

Supporting information for:

On the Variation of Cluster Core Characteristics by Endohedral Atom. Shape Variation in 8-*ce* [EAu₄(PPh₃)₄]²⁺ (E=N, P, As, Sb) Clusters

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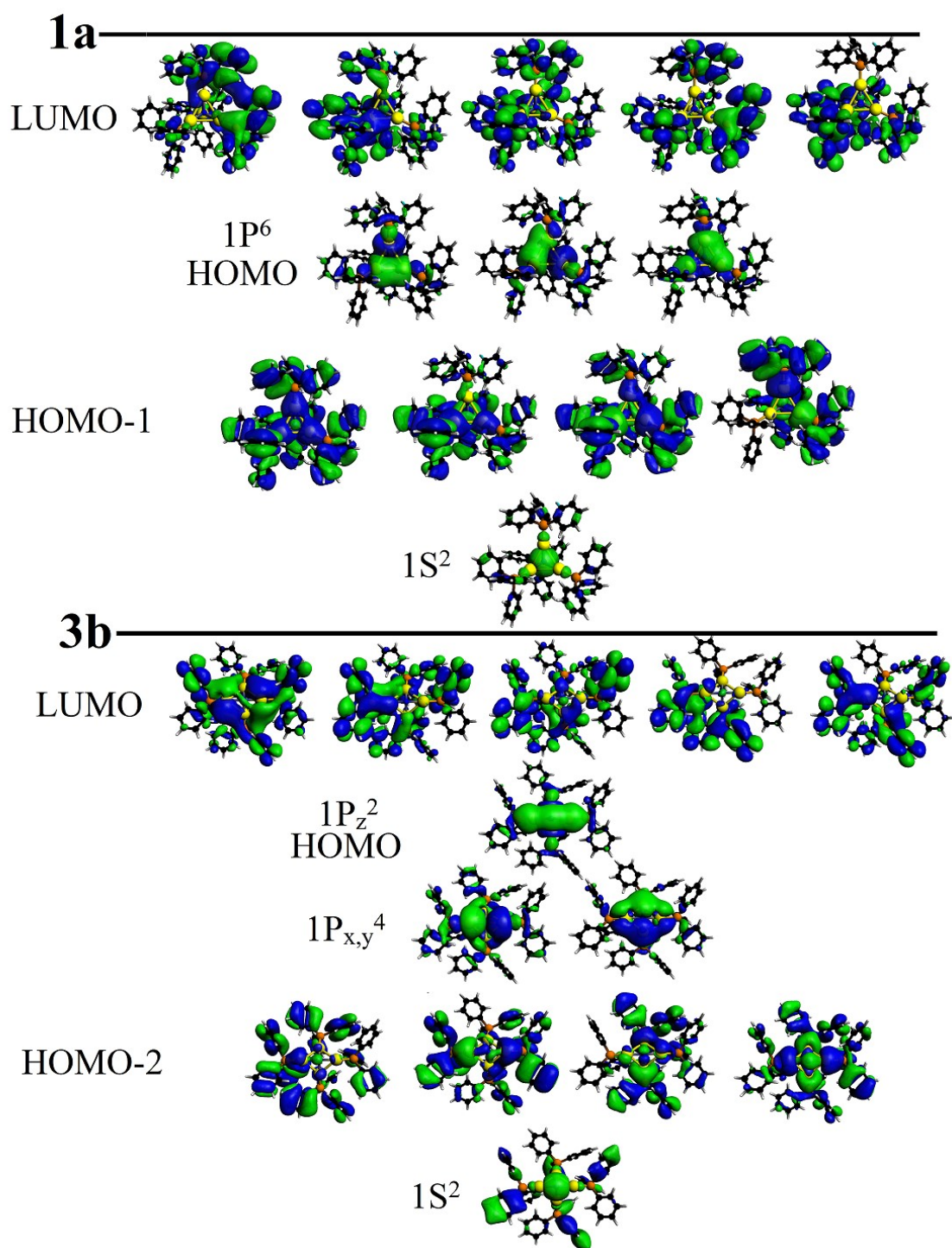
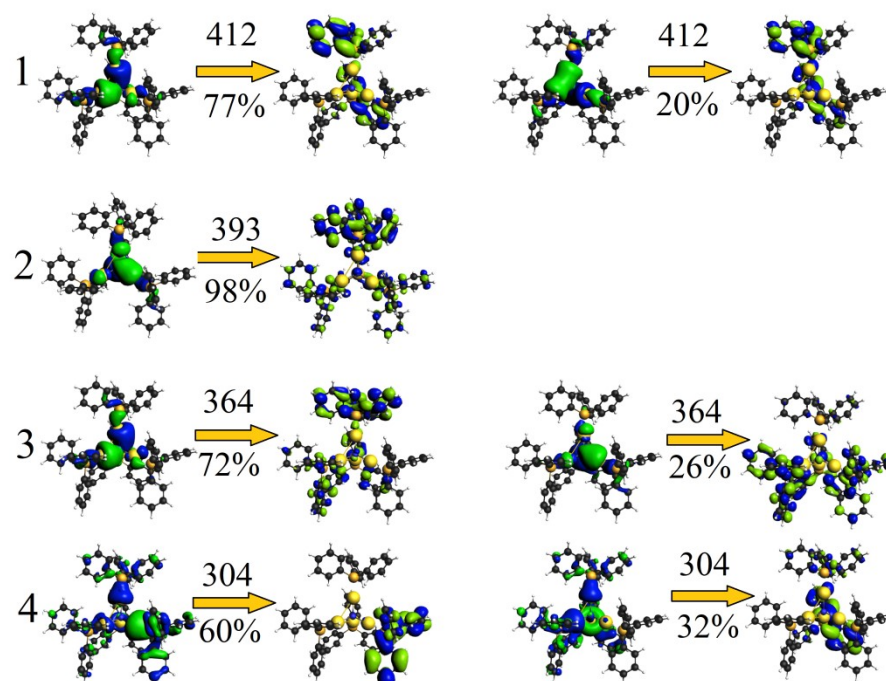


Figure S1. Extended picture for the isosurfaces for $1S^2$, $1P^6$ and frontier orbitals for **1a** and **3b**.

1a



3b

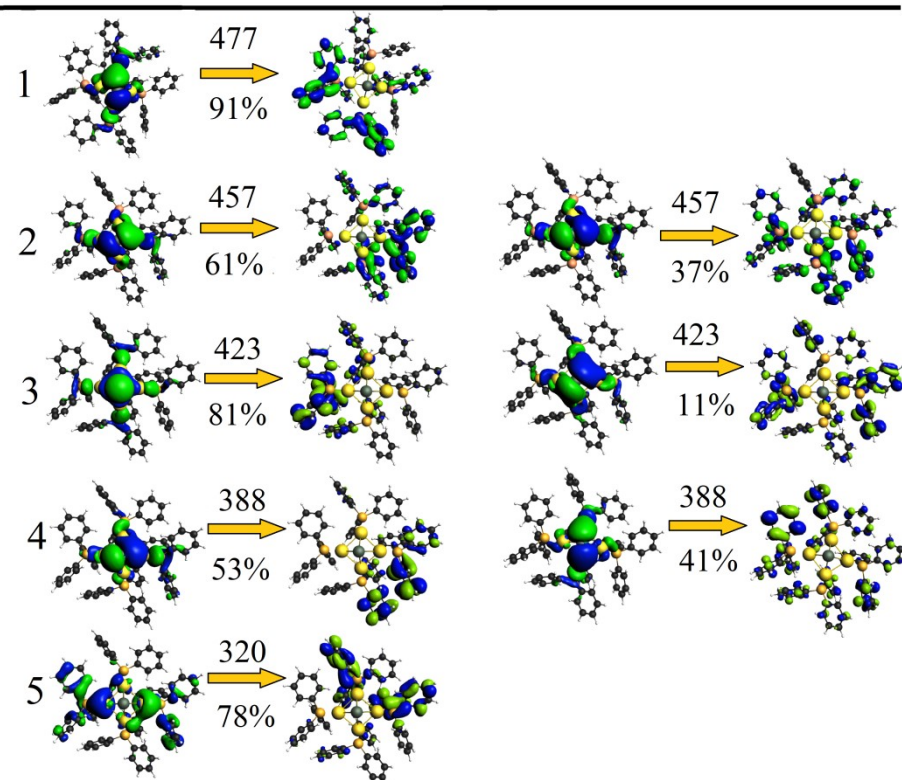
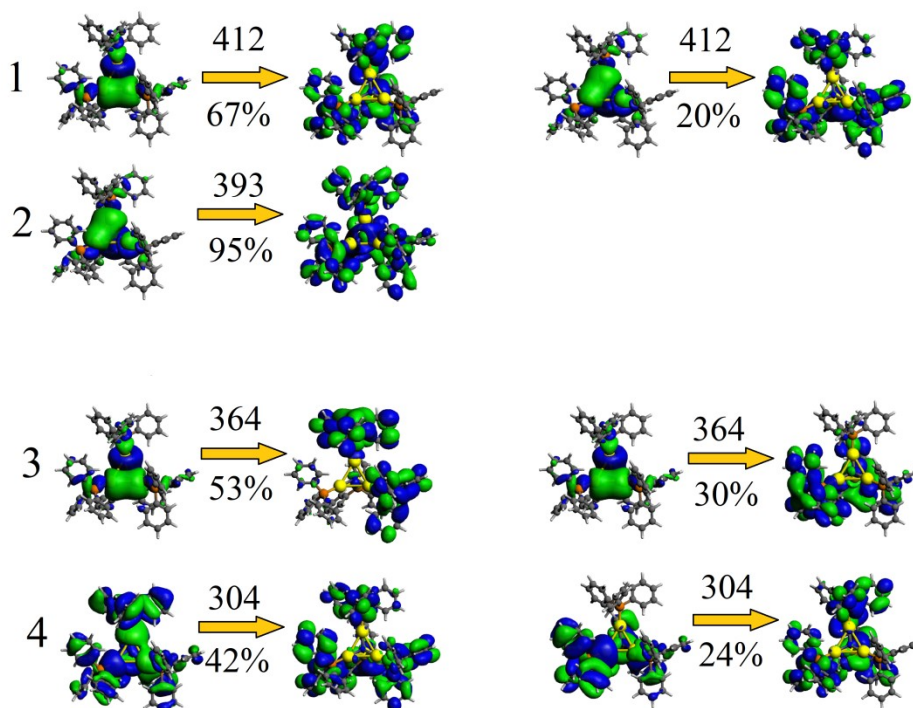


Figure S2. Natural transition orbitals (NTOs) representation of the *electron*→*hole* transition, involving occupied (*electron*) and unoccupied NTOs (*hole*) leading to the four and five main transitions discussed for **1a** and **3b**, respectively, denoting their percentage contribution. Wavelength for each transition given in nm.

