13.60643675502539	2.97090451583443	16.22797341056878	c
12.26804335746478	4.26999853463675	19.86794652119249	h
14.39572274303805	1.73765012311878	12.41580577080600	h
15.54752357016844	2.68521879019051	16.87942382432729	h
-7.53114084832963	5.63851741026293	14.56096574975641	c
-8.29812168328602	5.94582151025993	17.08050894038123	c
-7.67436160294017	7.68058831496399	12.88857269768702	c
-9.22906562714198	8.26365402721646	17.90380826854436	c
-8.16116453274519	4.36051989574602	18.40576856440853	h

-8.59389218047363	10.00573735778812	13.72961956077582	c
-7.06432765393033	7.46838545270391	10.92524761835256	h
-9.37609716044319	10.29806762692104	16.22797341056878	c
-9.83194888385015	8.48943793497505	19.86794652119249	h
-8.70271052102901	11.59823653974891	12.41580577080600	h
-10.09922947210850	12.12194098260790	16.87942382432729	h
-9.00010902203521	0.42135591704104	13.63152244608190	c
-11.48894860423395	1.30620013270722	13.47739402346138	c
-8.53297713255450	-2.18509077694056	13.72807265120073	c
-13.48982567922615	-0.40793625973386	13.39859883381835	c
-11.87032669022366	3.33910085475591	13.44410370823315	h
-10.53751108036675	-3.88774486648206	13.63767223816742	c
-6.59141795208240	-2.88512964350831	13.90224234202278	h
-13.01673428381913	-3.00026260750888	13.47248127827735	c
-15.43295965840773	0.28949491733762	13.29269820973388	h
-10.16164180739200	-5.91886285129436	13.72461716928368	h
-14.59233166126086	-4.33800415838847	13.42356420498361	h
4.13514958282513	8.00500100843253	-13.63152244608190	c
4.61327180476589	10.60282142039399	-13.47739402346138	c
6.15883268868285	6.29722957823365	-13.72807265120073	c
7.09819600366739	11.47856360096661	-13.39859883381835	c
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5.79430454053091	4.26577057171008	-13.90224234202278	h
9.10667077803678	9.77269126034477	-13.47248127827735	c
7.46576987652302	13.51008257843035	-13.29269820973388	h
10.20670649443289	5.84080852371227	-13.72461716928368	h
11.05298763351739	10.46832783990568	-13.42356420498361	h
-1.11752889280373	9.34141799926360	-14.56096574975641	c
-1.00017163261000	10.15929493655009	-17.08050894038123	c
-2.81440379529865	10.48648626345600	-12.88857269768702	c
-2.54200150208402	12.12443229990698	-17.90380826854436	h
0.30426126294907	9.24803575769483	-18.40576856440853	h
-4.36827664520274	12.44539762456872	-13.72961956077582	c
-2.93564770033055	9.85207993531254	-10.92524761835256	h
-4.23033959458219	13.26897214275554	-16.22797341056878	c
-2.43609447361467	12.75943646961179	-19.86794652119249	h
-5.69301222200901	13.33588666286772	-12.41580577080600	h
-5.44829409805992	14.80715977279853	-16.87942382432729	h
-7.53114084832963	-5.63851741026293	-14.56096574975641	c
-8.29812168328602	-5.94582151025993	-17.08050894038123	c
-7.67436160294017	-7.68058831496399	-12.88857269768702	c
-9.22906562714198	-8.26365402721646	-17.90380826854436	c
-8.16116453274519	-4.36051989574602	-18.40576856440853	h
-8.59389218047363	-10.00573735778812	-13.72961956077582	c
-7.06432765393033	-7.46838545270391	-10.92524761835256	h
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-9.83194888385015	-8.48943793497510	-19.86794652119249	h
-8.70271052102901	-11.59823653974891	-12.41580577080600	h
-10.09922947210850	-12.12194098260790	-16.87942382432729	h
-9.00010902203521	-0.42135591704104	-13.63152244608190	c
-11.48894860423395	-1.30620013270722	-13.47739402346138	c
-8.53297713255450	2.18509077694058	-13.72807265120073	c
-13.48982567922615	0.40793625973386	-13.39859883381835	c
-11.87032669022366	-3.33910085475591	-13.44410370823315	h
-10.53751108036675	3.88774486648206	-13.63767223816742	c
