Supplementary Information For:

Tetranuclear Ag(I) and Au(I) nano-sized $[L_2(R)_8 \rightarrow M_4]^{4+}$ (M = Ag(I) and Au(I); R = C_2H_5, CH_3, H, F, Cl, Br, Ph and SiH_3) complexes: Nature and cooperativity of metal-ligand bonds

Supporting Information – Table of Contents

Section S1: Detailed derivations, mathematical expressions, and example calculations of Cooperativity

Overview of Cooperativity Concept

Cooperativity refers to nonadditive effects in multicomponent systems where the formation of one bond influences subsequent interactions. Early theoretical studies [51–54] introduced the concept of pairwise nonadditivity and triad models. Full details and conceptual background are provided here for clarity.

Mathematical Formulation – Equations 4 & 5

For a noncyclic A–B–C arrangement, cooperative energy is defined as:

$E_{coop}=SE_{ABC}-SE_{AB}-SE_{BC}-SE_{(AC,T)}$ (eq. S1)

or alternatively:

$E_{coop}=SE_{ABC}-SE_{AB}-SE_{BC}$ (eq. S2)

See also refs [51–54] for the original derivations.

Interaction-Energy-Based Cooperativity (Equation 6)

To overcome limitations of Eqs. 4 & 5 for covalent bonds in metal complexes, the following approach was used [47, 59 and 60]:

$\Delta IE_{coop}=\Delta IE_{A-B}=\Delta IE_{B-C}$ (eq. S3)

where: $\Delta IE_{A-B}= IE_{A-BC}^{ABC}-IE_{A-B}^{AB}$ and $\Delta IE_{B-C}= IE_{AB-C}^{ABC}-IE_{B-C}^{ABC}$

Positive values indicate anti-cooperativity.

ABA′ Fragmentation Scheme

In tetranuclear NHC complexes, fragments A and C are identical ligands, allowing ABC → ABA′ redefinition:

$IE_{A-B}^{ABA'}$, $IE_{B-A'}^{ABA'}$, $IE_{A-BA'}^{ABA'}$ and $IE_{AB-A'}^{ABA'}$

This preserves chemical equivalence and allows meaningful decomposition of interaction energies.

Alternative schemes (ligand-only or full-core) were tested but provided less clarity.

Calculated Cooperativity Energies (Table S1)

All ΔIE_{coop} values for $[L_2(R)_8 \rightarrow M_4]^{4+}$ complexes are summarized here. Positive values indicate anti-cooperativity.

Examples:

$[L_2(F)_8 \rightarrow Ag_4]^{4+}$: 175.85 kcal/mol

$[L_2(F)_8 \rightarrow Au_4]^{4+}$: 229.49 kcal/mol

Cooperativity Data

Key ΔIE_{coop} values for all $[L_2(R)_8 \rightarrow M_4]^{4+}$ complexes are summarized in Table 2 of the main text.

Table S1. The calculated M–C bond lengths (Å) of $[L_2(R)_8 \rightarrow M_3]^{4+}$; M= Ag(I), Au(I); R = C_2H_5, CH_3, H, F, Cl, Br, Ph, and SiH_3 at the PBE-D3/def2-SVP level of theory.

R	M-$C_{(NHC)}$ bond Length					
	Ag_1-$C_{(NHC)1}$	Ag_2-$C_{(NHC)1}$	Ag_2-$C_{(NHC)2}$	Au_1-$C_{(NHC)1}$	Au_2-$C_{(NHC)1}$	Au_2-$C_{(NHC)2}$
C_2H_5	2.09	2.67	2.10	2.05	2.71	2.05
CH_3	2.10	2.66	2.13	2.06	2.73	2.06
H	2.11	2.68	2.13	2.06	2.73	2.06
F	2.11	2.70	2.13	2.06	2.76	2.06
Cl	2.10	2.69	2.13	2.06	2.74	2.06
Br	2.10	2.68	2.13	2.05	2.74	2.06
SiH_3	2.10	2.67	2.12	2.05	2.73	2.06
Ph	2.10	2.70	2.14	2.05	2.76	2.07

Table S2. Comparison of gas-phase and acetonitrile-calculated interaction energies for $[L_2(Ph)_8 \rightarrow Au_4]^{4+}$ and $[L_2(Ph)_8 \rightarrow Ag_4]^{4+}$complexes.

Complex	IE-AB	IE-BA'	IE-A-BA'	IE-AB-A'	IE-Tot
$[L_2(Ph)_8 \rightarrow Au_4]^{4+}$-Gas	-702.36	-702.36	-414.70	-414.70	-1117.06
$[L_2(Ph)_8 \rightarrow Au_4]^{4+}$-Acetonitrile-CPCM	-926.25	-926.25	-897.01	-897.01	-1823.27
$[L_2(Ph)_8 \rightarrow Au_4]^{4+}$-Acetonitrile-IEFCPCM	-927.10	-927.10	-898.3197961	-898.32	-1825.42
$[L_2(Ph)_8 \rightarrow Au_4]^{4+}$-Acetonitrile-SMD	-876.21	-876.21	-846.49	-846.49	-1722.7
$[L_2(Ph)_8 \rightarrow Ag_4]^{4+}$-Gas	-580.32	-580.32	-347.18	-347.18	-927.498
$[L_2(Ph)_8 \rightarrow Ag_4]^{4+}$-Acetonitrile-SMD	-767.567	-767.57	-765.86	-765.86	-1533.43

Atomic coordinates

$[L_2(C_2H_5)_8 \rightarrow Ag_4]^{4+}$

Ag	0.101034000	-0.159966000	-2.738074000
N	-2.530391000	-2.998900000	0.966791000
C	-2.280683000	-2.205926000	-0.114397000
Ag	-1.820604000	-0.154660000	-0.129629000
N	-2.501158000	-3.019992000	-1.186558000
C	-2.853445000	-4.314928000	0.589985000
N	-2.864509000	-1.223842000	-2.792385000
N	-2.808342000	0.942054000	-2.806544000
C	-2.154733000	1.920431000	-0.146617000
C	-2.514811000	4.085675000	0.527575000
C	-2.288000000	2.317459000	2.335777000
H	-1.244867000	2.325044000	2.712380000
H	-2.877128000	3.040582000	2.926729000
C	-2.001194000	-0.126397000	2.532010000
C	-4.170415000	0.634989000	2.494929000
C	-4.214216000	-0.745898000	2.507587000
C	-2.441285000	-2.549038000	2.370852000
H	-3.062132000	-3.224698000	2.985046000
H	-1.393353000	-2.613582000	2.727488000
N	-2.304332000	2.735753000	-1.230045000
N	-2.321421000	2.750064000	0.923202000
C	-2.833536000	-4.328644000	-0.793515000
N	-2.809504000	0.983070000	2.533818000
C	-2.411166000	-2.584883000	-2.595215000
H	-1.360988000	-2.638774000	-2.946758000
H	-3.019350000	-3.275857000	-3.205164000
N	-2.877832000	-1.180187000	2.552274000
C	-1.995259000	-0.163621000	-2.771269000
C	-4.203641000	-0.796385000	-2.803414000
C	-2.285402000	2.279192000	-2.636017000
H	-2.881087000	2.992509000	-3.232529000
H	-1.246447000	2.281507000	-3.023883000
C	-4.167850000	0.585901000	-2.812040000
C	-2.503360000	4.076416000	-0.855611000
Ag	0.094508000	-0.132973000	2.509600000
N	2.291709000	2.894138000	-1.215952000
C	2.133005000	2.073154000	-0.136028000
Ag	1.902101000	-0.035173000	-0.126858000
N	2.306963000	2.901462000	0.935449000
C	2.537630000	4.226567000	-0.837033000
N	2.904754000	1.187657000	2.555338000
N	3.141792000	-0.958649000	2.572490000
C	2.588350000	-2.043487000	-0.115585000
C	3.649981000	-3.967396000	-0.798043000
C	2.810743000	-2.375128000	-2.589983000
H	1.754079000	-2.510825000	-2.894227000
H	3.441427000	-3.024032000	-3.222111000
C	2.193047000	-0.002678000	-2.775622000
C	4.446537000	-0.447097000	-2.834698000
C	4.294629000	0.927907000	-2.838289000
C	2.273513000	2.447396000	-2.620762000
H	2.781159000	3.217488000	-3.227883000
H	1.228670000	2.354695000	-2.979164000
N	3.003094000	-2.769955000	0.963080000
N	2.992790000	-2.785729000	-1.188167000
C	2.548161000	4.231217000	0.544165000
N	3.147956000	-0.983701000	-2.807268000
C	2.277036000	2.471353000	2.344637000
H	1.229420000	2.389300000	2.697760000
H	2.786750000	3.244363000	2.946018000
N	2.910284000	1.165307000	-2.813194000
C	2.185719000	0.020674000	2.548912000
C	4.289166000	0.950715000	2.526566000
C	2.814964000	-2.353435000	2.362208000
H	3.452483000	-2.992391000	2.997488000
H	1.759271000	-2.497307000	2.666166000
C	4.441034000	-0.422988000	2.539317000
C	3.657710000	-3.956852000	0.584041000
C	4.159901000	-5.005051000	-1.749647000
H	4.778951000	-4.525265000	-2.539817000
H	4.869432000	-5.649140000	-1.193522000
C	3.061137000	-5.876979000	-2.382974000
H	2.347473000	-5.280791000	-2.988731000
H	2.480958000	-6.409859000	-1.603817000
H	3.508440000	-6.636891000	-3.052240000
C	4.173938000	-4.981617000	1.546888000
H	4.889480000	-5.625776000	0.998513000
H	4.786845000	-4.490134000	2.334919000
C	3.080225000	-5.855810000	2.186100000
H	2.505260000	-6.399969000	1.410901000
H	2.361434000	-5.258867000	2.784995000
H	3.531703000	-6.606434000	2.863036000
C	5.679579000	-1.260415000	2.608328000
H	5.601914000	-2.096278000	1.879529000
H	6.525392000	-0.641287000	2.247709000
C	5.997906000	-1.797243000	4.016600000
H	5.189709000	-2.443364000	4.417086000
H	6.141999000	-0.967811000	4.736218000
H	6.928495000	-2.396716000	4.000077000
C	5.310895000	2.043345000	2.575911000
H	6.269826000	1.625989000	2.208231000
H	5.040406000	2.835310000	1.843631000
C	5.516426000	2.648199000	3.977662000
H	5.846912000	1.876330000	4.699851000
H	4.588964000	3.102390000	4.383643000
H	6.291302000	3.438325000	3.948131000
C	2.688847000	5.376658000	1.498458000
H	3.434256000	5.132257000	2.287361000
H	3.137112000	6.225040000	0.944767000
C	1.360582000	5.822801000	2.136534000
H	0.899490000	5.020013000	2.749482000
H	0.628681000	6.117675000	1.357819000
H	1.521188000	6.693464000	2.801199000
C	2.669624000	5.364950000	-1.800457000
H	3.112127000	6.220735000	-1.253625000
H	3.417232000	5.119516000	-2.586809000
C	1.338618000	5.796635000	-2.442281000
H	0.604738000	6.093163000	-1.666099000
H	0.882803000	4.985697000	-3.048403000
H	1.493523000	6.662520000	-3.114464000
C	5.339383000	2.000445000	-2.871449000
H	6.214816000	1.595273000	-3.418691000
H	4.983857000	2.847932000	-3.495630000

C	5.797351000	2.511938000	-1.492050000
H	6.200116000	1.684853000	-0.874732000
H	4.970920000	2.984978000	-0.925305000
H	6.599776000	3.265119000	-1.612778000
C	5.703973000	-1.260899000	-2.854659000
H	5.525553000	-2.211073000	-3.400497000
H	6.446698000	-0.716270000	-3.473077000
C	6.311597000	-1.548504000	-1.468382000
H	5.626274000	-2.138528000	-0.828157000
H	6.546968000	-0.606957000	-0.934251000
H	7.253792000	-2.119924000	-1.575807000
C	-5.391098000	-1.707507000	-2.799692000
H	-6.208125000	-1.193869000	-3.345743000
H	-5.171051000	-2.610755000	-3.406718000
C	-5.892285000	-2.113064000	-1.400680000
H	-6.151851000	-1.219541000	-0.799152000
H	-5.134023000	-2.691881000	-0.837458000
H	-6.800177000	-2.740576000	-1.488296000
C	-5.304447000	1.559869000	-2.823931000
H	-5.050046000	2.423818000	-3.474118000
H	-6.158675000	1.068384000	-3.331843000
C	-5.754992000	2.050686000	-1.435072000
H	-4.957872000	2.614853000	-0.911913000
H	-6.044891000	1.198338000	-0.789290000
H	-6.632536000	2.718567000	-1.533136000
C	-2.687846000	5.215097000	-1.815040000
H	-2.341651000	6.135539000	-1.301691000
H	-1.998350000	5.095090000	-2.678443000
C	-4.130802000	5.432151000	-2.307247000
H	-4.822520000	5.595061000	-1.457781000
H	-4.514991000	4.569886000	-2.888514000
H	-4.184122000	6.321615000	-2.963982000
C	-2.713302000	5.237891000	1.467619000
H	-2.014982000	5.147918000	2.327825000
H	-2.389445000	6.154186000	0.933048000
C	-4.156598000	5.436815000	1.967441000
H	-4.512502000	4.591515000	2.589894000
H	-4.860240000	5.549433000	1.119396000
H	-4.225824000	6.350672000	2.588324000
C	-5.281085000	1.636263000	2.536602000
H	-5.065964000	2.455388000	1.816891000
H	-6.195053000	1.143332000	2.148828000
C	-5.560474000	2.206925000	3.939685000
H	-4.676682000	2.719665000	4.372138000
H	-5.851473000	1.405082000	4.645978000
H	-6.388357000	2.940978000	3.901068000
C	-5.388476000	-1.670248000	2.569225000
H	-6.267808000	-1.126482000	2.169345000
H	-5.228347000	-2.517776000	1.868894000
C	-5.704152000	-2.189457000	3.984563000
H	-5.940663000	-1.354522000	4.672657000
H	-4.856135000	-2.750453000	4.428246000
H	-6.579082000	-2.867430000	3.961460000
C	-3.159137000	-5.433427000	1.541928000
H	-2.916068000	-6.380005000	1.017878000
H	-2.459402000	-5.398658000	2.404600000
C	-4.615796000	-5.499337000	2.037898000
H	-5.326129000	-5.541068000	1.188874000
H	-4.891744000	-4.629837000	2.667095000
H	-4.769866000	-6.407068000	2.652452000
C	-3.111097000	-5.465531000	-1.732582000
H	-2.418225000	-5.416205000	-2.599810000
H	-2.834388000	-6.400266000	-1.203496000
C	-4.567853000	-5.581277000	-2.217636000
H	-4.884051000	-4.707927000	-2.822421000
H	-5.268810000	-5.668010000	-1.364501000
H	-4.690987000	-6.481215000	-2.850237000

$[L_2(CH_3)_8 \rightarrow Ag_4]^{4+}$

Ag	-0.000061000	-0.000022000	-2.578580000
N	2.696877000	2.833795000	1.075498000
C	2.352385000	2.066729000	0.000061000
Ag	1.852437000	0.000053000	0.000012000
N	2.696777000	2.833834000	-1.075386000
C	3.240677000	4.073863000	0.691008000
N	2.943270000	1.079826000	-2.736668000
N	2.943649000	-1.079147000	-2.736707000
C	2.352867000	-2.066554000	-0.000054000
C	3.242361000	-4.073184000	0.690842000
C	2.496350000	-2.430192000	2.478573000
H	1.419753000	-2.481309000	2.736589000
H	3.043438000	-3.140932000	3.122439000
C	2.103168000	0.000072000	2.650745000
C	4.289849000	-0.690073000	2.841132000
C	4.289667000	0.690810000	2.841204000
C	2.495698000	2.430467000	2.478734000
H	3.042806000	3.141296000	3.122492000
H	1.419145000	2.481411000	2.736992000
N	2.697835000	-2.833392000	-1.075518000
N	2.697833000	-2.833453000	1.075361000
C	3.240543000	4.073922000	-0.690900000
N	2.943730000	-1.079294000	2.736631000
C	2.495485000	2.430575000	-2.478615000
H	1.418897000	2.481439000	-2.736740000
H	3.042451000	3.141497000	-3.122402000
N	2.943430000	1.079675000	2.736677000
C	2.103051000	0.000190000	-2.650743000
C	4.289508000	0.691023000	-2.841202000
C	2.496320000	-2.430080000	-2.478714000
H	3.043457000	-3.140759000	-3.122607000
H	1.419726000	-2.481243000	-2.736744000
C	4.289762000	-0.689860000	-2.841269000
C	3.242423000	-4.073118000	-0.691064000
Ag	0.000058000	-0.000267000	2.578562000
N	-2.697174000	-2.833781000	-1.075576000
C	-2.352590000	-2.066783000	-0.000122000
Ag	-1.852451000	-0.000154000	-0.000008000
N	-2.697063000	-2.833872000	1.075310000
C	-3.241122000	-4.073792000	-0.691112000
N	-2.943376000	-1.079875000	2.736631000
N	-2.943544000	1.079100000	2.736746000
C	-2.352667000	2.066502000	0.000114000
C	-3.241872000	4.073275000	-0.690735000
C	-2.496075000	2.430226000	-2.478504000
H	-1.419467000	2.481218000	-2.736499000
H	-3.043064000	3.141055000	-3.122356000