1a



3b

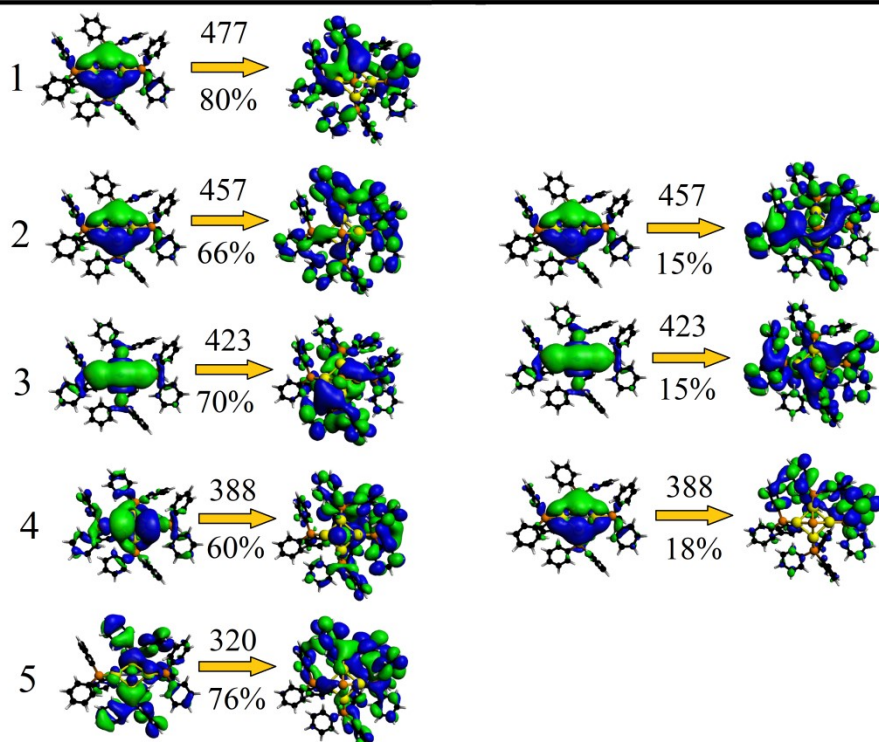


Figure S3. Canonical molecular orbitals involved in the discussed four and five main transitions discussed for **1a** and **3b**, respectively, denoting their percentage contribution. Wavelength for each transition given in nm.

Table S1. Cartesian coordinates for the optimized geometries in Angstrom (Å) in a multipleXYZ format.

```

141
[NAu4(PPh3)4]+ Tetrahedro
Au      11.763368000    11.666633000    5.621714000
Au      8.574031000    11.726962000    4.656727000
Au      9.650241000    9.362548000    6.737444000
Au      10.575427000    9.364479000    3.550639000
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C       12.562937000    6.994233000    2.144551000
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141			
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H	1.989914000	11.337473000	-0.155662000
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H	6.459249000	12.431373000	1.473832000
H	4.285550000	13.253234000	0.597337000

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[PAu4(PPh3)4]+ Tetrahedro

Au	11.915477000	11.855685000	5.698272000
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Au	9.673985000	9.131647000	6.976132000
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H	8.495669000	4.168129000	-0.887829000
H	7.399148000	3.302811000	1.171532000
H	7.867274000	4.368521000	3.371326000
H	9.433443000	6.298595000	3.510092000
H	13.510443000	8.657958000	2.646071000
H	15.775916000	7.655803000	2.903285000
H	16.202379000	5.329209000	2.133046000
H	14.367645000	4.008044000	1.095421000
H	12.109424000	5.003486000	0.836818000
H	12.644730000	7.322891000	-0.918052000
H	12.496045000	8.391925000	-3.155875000
H	10.804348000	10.165210000	-3.581486000
H	9.263245000	10.875507000	-1.761834000
H	9.413327000	9.811777000	0.484895000
P	9.188160000	7.765763000	8.775193000
C	10.382911000	6.414852000	9.018268000
C	10.641904000	5.887307000	10.290566000
C	11.534076000	4.824340000	10.433170000
C	12.174036000	4.290814000	9.311752000
C	11.926033000	4.823044000	8.042639000
C	11.035400000	5.884845000	7.893698000
C	7.572019000	6.950144000	8.572715000
C	6.565393000	7.641238000	7.879318000
C	5.317712000	7.048512000	7.691831000

C	5.069640000	5.764747000	8.187088000
C	6.0712211000	5.074707000	8.873610000
C	7.322277000	5.662682000	9.065790000
C	9.126713000	8.613303000	10.385064000
C	8.189193000	8.272308000	11.367970000
C	8.219111000	8.910752000	12.609501000
C	9.179717000	9.889333000	12.871060000
C	10.110794000	10.236404000	11.887281000
C	10.085082000	9.605825000	10.644767000
H	10.152768000	6.312974000	11.166521000
H	11.735665000	4.419062000	11.424007000
H	12.875968000	3.466255000	9.428674000
H	12.436524000	4.417551000	7.170318000
H	10.849907000	6.317483000	6.909006000
H	6.774913000	8.634435000	7.478365000
H	4.539687000	7.583208000	7.149533000
H	4.097630000	5.298267000	8.030172000
H	5.882625000	4.072155000	9.254131000
H	8.108773000	5.117323000	9.586418000
H	7.437036000	7.511898000	11.160645000
H	7.488234000	8.644157000	13.371454000
H	9.198941000	10.387499000	13.840203000
H	10.855868000	11.003996000	12.089528000
H	10.803845000	9.877814000	9.870871000
P	13.669095000	13.244683000	6.277196000
C	15.195385000	12.884649000	5.352622000
C	16.111920000	13.883442000	4.999687000
C	17.288641000	13.542357000	4.331891000
C	17.553092000	12.209084000	4.011653000
C	16.635231000	11.212053000	4.354348000
C	15.457309000	11.546001000	5.019767000
C	14.148190000	13.147671000	8.032599000
C	13.128534000	13.008059000	8.987912000
C	13.446331000	12.982399000	10.344431000
C	14.777997000	13.086866000	10.754747000
C	15.794123000	13.214114000	9.805260000
C	15.483381000	13.241701000	8.445252000
C	13.293795000	15.006082000	6.001419000
C	13.934109000	16.017571000	6.731797000
C	13.619195000	17.354383000	6.490331000
C	12.659109000	17.686664000	5.530664000
C	12.011120000	16.680721000	4.809114000
C	12.325702000	15.342632000	5.042283000
H	15.901959000	14.924998000	5.239455000
H	17.996563000	14.321689000	4.055373000
H	18.469814000	11.947672000	3.484693000
H	16.837009000	10.173488000	4.096021000
H	14.729124000	10.776550000	5.279677000
H	12.092018000	12.916144000	8.659692000
H	12.655665000	12.879764000	11.085707000
H	15.024085000	13.063369000	11.815591000
H	16.833059000	13.290028000	10.122397000
H	16.277741000	13.330926000	7.704359000
H	14.663799000	15.757945000	7.498314000
H	14.118465000	18.137255000	7.059131000
H	12.410333000	18.731798000	5.350624000
H	11.252457000	16.936749000	4.071803000
H	11.812499000	14.550365000	4.495803000
P	6.633190000	13.277177000	3.957332000
C	5.074290000	12.944592000	4.835754000
C	4.202840000	13.965505000	5.235427000
C	3.004080000	13.644855000	5.874267000
C	2.674408000	12.310462000	6.118218000
C	3.546000000	11.290221000	5.726323000
C	4.744265000	11.603024000	5.089654000
C	6.191485000	13.249202000	2.189794000
C	7.227710000	13.121838000	1.250677000
C	6.936282000	13.148549000	-0.111777000

C	5.613683000	13.292643000	-0.544065000
C	4.581081000	13.406899000	0.389110000
C	4.866195000	13.384358000	1.754956000
C	7.065061000	15.014951000	4.293668000
C	6.473421000	16.068013000	3.580742000
C	6.834981000	17.385783000	3.859967000
C	7.790502000	17.657604000	4.843254000
C	8.387152000	16.610240000	5.550399000
C	8.028015000	15.290683000	5.277109000
H	4.464561000	15.007452000	5.055028000
H	2.329432000	14.440607000	6.186025000
H	1.740834000	12.064573000	6.621943000
H	3.292569000	10.249904000	5.924013000
H	5.437008000	10.813886000	4.792792000
H	8.256529000	13.000660000	1.595657000
H	7.740473000	13.057495000	-0.840746000
H	5.388717000	13.311968000	-1.609503000
H	3.549326000	13.511443000	0.055358000
H	4.060212000	13.466014000	2.483741000
H	5.744785000	15.854853000	2.798486000
H	6.376501000	18.200433000	3.301661000
H	8.075940000	18.688168000	5.052824000
H	9.142036000	16.819110000	6.306488000
H	8.504447000	14.465763000	5.809056000
P	10.132831000	10.469362000	5.133395000
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[PAu4(PPh3)4]+ Planar			
Au	1.535564000	16.829212000	1.977072000
Au	2.205553000	14.851852000	0.016455000
Au	1.014464000	13.034666000	1.842715000
Au	-0.052354000	15.018859000	3.537698000
P	0.023909000	15.139917000	1.104760000
P	3.030827000	18.378726000	2.782500000
C	2.576196000	19.145436000	4.368152000
C	1.744247000	18.412325000	5.226835000
C	1.440168000	18.906219000	6.493191000
C	1.952011000	20.140277000	6.900124000
C	2.760476000	20.885498000	6.037042000
C	3.074824000	20.391715000	4.770551000
C	3.391133000	19.769953000	1.660418000
