

Understanding the Role of Frustrated Lewis Pairs as ligands in transition metal-catalyzed reactions

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Table S1. EDA-NOCV analyses of the bonding situation of L–AuCl complexes. Energy values (in kcal/mol) were computed at the ZORA-BP86-D3/TZ2P//PCM(DCM)-BP86-D3/6-31G(d)&SDD(f) level.

L–AuCl	L = PPh ₃	L = FLP 1	L = FLP 2	L = FLP 3	L = FLP 4	L = FLP 5	L = FLP 6
ΔE_{int}	-74.2	-87.6	-89.4	-89.3	-88.8	-87.7	-92.8
ΔE_{Pauli}	169.6	215.8	200.7	217.3	192.6	221.9	246.4
ΔE_{elstat}	-163.5 (61.1%)	-188.3 (62.1%)	-192.1 (66.2%)	-199.9 (65.2%)	-188.2 (66.9%)	-194.4 (62.8%)	-205.7 (60.7%)
ΔE_{orb}	-72.0 (29.5%)	-94.8 (31.2%)	-80.1 (27.6%)	-89.7 (29.3%)	-76.9 (27.3%)	-100.4 (32.4%)	-111.1 (32.7%)
ΔE_{dispa}	-8.3 (3.4%)	-20.3 (6.7%)	-17.9 (6.2%)	-17.0 (5.6%)	-16.4 (5.8%)	-14.9 (4.8%)	-22.4 (6.6%)
ΔE_{orb1b}	-43.1 (59.8%)	-44.6 (47.1%)	-43.3 (54.1%)	-42.5 (47.4%)	-44.0 (57.2%)	-42.6 (42.5%)	-44.6 (40.2%)
ΔE_{orb2b}	–	-20.8 (21.9%)	-10.4 (13.0%)	-17.8 (19.8%)	-8.0 (10.4%)	-27.3 (27.2%)	-34.5 (31.0%)
ΔE_{orb3b}	-8.7 (12.1%)	-7.0 (7.4%)	-8.1 (10.1%)	-8.0 (9.0%)	-8.0 (10.4%)	-8.5 (8.4%)	-7.7 (6.9%)
ΔE_{orb4b}	-8.7 (12.1%)	-6.9 (7.3%)	-7.3 (9.1%)	-8.3 (9.2%)	-7.3 (9.4%)	-7.5 (7.4%)	-6.8 (6.2%)
$\Delta E_{\text{orb(rest)[b]}}$	-11.5 (16.0%)	-15.5 (16.4%)	-11.0 (13.7%)	-13.0 (14.5%)	-9.5 (12.4%)	-14.5 (14.5%)	-17.4 (15.7%)
$q(\text{Au})^c$	0.280	0.453	0.343	0.432	0.305	0.514	0.548
$r(\text{Au} \cdots \text{B}) / \text{\AA}_d$	–	2.592 (2.347)	2.963 (2.903)	2.610 (2.663)	3.126	2.416	2.322

^a The values in parentheses give the percentage contribution to the total attractive interactions $\Delta E_{\text{elstat}} + \Delta E_{\text{orb}} + \Delta E_{\text{disp}}$. ^b The values in parentheses give the percentage contribution to the total orbital interactions ΔE_{orb} . ^c Natural charges computed at the PCM(DCM)-BP86-D3/6-31G(d)&SDD(f) level. ^d Experimental values are given within parentheses.

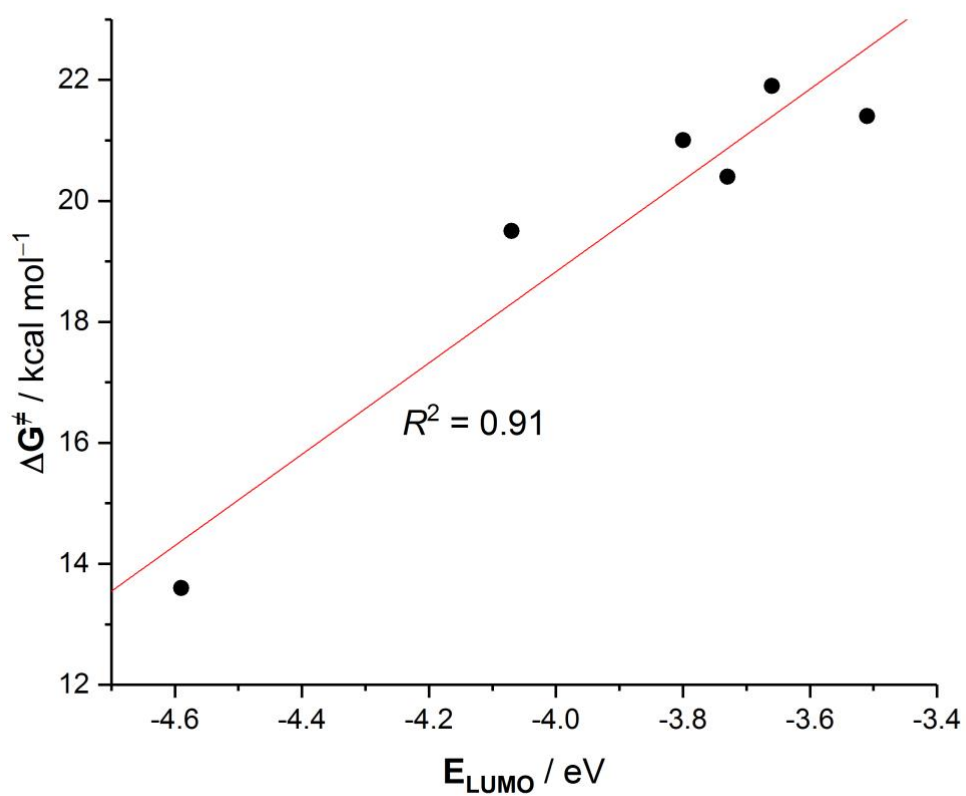


Figure S1. Plot of the computed free energies barriers of the hydroarylation reaction involving the π -complexes $[\text{L-Au-phenylacetylene}]^+$ and mesitylene versus the energy of the LUMO of the reactive π -complexes.

Cartesian coordinates (in Å) and total energies (in a.u., noncorrected ZVPE included) of all the stationary points discussed in the text. All calculations have been performed at the PCM(DCM)-BP86-D3/6-31G(d)&SDD(f) level.

L-AuNTf₂

Ph₃P-AuNTf₂: E= -2999.223824

Au	-0.186429000	-0.030308000	0.034997000
P	2.074499000	-0.012397000	0.000021000
C	2.769030000	-1.349715000	-1.043874000
C	3.945600000	-1.160022000	-1.797985000
C	4.472620000	-2.225917000	-2.545265000
H	5.384395000	-2.075983000	-3.132933000
C	3.831212000	-3.476021000	-2.542156000
C	2.656619000	-3.664836000	-1.792240000
H	2.151234000	-4.636261000	-1.794353000
C	2.121843000	-2.604989000	-1.045573000
C	2.731129000	1.564538000	-0.666160000
C	1.989598000	2.248186000	-1.655014000
C	2.496799000	3.430973000	-2.213217000
H	1.917697000	3.961330000	-2.976377000
C	3.737211000	3.937038000	-1.786552000
C	4.472648000	3.260740000	-0.798308000
H	5.435892000	3.657084000	-0.460308000
C	3.973316000	2.075837000	-0.234428000
N	-2.283588000	-0.005812000	0.016822000
S	-3.052574000	1.203143000	-0.873779000
O	-4.463647000	0.902081000	-1.185166000
O	-2.106329000	1.622594000	-1.932678000
C	-3.051011000	2.602628000	0.408415000
F	-3.636401000	2.174975000	1.540143000
F	-1.777659000	2.963857000	0.671822000
S	-3.119052000	-1.181980000	0.890112000
O	-4.516581000	-0.815720000	1.193197000
O	-2.201793000	-1.653266000	1.952391000
C	-3.174028000	-2.569168000	-0.403074000
F	-1.915033000	-2.965581000	-0.683826000
F	-3.872742000	-3.605081000	0.090408000
F	-3.758912000	-2.113863000	-1.524133000
F	-3.723787000	3.654653000	-0.086735000
C	2.824903000	-0.222989000	1.658850000
C	4.055540000	-0.892783000	1.823738000
C	2.170816000	0.340695000	2.776083000
C	4.629764000	-0.989157000	3.101492000
C	2.752169000	0.241004000	4.048580000
C	3.980865000	-0.423016000	4.211882000
H	4.560076000	-1.339992000	0.960486000
H	1.207822000	0.849307000	2.648325000
H	5.583885000	-1.511475000	3.228006000
H	2.240734000	0.675193000	4.914000000
H	4.429745000	-0.504767000	5.207481000
H	1.200494000	-2.747198000	-0.468307000
H	4.243380000	-4.303288000	-3.129642000
H	4.445352000	-0.185514000	-1.805204000
H	4.545091000	1.554521000	0.540870000
H	1.015708000	1.861367000	-1.978279000
H	4.127823000	4.863754000	-2.220186000

FLP1-AuNTf₂: E= -4969.756390

Au	0.429365000	0.445058000	-0.336874000
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P	-1.815633000	0.922130000	-0.115438000
C	-2.194085000	0.786437000	1.687567000
C	-1.421845000	-0.127366000	2.336001000
H	-1.561313000	-0.224150000	3.427554000
Si	-3.369548000	1.900578000	2.719873000
C	-2.264217000	3.006449000	3.793238000
H	-1.837408000	3.834023000	3.201174000
H	-1.427324000	2.428471000	4.224037000
H	-2.848545000	3.444876000	4.622507000
C	-4.540219000	2.986645000	1.701627000
H	-5.281473000	3.432421000	2.390958000
H	-5.099575000	2.429859000	0.930029000
H	-3.999043000	3.807079000	1.201387000
C	-4.383426000	0.748796000	3.838206000
H	-4.903078000	1.344241000	4.611065000
H	-3.747549000	0.006452000	4.352183000
H	-5.147440000	0.197789000	3.262832000
C	-2.191363000	2.665829000	-0.604323000
C	-3.277766000	3.031887000	-1.460019000
C	-3.495886000	4.399053000	-1.717424000
H	-4.333502000	4.675573000	-2.369228000
C	-2.710690000	5.417928000	-1.156174000
C	-1.673018000	5.035370000	-0.292399000
H	-1.058709000	5.810453000	0.182155000
C	-1.385167000	3.688237000	-0.008144000
C	-4.270240000	2.072115000	-2.089363000
H	-5.086002000	2.642791000	-2.562597000
H	-4.726608000	1.392435000	-1.351774000
H	-3.813850000	1.436701000	-2.866624000
C	-2.967398000	6.872763000	-1.476614000
H	-2.689982000	7.528131000	-0.633014000
H	-4.027149000	7.052780000	-1.726258000
H	-2.365504000	7.190325000	-2.349466000
C	-0.216055000	3.432856000	0.921189000
H	-0.021162000	4.325843000	1.539472000
H	0.710034000	3.233291000	0.356716000
H	-0.359814000	2.585274000	1.607716000
C	-2.722039000	-0.316356000	-1.149840000
C	-2.214791000	-0.549386000	-2.464321000
C	-2.713043000	-1.638336000	-3.200940000
H	-2.307318000	-1.818677000	-4.203998000
C	-3.707561000	-2.491666000	-2.698669000
C	-4.261270000	-2.177669000	-1.446534000
H	-5.080597000	-2.794701000	-1.057484000
C	-3.802217000	-1.106299000	-0.659390000
C	-1.188815000	0.336436000	-3.146521000
H	-0.158860000	-0.025046000	-2.967696000
H	-1.239343000	1.389529000	-2.820282000
H	-1.351794000	0.322100000	-4.238429000
C	-4.146955000	-3.721634000	-3.457753000
H	-3.991941000	-3.609087000	-4.544299000
H	-5.209958000	-3.955934000	-3.275158000
H	-3.555256000	-4.594005000	-3.125375000
C	-4.539976000	-0.836873000	0.634262000
H	-5.486515000	-1.402033000	0.655221000
H	-4.793145000	0.231143000	0.745063000
H	-3.959989000	-1.123630000	1.524950000
B	-0.393139000	-1.157611000	1.701328000
C	1.110126000	-1.153279000	2.142667000
F	0.894521000	1.022838000	3.132857000
C	1.667646000	-0.042765000	2.823832000

F	3.508136000	1.142584000	3.775931000
C	3.020737000	0.054104000	3.156952000
F	5.191052000	-0.912579000	3.094259000
C	3.884135000	-0.996015000	2.809310000
F	4.204163000	-3.159127000	1.874694000
C	3.376843000	-2.140623000	2.174208000
F	1.589156000	-3.350176000	1.289040000
C	2.014375000	-2.208937000	1.870523000
C	-1.082012000	-2.415708000	1.006288000
F	-2.575822000	-2.593793000	2.869407000
C	-2.170715000	-3.035347000	1.647099000
F	-3.946085000	-4.634672000	1.743171000
C	-2.897238000	-4.095184000	1.090894000
C	-2.535916000	-4.573257000	-0.175681000
F	-3.245810000	-5.558244000	-0.756583000
F	-1.139285000	-4.419971000	-2.093590000
C	-1.458619000	-3.990143000	-0.856014000
F	0.272294000	-2.421890000	-0.970314000
C	-0.749369000	-2.946387000	-0.252824000
N	2.546353000	0.326418000	-0.707798000
S	3.104997000	-0.463053000	-2.097796000
O	4.093871000	0.347138000	-2.845910000
O	1.936929000	-1.056760000	-2.783178000
C	4.059715000	-1.926634000	-1.352487000
F	4.900001000	-1.493606000	-0.398418000
F	3.184212000	-2.800063000	-0.824003000
S	3.455213000	1.643100000	-0.143667000
O	4.909557000	1.386178000	-0.142686000
O	2.767480000	2.116267000	1.077784000
C	3.124404000	3.021652000	-1.458729000
F	2.072155000	2.682641000	-2.238670000
F	2.828351000	4.155858000	-0.797650000
F	4.208698000	3.206481000	-2.216910000
F	4.755019000	-2.523428000	-2.335650000

FLP2-AuNTf₂: E= -3267.534796

P	2.048289000	-1.751204000	-0.514997000
C	3.214621000	0.739603000	0.020441000
C	1.438853000	1.039656000	2.077743000
H	1.488891000	-0.063051000	2.241486000
B	1.823951000	1.296263000	0.550606000
C	4.683776000	-0.919366000	-1.068868000
H	4.826641000	-1.902809000	-1.529128000
C	4.333140000	1.609422000	0.073342000
H	4.215894000	2.606457000	0.513549000
C	0.613812000	4.836176000	-0.677422000
H	-0.467441000	4.683576000	-0.484783000
H	0.868480000	5.851110000	-0.315238000
C	1.310942000	2.223553000	-1.893511000
H	2.400602000	2.319443000	-2.078853000
H	1.019274000	1.215642000	-2.247817000
C	2.393508000	-2.807455000	1.005275000
H	2.722337000	-2.041768000	1.735580000
C	0.553728000	3.298619000	-2.694738000
H	0.789533000	3.208685000	-3.773030000
H	-0.532301000	3.119158000	-2.589839000
C	2.525117000	1.641198000	3.024981000
H	3.528820000	1.271810000	2.743354000
H	2.547221000	2.743705000	2.899257000
C	3.423690000	-0.543377000	-0.550004000
C	1.410213000	3.778990000	0.114328000