C	-2.103171000	-0.000073000	-2.650750000
C	-4.289774000	0.690321000	-2.841120000
C	-4.289752000	-0.690561000	-2.841216000
C	-2.495985000	-2.430435000	-2.478805000
H	-3.043197000	-3.141179000	-3.122567000
H	-1.419445000	-2.481497000	-2.737096000
N	-2.697540000	2.833357000	1.075596000
N	-2.697528000	2.833474000	-1.075282000
C	-3.240977000	-4.073888000	0.690796000
N	-2.943610000	1.079389000	-2.736611000
C	-2.495728000	-2.430666000	2.478547000
H	-1.419146000	-2.481647000	2.736677000
H	-3.042773000	-3.141544000	3.122316000
N	-2.943556000	-1.079581000	-2.736699000
C	-2.103056000	-0.000317000	2.650739000
C	-4.289576000	-0.690943000	2.841189000
C	-2.496074000	2.429988000	2.478785000
H	-3.043141000	3.140707000	3.122694000
H	-1.419474000	2.481042000	2.736821000
C	-4.289697000	0.689940000	2.841296000
C	-3.241955000	4.073168000	0.691173000
C	3.699986000	-5.117063000	1.653071000
H	4.082738000	-5.998361000	1.107030000
H	4.527931000	-4.761041000	2.301645000
H	2.880896000	-5.475104000	2.310677000
C	3.700101000	-5.116945000	-1.653332000
H	4.528141000	-4.760905000	-2.301766000
H	4.082754000	-5.998297000	-1.107311000
H	2.881081000	-5.474906000	-2.311077000
C	-3.698476000	-5.117744000	-1.653402000
H	-2.879467000	-5.475229000	-2.311416000
H	-4.080535000	-5.999366000	-1.107402000
H	-4.526865000	-4.762000000	-2.301550000
C	-3.698168000	-5.117891000	1.653080000
H	-4.080569000	-5.999356000	1.107067000
H	-2.878965000	-5.475597000	2.310710000
H	-4.526272000	-4.762133000	2.301612000
C	-3.699344000	5.117245000	-1.652940000
H	-4.082008000	5.998570000	-1.106880000
H	-2.880192000	5.475212000	-2.310513000
H	-4.527310000	4.761342000	-2.301549000
C	-3.699503000	5.117026000	1.653468000
H	-4.527575000	4.761064000	2.301902000
H	-2.880435000	5.474879000	2.311212000
H	-4.082061000	5.998435000	1.107472000
C	3.697588000	5.117970000	-1.653206000
H	4.079925000	5.999476000	-1.107214000
H	4.525699000	4.762289000	-2.301766000
H	2.878324000	5.475590000	-2.310813000
C	3.697883000	5.117896000	1.653278000
H	2.878794000	5.475362000	2.311206000
H	4.526240000	4.762241000	2.301515000
H	4.079933000	5.999511000	1.107262000
C	5.408225000	1.666195000	-2.966737000
H	5.484414000	2.327066000	-2.078389000
H	6.373360000	1.137480000	-3.067075000
H	5.296630000	2.306986000	-3.866656000
C	5.408818000	-1.664626000	-2.966913000
H	6.373755000	-1.135571000	-3.067396000
H	5.485336000	-2.325358000	-2.078513000
H	5.297388000	-2.305545000	-3.866778000
C	-5.408700000	1.665272000	-2.966510000
H	-6.373703000	1.136362000	-3.067107000
H	-5.485155000	2.325880000	-2.077983000
H	-5.297151000	2.306322000	-3.866242000
C	-5.408625000	-1.665551000	-2.966764000
H	-5.297128000	-2.306466000	-3.866620000
H	-5.484958000	-2.326287000	-2.078345000
H	-6.373668000	-1.136683000	-3.067189000
C	5.408888000	-1.664893000	2.966526000
H	6.373833000	-1.135872000	3.067101000
H	5.297431000	-2.305940000	3.866269000
H	5.485402000	-2.325507000	2.078008000
C	5.408426000	1.665931000	2.966755000
H	5.296839000	2.306842000	3.866603000
H	6.373528000	1.137175000	3.067201000
H	5.484699000	2.326671000	2.078333000
C	-5.408657000	1.664807000	2.966991000
H	-6.373642000	1.135835000	3.067448000
H	-5.297167000	2.305666000	3.866892000
H	-5.485117000	2.325594000	2.078628000
C	-5.408382000	-1.666015000	2.966696000
H	-5.484627000	-2.326854000	2.078329000
H	-5.296846000	-2.306841000	3.866596000
H	-6.373470000	-1.137217000	3.067046000

$[L_2(H)_8 \rightarrow Ag_4]^{4+}$

Ag	-0.000061000	-2.584132000	0.000237000
N	2.737755000	1.077043000	-2.813195000
C	2.355157000	0.000009000	-2.061288000
Ag	1.830227000	-0.000036000	0.000058000
N	2.737564000	-1.077015000	-2.813286000
C	3.337807000	0.684550000	-4.008242000
N	2.950767000	-2.764192000	-1.081683000
N	2.951011000	-2.764161000	1.081391000
C	2.354774000	-0.000067000	2.061485000
C	3.338420000	0.684428000	4.007964000
C	2.525963000	2.488898000	2.439445000
H	1.451039000	2.743455000	2.519128000
H	3.092145000	3.120523000	3.149110000
C	2.110191000	2.660615000	0.000058000
C	4.279494000	2.906056000	0.683920000
C	4.279464000	2.906126000	-0.683879000
C	2.525895000	2.488979000	-2.439331000
H	3.091911000	3.120736000	-3.149018000
H	1.450914000	2.743323000	-2.518908000
N	2.737760000	-1.077121000	2.813191000
N	2.737697000	1.076944000	2.813257000
C	3.337622000	-0.684527000	-4.008333000
N	2.950992000	2.764078000	1.081585000
C	2.525594000	-2.488938000	-2.439490000
H	1.450588000	-2.743224000	-2.518960000
H	3.091521000	-3.120699000	-3.149237000
N	2.950933000	2.764159000	-1.081481000
C	2.110119000	-2.660582000	-0.000038000
C	4.279308000	-2.906220000	-0.684191000

C	2.526076000	-2.489069000	2.439295000
H	3.092285000	-3.120727000	3.148908000
H	1.451157000	-2.743636000	2.519002000
C	4.279463000	-2.906239000	0.683614000
C	3.338553000	-0.684643000	4.007873000
Ag	0.000002000	2.584295000	0.000023000
N	-2.737761000	-1.077074000	2.813204000
C	-2.354761000	-0.000031000	2.061491000
Ag	-1.830042000	-0.000024000	0.000046000
N	-2.737648000	1.076993000	2.813265000
C	-3.338564000	-0.684580000	4.007875000
N	-2.950987000	2.764125000	1.081583000
N	-2.950933000	2.764175000	-1.081479000
C	-2.354905000	0.000028000	-2.061372000
C	-3.337868000	-0.684477000	-4.008186000
C	-2.525743000	-2.488931000	-2.439471000
H	-1.450787000	-2.743408000	-2.519026000
H	-3.091797000	-3.120605000	-3.149192000
C	-2.110241000	-2.660578000	-0.000025000
C	-4.279446000	-2.906145000	-0.684156000
C	-4.279591000	-2.906192000	0.683642000
C	-2.526180000	-2.489037000	2.439308000
H	-3.092444000	-3.120645000	3.148921000
H	-1.451285000	-2.743704000	2.519032000
N	-2.737616000	1.077076000	-2.813215000
N	-2.737525000	-1.076983000	-2.813285000
C	-3.338402000	0.684491000	4.007961000
N	-2.950892000	-2.764123000	-1.081653000
C	-2.525961000	2.488954000	2.439444000
H	-1.451050000	2.743565000	2.519145000
H	-3.092169000	3.120554000	3.149108000
N	-2.951125000	-2.764113000	1.081411000
C	-2.110187000	2.660682000	0.000059000
C	-4.279487000	2.906151000	0.683921000
C	-2.525887000	2.489022000	-2.439330000
H	-3.091979000	3.120718000	-3.149006000
H	-1.450942000	2.743516000	-2.518936000
C	-4.279456000	2.906223000	-0.683877000
C	-3.337989000	0.684596000	-4.008104000
H	3.719148000	1.393146000	4.753260000
H	3.719345000	-1.393357000	4.753141000
H	-3.719311000	-1.393281000	4.753179000
H	-3.719068000	1.393217000	4.753281000
H	-3.718472000	-1.393214000	-4.753526000
H	-3.718698000	1.393324000	-4.753400000
H	3.718208000	-1.393251000	-4.753697000
H	3.718634000	1.393236000	-4.753518000
H	5.105055000	-3.027231000	-1.395043000
H	5.105285000	-3.027330000	1.394365000
H	-5.105134000	-3.027151000	-1.395077000
H	-5.105405000	-3.027269000	1.394407000
H	5.105293000	3.027008000	1.394723000
H	5.105177000	3.027174000	-1.394762000
H	-5.105161000	3.027287000	-1.394767000
H	-5.105272000	3.027125000	1.394736000

$[L_2(F)_8 \rightarrow Ag_4]^{4+}$

Ag	1.994497000	1.707172000	-0.163786000
N	1.004495000	-2.546488000	3.019585000
C	1.550741000	-1.598219000	2.194084000
Ag	1.186707000	-1.371111000	0.107760000
N	2.642799000	-1.142315000	2.885928000
C	1.739736000	-2.685532000	4.198118000
N	4.042086000	-0.339041000	1.083416000
N	4.023990000	-0.523621000	-1.078022000
C	1.514072000	-1.946227000	-1.917151000
C	1.667929000	-3.356368000	-3.712150000
C	-0.250141000	-3.759609000	-2.134832000
H	-1.154502000	-3.138572000	-2.281697000
H	-0.330488000	-4.665959000	-2.765223000
C	-0.659079000	-3.339389000	0.291329000
C	0.615163000	-5.162339000	-0.255450000
C	0.627701000	-5.046948000	1.112433000
C	-0.204792000	-3.348080000	2.745948000
H	-0.270218000	-4.136397000	3.520272000
H	-1.108110000	-2.711261000	2.804894000
N	2.593810000	-1.616603000	-2.694744000
N	0.953511000	-3.018634000	-2.561358000
C	2.780901000	-1.793178000	4.113173000
N	-0.184374000	-4.124505000	-0.735336000
C	3.585810000	-0.099102000	2.436289000
H	3.097775000	0.894029000	2.459329000
H	4.443482000	-0.094129000	3.136062000
N	-0.164295000	-3.941873000	1.426213000
C	3.416821000	0.149632000	-0.041784000
C	4.983557000	-1.316456000	0.759245000
C	3.544856000	-0.515267000	-2.444163000
H	4.390568000	-0.631828000	-3.148780000
H	3.057106000	0.461297000	-2.627171000
C	4.971965000	-1.433407000	-0.608521000
C	2.710246000	-2.465343000	-3.796963000
Ag	-1.994497000	-1.707172000	0.163786000
N	-1.004495000	2.546488000	-3.019585000
C	-1.550741000	1.598219000	-2.194084000
Ag	-1.186707000	1.371111000	-0.107760000
N	-2.642799000	1.142315000	-2.885928000
C	-1.739736000	2.685532000	-4.198118000
N	-4.042086000	0.339041000	-1.083416000
N	-4.023990000	0.523621000	1.078022000
C	-1.514072000	1.946227000	1.917151000
C	-1.667929000	3.356368000	3.712150000
C	0.250141000	3.759609000	2.134832000
H	1.154502000	3.138572000	2.281697000
H	0.330488000	4.665959000	2.765223000
C	0.659079000	3.339389000	-0.291329000
C	-0.615163000	5.162339000	0.255450000
C	-0.627701000	5.046948000	-1.112433000
C	0.204792000	3.348080000	-2.745948000
H	0.270218000	4.136397000	-3.520272000
H	1.108110000	2.711261000	-2.804894000
N	-2.593810000	1.616603000	2.694744000
N	-0.953511000	3.018634000	2.561358000
C	-2.780901000	1.793178000	-4.113173000
N	0.184374000	4.124505000	0.735336000
C	-3.585810000	0.099102000	-2.436289000
H	-3.097775000	-0.894029000	-2.459329000

H	-4.443482000	0.094129000	-3.136062000
N	0.164295000	3.941873000	-1.426213000
C	-3.416821000	-0.149632000	0.041784000
C	-4.983557000	1.316456000	-0.759245000
C	-3.544856000	0.515267000	2.444163000
H	-4.390568000	0.631828000	3.148780000
H	-3.057106000	-0.461297000	2.627171000
C	-4.971965000	1.433407000	0.608521000
C	-2.710246000	2.465343000	3.796963000
F	1.310744000	-4.351998000	-4.476192000
F	3.672419000	-2.333093000	-4.668371000
F	-1.398764000	3.538426000	-5.124999000
F	-3.758002000	1.516336000	-4.932554000
F	-1.310744000	4.351998000	4.476192000
F	-3.672419000	2.333093000	4.668371000
F	3.758002000	-1.516336000	4.932554000
F	1.398764000	-3.538426000	5.124999000
F	5.680510000	-1.916996000	1.684156000
F	5.654233000	-2.183134000	-1.429640000
F	-1.174675000	6.015872000	1.068092000
F	-1.203285000	5.753264000	-2.046027000
F	1.174675000	-6.015872000	-1.068092000
F	1.203285000	-5.753264000	2.046027000
F	-5.654233000	2.183134000	1.429640000
F	-5.680510000	1.916996000	-1.684156000

$[L_2(Cl)_8 \rightarrow Ag_4]^{4+}$

Ag	1.991796000	1.705354000	-0.164310000
N	0.969235000	-2.504753000	3.042757000
C	1.543350000	-1.589115000	2.203655000
Ag	1.198952000	-1.385529000	0.107994000
N	2.608210000	-1.098432000	2.908953000
C	1.660956000	-2.593828000	4.259845000
N	4.009159000	-0.354813000	1.084126000
N	3.991032000	-0.539754000	-1.077838000
C	1.506474000	-1.938836000	-1.929818000
C	1.585957000	-3.275149000	-3.789730000
C	-0.273916000	-3.717227000	-2.130822000
H	-1.179658000	-3.090106000	-2.240282000
H	-0.378749000	-4.616971000	-2.766808000
C	-0.653784000	-3.328809000	0.289741000
C	0.673267000	-5.113900000	-0.266500000
C	0.686482000	-4.998283000	1.110447000
C	-0.227190000	-3.309011000	2.733698000
H	-0.315758000	-4.090456000	3.512476000
H	-1.133147000	-2.673213000	2.756054000
N	2.558701000	-1.577631000	-2.726289000
N	0.916550000	-2.980323000	-2.592784000
C	2.708019000	-1.695505000	4.174341000
N	-0.164035000	-4.095087000	-0.739378000
C	3.547740000	-0.070545000	2.424743000
H	3.056771000	0.921578000	2.410442000
H	4.402369000	-0.040000000	3.127366000
N	-0.143120000	-3.913308000	1.422781000
C	3.404238000	0.145917000	-0.042643000
C	4.925415000	-1.366271000	0.767494000
C	3.507242000	-0.485861000	-2.439379000
H	4.349877000	-0.578531000	-3.150972000
H	3.017580000	0.496145000	-2.585900000
C	4.913813000	-1.484097000	-0.609287000
C	2.634925000	-2.379023000	-3.875060000
Ag	-1.991796000	-1.705354000	0.164310000
N	-0.969235000	2.504753000	-3.042757000
C	-1.543350000	1.589115000	-2.203655000
Ag	-1.198952000	1.385529000	-0.107994000
N	-2.608210000	1.098432000	-2.908953000
C	-1.660956000	2.593828000	-4.259845000
N	-4.009159000	0.354813000	-1.084126000
N	-3.991032000	0.539754000	1.077838000
C	-1.506474000	1.938836000	1.929818000
C	-1.585957000	3.275149000	3.789730000
C	0.273916000	3.717227000	2.130822000
H	1.179658000	3.090106000	2.240282000
H	0.378749000	4.616971000	2.766808000
C	0.653784000	3.328809000	-0.289741000
C	-0.673267000	5.113900000	0.266500000
C	-0.686482000	4.998283000	-1.110447000
C	0.227190000	3.309011000	-2.733698000
H	0.315758000	4.090456000	-3.512476000
H	1.133147000	2.673213000	-2.756054000
N	-2.558701000	1.577631000	2.726289000
N	-0.916550000	2.980323000	2.592784000
C	-2.708019000	1.695505000	-4.174341000
N	0.164035000	4.095087000	0.739378000
C	-3.547740000	0.070545000	-2.424743000
H	-3.056771000	-0.921578000	-2.410442000
H	-4.402369000	0.040000000	-3.127366000
N	0.143120000	3.913308000	-1.422781000
C	-3.404238000	-0.145917000	0.042643000
C	-4.925415000	1.366271000	-0.767494000
C	-3.507242000	0.485861000	2.439379000
H	-4.349877000	0.578531000	3.150972000
H	-3.017580000	-0.496145000	2.585900000
C	-4.913813000	1.484097000	0.609287000
C	-2.634925000	2.379023000	3.875060000
Cl	1.139417000	-4.502240000	-4.867101000
Cl	3.809441000	-2.221638000	-5.084005000
Cl	-1.238634000	3.623319000	-5.535746000
Cl	-3.903359000	1.336734000	-5.318239000
Cl	-1.139417000	4.502240000	4.867101000
Cl	-3.809441000	2.221638000	5.084005000
Cl	3.903359000	-1.336734000	5.318239000
Cl	1.238634000	-3.623319000	5.535746000
Cl	5.830156000	-2.205105000	1.923205000
Cl	5.800358000	-2.508335000	-1.620649000
Cl	-1.453812000	6.226285000	1.272148000
Cl	-1.488375000	5.928558000	-2.272083000
Cl	1.453812000	-6.226285000	-1.272148000
Cl	1.488375000	-5.928558000	2.272083000
Cl	-5.800358000	2.508335000	1.620649000
Cl	-5.830156000	2.205105000	-1.923205000