C	2.322568000	20.294447000	0.917731000
C	2.522542000	21.397370000	0.090341000
C	3.790118000	21.976857000	-0.008078000
C	4.859870000	21.444661000	0.713284000
C	4.664506000	20.341031000	1.545406000
C	4.637015000	17.572620000	3.103332000
C	4.956231000	16.417040000	2.375316000
C	6.164296000	15.761766000	2.599500000
C	7.058019000	16.250987000	3.555066000
C	6.740173000	17.396237000	4.289678000
C	5.530926000	18.055199000	4.068341000
P	3.995740000	14.704445000	-1.413690000
C	5.568366000	14.155577000	-0.670636000
C	5.544293000	13.024803000	0.158307000
C	6.719652000	12.570566000	0.752078000
C	7.924920000	13.240872000	0.521881000
C	7.949886000	14.369644000	-0.299258000
C	6.774395000	14.832193000	-0.893918000
C	4.384786000	16.309284000	-2.170424000
C	4.856083000	16.422136000	-3.484640000
C	5.182020000	17.678515000	-3.997014000
C	5.043322000	18.817581000	-3.199942000
C	4.568065000	18.706296000	-1.890302000
C	4.231986000	17.456659000	-1.376788000
C	3.689004000	13.541352000	-2.781317000
C	2.362714000	13.332022000	-3.187588000
C	2.083635000	12.453552000	-4.233028000
C	3.125130000	11.775647000	-4.872729000

C	4.445947000	11.978336000	-4.465783000
C	4.730709000	12.858150000	-3.420921000
P	2.122766000	11.121994000	2.448301000
C	3.112176000	10.505286000	1.046441000
C	2.630321000	10.737308000	-0.251437000
C	3.362962000	10.308235000	-1.355686000
C	4.582188000	9.653394000	-1.171709000
C	5.066319000	9.420594000	0.117663000
C	4.336537000	9.846229000	1.226914000
C	1.155640000	9.714058000	3.064213000
C	1.687715000	8.416185000	3.094332000
C	0.917185000	7.362397000	3.580616000
C	-0.388678000	7.597030000	4.024488000
C	-0.920015000	8.887058000	3.990174000
C	-0.150142000	9.949252000	3.515543000
C	3.371894000	11.471758000	3.726944000
C	3.432233000	10.766570000	4.933523000
C	4.429899000	11.065706000	5.864520000
C	5.375965000	12.052437000	5.585869000
C	5.310514000	12.762822000	4.382663000
C	4.301527000	12.492290000	3.465528000
P	0.025185000	14.716072000	5.808707000
C	-0.312311000	12.998254000	6.306359000
C	-1.623479000	12.510393000	6.172391000
C	-1.916049000	11.198868000	6.534448000
C	-0.901996000	10.360190000	7.009786000
C	0.404650000	10.835679000	7.114841000
C	0.704823000	12.154109000	6.764970000
C	-1.089173000	15.728557000	6.826485000
C	-1.513556000	16.963766000	6.316608000
C	-2.317861000	17.798382000	7.091337000
C	-2.708857000	17.398686000	8.371511000
C	-2.299121000	16.161880000	8.876529000
C	-1.491442000	15.325270000	8.107473000
C	1.705389000	15.099264000	6.398209000
C	1.949386000	15.468635000	7.728236000
C	3.235915000	15.831025000	8.123453000
C	4.279977000	15.826837000	7.195009000
C	4.041952000	15.444257000	5.874993000
C	2.760045000	15.079454000	5.473187000
H	2.566574000	14.800015000	4.436643000
H	4.852138000	15.441588000	5.149868000
H	5.280882000	16.129353000	7.500434000
H	3.420041000	16.128875000	9.154400000
H	1.131859000	15.494061000	8.447371000
H	1.724769000	12.527974000	6.851629000
H	1.195239000	10.180844000	7.477841000
H	-1.131360000	9.333222000	7.289957000
H	-2.936873000	10.829137000	6.445580000
H	-2.411715000	13.164640000	5.798229000
H	-1.181783000	14.354470000	8.492900000
H	-2.614358000	15.845666000	9.869668000
H	-3.344073000	18.047034000	8.973432000
H	-2.647601000	18.755587000	6.691065000
H	-1.214469000	17.261437000	5.310712000
H	8.001207000	15.734495000	3.731691000
H	6.402042000	14.864247000	2.032437000
H	4.241531000	16.017093000	1.652513000
H	7.429889000	17.773622000	5.043187000
H	5.268781000	18.929411000	4.663252000
H	1.339966000	17.456931000	4.890635000
H	0.797472000	18.329738000	7.157027000
H	1.709992000	20.528417000	7.888784000
H	3.143765000	21.856344000	6.347800000
H	3.696587000	20.977052000	4.093187000
H	5.502638000	19.918709000	2.097500000
H	5.851475000	21.884879000	0.624702000
H	3.945311000	22.836960000	-0.658056000

H	1.690696000	21.800245000	-0.483900000
H	1.338751000	19.828727000	0.988101000
H	3.835708000	17.368729000	-0.364614000
H	4.446491000	19.593274000	-1.271488000
H	5.294830000	19.797450000	-3.604321000
H	5.540052000	17.766913000	-5.021768000
H	4.958049000	15.533453000	-4.106872000
H	5.759340000	13.004182000	-3.092257000
H	5.257153000	11.446879000	-4.960576000
H	2.905436000	11.084600000	-5.685665000
H	1.052731000	12.291711000	-4.544076000
H	1.553862000	13.851345000	-2.670685000
H	1.691785000	11.276346000	-0.387063000
H	2.988265000	10.498802000	-2.359846000
H	5.160747000	9.331271000	-2.036487000
H	6.020249000	8.915093000	0.259250000
H	4.726239000	9.690267000	2.232827000
H	2.700654000	9.987281000	5.141495000
H	6.158879000	12.278061000	6.309107000
H	6.035775000	13.544170000	4.166110000
H	4.231206000	13.069416000	2.543196000
H	4.470495000	10.519295000	6.805780000
H	2.696195000	8.230153000	2.726882000
H	1.329292000	6.354251000	3.599290000
H	-0.994988000	6.767550000	4.387383000
H	-1.938972000	9.068545000	4.326900000
H	-0.556570000	10.961973000	3.487555000
H	6.792577000	15.719696000	-1.525162000
H	8.885328000	14.898086000	-0.476334000
H	8.843299000	12.886779000	0.988351000
H	6.687367000	11.698179000	1.401474000
H	4.603213000	12.503141000	0.333068000

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[AsAu4 (PPh3)4]+ Tetrahedro

Au	12.074520000	11.949428000	5.726684000
Au	8.285450000	11.990409000	4.469078000
Au	9.552482000	9.151104000	7.078340000
Au	10.730415000	9.058389000	3.262715000
P	11.210517000	7.634550000	1.529672000
C	9.937870000	6.349524000	1.316382000
C	9.644556000	5.807420000	0.057876000
C	8.669507000	4.816675000	-0.062743000
C	7.984452000	4.367424000	1.068235000
C	8.271889000	4.910264000	2.324201000
C	9.243161000	5.902127000	2.450831000
C	12.783848000	6.739544000	1.735488000
C	13.878691000	7.444373000	2.260668000
C	15.106410000	6.803917000	2.417311000
C	15.245854000	5.458356000	2.063716000
C	14.155877000	4.754383000	1.549990000
C	12.924952000	5.391386000	1.384046000
C	11.338001000	8.442734000	-0.097617000
C	12.265511000	8.025772000	-1.060876000
C	12.299338000	8.650260000	-2.309192000
C	11.411714000	9.687422000	-2.597509000
C	10.488904000	10.108329000	-1.634661000
C	10.452866000	9.493161000	-0.384959000
H	10.169667000	6.169306000	-0.824987000
H	8.437114000	4.404010000	-1.043120000
H	7.215820000	3.602384000	0.968705000
H	7.728549000	4.569632000	3.204018000
H	9.457209000	6.347840000	3.423542000
H	13.757358000	8.489035000	2.549191000
H	15.955384000	7.349971000	2.826208000
H	16.203561000	4.957392000	2.196425000
H	14.259168000	3.704968000	1.279487000
H	12.071744000	4.839757000	0.989448000
H	12.961572000	7.219245000	-0.833000000

