

## *Supporting Information*

### **Theoretical investigations on the structure-property relationships of Au<sub>13</sub> and Au<sub>x</sub>M<sub>13-x</sub> nanoclusters**

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## Cartesian coordinates of optimized structures calculated at PBE/TZP level

[Au<sub>9</sub>Ag<sub>4</sub>(PPh<sub>2</sub>Me)<sub>8</sub>Cl<sub>4</sub>]<sup>+</sup> (-1398.97040560 eV)

Au	27.240963000	5.194708000	-1.318941000
Au	24.883680000	3.419612000	-1.329625000
Au	25.856201000	0.621040000	-1.104264000
Au	28.827804000	0.803253000	-1.004047000
Au	28.423434000	4.974279000	1.389247000
Au	24.740337000	2.046843000	1.294298000
Au	29.515564000	2.133045000	1.536890000
Au	27.034740000	2.834616000	2.918029000
Au	27.181942000	2.792279000	0.125253000
Ag	27.380940000	2.636542000	-2.714285000
Ag	29.668014000	3.637910000	-0.963142000
Ag	25.541842000	4.877971000	1.169169000
Ag	27.207996000	0.255445000	1.430356000
P	27.586990000	7.119243000	-2.613890000
P	22.986143000	4.194385000	-2.474330000
P	25.148262000	-1.471846000	-1.913553000
P	30.369882000	-0.395065000	-2.296759000
P	29.023027000	7.070834000	2.273084000
P	22.721464000	1.375369000	2.294788000
P	31.614337000	1.672472000	2.475265000
P	27.060721000	2.859531000	5.263008000
Cl	27.733607000	2.235966000	-5.062203000
Cl	31.951865000	4.163509000	-1.502399000
Cl	24.372708000	6.823489000	2.020418000
Cl	27.033377000	-2.044547000	2.156136000
C	27.203588000	6.916344000	-4.394695000
C	27.906713000	5.942317000	-5.124404000
C	27.658687000	5.774595000	-6.487137000
C	26.701279000	6.564081000	-7.130068000
C	25.980337000	7.514788000	-6.403109000
C	26.226273000	7.692293000	-5.039303000
C	26.702219000	8.633819000	-2.086836000
C	25.641238000	8.527996000	-1.175495000
C	24.946252000	9.669140000	-0.764702000
C	25.305939000	10.923047000	-1.263201000
C	26.367464000	11.038024000	-2.168387000
C	27.063812000	9.900917000	-2.581261000
C	29.372419000	7.557731000	-2.592568000
C	21.424421000	3.338243000	-2.037580000
C	21.052024000	2.170610000	-2.727790000

C	19.880209000	1.494602000	-2.383619000
C	19.073106000	1.966564000	-1.342722000
C	19.446866000	3.116239000	-0.642157000
C	20.617205000	3.799534000	-0.984407000
C	23.043425000	4.136630000	-4.303364000
C	24.216442000	3.730938000	-4.953119000
C	24.276022000	3.711992000	-6.349701000
C	23.165277000	4.098730000	-7.101661000
C	21.990365000	4.506990000	-6.457989000
C	21.925650000	4.525949000	-5.064806000
C	22.684135000	5.963099000	-2.078182000
C	24.789453000	-1.549509000	-3.708701000
C	24.911037000	-0.396395000	-4.495611000
C	24.659513000	-0.452512000	-5.869971000
C	24.285797000	-1.659515000	-6.463579000
C	24.168545000	-2.816760000	-5.683574000
C	24.419195000	-2.765049000	-4.312609000
C	23.665772000	-2.211673000	-1.122132000
C	22.398033000	-2.076315000	-1.713366000
C	21.276242000	-2.654327000	-1.115872000
C	21.405507000	-3.369854000	0.078186000
C	22.661194000	-3.490813000	0.680710000
C	23.789147000	-2.910233000	0.093234000
C	26.464796000	-2.712748000	-1.622369000
C	29.688371000	-1.673013000	-3.424241000
C	29.983897000	-3.036007000	-3.257784000
C	29.446199000	-3.980652000	-4.136327000
C	28.614314000	-3.574432000	-5.182691000
C	28.314211000	-2.218399000	-5.346193000
C	28.841192000	-1.266362000	-4.471722000
C	31.637427000	-1.269134000	-1.308513000
C	31.259433000	-1.839497000	-0.080778000
C	32.191163000	-2.548807000	0.680876000
C	33.507052000	-2.685670000	0.229239000
C	33.891215000	-2.113672000	-0.987233000
C	32.961286000	-1.411073000	-1.757656000
C	31.240801000	0.770043000	-3.408170000
C	30.695577000	7.687030000	1.844057000
C	31.465380000	6.985561000	0.905324000
C	32.705872000	7.485426000	0.496162000
C	33.188071000	8.682114000	1.030626000
C	32.425634000	9.385421000	1.971539000
C	31.182757000	8.895640000	2.374969000
C	28.851604000	7.283672000	4.087300000