H	1.217766000	3.889465000	1.197266000
H	2.493969000	3.960432000	-0.037624000
C	5.588831000	1.234946000	-0.427591000
H	6.428775000	1.936277000	-0.371053000
C	0.034578000	1.508831000	2.518400000
H	-0.046840000	2.605939000	2.380491000
H	-0.734719000	1.056719000	1.872290000
C	1.049897000	2.335312000	-0.373179000
H	-0.039013000	2.226790000	-0.195353000
C	2.175493000	-2.780043000	-2.068180000
H	3.180057000	-3.243665000	-2.061852000
C	5.765687000	-0.030587000	-1.011523000
H	6.738158000	-0.325448000	-1.419391000
C	1.127075000	-3.489478000	1.558275000
H	0.701331000	-4.213638000	0.842946000
H	0.341850000	-2.753250000	1.805036000
H	1.385554000	-4.040104000	2.481015000
C	2.043732000	-1.850062000	-3.291034000
H	2.159081000	-2.441103000	-4.217179000
H	2.806692000	-1.053149000	-3.291115000
H	1.047007000	-1.371963000	-3.311500000
C	0.882808000	4.715982000	-2.189062000
H	1.952939000	4.938080000	-2.383153000
H	0.295362000	5.471543000	-2.745354000
C	2.231865000	1.305806000	4.501268000
H	2.997701000	1.768438000	5.153735000
H	2.315654000	0.207623000	4.638209000
C	3.551212000	-3.794901000	0.772357000
H	3.798147000	-4.297392000	1.724595000
H	4.464627000	-3.288240000	0.416087000
H	3.277015000	-4.578573000	0.044165000
C	1.109040000	-3.891585000	-2.086467000
H	0.092147000	-3.463884000	-2.017119000
H	1.237157000	-4.614108000	-1.263500000
H	1.179963000	-4.449074000	-3.037661000
C	0.820598000	1.759431000	4.920360000
H	0.767891000	2.867017000	4.870137000
H	0.624498000	1.479980000	5.973308000
C	-0.252059000	1.163270000	3.989809000
H	-1.259212000	1.520755000	4.278404000
H	-0.266192000	0.059639000	4.098731000
N	-2.008558000	-0.169849000	-0.153976000
S	-2.761821000	0.717939000	-1.377628000
O	-4.090545000	0.185587000	-1.749453000
O	-1.713796000	0.947753000	-2.396349000
C	-3.084788000	2.426874000	-0.552006000
F	-4.366344000	2.505448000	-0.176084000
F	-2.286553000	2.595085000	0.519590000
S	-2.916594000	-0.840797000	1.094670000
O	-4.115660000	-0.028493000	1.394969000
O	-1.958334000	-1.231703000	2.153147000
C	-3.523432000	-2.500894000	0.369486000
F	-2.534989000	-3.056107000	-0.368751000
F	-3.822961000	-3.317233000	1.394866000
F	-4.603909000	-2.314869000	-0.398025000
F	-2.815777000	3.383022000	-1.461551000
Au	-0.014241000	-0.824411000	-0.368935000

FLP3-AuNTf₂: E= -3259.248010

Au	0.281904000	-0.518386000	-0.260046000
B	1.665119000	1.448302000	0.777225000

C	3.189466000	1.058925000	0.634766000
C	3.654842000	-0.169604000	0.105243000
C	5.025050000	-0.512443000	0.120013000
H	5.363490000	-1.478846000	-0.268603000
C	5.959515000	0.390153000	0.645658000
H	7.022846000	0.129071000	0.661941000
C	5.523649000	1.631042000	1.146106000
H	6.252378000	2.342978000	1.549437000
C	4.159194000	1.957607000	1.142127000
H	3.834527000	2.921507000	1.551997000
C	2.616284000	-2.965530000	0.024043000
H	3.664619000	-3.252621000	-0.187893000
C	1.657061000	-3.945193000	-0.677466000
H	1.786425000	-4.955674000	-0.250456000
H	1.841366000	-4.011955000	-1.763622000
H	0.605174000	-3.642191000	-0.522043000
C	2.394640000	-2.933382000	1.549260000
H	1.359448000	-2.627083000	1.788907000
H	3.085769000	-2.232704000	2.049090000
H	2.561114000	-3.941286000	1.969346000
C	2.683698000	-1.263906000	-2.501164000
H	1.843611000	-1.873543000	-2.885545000
C	4.020021000	-1.909723000	-2.906633000
H	4.076591000	-1.960966000	-4.008776000
H	4.131787000	-2.936877000	-2.518032000
H	4.875238000	-1.305537000	-2.557220000
C	2.545111000	0.172158000	-3.044071000
H	3.329208000	0.829005000	-2.625842000
H	1.561594000	0.609722000	-2.797923000
H	2.655105000	0.163956000	-4.142972000
C	0.818192000	1.264715000	2.097113000
C	0.990306000	0.455455000	3.229626000
H	1.824292000	-0.255934000	3.269546000
C	0.085889000	0.552134000	4.305364000
H	0.213246000	-0.080236000	5.191017000
C	-0.992650000	1.450310000	4.237974000
H	-1.699733000	1.511982000	5.073030000
C	-1.176764000	2.283058000	3.112515000
H	-2.012302000	2.992342000	3.085473000
C	-0.267198000	2.197102000	2.053650000
C	-0.193243000	3.015895000	0.814531000
C	-0.984786000	4.105240000	0.434882000
H	-1.829065000	4.432810000	1.052114000
C	-0.671401000	4.794673000	-0.756477000
H	-1.284835000	5.650983000	-1.059272000
C	0.413649000	4.399273000	-1.557885000
H	0.640910000	4.949241000	-2.477875000
C	1.207541000	3.298506000	-1.174674000
H	2.060499000	2.993029000	-1.792748000
C	0.916579000	2.602912000	0.008396000
N	-1.827292000	-0.314408000	-0.170881000
S	-2.662640000	-0.145741000	-1.623975000
O	-3.998426000	-0.783313000	-1.579434000
O	-1.719528000	-0.432255000	-2.730907000
C	-2.941149000	1.730380000	-1.676880000
F	-3.327626000	2.174368000	-0.470549000
F	-1.791178000	2.320478000	-2.040652000
S	-2.625517000	-0.938381000	1.184189000
O	-3.938717000	-0.303914000	1.421046000
O	-1.603689000	-1.021356000	2.246974000
C	-2.962979000	-2.772071000	0.693968000

F	-2.156031000	-3.132087000	-0.331267000
F	-2.681055000	-3.539002000	1.762309000
F	-4.242026000	-2.940983000	0.340560000
F	-3.895687000	1.998496000	-2.587214000
P	2.396296000	-1.242948000	-0.651527000

FLP4-AuNTf₂: E= -3147.299500

B	-2.245203000	-0.228072000	1.757444000
C	-3.077305000	-1.157122000	0.754301000
P	-2.132823000	-1.054466000	-0.854770000
H	-3.097002000	-2.221730000	1.040163000
C	-2.684000000	1.275220000	1.866028000
C	-4.032764000	1.552641000	2.207886000
C	-4.509028000	2.869393000	2.304573000
C	-3.652676000	3.947905000	2.020878000
C	-2.317477000	3.697021000	1.661252000
C	-1.837086000	2.379249000	1.600569000
C	-1.075171000	-0.845526000	2.600962000
C	0.033939000	-0.062463000	3.022639000
C	1.112036000	-0.630180000	3.714057000
C	1.090348000	-1.994489000	4.052524000
C	-0.014276000	-2.785331000	3.691740000
C	-1.071024000	-2.217720000	2.965040000
H	-4.114612000	-0.826565000	0.573658000
H	-4.723907000	0.722710000	2.404380000
H	-5.552637000	3.054239000	2.583959000
H	-4.026203000	4.976696000	2.075378000
H	-1.644574000	4.529724000	1.425944000
H	-0.800711000	2.209429000	1.295174000
H	-1.923204000	-2.853590000	2.697252000
H	-0.046422000	-3.845051000	3.968740000
H	1.928726000	-2.439042000	4.600517000
H	1.969913000	-0.008090000	3.990287000
H	0.073010000	1.000548000	2.772509000
C	-3.146852000	0.004164000	-2.074082000
C	-1.877046000	-2.866153000	-1.418795000
C	-1.321871000	-2.889764000	-2.858909000
H	-0.438618000	-2.235067000	-2.965735000
H	-1.005907000	-3.922736000	-3.096398000
H	-2.080104000	-2.598524000	-3.604824000
C	-0.814318000	-3.479011000	-0.472217000
H	-1.093192000	-3.401325000	0.591484000
H	-0.709089000	-4.553269000	-0.715056000
H	0.172048000	-3.000756000	-0.600718000
C	-3.177244000	-3.694477000	-1.331146000
H	-3.973702000	-3.312340000	-1.987541000
H	-2.950435000	-4.728874000	-1.649758000
H	-3.572881000	-3.750573000	-0.302609000
C	-2.268546000	0.361390000	-3.297212000
H	-1.357431000	0.905540000	-2.990882000
H	-1.964231000	-0.518151000	-3.883772000
H	-2.853654000	1.022366000	-3.963683000
C	-3.504832000	1.321760000	-1.349551000
H	-4.007353000	1.987366000	-2.076053000
H	-4.189650000	1.175823000	-0.498795000
H	-2.607014000	1.841128000	-0.973437000
C	-4.435888000	-0.712431000	-2.524252000
H	-4.223638000	-1.571759000	-3.181885000
H	-5.042768000	-1.061653000	-1.670129000
H	-5.054534000	-0.000452000	-3.101584000
N	1.964187000	0.432601000	-0.359804000

S	3.088315000	-0.715273000	-0.875124000
O	4.401342000	-0.153198000	-1.249190000
O	2.375348000	-1.643772000	-1.783977000
C	3.327695000	-1.667614000	0.748289000
F	3.649946000	-0.806670000	1.730192000
F	2.182240000	-2.303073000	1.061440000
S	2.400816000	1.974427000	0.141715000
O	3.844963000	2.134583000	0.403795000
O	1.403323000	2.422984000	1.138925000
C	2.011305000	2.945930000	-1.442853000
F	0.678393000	2.932223000	-1.663769000
F	2.428861000	4.214485000	-1.300100000
F	2.638810000	2.371534000	-2.485130000
F	4.313680000	-2.567785000	0.590327000
Au	-0.066101000	-0.146315000	-0.539145000

FLP5-AuNTf₂: E= -3260.344058

Au	0.289344000	-0.310893000	0.395013000
B	0.430605000	-1.300849000	2.584388000
C	-2.166420000	-1.147999000	2.489471000
P	-1.950021000	-0.450961000	0.827504000
C	-1.034380000	-1.534693000	3.119559000
H	-1.141930000	-2.035853000	4.096955000
C	-2.480113000	1.296597000	0.568689000
C	-2.631862000	1.746365000	-0.777679000
C	-3.027302000	3.077625000	-0.998984000
H	-3.150936000	3.420079000	-2.033917000
C	-3.249485000	3.981652000	0.052342000
C	-3.036362000	3.525565000	1.364677000
H	-3.172312000	4.223523000	2.200058000
C	-2.641793000	2.207122000	1.652329000
C	-3.033942000	-1.521230000	-0.212500000
C	-4.442720000	-1.302175000	-0.155125000
C	-5.280606000	-2.117515000	-0.940626000
H	-6.363344000	-1.946470000	-0.897647000
C	-4.781197000	-3.133743000	-1.768908000
C	-3.391879000	-3.350086000	-1.776357000
H	-2.982581000	-4.158108000	-2.395138000
C	-2.501973000	-2.574345000	-1.013468000
C	1.415287000	-0.189780000	3.179837000
C	2.663657000	-0.734715000	3.129048000
C	2.663381000	-2.082437000	2.477040000
C	1.414449000	-2.460289000	2.082656000
H	-3.182021000	-1.323769000	2.864272000
C	-2.381983000	0.879438000	-1.998002000
H	-1.490804000	0.235219000	-1.886713000
H	-3.236076000	0.213373000	-2.213953000
H	-2.214423000	1.515822000	-2.882520000
C	-2.390728000	1.842712000	3.101449000
H	-3.118682000	1.104254000	3.481913000
H	-1.386709000	1.407589000	3.244944000
H	-2.466448000	2.740666000	3.736795000
C	-3.646362000	5.415382000	-0.219865000
H	-2.750060000	6.059263000	-0.304227000
H	-4.207135000	5.508264000	-1.165808000
H	-4.266757000	5.825224000	0.595861000
C	-5.114855000	-0.223861000	0.677195000
H	-5.082386000	0.755241000	0.165893000
H	-6.174007000	-0.482200000	0.842721000
H	-4.653701000	-0.077311000	1.667725000
C	-5.698312000	-3.977051000	-2.626184000

H	-5.552651000	-3.748504000	-3.698680000
H	-5.488842000	-5.054077000	-2.496206000
H	-6.759812000	-3.799602000	-2.385016000
C	-1.029334000	-2.916266000	-1.093471000
H	-0.580151000	-3.078862000	-0.098459000
H	-0.879111000	-3.837737000	-1.680337000
H	-0.438705000	-2.120042000	-1.583996000
H	1.194853000	-3.407590000	1.582321000
H	3.586131000	-2.658509000	2.339532000
H	3.587704000	-0.273374000	3.500171000
H	1.192737000	0.787937000	3.616576000
N	2.203556000	0.162768000	-0.359698000
S	2.665951000	1.778316000	-0.367519000
O	4.051688000	1.943451000	-0.859590000
O	2.222449000	2.386708000	0.904449000
C	1.510286000	2.514923000	-1.696630000
F	1.468738000	1.712828000	-2.774583000
S	3.050305000	-0.970498000	-1.291152000
O	3.450074000	-0.458927000	-2.620092000
O	2.296859000	-2.236772000	-1.162969000
C	4.685294000	-1.194432000	-0.288372000
F	4.649349000	-0.485323000	0.853742000
F	4.822576000	-2.500892000	-0.000878000
F	5.715209000	-0.783842000	-1.040000000
F	1.969974000	3.727744000	-2.046632000
F	0.265184000	2.633270000	-1.187216000

FLP6-AuNTf₂: E= -6577.641104

Au	-1.211409000	-0.229689000	0.645629000
P	-2.690722000	0.905909000	-0.731905000
C	-2.018088000	0.935139000	-2.426732000
C	-0.677840000	0.693142000	-2.412721000
H	-0.132247000	0.730012000	-3.368987000
Si	-3.023946000	0.973432000	-4.059473000
C	-3.116325000	-0.813506000	-4.689274000
H	-3.815592000	-1.403548000	-4.070600000
H	-2.133816000	-1.313645000	-4.670835000
H	-3.493536000	-0.822614000	-5.728461000
C	-4.808146000	1.585297000	-3.879185000
H	-5.262104000	1.598403000	-4.887713000
H	-4.905989000	2.601854000	-3.462511000
H	-5.400776000	0.898187000	-3.251750000
C	-2.057760000	2.057760000	-5.275475000
H	-2.543419000	2.033762000	-6.267915000
H	-1.019383000	1.702589000	-5.399833000
H	-2.020572000	3.108023000	-4.937065000
C	-4.309080000	0.025331000	-0.788191000
C	-5.566852000	0.680198000	-0.587114000
C	-6.740546000	-0.088397000	-0.693498000
H	-7.703733000	0.415767000	-0.549421000
C	-6.732535000	-1.459551000	-0.999902000
C	-5.490222000	-2.065444000	-1.243031000
H	-5.456245000	-3.124900000	-1.524274000
C	-4.276908000	-1.361877000	-1.145429000
C	-5.758396000	2.162777000	-0.329161000
H	-6.817311000	2.428858000	-0.480088000
H	-5.158052000	2.791080000	-1.005308000
H	-5.486638000	2.451037000	0.700361000
C	-8.016871000	-2.252522000	-1.067139000
H	-7.935144000	-3.096796000	-1.772939000
H	-8.868933000	-1.620796000	-1.371598000

H	-8.260958000	-2.677041000	-0.074576000
C	-3.011150000	-2.132051000	-1.448467000
H	-3.250413000	-3.053700000	-2.004335000
H	-2.484286000	-2.434733000	-0.527014000
H	-2.300645000	-1.557000000	-2.059107000
C	-2.804660000	2.555448000	0.097664000
C	-3.054739000	2.555606000	1.505865000
C	-2.907520000	3.755551000	2.222170000
H	-3.083760000	3.738553000	3.304823000
C	-2.549631000	4.961829000	1.601663000
C	-2.418806000	4.955919000	0.203580000
H	-2.195631000	5.897914000	-0.311631000
C	-2.536383000	3.787755000	-0.571060000
C	-3.510727000	1.350213000	2.309091000
H	-2.680261000	0.947227000	2.911442000
H	-3.929991000	0.532419000	1.702897000
H	-4.300413000	1.659205000	3.017344000
C	-2.287027000	6.214183000	2.404011000
H	-2.875855000	6.232154000	3.336931000
H	-2.513357000	7.124849000	1.823767000
H	-1.218773000	6.260860000	2.684031000
C	-2.433305000	3.953890000	-2.071665000
H	-2.269850000	5.012866000	-2.326232000
H	-3.359665000	3.629860000	-2.574939000
H	-1.608655000	3.376912000	-2.511353000
N	-0.787688000	-1.305965000	2.455775000
S	-0.150418000	-0.488846000	3.787505000
O	-0.462625000	-1.172158000	5.062749000
O	-0.436997000	0.951528000	3.603014000
C	1.702898000	-0.680379000	3.451311000
F	2.076152000	-1.950417000	3.658966000
F	1.915461000	-0.339571000	2.168981000
S	-1.329324000	-2.900117000	2.648499000
O	-0.392536000	-3.751695000	3.407619000
O	-1.845625000	-3.313072000	1.324248000
C	-2.909838000	-2.705801000	3.735205000
F	-3.338191000	-1.426420000	3.708776000
F	-3.859464000	-3.500100000	3.212270000
F	-2.652164000	-3.072631000	4.994656000
F	2.390933000	0.140688000	4.262324000
C	0.007669000	-2.642501000	-2.872824000
C	-0.211662000	-4.694193000	-1.000368000
C	-0.624070000	-3.837903000	-3.232933000
C	-0.740125000	-4.869214000	-2.288096000
F	6.781332000	-4.182182000	-1.561073000
F	0.102594000	-1.673202000	-3.817567000
F	-1.127827000	-3.995519000	-4.473960000
F	-1.358631000	-6.018536000	-2.616114000
F	-0.323750000	-5.677534000	-0.089140000
C	1.014445000	-1.094468000	-1.160761000
C	2.304763000	-0.795437000	-0.814965000
C	4.726903000	0.847584000	0.680278000
C	5.986775000	1.441271000	0.835029000
C	0.517145000	-2.416199000	-1.580516000
C	0.420906000	-3.488117000	-0.673649000
C	3.472375000	-1.703911000	-0.955457000
C	4.197572000	-1.677901000	-2.161434000
C	3.917630000	-2.579475000	0.049344000
C	5.307512000	-2.503234000	-2.381910000
C	5.024403000	-3.419202000	-0.148764000
C	5.718739000	-3.381185000	-1.366852000