$[L_2(Br)_8 \rightarrow Ag_4]^{4+}$

Ag	1.986954000	1.701097000	-0.163272000
N	0.948273000	-2.479941000	3.054937000
C	1.539573000	-1.584536000	2.206338000

Ag	1.203213000	-1.390307000	0.108879000
N	2.588740000	-1.074431000	2.920872000
C	1.608707000	-2.531271000	4.291440000
N	3.996516000	-0.362707000	1.086119000
N	3.978138000	-0.547253000	-1.077049000
C	1.503900000	-1.935675000	-1.931727000
C	1.535114000	-3.219286000	-3.829163000
C	-0.282778000	-3.701670000	-2.128594000
H	-1.191673000	-3.075930000	-2.221915000
H	-0.396008000	-4.599313000	-2.766621000
C	-0.648487000	-3.321543000	0.289335000
C	0.692028000	-5.095853000	-0.266960000
C	0.704340000	-4.979548000	1.111292000
C	-0.238784000	-3.291494000	2.730031000
H	-0.337396000	-4.069676000	3.511276000
H	-1.147689000	-2.658994000	2.734938000
N	2.539378000	-1.555421000	-2.740781000
N	0.897695000	-2.959490000	-2.606873000
C	2.657074000	-1.633058000	4.205781000
N	-0.153627000	-4.083690000	-0.740122000
C	3.533497000	-0.058751000	2.421682000
H	3.045797000	0.934972000	2.390878000
H	4.386892000	-0.019432000	3.125824000
N	-0.134266000	-3.900943000	1.423138000
C	3.396766000	0.141940000	-0.041434000
C	4.905200000	-1.381586000	0.769928000
C	3.492549000	-0.472580000	-2.436804000
H	4.333939000	-0.555520000	-3.151521000
H	3.005476000	0.513430000	-2.566495000
C	4.893262000	-1.499327000	-0.608214000
C	2.584235000	-2.321926000	-3.914747000
Ag	-1.986954000	-1.701097000	0.163272000
N	-0.948273000	2.479941000	-3.054937000
C	-1.539573000	1.584536000	-2.206338000
Ag	-1.203213000	1.390307000	-0.108879000
N	-2.588740000	1.074431000	-2.920872000
C	-1.608707000	2.531271000	-4.291440000
N	-3.996516000	0.362707000	-1.086119000
N	-3.978138000	0.547253000	1.077049000
C	-1.503900000	1.935675000	1.931727000
C	-1.535114000	3.219286000	3.829163000
C	0.282778000	3.701670000	2.128594000
H	1.191673000	3.075930000	2.221915000
H	0.396008000	4.599313000	2.766621000
C	0.648487000	3.321543000	-0.289335000
C	-0.692028000	5.095853000	0.266960000
C	-0.704340000	4.979548000	-1.111292000
C	0.238784000	3.291494000	-2.730031000
H	0.337396000	4.069676000	-3.511276000
H	1.147689000	2.658994000	-2.734938000
N	-2.539378000	1.555421000	2.740781000
N	-0.897695000	2.959490000	2.606873000
C	-2.657074000	1.633058000	-4.205781000
N	0.153627000	4.083690000	0.740122000
C	-3.533497000	0.058751000	-2.421682000
H	-3.045797000	-0.934972000	-2.390878000
H	-4.386892000	0.019432000	-3.125824000
N	0.134266000	3.900943000	-1.423138000
C	-3.396766000	-0.141940000	0.041434000
C	-4.905200000	1.381586000	-0.769928000
C	-3.492549000	0.472580000	2.436804000
H	-4.333939000	0.555520000	3.151521000
H	-3.005476000	-0.513430000	2.566495000
C	-4.893262000	1.499327000	0.608214000
C	-2.584235000	2.321926000	3.914747000
Br	1.026168000	-4.521014000	-5.045102000
Br	3.827128000	-2.123924000	-5.274227000
Br	-1.125177000	3.609832000	-5.718227000
Br	-3.925099000	1.211935000	-5.489255000
Br	-1.026168000	4.521014000	5.045102000
Br	-3.827128000	2.123924000	5.274227000
Br	3.925099000	-1.211935000	5.489255000
Br	1.125177000	-3.609832000	5.718227000
Br	5.906994000	-2.303383000	2.020491000
Br	5.873751000	-2.621913000	-1.701720000
Br	-1.548635000	6.323479000	1.351660000
Br	-1.580983000	6.010127000	-2.370944000
Br	1.548635000	-6.323479000	-1.351660000
Br	1.580983000	-6.010127000	2.370944000
Br	-5.873751000	2.621913000	1.701720000
Br	-5.906994000	2.303383000	-2.020491000

$[L_2(SiH_3)_8 \rightarrow Ag_4]^{4+}$

Ag	1.984879000	1.713604000	-0.207165000
N	0.944333000	-2.423986000	3.066345000
C	1.538019000	-1.555011000	2.199364000
Ag	1.215950000	-1.385738000	0.107377000
N	2.537639000	-0.984488000	2.935336000
C	1.535041000	-2.391706000	4.342470000
N	3.967247000	-0.338844000	1.080624000
N	3.972456000	-0.562190000	-1.068820000
C	1.495954000	-1.909362000	-1.931822000
C	1.419571000	-3.094259000	-3.908678000
C	-0.316518000	-3.622920000	-2.115938000
H	-1.216680000	-2.977267000	-2.142741000
H	-0.490542000	-4.493988000	-2.771168000
C	-0.628433000	-3.317424000	0.304271000
C	0.759795000	-5.049222000	-0.308664000
C	0.800273000	-4.947266000	1.076248000
C	-0.193336000	-3.300558000	2.727348000
H	-0.249784000	-4.097033000	3.494273000
H	-1.140292000	-2.725057000	2.752519000
N	2.504585000	-1.516993000	-2.761207000
N	0.849790000	-2.885774000	-2.635726000
C	2.563782000	-1.460573000	4.262442000
N	-0.129177000	-4.047466000	-0.741627000
C	3.470779000	0.021462000	2.395140000
H	2.960298000	1.000340000	2.299473000
H	4.305873000	0.130890000	3.108550000
N	-0.070433000	-3.895591000	1.412851000
C	3.392795000	0.158590000	-0.059261000
C	4.869541000	-1.383077000	0.803452000
C	3.500352000	-0.477749000	-2.435333000
H	4.352473000	-0.591463000	-3.132946000
H	3.062129000	0.529769000	-2.581522000
C	4.868610000	-1.528016000	-0.578142000
C	2.489463000	-2.210306000	-3.985009000

Ag	-1.984879000	-1.713604000	0.207165000
N	-0.944333000	2.423986000	-3.066345000
C	-1.538019000	1.555011000	-2.199364000
Ag	-1.215950000	1.385738000	-0.107377000
N	-2.537639000	0.984488000	-2.935336000
C	-1.535041000	2.391706000	-4.342470000
N	-3.967247000	0.338844000	-1.080624000
N	-3.972456000	0.562190000	1.068820000
C	-1.495954000	1.909362000	1.931822000
C	-1.419571000	3.094259000	3.908678000
C	0.316518000	3.622920000	2.115938000
H	1.216680000	2.977267000	2.142741000
H	0.490542000	4.493988000	2.771168000
C	0.628433000	3.317424000	-0.304271000
C	-0.759795000	5.049222000	0.308664000
C	-0.800273000	4.947266000	-1.076248000
C	0.193336000	3.300558000	-2.727348000
H	0.249784000	4.097033000	-3.494273000
H	1.140292000	2.725057000	-2.752519000
N	-2.504585000	1.516993000	2.761207000
N	-0.849790000	2.885774000	2.635726000
C	-2.563782000	1.460573000	-4.262442000
N	0.129177000	4.047466000	0.741627000
C	-3.470779000	-0.021462000	-2.395140000
H	-2.960298000	-1.000340000	-2.299473000
H	-4.305873000	-0.130890000	-3.108550000
N	0.070433000	3.895591000	-1.412851000
C	-3.392795000	-0.158590000	0.059261000
C	-4.869541000	1.383077000	-0.803452000
C	-3.500352000	0.477749000	2.435333000
H	-4.352473000	0.591463000	3.132946000
H	-3.062129000	-0.529769000	2.581522000
C	-4.868610000	1.528016000	0.578142000
C	-2.489463000	2.210306000	3.985009000
Si	3.738876000	-0.930391000	5.688145000
H	2.873624000	-0.470105000	6.818809000
H	4.590998000	-2.101757000	6.059650000
H	4.574051000	0.205286000	5.176804000
Si	0.979861000	-3.405984000	5.865427000
H	0.932441000	-4.851196000	5.466347000
H	1.997425000	-3.146893000	6.927224000
H	-0.390590000	-2.934316000	6.252081000
Si	-0.842504000	4.311671000	5.279627000
H	-0.607789000	3.499462000	6.514111000
H	0.440858000	4.930909000	4.812471000
H	-1.903684000	5.348110000	5.469391000
Si	-3.686511000	1.934100000	5.450385000
H	-5.088700000	2.037296000	4.927706000
H	-3.438275000	0.555903000	5.987919000
H	-3.375224000	3.003557000	6.445036000
Si	-3.738876000	0.930391000	-5.688145000
H	-4.574051000	-0.205286000	-5.176804000
H	-4.590998000	2.101757000	-6.059650000
H	-2.873624000	0.470105000	-6.818809000
Si	-0.979861000	3.405984000	-5.865427000
H	0.390590000	2.934316000	-6.252081000
H	-1.997425000	3.146893000	-6.927224000
H	-0.932441000	4.851196000	-5.466347000
Si	3.686511000	-1.934100000	-5.450385000
H	3.375224000	-3.003557000	-6.445036000
H	3.438275000	-0.555903000	-5.987919000
H	5.088700000	-2.037296000	-4.927706000
Si	0.842504000	-4.311671000	-5.279627000
H	1.903684000	-5.348110000	-5.469391000
H	-0.440858000	-4.930909000	-4.812471000
H	0.607789000	-3.499462000	-6.514111000
Si	5.863831000	-2.764168000	-1.640944000
H	6.630883000	-3.605533000	-0.673706000
H	4.866945000	-3.581503000	-2.411140000
H	6.742393000	-1.991083000	-2.575572000
Si	5.877193000	-2.376429000	2.095639000
H	5.279257000	-3.748945000	2.177467000
H	7.308041000	-2.399265000	1.670563000
H	5.705726000	-1.665861000	3.404204000
Si	1.700812000	-6.277936000	-1.438113000
H	1.567459000	-7.649851000	-0.865755000
H	1.063217000	-6.183397000	-2.791452000
H	3.127509000	-5.821995000	-1.513778000
Si	1.814359000	-5.988668000	2.315661000
H	0.867118000	-6.685877000	3.242799000
H	2.628497000	-6.929098000	1.488676000
H	2.686756000	-5.032245000	3.076970000
Si	-1.814359000	5.988668000	-2.315661000
H	-2.686756000	5.032245000	-3.076970000
H	-2.628497000	6.929098000	-1.488676000
H	-0.867118000	6.685877000	-3.242799000
Si	-1.700812000	6.277936000	1.438113000
H	-3.127509000	5.821995000	1.513778000
H	-1.063217000	6.183397000	2.791452000
H	-1.567459000	7.649851000	0.865755000
Si	-5.877193000	2.376429000	-2.095639000
H	-5.705726000	1.665861000	-3.404204000
H	-7.308041000	2.399265000	-1.670563000
H	-5.279257000	3.748945000	-2.177467000
Si	-5.863831000	2.764168000	1.640944000
H	-6.742393000	1.991083000	2.575572000
H	-4.866945000	3.581503000	2.411140000
H	-6.630883000	3.605533000	0.673706000

$[L_2(Ph)_8 \rightarrow Ag_4]^{4+}$

Ag	1.998977000	1.710841000	-0.162918000
N	0.942183000	-2.481738000	3.046165000
C	1.529718000	-1.572144000	2.210645000
Ag	1.188239000	-1.372918000	0.107583000
N	2.591896000	-1.070689000	2.911346000
C	1.620066000	-2.569818000	4.275592000
N	4.005547000	-0.338976000	1.090364000
C	1.410448000	-3.349008000	5.425559000
H	0.575943000	-4.058770000	5.521262000
N	3.986130000	-0.523437000	-1.085428000
C	2.320538000	-3.179864000	6.477302000
H	2.194958000	-3.771898000	7.395863000
C	1.493045000	-1.924157000	-1.937894000
C	3.287444000	-3.313907000	-5.970619000
H	3.960606000	-3.356689000	-6.839554000
C	2.214555000	-4.232835000	-5.883019000
H	2.074704000	-4.971988000	-6.685592000
C	1.322675000	-4.220382000	-4.802528000
H	0.488134000	-4.935402000	-4.762276000
C	1.550039000	-3.257629000	-3.805040000

C	-0.295560000	-3.686758000	-2.126604000
H	-1.198061000	-3.050523000	-2.220911000
H	-0.428870000	-4.577120000	-2.767933000
C	-0.665205000	-3.333528000	0.290518000
C	0.670582000	-5.107055000	-0.279328000
C	1.405632000	-6.100731000	-0.942489000
H	1.403790000	-6.204748000	-2.036859000
C	2.146616000	-6.974108000	-0.134523000
H	2.728804000	-7.778628000	-0.607576000
C	2.158698000	-6.854099000	1.276258000
H	2.750009000	-7.567983000	1.868449000
C	1.430276000	-5.855690000	1.937493000
H	1.447123000	-5.773311000	3.033578000
C	0.682623000	-4.987360000	1.128567000
C	-0.253158000	-3.274373000	2.726038000
H	-0.373249000	-4.043830000	3.510477000
H	-1.155060000	-2.630474000	2.728177000
C	5.739778000	-2.168192000	1.584417000
H	5.759566000	-2.084284000	2.680340000
C	6.552647000	-3.093601000	0.915461000
H	7.223846000	-3.739416000	1.500601000
N	2.542020000	-1.549741000	-2.731615000
C	3.394021000	-2.261633000	6.389586000
H	4.081896000	-2.157830000	7.241689000
N	0.892964000	-2.961655000	-2.596918000
C	3.598586000	-1.477382000	5.246738000
H	4.431687000	-0.760700000	5.206124000
C	2.692063000	-1.652873000	4.187991000
N	-0.178928000	-4.088907000	-0.745222000
C	3.521568000	-0.044891000	2.418045000
H	3.023630000	0.944716000	2.388105000
H	4.370655000	0.014325000	3.123279000
N	-0.160172000	-3.903847000	1.430471000
C	3.411724000	0.155806000	-0.042148000
C	4.919125000	-1.361675000	0.782189000
C	6.539644000	-3.213354000	-0.495337000
H	7.200967000	-3.949626000	-0.975466000
C	3.478306000	-0.456520000	-2.434891000
H	4.314650000	-0.517835000	-3.155008000
H	2.979179000	0.524599000	-2.563012000
C	4.906276000	-1.481183000	-0.625713000
C	5.713247000	-2.412517000	-1.295573000
H	5.712704000	-2.514388000	-2.390147000
C	3.509613000	-2.347343000	-4.980978000
H	4.341703000	-1.634731000	-5.076673000
C	2.621539000	-2.340089000	-3.892522000
Ag	-1.998977000	-1.710841000	0.162918000
N	-0.942183000	2.481738000	-3.046165000
C	-1.529718000	1.572144000	-2.210645000
Ag	-1.188239000	1.372918000	-0.107583000
N	-2.591896000	1.070689000	-2.911346000
C	-1.620066000	2.569818000	-4.275592000
N	-4.005547000	0.338976000	-1.090364000
C	-1.410448000	3.349008000	-5.425559000
H	-0.575943000	4.058770000	-5.521262000
N	-3.986130000	0.523437000	1.085428000
C	-2.320538000	3.179864000	-6.477302000
H	-2.194958000	3.771898000	-7.395863000
C	-1.493045000	1.924157000	1.937894000
C	-3.287444000	3.313907000	5.970619000
H	-3.960606000	3.356689000	6.839554000
C	-2.214555000	4.232835000	5.883019000
H	-2.074704000	4.971988000	6.685592000
C	-1.322675000	4.220382000	4.802528000
H	-0.488134000	4.935402000	4.762276000
C	-1.550039000	3.257629000	3.805040000
C	0.295560000	3.686758000	2.126604000
H	1.198061000	3.050523000	2.220911000
H	0.428870000	4.577120000	2.767933000
C	0.665205000	3.333528000	-0.290518000
C	-0.670582000	5.107055000	0.279328000
C	-1.405632000	6.100731000	0.942489000
H	-1.403790000	6.204748000	2.036859000
C	-2.146616000	6.974108000	0.134523000
H	-2.728804000	7.778628000	0.607576000
C	-2.158698000	6.854099000	-1.276258000
H	-2.750009000	7.567983000	-1.868449000
C	-1.430276000	5.855690000	-1.937493000
H	-1.447123000	5.773311000	-3.033578000
C	-0.682623000	4.987360000	-1.128567000
C	0.253158000	3.274373000	-2.726038000
H	0.373249000	4.043830000	-3.510477000
H	1.155060000	2.630474000	-2.728177000
C	-5.739778000	2.168192000	-1.584417000
H	-5.759566000	2.084284000	-2.680340000
C	-6.552647000	3.093601000	-0.915461000
H	-7.223846000	3.739416000	-1.500601000
N	-2.542020000	1.549741000	2.731615000
C	-3.394021000	2.261633000	-6.389586000
H	-4.081896000	2.157830000	-7.241689000
N	-0.892964000	2.961655000	2.596918000
C	-3.598586000	1.477382000	-5.246738000
H	-4.431687000	0.760700000	-5.206124000
C	-2.692063000	1.652873000	-4.187991000
N	0.178928000	4.088907000	0.745222000
C	-3.521568000	0.044891000	-2.418045000
H	-3.023630000	-0.944716000	-2.388105000
H	-4.370655000	-0.014325000	-3.123279000
N	0.160172000	3.903847000	-1.430471000
C	-3.411724000	-0.155806000	0.042148000
C	-4.919125000	1.361675000	-0.782189000
C	-6.539644000	3.213354000	0.495337000
H	-7.200967000	3.949626000	0.975466000
C	-3.478306000	0.456520000	2.434891000
H	-4.314650000	0.517835000	3.155008000
H	-2.979179000	-0.524599000	2.563012000
C	-4.906276000	1.481183000	0.625713000
C	-5.713247000	2.412517000	1.295573000
H	-5.712704000	2.514388000	2.390147000
C	-3.509613000	2.347343000	4.980978000
H	-4.341703000	1.634731000	5.076673000
C	-2.621539000	2.340089000	3.892522000