H	13.025070000	8.327032000	-3.054304000
H	11.443972000	10.174219000	-3.571421000
H	9.802097000	10.922948000	-1.857044000
H	9.745340000	9.824475000	0.376574000
P	8.985244000	7.760466000	8.813623000
C	10.218565000	6.466635000	9.163594000
C	10.402104000	5.962777000	10.457489000
C	11.323576000	4.939155000	10.681015000
C	12.065172000	4.419187000	9.618450000
C	11.889844000	4.925911000	8.327999000
C	10.972340000	5.951058000	8.098402000
C	7.440037000	6.854796000	8.473281000
C	6.444714000	7.498945000	7.721573000
C	5.259148000	6.831119000	7.420140000
C	5.062531000	5.518635000	7.860798000
C	6.051933000	4.875963000	8.607853000
C	7.240891000	5.539929000	8.913045000
C	8.739891000	8.595305000	10.412796000
C	7.742891000	8.200786000	11.312679000
C	7.635512000	8.835273000	12.551653000
C	8.518544000	9.861301000	12.893569000
C	9.508560000	10.261403000	11.991688000
C	9.618668000	9.635879000	10.751767000
H	9.829993000	6.373897000	11.288369000
H	11.466152000	4.552357000	11.689018000
H	12.788446000	3.624649000	9.798192000
H	12.476995000	4.528009000	7.501597000
H	10.841978000	6.364009000	7.097458000
H	6.616684000	8.515297000	7.363145000
H	4.491459000	7.328743000	6.828653000
H	4.141172000	4.993199000	7.614215000
H	5.903245000	3.851124000	8.948503000
H	8.019826000	5.032070000	9.480366000
H	7.051515000	7.403386000	11.042297000
H	6.857085000	8.529690000	13.248401000
H	8.428602000	10.356152000	13.859219000
H	10.190477000	11.067998000	12.252756000
H	10.380866000	9.951167000	10.038908000
P	13.861575000	13.271167000	6.301564000
C	15.332955000	12.971777000	5.271928000
C	16.316817000	13.951252000	5.084798000
C	17.452327000	13.660111000	4.329582000
C	17.606974000	12.395559000	3.754288000
C	16.624039000	11.419297000	3.933908000
C	15.487525000	11.704170000	4.690196000
C	14.442123000	13.065977000	8.017002000
C	13.485771000	13.108656000	9.044562000
C	13.883139000	12.961971000	10.371777000
C	15.232822000	12.761433000	10.682562000
C	16.182505000	12.708124000	9.661925000
C	15.791049000	12.859299000	8.329646000
C	13.478122000	15.047191000	6.160824000
C	14.101175000	16.003562000	6.974364000
C	13.782167000	17.353466000	6.828749000
C	12.842056000	17.752399000	5.874887000
C	12.213136000	16.800221000	5.067901000
C	12.524575000	15.449010000	5.212516000
H	16.190567000	14.939626000	5.524513000
H	18.214861000	14.424358000	4.185481000
H	18.491946000	12.174596000	3.158485000
H	16.739125000	10.437935000	3.476298000
H	14.707692000	10.953677000	4.828919000
H	12.433485000	13.255012000	8.796814000
H	13.139361000	12.998729000	11.167607000
H	15.541929000	12.640202000	11.720168000
H	17.233284000	12.544069000	9.898516000
H	16.533737000	12.812678000	7.534759000
H	14.821956000	15.688761000	7.728946000

H	14.265539000	18.093592000	7.464753000
H	12.595346000	18.807380000	5.765407000
H	11.473358000	17.107685000	4.330425000
H	12.023869000	14.696264000	4.601687000
P	6.545099000	13.386117000	3.917833000
C	5.060447000	13.058541000	4.918850000
C	4.191117000	14.076082000	5.329967000
C	3.042728000	13.758426000	6.057056000
C	2.761689000	12.428970000	6.378038000
C	3.633715000	11.412985000	5.977449000
C	4.783186000	11.724280000	5.253390000
C	5.967954000	13.291167000	2.191033000
C	6.932861000	13.257996000	1.171752000
C	6.533431000	13.205740000	-0.161731000
C	5.173519000	13.175784000	-0.486854000
C	4.213482000	13.201106000	0.525251000
C	4.606624000	13.258349000	1.863558000
C	6.962390000	15.142788000	4.164726000
C	6.283169000	16.161022000	3.480134000
C	6.629973000	17.495262000	3.695933000
C	7.658606000	17.817050000	4.585408000
C	8.342755000	16.804283000	5.262832000
C	7.997636000	15.468936000	5.053751000
H	4.413889000	15.114424000	5.088955000
H	2.369671000	14.552839000	6.377464000
H	1.868045000	12.185442000	6.951518000
H	3.421057000	10.377173000	6.238680000
H	5.476495000	10.939146000	4.948605000
H	7.992944000	13.267629000	1.430831000
H	7.282842000	13.183247000	-0.951966000
H	4.863126000	13.126329000	-1.529661000
H	3.153916000	13.172091000	0.275489000
H	3.857348000	13.269928000	2.653435000
H	5.496785000	15.907353000	2.768989000
H	6.102894000	18.284307000	3.161843000
H	7.932792000	18.859946000	4.743331000
H	9.152163000	17.051261000	5.947985000
H	8.536475000	14.670232000	5.565296000
As	10.151463000	10.542107000	5.141028000
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[AsAu4(PPh3)4]+ Planar			
Au	1.465575000	16.837263000	1.937859000
Au	2.191000000	14.841377000	-0.000474000
Au	0.944489000	13.022636000	1.790143000
Au	-0.105746000	15.003083000	3.514122000
As	-0.203658000	15.166081000	0.952305000
P	2.990037000	18.344391000	2.768372000
C	2.562582000	19.105896000	4.364248000
C	1.740244000	18.375576000	5.232854000
C	1.471165000	18.859175000	6.511366000
C	2.006272000	20.082424000	6.919367000
C	2.802457000	20.827456000	6.045365000
C	3.082430000	20.343218000	4.767471000
C	3.340767000	19.748709000	1.658004000
C	2.264228000	20.283051000	0.932986000
C	2.453218000	21.400768000	0.122842000
C	3.717767000	21.987217000	0.024160000
C	4.795118000	21.445779000	0.727922000
C	4.610656000	20.326855000	1.542154000
C	4.599863000	17.540113000	3.068102000
C	4.902878000	16.370890000	2.356270000
C	6.120497000	15.727037000	2.559639000
C	7.041356000	16.243065000	3.474386000
C	6.739563000	17.401416000	4.194220000
C	5.519671000	18.047331000	3.996500000
P	4.026143000	14.698224000	-1.371896000
C	5.602267000	14.146256000	-0.640515000
C	5.591197000	12.992032000	0.156037000

C	6.771182000	12.536003000	0.739440000
C	7.968922000	13.226437000	0.529271000
C	7.981366000	14.376562000	-0.262027000
C	6.801065000	14.841609000	-0.844401000
C	4.404352000	16.311322000	-2.118738000
C	4.912192000	16.429735000	-3.419523000
C	5.219441000	17.691264000	-3.930045000
C	5.025006000	18.831159000	-3.145289000
C	4.514436000	18.714695000	-1.849741000
C	4.196896000	17.459027000	-1.337873000
C	3.731958000	13.547242000	-2.753795000
C	2.411546000	13.360916000	-3.190073000
C	2.141560000	12.495030000	-4.247982000
C	3.186521000	11.807265000	-4.871982000
C	4.501387000	11.987666000	-4.435973000
C	4.776660000	12.854328000	-3.377728000
P	2.095605000	11.151267000	2.436167000
C	3.096203000	10.517121000	1.048961000
C	2.639139000	10.751514000	-0.257035000
C	3.385717000	10.312365000	-1.348521000
C	4.594722000	9.645200000	-1.143136000
C	5.054815000	9.409970000	0.154941000
C	4.311061000	9.845533000	1.250889000
C	1.125401000	9.753562000	3.072707000
C	1.655896000	8.456699000	3.130346000
C	0.886284000	7.413880000	3.642254000
C	-0.417597000	7.657843000	4.083814000
C	-0.949305000	8.946140000	4.019628000
C	-0.179770000	9.997669000	3.519538000