F	6.832803000	1.004301000	1.786633000
F	4.416587000	-0.161768000	1.519782000
F	3.308213000	-2.619018000	1.247727000
F	5.432424000	-4.250892000	0.829187000
F	5.976379000	-2.463151000	-3.550661000
F	3.815750000	-0.833422000	-3.145172000
F	0.899256000	-3.343218000	0.579836000
C	2.473838000	0.662302000	-0.496312000
C	3.801338000	1.284495000	-0.289682000
C	4.222106000	2.343328000	-1.125715000
C	5.474301000	2.956021000	-0.987850000
C	6.361991000	2.503017000	-0.000895000
F	3.427293000	2.780733000	-2.124718000
F	5.837218000	3.960036000	-1.808234000
F	7.565872000	3.081419000	0.141411000
C	1.281720000	1.332850000	-0.586438000
C	1.094340000	2.763444000	-0.298940000
C	0.786254000	3.688569000	-1.312716000
C	1.194389000	3.267067000	1.012155000
C	0.558965000	5.042043000	-1.044717000
C	0.949883000	4.614326000	1.310652000
C	0.635389000	5.504724000	0.276079000
F	0.698876000	3.268693000	-2.597948000
F	1.505350000	2.435265000	2.027164000
F	0.986448000	5.055158000	2.585925000
F	0.339204000	6.789208000	0.556062000
F	0.204758000	5.892432000	-2.031475000
B	0.197851000	0.298924000	-1.152480000

L-AuCl

Ph₃P-AuCl: E= -1632.282728

Au	-1.847349000	0.002002000	0.003363000
P	0.419064000	-0.000224000	0.000219000
C	1.135650000	0.222211000	-1.674876000
C	2.337334000	0.934486000	-1.871648000
C	2.883634000	1.037267000	-3.161292000
H	3.815098000	1.593177000	-3.311732000
C	2.236839000	0.433275000	-4.252725000
C	1.038105000	-0.275470000	-4.057903000
H	0.528684000	-0.741274000	-4.907998000
C	0.484554000	-0.380094000	-2.773391000
C	1.140742000	1.337358000	1.029535000
C	0.491725000	2.590988000	1.061517000
C	1.050294000	3.649252000	1.793277000
H	0.542431000	4.619102000	1.818365000
C	2.251970000	3.460963000	2.498791000
C	2.896528000	2.212742000	2.471893000
H	3.830494000	2.062939000	3.023794000
C	2.345152000	1.149034000	1.739310000
C	1.137404000	-1.562297000	0.642724000
C	2.341084000	-2.085127000	0.125242000
C	0.485059000	-2.216982000	1.710070000
C	2.888692000	-3.253624000	0.679222000
C	1.039969000	-3.381964000	2.259942000
C	2.241097000	-3.900921000	1.745045000
H	2.846666000	-1.584110000	-0.707040000
H	-0.456519000	-1.815675000	2.103600000
H	3.821739000	-3.658945000	0.273670000
H	0.529603000	-3.888727000	3.085703000
H	2.669466000	-4.814148000	2.171630000

H	-0.454774000	-0.924661000	-2.620395000
H	2.664250000	0.518970000	-5.257450000
H	2.842606000	1.407489000	-1.022910000
H	2.848868000	0.176792000	1.721002000
H	-0.449735000	2.733867000	0.517803000
H	2.683237000	4.286857000	3.074488000
Cl	-4.186030000	0.002762000	-0.001170000

FLP1-AuCl: E= -3602.805729

Au	0.357766000	-0.943049000	-1.237265000
B	1.362444000	-0.097718000	0.998121000
C	-1.189579000	-0.426220000	1.636101000
Cl	1.991947000	-2.007491000	-2.585438000
P	-1.486531000	-0.080293000	-0.152561000
Si	-2.480674000	-0.942210000	2.956197000
C	0.134239000	-0.460867000	1.949457000
H	0.404175000	-0.711711000	2.990542000
C	-4.286803000	-0.657485000	2.461223000
H	-4.917938000	-0.809289000	3.356740000
H	-4.609157000	-1.375056000	1.688177000
H	-4.488127000	0.359672000	2.083168000
C	-2.215838000	-2.793736000	3.273197000
H	-1.140057000	-3.030652000	3.354296000
H	-2.637470000	-3.397242000	2.450556000
H	-2.712748000	-3.100302000	4.211554000
C	-2.087341000	0.036132000	4.534347000
H	-2.665037000	-0.374073000	5.382815000
H	-2.354404000	1.101561000	4.423809000
H	-1.015623000	-0.017974000	4.795372000
C	-1.549377000	1.726393000	-0.552577000
C	-1.377966000	2.085276000	-1.924646000
C	-1.172837000	3.435830000	-2.255252000
H	-1.030504000	3.699796000	-3.310469000
C	-1.141709000	4.448747000	-1.283879000
C	-1.406788000	4.081647000	0.045218000
H	-1.440791000	4.862130000	0.815418000
C	-1.620214000	2.747623000	0.438783000
C	-1.435404000	1.092045000	-3.070873000
H	-1.780214000	1.596591000	-3.989888000
H	-2.119731000	0.248107000	-2.877860000
H	-0.436985000	0.664839000	-3.287187000
C	-0.798509000	5.874535000	-1.646590000
H	-1.094731000	6.116066000	-2.681773000
H	0.293958000	6.023932000	-1.569740000
H	-1.279034000	6.596729000	-0.964409000
C	-1.963903000	2.506465000	1.893096000
H	-2.842840000	1.848874000	2.002856000
H	-2.204877000	3.461553000	2.388613000
H	-1.140376000	2.037507000	2.453454000
C	-3.044156000	-0.967137000	-0.606256000
C	-4.274053000	-0.303281000	-0.906576000
C	-5.415076000	-1.088757000	-1.162720000
H	-6.356625000	-0.574956000	-1.391641000
C	-5.404560000	-2.490585000	-1.110832000
C	-4.188657000	-3.119966000	-0.799494000
H	-4.152328000	-4.215033000	-0.747638000
C	-3.006508000	-2.398885000	-0.555840000
C	-4.481142000	1.199455000	-0.932990000
H	-4.142931000	1.688233000	-0.004844000
H	-5.553982000	1.423035000	-1.052226000
H	-3.943940000	1.688533000	-1.762799000

C	-6.663934000	-3.295021000	-1.340702000
H	-7.161111000	-3.523654000	-0.378678000
H	-6.443317000	-4.259353000	-1.830371000
H	-7.389187000	-2.744480000	-1.963817000
C	-1.762147000	-3.215121000	-0.262673000
H	-2.037728000	-4.252770000	-0.009175000
H	-1.162281000	-2.818899000	0.571077000
H	-1.096080000	-3.258896000	-1.146310000
C	1.587455000	1.476039000	0.808314000
C	1.426799000	2.320364000	1.922753000
F	1.163445000	1.783952000	3.146436000
C	1.499632000	3.717313000	1.859489000
F	1.306739000	4.472015000	2.959999000
C	1.745771000	4.327444000	0.623223000
F	1.771026000	5.669704000	0.520434000
C	1.922620000	3.532653000	-0.516728000
F	2.118033000	4.120996000	-1.714954000
C	1.863380000	2.139260000	-0.401915000
F	2.046218000	1.439329000	-1.549270000
C	2.526565000	-1.140820000	0.812254000
C	3.811131000	-0.812573000	0.322023000
F	4.139229000	0.467750000	0.042705000
C	4.798147000	-1.770520000	0.066021000
F	6.002599000	-1.410057000	-0.417147000
C	4.525278000	-3.124315000	0.313006000
F	5.458795000	-4.055049000	0.064767000
C	3.272107000	-3.503229000	0.819781000
F	3.004744000	-4.804171000	1.045633000
C	2.315837000	-2.517140000	1.069287000
F	1.109821000	-2.952252000	1.513135000

FLP2-AuCl: E= -1900.585543

Au	-0.691535000	-0.977488000	-1.082307000
P	-1.960167000	0.232637000	0.361421000
Cl	0.516584000	-2.304808000	-2.597687000
C	0.351903000	0.831274000	1.833841000
C	1.418776000	1.683384000	-0.525080000
H	0.393756000	2.010893000	-0.814605000
B	1.259156000	0.526886000	0.563378000
C	-1.774736000	0.982778000	3.078250000
H	-2.862061000	0.857758000	3.118540000
C	1.004575000	1.274787000	3.011846000
H	2.094116000	1.394210000	3.007645000
C	4.596695000	-1.540497000	1.020359000
H	4.725463000	-1.835865000	-0.040920000
H	5.594450000	-1.236608000	1.392397000
C	1.688522000	-1.950658000	1.424201000
H	1.563553000	-1.627021000	2.478241000
H	0.681652000	-2.252599000	1.071779000
C	-2.525381000	1.880563000	-0.355093000
H	-1.634483000	2.516284000	-0.184638000
C	2.653650000	-3.147850000	1.361069000
H	2.272606000	-3.986190000	1.975751000
H	2.700421000	-3.514458000	0.314563000
C	2.077750000	2.939561000	0.130084000
H	1.516061000	3.239412000	1.034528000
H	3.102946000	2.680865000	0.466638000
C	-1.061777000	0.702211000	1.890668000
C	3.624211000	-0.344348000	1.085805000
H	4.021566000	0.498835000	0.490758000
H	3.561806000	0.007586000	2.135735000

C	0.298187000	1.567802000	4.188227000
H	0.839424000	1.906937000	5.078556000
C	2.165980000	1.306908000	-1.824051000
H	3.198229000	0.986494000	-1.574129000
H	1.678584000	0.435946000	-2.301538000
C	2.200085000	-0.755710000	0.586326000
H	2.333959000	-1.100393000	-0.461130000
C	-3.451769000	-0.763782000	0.889622000
H	-4.038105000	-0.122495000	1.574483000
C	-1.097275000	1.414097000	4.227226000
H	-1.656254000	1.626011000	5.144724000
C	-2.782891000	1.808392000	-1.871437000
H	-3.624675000	1.138872000	-2.117180000
H	-1.891751000	1.446880000	-2.414327000
H	-3.032478000	2.816632000	-2.248946000
C	-2.977189000	-2.021520000	1.644191000
H	-3.854695000	-2.597729000	1.988566000
H	-2.361216000	-1.770486000	2.524384000
H	-2.378769000	-2.672028000	0.979971000
C	4.067507000	-2.744334000	1.823196000
H	4.030956000	-2.471742000	2.898524000
H	4.764668000	-3.599576000	1.736164000
C	2.154723000	4.117296000	-0.861975000
H	2.652614000	4.983171000	-0.383930000
H	1.122429000	4.439467000	-1.111675000
C	-3.707940000	2.483177000	0.424377000
H	-3.909801000	3.502662000	0.049656000
H	-3.495499000	2.560492000	1.504713000
H	-4.630067000	1.890900000	0.288975000
C	-4.327262000	-1.129651000	-0.324001000
H	-3.746775000	-1.698563000	-1.073331000
H	-4.753400000	-0.241510000	-0.819433000
H	-5.168138000	-1.763985000	0.009736000
C	2.887444000	3.721828000	-2.157684000
H	3.944641000	3.484875000	-1.916998000
H	2.905879000	4.573295000	-2.864636000
C	2.233845000	2.488564000	-2.809762000
H	2.785447000	2.196562000	-3.724057000
H	1.203186000	2.749912000	-3.130057000

FLP3-AuCl: E= -1892.303021

Au	-0.048426000	-1.168866000	-0.450937000
B	-0.670902000	1.207067000	0.433177000
Cl	-1.947736000	-2.469535000	-0.965880000
P	2.030689000	-0.295212000	-0.137379000
C	0.686876000	1.948007000	0.751732000
C	1.968507000	1.356661000	0.631105000
C	3.135894000	2.032795000	1.050922000
H	4.116695000	1.550350000	0.981549000
C	3.038793000	3.330137000	1.572426000
H	3.941302000	3.856699000	1.900225000
C	1.779085000	3.949426000	1.668558000
H	1.699652000	4.966722000	2.067860000
C	0.621786000	3.265506000	1.267303000
H	-0.354533000	3.755039000	1.366859000
C	3.075304000	-1.379373000	0.962888000
H	4.047742000	-0.861581000	1.073832000
C	3.295616000	-2.757520000	0.313041000
H	3.889845000	-3.395358000	0.991482000
H	3.837555000	-2.688768000	-0.646078000
H	2.329383000	-3.262975000	0.129599000

C	2.400509000	-1.488516000	2.343692000
H	1.412573000	-1.977368000	2.259310000
H	2.255768000	-0.497017000	2.807027000
H	3.029514000	-2.096481000	3.018246000
C	2.889758000	-0.124966000	-1.794259000
H	2.825425000	-1.144132000	-2.221573000
C	4.366146000	0.296164000	-1.690347000
H	4.816848000	0.283212000	-2.699052000
H	4.959292000	-0.380502000	-1.051257000
H	4.459970000	1.323750000	-1.298421000
C	2.078760000	0.838485000	-2.682509000
H	2.067030000	1.855695000	-2.250589000
H	1.033391000	0.503352000	-2.801761000
H	2.540627000	0.897351000	-3.684148000
C	-1.585123000	0.505137000	1.515326000
C	-1.318290000	-0.017666000	2.789833000
H	-0.297627000	0.015812000	3.190276000
C	-2.358704000	-0.601365000	3.541904000
H	-2.155354000	-1.017011000	4.535149000
C	-3.662303000	-0.650988000	3.016268000
H	-4.467065000	-1.105756000	3.605132000
C	-3.953012000	-0.118190000	1.740770000
H	-4.976058000	-0.161448000	1.349180000
C	-2.917352000	0.454201000	0.995122000
C	-2.963489000	1.052098000	-0.364262000
C	-4.055945000	1.186597000	-1.227142000
H	-5.053570000	0.836824000	-0.936953000
C	-3.857109000	1.781932000	-2.492651000
H	-4.706659000	1.886592000	-3.177179000
C	-2.588555000	2.246789000	-2.882635000
H	-2.456932000	2.711598000	-3.866109000
C	-1.490445000	2.114082000	-2.007283000
H	-0.499744000	2.474895000	-2.308454000
C	-1.663996000	1.511539000	-0.752366000

FLP4-AuCl: E= -1780.350804

B	1.124677000	0.278852000	1.421569000
C	-0.350728000	0.290631000	2.042768000
P	-1.487904000	0.072943000	0.572439000
H	-0.554404000	-0.540320000	2.737226000
C	1.735625000	1.659601000	0.976374000
C	1.782132000	2.700878000	1.938813000
C	2.308483000	3.965321000	1.631603000
C	2.773013000	4.235102000	0.332676000
C	2.725570000	3.225593000	-0.643997000
C	2.229681000	1.952684000	-0.320142000
C	1.935251000	-1.063547000	1.358362000
C	3.014677000	-1.241890000	0.451716000
C	3.716924000	-2.452011000	0.370441000
C	3.385805000	-3.515135000	1.229895000
C	2.352232000	-3.355984000	2.169616000
C	1.636769000	-2.151008000	2.221672000
H	-0.620194000	1.232657000	2.550435000
H	1.399782000	2.518708000	2.951559000
H	2.340361000	4.745703000	2.400541000
H	3.165347000	5.227164000	0.082325000
H	3.075782000	3.428625000	-1.662517000
H	2.182037000	1.188772000	-1.104826000
H	0.842779000	-2.048523000	2.970429000
H	2.103345000	-4.171788000	2.857466000
H	3.939458000	-4.459250000	1.176126000