$[L_2(C_2H_5)_8 \rightarrow Au_4]^{4+}$

Au	0.089190000	0.076891000	-2.829569000
N	-2.343912000	-2.760432000	0.966543000

C	-2.176408000	-1.939176000	-0.113278000
Au	-1.948099000	0.094718000	-0.107389000
N	-2.326510000	-2.757610000	-1.197868000
C	-2.536169000	-4.096118000	0.572283000
N	-2.797849000	-0.992864000	-2.834201000
N	-2.809389000	1.179817000	-2.831442000
C	-2.212388000	2.124272000	-0.103047000
C	-2.649244000	4.263524000	0.592981000
C	-2.329132000	2.512422000	2.398944000
H	-1.277749000	2.556899000	2.747918000
H	-2.928919000	3.224827000	2.991804000
C	-1.957693000	0.085660000	2.623178000
C	-4.150830000	0.761334000	2.569407000
C	-4.142187000	-0.619310000	2.563746000
C	-2.299573000	-2.345694000	2.388886000
H	-2.904769000	-3.067571000	2.964439000
H	-1.255396000	-2.384444000	2.759291000
N	-2.388360000	2.942537000	-1.183783000
N	-2.407361000	2.933949000	0.980778000
C	-2.524494000	-4.094283000	-0.810509000
N	-2.803959000	1.164883000	2.627955000
C	-2.299579000	-2.332429000	-2.618160000
H	-1.259757000	-2.365581000	-3.000940000
H	-2.908879000	-3.052702000	-3.191616000
N	-2.790614000	-1.005560000	2.620084000
C	-1.965127000	0.098680000	-2.818641000
C	-4.150204000	-0.605030000	-2.822598000
C	-2.324551000	2.523634000	-2.603785000
H	-2.924280000	3.241603000	-3.190038000
H	-1.276069000	2.562341000	-2.961852000
C	-4.157570000	0.776831000	-2.821423000
C	-2.636116000	4.269048000	-0.790080000
Au	0.096096000	0.060157000	2.630898000
N	2.812832000	2.768248000	-1.181497000
C	2.497103000	1.988241000	-0.102755000
Au	2.047824000	-0.017461000	-0.114705000
N	2.839224000	2.748595000	0.981424000
C	3.341345000	4.010372000	-0.786187000
N	3.068633000	0.967438000	2.634386000
N	2.903881000	-1.192479000	2.614830000
C	2.184720000	-2.067294000	-0.129471000
C	2.563248000	-4.219017000	-0.832200000
C	2.314700000	-2.460543000	-2.632874000
H	1.269847000	-2.416317000	-2.999412000
H	2.857787000	-3.225529000	-3.215265000
C	2.143358000	-0.020204000	-2.835845000
C	4.278409000	-0.864664000	-2.848577000
C	4.375042000	0.514445000	-2.842755000
C	2.657937000	2.369952000	-2.595208000
H	3.264155000	3.061343000	-3.205935000
H	1.597363000	2.465734000	-2.901545000
N	2.351825000	-2.894617000	0.947299000
N	2.334598000	-2.885414000	-1.215994000
C	3.359547000	3.997468000	0.595708000
N	2.903887000	-1.161320000	-2.855926000
C	2.687919000	2.341939000	2.393370000
H	1.631049000	2.452665000	2.707592000
H	3.310469000	3.018692000	3.003848000
N	3.055849000	1.002088000	-2.847094000
C	2.149127000	-0.047792000	2.625386000
C	4.384505000	0.472995000	2.574487000
C	2.314605000	-2.487817000	2.368219000
H	2.848887000	-3.260491000	2.948162000
H	1.265022000	-2.444965000	2.721234000
C	4.279308000	-0.904185000	2.560613000
C	2.575051000	-4.224802000	0.548978000
C	2.675038000	-5.362681000	-1.792244000
H	3.421058000	-5.131036000	-2.584081000
H	3.109768000	-6.221372000	-1.243919000
C	1.334727000	-5.780956000	-2.423806000
H	0.885671000	-4.968525000	-3.032771000
H	0.601913000	-6.063987000	-1.641524000
H	1.475407000	-6.652737000	-3.091472000
C	2.698181000	-5.376919000	1.497918000
H	3.138993000	-6.226867000	0.940821000
H	3.443262000	-5.146282000	2.291040000
C	1.362063000	-5.812376000	2.127196000
H	0.630371000	-6.093528000	1.343162000
H	0.907280000	-5.009560000	2.744597000
H	1.510665000	-6.689742000	2.785799000
C	5.336522000	-1.962796000	2.586219000
H	5.085715000	-2.752863000	1.844738000
H	6.278017000	-1.508956000	2.217053000
C	5.571879000	-2.580034000	3.977778000
H	4.662140000	-3.068620000	4.383811000
H	5.883202000	-1.807901000	4.708125000
H	6.371022000	-3.344745000	3.931551000
C	5.591837000	1.355774000	2.620645000
H	6.454975000	0.766963000	2.250627000
H	5.471825000	2.184304000	1.888765000
C	5.908542000	1.912567000	4.021501000
H	6.092593000	1.093279000	4.743595000
H	5.081751000	2.530312000	4.428815000
H	6.815882000	2.546046000	3.989347000
C	3.770147000	5.071706000	1.555494000
H	4.441954000	4.649573000	2.335632000
H	4.404963000	5.790626000	1.000937000
C	2.594162000	5.821259000	2.207016000
H	1.953340000	5.150921000	2.816735000
H	1.953605000	6.296248000	1.437564000
H	2.968176000	6.619222000	2.877008000
C	3.726069000	5.102893000	-1.735360000
H	4.361587000	5.820283000	-1.179727000
H	4.390526000	4.700367000	-2.531701000
C	2.531715000	5.848593000	-2.357127000
H	1.898570000	6.305283000	-1.570622000
H	1.888280000	5.179943000	-2.966052000
H	2.886158000	6.659956000	-3.021618000
C	5.597922000	1.379265000	-2.828184000
H	6.377927000	0.866050000	-3.427210000
H	5.395972000	2.322615000	-3.377817000
C	6.157466000	1.687133000	-1.425982000
H	6.396631000	0.753295000	-0.880104000
H	5.440773000	2.264002000	-0.808646000
H	7.088932000	2.279830000	-1.508529000
C	5.366057000	-1.893909000	-2.854891000

H	5.066039000	-2.750057000	-3.496242000
H	6.240349000	-1.447764000	-3.371064000
C	5.802245000	-2.396157000	-1.465045000
H	4.988265000	-2.932083000	-0.937932000
H	6.122720000	-1.553621000	-0.821006000
H	6.656457000	-3.093495000	-1.563445000
C	-5.305785000	-1.556462000	-2.813246000
H	-6.153747000	-1.054090000	-3.321075000
H	-5.073283000	-2.432718000	-3.455090000
C	-5.756856000	-2.021480000	-1.415647000
H	-6.027207000	-1.156143000	-0.778839000
H	-4.967256000	-2.593578000	-0.889663000
H	-6.646874000	-2.674491000	-1.500520000
C	-5.324351000	1.714466000	-2.809522000
H	-5.091546000	2.607254000	-3.427459000
H	-6.158752000	1.214628000	-3.341928000
C	-5.801655000	2.142748000	-1.408939000
H	-5.024267000	2.706803000	-0.856899000
H	-6.077066000	1.260669000	-0.797765000
H	-6.694566000	2.791887000	-1.492993000
C	-2.856839000	5.415454000	-1.732622000
H	-2.547219000	6.338635000	-1.201882000
H	-2.159476000	5.336533000	-2.594205000
C	-4.304656000	5.588265000	-2.228284000
H	-5.006327000	5.707968000	-1.379762000
H	-4.653606000	4.725160000	-2.830084000
H	-4.386962000	6.488864000	-2.866530000
C	-2.887867000	5.402846000	1.539482000
H	-2.183788000	5.338015000	2.396945000
H	-2.601896000	6.332525000	1.007159000
C	-4.336150000	5.544104000	2.044760000
H	-4.655931000	4.686591000	2.669985000
H	-5.047363000	5.628574000	1.199724000
H	-4.437983000	6.455294000	2.665032000
C	-5.298819000	1.719065000	2.606171000
H	-5.112257000	2.545823000	1.887119000
H	-6.191545000	1.191439000	2.214745000
C	-5.603478000	2.278628000	4.008397000
H	-4.740421000	2.823567000	4.443096000
H	-5.866444000	1.466053000	4.713421000
H	-6.457912000	2.981418000	3.967265000
C	-5.276536000	-1.593702000	2.591406000
H	-6.176840000	-1.075139000	2.205316000
H	-5.078232000	-2.410445000	1.863757000
C	-5.573411000	-2.171725000	3.987808000
H	-5.847889000	-1.370091000	4.700915000
H	-4.702796000	-2.708567000	4.417703000
H	-6.417817000	-2.886095000	3.939508000
C	-2.738367000	-5.244728000	1.516061000
H	-2.423038000	-6.164422000	0.982555000
H	-2.036595000	-5.158117000	2.373698000
C	-4.182116000	-5.431388000	2.019858000
H	-4.887639000	-5.546248000	1.173725000
H	-4.532948000	-4.579401000	2.636307000
H	-4.255350000	-6.340192000	2.647641000
C	-2.712150000	-5.239982000	-1.761085000
H	-2.019544000	-5.132141000	-2.623474000
H	-2.373328000	-6.157856000	-1.238612000
C	-4.155800000	-5.451780000	-2.254140000
H	-4.534751000	-4.591418000	-2.841790000
H	-4.849519000	-5.604803000	-1.404493000
H	-4.213175000	-6.345424000	-2.904810000

$[L_2(CH_3)_8 \rightarrow Au_4]^{4+}$

Au	-0.000612000	-0.000136000	-2.697422000
N	2.643284000	2.809488000	1.080930000
C	2.335057000	2.029650000	-0.000223000
Au	1.988766000	0.000110000	-0.000036000
N	2.642752000	2.809334000	-1.081665000
C	3.130635000	4.070202000	0.690290000
N	2.899433000	1.082538000	-2.785188000
N	2.899564000	-1.082508000	-2.785126000
C	2.335035000	-2.029456000	-0.000141000
C	3.131037000	-4.069765000	0.690664000
C	2.448147000	-2.424154000	2.494892000
H	1.371473000	-2.475216000	2.752325000
H	2.994676000	-3.151626000	3.120010000
C	2.061022000	0.000271000	2.725199000
C	4.249757000	-0.689784000	2.846037000
C	4.249838000	0.690112000	2.845954000
C	2.448430000	2.424657000	2.494809000
H	2.995383000	3.152054000	3.119643000
H	1.371866000	2.476048000	2.752644000
N	2.642993000	-2.809212000	-1.081454000
N	2.643395000	-2.809128000	1.081120000
C	3.130271000	4.070142000	-0.691419000
N	2.900683000	-1.082296000	2.784462000
C	2.447019000	2.424375000	-2.495371000
H	1.370276000	2.475537000	-2.752511000
H	2.993416000	3.151838000	-3.120618000
N	2.900782000	1.082753000	2.784389000
C	2.059797000	-0.000046000	-2.725786000
C	4.248488000	0.690051000	-2.847250000
C	2.447281000	-2.424385000	-2.495218000
H	2.993717000	-3.151865000	-3.120406000
H	1.370538000	-2.475628000	-2.752331000
C	4.248595000	-0.689848000	-2.847202000
C	3.130771000	-4.069817000	-0.691070000
Au	0.000614000	0.000404000	2.697478000
N	-2.642956000	-2.809528000	-1.080914000
C	-2.334814000	-2.029647000	0.000232000
Au	-1.988766000	-0.000064000	0.000015000
N	-2.642453000	-2.809337000	1.081684000
C	-3.130206000	-4.070276000	-0.690260000
N	-2.899312000	-1.082560000	2.785199000
N	-2.899682000	1.082486000	2.785113000
C	-2.335266000	2.029462000	0.000106000
C	-3.131487000	4.069679000	-0.690717000
C	-2.448424000	2.424127000	-2.494932000
H	-1.371756000	2.475321000	-2.752364000
H	-2.995042000	3.151529000	-3.120053000
C	-2.061016000	-0.000256000	-2.725190000
C	-4.249829000	0.689542000	-2.846078000
C	-4.249748000	-0.690353000	-2.845974000
C	-2.448139000	-2.424686000	-2.494794000
H	-2.994991000	-3.152157000	-3.119629000

H	-1.371565000	-2.475948000	-2.752613000
N	-2.643300000	2.809196000	1.081413000
N	-2.643717000	2.809088000	-1.081161000
C	-3.129846000	-4.070205000	0.691447000
N	-2.900800000	1.082213000	-2.784488000
C	-2.446762000	-2.424350000	2.495386000
H	-1.370016000	-2.475409000	2.752535000
H	-2.993090000	-3.151865000	3.120635000
N	-2.900646000	-1.082837000	-2.784387000
C	-2.059796000	0.000119000	2.725792000
C	-4.248412000	-0.690219000	2.847261000
C	-2.447542000	2.424407000	2.495183000
H	-2.994055000	3.151839000	3.120360000
H	-1.370805000	2.475769000	2.752294000
C	-4.248672000	0.689679000	2.847197000
C	-3.131217000	4.069744000	0.691017000
C	3.547701000	-5.133131000	1.650195000
H	3.890698000	-6.029002000	1.101637000
H	4.393402000	-4.812196000	2.294365000
H	2.717914000	-5.457108000	2.311913000
C	3.547003000	-5.133282000	-1.650673000
H	4.392597000	-4.812526000	-2.295069000
H	3.889988000	-6.029189000	-1.102170000
H	2.716984000	-5.457130000	-2.312170000
C	-3.546753000	-5.133856000	-1.649621000
H	-2.717264000	-5.457091000	-2.312069000
H	-3.888560000	-6.030087000	-1.100900000
H	-4.393257000	-4.813491000	-2.293018000
C	-3.545771000	-5.133664000	1.651194000
H	-3.888012000	-6.029942000	1.102809000
H	-2.715818000	-5.456801000	2.313080000
H	-4.391844000	-4.813246000	2.295138000
C	-3.548283000	5.132986000	-1.650257000
H	-3.891357000	6.028831000	-1.101705000
H	-2.718548000	5.457038000	-2.312004000
H	-4.393969000	4.811950000	-2.294395000
C	-3.547546000	5.133178000	1.650612000
H	-4.393091000	4.812345000	2.295033000
H	-2.717546000	5.457121000	2.312086000
H	-3.890638000	6.029041000	1.102104000
C	3.546306000	5.133572000	-1.651152000
H	3.888626000	6.029810000	-1.102753000
H	4.392350000	4.813068000	-2.295091000
H	2.716396000	5.456809000	-2.313047000
C	3.547280000	5.133731000	1.649663000
H	2.717826000	5.457033000	2.312119000
H	4.393761000	4.813281000	2.293050000
H	3.889166000	6.029940000	1.100953000
C	5.368821000	1.666978000	-2.936795000
H	5.416204000	2.326814000	-2.045537000
H	6.337542000	1.140174000	-3.007947000
H	5.283124000	2.308747000	-3.838845000
C	5.369044000	-1.666644000	-2.936698000
H	6.337659000	-1.139742000	-3.008568000
H	5.416910000	-2.325953000	-2.045086000
H	5.283071000	-2.308931000	-3.838360000
C	-5.370341000	1.666303000	-2.935281000
H	-6.339004000	1.139361000	-3.006201000
H	-5.417586000	2.326077000	-2.043974000
H	-5.284987000	2.308124000	-3.837327000
C	-5.370095000	-1.667299000	-2.935057000
H	-5.284434000	-2.309494000	-3.836817000
H	-5.417484000	-2.326696000	-2.043482000
H	-6.338810000	-1.140518000	-3.006448000
C	5.370154000	-1.666678000	2.935224000
H	6.338882000	-1.139852000	3.006112000
H	5.284739000	-2.308479000	3.837279000
H	5.417303000	-2.326471000	2.043926000
C	5.370299000	1.666928000	2.935018000
H	5.284741000	2.309123000	3.836788000
H	6.338955000	1.140034000	3.006375000
H	5.417735000	2.326331000	2.043449000
C	-5.369227000	1.666354000	2.936694000
H	-6.337785000	1.139346000	3.008540000
H	-5.283332000	2.308635000	3.838367000
H	-5.417155000	2.325671000	2.045092000
C	-5.368639000	-1.667268000	2.936799000
H	-5.415929000	-2.327120000	2.045549000
H	-5.282890000	-2.309016000	3.838860000
H	-6.337420000	-1.140573000	3.007931000