C	3.345535000	11.507396000	3.710508000
C	3.406468000	10.806727000	4.919489000
C	4.413741000	11.098002000	5.842018000
C	5.369378000	12.071413000	5.551762000
C	5.303373000	12.777281000	4.346737000
C	4.284046000	12.515542000	3.437992000
P	0.032574000	14.694692000	5.780395000
C	-0.316989000	12.988852000	6.307685000
C	-1.635114000	12.514574000	6.204415000
C	-1.935262000	11.210951000	6.588729000
C	-0.922163000	10.365827000	7.054502000
C	0.390884000	10.827248000	7.129249000
C	0.698564000	12.138041000	6.758480000
C	-1.061026000	15.732885000	6.797664000
C	-1.477006000	16.965467000	6.274603000
C	-2.258219000	17.823561000	7.047458000
C	-2.635279000	17.449828000	8.339385000
C	-2.235331000	16.215072000	8.858021000
C	-1.450098000	15.355676000	8.091130000
C	1.718828000	15.065255000	6.355520000
C	1.979159000	15.382570000	7.696277000
C	3.269981000	15.728801000	8.090805000
C	4.302015000	15.761699000	7.149802000
C	4.046665000	15.435128000	5.817834000
C	2.759575000	15.086407000	5.416640000
H	2.550393000	14.851328000	4.371614000
H	4.848301000	15.462123000	5.084352000
H	5.307216000	16.050748000	7.455275000
H	3.467180000	15.984637000	9.130930000
H	1.171118000	15.377209000	8.425886000
H	1.723355000	12.501689000	6.821484000
H	1.181231000	10.166864000	7.482800000
H	-1.158122000	9.344685000	7.350152000
H	-2.960882000	10.851895000	6.523277000
H	-2.422617000	13.173589000	5.837275000
H	-1.149507000	14.386230000	8.487649000
H	-2.540175000	15.918290000	9.860266000
H	-3.254037000	18.115571000	8.939264000
H	-2.580287000	18.778798000	6.636448000

H	-1.188749000	17.242084000	5.259498000
H	7.992861000	15.736243000	3.630806000
H	6.346587000	14.817253000	2.008115000
H	4.169830000	15.953675000	1.661730000
H	7.450961000	17.799779000	4.916851000
H	5.270615000	18.931500000	4.581393000
H	1.317880000	17.429286000	4.895443000
H	0.837866000	18.283078000	7.183966000
H	1.791858000	20.462513000	7.917506000
H	3.203720000	21.790401000	6.357025000
H	3.694847000	20.928770000	4.082313000
H	5.455292000	19.898731000	2.079843000
H	5.784300000	21.891304000	0.639887000
H	3.864726000	22.859480000	-0.611567000
H	1.614858000	21.810555000	-0.437395000
H	1.282341000	19.813404000	1.003877000
H	3.770705000	17.366729000	-0.337870000
H	4.349736000	19.601579000	-1.240981000
H	5.261191000	19.815339000	-3.549011000
H	5.605756000	17.783399000	-4.943992000
H	5.056593000	15.540442000	-4.032474000
H	5.800251000	12.983261000	-3.027569000
H	5.315656000	11.449882000	-4.918990000
H	2.974101000	11.127040000	-5.695784000
H	1.114996000	12.351634000	-4.581895000
H	1.600330000	13.888848000	-2.686190000
H	1.708913000	11.301024000	-0.408332000
H	3.029994000	10.505354000	-2.359151000
H	5.184446000	9.315034000	-1.997339000
H	6.000835000	8.894209000	0.313589000
H	4.683250000	9.688281000	2.263140000
H	2.669130000	10.036019000	5.134980000
H	6.160830000	12.289511000	6.267551000
H	6.036554000	13.548091000	4.122422000
H	4.214619000	13.087573000	2.512553000
H	4.455551000	10.554529000	6.784943000
H	2.663001000	8.262785000	2.765570000
H	1.297772000	6.406640000	3.682942000
H	-1.022271000	6.836940000	4.467879000
H	-1.967684000	9.134552000	4.353157000
H	-0.585337000	11.009340000	3.467939000
H	6.809822000	15.745545000	-1.451806000
H	8.910220000	14.920538000	-0.424928000
H	8.891517000	12.869728000	0.985831000
H	6.748753000	11.644938000	1.363606000
H	4.657294000	12.452610000	0.314437000

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[SbAu4 (PPh3)4]+ Tetrahedro

Au	12.248411000	12.024036000	5.798302000
Au	8.194126000	12.090095000	4.503310000
Au	9.513729000	9.023177000	7.239927000
Au	10.756646000	8.946529000	3.181946000
P	11.218259000	7.542338000	1.407720000
C	9.970393000	6.235541000	1.181012000
C	9.612503000	5.770913000	-0.091588000
C	8.661214000	4.758715000	-0.219751000
C	8.067926000	4.207343000	0.918188000
C	8.420844000	4.671353000	2.188880000
C	9.366018000	5.687044000	2.323047000
C	12.808988000	6.666188000	1.551611000
C	13.924472000	7.389621000	2.003371000
C	15.162184000	6.758856000	2.115580000
C	15.290808000	5.403853000	1.793533000
C	14.180274000	4.681857000	1.353578000
C	12.939346000	5.309674000	1.230467000
C	11.290297000	8.398182000	-0.197494000
C	12.147309000	7.974016000	-1.221109000
C	12.127557000	8.622603000	-2.456853000

C	11.257556000	9.693896000	-2.671488000
C	10.408605000	10.124041000	-1.647919000
C	10.424435000	9.481941000	-0.4111073000
H	10.069083000	6.208174000	-0.979657000
H	8.378747000	4.406116000	-1.211061000
H	7.320648000	3.421788000	0.813926000
H	7.948455000	4.250821000	3.075670000
H	9.630870000	6.071069000	3.309824000
H	13.813428000	8.441897000	2.269638000
H	16.027942000	7.321100000	2.463169000
H	16.256343000	4.908949000	1.891466000
H	14.277368000	3.625237000	1.105903000
H	12.071390000	4.745911000	0.890381000
H	12.828725000	7.141184000	-1.049191000
H	12.795286000	8.291991000	-3.251796000
H	11.248214000	10.200776000	-3.635603000
H	9.739028000	10.967131000	-1.812492000
H	9.773814000	9.817777000	0.397446000
P	8.903532000	7.622258000	8.968842000
C	10.112249000	6.305788000	9.313726000
C	10.317596000	5.807369000	10.606411000
C	11.222515000	4.765364000	10.813646000
C	11.922444000	4.220629000	9.735287000
C	11.724811000	4.721225000	8.445342000
C	10.825498000	5.765295000	8.232656000
C	7.347509000	6.742277000	8.618237000
C	6.329070000	7.443748000	7.954153000
C	5.126590000	6.806316000	7.655619000
C	4.937699000	5.466177000	8.007013000
C	5.951460000	4.765800000	8.662553000
C	7.156503000	5.400492000	8.969521000
C	8.638939000	8.473161000	10.554900000
C	7.717905000	8.003337000	11.500251000
C	7.573975000	8.667370000	12.719387000
C	8.341768000	9.801132000	12.995283000
C	9.254027000	10.276264000	12.049579000
C	9.401960000	9.618178000	10.829398000
H	9.777010000	6.237652000	11.448263000
H	11.384125000	4.383831000	11.820484000
H	12.632675000	3.410748000	9.901488000
H	12.281535000	4.305829000	7.606466000
H	10.678284000	6.174598000	7.232408000
H	6.492907000	8.482467000	7.663912000
H	4.339156000	7.350127000	7.136326000
H	4.001856000	4.965318000	7.761091000
H	5.810170000	3.720114000	8.931058000
H	7.952147000	4.850762000	9.471137000
H	7.109487000	7.126461000	11.277684000
H	6.855179000	8.302839000	13.451220000
H	8.219942000	10.322208000	13.944496000
H	9.843077000	11.168265000	12.259061000
H	10.099370000	9.991373000	10.077927000
P	14.055625000	13.355296000	6.347528000
C	15.557373000	12.913955000	5.418093000
C	16.540727000	13.855531000	5.089547000
C	17.696156000	13.448969000	4.422440000
C	17.870659000	12.106828000	4.076452000