H	4.529980000	-2.564854000	-0.355253000
H	3.300773000	-0.419909000	-0.210966000
C	-2.417717000	1.723927000	0.340338000
C	-2.620149000	-1.402553000	1.011312000
C	-3.767346000	-1.497418000	-0.017124000
H	-3.390015000	-1.463424000	-1.055049000
H	-4.288879000	-2.462822000	0.121961000
H	-4.514792000	-0.697729000	0.117636000
C	-1.740179000	-2.671457000	0.892868000
H	-0.845074000	-2.630331000	1.534761000
H	-2.339589000	-3.547733000	1.203829000
H	-1.401703000	-2.835565000	-0.145309000
C	-3.195829000	-1.314306000	2.441543000
H	-3.834657000	-0.430717000	2.591125000
H	-3.818382000	-2.210635000	2.621220000
H	-2.408050000	-1.305957000	3.213951000
C	-3.160717000	1.716123000	-1.016427000
H	-2.462266000	1.551790000	-1.856195000
H	-3.951272000	0.952720000	-1.070467000
H	-3.639185000	2.703372000	-1.157889000
C	-1.349442000	2.841923000	0.292070000
H	-1.855441000	3.791205000	0.035094000
H	-0.836419000	2.987806000	1.256008000
H	-0.577432000	2.645673000	-0.472366000
C	-3.405676000	1.997653000	1.492253000
H	-4.273830000	1.318044000	1.462745000
H	-2.927202000	1.917647000	2.484624000
H	-3.791621000	3.029338000	1.392093000
Au	-0.263116000	-0.382682000	-1.299970000
Cl	1.023639000	-0.798291000	-3.226286000

FLP5-AuCl: E= -1893.396261

Au	-1.475494000	0.047673000	-0.614238000
B	-2.453459000	0.608367000	1.522994000
C	0.006134000	0.413093000	2.364630000
P	0.448295000	0.095126000	0.633616000
C	-1.297601000	0.684197000	2.595353000
H	-1.586321000	0.967044000	3.622537000
C	1.186613000	-1.553990000	0.255848000
C	1.875214000	-1.705902000	-0.985920000
C	2.443074000	-2.956420000	-1.290309000
H	2.977070000	-3.069761000	-2.241988000
C	2.338761000	-4.060687000	-0.428272000
C	1.596502000	-3.899440000	0.754283000
H	1.460959000	-4.760749000	1.420119000
C	1.003072000	-2.676304000	1.114241000
C	1.754059000	1.366644000	0.327945000
C	3.061026000	1.134636000	0.854062000
C	4.056216000	2.105856000	0.632291000
H	5.060347000	1.924508000	1.035349000
C	3.809202000	3.290600000	-0.078280000
C	2.502390000	3.512891000	-0.544737000
H	2.277229000	4.448234000	-1.071762000
C	1.463494000	2.584526000	-0.353312000
Cl	-3.103413000	-0.279946000	-2.287874000
C	-3.550879000	-0.556982000	1.539079000
C	-4.737726000	0.049939000	1.251737000
C	-4.566352000	1.502511000	0.938808000
C	-3.262245000	1.893360000	1.012159000
H	0.802892000	0.483253000	3.115224000
C	2.031088000	-0.597321000	-2.011178000

H	1.104713000	-0.008989000	-2.144007000
H	2.828035000	0.114342000	-1.731576000
H	2.290072000	-1.026275000	-2.993495000
C	0.176427000	-2.637827000	2.383899000
H	0.636321000	-2.008613000	3.166390000
H	-0.835059000	-2.234788000	2.202405000
H	0.069051000	-3.654624000	2.796800000
C	3.000675000	-5.378708000	-0.762201000
H	3.086700000	-5.524372000	-1.852809000
H	4.024925000	-5.418189000	-0.344131000
H	2.442251000	-6.231662000	-0.339373000
C	3.474477000	-0.106315000	1.626809000
H	3.714353000	-0.942594000	0.945601000
H	4.375020000	0.107822000	2.226234000
H	2.699247000	-0.475653000	2.317806000
C	4.909052000	4.295381000	-0.338854000
H	5.319121000	4.169150000	-1.359023000
H	4.534466000	5.331532000	-0.266590000
H	5.745306000	4.176654000	0.370959000
C	0.091253000	2.955788000	-0.876251000
H	-0.685894000	2.876779000	-0.096478000
H	0.089554000	3.994207000	-1.247520000
H	-0.223872000	2.305928000	-1.714486000
H	-2.924087000	2.920438000	0.842896000
H	-5.421853000	2.145116000	0.691127000
H	-5.725598000	-0.430027000	1.243667000
H	-3.453560000	-1.611713000	1.814584000

FLP6-AuCl: E= -5210.703026

Au	-0.899751000	-0.172525000	-1.385499000
B	0.034565000	-0.138670000	0.739749000
C	-2.399679000	-0.492756000	1.628719000
P	-2.808016000	0.000187000	-0.080968000
Si	-3.567715000	-1.304339000	2.904621000
C	-1.064248000	-0.343691000	1.851704000
H	-0.682388000	-0.495510000	2.873766000
C	-5.383073000	-0.775498000	2.769646000
H	-5.938702000	-1.262315000	3.592720000
H	-5.823191000	-1.120782000	1.818746000
H	-5.551733000	0.311427000	2.856304000
C	-3.506292000	-3.176905000	2.617706000
H	-2.477571000	-3.567034000	2.684809000
H	-3.919087000	-3.438381000	1.627528000
H	-4.116567000	-3.688048000	3.385106000
C	-2.872931000	-0.877906000	4.614601000
H	-3.533438000	-1.286701000	5.400605000
H	-2.800838000	0.214668000	4.760008000
H	-1.868170000	-1.311882000	4.761907000
C	-3.235349000	1.799237000	-0.227784000
C	-3.420698000	2.298567000	-1.556325000
C	-3.689431000	3.665563000	-1.744398000
H	-3.829975000	4.033610000	-2.767784000
C	-3.780956000	4.566402000	-0.674059000
C	-3.601431000	4.053030000	0.619684000
H	-3.662523000	4.741538000	1.471247000
C	-3.322792000	2.698182000	0.881065000
C	-3.353535000	1.441372000	-2.807980000
H	-3.883511000	1.936996000	-3.638691000
H	-3.800476000	0.441216000	-2.681627000
H	-2.304645000	1.298693000	-3.136143000
C	-4.008767000	6.043690000	-0.891858000

H	-4.367503000	6.256394000	-1.912737000
H	-3.061616000	6.592013000	-0.743147000
H	-4.739630000	6.450045000	-0.170639000
C	-3.155024000	2.333632000	2.343452000
H	-3.831585000	1.522196000	2.652879000
H	-3.380595000	3.210497000	2.972195000
H	-2.133064000	2.002379000	2.583292000
C	-4.183428000	-1.086303000	-0.662351000
C	-5.545126000	-0.657454000	-0.748189000
C	-6.518369000	-1.598894000	-1.136192000
H	-7.563064000	-1.269658000	-1.191596000
C	-6.211747000	-2.935848000	-1.434340000
C	-4.872317000	-3.339787000	-1.313074000
H	-4.608849000	-4.385927000	-1.510574000
C	-3.849621000	-2.451632000	-0.937206000
C	-6.050927000	0.734394000	-0.417887000
H	-5.624646000	1.133304000	0.515226000
H	-7.146964000	0.711975000	-0.302801000
H	-5.812141000	1.462041000	-1.213022000
C	-7.282895000	-3.906459000	-1.875767000
H	-8.278428000	-3.609514000	-1.504113000
H	-7.069281000	-4.930927000	-1.525118000
H	-7.340449000	-3.944763000	-2.980301000
C	-2.450303000	-3.021861000	-0.827665000
H	-2.482596000	-4.123807000	-0.835173000
H	-1.938540000	-2.714478000	0.098612000
H	-1.810351000	-2.704145000	-1.673164000
C1	0.584828000	-0.222841000	-3.215807000
C	0.894664000	1.184988000	0.510110000
C	2.195687000	0.784628000	0.340287000
C	2.314342000	-0.712952000	0.308282000
C	3.591586000	-1.404273000	0.054298000
C	4.070558000	-2.408181000	0.918721000
C	4.382141000	-1.091100000	-1.068498000
C	5.278217000	-3.076154000	0.678592000
C	5.595852000	-1.740318000	-1.327371000
C	6.044585000	-2.737849000	-0.447779000
C	0.401194000	2.572479000	0.627886000
C	-0.015152000	3.333535000	-0.481868000
C	0.218137000	3.154243000	1.895184000
C	-0.519119000	4.632464000	-0.344362000
C	-0.313009000	4.439760000	2.064592000
C	-0.673527000	5.184960000	0.933396000
C	3.394446000	1.646666000	0.295574000
C	3.578469000	2.644507000	-0.678758000
C	4.430389000	1.468110000	1.234326000
C	4.731744000	3.439709000	-0.716582000
C	5.594892000	2.245582000	1.215969000
C	5.743117000	3.239011000	0.235390000
F	3.373201000	-2.737839000	2.026852000
F	5.716085000	-4.027117000	1.526487000
F	7.205655000	-3.372385000	-0.686125000
F	6.323916000	-1.427227000	-2.416137000
F	3.955506000	-0.162109000	-1.950914000
F	4.299485000	0.535119000	2.204326000
F	6.560873000	2.058600000	2.135571000
F	6.852894000	3.996917000	0.208429000
F	4.884216000	4.379656000	-1.668714000
F	2.652375000	2.828432000	-1.640337000
F	0.021627000	2.810561000	-1.727026000
F	0.518979000	2.434515000	3.002389000

F	-0.507327000	4.948937000	3.297958000
F	-1.220967000	6.408775000	1.076539000
F	-0.909791000	5.333774000	-1.428202000
C	1.103170000	-1.318193000	0.514987000
C	0.837488000	-2.762849000	0.462476000
C	0.238708000	-3.450756000	1.536967000
C	1.091780000	-3.522392000	-0.698876000
C	-0.145725000	-4.793753000	1.450647000
C	0.708873000	-4.865818000	-0.815213000
C	0.082805000	-5.506448000	0.264564000
F	0.016424000	-2.817136000	2.714053000
F	1.671762000	-2.942115000	-1.769483000
F	0.929536000	-5.542068000	-1.959651000
F	-0.292704000	-6.794324000	0.164271000
F	-0.737130000	-5.400536000	2.500742000

Hydroarylation

Mesitylene: E= -350.024527

C	-0.750631000	-1.204024000	-0.008172000
C	0.661070000	-1.231592000	-0.003744000
C	-1.397004000	0.043356000	-0.004603000
H	1.177735000	-2.200588000	-0.006835000
H	-2.494514000	0.080395000	-0.007477000
C	1.418136000	-0.048162000	0.006906000
C	-0.667320000	1.252117000	0.006090000
C	0.736112000	1.188147000	0.014249000
H	1.316917000	2.120044000	0.025353000
C	2.933035000	-0.085116000	-0.005302000
H	3.316743000	-1.105321000	0.167058000
H	3.333604000	0.262997000	-0.976393000
H	3.358704000	0.576050000	0.771503000
C	-1.392818000	2.582535000	-0.004812000
H	-0.699845000	3.425387000	0.159863000
H	-1.902099000	2.752092000	-0.972487000
H	-2.172322000	2.623321000	0.777902000
C	-1.540369000	-2.497330000	0.003929000
H	-2.613487000	-2.320631000	-0.183078000
H	-1.171176000	-3.202575000	-0.762898000
H	-1.451525000	-3.010746000	0.980250000

[PPh3-Au-phenylacetylene]⁺: E= -1480.150106

P	1.088270000	0.111535000	-0.019593000
C	2.418737000	-0.133953000	1.211895000
C	3.754708000	0.215366000	0.924916000
C	4.738611000	0.068313000	1.916038000
H	5.776025000	0.337639000	1.692295000
C	4.394175000	-0.423693000	3.186219000
C	3.062168000	-0.773422000	3.471444000
H	2.793786000	-1.162280000	4.459175000
C	2.073299000	-0.632704000	2.487252000
C	1.892283000	0.234501000	-1.657065000
C	2.096302000	-0.945392000	-2.404935000
C	2.761900000	-0.882238000	-3.637938000
H	2.917535000	-1.797243000	-4.218734000
C	3.219024000	0.353832000	-4.128306000
C	3.010971000	1.529319000	-3.386575000
H	3.362727000	2.492464000	-3.770582000
C	2.347490000	1.475552000	-2.150585000
C	0.348048000	1.753569000	0.334692000
C	1.087220000	2.743815000	1.016032000

C	-0.963747000	2.031580000	-0.109727000
C	0.514362000	4.005473000	1.244527000
C	-1.527331000	3.293961000	0.123253000
C	-0.789897000	4.281185000	0.800216000
H	2.101269000	2.529997000	1.370070000
H	-1.550296000	1.265098000	-0.629709000
H	1.089152000	4.771675000	1.775008000
H	-2.548080000	3.497414000	-0.215558000
H	-1.234500000	5.264337000	0.986987000
H	1.034870000	-0.908941000	2.706217000
H	5.165563000	-0.539459000	3.954759000
H	4.025115000	0.598832000	-0.064529000
H	2.182717000	2.392549000	-1.574832000
H	1.731869000	-1.906850000	-2.023165000
H	3.733687000	0.401473000	-5.093696000
C	-2.157354000	-2.964349000	0.172575000
C	-2.871325000	-1.931665000	0.107018000
Au	-0.564919000	-1.493024000	0.071198000
H	-2.020301000	-4.037437000	0.243573000
C	-3.623371000	-0.722398000	0.031516000
C	-3.940081000	-0.015209000	1.221430000
C	-3.968641000	-0.185978000	-1.237479000
C	-4.598228000	1.215088000	1.134308000
C	-4.626553000	1.046646000	-1.305556000
C	-4.939729000	1.745886000	-0.124228000
H	-3.650447000	-0.433945000	2.189622000
H	-3.703337000	-0.735696000	-2.145263000
H	-4.839531000	1.767692000	2.047257000
H	-4.891712000	1.467317000	-2.280221000
H	-5.449835000	2.712703000	-0.185005000

[FLP1'-Au-phenylacetylene]⁺: E= -3214.938916

Au	-0.008876000	-0.091082000	-1.433397000
B	0.443712000	0.715977000	1.503009000
C	-1.644094000	-0.970554000	1.583585000
P	-1.804082000	-0.912309000	-0.236360000
C	-0.645848000	-0.231772000	2.137994000
H	-0.563065000	-0.272701000	3.240345000
C	-3.207079000	0.180722000	-0.670461000
C	-3.660800000	0.214102000	-2.009087000
C	-4.647108000	1.136393000	-2.386197000
H	-5.003028000	1.155817000	-3.421483000
C	-5.168507000	2.039366000	-1.441063000
C	-4.709763000	2.012746000	-0.114081000
H	-5.100880000	2.721419000	0.622205000
C	-3.732693000	1.082511000	0.275072000
H	-3.242433000	-0.476508000	-2.750373000
H	-5.930103000	2.765911000	-1.742818000
H	-3.373677000	1.067647000	1.306533000
C	-2.207056000	-2.602288000	-0.812402000
C	-3.526202000	-3.000968000	-1.110698000
C	-3.788126000	-4.336460000	-1.456485000
C	-2.740784000	-5.271919000	-1.508132000
C	-1.422946000	-4.871509000	-1.223594000
H	-0.604298000	-5.597104000	-1.268890000
C	-1.152081000	-3.539755000	-0.880348000
H	-4.346114000	-2.276978000	-1.075651000
H	-2.950232000	-6.312864000	-1.775458000
H	-0.126691000	-3.229926000	-0.651263000
C	0.012854000	2.165372000	1.091867000
C	-1.196693000	2.730589000	1.556534000

F	-1.849056000	2.171171000	2.603284000
C	-1.786265000	3.862334000	0.984386000
F	-2.958624000	4.336802000	1.442122000
C	-1.141160000	4.498424000	-0.088304000
F	-1.693882000	5.574781000	-0.661429000
C	0.092795000	4.010375000	-0.551681000
F	0.711662000	4.619309000	-1.579320000
C	0.659554000	2.889495000	0.061894000
F	1.842317000	2.464148000	-0.439814000
C	1.930174000	0.218376000	1.496477000
C	3.005348000	1.067244000	1.843907000
F	2.785125000	2.372771000	2.107112000
C	4.323375000	0.611514000	1.966014000
F	5.322351000	1.454416000	2.284038000
C	4.604471000	-0.742907000	1.731992000
F	5.866293000	-1.188463000	1.811400000
C	3.573809000	-1.624219000	1.371413000
F	3.855219000	-2.913317000	1.109078000
C	2.269002000	-1.134520000	1.272114000
F	1.316153000	-2.023561000	0.896058000
H	-4.813842000	-4.644196000	-1.684164000
C	2.107070000	0.296233000	-2.584889000
C	1.079995000	0.867535000	-3.021439000
H	0.545940000	1.468512000	-3.749427000
C	3.301400000	-0.299456000	-2.095761000
C	4.324199000	0.531043000	-1.567641000
C	3.489761000	-1.704028000	-2.185320000
C	5.536369000	-0.044302000	-1.171752000
C	4.701904000	-2.262554000	-1.768994000
C	5.727405000	-1.434875000	-1.273809000
H	4.154950000	1.607642000	-1.482046000
H	2.682725000	-2.329740000	-2.578221000
H	6.327443000	0.589633000	-0.759837000
H	4.849768000	-3.344750000	-1.826913000
H	6.672508000	-1.877639000	-0.945625000
Si	-2.826195000	-2.048870000	2.644626000
C	-4.624557000	-1.650236000	2.205039000
H	-5.295330000	-2.304929000	2.791061000
H	-4.876889000	-0.601884000	2.440226000
H	-4.839019000	-1.818996000	1.136473000
C	-2.467361000	-3.887071000	2.360668000
H	-2.962285000	-4.480116000	3.151731000
H	-2.843213000	-4.235410000	1.384159000
H	-1.383510000	-4.093002000	2.404430000
C	-2.493136000	-1.598699000	4.453350000
H	-1.476450000	-1.889745000	4.772567000
H	-2.621191000	-0.517063000	4.636410000
H	-3.211890000	-2.138835000	5.096221000