$[L_2(H)_8 \rightarrow Au_4]^{4+}$

Au	0.000633000	-2.698464000	0.000011000
N	2.664337000	1.083568000	-2.796314000
C	2.332037000	0.000391000	-2.024428000
Au	1.967952000	0.000293000	0.000009000
N	2.664857000	-1.082605000	-2.796328000
C	3.184700000	0.685073000	-4.025396000
N	2.904830000	-2.803614000	-1.085099000
N	2.904816000	-2.803605000	1.085105000
C	2.331781000	0.000376000	2.024480000
C	3.184410000	0.685024000	4.025483000
C	2.469528000	2.506372000	2.434310000
H	1.396169000	2.768553000	2.510871000
H	3.038632000	3.117717000	3.159367000
C	2.062382000	2.734243000	0.000032000
C	4.236593000	2.893248000	0.683540000
C	4.236598000	2.893240000	-0.683476000
C	2.469531000	2.506366000	-2.434234000
H	3.038476000	3.117839000	-3.159310000
H	1.396108000	2.768309000	-2.510734000
N	2.664618000	-1.082641000	2.796375000
N	2.664100000	1.083537000	2.796380000
C	3.184997000	-0.683843000	-4.025424000
N	2.903493000	2.804633000	1.085136000
C	2.470749000	-2.505503000	-2.434278000
H	1.397456000	-2.767969000	-2.510779000
H	3.040004000	-3.116694000	-3.159347000
N	2.903481000	2.804674000	-1.085066000
C	2.063688000	-2.733501000	0.000000000
C	4.237961000	-2.891655000	-0.683498000
C	2.470697000	-2.505557000	2.434274000
H	3.040027000	-3.116669000	3.159353000
H	1.397446000	-2.768192000	2.510792000
C	4.237964000	-2.891641000	0.683522000
C	3.184669000	-0.683889000	4.025503000

Au	-0.000665000	2.698461000	0.000011000
N	-2.664168000	-1.083545000	2.796317000
C	-2.331801000	-0.000366000	2.024447000
Au	-1.967899000	-0.000260000	-0.000020000
N	-2.664698000	1.082631000	2.796325000
C	-3.184513000	-0.685041000	4.025403000
N	-2.904882000	2.803590000	1.085064000
N	-2.904814000	2.803600000	-1.085137000
C	-2.331857000	-0.000386000	-2.024482000
C	-3.184588000	-0.685054000	-4.025430000
C	-2.469515000	-2.506376000	-2.434290000
H	-1.396124000	-2.768443000	-2.510808000
H	-3.038527000	-3.117777000	-3.159372000
C	-2.062410000	-2.734298000	-0.000007000
C	-4.236605000	-2.893325000	-0.683566000
C	-4.236641000	-2.893303000	0.683451000
C	-2.469590000	-2.506381000	2.434241000
H	-3.038675000	-3.117724000	3.159315000
H	-1.396228000	-2.768549000	2.510802000
N	-2.664709000	1.082619000	-2.796375000
N	-2.664197000	-1.083555000	-2.796355000
C	-3.184895000	0.683871000	4.025393000
N	-2.903492000	-2.804693000	-1.085131000
C	-2.470819000	2.505558000	2.434255000
H	-1.397588000	2.768257000	2.510843000
H	-3.040231000	3.116635000	3.159296000
N	-2.903542000	-2.804674000	1.085072000
C	-2.063720000	2.733497000	-0.000015000
C	-4.238011000	2.891612000	0.683433000
C	-2.470685000	2.505521000	-2.434296000
H	-3.039936000	3.116684000	-3.159392000
H	-1.397405000	2.768048000	-2.510774000
C	-4.237979000	2.891597000	-0.683584000
C	-3.184858000	0.683859000	-4.025461000
H	3.517735000	1.392339000	4.794388000
H	3.518253000	-1.391067000	4.794423000
H	-3.517790000	-1.392377000	4.794311000
H	-3.518584000	1.391025000	4.794290000
H	-3.517912000	-1.392379000	-4.794328000
H	-3.518465000	1.391028000	-4.794379000
H	3.518611000	-1.391001000	-4.794349000
H	3.518014000	1.392421000	-4.794277000
H	5.068100000	-2.979056000	-1.394027000
H	5.068125000	-2.979063000	1.394023000
H	-5.066703000	-2.981084000	-1.394099000
H	-5.066777000	-2.981057000	1.393940000
H	5.066704000	2.980995000	1.394061000
H	5.066726000	2.980999000	-1.393973000
H	-5.068125000	2.979005000	-1.394104000
H	-5.068179000	2.979019000	1.393929000

$[L_2(F)_8 \rightarrow Au_4]^{4+}$

Au	2.073820000	1.776228000	-0.171457000
N	0.944710000	-2.489034000	2.997325000
C	1.524313000	-1.572509000	2.153847000
Au	1.263458000	-1.461683000	0.114233000
N	2.591044000	-1.075943000	2.862956000
C	1.639025000	-2.567413000	4.205935000
N	4.036474000	-0.274457000	1.080969000
N	4.019470000	-0.460624000	-1.087057000
C	1.489854000	-1.915653000	-1.881664000
C	1.566941000	-3.241617000	-3.739051000
C	-0.303720000	-3.723631000	-2.132035000
H	-1.214784000	-3.111017000	-2.273583000
H	-0.366572000	-4.619270000	-2.779455000
C	-0.747036000	-3.350390000	0.292776000
C	0.598235000	-5.115905000	-0.259012000
C	0.610681000	-5.000615000	1.107926000
C	-0.258696000	-3.312741000	2.737400000
H	-0.306739000	-4.087249000	3.526748000
H	-1.168684000	-2.684907000	2.791763000
N	2.543887000	-1.549010000	-2.682893000
N	0.894639000	-2.958909000	-2.548636000
C	2.679191000	-1.674555000	4.121069000
N	-0.246990000	-4.112505000	-0.739384000
C	3.555023000	-0.039947000	2.425283000
H	3.075451000	0.957587000	2.442085000
H	4.397952000	-0.047583000	3.142698000
N	-0.226943000	-3.929510000	1.428840000
C	3.438195000	0.234543000	-0.050174000
C	4.937610000	-1.291999000	0.757650000
C	3.516441000	-0.457344000	-2.443750000
H	4.347552000	-0.590899000	-3.162546000
H	3.038450000	0.524888000	-2.623027000
C	4.926753000	-1.409503000	-0.609123000
C	2.608910000	-2.350875000	-3.823856000
Au	-2.073820000	-1.776228000	0.171457000
N	-0.944710000	2.489034000	-2.997325000
C	-1.524313000	1.572509000	-2.153847000
Au	-1.263458000	1.461683000	-0.114233000
N	-2.591044000	1.075943000	-2.862956000
C	-1.639025000	2.567413000	-4.205935000
N	-4.036474000	0.274457000	-1.080969000
N	-4.019470000	0.460624000	1.087057000
C	-1.489854000	1.915653000	1.881664000
C	-1.566941000	3.241617000	3.739051000
C	0.303720000	3.723631000	2.132035000
H	1.214784000	3.111017000	2.273583000
H	0.366572000	4.619270000	2.779455000
C	0.747036000	3.350390000	-0.292776000
C	-0.598235000	5.115905000	0.259012000
C	-0.610681000	5.000615000	-1.107926000
C	0.258696000	3.312741000	-2.737400000
H	0.306739000	4.087249000	-3.526748000
H	1.168684000	2.684907000	-2.791763000
N	-2.543887000	1.549010000	2.682893000
N	-0.894639000	2.958909000	2.548636000
C	-2.679191000	1.674555000	-4.121069000
N	0.246990000	4.112505000	0.739384000
C	-3.555023000	0.039947000	-2.425283000
H	-3.075451000	-0.957587000	-2.442085000
H	-4.397952000	0.047583000	-3.142698000
N	0.226943000	3.929510000	-1.428840000
C	-3.438195000	-0.234543000	0.050174000
C	-4.937610000	1.291999000	-0.757650000
C	-3.516441000	0.457344000	2.443750000

H	-4.347552000	0.590899000	3.162546000
H	-3.038450000	-0.524888000	2.623027000
C	-4.926753000	1.409503000	0.609123000
C	-2.608910000	2.350875000	3.823856000
F	1.175769000	-4.197017000	-4.536175000
F	3.533530000	-2.181462000	-4.728065000
F	-1.265327000	3.375558000	-5.158980000
F	-3.619118000	1.355096000	-4.966946000
F	-1.175769000	4.197017000	4.536175000
F	-3.533530000	2.181462000	4.728065000
F	3.619118000	-1.355096000	4.966946000
F	1.265327000	-3.375558000	5.158980000
F	5.606401000	-1.917511000	1.686416000
F	5.581929000	-2.184987000	-1.427932000
F	-1.187210000	5.946060000	1.074526000
F	-1.215731000	5.683197000	-2.040224000
F	1.187210000	-5.946060000	-1.074526000
F	1.215731000	-5.683197000	2.040224000
F	-5.581929000	2.184987000	1.427932000
F	-5.606401000	1.917511000	-1.686416000

$[L_2(Cl)_8 \rightarrow Au_4]^{4+}$

Au	2.071252000	1.774217000	-0.171434000
N	0.920461000	-2.460236000	3.014871000
C	1.525395000	-1.572828000	2.161419000
Au	1.278729000	-1.479527000	0.114776000
N	2.568124000	-1.045851000	2.880277000
C	1.575570000	-2.494886000	4.254399000
N	4.012417000	-0.287195000	1.080889000
N	3.994344000	-0.472640000	-1.087095000
C	1.489493000	-1.916289000	-1.891077000
C	1.499769000	-3.175656000	-3.800838000
C	-0.322979000	-3.686969000	-2.127154000
H	-1.231598000	-3.063934000	-2.236497000
H	-0.411128000	-4.575552000	-2.780864000
C	-0.738861000	-3.341067000	0.291228000
C	0.637841000	-5.083407000	-0.268477000
C	0.651125000	-4.967693000	1.107513000
C	-0.276630000	-3.278920000	2.724921000
H	-0.349790000	-4.045683000	3.519524000
H	-1.184636000	-2.645951000	2.746315000
N	2.518702000	-1.520685000	-2.707138000
N	0.868166000	-2.931828000	-2.572644000
C	2.622047000	-1.596535000	4.168934000
N	-0.231353000	-4.090117000	-0.742549000
C	3.523638000	-0.017845000	2.413824000
H	3.036233000	0.976112000	2.399171000
H	4.363396000	0.000266000	3.134358000
N	-0.210456000	-3.907776000	1.425634000
C	3.427575000	0.228201000	-0.050349000
C	4.898903000	-1.326579000	0.763405000
C	3.483233000	-0.432067000	-2.438011000
H	4.310588000	-0.540047000	-3.164986000
H	2.997421000	0.551974000	-2.584397000
C	4.887251000	-1.444425000	-0.612419000
C	2.548075000	-2.279435000	-3.886231000
Au	-2.071252000	-1.774217000	0.171434000
N	-0.920461000	2.460236000	-3.014871000
C	-1.525395000	1.572828000	-2.161419000
Au	-1.278729000	1.479527000	-0.114776000
N	-2.568124000	1.045851000	-2.880277000
C	-1.575570000	2.494886000	-4.254399000
N	-4.012417000	0.287195000	-1.080889000
N	-3.994344000	0.472640000	1.087095000
C	-1.489493000	1.916289000	1.891077000
C	-1.499769000	3.175656000	3.800838000
C	0.322979000	3.686969000	2.127154000
H	1.231598000	3.063934000	2.236497000
H	0.411128000	4.575552000	2.780864000
C	0.738861000	3.341067000	-0.291228000
C	-0.637841000	5.083407000	0.268477000
C	-0.651125000	4.967693000	-1.107513000
C	0.276630000	3.278920000	-2.724921000
H	0.349790000	4.045683000	-3.519524000
H	1.184636000	2.645951000	-2.746315000
N	-2.518702000	1.520685000	2.707138000
N	-0.868166000	2.931828000	2.572644000
C	-2.622047000	1.596535000	-4.168934000
N	0.231353000	4.090117000	0.742549000
C	-3.523638000	0.017845000	-2.413824000
H	-3.036233000	-0.976112000	-2.399171000
H	-4.363396000	-0.000266000	-3.134358000
N	0.210456000	3.907776000	-1.425634000
C	-3.427575000	-0.228201000	0.050349000
C	-4.898903000	1.326579000	-0.763405000
C	-3.483233000	0.432067000	2.438011000
H	-4.310588000	0.540047000	3.164986000
H	-2.997421000	-0.551974000	2.584397000
C	-4.887251000	1.444425000	0.612419000
C	-2.548075000	2.279435000	3.886231000
Cl	1.015143000	-4.353985000	-4.914858000
Cl	3.676532000	-2.078765000	-5.131515000
Cl	-1.115754000	3.470467000	-5.558759000
Cl	-3.772273000	1.189571000	-5.341864000
Cl	-1.015143000	4.353985000	4.914858000
Cl	-3.676532000	2.078765000	5.131515000
Cl	3.772273000	-1.189571000	5.341864000
Cl	1.115754000	-3.470467000	5.558759000
Cl	5.774095000	-2.188948000	1.923971000
Cl	5.744271000	-2.492687000	-1.623986000
Cl	-1.446254000	6.170669000	1.278928000
Cl	-1.480788000	5.872183000	-2.269447000
Cl	1.446254000	-6.170669000	-1.278928000
Cl	1.480788000	-5.872183000	2.269447000
Cl	-5.744271000	2.492687000	1.623986000
Cl	-5.774095000	2.188948000	-1.923971000

$[L_2(Br)_8 \rightarrow Au_4]^{4+}$

Au	2.070400000	1.773106000	-0.169813000
N	0.900588000	-2.436509000	3.027409000
C	1.520155000	-1.566128000	2.167285000
Au	1.283273000	-1.483473000	0.118155000
N	2.549139000	-1.022808000	2.893313000
C	1.528055000	-2.438819000	4.281732000
N	4.001539000	-0.292562000	1.087006000
N	3.985637000	-0.479596000	-1.081698000
C	1.489438000	-1.914610000	-1.890307000
C	1.462750000	-3.133073000	-3.826094000
C	-0.327928000	-3.674477000	-2.121666000

H	-1.238239000	-3.051335000	-2.218132000
H	-0.424201000	-4.561091000	-2.777303000
C	-0.735342000	-3.336037000	0.293226000
C	0.655617000	-5.067319000	-0.263539000
C	0.666468000	-4.949820000	1.113546000
C	-0.289180000	-3.260171000	2.723624000
H	-0.373409000	-4.022387000	3.521840000
H	-1.198799000	-2.628714000	2.727703000
N	2.506259000	-1.504880000	-2.714492000
N	0.856086000	-2.916696000	-2.580171000
C	2.575395000	-1.540193000	4.196636000
N	-0.221519000	-4.081633000	-0.739532000
C	3.508571000	-0.004820000	2.414260000
H	3.022754000	0.989826000	2.383315000
H	4.345916000	0.023132000	3.137668000
N	-0.204301000	-3.896314000	1.429266000
C	3.423134000	0.225574000	-0.045970000
C	4.880037000	-1.339849000	0.772051000
C	3.472893000	-0.422328000	-2.431175000
H	4.299376000	-0.520833000	-3.160848000
H	2.987782000	0.564284000	-2.563856000
C	4.869882000	-1.458629000	-0.604928000
C	2.511553000	-2.236141000	-3.911288000
Au	-2.070400000	-1.773106000	0.169813000
N	-0.900588000	2.436509000	-3.027409000
C	-1.520155000	1.566128000	-2.167285000
Au	-1.283273000	1.483473000	-0.118155000
N	-2.549139000	1.022808000	-2.893313000
C	-1.528055000	2.438819000	-4.281732000
N	-4.001539000	0.292562000	-1.087006000
N	-3.985637000	0.479596000	1.081698000
C	-1.489438000	1.914610000	1.890307000
C	-1.462750000	3.133073000	3.826094000
C	0.327928000	3.674477000	2.121666000
H	1.238239000	3.051335000	2.218132000
H	0.424201000	4.561091000	2.777303000
C	0.735342000	3.336037000	-0.293226000
C	-0.655617000	5.067319000	0.263539000
C	-0.666468000	4.949820000	-1.113546000
C	0.289180000	3.260171000	-2.723624000
H	0.373409000	4.022387000	-3.521840000
H	1.198799000	2.628714000	-2.727703000
N	-2.506259000	1.504880000	2.714492000
N	-0.856086000	2.916696000	2.580171000
C	-2.575395000	1.540193000	-4.196636000
N	0.221519000	4.081633000	0.739532000
C	-3.508571000	0.004820000	-2.414260000
H	-3.022754000	-0.989826000	-2.383315000
H	-4.345916000	-0.023132000	-3.137668000
N	0.204301000	3.896314000	-1.429266000
C	-3.423134000	-0.225574000	0.045970000
C	-4.880037000	1.339849000	-0.772051000
C	-3.472893000	0.422328000	2.431175000
H	-4.299376000	0.520833000	3.160848000
H	-2.987782000	-0.564284000	2.563856000
C	-4.869882000	1.458629000	0.604928000
C	-2.511553000	2.236141000	3.911288000
Br	0.922193000	-4.392630000	-5.071952000
Br	3.716150000	-2.003301000	-5.299069000
Br	-1.012485000	3.470452000	-5.731471000
Br	-3.801666000	1.075578000	-5.505208000
Br	-0.922193000	4.392630000	5.071952000
Br	-3.716150000	2.003301000	5.299069000
Br	3.801666000	-1.075578000	5.505208000
Br	1.012485000	-3.470452000	5.731471000
Br	5.844720000	-2.288969000	2.030559000
Br	5.817068000	-2.610370000	-1.696696000
Br	-1.546575000	6.265954000	1.352112000
Br	-1.574893000	5.948703000	-2.375452000
Br	1.546575000	-6.265954000	-1.352112000
Br	1.574893000	-5.948703000	2.375452000
Br	-5.817068000	2.610370000	1.696696000
Br	-5.844720000	2.288969000	-2.030559000