C	16.885090000	11.168019000	4.391568000
C	15.729096000	11.567878000	5.058414000
C	14.554670000	13.302221000	8.099221000
C	13.544179000	13.227906000	9.070348000
C	13.877212000	13.239046000	10.423084000
C	15.217015000	13.316701000	10.813538000
C	16.223760000	13.379510000	9.849476000
C	15.896540000	13.370022000	8.492694000
C	13.737681000	15.120698000	6.021365000
C	14.379651000	16.134856000	6.744786000
C	14.091335000	17.472070000	6.472100000

C	13.158968000	17.801914000	5.485306000
C	12.512055000	16.793239000	4.767015000
C	12.797694000	15.455018000	5.034129000
H	16.400289000	14.903985000	5.349900000
H	18.458820000	14.182974000	4.167779000
H	18.772244000	11.793039000	3.552236000
H	17.014393000	10.123232000	4.110593000
H	14.948380000	10.844458000	5.298190000
H	12.501873000	13.156216000	8.758035000
H	13.092702000	13.178093000	11.175129000
H	15.476822000	13.317223000	11.871751000
H	17.268474000	13.429118000	10.150834000
H	16.683728000	13.406863000	7.740954000
H	15.087642000	15.877807000	7.532451000
H	14.588193000	18.256960000	7.039349000
H	12.929522000	18.847357000	5.281952000
H	11.775682000	17.047769000	4.006273000
H	12.282316000	14.660326000	4.493262000
P	6.451566000	13.495399000	3.936308000
C	4.958809000	13.201087000	4.937192000
C	4.066392000	14.224041000	5.280544000
C	2.914747000	13.924967000	6.009207000
C	2.653311000	12.609735000	6.399999000
C	3.547093000	11.588754000	6.067143000
C	4.699548000	11.881281000	5.340705000
C	5.889515000	13.352108000	2.208552000
C	6.864948000	13.188884000	1.212200000
C	6.485526000	13.100708000	-0.125137000
C	5.133826000	13.168513000	-0.475306000
C	4.161743000	13.321755000	0.514824000
C	4.535911000	13.411471000	1.856669000
C	6.891838000	15.251628000	4.138724000
C	6.225960000	16.266432000	3.437352000
C	6.602955000	17.597008000	3.617497000
C	7.650915000	17.917411000	4.485834000
C	8.323496000	16.907768000	5.177494000
C	7.945591000	15.576576000	5.007326000
H	4.274676000	15.252370000	4.986605000
H	2.223763000	14.722558000	6.277532000
H	1.758108000	12.381955000	6.976382000
H	3.351733000	10.565698000	6.385486000
H	5.413164000	11.094595000	5.091118000
H	7.916622000	13.123870000	1.494675000
H	7.243248000	12.972302000	-0.897175000
H	4.837703000	13.092756000	-1.521075000
H	3.107423000	13.364676000	0.245786000
H	3.775709000	13.518290000	2.629966000
H	5.429041000	16.013163000	2.738054000
H	6.085071000	18.384466000	3.071499000
H	7.949319000	18.957013000	4.615846000
H	9.148722000	17.154781000	5.844200000
H	8.474831000	14.778194000	5.530439000
Sb	10.180671000	10.529162000	5.197961000
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[SbAu4 (PPh3)4]+ Planar			
Au	1.417714000	16.858934000	1.902728000
Au	2.217164000	14.830245000	-0.016037000
Au	0.922411000	13.046711000	1.785294000
Au	-0.210477000	15.028832000	3.488431000
Sb	-0.413772000	15.208627000	0.770642000
P	2.975670000	18.328278000	2.763375000
C	2.547051000	19.074034000	4.365694000
C	1.752752000	18.316442000	5.237938000
C	1.491266000	18.780162000	6.525246000
C	2.001793000	20.013135000	6.936870000
C	2.765980000	20.786844000	6.058292000
C	3.042590000	20.320562000	4.772632000
C	3.326788000	19.737750000	1.659935000

C	2.246881000	20.288240000	0.951742000
C	2.440644000	21.400790000	0.136140000
C	3.713308000	21.965663000	0.014882000
C	4.792928000	21.409643000	0.703673000
C	4.603870000	20.295772000	1.523715000
C	4.584710000	17.522022000	3.056641000
C	4.897076000	16.370490000	2.319712000
C	6.114786000	15.725693000	2.518650000
C	7.024968000	16.221496000	3.454872000
C	6.712738000	17.360865000	4.200564000
C	5.493372000	18.009013000	4.006232000
P	4.069161000	14.687658000	-1.379271000
C	5.658274000	14.147632000	-0.667909000
C	5.673232000	12.971056000	0.095946000
C	6.858603000	12.534943000	0.682777000
C	8.037191000	13.267051000	0.508428000
C	8.025129000	14.437402000	-0.252843000
C	6.838430000	14.882884000	-0.838480000
C	4.423106000	16.303689000	-2.132564000
C	4.943091000	16.421589000	-3.429208000
C	5.228513000	17.684589000	-3.948941000
C	4.999938000	18.826934000	-3.177289000
C	4.477565000	18.710969000	-1.885922000
C	4.182233000	17.453430000	-1.365004000
C	3.760285000	13.535627000	-2.757043000
C	2.435987000	13.363874000	-3.188577000
C	2.151877000	12.498144000	-4.242507000
C	3.186329000	11.794104000	-4.866349000
C	4.504721000	11.960768000	-4.436064000
C	4.794711000	12.828997000	-3.382656000
P	2.134253000	11.221058000	2.483379000
C	3.119245000	10.565063000	1.093418000
C	2.657617000	10.796404000	-0.211693000
C	3.388456000	10.335623000	-1.305202000
C	4.585930000	9.647688000	-1.103181000
C	5.050157000	9.414030000	0.193904000
C	4.322342000	9.871687000	1.291516000
C	1.160817000	9.838503000	3.152554000
C	1.726882000	8.570139000	3.354180000
C	0.949116000	7.537726000	3.873545000
C	-0.397236000	7.762030000	4.180660000
C	-0.962796000	9.021384000	3.976354000
C	-0.185961000	10.063336000	3.467823000
C	3.398501000	11.589137000	3.739550000
C	3.379068000	11.011596000	5.013541000
C	4.390901000	11.311416000	5.928162000
C	5.430809000	12.168255000	5.567752000
C	5.443696000	12.754330000	4.298670000
C	4.420625000	12.488445000	3.395695000
P	-0.003081000	14.673287000	5.750614000
C	-0.398803000	12.974831000	6.269538000
C	-1.722177000	12.526490000	6.118553000
C	-2.068753000	11.239155000	6.517254000
C	-1.095684000	10.382523000	7.043702000
C	0.223465000	10.817340000	7.167497000
C	0.575839000	12.113659000	6.784832000
C	-1.053277000	15.723823000	6.801356000
C	-1.462059000	16.967313000	6.299200000
C	-2.218794000	17.826962000	7.094549000
C	-2.578314000	17.444012000	8.388377000
C	-2.186025000	16.197773000	8.886563000
C	-1.427178000	15.336212000	8.095836000
C	1.703997000	14.984527000	6.296631000
C	2.005756000	15.241016000	7.641321000
C	3.314705000	15.540366000	8.015188000
C	4.322564000	15.591215000	7.049299000
C	4.025275000	15.329621000	5.712117000
C	2.721006000	15.022988000	5.331890000

H	2.480400000	14.836690000	4.283607000
H	4.807263000	15.371008000	4.958595000
H	5.342289000	15.843608000	7.339571000
H	3.544470000	15.746997000	9.059720000
H	1.216377000	15.224255000	8.391043000
H	1.603718000	12.459998000	6.887290000
H	0.982019000	10.147903000	7.570890000
H	-1.367368000	9.373286000	7.349788000
H	-3.099030000	10.900738000	6.414716000
H	-2.477855000	13.194236000	5.703041000
H	-1.136692000	14.356679000	8.474981000
H	-2.479075000	15.892599000	9.890141000
H	-3.177357000	18.111603000	9.006467000
H	-2.534043000	18.791489000	6.699845000
H	-1.187065000	17.252101000	5.282952000
H	7.975973000	15.712460000	3.608951000
H	6.348784000	14.829168000	1.949037000