-6.59141795208240	2.88512964350831	-13.90224234202278	h
-13.01673428381913	3.00026260750888	-13.47248127827735	c
-15.43295965840773	-0.28949491733762	-13.29269820973388	h
-10.16164180739200	5.91886285129436	-13.72461716928368	h
-14.59233166126086	4.33800415838847	-13.42356420498361	h
-1.11752889280373	-9.34141799926360	14.56096574975641	c
-1.00017163261000	-10.15929493655009	17.08050894038123	c
-2.81440379529865	-10.48648626345600	12.88857269768702	c
-2.54200150208402	-12.12443229990695	17.90380826854436	c
0.30426126294907	-9.24803575769483	18.40576856440853	h
-4.36827664520274	-12.44539762456877	13.72961956077582	c
-2.93564770033055	-9.85207993531254	10.92524761835256	h
-4.23033959458219	-13.26897214275554	16.22797341056878	c
-2.43609447361467	-12.75943646961179	19.86794652119249	h
-5.69301222200901	-13.33588666286772	12.41580577080600	h
-5.44829409805992	-14.80715977279853	16.87942382432729	h
4.13514958282513	-8.00500100843253	13.63152244608190	c
4.61327180476589	-10.60282142039399	13.47739402346138	c
6.15883268868285	-6.29722957823365	13.72807265120073	c
7.09819600366739	-11.47856360096661	13.39859883381835	c
3.04341717909489	-11.94955489233224	13.44410370823315	h

8.63564135798937	-7.18187985501657	13.63767223816742	c
5.79430454053091	-4.26577057171008	13.90224234202278	h
9.10667077803678	-9.77269126034477	13.47248127827735	c
7.46576987652302	-13.51008257843035	13.29269820973388	h
10.20670649443289	-5.84080852371227	13.72461716928368	h
11.05298763351742	-10.46832783990568	13.42356420498361	h
-3.94911910555959	-3.57258486181330	-5.23862770140912	c
-2.12609176834684	-3.43537345756662	-7.16471564806119	c
-6.50040715685922	-3.29933562892861	-5.93174678697239	c
-2.82456651750295	-3.09353059258590	-9.67810178109514	c
-0.11446917116543	-3.54295041002008	-6.70537030515941	h
-7.20467053872540	-2.92622321240552	-8.43344325977817	c
-7.98010657860321	-3.43578075687421	-4.49728293956584	h
-5.37451508384342	-2.85167681833198	-10.34535542421180	c
-1.35545003652858	-2.98962400559618	-11.13456122341222	h
-9.20795494183245	-2.71713445758260	-8.90351487688694	h
-1.11938969472625	5.20632989889173	-5.23862770140912	c
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0.39289510816631	7.27918554724655	-5.93174678697239	c
-1.26679282181220	3.99291165512942	-9.67810178109514	c
-3.01105047384307	1.87060841518946	-6.70537030515941	h
1.06815163027583	7.70253931863624	-8.43344325977817	c
1.01457987201481	8.62886540041480	-4.49728293956584	h
0.21763297386299	6.08030500479711	-10.34535542421180	c
-1.91136531834572	2.66866616799242	-11.13456122341222	h
2.25087000515169	9.33289012532073	-8.90351487688694	h
5.06850880028585	-1.63374503707839	-5.23862770140912	c
4.03816656991288	-0.12356275338211	-7.16471564806119	c
6.10751204869284	-3.97984991831794	-5.93174678697239	c
4.09135933931516	-0.89938106254358	-9.67810178109514	c
3.12551964500857	1.67234199483059	-6.70537030515941	h
6.13651890844955	-4.77631610623075	-8.43344325977817	c
6.96552670658836	-5.19308464354062	-4.49728293956584	h
5.15688210998038	-3.22862818646502	-10.34535542421180	c
3.26681535487437	0.32095783760375	-11.13456122341222	h
6.95708493668084	-6.61575566773820	-8.90351487688694	h
5.06850880028585	1.63374503707839	5.23862770140912	c
6.10751204869284	3.97984991831794	5.93174678697239	c
4.03816656991288	0.12356275338211	7.16471564806119	c
6.13651890844955	4.77631610623075	8.43344325977817	c
6.96552670658836	5.19308464354062	4.49728293956584	h
4.09135933931516	0.89938106254358	9.67810178109514	c
3.12551964500857	-1.67234199483059	6.70537030515941	h