$[L_2(SiH_3)_8 \rightarrow Au_4]^{4+}$

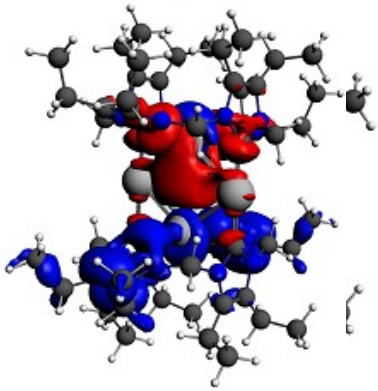
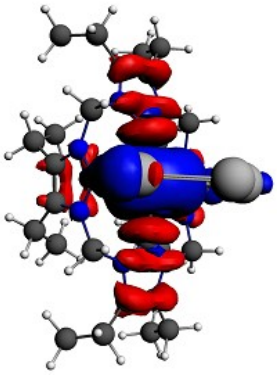
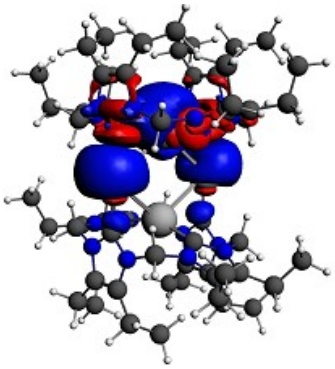
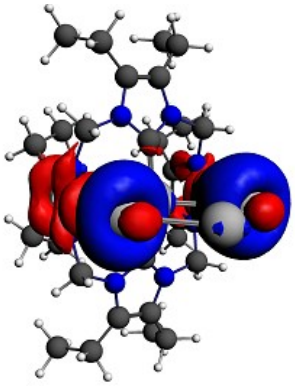
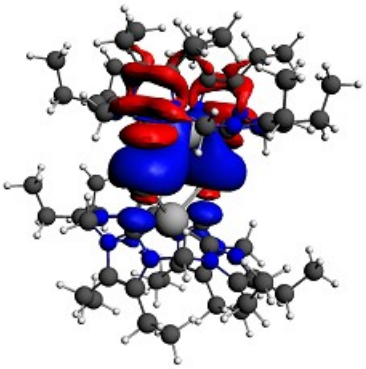
Au	2.050000000	1.805043000	-0.131964000
N	0.864507000	-2.387095000	3.042671000
C	1.514275000	-1.558028000	2.167504000
Au	1.299796000	-1.497312000	0.120650000
N	2.505957000	-0.985492000	2.912816000
C	1.419034000	-2.321645000	4.336441000
N	3.980977000	-0.290765000	1.090865000
N	3.947120000	-0.444790000	-1.070225000
C	1.493653000	-1.897720000	-1.889517000
C	1.400956000	-3.016519000	-3.892139000
C	-0.278290000	-3.693539000	-2.125815000
H	-1.222457000	-3.122431000	-2.230254000
H	-0.338544000	-4.591511000	-2.770615000
C	-0.700331000	-3.353974000	0.273988000
C	0.744500000	-5.060306000	-0.254415000
C	0.739065000	-4.931283000	1.127758000
C	-0.303923000	-3.225855000	2.697038000
H	-0.431830000	-3.968215000	3.503553000
H	-1.216276000	-2.599179000	2.647853000
N	2.462112000	-1.430107000	-2.736932000
N	0.861158000	-2.877493000	-2.601876000
C	2.474366000	-1.421951000	4.248484000
N	-0.155622000	-4.095398000	-0.741239000
C	3.495524000	0.000086000	2.422749000
H	3.044680000	1.012323000	2.407486000
H	4.343327000	0.003699000	3.134928000
N	-0.163727000	-3.889651000	1.416194000
C	3.399291000	0.252211000	-0.024692000
C	4.855564000	-1.342590000	0.761291000
C	3.404633000	-0.338259000	-2.410198000
H	4.214711000	-0.361294000	-3.159347000
H	2.886001000	0.638687000	-2.478261000
C	4.837817000	-1.440140000	-0.623434000
C	2.429320000	-2.086204000	-3.983580000
Au	-2.050000000	-1.805043000	0.131964000
N	-0.864507000	2.387095000	-3.042671000
C	-1.514275000	1.558028000	-2.167504000
Au	-1.299796000	1.497312000	-0.120650000
N	-2.505957000	0.985492000	-2.912816000
C	-1.419034000	2.321645000	-4.336441000
N	-3.980977000	0.290765000	-1.090865000
N	-3.947120000	0.444790000	1.070225000
C	-1.493653000	1.897720000	1.889517000
C	-1.400956000	3.016519000	3.892139000
C	0.278290000	3.693539000	2.125815000
H	1.222457000	3.122431000	2.230254000

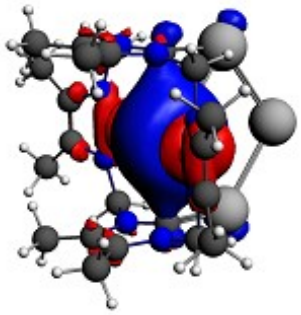
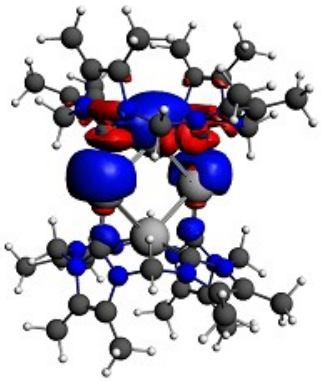
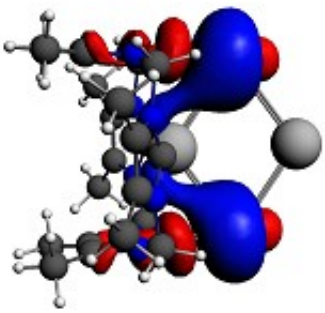
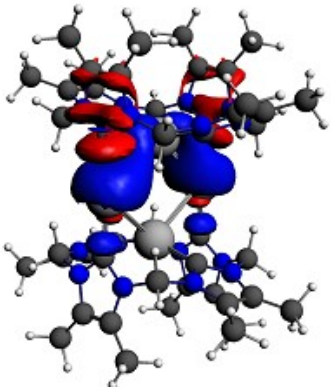
H	0.338544000	4.591511000	2.770615000
C	0.700331000	3.353974000	-0.273988000
C	-0.744500000	5.060306000	0.254415000
C	-0.739065000	4.931283000	-1.127758000
C	0.303923000	3.225855000	-2.697038000
H	0.431830000	3.968215000	-3.503553000
H	1.216276000	2.599179000	-2.647853000
N	-2.462112000	1.430107000	2.736932000
N	-0.861158000	2.877493000	2.601876000
C	-2.474366000	1.421951000	-4.248484000
N	0.155622000	4.095398000	0.741239000
C	-3.495524000	-0.000086000	-2.422749000
H	-3.044680000	-1.012323000	-2.407486000
H	-4.343327000	-0.003699000	-3.134928000
N	0.163727000	3.889651000	-1.416194000
C	-3.399291000	-0.252211000	0.024692000
C	-4.855564000	1.342590000	-0.761291000
C	-3.404633000	0.338259000	2.410198000
H	-4.214711000	0.361294000	3.159347000
H	-2.886001000	-0.638687000	2.478261000
C	-4.837817000	1.440140000	0.623434000
C	-2.429320000	2.086204000	3.983580000
Si	3.652989000	-0.847650000	5.641055000
H	3.300703000	-1.663450000	6.840946000
H	5.060355000	-1.087522000	5.180834000
H	3.423064000	0.619556000	5.854573000
Si	0.849307000	-3.254522000	5.919160000
H	-0.392679000	-4.017366000	5.568443000
H	1.948370000	-4.176306000	6.341241000
H	0.544597000	-2.214132000	6.950809000
Si	-0.789803000	4.237073000	5.232184000
H	-1.715226000	4.071627000	6.392262000
H	0.625300000	3.867613000	5.567334000
H	-0.838898000	5.620602000	4.655044000
Si	-3.554140000	1.780088000	5.513790000
H	-4.437350000	0.611862000	5.193948000
H	-2.652450000	1.449024000	6.661275000
H	-4.359254000	3.016790000	5.755295000
Si	-3.652989000	0.847650000	-5.641055000
H	-3.423064000	-0.619556000	-5.854573000
H	-5.060355000	1.087522000	-5.180834000
H	-3.300703000	1.663450000	-6.840946000
Si	-0.849307000	3.254522000	-5.919160000
H	-0.544597000	2.214132000	-6.950809000
H	-1.948370000	4.176306000	-6.341241000
H	0.392679000	4.017366000	-5.568443000
Si	3.554140000	-1.780088000	-5.513790000
H	4.359254000	-3.016790000	-5.755295000
H	2.652450000	-1.449024000	-6.661275000
H	4.437350000	-0.611862000	-5.193948000
Si	0.789803000	-4.237073000	-5.232184000
H	0.838898000	-5.620602000	-4.655044000
H	-0.625300000	-3.867613000	-5.567334000
H	1.715226000	-4.071627000	-6.392262000
Si	5.791754000	-2.670133000	-1.739757000
H	5.160749000	-4.019055000	-1.564417000
H	5.599314000	-2.198129000	-3.149800000
H	7.232549000	-2.656746000	-1.349474000
Si	5.827376000	-2.403718000	2.015566000
H	4.809666000	-3.098831000	2.874874000
H	6.616584000	-3.377620000	1.203077000
H	6.682631000	-1.498497000	2.847490000
Si	1.737196000	-6.287339000	-1.328270000
H	2.525310000	-7.119643000	-0.369948000
H	0.771748000	-7.087240000	-2.147751000
H	2.630483000	-5.471514000	-2.218896000
Si	1.737390000	-5.944080000	2.411786000
H	1.463406000	-7.396258000	2.197413000
H	3.184605000	-5.597890000	2.231337000
H	1.269550000	-5.491041000	3.762473000
Si	-1.737390000	5.944080000	-2.411786000
H	-1.269550000	5.491041000	-3.762473000
H	-3.184605000	5.597890000	-2.231337000
H	-1.463406000	7.396258000	-2.197413000
Si	-1.737196000	6.287339000	1.328270000
H	-2.630483000	5.471514000	2.218896000
H	-0.771748000	7.087240000	2.147751000
H	-2.525310000	7.119643000	0.369948000
Si	-5.827376000	2.403718000	-2.015566000
H	-6.682631000	1.498497000	-2.847490000
H	-6.616584000	3.377620000	-1.203077000
H	-4.809666000	3.098831000	-2.874874000
Si	-5.791754000	2.670133000	1.739757000
H	-7.232549000	2.656746000	1.349474000
H	-5.599314000	2.198129000	3.149800000
H	-5.160749000	4.019055000	1.564417000

$[L_2(Ph)_8{\rightarrow}Au_4]^{4+}$

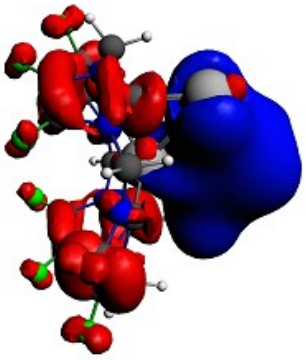
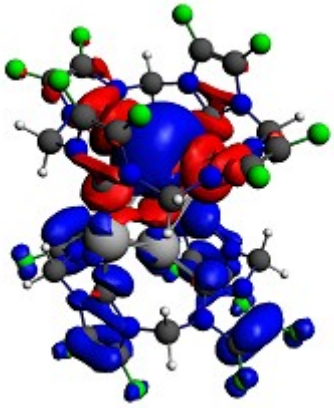
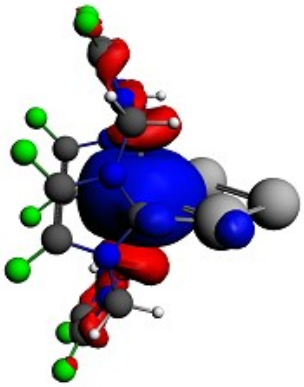
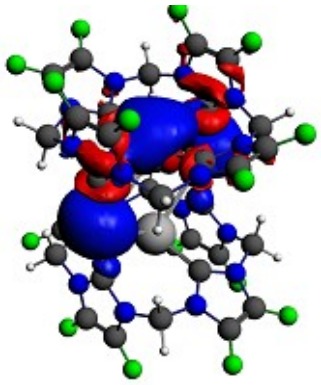
Au	2.084409000	1.784927000	-0.170361000
N	0.891868000	-2.434385000	3.017379000
C	1.514864000	-1.559136000	2.165539000
Au	1.270880000	-1.469552000	0.113818000
N	2.549642000	-1.015379000	2.882006000
C	1.521298000	-2.454253000	4.274374000
N	4.008815000	-0.275116000	1.086660000
C	1.266336000	-3.177365000	5.451773000
H	0.432052000	-3.887219000	5.547268000
N	3.989179000	-0.459820000	-1.095608000
C	2.131367000	-2.953323000	6.530696000
H	1.970420000	-3.502474000	7.470162000
C	1.478920000	-1.903637000	-1.897494000
C	3.090006000	-3.092141000	-6.065223000
H	3.726293000	-3.094048000	-6.962554000
C	2.017462000	-4.011320000	-5.977448000
H	1.840450000	-4.710290000	-6.808213000
C	1.172967000	-4.050223000	-4.860345000
H	0.338685000	-4.765324000	-4.819806000
C	1.447960000	-3.139926000	-3.825983000
C	-0.343604000	-3.657334000	-2.124162000
H	-1.252649000	-3.030691000	-2.219082000
H	-0.454349000	-4.538132000	-2.782651000
C	-0.748332000	-3.347311000	0.291173000
C	0.643308000	-5.071366000	-0.284033000
C	1.412060000	-6.036248000	-0.950208000
H	1.408616000	-6.140466000	-2.044589000
C	2.187547000	-6.882752000	-0.145448000
H	2.795978000	-7.665940000	-0.621257000
C	2.200064000	-6.763163000	1.264913000
H	2.817955000	-7.455955000	1.855004000
C	1.437609000	-5.792039000	1.929115000
H	1.453514000	-5.710398000	3.025304000