H	4.170128000	15.966307000	1.610498000
H	7.415043000	17.742297000	4.940997000
H	5.236339000	18.879536000	4.608422000
H	1.346470000	17.364443000	4.896632000
H	0.882370000	18.181726000	7.201507000
H	1.793076000	20.378281000	7.941681000
H	3.146620000	21.757105000	6.374087000
H	3.634316000	20.925057000	4.085227000
H	5.449936000	19.855372000	2.049589000
H	5.787883000	21.838831000	0.598421000
H	3.864556000	22.832658000	-0.626864000
H	1.599901000	21.822794000	-0.411366000
H	1.258988000	19.833614000	1.039499000
H	3.747124000	17.361048000	-0.368678000
H	4.286082000	19.599372000	-1.287475000
H	5.218498000	19.812517000	-3.587733000
H	5.623386000	17.775638000	-4.960128000
H	5.114087000	15.530264000	-4.032281000
H	5.821207000	12.948274000	-3.037450000
H	5.310568000	11.411123000	-4.920052000
H	2.962745000	11.113103000	-5.686594000
H	1.122936000	12.367828000	-4.574485000
H	1.633107000	13.904540000	-2.684736000
H	1.736435000	11.361032000	-0.361439000
H	3.029074000	10.527293000	-2.314781000
H	5.163514000	9.300184000	-1.958794000
H	5.986418000	8.880191000	0.350229000
H	4.699790000	9.716114000	2.301517000
H	2.578335000	10.325904000	5.283920000
H	6.225287000	12.389846000	6.279199000
H	6.241700000	13.438358000	4.018730000
H	4.416824000	12.969185000	2.417726000
H	4.371681000	10.863609000	6.920893000
H	2.769445000	8.389081000	3.096626000
H	1.387565000	6.552215000	4.024124000
H	-1.006716000	6.947781000	4.571485000
H	-2.011826000	9.195022000	4.207629000
H	-0.618093000	11.053298000	3.306785000
H	6.827109000	15.803451000	-1.420388000
H	8.939454000	15.013064000	-0.387430000
H	8.963104000	12.926527000	0.970046000
H	6.855603000	11.626889000	1.282992000
H	4.754127000	12.400202000	0.227439000
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[BiAu4(PPh3)4]+ Tetrahedro			
Au	12.212362000	11.958320000	5.748723000
Au	8.002855000	12.046818000	4.492675000
Au	9.368018000	8.813926000	7.279845000
Au	10.699722000	8.766182000	3.068230000
P	11.226860000	7.475459000	1.233679000
C	10.029021000	6.155242000	0.869958000

C	9.717766000	5.779973000	-0.442705000
C	8.828921000	4.729432000	-0.672789000
C	8.249253000	4.054038000	0.402748000
C	8.553148000	4.431469000	1.714151000
C	9.437664000	5.482705000	1.950296000
C	12.825928000	6.618461000	1.400971000
C	13.883342000	7.305934000	2.016922000
C	15.123064000	6.686897000	2.160576000
C	15.311738000	5.379217000	1.703684000
C	14.259045000	4.692609000	1.096276000
C	13.016626000	5.309368000	0.942711000
C	11.358142000	8.441935000	-0.304125000
C	12.238819000	8.071532000	-1.329010000
C	12.285906000	8.815751000	-2.507757000
C	11.459300000	9.929865000	-2.666400000
C	10.583030000	10.303571000	-1.643881000
C	10.531977000	9.564964000	-0.462426000
H	10.165580000	6.309979000	-1.282430000
H	8.587736000	4.442024000	-1.694925000
H	7.552691000	3.237262000	0.217686000
H	8.091769000	3.912850000	2.553365000
H	9.668058000	5.795117000	2.969684000
H	13.723094000	8.319011000	2.388369000
H	15.942506000	7.219286000	2.640086000
H	16.278375000	4.892695000	1.828710000
H	14.400901000	3.671609000	0.744864000
H	12.193217000	4.770753000	0.474588000
H	12.890461000	7.207995000	-1.199983000
H	12.975014000	8.528896000	-3.300037000
H	11.506559000	10.513910000	-3.584970000
H	9.947250000	11.179750000	-1.762978000
H	9.863035000	9.858722000	0.347474000
P	8.810979000	7.425718000	9.036577000
C	9.986967000	6.058606000	9.287228000
C	10.283343000	5.566210000	10.565053000
C	11.148500000	4.480784000	10.707842000
C	11.720910000	3.887341000	9.580016000
C	11.434142000	4.382897000	8.304899000
C	10.572127000	5.468573000	8.156092000
C	7.193984000	6.612487000	8.822841000
C	6.150397000	7.349811000	8.241164000
C	4.897877000	6.763515000	8.068539000
C	4.683237000	5.439786000	8.463631000
C	5.721441000	4.703948000	9.038558000
C	6.976180000	5.287120000	9.220048000
C	8.718364000	8.260293000	10.649695000
C	7.799542000	7.866685000	11.631381000
C	7.796026000	8.501492000	12.874049000
C	8.703135000	9.529696000	13.138626000
C	9.615643000	9.928343000	12.157100000
C	9.623319000	9.299356000	10.912619000
H	9.840890000	6.032538000	11.444284000
H	11.378471000	4.101689000	11.703082000
H	12.399493000	3.042625000	9.695095000
H	11.891640000	3.930461000	7.426573000
H	10.354602000	5.871869000	7.165667000
H	6.331091000	8.375326000	7.916790000
H	4.088727000	7.335405000	7.616079000
H	3.706768000	4.979215000	8.316802000
H	5.558176000	3.670897000	9.342713000
H	7.788378000	4.710652000	9.661291000
H	7.087573000	7.069472000	11.421618000
H	7.078966000	8.194456000	13.634380000
H	8.692776000	10.027528000	14.108452000
H	10.315854000	10.738092000	12.359513000
H	10.323476000	9.612472000	10.136889000
P	14.033620000	13.290226000	6.220681000
C	15.483105000	12.900997000	5.190669000

C	16.383858000	13.884710000	4.764228000
C	17.514577000	13.519620000	4.031800000
C	17.744989000	12.177965000	3.717986000
C	16.838800000	11.196802000	4.130043000
C	15.708436000	11.554363000	4.863019000
C	14.649185000	13.196193000	7.933416000
C	13.708814000	13.141848000	8.974259000
C	14.138881000	13.128631000	10.299827000
C	15.505813000	13.160362000	10.593741000
C	16.442343000	13.199230000	9.559382000
C	16.017777000	13.215720000	8.229162000
C	13.670059000	15.058401000	5.968658000
C	14.358242000	16.058095000	6.671043000
C	14.037891000	17.399301000	6.462044000
C	13.028911000	17.747260000	5.560281000
C	12.336332000	16.753160000	4.864114000
C	12.653482000	15.410864000	5.067495000
H	16.199192000	14.932761000	5.001313000
H	18.214607000	14.285890000	3.701702000
H	18.626409000	11.898579000	3.141976000
H	17.011301000	10.152121000	3.875178000
H	14.990575000	10.797007000	5.181983000
H	12.644143000	13.107077000	8.737967000
H	13.407719000	13.087379000	11.106010000
H	15.839914000	13.147088000	11.630668000
H	17.507799000	13.214015000	9.784713000
H	16.748401000	13.242833000	7.422137000
H	15.129468000	15.784988000	7.391247000
H	14.570320000	18.172873000	7.012728000
H	12.777154000	18.795744000	5.406073000
H	11.539913000	17.021176000	4.170964000
H	12.103552000	14.626803000	4.544392000
P	6.367377000	13.623289000	4.081218000
C	4.865093000	13.377096000	5.081667000
C	4.065351000	14.447079000	5.503754000
C	2.887689000	14.197960000	6.209126000
C	2.508098000	12.885784000	6.499611000
C	3.309508000	11.817093000	6.088615000
C	4.487313000	12.059526000	5.382700000
C	5.765365000	13.729627000	2.363658000
C	6.720473000	13.748512000	1.334420000
C	6.311023000	13.872493000	0.008683000
C	4.949805000	13.966991000	-0.298880000
C	3.999913000	13.935364000	0.722410000
C	4.403625000	13.815643000	2.053686000