C	27.576239000	7.517235000	4.636169000
C	27.428403000	7.685643000	6.015341000
C	28.541463000	7.619477000	6.858831000
C	29.805495000	7.362690000	6.319615000
C	29.962155000	7.187957000	4.942416000
C	27.902024000	8.361248000	1.602904000
C	21.566266000	2.721943000	2.756921000
C	20.282848000	2.427331000	3.253667000
C	19.395650000	3.460813000	3.557481000
C	19.778566000	4.795384000	3.371330000
C	21.054054000	5.093106000	2.887086000
C	21.944261000	4.058813000	2.582099000
C	22.904394000	0.354328000	3.807006000
C	22.679073000	0.889290000	5.085951000
C	22.819222000	0.080757000	6.216711000
C	23.190636000	-1.259437000	6.084889000
C	23.444878000	-1.787483000	4.815510000
C	23.311740000	-0.985703000	3.681434000
C	21.738548000	0.325390000	1.156016000
C	32.274449000	2.984475000	3.574197000
C	32.777008000	4.165403000	2.999467000
C	33.283628000	5.181363000	3.812508000
C	33.285971000	5.035809000	5.203415000
C	32.767199000	3.873213000	5.780401000
C	32.259865000	2.851736000	4.972672000
C	31.721163000	0.118689000	3.439624000
C	32.944257000	-0.313743000	3.984370000
C	33.014085000	-1.527879000	4.668646000
C	31.869431000	-2.322153000	4.811729000
C	30.653531000	-1.898319000	4.271568000
C	30.578814000	-0.679378000	3.591205000
C	32.886457000	1.510720000	1.162890000
C	27.352562000	1.225591000	6.036250000
C	26.909792000	0.075043000	5.365683000
C	27.129282000	-1.190596000	5.912211000
C	27.786680000	-1.319265000	7.137870000
C	28.231689000	-0.178720000	7.814117000
C	28.020932000	1.088796000	7.266584000
C	25.539151000	3.543657000	6.030946000
C	24.828472000	4.537969000	5.339946000
C	23.699297000	5.123613000	5.916199000
C	23.266740000	4.716136000	7.181305000
C	23.967493000	3.720942000	7.870327000
C	25.099627000	3.133958000	7.300050000

C	28.390603000	3.943592000	5.907625000
H	28.637333000	5.294078000	-4.636487000
H	28.207935000	5.008214000	-7.036463000
H	26.510685000	6.432434000	-8.197080000
H	25.224298000	8.127858000	-6.897815000
H	25.664734000	8.444085000	-4.482837000
H	25.372788000	7.556086000	-0.754500000
H	24.136566000	9.566237000	-0.039701000
H	24.765864000	11.815942000	-0.942006000
H	26.653777000	12.017599000	-2.556439000
H	27.882903000	10.005193000	-3.295552000
H	29.580905000	8.399405000	-3.266315000
H	29.958665000	6.683742000	-2.906788000
H	29.667567000	7.813588000	-1.566246000
H	21.668774000	1.802550000	-3.550368000
H	19.590236000	0.600275000	-2.938907000
H	18.153150000	1.440290000	-1.080888000
H	18.827662000	3.488804000	0.176019000
H	20.891959000	4.693543000	-0.422905000
H	25.095167000	3.428907000	-4.378632000
H	25.202652000	3.396380000	-6.832719000
H	23.209661000	4.084058000	-8.192856000
H	21.119933000	4.808979000	-7.043961000
H	21.000113000	4.831395000	-4.571599000
H	21.730699000	6.307710000	-2.501290000
H	23.509116000	6.542330000	-2.513230000
H	22.696801000	6.114428000	-0.990285000
H	25.225385000	0.545114000	-4.040087000
H	24.767282000	0.452484000	-6.470528000
H	24.087040000	-1.704289000	-7.536505000
H	23.878833000	-3.762534000	-6.145940000
H	24.316209000	-3.671411000	-3.711871000
H	22.290941000	-1.535547000	-2.655436000
H	20.298488000	-2.554365000	-1.591935000
H	20.530246000	-3.834401000	0.536829000
H	22.768341000	-4.047892000	1.613914000
H	24.759470000	-2.998567000	0.589521000
H	26.127025000	-3.714557000	-1.920733000
H	27.340257000	-2.423480000	-2.217207000
H	26.737966000	-2.703510000	-0.556595000
H	30.637919000	-3.363067000	-2.448207000
H	29.686753000	-5.037365000	-4.003262000
H	28.199149000	-4.313844000	-5.870657000
H	27.661132000	-1.892704000	-6.158237000