[FLP3'-Au-phenylacetylene]⁺: E= -1966.406499

B	0.304662000	-1.978255000	1.020905000
C	-1.225724000	-2.207069000	1.311227000
C	-2.260796000	-1.319050000	0.914387000
C	-3.616092000	-1.581678000	1.194311000
H	-4.394190000	-0.889564000	0.853512000
C	-3.963959000	-2.742582000	1.902438000
H	-5.015517000	-2.952321000	2.123552000
C	-2.959314000	-3.636215000	2.309644000
H	-3.226956000	-4.550279000	2.850624000
C	-1.611672000	-3.375611000	2.008495000
H	-0.844323000	-4.095976000	2.315317000

C	1.342243000	-1.088424000	1.802661000
C	1.208036000	-0.108013000	2.798319000
H	0.215334000	0.177468000	3.161851000
C	2.355031000	0.524040000	3.324628000
H	2.248311000	1.298417000	4.091392000
C	3.632697000	0.161796000	2.865011000
H	4.519099000	0.654878000	3.278697000
C	3.791801000	-0.825234000	1.864333000
H	4.794774000	-1.091714000	1.512538000
C	2.652026000	-1.438254000	1.334604000
C	2.562236000	-2.463427000	0.261770000
C	3.581755000	-3.013697000	-0.519439000
H	4.630772000	-2.739682000	-0.361205000
C	3.237218000	-3.924997000	-1.545188000
H	4.028972000	-4.353197000	-2.169627000
C	1.897837000	-4.290684000	-1.774799000
H	1.656463000	-5.000686000	-2.572790000
C	0.872557000	-3.744975000	-0.974079000
H	-0.174145000	-4.021200000	-1.148951000
C	1.193753000	-2.825365000	0.038125000
P	-1.754558000	0.201048000	0.035075000
Au	0.176795000	-0.197768000	-1.160244000
C	2.311726000	0.587718000	-1.914599000
C	2.000056000	-0.566464000	-2.297130000
H	2.217733000	-1.543916000	-2.717269000
C	2.646951000	1.891025000	-1.445837000
C	2.798840000	2.970743000	-2.354010000
C	2.800181000	2.101138000	-0.048853000
C	3.112122000	4.242259000	-1.859960000
C	3.108365000	3.378459000	0.426641000
C	3.264438000	4.448123000	-0.475313000
H	2.672298000	2.798564000	-3.426934000
H	2.653010000	1.264510000	0.637919000
H	3.233340000	5.078588000	-2.555308000
H	3.221835000	3.537836000	1.503502000
H	3.503244000	5.447934000	-0.098245000
C	-1.445813000	1.466128000	1.322909000
C	-2.117257000	1.401949000	2.562594000
C	-0.478333000	2.466898000	1.094594000
C	-1.812391000	2.334221000	3.567308000
C	-0.175214000	3.390050000	2.104590000
C	-0.837556000	3.321882000	3.342642000
H	-2.853636000	0.613855000	2.751861000
H	0.058827000	2.509204000	0.140502000
H	-2.328402000	2.278433000	4.531282000
H	0.590788000	4.151507000	1.925794000
H	-0.590670000	4.035694000	4.135452000
C	-3.167435000	0.757183000	-0.977783000
C	-4.090672000	1.704070000	-0.487362000
C	-3.349350000	0.179173000	-2.253400000
C	-5.196785000	2.064212000	-1.273956000
C	-4.458051000	0.543669000	-3.030432000
C	-5.380930000	1.485758000	-2.541226000
H	-3.945927000	2.157157000	0.499086000
H	-2.623442000	-0.549793000	-2.633524000
H	-5.913423000	2.800093000	-0.894848000
H	-4.598128000	0.097718000	-4.020493000
H	-6.242937000	1.773205000	-3.152287000

[FLP4-Au-phenylacetylene] +: E= -1628.228545

B	0.344911000	0.960635000	1.683030000
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C	-1.255166000	1.031626000	1.786706000
H	-1.622532000	0.412909000	2.624627000
C	1.129385000	2.200073000	1.146095000
C	0.819360000	3.527568000	1.537807000
C	1.510190000	4.625054000	1.004106000
C	2.504089000	4.422141000	0.028289000
C	2.822521000	3.117184000	-0.385552000
C	2.158660000	2.021913000	0.186444000
C	1.140693000	-0.308254000	2.143971000
C	2.506491000	-0.187008000	2.520332000
C	3.246363000	-1.285964000	2.982063000
C	2.649480000	-2.556974000	3.045120000
C	1.300563000	-2.713712000	2.673564000
C	0.559751000	-1.600524000	2.254082000
H	-1.625043000	2.062166000	1.943864000
H	0.029767000	3.703423000	2.279115000
H	1.266917000	5.640579000	1.335842000
H	3.029955000	5.280364000	-0.404783000
H	3.594822000	2.948294000	-1.144048000
H	2.422814000	1.007827000	-0.128042000
H	-0.491091000	-1.745137000	1.990541000
H	0.826612000	-3.700096000	2.724469000
H	3.228743000	-3.421190000	3.388338000
H	4.292137000	-1.155310000	3.281189000
H	2.991073000	0.793050000	2.459053000
C	-2.560522000	1.823599000	-0.886570000
C	-3.654470000	-0.560685000	0.935999000
C	-4.560367000	-0.977730000	-0.242512000
H	-3.997877000	-1.524639000	-1.021024000
H	-5.348975000	-1.651500000	0.140078000
H	-5.065175000	-0.114744000	-0.706303000
C	-3.150013000	-1.839997000	1.646264000
H	-2.522088000	-1.616924000	2.526058000
H	-4.027499000	-2.403908000	2.012928000
H	-2.584631000	-2.499970000	0.963725000
C	-4.448148000	0.291549000	1.951650000
H	-4.894227000	1.188993000	1.498833000
H	-5.274575000	-0.325803000	2.349726000
H	-3.830614000	0.605708000	2.810267000
C	-2.980976000	1.270813000	-2.269825000
H	-2.170483000	0.678525000	-2.731588000
H	-3.886495000	0.647478000	-2.233785000
H	-3.192888000	2.129855000	-2.933107000
C	-1.272312000	2.654504000	-1.074505000
H	-1.451499000	3.394498000	-1.876343000
H	-0.991784000	3.206369000	-0.165217000
H	-0.409908000	2.032072000	-1.373521000
C	-3.672713000	2.723101000	-0.309255000
H	-4.657417000	2.227593000	-0.323492000
H	-3.455659000	3.054440000	0.721454000
H	-3.751737000	3.629261000	-0.937871000
Au	-0.729431000	-1.075610000	-0.895919000
C	1.281421000	-2.019167000	-1.869206000
C	0.206065000	-2.636606000	-2.058286000
H	-0.369098000	-3.462069000	-2.463011000
C	2.499199000	-1.316627000	-1.653196000
C	2.946174000	-0.365658000	-2.609586000
C	3.257651000	-1.567391000	-0.480210000
C	4.152553000	0.308380000	-2.395791000
C	4.461239000	-0.882551000	-0.283194000
C	4.910015000	0.049644000	-1.236782000

H	2.341918000	-0.172798000	-3.500886000
H	2.882632000	-2.272277000	0.267443000
H	4.502886000	1.040881000	-3.129525000
H	5.040271000	-1.063740000	0.626729000
H	5.849652000	0.586500000	-1.071767000
P	-2.121432000	0.369302000	0.268959000

[FLP5-Au-phenylacetylene]⁺: E= -1741.269354

Au	0.743061000	-1.061161000	0.186723000
B	1.149649000	-1.758168000	-2.105512000
C	-1.100800000	-0.506841000	-2.544783000
P	-1.085765000	-0.019640000	-0.795792000
C	-0.036667000	-1.213934000	-2.986666000
H	0.008099000	-1.435560000	-4.066982000
C	-2.466471000	-0.626005000	0.262248000
C	-2.597578000	-0.034296000	1.556285000
C	-3.627045000	-0.487906000	2.400004000
H	-3.730633000	-0.029509000	3.391251000
C	-4.516506000	-1.507117000	2.019882000
C	-4.329507000	-2.105032000	0.761485000
H	-4.991216000	-2.925661000	0.458541000
C	-3.318789000	-1.699104000	-0.127953000
C	-1.185832000	1.821468000	-0.861275000
C	-2.460932000	2.408553000	-1.127638000
C	-2.552167000	3.811360000	-1.187265000
H	-3.531132000	4.261088000	-1.393408000
C	-1.441371000	4.649128000	-0.997691000
C	-0.194537000	4.041885000	-0.774170000
H	0.692347000	4.675630000	-0.653590000
C	-0.033344000	2.646152000	-0.705595000
C	1.296057000	-3.279671000	-1.635398000
C	2.637301000	-3.543823000	-1.650161000
C	3.446707000	-2.332444000	-1.991113000
C	2.662052000	-1.238217000	-2.206987000
H	-1.897363000	-0.121766000	-3.192316000
C	-1.692996000	1.066714000	2.079521000
H	-0.627509000	0.897887000	1.833703000
H	-1.964802000	2.052494000	1.662095000
H	-1.770133000	1.130600000	3.177491000
C	-3.197078000	-2.439525000	-1.444564000
H	-3.443729000	-1.796238000	-2.308045000
H	-2.177451000	-2.826361000	-1.611651000
H	-3.892472000	-3.294660000	-1.464420000
C	-5.641774000	-1.942276000	2.930765000
H	-5.381601000	-1.799664000	3.993634000
H	-6.553466000	-1.346510000	2.733423000
H	-5.903794000	-3.002643000	2.773480000
C	-3.745157000	1.624794000	-1.335009000
H	-4.184326000	1.309320000	-0.371601000
H	-4.488404000	2.252526000	-1.853587000
H	-3.612612000	0.711106000	-1.937797000
C	-1.584464000	6.154007000	-1.023545000
H	-1.800679000	6.540855000	-0.009352000
H	-0.658172000	6.643695000	-1.369870000
H	-2.414169000	6.471248000	-1.678284000
C	1.365680000	2.121965000	-0.462287000
H	1.664351000	1.347783000	-1.189563000
H	2.104005000	2.937940000	-0.526370000
H	1.467559000	1.680828000	0.546815000
H	3.050967000	-0.254064000	-2.485332000
H	4.542032000	-2.368385000	-2.053183000

H	3.106355000	-4.516728000	-1.454678000
H	0.526349000	-4.031215000	-1.436599000
C	2.836075000	-1.121154000	1.491964000
C	2.154205000	-2.173071000	1.432412000
H	1.995097000	-3.221674000	1.652342000
C	3.528856000	0.117275000	1.555927000
C	3.308125000	0.988335000	2.656694000
C	3.941861000	2.234605000	2.683919000
C	4.787397000	2.619100000	1.626010000
H	2.638484000	0.677298000	3.464065000
H	3.773780000	2.911461000	3.527170000
H	5.273981000	3.599590000	1.649613000
C	4.386343000	0.505597000	0.492881000
C	5.010630000	1.755167000	0.536261000
H	4.519828000	-0.170874000	-0.355441000
H	5.667232000	2.063211000	-0.283206000

[FLP6-Au-phenylacetylene]⁺: E= -5058.580174

P	2.492624000	0.803452000	0.269945000
C	2.201968000	0.531111000	2.056228000
C	0.887837000	0.290390000	2.320889000
H	0.596472000	0.159300000	3.375091000
Si	3.535874000	0.278435000	3.413125000
C	3.573293000	-1.589877000	3.735105000
H	3.973383000	-2.136215000	2.862670000
H	2.564369000	-1.979618000	3.957031000
H	4.224367000	-1.811381000	4.600404000
C	5.268278000	0.839064000	2.898332000
H	5.953518000	0.659719000	3.747325000
H	5.335491000	1.910611000	2.643531000
H	5.637063000	0.256957000	2.036840000
C	2.948639000	1.189457000	4.965185000
H	3.639964000	0.979779000	5.801566000
H	1.941086000	0.856463000	5.271615000
H	2.916526000	2.282058000	4.812974000
C	4.001935000	-0.119583000	-0.242171000
C	5.216750000	0.517066000	-0.649092000
C	6.272705000	-0.296279000	-1.102818000
H	7.202794000	0.192487000	-1.417012000
C	6.193432000	-1.697485000	-1.149302000
C	5.022417000	-2.300332000	-0.664315000
H	4.949548000	-3.393775000	-0.647793000
C	3.922485000	-1.551102000	-0.218069000
C	5.490524000	2.008104000	-0.592035000
H	6.578592000	2.182992000	-0.614690000
H	5.096484000	2.479846000	0.320952000
H	5.050054000	2.548696000	-1.447917000
C	7.318524000	-2.532836000	-1.711073000
H	7.431629000	-3.483111000	-1.161113000
H	8.281053000	-1.994942000	-1.687237000
H	7.108993000	-2.791512000	-2.767084000
C	2.712956000	-2.327177000	0.249065000
H	2.977143000	-3.381817000	0.427226000
H	1.916277000	-2.321384000	-0.517322000
H	2.268210000	-1.929546000	1.173779000
C	2.537295000	2.576841000	-0.251999000
C	2.517521000	2.839736000	-1.660395000
C	2.420092000	4.167655000	-2.105862000
H	2.402718000	4.354318000	-3.186457000
C	2.350092000	5.255143000	-1.221018000
C	2.419240000	4.975871000	0.152318000

H	2.381840000	5.809452000	0.863460000
C	2.506378000	3.668763000	0.667574000
C	2.620471000	1.777514000	-2.741789000
H	1.617665000	1.460189000	-3.086285000
H	3.173707000	0.878127000	-2.428760000
H	3.143525000	2.187725000	-3.622871000
C	2.160065000	6.664298000	-1.727854000
H	2.700197000	6.831329000	-2.675616000
H	2.497659000	7.411595000	-0.990699000
H	1.087502000	6.847206000	-1.919887000
C	2.597641000	3.545927000	2.173848000
H	2.578058000	4.545895000	2.635829000
H	3.536927000	3.058694000	2.484565000
H	1.770671000	2.964478000	2.607222000
C	0.050547000	-2.956614000	2.640671000
C	0.354089000	-4.845315000	0.616888000
C	0.750970000	-4.141177000	2.899520000
C	0.910914000	-5.093366000	1.880268000
F	-6.631994000	-4.565333000	-0.129779000
F	-0.081027000	-2.078887000	3.662296000
F	1.277332000	-4.362858000	4.118206000
F	1.593985000	-6.225881000	2.110600000
F	0.532978000	-5.725643000	-0.389514000
C	-1.034219000	-1.324933000	1.060235000
C	-2.260480000	-1.024013000	0.514867000
C	-4.266044000	0.873190000	-1.360901000
C	-5.452328000	1.498157000	-1.762043000
C	-0.500150000	-2.658299000	1.376082000
C	-0.346698000	-3.655047000	0.391931000
C	-3.383556000	-1.970713000	0.294402000
C	-4.258639000	-2.233164000	1.366223000
C	-3.653509000	-2.607691000	-0.929406000
C	-5.351330000	-3.101203000	1.240425000
C	-4.738629000	-3.483581000	-1.079673000
C	-5.590108000	-3.728731000	0.007881000
F	-5.973115000	1.264811000	-2.979589000
F	-3.651785000	0.055771000	-2.249084000
F	-2.867351000	-2.400642000	-2.006130000
F	-4.968223000	-4.086307000	-2.261214000
F	-6.167530000	-3.334946000	2.284424000
F	-4.047590000	-1.633357000	2.556801000
F	-0.792356000	-3.428589000	-0.866008000
C	-2.426102000	0.460181000	0.331448000
C	-3.679966000	1.104020000	-0.104195000
C	-4.335545000	2.018925000	0.748081000
C	-5.525813000	2.656804000	0.374505000
C	-6.087333000	2.391980000	-0.884714000
F	-3.829117000	2.286756000	1.968568000
F	-6.135320000	3.512568000	1.213641000
F	-7.224395000	3.000647000	-1.254327000
C	-1.304844000	1.146122000	0.744032000
C	-1.110945000	2.596540000	0.635043000
C	-0.777549000	3.373452000	1.759812000
C	-1.173170000	3.262464000	-0.605220000
C	-0.527454000	4.746729000	1.668898000
C	-0.917296000	4.632248000	-0.726912000
C	-0.608447000	5.378691000	0.419645000
F	-0.664161000	2.777863000	2.969909000
F	-1.417364000	2.555026000	-1.735831000
F	-0.917187000	5.229745000	-1.935010000
F	-0.312965000	6.686468000	0.309784000