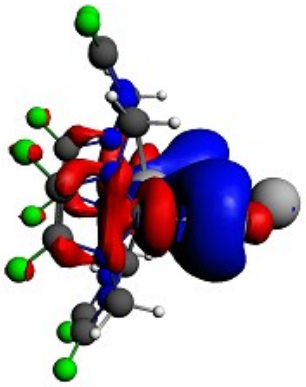
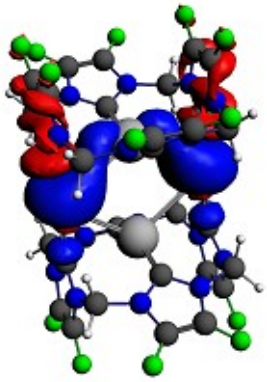
C	0.655788000	-4.952059000	1.123594000
C	-0.300372000	-3.246962000	2.716673000
H	-0.398072000	-4.004224000	3.515858000
H	-1.208341000	-2.611712000	2.720963000
C	5.673035000	-2.165603000	1.582600000
H	5.693651000	-2.080508000	2.678448000
C	6.453207000	-3.121269000	0.916548000
H	7.098940000	-3.790408000	1.504122000
N	2.498999000	-1.488864000	-2.714246000
C	3.204577000	-2.034903000	6.443031000
H	3.857468000	-1.887626000	7.316018000
N	0.841845000	-2.908675000	-2.578651000
C	3.453495000	-1.305606000	5.273102000
H	4.286363000	-0.588857000	5.232419000
C	2.592924000	-1.537130000	4.186838000
N	-0.242264000	-4.083708000	-0.749945000
C	3.499751000	0.006244000	2.406633000
H	3.011234000	1.000537000	2.378014000
H	4.335054000	0.046675000	3.129345000
N	-0.222885000	-3.898740000	1.432262000
C	3.436732000	0.236590000	-0.050565000
C	4.886377000	-1.329373000	0.777838000
C	6.440073000	-3.240891000	-0.493802000
H	7.075838000	-4.000468000	-0.972138000
C	3.456237000	-0.403459000	-2.434714000
H	4.278346000	-0.486787000	-3.168798000
H	2.967348000	0.582567000	-2.564796000
C	4.873390000	-1.448717000	-0.629767000
C	5.646315000	-2.409688000	-1.296688000
H	5.646324000	-2.510325000	-2.391409000
C	3.358822000	-2.176981000	-5.039183000
H	4.190563000	-1.464173000	-5.134899000
C	2.519033000	-2.222175000	-3.913621000
Au	-2.084409000	-1.784927000	0.170361000
N	-0.891868000	2.434385000	-3.017379000
C	-1.514864000	1.559136000	-2.165539000
Au	-1.270880000	1.469552000	-0.113818000
N	-2.549642000	1.015379000	-2.882006000
C	-1.521298000	2.454253000	-4.274374000
N	-4.008815000	0.275116000	-1.086660000
C	-1.266336000	3.177365000	-5.451773000
H	-0.432052000	3.887219000	-5.547268000
N	-3.989179000	0.459820000	1.095608000
C	-2.131367000	2.953323000	-6.530696000
H	-1.970420000	3.502474000	-7.470162000
C	-1.478920000	1.903637000	1.897494000
C	-3.090006000	3.092141000	6.065223000
H	-3.726293000	3.094048000	6.962554000
C	-2.017462000	4.011320000	5.977448000
H	-1.840450000	4.710290000	6.808213000
C	-1.172967000	4.050223000	4.860345000
H	-0.338685000	4.765324000	4.819806000
C	-1.447960000	3.139926000	3.825983000
C	0.343604000	3.657334000	2.124162000
H	1.252649000	3.030691000	2.219082000
H	0.454349000	4.538132000	2.782651000
C	0.748332000	3.347311000	-0.291173000
C	-0.643308000	5.071366000	0.284033000
C	-1.412060000	6.036248000	0.950208000
H	-1.408616000	6.140466000	2.044589000
C	-2.187547000	6.882752000	0.145448000
H	-2.795978000	7.665940000	0.621257000
C	-2.200064000	6.763163000	-1.264913000
H	-2.817955000	7.455955000	-1.855004000
C	-1.437609000	5.792039000	-1.929115000
H	-1.453514000	5.710398000	-3.025304000
C	-0.655788000	4.952059000	-1.123594000
C	0.300372000	3.246962000	-2.716673000
H	0.398072000	4.004224000	-3.515858000
H	1.208341000	2.611712000	-2.720963000
C	-5.673035000	2.165603000	-1.582600000
H	-5.693651000	2.080508000	-2.678448000
C	-6.453207000	3.121269000	-0.916548000
H	-7.098940000	3.790408000	-1.504122000
N	-2.498999000	1.488864000	2.714246000
C	-3.204577000	2.034903000	-6.443031000
H	-3.857468000	1.887626000	-7.316018000
N	-0.841845000	2.908675000	2.578651000
C	-3.453495000	1.305606000	-5.273102000
H	-4.286363000	0.588857000	-5.232419000
C	-2.592924000	1.537130000	-4.186838000
N	0.242264000	4.083708000	0.749945000
C	-3.499751000	-0.006244000	-2.406633000
H	-3.011234000	-1.000537000	-2.378014000
H	-4.335054000	-0.046675000	-3.129345000
N	0.222885000	3.898740000	-1.432262000
C	-3.436732000	-0.236590000	0.050565000
C	-4.886377000	1.329373000	-0.777838000
C	-6.440073000	3.240891000	0.493802000
H	-7.075838000	4.000468000	0.972138000
C	-3.456237000	0.403459000	2.434714000
H	-4.278346000	0.486787000	3.168798000
H	-2.967348000	-0.582567000	2.564796000
C	-4.873390000	1.448717000	0.629767000
C	-5.646315000	2.409688000	1.296688000
H	-5.646324000	2.510325000	2.391409000
C	-3.358822000	2.176981000	5.039183000
H	-4.190563000	1.464173000	5.134899000
C	-2.519033000	2.222175000	3.913621000

	Component A-B of $[L_2(C_2H_5)_8 \rightarrow Ag_4]^{4+}$	Component A-BA′ of $[L_2(C_2H_5)_8 \rightarrow Ag_4]^{4+}$
Δρ1	ΔE =-85.79 kcal/mol ν: 1.47280	ΔE = -107.20 kcal/mol ν: 1.17807 
Δρ2	ΔE =-45.67 kcal/mol ν: 0.67486 	ΔE = -32.61 kcal/mol ν: 0.59308 
Δρ3	ΔE =-44.44 kcal/mol ν: 0.65278 	ΔE = -29.20 kcal/mol ν: 0.49719 

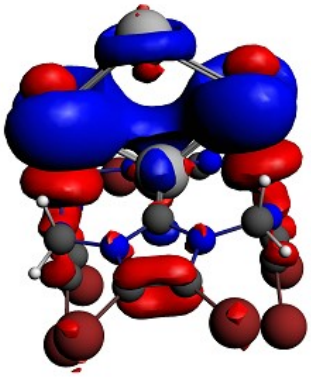
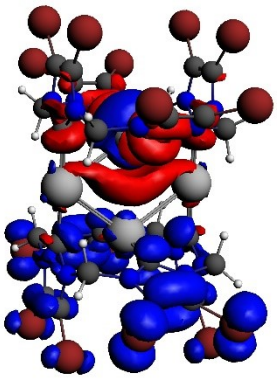
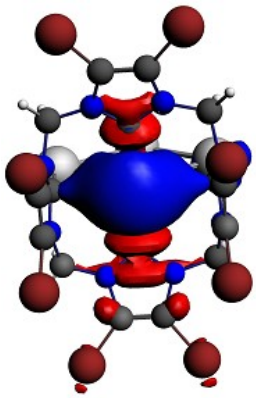
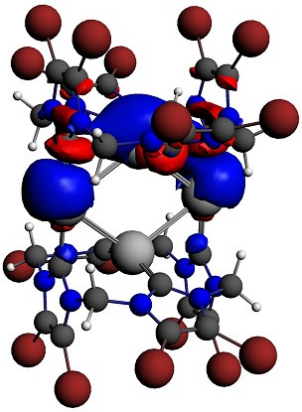
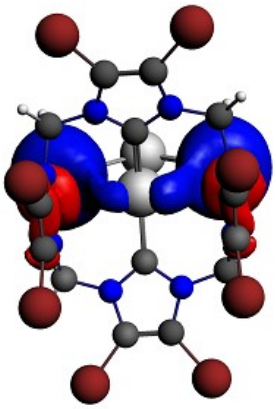
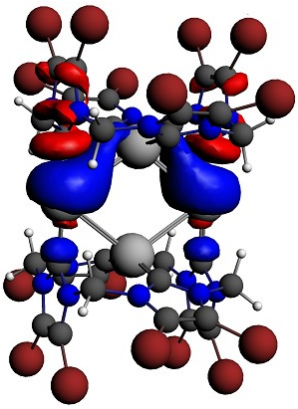
Δρ2	ΔE =-46.59 kcal/mol ν: 0.67967 	ΔE =-34.04 kcal/mol ν: 0.60581 	Component A-B of $[L_2(CH_3)_8 \rightarrow Ag_4]^{4+}$ Component A-BA′ of $[L_2(CH_3)_8 \rightarrow Ag_4]^{4+}$
Δρ3	ΔE =-44.83 kcal/mol ν: 0.64329 	ΔE =-31.10 kcal/mol ν: 0.50318 	

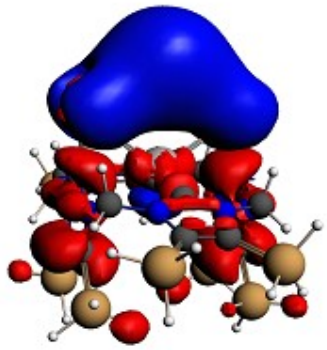
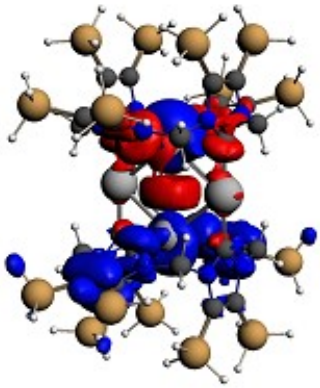
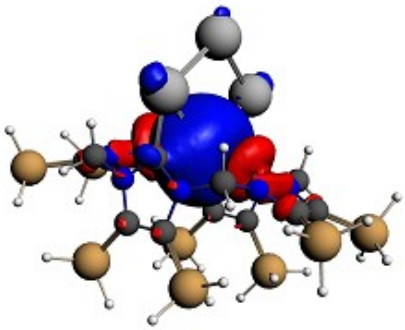
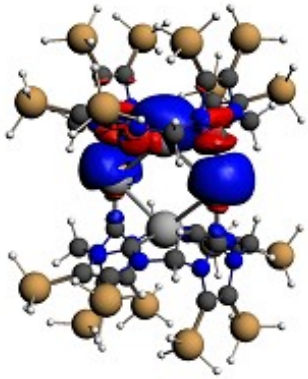
Δρ1	ΔE = -69.69 kcal/mol ν: 1.12198	ΔE = -93.24 kcal/mol ν: 1.07052	Component A-B of $[L_2(H)_8 \rightarrow Ag_4]^{4+}$ Component A-BA′ of $[L_2(H)_8 \rightarrow Ag_4]^{4+}$
Δρ2	ΔE =-58.29 kcal/mol ν: 0.71759	ΔE =-33.49 kcal/mol ν: 0.61400	
Δρ3	ΔE =-43.52 kcal/mol ν: 0.64052	ΔE = -31.11 kcal/mol ν: 0.50231	

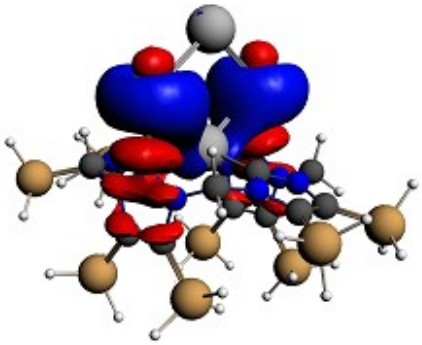
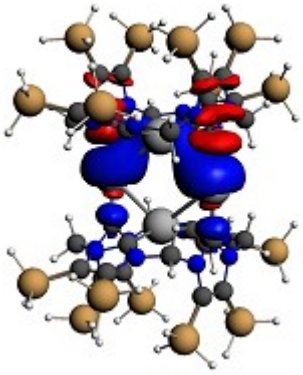
Δρ1	ΔE = -82.06 kcal/mol v: 1.27906 	ΔE = -83.86 kcal/mol v: 1.03902 
Δρ2	ΔE = -53.91 kcal/mol v: 0.70791 	ΔE = -32.92 kcal/mol v: 0.60083 

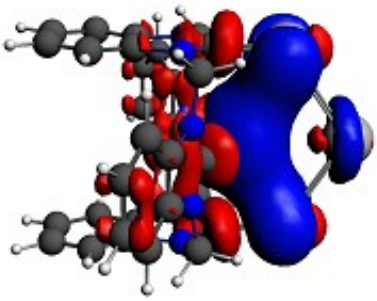
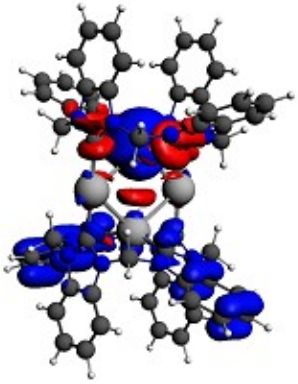
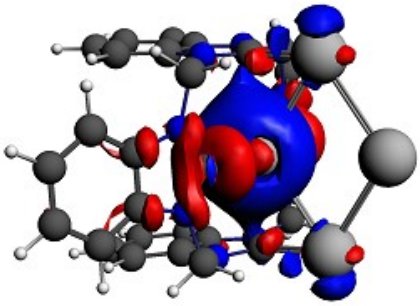
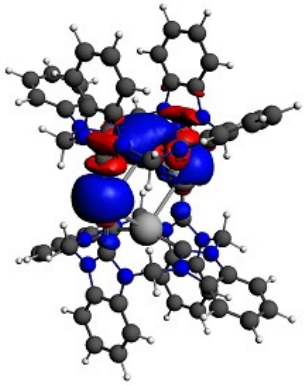
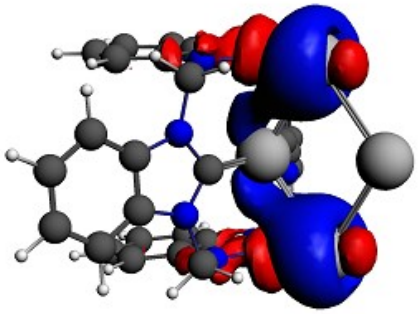
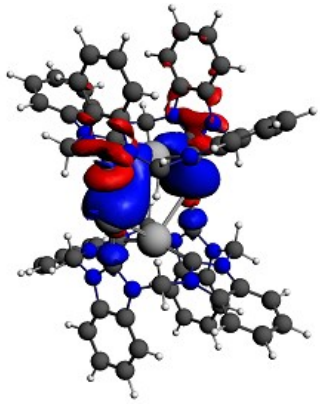
Δρ3	ΔE =-42.41 kcal/mol v: 0.63868 	ΔE = -31.89 kcal/mol 0v: 0.50825 	Component A-B of $[L_2(F)_8 \rightarrow Ag_4]^{4+}$ Component A-BA' of $[L_2(F_3)_8 \rightarrow Ag_4]^{4+}$

Δρ1	ΔE = -94.08 kcal/mol v: 1.37914	ΔE = -93.52 kcal/mol v: 1.13961	Component A-B of $[L_2(Cl)_8 \rightarrow Ag_4]^{4+}$ Component A-BA′ of $[L_2(Cl)_8 \rightarrow Ag_4]^{4+}$
Δρ2	ΔE =-55.57 kcal/mol v: 0.72075	ΔE = -34.29 kcal/mol v: 0.61574	
Δρ3	ΔE =-43.31 kcal/mol v: 0.64915	ΔE = -34.46 kcal/mol v: 0.51918	

Δρ1	ΔE = -100.51 kcal/mol v: 1.47959 	ΔE = ΔE = -112.42 kcal/mol v: 1.25546 	Component A-B of $[L_2(Br)_8 \rightarrow Ag_4]^{4+}$ Component A-BA′ of $[L_2(Br)_8 \rightarrow Ag_4]^{4+}$
Δρ2	ΔE =-56.97 kcal/mol v:0.72818 	ΔE = -35.68 kcal/mol v: 0.62891 	
Δρ3	ΔE =-40.02 kcal/mol v: 0.65966 	ΔE = -33.21 kcal/mol v: 0.52862 	

Δρ1	ΔE = -80.39 kcal/mol ν: 1.08128	ΔE = -115.27 kcal/mol ν: 1.21311
		
Δρ2	ΔE =-55.65 kcal/mol ν: 0.71140	ΔE = -33.48 kcal/mol ν: 0.60501
		

Δρ3	ΔE =-47.52 kcal/mol v: 0.67435 	ΔE = -31.63 kcal/mol v: 0.51475 	Component A-B of $[L_2(SiH_3)_8 \rightarrow Ag_4]^{4+}$ Component A-BA' of $[L_2(SiH_3)_8 \rightarrow Ag_4]^{4+}$

Δρ1	ΔE = -77.56 kcal/mol v: 0.84790	ΔE = -85.38 kcal/mol v: 1.06442	Component A-B of $[L_2(Ph)_8 \rightarrow Ag_4]^{4+}$ Component A-BA′ of $[L_2(Ph)_8 \rightarrow Ag_4]^{4+}$
			