H	28.582808000	-0.211839000	-4.612370000
H	30.235541000	-1.720540000	0.283886000
H	31.888143000	-2.982478000	1.635431000
H	34.236288000	-3.234960000	0.828167000
H	34.918533000	-2.216861000	-1.342007000
H	33.275207000	-0.974011000	-2.706546000
H	31.960352000	0.244965000	-4.050377000
H	30.481411000	1.252878000	-4.040521000
H	31.737387000	1.548931000	-2.810784000
H	31.106186000	6.045444000	0.478052000
H	33.282504000	6.925683000	-0.243301000
H	34.157498000	9.073041000	0.714290000
H	32.798622000	10.322853000	2.389608000
H	30.596056000	9.452643000	3.108863000
H	26.692322000	7.564174000	3.995380000
H	26.435617000	7.872618000	6.429060000
H	28.422827000	7.765240000	7.934245000
H	30.678642000	7.301901000	6.972542000
H	30.953330000	6.985941000	4.533371000
H	28.117557000	9.331629000	2.070683000
H	28.064720000	8.431249000	0.520462000
H	26.854068000	8.076735000	1.776185000
H	19.975763000	1.391731000	3.414977000
H	18.402648000	3.224752000	3.945581000
H	19.080370000	5.600317000	3.611128000
H	21.379111000	6.126179000	2.745652000
H	22.939895000	4.307349000	2.208404000
H	22.384258000	1.933346000	5.202934000
H	22.632796000	0.504308000	7.205461000
H	23.291129000	-1.889547000	6.970696000
H	23.756449000	-2.827816000	4.703680000
H	23.536349000	-1.409253000	2.701416000
H	20.816195000	-0.021961000	1.640040000
H	21.490516000	0.921207000	0.268077000
H	22.336340000	-0.539103000	0.844235000
H	32.778994000	4.296650000	1.915082000
H	33.680862000	6.088408000	3.351706000
H	33.697632000	5.824849000	5.836208000
H	32.769114000	3.751869000	6.865704000
H	31.875131000	1.938848000	5.431610000
H	33.842974000	0.298473000	3.881711000
H	33.965570000	-1.856022000	5.092175000
H	31.930374000	-3.272580000	5.346200000
H	29.753833000	-2.509267000	4.365300000

H	29.625238000	-0.359392000	3.164374000
H	33.890380000	1.427133000	1.600423000
H	32.830950000	2.378664000	0.488981000
H	32.656555000	0.607469000	0.582985000
H	26.408299000	0.159081000	4.398925000
H	26.799068000	-2.069216000	5.355434000
H	27.963334000	-2.308903000	7.564382000
H	28.751518000	-0.274362000	8.769690000
H	28.384980000	1.965652000	7.804260000
H	25.146478000	4.856850000	4.343568000
H	23.157033000	5.892350000	5.362259000
H	22.380493000	5.170024000	7.630005000
H	23.631116000	3.398025000	8.858099000
H	25.632243000	2.348753000	7.840178000
H	28.357096000	4.011008000	7.003145000
H	28.239743000	4.945894000	5.490081000
H	29.366713000	3.563227000	5.577969000

[Au<sub>9</sub>Cu<sub>4</sub>(PPh<sub>2</sub>Me)<sub>8</sub>Cl<sub>4</sub>]<sup>+</sup> (-1403.39989663 eV)

Cu	2.796383270	-0.482579330	0.925152610
Cu	2.397969670	1.790222110	-0.455784470
Au	2.363071530	-0.578958160	-1.824425170
Au	1.131407730	-2.531286070	-0.011266390
Au	0.581282270	-1.064728970	2.574152360
Au	1.549053780	1.673704710	2.149780360
Au	0.381573620	1.498525080	-2.422349080
Cu	-0.396933580	-1.124648010	-2.022902850
Au	-1.652147710	-1.589647930	0.558024100
Cu	-1.201705880	0.961039210	1.896348290
Au	-0.165776590	2.890009910	0.129059680
Au	-2.087759360	0.859287490	-0.897861990
Au	0.421016970	0.157425040	0.062621820
Cl	4.733989880	-1.088358110	1.646240590
Cl	4.039622890	3.112088080	-0.921956300
P	4.151362200	-1.229005260	-3.181852650
P	1.636741830	-4.818067780	0.051496450
P	0.582692770	-1.580198150	4.862844110
P	2.767164170	3.011191240	3.642693400
P	0.388396920	2.364961920	-4.602325190
Cl	-1.047079060	-2.084791790	-3.859860010
P	-3.436253040	-3.049730370	0.999276990
Cl	-2.380387110	1.593991150	3.607921850
P	-4.273952830	1.502491500	-1.469041170
P	-0.622461180	5.185653840	-0.004023380