F	-0.153891000	5.452254000	2.753564000
B	-0.258609000	0.071583000	1.269485000
C	0.464106000	-1.449670000	-3.027454000
C	-0.496808000	-0.724107000	-2.668875000
H	-1.500174000	-0.349434000	-2.834240000
C	1.633499000	-2.202663000	-3.305118000
C	1.754794000	-3.539089000	-2.832842000
C	2.955718000	-4.228333000	-3.021697000
C	4.033816000	-3.605180000	-3.678044000
H	0.920081000	-4.004957000	-2.305512000
H	3.055383000	-5.250872000	-2.645292000
H	4.975808000	-4.147366000	-3.809195000
C	2.720662000	-1.584798000	-3.984724000
C	3.913119000	-2.289084000	-4.164030000
H	2.611862000	-0.560834000	-4.351971000
H	4.755897000	-1.812197000	-4.673184000
Au	0.652581000	-0.042810000	-0.916185000

RC-PPh₃: E= -1830.181783

Au	0.015133000	-0.744552000	-0.176805000
P	2.259971000	-0.238234000	-0.004455000
C	2.937809000	-0.511211000	1.673396000
C	2.507702000	-1.641533000	2.402052000
C	3.050694000	-1.902582000	3.668608000
H	2.714811000	-2.778243000	4.233709000
C	4.016553000	-1.037038000	4.212354000
C	4.441975000	0.090216000	3.489156000
H	5.191699000	0.766171000	3.913300000
C	3.905717000	0.357938000	2.219414000
H	1.750599000	-2.312435000	1.978669000
H	4.434756000	-1.239507000	5.203953000
H	4.236499000	1.237782000	1.657400000
C	3.330252000	-1.169181000	-1.160016000
C	4.649958000	-1.523327000	-0.809396000
C	5.461377000	-2.189031000	-1.742121000
C	4.961634000	-2.500966000	-3.017869000
C	3.645366000	-2.149692000	-3.366652000
H	3.252979000	-2.397627000	-4.358353000
C	2.826855000	-1.486986000	-2.440544000
H	5.040326000	-1.282381000	0.185059000
H	5.597146000	-3.023172000	-3.740743000
H	1.798192000	-1.216678000	-2.707772000
H	6.485029000	-2.465354000	-1.468828000
C	-2.205076000	0.167208000	-0.201720000
C	-2.090259000	-1.083802000	-0.317796000
H	-2.633449000	-2.023146000	-0.393501000
C	-2.201755000	1.583887000	-0.078786000
C	-2.219066000	2.178207000	1.211311000
C	-2.113475000	2.394637000	-1.240958000
C	-2.147595000	3.569317000	1.328527000
C	-2.044424000	3.785484000	-1.105818000
C	-2.059784000	4.371729000	0.173597000
H	-2.284321000	1.537417000	2.095331000
H	-2.085672000	1.919712000	-2.225948000
H	-2.157602000	4.032632000	2.319766000
H	-1.971176000	4.414755000	-1.997845000
H	-2.000471000	5.460446000	0.272573000
C	-5.155215000	0.271695000	0.589355000
C	-5.431825000	0.067028000	-0.781607000
C	-4.945226000	-0.806312000	1.467708000
C	-5.503331000	-1.252364000	-1.261045000

C	-5.035711000	-2.116998000	0.956468000
C	-5.317809000	-2.358347000	-0.403431000
H	-5.713133000	-1.428080000	-2.323896000
H	-4.874892000	-2.968416000	1.630427000
C	-4.554767000	-0.566290000	2.910342000
H	-5.012494000	-1.308212000	3.588058000
H	-3.456763000	-0.650919000	3.032750000
H	-4.848276000	0.441746000	3.250621000
C	-5.447185000	-3.771881000	-0.932995000
H	-4.921432000	-4.497930000	-0.289151000
H	-6.509298000	-4.080060000	-0.977683000
H	-5.042408000	-3.858976000	-1.956835000
C	-5.638416000	1.253616000	-1.697757000
H	-4.791507000	1.961888000	-1.627557000
H	-5.739435000	0.943314000	-2.751504000
H	-6.549033000	1.817242000	-1.421080000
H	-5.085581000	1.297951000	0.971568000
C	2.503068000	1.542448000	-0.382781000
C	1.519050000	2.472588000	0.021263000
C	3.667586000	1.989828000	-1.041731000
C	1.703507000	3.839349000	-0.230894000
C	3.843928000	3.360875000	-1.289994000
C	2.864688000	4.284495000	-0.887071000
H	0.606268000	2.134472000	0.525965000
H	4.430191000	1.272196000	-1.362460000
H	0.931045000	4.551862000	0.075979000
H	4.747699000	3.704954000	-1.803561000
H	3.003832000	5.351692000	-1.089400000

RC-FLP1' : E= -3564.976888

Au	-0.056071000	-0.283027000	-0.973874000
B	-0.575016000	0.336918000	1.943976000
C	-2.844213000	-0.810939000	1.118450000
P	-2.322511000	-0.547737000	-0.612329000
C	-1.968712000	-0.396649000	2.073232000
H	-2.274934000	-0.549262000	3.124587000
C	-3.156370000	0.947212000	-1.255770000
C	-3.030279000	1.265089000	-2.627250000
C	-3.556725000	2.470261000	-3.112901000
H	-3.464936000	2.712001000	-4.176836000
C	-4.188456000	3.370282000	-2.234210000
C	-4.304799000	3.058224000	-0.870018000
H	-4.778304000	3.761306000	-0.177761000
C	-3.794912000	1.845546000	-0.379120000
H	-2.521649000	0.573278000	-3.308618000
H	-4.585379000	4.317028000	-2.615105000
H	-3.879273000	1.607443000	0.684089000
C	-2.884079000	-1.990529000	-1.586918000
C	-4.043268000	-1.958507000	-2.387589000
C	-4.466770000	-3.125966000	-3.043742000
C	-3.736812000	-4.318920000	-2.906967000
C	-2.573002000	-4.347752000	-2.117275000
H	-2.000664000	-5.275094000	-2.011718000
C	-2.142785000	-3.187367000	-1.459891000
H	-4.613018000	-1.030761000	-2.501710000
H	-4.072233000	-5.226369000	-3.419690000
H	-1.242751000	-3.212228000	-0.834592000
C	-0.623667000	1.890249000	1.697671000
C	-1.783569000	2.640049000	2.000511000
F	-2.797428000	2.080961000	2.704201000
C	-1.972654000	3.966443000	1.597563000

F	-3.120135000	4.612495000	1.873358000
C	-0.956669000	4.614816000	0.880409000
F	-1.118326000	5.880890000	0.476856000
C	0.233686000	3.928591000	0.588727000
F	1.212049000	4.557921000	-0.093940000
C	0.385779000	2.605120000	1.011963000
F	1.541924000	1.992482000	0.669037000
C	0.730729000	-0.469293000	2.271868000
C	1.869835000	0.103740000	2.882961000
F	1.884795000	1.412853000	3.217611000
C	3.018030000	-0.632966000	3.199151000
F	4.085202000	-0.040041000	3.765759000
C	3.050295000	-2.009265000	2.925598000
F	4.151728000	-2.724021000	3.195133000
C	1.931893000	-2.635048000	2.354083000
F	1.959518000	-3.952607000	2.091579000
C	0.812217000	-1.862955000	2.034657000
F	-0.204111000	-2.513548000	1.417888000
H	-5.369899000	-3.100601000	-3.662102000
C	2.216498000	-0.903103000	-1.397744000
C	1.903519000	0.282149000	-1.659103000
H	2.128764000	1.278652000	-2.032137000
C	2.638702000	-2.223942000	-1.076644000
C	3.779114000	-2.396364000	-0.249818000
C	1.942307000	-3.353105000	-1.579341000
C	4.224008000	-3.687956000	0.049920000
C	2.393002000	-4.637901000	-1.258612000
C	3.534109000	-4.806340000	-0.452801000
H	4.291645000	-1.514428000	0.142252000
H	1.054476000	-3.203530000	-2.202347000
H	5.097626000	-3.822004000	0.694307000
H	1.854514000	-5.511665000	-1.638429000
H	3.881041000	-5.814758000	-0.205680000
C	5.242295000	0.847749000	-1.100115000
C	5.113249000	0.881779000	-2.504308000
C	4.676797000	1.841307000	-0.280520000
C	4.428444000	1.963692000	-3.087845000
C	3.984358000	2.904454000	-0.895502000
C	3.860270000	2.987561000	-2.296715000
H	4.318478000	2.006243000	-4.179006000
H	3.513118000	3.670082000	-0.269857000
C	4.796871000	1.773512000	1.226725000
H	5.498647000	2.539518000	1.607567000
H	3.824971000	1.957704000	1.714645000
H	5.166347000	0.790963000	1.564968000
C	3.133965000	4.153121000	-2.937936000
H	2.280751000	4.480820000	-2.320020000
H	3.806910000	5.024287000	-3.053042000
H	2.758207000	3.894900000	-3.943299000
C	5.659161000	-0.253264000	-3.344784000
H	5.070135000	-1.176407000	-3.181809000
H	5.624828000	-0.018205000	-4.422084000
H	6.704993000	-0.489061000	-3.076810000
H	5.794510000	0.019465000	-0.637519000
Si	-4.528704000	-1.621697000	1.545355000
C	-5.916838000	-0.722101000	0.621926000
H	-6.880111000	-1.218804000	0.839544000
H	-5.997243000	0.333150000	0.935176000
H	-5.768145000	-0.741871000	-0.470937000
C	-4.518877000	-3.457643000	1.081233000
H	-5.386180000	-3.956991000	1.551087000

H	-4.586982000	-3.604396000	-0.009820000
H	-3.600463000	-3.956349000	1.437381000
C	-4.760951000	-1.416560000	3.413379000
H	-4.006086000	-1.980750000	3.989869000
H	-4.706280000	-0.354694000	3.712798000
H	-5.756556000	-1.799772000	3.701933000

RC-FLP3' : E= -2316.444123

B	-0.915806000	-1.730591000	-1.540919000
C	-2.394384000	-2.164790000	-1.209108000
C	-3.233771000	-1.499084000	-0.277520000
C	-4.547377000	-1.932158000	-0.012938000
H	-5.159746000	-1.412440000	0.732553000
C	-5.059597000	-3.043585000	-0.700461000
H	-6.079853000	-3.386811000	-0.500515000
C	-4.251621000	-3.718709000	-1.630992000
H	-4.642305000	-4.595026000	-2.159517000
C	-2.935135000	-3.290392000	-1.873110000
H	-2.312732000	-3.844136000	-2.585784000
C	0.383197000	-2.553257000	-1.206189000
C	0.630711000	-3.618879000	-0.325088000
H	-0.193495000	-4.049892000	0.255806000
C	1.943345000	-4.115100000	-0.178839000
H	2.148820000	-4.940311000	0.511304000
C	2.992718000	-3.553365000	-0.927735000
H	4.008342000	-3.945518000	-0.810891000
C	2.760846000	-2.489386000	-1.829446000
H	3.592696000	-2.062068000	-2.399172000
C	1.463944000	-1.990495000	-1.960664000
C	0.979747000	-0.852629000	-2.782767000
C	1.699389000	-0.054967000	-3.679234000
H	2.761635000	-0.238947000	-3.875745000
C	1.032780000	1.007059000	-4.333774000
H	1.590296000	1.644729000	-5.028369000
C	-0.329475000	1.257782000	-4.095991000
H	-0.828602000	2.091103000	-4.601430000
C	-1.057635000	0.434656000	-3.210122000
H	-2.121150000	0.630451000	-3.037451000
C	-0.415641000	-0.622524000	-2.546410000
P	-2.520509000	-0.038089000	0.554885000
Au	-0.231866000	-0.295479000	0.712936000
C	1.921535000	0.803380000	0.601346000
C	1.821876000	2.174912000	0.235897000
C	1.459568000	2.501338000	-1.097494000
C	2.049145000	3.202261000	1.187925000
C	1.339498000	3.842792000	-1.472416000
C	1.925440000	4.539273000	0.796623000
C	1.571439000	4.860975000	-0.529024000
H	2.326965000	2.936348000	2.211351000
H	1.054847000	4.090205000	-2.499883000
H	2.103229000	5.336221000	1.525273000
H	1.473433000	5.910633000	-0.824707000
C	4.931549000	1.225962000	0.877436000
C	4.933057000	0.800655000	2.219264000
C	5.056320000	0.308491000	-0.187745000
C	5.067810000	-0.576090000	2.488356000
C	5.224244000	-1.053075000	0.117440000
C	5.220744000	-1.516042000	1.450629000
H	5.066840000	-0.922446000	3.530072000
H	5.359585000	-1.772577000	-0.698481000
C	4.933849000	0.779766000	-1.619897000

H	5.416277000	1.760955000	-1.774311000
H	5.375225000	0.058925000	-2.329899000
H	3.865594000	0.899810000	-1.889215000
C	5.345248000	-2.994723000	1.754585000
H	4.354667000	-3.488691000	1.721957000
H	5.986042000	-3.507829000	1.016016000
H	5.767031000	-3.170256000	2.759199000
C	4.764516000	1.790671000	3.353106000
H	4.834795000	2.832869000	2.997616000
H	3.780232000	1.666973000	3.844746000
H	4.819533000	2.293827000	0.652410000
H	1.255780000	1.696748000	-1.807073000
C	1.914657000	-0.425123000	0.874202000
H	2.491391000	-1.335086000	1.019815000
H	5.530909000	1.644672000	4.135620000
C	-3.380093000	0.172154000	2.151415000
C	-2.924974000	-0.573102000	3.261373000
C	-4.503096000	1.016981000	2.274206000
C	-3.599619000	-0.478365000	4.486916000
C	-5.170667000	1.106882000	3.506378000
C	-4.721546000	0.361152000	4.609442000
H	-2.045428000	-1.221083000	3.163208000
H	-4.852012000	1.600726000	1.415714000
H	-3.245607000	-1.054367000	5.348161000
H	-6.041812000	1.763127000	3.602912000
H	-5.243405000	0.437773000	5.569088000
C	-2.919236000	1.405928000	-0.499315000
C	-2.024791000	2.495658000	-0.550776000
C	-4.072899000	1.399965000	-1.312476000
C	-2.279785000	3.569520000	-1.414835000
C	-4.323463000	2.481250000	-2.172298000
C	-3.425764000	3.561720000	-2.228723000
H	-1.114463000	2.493081000	0.058997000
H	-4.756994000	0.544742000	-1.294191000
H	-1.570401000	4.401867000	-1.461787000
H	-5.214850000	2.471683000	-2.807952000
H	-3.616832000	4.395038000	-2.912958000

RC-FLP4: E= -1978.262969

Au	0.161182000	-1.003271000	-0.478846000
B	-2.954992000	1.204613000	-0.777457000
C	-3.199602000	-0.334907000	-1.124636000
P	-2.076489000	-1.589966000	-0.350633000
H	-4.241172000	-0.665045000	-0.970664000
C	-1.525915000	1.815508000	-0.987405000
C	-0.720729000	1.486168000	-2.111988000
C	0.565066000	2.026519000	-2.276865000
C	1.097092000	2.880019000	-1.295609000
C	0.330932000	3.209868000	-0.165647000
C	-0.968332000	2.695118000	-0.024169000
C	-4.145157000	2.105463000	-0.313534000
C	-4.079424000	3.519988000	-0.449187000
C	-5.142860000	4.347276000	-0.061014000
C	-6.304344000	3.780872000	0.492680000
C	-6.401490000	2.384966000	0.642225000
C	-5.342145000	1.565639000	0.232163000
C	2.198524000	-0.303705000	0.548842000
C	2.233106000	-0.487307000	-0.693912000
H	2.780187000	-0.376381000	-1.625666000
C	2.146301000	-0.120374000	1.959768000
C	1.319354000	0.895166000	2.507254000