5.15688210998038	3.22862818646502	10.34535542421180	c
6.95708493668084	6.61575566773820	8.90351487688694	h
3.26681535487437	-0.32095783760375	11.13456122341222	h
-1.11938969472625	-5.20632989889173	5.23862770140912	c
0.39289510816631	-7.27918554724655	5.93174678697239	c
-1.91207480156600	-3.55893621094875	7.16471564806119	c
1.06815163027583	-7.70253931863624	8.43344325977817	c
1.01457987201481	-8.62886540041480	4.49728293956584	h
-1.26679282181220	-3.99291165512942	9.67810178109514	c
-3.01105047384307	-1.87060841518946	6.70537030515941	h
0.21763297386299	-6.08030500479711	10.34535542421180	c
2.25087000515169	-9.33289012532073	8.90351487688694	h
-1.91136531834572	-2.66866616799242	11.13456122341222	h
-3.94911910555959	3.57258486181330	5.23862770140912	c
-6.50040715685922	3.29933562892861	5.93174678697239	c
-2.12609176834684	3.43537345756662	7.16471564806119	c
-7.20467053872540	2.92622321240552	8.43344325977817	c
-7.98010657860321	3.43578075687421	4.49728293956584	h
-2.82456651750295	3.09353059258590	9.67810178109514	c
-0.11446917116543	3.54295041002008	6.70537030515941	h
-5.37451508384342	2.85167681833198	10.34535542421180	c
-9.20795494183245	2.71713445758260	8.90351487688694	h
-1.35545003652858	2.98962400559620	11.13456122341222	h

$[(\mu_3\text{-Bu}^t\text{NAu}_3)_4\{(\text{PPh}_2\text{C}_6\text{H}_4)_3\text{C}_6\text{H}_3\}_3]^{4+}$ (4)

-8.96183071402911	8.35798996565733	12.71217605308315	au
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-6.39724943781630	5.05729780897629	13.71773777386502	p
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11.18835173096916	-11.18835173096916	11.18835173096916	n
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6.39724943781630	-5.05729780897629	13.71773777386502	p
6.39724943781630	5.05729780897629	-13.71773777386502	p
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8.35798996565730	-12.71217605308315	8.96183071402911	au
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-5.04206620184753	-11.68765303202173	-3.59061755459760	c
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-6.19418303039334	-9.31617510398146	-3.76369666442265	c
-3.71276735096184	-10.59264772657551	0.65304652100808	c
-6.05594955050423	-7.58488583038511	-1.79781244139128	c
-4.81019230262172	-8.17939806939267	0.46272339861967	c
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-9.31617510398146	3.76369666442265	6.19418303039334	c
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-7.58488583038511	1.79781244139128	6.05594955050423	c
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-8.17939806939267	-0.46272339861967	4.81019230262172	c
3.59061755459760	-5.04206620184753	11.68765303202173	c
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-0.65304652100808	-3.71276735096184	10.59264772657551	c
1.79781244139128	-6.05594955050423	7.58488583038511	c
-0.46272339861967	-4.81019230262172	8.17939806939267	c
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-3.76369666442265	6.19418303039334	9.31617510398146	c
-1.33124237576697	3.81298602826709	12.31723785580189	c
-1.79781244139128	6.05594955050423	7.58488583038511	c
0.65304652100808	3.71276735096184	10.59264772657551	c
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1.99745854437807	-13.05965438263838	7.86544487861642	c
-0.25434196358701	-13.36251262702679	6.49963309619870	c
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-2.56104634584348	-12.70908521599581	7.58226815783229	c
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21.93339972260438	3.51294697977221	-5.06080714341443	c
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