C	3.958900420	-2.879067850	-3.946908130
C	5.055572630	-3.722461500	-4.189288790
C	4.869414360	-4.945259570	-4.838358800
C	3.592503030	-5.333127710	-5.254388390
C	2.497059990	-4.500665940	-5.008258030
C	2.674961160	-3.280468490	-4.352753890
C	4.541421100	-0.105887350	-4.582048680
C	4.648827030	-0.577082550	-5.900414320
C	4.988513980	0.301713930	-6.932957590
C	5.225788750	1.650422380	-6.657728520
C	5.109921510	2.124132810	-5.346784220
C	4.760649860	1.256849880	-4.310105250
C	5.702262860	-1.254999010	-2.204630250
C	0.570722150	-5.870619650	-1.003655560
C	0.397668570	-7.243887520	-0.754863750
C	-0.411786280	-8.013149150	-1.593521570
C	-1.059424190	-7.420973620	-2.682958160
C	-0.895379600	-6.055759220	-2.930962520
C	-0.084389770	-5.282967900	-2.096361320
C	3.371877540	-5.259224200	-0.362417020
C	3.698312970	-6.360316460	-1.168814760
C	5.037926480	-6.697573250	-1.383214410
C	6.057565970	-5.941681710	-0.799411680
C	5.735226600	-4.832329000	-0.010770760
C	4.399722640	-4.484768880	0.203452370
C	1.440058200	-5.482868110	1.754528920
C	2.038537360	-2.504715240	5.482458470
C	3.045550030	-2.883284360	4.583048360
C	4.186876910	-3.547170000	5.043493120
C	4.328767320	-3.836660010	6.402337380
C	3.333484900	-3.449232810	7.307344720
C	2.194518140	-2.783682270	6.852749730
C	-0.897683500	-2.440277050	5.533552910
C	-0.847845100	-3.738617800	6.066174790
C	-1.998164260	-4.321893990	6.606591470
C	-3.207615700	-3.623051470	6.611669660
C	-3.265845210	-2.336827350	6.065019590
C	-2.122553880	-1.745566120	5.523743890
C	0.580328690	-0.015420230	5.823396440
C	3.541424050	2.130207770	5.058133420
C	3.423528620	2.590396700	6.379578930
C	4.058524690	1.904059090	7.418813390
C	4.814047820	0.760563480	7.147834580
C	4.929058720	0.298078940	5.832966470



C	4.293578320	0.972457110	4.788915340
C	1.815658960	4.381748990	4.394517320
C	2.426531310	5.586783550	4.779959980
C	1.677971240	6.582297200	5.412094490
C	0.318212150	6.382795960	5.668055180
C	-0.296535540	5.189798920	5.277531240
C	0.444860620	4.193590000	4.638109550
C	4.207728390	3.758686950	2.791343150
C	-1.223722790	3.020147820	-5.187355690
C	-1.479087080	4.402282190	-5.204603310
C	-2.721468220	4.885568670	-5.622578220
C	-3.721783680	3.996689590	-6.026043540
C	-3.477069620	2.620844740	-6.001771330
C	-2.239245770	2.131402590	-5.579154930
C	1.570407020	3.720240210	-4.956914680
C	1.692250690	4.240431980	-6.258544340
C	2.597258620	5.269837430	-6.518725000
C	3.386088520	5.790454690	-5.485130860
C	3.273689990	5.271373450	-4.194034660
C	2.369667260	4.237070350	-3.929154520
C	0.813976510	1.034981610	-5.795115920
C	-2.987548840	-4.730372950	1.600279570
C	-3.169124420	-5.868163930	0.797854320
C	-2.831240140	-7.133819470	1.283886550
C	-2.308599690	-7.278674710	2.570725470
C	-2.113269790	-6.147399480	3.368905380
C	-2.441473760	-4.878499970	2.887354370
C	-4.530704210	-3.389255500	-0.429308530
C	-3.980410320	-3.382796130	-1.720169450
C	-4.767745400	-3.733536130	-2.819741460
C	-6.110087610	-4.076103780	-2.643324000
C	-6.667678410	-4.069522620	-1.360420610
C	-5.882430830	-3.733529590	-0.256152140
C	-4.518994630	-2.386463700	2.323009610
C	-4.990256210	0.835206000	-3.018677850
C	-6.199360330	1.334201840	-3.537937900
C	-6.724481330	0.813896760	-4.721819500
C	-6.045916490	-0.204614660	-5.401620370
C	-4.841836450	-0.697036660	-4.893775710
C	-4.314405350	-0.182580520	-3.705251320
C	-5.480617180	1.099541610	-0.141203510
C	-5.204850000	1.571752900	1.154351740
C	-6.093828850	1.318292840	2.199449120
C	-7.260325320	0.581845780	1.967806740