C	2.922053000	-0.947442000	2.812218000
C	1.277022000	1.079194000	3.893142000
C	2.874930000	-0.744947000	4.195742000
C	2.053667000	0.263084000	4.736608000
H	0.721409000	1.512421000	1.830127000
H	3.557326000	-1.723962000	2.376737000
H	0.637709000	1.859458000	4.317942000
H	3.477171000	-1.376002000	4.856810000
H	2.018328000	0.411414000	5.820840000
C	5.112626000	0.772886000	0.637852000
C	5.559596000	-0.333275000	-0.105853000
C	4.630007000	1.941055000	0.008080000
C	5.532161000	-0.253528000	-1.514243000
C	4.631141000	1.993669000	-1.396036000
C	5.075856000	0.903321000	-2.175202000
H	5.874827000	-1.111173000	-2.107458000
H	4.286186000	2.903578000	-1.903678000
C	4.068956000	3.074242000	0.838567000
H	4.013977000	4.016685000	0.266874000
H	3.043185000	2.828529000	1.176667000
H	4.672351000	3.253288000	1.745969000
C	5.072421000	0.993921000	-3.687623000
H	5.880723000	1.658024000	-4.048143000
H	5.220476000	0.005363000	-4.154839000
H	4.121072000	1.413426000	-4.062705000
C	6.005088000	-1.605846000	0.583038000
H	6.214641000	-1.437609000	1.653359000
H	5.218723000	-2.382736000	0.514637000
H	6.912937000	-2.027356000	0.115876000
H	5.118671000	0.721554000	1.733771000
H	-3.002539000	-0.434827000	-2.212405000
H	-1.114249000	0.812327000	-2.882773000
H	1.161565000	1.763854000	-3.157535000
H	2.107016000	3.282808000	-1.409156000
H	0.742282000	3.878251000	0.599164000
H	-1.561700000	2.965866000	0.857123000
H	-3.180947000	3.973026000	-0.882485000
H	-5.067757000	5.432950000	-0.186950000
H	-7.134836000	4.424350000	0.803834000
H	-7.304908000	1.940232000	1.073644000
C	-2.403920000	-3.194005000	-1.322284000
C	-2.542628000	-1.666684000	1.496110000
C	-2.461217000	-0.214605000	2.025338000
H	-1.477441000	0.244424000	1.818973000
H	-3.248326000	0.435537000	1.609157000
H	-2.599480000	-0.230183000	3.122334000
C	-1.506936000	-2.512103000	2.275948000
H	-1.782643000	-2.496999000	3.346759000
H	-1.479143000	-3.564056000	1.954735000
H	-0.488493000	-2.093154000	2.184880000
C	-3.961743000	-2.231431000	1.712644000
H	-4.235963000	-2.109891000	2.776862000
H	-4.724743000	-1.704218000	1.113647000
H	-4.015883000	-3.307733000	1.478279000
C	-1.777598000	-4.391500000	-0.577274000
H	-1.800554000	-5.276702000	-1.239535000
H	-0.723474000	-4.198940000	-0.306152000
H	-2.338945000	-4.649677000	0.336201000
C	-3.908370000	-3.440462000	-1.572098000
H	-4.486694000	-3.530269000	-0.639054000
H	-4.361573000	-2.646430000	-2.189469000

H	-4.019893000	-4.391346000	-2.125385000
C	-1.686044000	-3.020980000	-2.685048000
H	-1.883517000	-3.914828000	-3.305471000
H	-2.048838000	-2.143195000	-3.248824000
H	-0.591907000	-2.926153000	-2.561925000
H	-5.440878000	0.481288000	0.359144000

RC-FLP5: E= -2091.310558

P	1.896510000	-0.520649000	0.640777000
C	2.517896000	-1.369388000	2.141457000
C	1.710469000	-2.195215000	2.846635000
H	2.152162000	-2.680660000	3.733450000
C	3.292762000	-0.851356000	-0.526963000
C	4.532627000	-0.175673000	-0.305701000
C	5.608164000	-0.450778000	-1.174058000
H	6.559000000	0.068810000	-1.003340000
C	5.506934000	-1.350367000	-2.244606000
C	4.278717000	-2.008646000	-2.431016000
H	4.178834000	-2.724845000	-3.255721000
C	3.170346000	-1.786482000	-1.596908000
C	4.788099000	0.871408000	0.766232000
H	5.868575000	0.934675000	0.976750000
H	4.275714000	0.680531000	1.721571000
H	4.452560000	1.868629000	0.427413000
C	6.672474000	-1.614332000	-3.170866000
H	6.425117000	-1.323928000	-4.208705000
H	6.927569000	-2.689625000	-3.190997000
H	7.571545000	-1.053911000	-2.865029000
C	1.906347000	-2.562238000	-1.902529000
H	2.062424000	-3.230771000	-2.765229000
H	1.058061000	-1.897610000	-2.151742000
H	1.594358000	-3.191401000	-1.050691000
C	1.781381000	1.308762000	0.798552000
C	1.856965000	2.086977000	-0.397929000
C	1.882617000	3.485802000	-0.284027000
H	1.940342000	4.083034000	-1.201884000
C	1.799829000	4.142915000	0.955495000
C	1.625528000	3.354633000	2.103330000
H	1.489816000	3.846926000	3.074115000
C	1.591244000	1.948836000	2.055944000
C	1.890286000	1.500083000	-1.796836000
H	1.253137000	0.603173000	-1.893824000
H	2.910621000	1.213504000	-2.106121000
H	1.512856000	2.245608000	-2.515932000
C	1.805132000	5.651587000	1.027620000
H	0.849935000	6.057042000	0.642824000
H	2.610730000	6.082129000	0.406783000
H	1.931819000	6.012435000	2.062021000
C	1.304503000	1.202234000	3.340552000
H	0.995468000	1.908763000	4.128690000
H	2.180400000	0.644459000	3.714224000
H	0.492664000	0.462648000	3.209831000
C	-0.304641000	-3.340123000	1.273185000
C	-1.694476000	-3.105258000	1.204599000
C	-2.151211000	-2.305448000	2.385508000
C	-1.106111000	-1.952757000	3.198786000
B	0.217051000	-2.478231000	2.498780000
C	-1.484061000	0.344883000	-0.992392000
C	-1.805935000	-0.832712000	-1.298347000
H	-2.510023000	-1.546620000	-1.710043000
C	-1.359553000	1.754962000	-0.815127000

C	-1.346008000	2.600028000	-1.952547000
C	-1.382270000	3.989064000	-1.779470000
C	-1.429081000	4.539320000	-0.486037000
H	-1.324926000	2.157439000	-2.952590000
H	-1.380403000	4.643631000	-2.656815000
H	-1.469437000	5.625965000	-0.357949000
C	-4.562997000	1.195336000	-0.515706000
C	-4.831840000	0.819240000	-1.848554000
C	-5.108461000	-0.532219000	-2.123095000
C	-4.864550000	-1.089282000	0.222015000
C	-5.135013000	-1.501246000	-1.095695000
H	-5.310879000	-0.841614000	-3.156828000
C	-5.452779000	-2.948887000	-1.412362000
H	-4.836874000	-3.322374000	-2.251089000
H	-5.276660000	-3.603094000	-0.541161000
H	-6.510200000	-3.070220000	-1.714159000
C	-4.822096000	1.859349000	-2.948944000
H	-5.758640000	2.449199000	-2.948377000
H	-3.989804000	2.572994000	-2.812505000
H	-4.722186000	1.397082000	-3.946142000
H	-4.318024000	2.241776000	-0.294607000
C	-1.370163000	2.313061000	0.486007000
C	-1.412589000	3.700690000	0.643827000
H	-1.348555000	1.645423000	1.351699000
H	-1.417588000	4.131513000	1.649259000
C	-4.564286000	0.254520000	0.528696000
H	-4.891004000	-1.834686000	1.026775000
C	-4.198442000	0.661388000	1.940152000
H	-4.850256000	0.175139000	2.688371000
H	-3.159233000	0.360223000	2.175912000
H	-4.263998000	1.753899000	2.079203000
Au	-0.319866000	-1.343119000	0.219592000
H	0.211472000	-4.062574000	0.632863000
H	-2.390599000	-3.564166000	0.494060000
H	-3.201784000	-2.032481000	2.521149000
H	-1.233475000	-1.333439000	4.091877000
H	3.581366000	-1.231371000	2.376046000

RC-FLP6: E= -5408.626720

P	-2.565761000	0.993311000	-0.460043000
C	-2.545963000	0.800493000	-2.280642000
C	-1.308895000	0.452130000	-2.733345000
H	-1.178615000	0.347290000	-3.822591000
Si	-4.061162000	0.727633000	-3.454346000
C	-4.250683000	-1.111604000	-3.877225000
H	-4.577577000	-1.689902000	-2.994853000
H	-3.297025000	-1.538151000	-4.234728000
H	-5.008016000	-1.248016000	-4.670421000
C	-5.665802000	1.352640000	-2.669262000
H	-6.477067000	1.251315000	-3.413582000
H	-5.626912000	2.414086000	-2.369404000
H	-5.941156000	0.755578000	-1.783403000
C	-3.635360000	1.715936000	-5.011529000
H	-2.688855000	1.371461000	-5.465150000
H	-3.538950000	2.794427000	-4.796861000
H	-4.435273000	1.586169000	-5.763039000
C	-4.062172000	0.171816000	0.230574000
C	-5.138189000	0.887310000	0.843231000
C	-6.172669000	0.144895000	1.444161000
H	-6.996456000	0.693991000	1.916007000
C	-6.201927000	-1.259026000	1.448300000

C	-5.180916000	-1.934362000	0.761197000
H	-5.202758000	-3.029155000	0.709838000
C	-4.110219000	-1.259017000	0.156121000
C	-5.288941000	2.396761000	0.864671000
H	-6.348312000	2.658239000	1.021816000
H	-4.963859000	2.872280000	-0.072786000
H	-4.707498000	2.864052000	1.678894000
C	-7.284260000	-2.025665000	2.169132000
H	-7.608866000	-2.908226000	1.590866000
H	-8.166164000	-1.397043000	2.376820000
H	-6.902984000	-2.397949000	3.139592000
C	-3.067030000	-2.114974000	-0.527249000
H	-3.490670000	-3.099896000	-0.783024000
H	-2.205638000	-2.303231000	0.139205000
H	-2.670100000	-1.672533000	-1.452642000
C	-2.371864000	2.723377000	0.164922000
C	-2.123453000	2.888903000	1.566263000
C	-1.846536000	4.174540000	2.060982000
H	-1.655695000	4.288006000	3.134816000
C	-1.817579000	5.309105000	1.236062000
C	-2.109095000	5.127170000	-0.125439000
H	-2.109212000	6.001373000	-0.787177000
C	-2.380334000	3.867299000	-0.689667000
C	-2.164508000	1.775331000	2.598865000
H	-1.149493000	1.409877000	2.841438000
H	-2.773033000	0.910149000	2.293925000
H	-2.595486000	2.156658000	3.541098000
C	-1.441376000	6.665751000	1.780835000
H	-1.730699000	6.773479000	2.839984000
H	-1.906979000	7.480670000	1.201310000
H	-0.346583000	6.799655000	1.718537000
C	-2.698046000	3.842384000	-2.169464000
H	-2.644916000	4.860909000	-2.585981000
H	-3.716206000	3.462119000	-2.360114000
H	-2.003666000	3.212171000	-2.744482000
C	-0.776552000	-2.846676000	-3.223876000
C	-0.966280000	-4.784253000	-1.234262000
C	-1.602451000	-3.960082000	-3.420252000
C	-1.704212000	-4.937310000	-2.417163000
F	6.213542000	-4.835216000	-0.791730000
F	-0.707251000	-1.942803000	-4.228896000
F	-2.300819000	-4.091738000	-4.563124000
F	-2.503065000	-6.002998000	-2.586489000
F	-1.082489000	-5.687475000	-0.238441000
C	0.634855000	-1.362926000	-1.767142000
C	1.930905000	-1.168626000	-1.342143000
C	4.148508000	0.646976000	0.435104000
C	5.356248000	1.248169000	0.801887000
C	-0.040417000	-2.641777000	-2.036746000
C	-0.144296000	-3.663369000	-1.071303000
C	2.997879000	-2.188055000	-1.170715000
C	3.803816000	-2.528183000	-2.273703000
C	3.323418000	-2.774682000	0.065123000
C	4.880601000	-3.419057000	-2.163363000
C	4.398147000	-3.662638000	0.204246000
C	5.181354000	-3.984693000	-0.914051000
F	5.862403000	1.076069000	2.040009000
F	3.495473000	-0.087865000	1.362397000
F	2.602211000	-2.503617000	1.173913000
F	4.681978000	-4.196399000	1.408117000
F	5.629987000	-3.726279000	-3.237921000

F	3.546983000	-1.975801000	-3.477878000
F	0.481051000	-3.527622000	0.120974000
C	2.233936000	0.291449000	-1.172284000
C	3.562667000	0.838293000	-0.826381000
C	4.247843000	1.674706000	-1.730439000
C	5.470458000	2.275417000	-1.398415000
C	6.026418000	2.060586000	-0.126542000
F	3.727067000	1.917499000	-2.949849000
F	6.111411000	3.057633000	-2.285011000
F	7.189791000	2.641465000	0.204714000
C	1.136914000	1.072967000	-1.455870000
C	1.081490000	2.526565000	-1.270350000
C	0.663153000	3.391523000	-2.298123000
C	1.373615000	3.117583000	-0.024441000
C	0.555309000	4.774542000	-2.110781000
C	1.261530000	4.492428000	0.196562000
C	0.864745000	5.326880000	-0.858799000
F	0.326970000	2.878471000	-3.504314000
F	1.711990000	2.329802000	1.026910000
F	1.478799000	5.011644000	1.421861000
F	0.709258000	6.646338000	-0.648989000
F	0.101805000	5.568691000	-3.099231000
B	-0.052268000	0.095164000	-1.857226000
Au	-0.680646000	-0.075040000	0.422125000
C	-0.471818000	-1.586696000	2.525127000
C	0.456794000	-0.866374000	2.074576000
H	1.448222000	-0.473500000	2.295564000
C	-1.628059000	-2.314054000	2.892188000
C	-2.623545000	-1.684815000	3.691489000
C	-1.831715000	-3.636835000	2.411571000
C	-3.804036000	-2.367676000	3.990717000
C	-3.022970000	-4.302857000	2.713961000
C	-4.006315000	-3.671932000	3.499483000
H	-2.444456000	-0.673146000	4.065163000
H	-1.068783000	-4.107634000	1.788073000
H	-4.573867000	-1.883847000	4.599322000
H	-3.188537000	-5.314604000	2.331441000
H	-4.938566000	-4.198877000	3.727604000
C	0.335625000	0.492263000	5.214432000
C	0.589677000	-0.861829000	5.523746000
C	1.281969000	1.284646000	4.539492000
C	1.822528000	-1.420563000	5.136373000
C	2.508115000	0.690579000	4.163130000
C	2.794958000	-0.660381000	4.456085000
H	2.031339000	-2.472691000	5.369674000
H	3.256320000	1.289267000	3.629496000
C	0.994258000	2.736383000	4.215731000
H	1.809468000	3.394449000	4.568003000
H	0.902952000	2.900891000	3.127867000
H	0.056158000	3.074547000	4.688266000
C	4.100007000	-1.300197000	4.026318000
H	4.795678000	-0.558310000	3.604550000
H	4.595563000	-1.802154000	4.876885000
H	3.925705000	-2.067293000	3.250074000
C	-0.424744000	-1.694762000	6.279417000
H	-0.654791000	-2.633102000	5.742947000
H	-0.040972000	-1.977437000	7.277416000
H	-1.372455000	-1.149523000	6.426433000
H	-0.620114000	0.939627000	5.517259000