C	6.965321000	15.308939000	4.436615000
C	6.394395000	16.431728000	3.819124000
C	6.876558000	17.707445000	4.113157000
C	7.935086000	17.866980000	5.012182000
C	8.512565000	16.750229000	5.621171000
C	8.030115000	15.472517000	5.336478000
H	4.364430000	15.471752000	5.284915000
H	2.267052000	15.031327000	6.533934000
H	1.590408000	12.697115000	7.054190000
H	3.018297000	10.794108000	6.322684000
H	5.124516000	11.232530000	5.064584000
H	7.780510000	13.668036000	1.579798000
H	7.052965000	13.892145000	-0.788376000
H	4.630963000	14.060372000	-1.336335000
H	2.939171000	14.002928000	0.486527000
H	3.660222000	13.790194000	2.848948000
H	5.587230000	16.304468000	3.097663000
H	6.431223000	18.577109000	3.632704000
H	8.314564000	18.864813000	5.232604000
H	9.345702000	16.871798000	6.311971000
H	8.484396000	14.592844000	5.796146000
Bi	10.060613000	10.388179000	5.166571000

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[BiAu4(PPh3)4]+ Planar

Au	1.434914000	16.818171000	1.919030000
Au	2.278453000	14.767937000	0.050256000
Au	0.938627000	13.070181000	1.889100000
Au	-0.327125000	15.065538000	3.472107000
Bi	-0.498346000	15.195925000	0.663436000
P	3.016248000	18.261935000	2.782029000
C	2.606753000	19.016618000	4.384772000
C	1.744627000	18.312376000	5.236910000
C	1.485006000	18.793036000	6.518445000
C	2.072176000	19.985575000	6.946317000
C	2.909916000	20.705015000	6.088784000
C	3.177315000	20.225551000	4.806860000
C	3.348600000	19.674733000	1.675248000
C	2.247466000	20.265414000	1.034522000
C	2.426772000	21.389167000	0.231051000
C	3.705655000	21.924504000	0.052924000
C	4.805128000	21.326282000	0.670648000
C	4.630423000	20.201395000	1.479083000
C	4.630417000	17.456502000	3.049574000
C	4.945843000	16.329763000	2.276896000
C	6.160234000	15.674816000	2.462443000
C	7.065027000	16.134799000	3.421390000
C	6.749988000	17.248859000	4.201915000
C	5.534509000	17.907893000	4.020054000
P	4.102493000	14.666518000	-1.358603000
C	5.722139000	14.138829000	-0.711992000
C	5.779239000	12.938978000	0.013642000
C	6.985306000	12.511331000	0.562737000
C	8.143156000	13.277634000	0.393508000
C	8.088636000	14.471863000	-0.327350000
C	6.881156000	14.907396000	-0.877905000
C	4.403841000	16.293924000	-2.110807000
C	5.024034000	16.420091000	-3.361691000
C	5.274065000	17.687515000	-3.886595000
C	4.902262000	18.827995000	-3.168400000
C	4.274805000	18.704111000	-1.926874000
C	4.022848000	17.439770000	-1.397883000
C	3.755812000	13.528042000	-2.740817000
C	2.423086000	13.394260000	-3.160412000
C	2.103833000	12.536026000	-4.210322000
C	3.110589000	11.799567000	-4.842307000
C	4.437143000	11.929029000	-4.425128000
C	4.762570000	12.792480000	-3.377604000
P	2.218519000	11.286882000	2.586841000
C	3.158714000	10.638908000	1.158536000
C	2.652612000	10.872289000	-0.129821000
C	3.334433000	10.397527000	-1.249045000
C	4.528933000	9.693555000	-1.089770000
C	5.038528000	9.458598000	0.190446000
C	4.359001000	9.929135000	1.313035000
C	1.271068000	9.886903000	3.261642000
C	1.883891000	8.659472000	3.557896000
C	1.121143000	7.602849000	4.049843000
C	-0.257251000	7.760748000	4.233377000
C	-0.869148000	8.978641000	3.934171000
C	-0.107258000	10.045183000	3.454973000
C	3.522408000	11.645232000	3.804062000
C	3.473178000	11.154272000	5.114499000
C	4.502510000	11.453306000	6.009369000
C	5.588031000	12.227284000	5.597234000
C	5.630052000	12.729593000	4.293238000
C	4.593025000	12.461360000	3.406086000
P	-0.121466000	14.705251000	5.736055000
C	-0.516415000	12.996737000	6.220736000
C	-1.832357000	12.544186000	6.029428000
C	-2.180717000	11.247547000	6.395967000
C	-1.216638000	10.387323000	6.931672000

C	0.096959000	10.826214000	7.094127000
C	0.450855000	12.131003000	6.742623000
C	-1.161150000	15.742610000	6.809195000
C	-1.547535000	17.005771000	6.337353000
C	-2.312423000	17.848097000	7.142712000
C	-2.704391000	17.428718000	8.416680000
C	-2.332429000	16.165360000	8.884378000
C	-1.562071000	15.321672000	8.085188000
C	1.592943000	15.006309000	6.259201000
C	1.904272000	15.359138000	7.579171000
C	3.220274000	15.663698000	7.924010000
C	4.223422000	15.621888000	6.953372000
C	3.916376000	15.262009000	5.639986000
C	2.606035000	14.951734000	5.288852000
H	2.357805000	14.695110000	4.257240000
H	4.694865000	15.231629000	4.881993000
H	5.248075000	15.879664000	7.219674000
H	3.458156000	15.948797000	8.948678000
H	1.117059000	15.415499000	8.329723000
H	1.474010000	12.481411000	6.876101000
H	0.850021000	10.152521000	7.501105000
H	-1.490299000	9.371276000	7.212916000
H	-3.204935000	10.904356000	6.259999000
H	-2.579773000	13.215005000	5.605816000
H	-1.281126000	14.331034000	8.443419000
H	-2.646555000	15.833691000	9.872801000
H	-3.310426000	18.082519000	9.042097000
H	-2.609960000	18.827842000	6.771796000
H	-1.250140000	17.318479000	5.336012000
H	8.013927000	15.618751000	3.564539000
H	6.396656000	14.797235000	1.864848000
H	4.222712000	15.952099000	1.549607000
H	7.447174000	17.602616000	4.959843000
H	5.276824000	18.758308000	4.648576000
H	1.283715000	17.389136000	4.884805000
H	0.818641000	18.238527000	7.177612000
H	1.866645000	20.363040000	7.947232000
H	3.352019000	21.644628000	6.416857000
H	3.821140000	20.790739000	4.133111000
H	5.490709000	19.729815000	1.952545000
H	5.803953000	21.732199000	0.520066000
H	3.844685000	22.802504000	-0.577210000
H	1.569124000	21.845179000	-0.260988000
H	1.253388000	19.837033000	1.168352000
H	3.509385000	17.336325000	-0.441147000
H	3.969144000	19.590161000	-1.374070000
H	5.090284000	19.817229000	-3.585292000
H	5.749776000	17.785013000	-4.861436000
H	5.300479000	15.530033000	-3.925831000
H	5.795515000	12.882278000	-3.043885000
H	5.221723000	11.354337000	-4.915073000
H	2.858395000	11.121862000	-5.657241000
H	1.068382000	12.434853000	-4.531425000
H	1.640132000	13.955603000	-2.647966000
H	1.732033000	11.445427000	-0.246611000
H	2.938310000	10.590008000	-2.244823000
H	5.068298000	9.334183000	-1.964913000
H	5.971765000	8.910834000	0.313237000
H	4.770890000	9.766992000	2.308637000
H	2.636052000	10.531338000	5.425420000
H	6.396344000	12.447575000	6.292859000
H	6.465063000	13.347418000	3.969739000
H	4.617509000	12.873818000	2.398541000
H	4.460255000	11.069354000	7.027671000
H	2.952472000	8.528450000	3.396331000
H	1.598600000	6.649721000	4.277294000
H	-0.853849000	6.926867000	4.603218000
H	-1.942165000	9.102321000	4.070743000

H	-0.574916000	11.004694000	3.225447000
H	6.837524000	15.847370000	-1.425650000
H	8.986063000	15.074355000	-0.457775000
H	9.086085000	12.946042000	0.827503000
H	7.014565000	11.582703000	1.129595000
H	4.874702000	12.346190000	0.146621000