C	-7.523464140	0.084057990	0.688896830
C	-6.637627040	0.336149950	-0.363246310
C	-4.433440150	3.328064520	-1.644707800
H	6.059601350	-3.432275360	-3.876412950
H	5.727478330	-5.594830040	-5.022194460
H	3.451403980	-6.287660260	-5.766150720
H	1.494683460	-4.800053250	-5.320313010
H	1.808150720	-2.643571640	-4.154423070
H	4.475167120	-1.630873740	-6.122281860
H	5.075025680	-0.075457050	-7.954126140
H	5.498008490	2.333859980	-7.464670990
H	5.282353970	3.179165080	-5.127608660
H	4.653271420	1.648701610	-3.293843530
H	6.569219450	-1.501672800	-2.832025320
H	5.837453650	-0.253469560	-1.774868500
H	5.597857060	-1.967530810	-1.376216630
H	0.892478830	-7.723342240	0.091489860
H	-0.536448710	-9.079542350	-1.394615040
H	-1.694173580	-8.025521960	-3.334425470
H	-1.401095720	-5.576580440	-3.771790080
H	0.024186800	-4.214483910	-2.296890690
H	2.911358670	-6.955467460	-1.633967980
H	5.281999600	-7.557582910	-2.010010550
H	7.102501010	-6.212378660	-0.964392990
H	6.523506890	-4.224660950	0.438944810
H	4.171813570	-3.595539660	0.798616330
H	1.727934450	-6.541401170	1.805968720
H	2.090837450	-4.904949750	2.423707170
H	0.396042510	-5.358516620	2.070741510
H	2.958839000	-2.622211940	3.525184610
H	4.969328100	-3.823589790	4.334195060
H	5.218944390	-4.357219440	6.761797770
H	3.445733370	-3.664638410	8.371822670
H	1.425153110	-2.486658010	7.568588700
H	0.092918290	-4.291355560	6.077028800
H	-1.943979310	-5.324778870	7.035209960
H	-4.101994280	-4.078145500	7.041635330
H	-4.206955690	-1.782510010	6.065481220
H	-2.190077600	-0.743032420	5.090761090
H	0.501978480	-0.222026440	6.899252320
H	1.513949990	0.520492410	5.613056570
H	-0.269544190	0.597854980	5.493530840
H	2.837106740	3.483372950	6.600927270
H	3.963312980	2.270833360	8.443028690

H	5.311135500	0.227895010	7.961014120
H	5.509958170	-0.599476190	5.612714200
H	4.380714740	0.581676500	3.770354630
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H	2.161622820	7.514861190	5.709690300
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H	0.693877310	1.378681160	-6.831249260
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H	0.177382040	0.160200570	-5.603746760
H	-3.585766180	-5.771119420	-0.205223280
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H	-4.323598290	-3.728047390	-3.816647490
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H	-7.717005220	-4.335636780	-1.217143740
H	-6.329463480	-3.749457470	0.738964230
H	-5.306722010	-3.099596040	2.599448900
H	-3.898046410	-2.177497740	3.203010380
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H	-7.666107720	1.203263230	-5.113857430
H	-6.457865290	-0.609072060	-6.328679630
H	-4.297703120	-1.482956410	-5.421588100
H	-3.365816510	-0.570559920	-3.326181600
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C	-2.200311990	5.685369630	0.781673960
C	-2.969940820	6.763400000	0.309637870
C	-2.648139980	4.956172710	1.895927600
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C	0.348127320	7.428529520	1.453218270
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C	1.358682340	8.303986180	1.861361340
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H	2.276142030	5.184635640	-0.276452830
C	2.684000940	8.076086040	1.482291260
H	1.105264360	9.169896410	2.476146370
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H	-0.908892190	6.819106540	-1.826328230
H	-5.857362950	1.685799090	3.199817490

[Au<sub>13</sub>(PPhMe<sub>2</sub>)<sub>10</sub>Cl<sub>2</sub>]<sup>3+</sup> (-1399.90925317 eV)

Au	2.558170171	0.959330025	-1.193527014
Au	1.789915399	-2.069377090	-1.307487024
Au	2.530825782	-0.703561435	1.449373557
Au	1.384552073	2.239940203	1.443782949
Au	-0.070418471	2.686251684	-1.329321805
Au	0.143418867	0.024052846	-3.015132385
Au	-0.013048806	-0.004186325	-0.000425987
Cl	4.802234116	1.436383176	-2.243471075
P	3.689769336	-3.377481017	-2.555235811
C	4.119136712	-5.026031293	-1.868474690