Δρ2	ΔE =-47.38 kcal/mol v: 0.69602	ΔE = -31.80 kcal/mol v: 0.59014	
			
Δρ3	ΔE =-45.95 kcal/mol v: 0.60411	ΔE = -30.99 kcal/mol v: 0.51014	
			

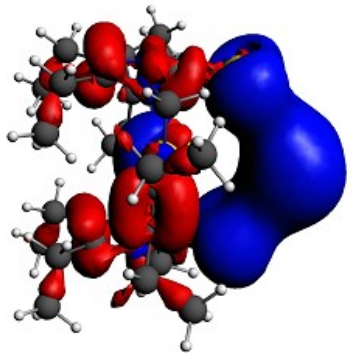
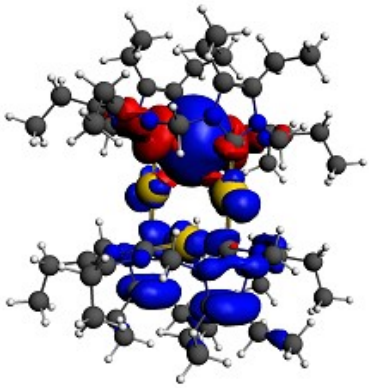
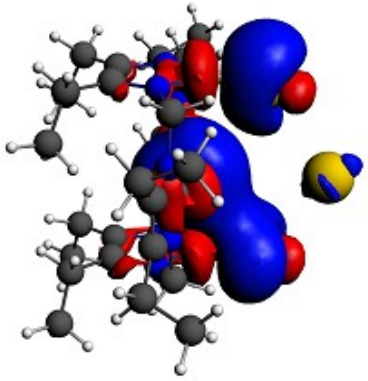
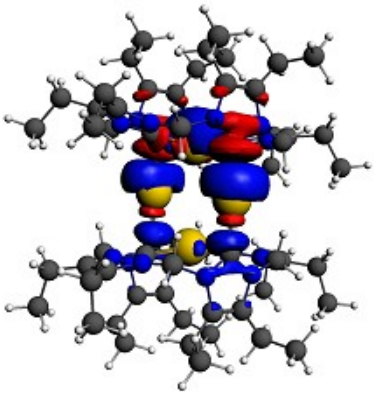
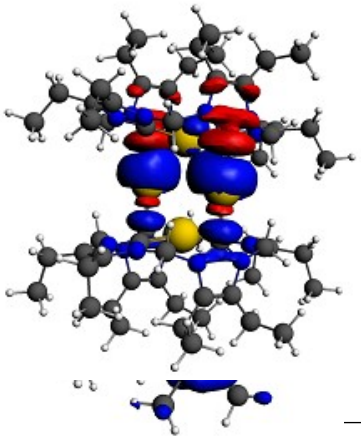
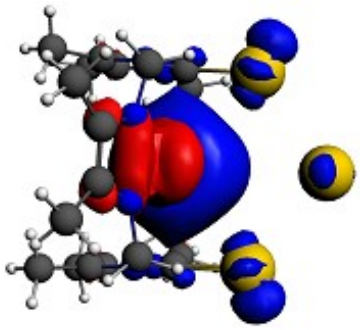
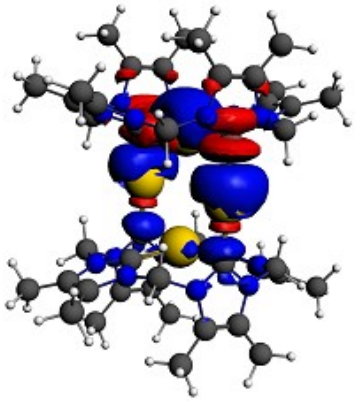
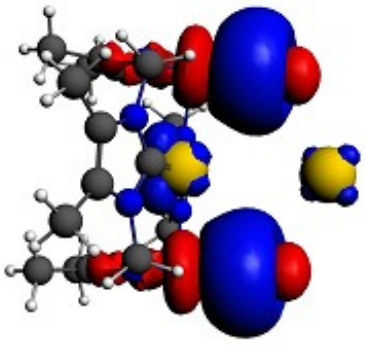
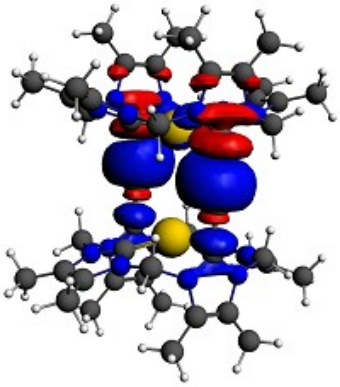
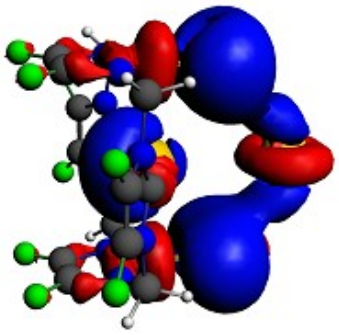
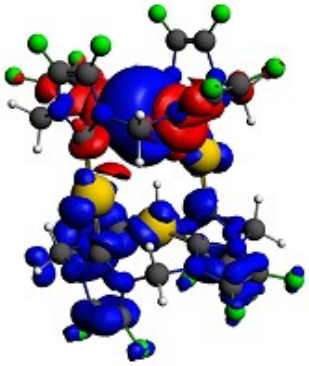
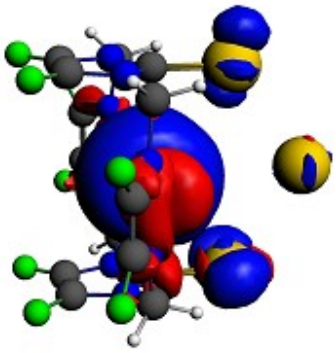
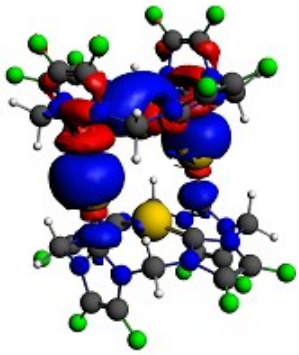
	Component A-B of $[L_2(C_2H_5)_8 \rightarrow Au_4]^{4+}$	Component A-BA′ of $[L_2(C_2H_5)_8 \rightarrow Au_4]^{4+}$
Δρ1	ΔE = -110.69 kcal/mol ν: 1.56918	ΔE = -153.43 kcal/mol ν: 1.27056
		
Δρ2	ΔE = -88.53 kcal/mol ν: 0.94413	ΔE = -57.11 kcal/mol ν: 0.72915
		

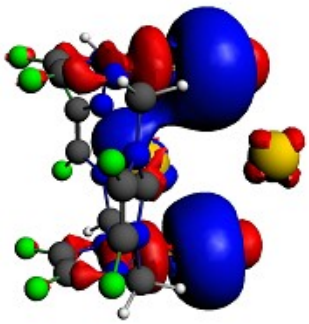
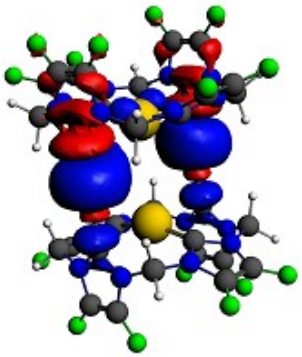
Figure S1: The deformation density between the M^{4+} and $L_2(R)_8$ fragments, along with the principal energy contributions in the $[L_2(R)_8 \rightarrow Ag_4]^{4+}$ complexes (where R = C_2H_5, CH_3, H, F, Cl, Br, SiH_3 and Ph), based on the A–B and A–BA′ components.

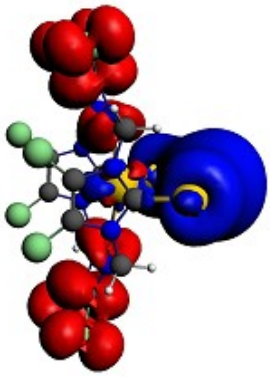
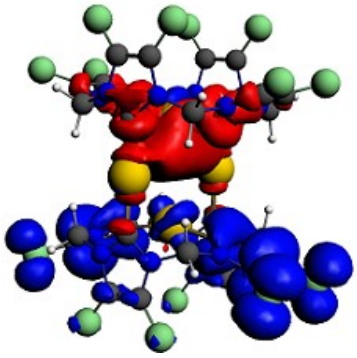
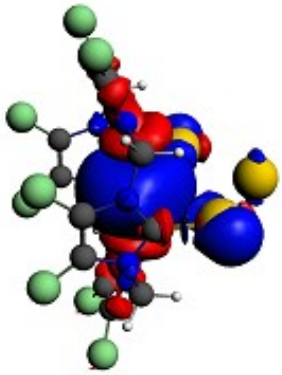
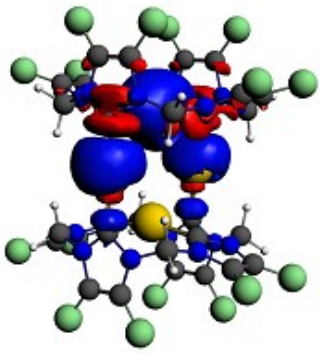
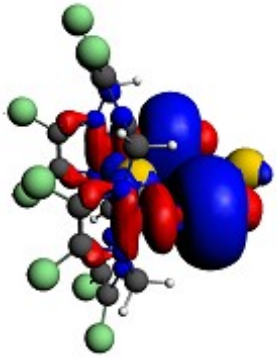
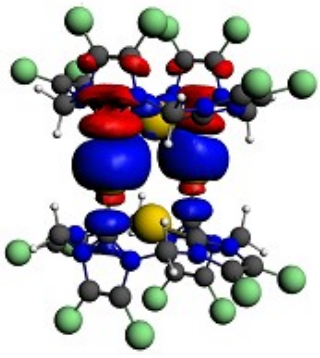
Δρ3	ΔE = -92.13 kcal/mol ν: 0.94391	ΔE = -46.21 kcal/mol ν: 0.58781
Δρ1	ΔE = -110.66 kcal/mol ν: 1.69066	

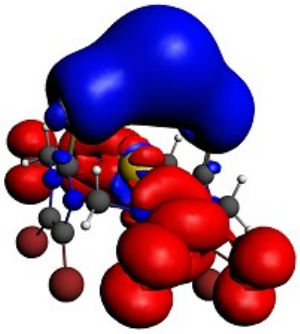
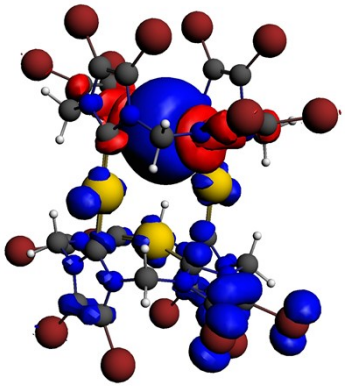
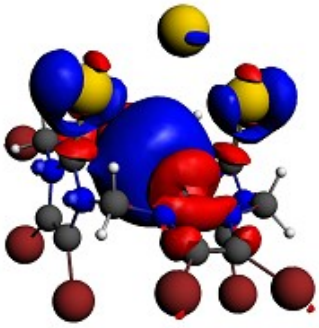
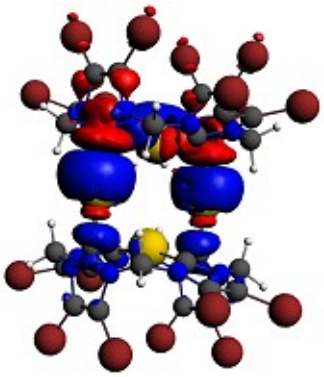
Δρ2	ΔE =-102.50 kcal/mol v: 0.93886 	ΔE = -60.67 kcal/mol v: 0.75611 	Component A-B of $[L_2(CH_3)_8 \rightarrow Au_4]^{4+}$ Component A-BA′ of $[L_2(CH_3)_8 \rightarrow Au_4]^{4+}$
Δρ3	ΔE =-68.00 kcal/mol v: 0.93312 	ΔE = -47.12 kcal/mol v: 0.59366 	

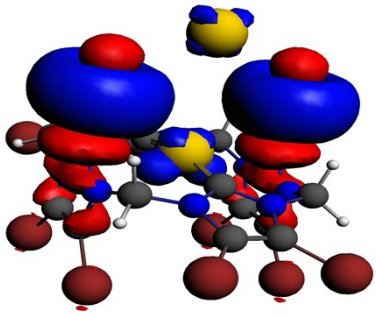
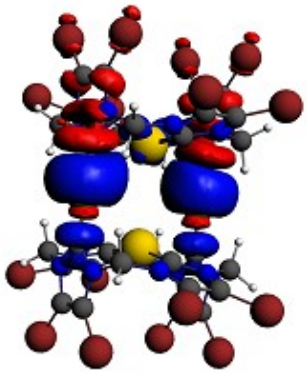
Δρ1	ΔE = -91.51 kcal/mol v: 1.66623	ΔE = -142.52 kcal/mol v: 1.21624	Component A-B of $[L_2(H)_8 \rightarrow Au_4]^{4+}$ Component A-BA′ of $[L_2(H)_8 \rightarrow Au_4]^{4+}$
Δρ2	ΔE =-100.63 kcal/mol v: 0.93416	ΔE = -59.29 kcal/mol v: 0.73997	
Δρ3	ΔE =-67.45 kcal/mol v: 0.92299	ΔE = -47.34 kcal/mol v: 0.59571	

Δρ1	ΔE = -97.71 kcal/mol ν: 1.53002	ΔE = -167.46 kcal/mol ν: 1.33239
		
Δρ2	ΔE = -106.69 kcal/mol ν: 0.94652	ΔE = -60.43 kcal/mol ν: 0.76330
		

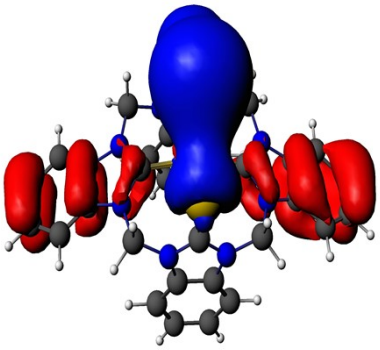
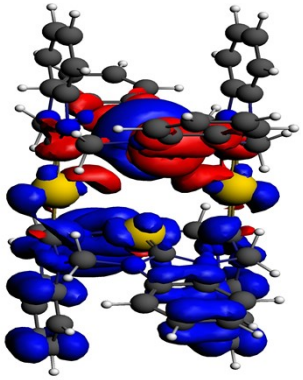
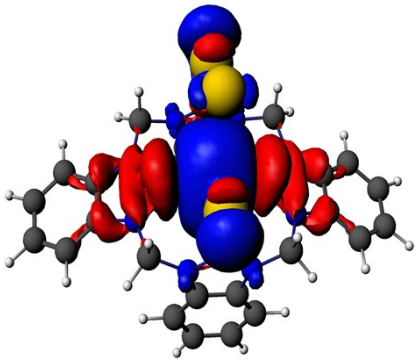
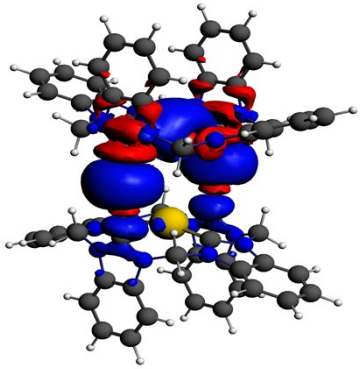
Δρ3	ΔE = -66.74 kcal/mol ν: 0.92077 	ΔE = -47.71 kcal/mol ν: 0.59789 	Component A-B of $[L_2(F)_8 \rightarrow Au_4]^{4+}$ Component A-BA′ of $[L_2(F_3)_8 \rightarrow Au_4]^{4+}$

Δρ1	ΔE = -113.59 kcal/mol v: 1.46234 	ΔE = -154.41 kcal/mol v: 1.31920 	Component A-B of $[L_2(Cl)_8 \rightarrow Au_4]^{4+}$ Component A-BA′ of $[L_2(Cl)_8 \rightarrow Au_4]^{4+}$
Δρ2	ΔE =-112.58 kcal/mol v: 0.95095 	ΔE = -59.35 kcal/mol v: 0.75836 	
Δρ3	ΔE =-69.06 kcal/mol v: 0.93004 	ΔE = -47.80 kcal/mol v: 0.59964 	

Δρ1	ΔE = -116.51 kcal/mol v: 1.54345	ΔE = -147.94 kcal/mol v: 1.30851
		
Δρ2	ΔE = -113.62 kcal/mol v: 0.96289	ΔE = -61.48 kcal/mol v: 0.78142
		

Δρ3	ΔE = -70.22 kcal/mol v: 0.94628 	ΔE = -49.81 kcal/mol v: 0.62236 	Component A-B of $[L_2(Br)_8 \rightarrow Au_4]^{4+}$ Component A-BA′ of $[L_2(Br)_8 \rightarrow Au_4]^{4+}$

Δρ1	ΔE = -104.58 kcal/mol ν: 1.59173	ΔE = -144.01 kcal/mol ν: 1.23766	Component A-B of $[L_2(SiH_3)_8 \rightarrow Au_4]^{4+}$ Component A-BA′ of $[L_2(SiH_3)_8 \rightarrow Au_4]^{4+}$
Δρ2	ΔE =-71.43 kcal/mol ν: 0.96357	ΔE = -54.41 kcal/mol ν: 0.73369	
Δρ3	ΔE =-110.28 kcal/mol ν: 0.94555	ΔE = -48.39 kcal/mol ν: 0.60803	

Δρ1	ΔE = -109.50 kcal/mol v: 1.49407 	ΔE = -183.92 kcal/mol v: 1.39900 
Δρ2	ΔE =-110.38 kcal/mol v: 0.94369 	ΔE = -59.52 kcal/mol v: -0.74611 

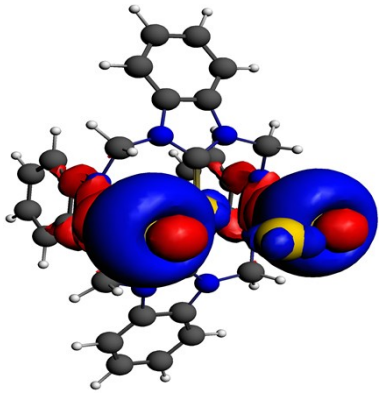
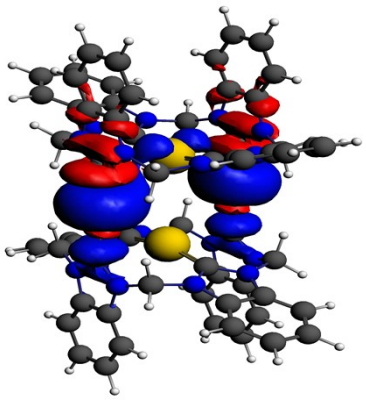
Δρ3	ΔE =-69.85 kcal/mol v: 0.94191 	ΔE = -46.74 kcal/mol v: 0.59253 	Component A-B of $[L_2(Ph)_8 \rightarrow Au_4]^{4+}$ Component A-BA′ of $[L_2(Ph)_8 \rightarrow Au_4]^{4+}$

Figure S2: The deformation density between the M^{4+} and $L_2(R)_8$ fragments, along with the principal energy contributions in the $[L_2(R)_8 \rightarrow Au_4]^{4+}$ complexes (where R = C_2H_5, CH_3, H, F, Cl, Br, SiH_3 and Ph), based on the A–B and A–BA′ components.