C	3.122649121	-5.759882684	-1.203581291
C	3.387768395	-7.045802493	-0.726501672
C	4.657288830	-7.606075553	-0.893909162
C	5.658768764	-6.877747623	-1.541697943
C	5.392573144	-5.596858695	-2.031283726
C	3.324185698	-3.723093355	-4.330262441
C	5.270938181	-2.439554654	-2.628701076
P	4.983339576	-1.095807150	2.243133423
C	5.317113169	-0.770643121	4.017619626
C	4.454113766	-1.346363002	4.967024003
C	4.682280902	-1.168689722	6.332109519
C	5.762759947	-0.393209883	6.765940792
C	6.614129373	0.196926742	5.829534097
C	6.398165305	0.007248148	4.461080280
C	5.630076255	-2.805642141	1.981337124
C	6.157930585	-0.040625842	1.302872913
P	2.586876043	4.245332605	2.612611531
C	3.732844889	5.127573599	1.486419982
C	4.320867118	4.396607487	0.440002612
C	5.236585263	5.001317428	-0.423484856
C	5.565660039	6.348987489	-0.254102876
C	4.979862439	7.087166889	0.779312478
C	4.070328607	6.482136691	1.650033005
C	1.466287409	5.529800578	3.312696699
C	3.629958965	3.793086184	4.067756569
P	0.238058440	5.014996507	-2.476614206
C	1.129660287	6.246574001	-1.430242718
C	-1.313481132	5.899155213	-2.921140350
P	0.400005788	0.089433604	-5.619839559
C	2.076225851	-0.341023693	-6.228363199
C	3.182897537	0.117104882	-5.492266190
C	4.481201564	-0.128982368	-5.943202636
C	4.688386643	-0.847849197	-7.124201020
C	3.593273283	-1.320027053	-7.853287662
C	2.291677420	-1.066716422	-7.412337970
C	-0.765905386	-0.995602820	-6.544944664
C	0.076343504	1.751239536	-6.352674423
Au	-1.396077882	-2.263673827	-1.425956141
Au	0.040224425	-2.699980964	1.316995191
Au	-0.150329209	-0.034380202	3.020122423
Au	-1.784709537	2.091523618	1.292151633
Au	-2.569469596	0.675254531	-1.438836468
Au	-2.568139222	-0.935082259	1.248266811
P	-2.703308463	-4.190344368	-2.623346814

P	-0.165749451	-5.027578630	2.493220910
P	-0.340097765	-0.107399517	5.627970427
P	-3.529610417	3.559558482	2.576101547
P	-5.041722609	0.711822943	-2.295843721
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C	-4.191495347	-4.768381087	-1.722603809
C	-1.712771677	-5.716286964	-2.932778139
C	-3.311713329	-3.766057781	-4.312960594
C	-1.012134848	-6.307802813	1.466068896
C	1.414107523	-5.853603887	2.950692512
C	-2.002644017	0.310076666	6.278929528
C	0.846369075	0.981454262	6.523412146
C	0.015168062	-1.769353635	6.346739997
C	-3.730965864	5.298066394	2.022371662
C	-3.209562666	3.709699837	4.386610403
C	-5.212799932	2.816879872	2.510109829
C	-5.251396626	0.280051781	-4.067930889
C	-5.926431242	2.322723549	-2.131264690
C	-6.105275649	-0.453496206	-1.358705447
C	-4.590685638	-4.090539540	-0.559980371
C	-4.953928677	-5.860356676	-2.175770800
C	-3.123046586	-0.092686311	5.531820112
C	-2.194906123	0.968982003	7.505177218
C	-2.730769787	5.886601281	1.232445707
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C	-4.530195002	1.020166902	-5.022314761
C	-6.094794369	-0.754242169	-4.503162546
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C	-6.091637335	-6.259561387	-1.472696247
C	-4.413396331	0.143640644	6.010450028
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C	-4.667995938	0.746433506	-6.383555288
C	-6.216452445	-1.037710862	-5.867449932
C	-6.483057170	-5.573793911	-0.316665389
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H	-5.268917776	-0.184603165	5.416902299
H	-3.627968477	1.720652628	8.930802847
H	-2.045939358	7.682583091	0.238320976
H	-5.809789981	7.994180743	2.314087429
H	-4.126491893	1.346161269	-7.118080155



H	-6.882166426	-1.838491925	-6.194788891
H	-7.375707796	-5.889826197	0.225970612
H	-5.604848269	0.980238166	7.610171808
H	-4.020022832	9.030022373	0.927912302
H	-5.620544574	-0.500597638	-7.873471234
C	-1.169957213	-4.965425437	4.025353247
C	-0.807958202	-5.640342588	5.202615817
C	-2.364716431	-4.223416335	3.997297797
C	-1.634597557	-5.578486624	6.328043703
H	0.111591748	-6.225113676	5.253214772
C	-3.191708215	-4.173172703	5.120210722
H	-2.664251932	-3.680717071	3.095780731
C	-2.826445345	-4.850103293	6.288247669
H	-1.348899293	-6.112048113	7.236271953
H	-4.119659440	-3.600555430	5.076899011
H	-3.472000064	-4.813000428	7.167365222
C	1.237626317	4.943773027	-4.011575054
C	0.864518918	5.602304719	-5.194643217
C	2.437937620	4.210766760	-3.980934458
C	1.686277267	5.534745607	-6.323504417
H	-0.059517925	6.179675559	-5.247175810
C	3.258836374	4.154292943	-5.107980697
H	2.749427810	3.680278187	-3.076361036
C	2.883657477	4.815821823	-6.281776123
H	1.392280968	6.056741679	-7.235822856
H	4.191085758	3.588807299	-5.061941224
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H	-0.951802228	2.058222171	-6.114318931
H	-0.091949427	-1.745395984	7.440493188

[Au<sub>12</sub>Pd(PPh<sub>3</sub>)<sub>8</sub>Cl<sub>4</sub>] (-1817.41738061 eV)

Au	9.868814033	15.179331130	8.649186644
Au	9.524514538	12.426916000	8.066262728
Au	7.763226352	14.528401050	6.766309532
Au	9.196413259	17.012143360	6.444962191
Au	12.009278450	16.526173500	7.341197029
Au	12.269091710	13.681461460	8.180661506
Au	11.541711970	11.816235070	5.920218294
Au	8.437350563	12.192796240	5.431269293
Au	8.673304757	15.516777690	4.032193341
Au	11.265296550	16.570333960	4.536538081
Au	13.207010500	14.597096420	5.527717712
Au	11.016049690	13.929249520	3.333361374
Pd	10.479464430	14.257694090	6.017776224

Cl	9.241273955	15.506501660	10.984513470
Cl	5.440900971	14.931727530	7.306362489
Cl	12.457484700	9.593845592	5.529854605
Cl	12.207424940	18.283168950	3.046830202
P	11.5598685200	13.1683689100	1.1909980340
P	8.6640280310	10.9679526100	9.6919201590
P	8.0572281150	19.0334342800	6.8967580070
P	13.1716173700	18.3078772500	8.4085133100
P	13.7036878100	12.8358159600	9.8616992010
P	6.9840678930	10.5739507800	4.6384778220
P	7.2085285400	16.3821464800	2.3824083610
P	15.4699950100	14.5121816400	4.8517846000
C	13.1376897500	12.2123397800	1.1388059440
C	13.9976432400	12.2351230300	0.0287750223
C	15.0978962300	11.3767829200	-0.0291859104
C	15.3493313400	10.4815803000	1.0134676480
C	14.5113707600	10.4693706700	2.1313922130
C	13.4170089200	11.3378489900	2.2015816870
C	10.4083409200	11.9588652000	0.3941877561
C	10.5412889600	10.5794890100	0.6287460704
C	9.7121565020	9.6665377090	-0.0269991102
C	8.7464004330	10.1125474200	-0.9330212239
C	8.5894667560	11.4833502400	-1.1479726420
C	9.3984340390	12.4026811200	-0.4742167635
C	11.7244940300	14.4888625000	-0.0815323765
C	11.7725009200	15.8193206300	0.3539848604
C	11.9270319300	16.8629303000	-0.5649418536
C	12.0387062700	16.5865168100	-1.9284323200
C	11.9812550600	15.2610641200	-2.3759238800
C	11.8200193000	14.2181415600	-1.4610212730
C	15.6678604100	14.8103473500	3.0372914150
C	16.6128421400	14.1304047000	2.2513460840
C	16.8096090900	14.4900520900	0.9159653885
C	16.0771636200	15.5369447800	0.3511918320
C	15.1231860900	16.2040234100	1.1226217930
C	14.9038828000	15.8323179900	2.4525049870
C	16.2922373000	12.8876922700	5.1343950070
C	17.6819478700	12.7014395500	4.9890753950
C	18.2413018500	11.4288340800	5.1126866300
C	17.4250898500	10.3238773100	5.3798125820
C	16.0494689300	10.5004847700	5.5347647290
C	15.4875247800	11.7755725900	5.4150443290
C	16.6765568300	15.7556846800	5.5128623740
C	16.7035077100	17.0520079700	4.9712854930

C	17.6584764500	17.9787847900	5.3922667240
C	18.6086778500	17.6248887300	6.3535855880
C	18.5624885800	16.3524936000	6.9255142030
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C	8.5121787240	9.2607464990	9.0199872350
C	7.5041833970	8.3567434000	9.3917502320
C	7.5027155730	7.0569552100	8.8789649580
C	8.4999900840	6.6462901990	7.9906662100
C	9.4931051120	7.5478364220	7.6000765120
C	9.4969278590	8.8480970840	8.1081402340
C	9.5779615390	10.7629556600	11.2782589600
C	9.8356468920	11.9265178600	12.0237164100
C	10.3297130400	11.8248591000	13.3244311000
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C	4.5932298300	12.2828964300	11.5132842000
C	5.1314669010	12.9648771100	10.4214101500
C	6.3421949630	12.5467437500	9.8599950040
C	6.6228533440	19.4925845100	5.8302598060
C	5.5114744160	18.6318982000	5.8035642460
C	4.3341028570	19.0392621600	5.1731204290
C	4.2511253690	20.2968730000	4.5666042510
C	5.3627340210	21.1415795300	4.5697526470
C	6.5467578670	20.7400328700	5.1940224460
C	9.1908812530	20.4689723000	6.7049410330
C	9.2033169680	21.5855386800	7.5551855810
C	10.0504205800	22.6639227500	7.2823538640
C	10.8874500300	22.6431227200	6.1624110390
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C	10.0506642300	20.4450743900	5.5927935250
C	7.2428136010	19.1697616700	8.5399429310
C	6.3584027180	20.2261908200	8.8328092130
C	5.7001502560	20.2683882600	10.0613546900
C	5.8962339720	19.2484111700	11.0012033400
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C	12.0686366500	19.3042951700	9.4968580130
C	11.1464419800	18.6076423300	10.2952603800
C	10.372206840	19.288234710	11.238554790
C	10.496245410	20.671820530	11.383787230

C	11.389052210	21.374655580	10.569562070
C	12.172548980	20.697805370	9.631449864
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C	16.693283590	17.467310770	11.351302070
C	16.918255730	17.563965990	9.975471621
C	15.850542380	17.745558460	9.093896869
C	14.031271430	19.516519410	7.317061174
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C	14.481057540	20.335416740	5.075366800
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C	16.186343250	11.659101340	9.106025423
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C	8.795425468	18.656141790	2.198103709
C	9.098742632	19.978124310	1.861840729
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C	6.755630741	20.411902370	1.476476948
C	6.448540034	19.090234400	1.808517162
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C	4.449831669	16.487093060	1.688826043
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H	11.601146480	15.771707390	13.257452740
H	11.763923790	14.686654440	11.064066510
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H	8.117762884	9.394460641	-1.463684957
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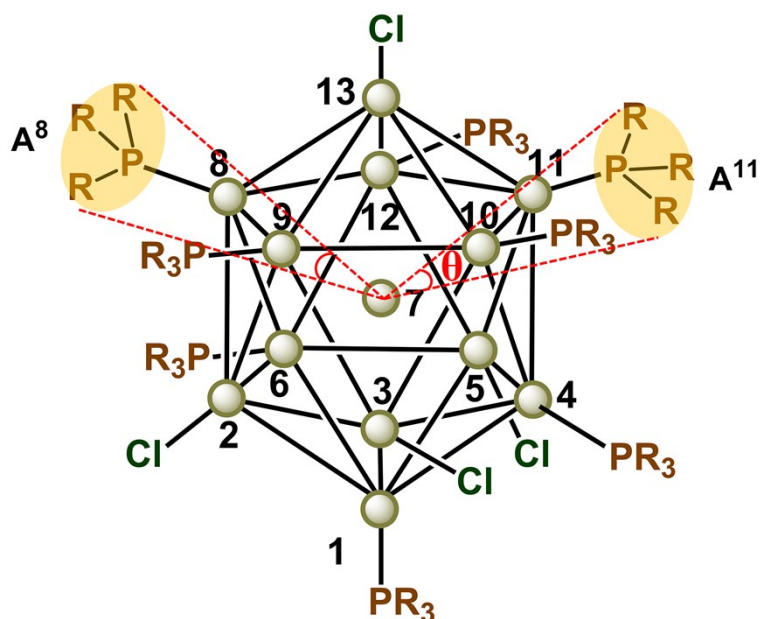


Figure S1: The diagram of cone angel  $\theta$  of  $\text{PR}_3$  ligands. The cone angle of the phosphine ligand connected to  $\text{M}^x$  is designated as  $\text{A}^x$ .

Table S1. The cone angel  $\theta$  of  $\text{PR}_3$  ligands in  $\text{M}_{13}$  NCs.

	Cone Angel ( $^\circ$ )											
	$\text{A}^1$	$\text{A}^2$	$\text{A}^3$	$\text{A}^4$	$\text{A}^5$	$\text{A}^6$	$\text{A}^8$	$\text{A}^9$	$\text{A}^{10}$	$\text{A}^{11}$	$\text{A}^{12}$	Average
NC0	46.4			46.1		46.6	46.9	48.0	46.0	46.5	46.5	46.7
NC1		61.5	58.3	59.5	61.4	61.7	59.6	61.3	61.5	62.6	58.5	60.9
NC2	76.2			76.1		74.0	73.5	71.0	76.7	74.8	76.7	74.7
NC3	79.1			71.5		78.5	77.8	79.3	76.3	71.4	80.0	76.4