TS-PPh₃: E= -1830.174437

Au	-0.069141000	-0.635736000	0.007873000
P	2.216066000	-0.259218000	0.005273000
C	3.002017000	-0.566765000	1.633293000
C	2.556480000	-1.672643000	2.390373000
C	3.166733000	-1.971948000	3.617272000
H	2.818296000	-2.829356000	4.202656000
C	4.215770000	-1.167257000	4.096535000
C	4.655605000	-0.062750000	3.347561000
H	5.469732000	0.567095000	3.721303000
C	4.052196000	0.241283000	2.116325000
H	1.732564000	-2.293639000	2.018515000
H	4.687151000	-1.398771000	5.057573000
H	4.395744000	1.103963000	1.535763000
C	3.150754000	-1.275478000	-1.200623000
C	4.475182000	-1.689906000	-0.946771000
C	5.174290000	-2.422886000	-1.919352000
C	4.557562000	-2.744227000	-3.140545000
C	3.236022000	-2.335315000	-3.392892000
H	2.751584000	-2.591318000	-4.341061000
C	2.530201000	-1.604900000	-2.425429000
H	4.956136000	-1.443198000	0.005965000
H	5.105224000	-3.318968000	-3.894943000
H	1.496528000	-1.291405000	-2.615793000
H	6.201841000	-2.744716000	-1.719993000
C	-2.724087000	0.364887000	0.106854000
C	-2.130470000	-0.793760000	0.004908000
H	-2.650545000	-1.759644000	-0.056906000
C	-2.472793000	1.791640000	0.060361000
C	-2.712673000	2.628204000	1.177971000
C	-1.899303000	2.342244000	-1.115753000
C	-2.363435000	3.982405000	1.125544000
C	-1.551696000	3.698720000	-1.157493000
C	-1.784597000	4.519999000	-0.040384000
H	-3.157495000	2.204661000	2.083916000
H	-1.704372000	1.684164000	-1.968180000
H	-2.538442000	4.622043000	1.996442000
H	-1.089926000	4.112363000	-2.059382000
H	-1.514046000	5.580487000	-0.075911000
C	-4.875989000	0.248963000	0.289876000
C	-5.059870000	-0.136048000	-1.081687000
C	-4.986635000	-0.714179000	1.349963000
C	-5.159846000	-1.501195000	-1.378835000
C	-5.101539000	-2.057551000	1.005438000
C	-5.168341000	-2.471151000	-0.354324000
H	-5.250806000	-1.822052000	-2.422569000
H	-5.143185000	-2.819188000	1.792918000
C	-4.868337000	-0.265710000	2.783567000
H	-5.229042000	-1.038080000	3.482243000
H	-3.806984000	-0.063461000	3.027243000
H	-5.430533000	0.666849000	2.965935000
C	-5.266969000	-3.940323000	-0.679354000
H	-4.349592000	-4.468745000	-0.359138000
H	-6.107385000	-4.406239000	-0.133040000
H	-5.407029000	-4.116174000	-1.757911000
C	-5.142811000	0.920810000	-2.149580000
H	-4.378927000	1.705080000	-1.998670000
H	-5.021362000	0.494542000	-3.158491000
H	-6.126429000	1.425950000	-2.106192000
H	-4.998719000	1.307379000	0.542590000
C	2.581975000	1.490067000	-0.419392000
C	1.649208000	2.489128000	-0.062966000

C	3.785423000	1.849855000	-1.063418000
C	1.926288000	3.836154000	-0.339120000
C	4.055084000	3.200458000	-1.336295000
C	3.128572000	4.193274000	-0.973627000
H	0.701960000	2.215924000	0.417454000
H	4.506671000	1.078120000	-1.353528000
H	1.192969000	4.602440000	-0.068082000
H	4.989305000	3.475477000	-1.837113000
H	3.340463000	5.245248000	-1.192656000

TS-FLP1': E= -3564.967962

Au	-0.108278000	-0.086458000	-0.912481000
B	-0.534297000	0.299548000	1.908267000
C	-2.862091000	-0.786859000	1.115938000
P	-2.365767000	-0.512088000	-0.623487000
C	-1.958338000	-0.379897000	2.047142000
H	-2.241724000	-0.526355000	3.106742000
C	-3.291339000	0.933084000	-1.264003000
C	-3.273667000	1.207308000	-2.650452000
C	-3.849133000	2.390982000	-3.135088000
H	-3.841586000	2.595936000	-4.210828000
C	-4.422261000	3.315972000	-2.242750000
C	-4.429315000	3.049917000	-0.863663000
H	-4.859151000	3.771137000	-0.161230000
C	-3.870808000	1.858693000	-0.373593000
H	-2.810240000	0.498392000	-3.346259000
H	-4.858679000	4.245044000	-2.624352000
H	-3.873606000	1.656278000	0.699712000
C	-2.875733000	-1.977446000	-1.596193000
C	-4.084030000	-2.027500000	-2.321507000
C	-4.460282000	-3.215000000	-2.969448000
C	-3.635416000	-4.350834000	-2.898532000
C	-2.422538000	-4.297675000	-2.188646000
H	-1.773551000	-5.178309000	-2.139306000
C	-2.037624000	-3.114122000	-1.543098000
H	-4.728939000	-1.145223000	-2.383037000
H	-3.934652000	-5.275825000	-3.402553000
H	-1.093364000	-3.072276000	-0.988935000
C	-0.486342000	1.867800000	1.738479000
C	-1.640628000	2.656090000	1.956033000
F	-2.721176000	2.132069000	2.584135000
C	-1.754056000	3.992574000	1.556265000
F	-2.898035000	4.674363000	1.750351000
C	-0.654706000	4.620689000	0.952082000
F	-0.736264000	5.900214000	0.563618000
C	0.539319000	3.903424000	0.773557000
F	1.606908000	4.513455000	0.214755000
C	0.611398000	2.568808000	1.182915000
F	1.788631000	1.944462000	0.959740000
C	0.715469000	-0.586172000	2.278875000
C	1.821860000	-0.100792000	3.009464000
F	1.851346000	1.176937000	3.446352000
C	2.929805000	-0.895267000	3.335378000
F	3.987114000	-0.368199000	3.982799000
C	2.937439000	-2.249502000	2.969417000
F	4.004809000	-3.017313000	3.241175000
C	1.836381000	-2.794583000	2.292974000
F	1.836795000	-4.094228000	1.946742000
C	0.765756000	-1.961967000	1.955288000
F	-0.232332000	-2.538112000	1.242651000
H	-5.401122000	-3.251397000	-3.528454000

C	2.791589000	-0.452434000	-1.231978000
C	1.835530000	0.422736000	-1.375767000
H	2.010993000	1.471078000	-1.656894000
C	3.037228000	-1.870960000	-1.103793000
C	3.915381000	-2.418127000	-0.136075000
C	2.307492000	-2.747618000	-1.951171000
C	4.049259000	-3.803770000	-0.008556000
C	2.441025000	-4.135189000	-1.809914000
C	3.313947000	-4.665244000	-0.844634000
H	4.473780000	-1.751922000	0.527854000
H	1.628503000	-2.318922000	-2.695033000
H	4.708925000	-4.213257000	0.761905000
H	1.866078000	-4.802559000	-2.460127000
H	3.419815000	-5.749715000	-0.738746000
C	4.754865000	0.436629000	-1.415898000
C	4.612160000	0.716668000	-2.816807000
C	4.624184000	1.475764000	-0.431456000
C	4.164938000	1.988432000	-3.192658000
C	4.177913000	2.723622000	-0.852949000
C	3.924426000	2.991489000	-2.226807000
H	3.995911000	2.212500000	-4.251891000
H	3.987301000	3.510596000	-0.116302000
C	4.822855000	1.150613000	1.024933000
H	4.887765000	2.059581000	1.643811000
H	3.957419000	0.565775000	1.386549000
H	5.727725000	0.540143000	1.191411000
C	3.416026000	4.351566000	-2.632122000
H	2.516712000	4.616346000	-2.048809000
H	4.174556000	5.126339000	-2.411781000
H	3.172794000	4.400619000	-3.705497000
C	4.909251000	-0.363235000	-3.823181000
H	4.372753000	-1.296347000	-3.566941000
H	4.622675000	-0.061472000	-4.843369000
H	5.987918000	-0.607349000	-3.822974000
H	5.298144000	-0.471416000	-1.136845000
Si	-4.518864000	-1.620422000	1.578990000
C	-5.945630000	-0.750475000	0.686442000
H	-6.898958000	-1.250285000	0.937997000
H	-6.023047000	0.309125000	0.985866000
H	-5.826432000	-0.783397000	-0.409652000
C	-4.464283000	-3.455963000	1.109119000
H	-5.332792000	-3.977998000	1.551420000
H	-4.494492000	-3.602382000	0.016201000
H	-3.545020000	-3.932885000	1.492721000
C	-4.726945000	-1.439177000	3.453024000
H	-3.949047000	-1.991996000	4.009682000
H	-4.691219000	-0.380016000	3.764716000
H	-5.708217000	-1.849092000	3.753952000

TS-FLP3' : E= -2316.435902

B	-0.611159000	-1.750702000	-1.414770000
C	-2.070607000	-2.304317000	-1.165404000
C	-3.048592000	-1.670438000	-0.354864000
C	-4.341222000	-2.203838000	-0.188316000
H	-5.061383000	-1.709259000	0.473672000
C	-4.692346000	-3.386055000	-0.859047000
H	-5.695281000	-3.807662000	-0.735090000
C	-3.744586000	-4.032933000	-1.670614000
H	-4.008851000	-4.965129000	-2.181881000
C	-2.449763000	-3.504935000	-1.810689000
H	-1.715197000	-4.036187000	-2.427319000

C	0.720762000	-2.547354000	-1.139916000
C	1.016321000	-3.643025000	-0.315684000
H	0.226112000	-4.096196000	0.295274000
C	2.330131000	-4.156413000	-0.274589000
H	2.568083000	-5.013774000	0.364669000
C	3.335735000	-3.576662000	-1.068247000
H	4.351720000	-3.985727000	-1.038613000
C	3.056391000	-2.474382000	-1.906330000
H	3.850223000	-2.039526000	-2.524645000
C	1.756904000	-1.960541000	-1.933762000
C	1.221957000	-0.820160000	-2.719933000
C	1.893985000	0.001974000	-3.632247000
H	2.957427000	-0.146926000	-3.850988000
C	1.178875000	1.037552000	-4.275389000
H	1.698688000	1.692229000	-4.983399000
C	-0.188626000	1.234220000	-4.016667000
H	-0.730674000	2.040222000	-4.523020000
C	-0.865904000	0.394741000	-3.106608000
H	-1.932096000	0.552706000	-2.914284000
C	-0.171842000	-0.630273000	-2.444030000
P	-2.510332000	-0.141694000	0.486681000
Au	-0.203669000	-0.200423000	0.702849000
C	2.306023000	1.129455000	0.754665000
C	1.910782000	2.436676000	0.265882000
C	1.345574000	2.513022000	-1.032966000
C	2.010334000	3.610534000	1.052533000
C	0.876101000	3.736630000	-1.525462000
C	1.537467000	4.828851000	0.551701000
C	0.971585000	4.896102000	-0.737248000
H	2.447786000	3.557534000	2.054219000
H	0.427641000	3.771689000	-2.523317000
H	1.607040000	5.731284000	1.167538000
H	0.606784000	5.853811000	-1.123453000
C	4.422721000	1.344998000	1.089262000
C	4.492993000	0.864173000	2.440366000
C	4.808009000	0.509023000	-0.015461000
C	4.771677000	-0.486562000	2.644961000
C	5.103598000	-0.830269000	0.244826000
C	5.061332000	-1.351461000	1.559265000
H	4.781740000	-0.890445000	3.663913000
H	5.375916000	-1.493780000	-0.581424000
C	4.818778000	1.068395000	-1.413356000
H	5.357202000	2.031354000	-1.459702000
H	5.282494000	0.366534000	-2.125521000
H	3.783836000	1.261712000	-1.756236000
C	5.312959000	-2.817333000	1.798141000
H	4.380600000	-3.386352000	1.615061000
H	6.072204000	-3.216652000	1.103930000
H	5.631517000	-3.017728000	2.834444000
C	4.170609000	1.786357000	3.588102000
H	4.547959000	2.808113000	3.409264000
H	3.073052000	1.855687000	3.719105000
H	4.421106000	2.427840000	0.930066000
H	1.252286000	1.599913000	-1.623894000
C	1.860309000	-0.085899000	0.916092000
H	2.467090000	-0.972950000	1.139420000
H	4.592503000	1.415395000	4.536625000
C	-3.436810000	-0.015522000	2.057662000
C	-2.938319000	-0.702498000	3.186494000
C	-4.640461000	0.714443000	2.147084000
C	-3.648808000	-0.666204000	4.395070000

C	-5.344535000	0.746781000	3.361766000
C	-4.851187000	0.058191000	4.483018000
H	-1.996086000	-1.259240000	3.114866000
H	-5.023793000	1.254998000	1.275052000
H	-3.260325000	-1.197456000	5.270269000
H	-6.279044000	1.313415000	3.430759000
H	-5.401552000	0.090047000	5.429263000
C	-3.034965000	1.268071000	-0.558966000
C	-2.274823000	2.456946000	-0.526767000
C	-4.137872000	1.159287000	-1.432461000
C	-2.620081000	3.530008000	-1.360483000
C	-4.476314000	2.238015000	-2.265154000
C	-3.717670000	3.421017000	-2.231913000
H	-1.396798000	2.534536000	0.125094000
H	-4.714614000	0.229465000	-1.479913000
H	-2.017807000	4.443821000	-1.338639000
H	-5.328168000	2.148869000	-2.947355000
H	-3.978224000	4.255787000	-2.891134000

TS-FLP4: E= -1978.249857

Au	-0.341167000	1.025095000	-0.425693000
B	2.908278000	-0.886531000	-1.039198000
C	3.115651000	0.693859000	-1.065070000
P	1.863496000	1.735974000	-0.170733000
H	4.125608000	1.019334000	-0.762642000
C	1.551129000	-1.480400000	-1.553259000
C	0.876723000	-0.923159000	-2.673523000
C	-0.319523000	-1.471313000	-3.159764000
C	-0.893883000	-2.580380000	-2.515103000
C	-0.263712000	-3.135404000	-1.388111000
C	0.944038000	-2.595114000	-0.919828000
C	4.081011000	-1.832097000	-0.612341000
C	4.111729000	-3.191471000	-1.030072000
C	5.165913000	-4.047395000	-0.679660000
C	6.221251000	-3.569473000	0.116560000
C	6.223600000	-2.229186000	0.545071000
C	5.176060000	-1.377275000	0.172279000
C	-2.550255000	-0.426724000	0.654675000
C	-2.296982000	0.351357000	-0.369870000
H	-3.038402000	0.602730000	-1.141247000
C	-1.884675000	-0.867351000	1.876620000
C	-1.390551000	-2.186276000	2.007733000
C	-1.658022000	0.066197000	2.917854000
C	-0.660162000	-2.553110000	3.145040000
C	-0.929594000	-0.308795000	4.054922000
C	-0.429311000	-1.617070000	4.170527000
H	-1.556743000	-2.903449000	1.199603000
H	-2.030991000	1.088508000	2.802390000
H	-0.262800000	-3.569877000	3.229678000
H	-0.742007000	0.425775000	4.844600000
H	0.144633000	-1.907582000	5.056613000
C	-4.425723000	-1.258162000	0.749117000
C	-5.090199000	-0.014472000	1.048637000
C	-4.558676000	-1.859742000	-0.556377000
C	-5.636886000	0.716803000	-0.011975000
C	-5.118244000	-1.099879000	-1.575164000
C	-5.633755000	0.204634000	-1.326742000
H	-6.088548000	1.696089000	0.181837000
H	-5.180043000	-1.509286000	-2.590061000
C	-4.026858000	-3.247637000	-0.782661000
H	-4.248878000	-3.610954000	-1.799038000

H	-2.930156000	-3.255867000	-0.648920000
H	-4.448663000	-3.960263000	-0.051317000
C	-6.193695000	1.011604000	-2.469740000
H	-6.879454000	0.402363000	-3.085503000
H	-6.731136000	1.907423000	-2.119107000
H	-5.376086000	1.343270000	-3.137587000
C	-5.181336000	0.461524000	2.472127000
H	-4.311585000	0.133573000	3.066878000
H	-5.269251000	1.558617000	2.534187000
H	-6.078540000	0.023779000	2.950952000
H	-4.212512000	-1.928882000	1.589300000
H	3.000421000	0.995651000	-2.126704000
H	1.306227000	-0.056742000	-3.189917000
H	-0.806750000	-1.031253000	-4.036894000
H	-1.827571000	-3.011137000	-2.892396000
H	-0.699219000	-4.008769000	-0.888390000
H	1.425762000	-3.037637000	-0.040508000
H	3.299196000	-3.575410000	-1.656499000
H	5.166066000	-5.087215000	-1.024961000
H	7.043380000	-4.236902000	0.398321000
H	7.045018000	-1.851626000	1.163951000
C	2.146407000	3.488162000	-0.864729000
C	2.276882000	1.545319000	1.684195000
C	2.145655000	0.031527000	1.987754000
H	1.148604000	-0.360927000	1.716212000
H	2.912787000	-0.573612000	1.476588000
H	2.275264000	-0.127099000	3.074406000
C	1.230330000	2.293250000	2.543099000
H	1.386532000	2.022566000	3.604041000
H	1.316098000	3.387260000	2.461047000
H	0.201794000	2.000793000	2.271146000
C	3.691446000	2.043816000	2.041240000
H	3.915206000	1.772314000	3.089808000
H	4.476452000	1.593024000	1.410237000
H	3.769500000	3.141320000	1.960735000
C	1.420447000	4.524047000	0.019261000
H	1.392720000	5.494142000	-0.511250000
H	0.378453000	4.222814000	0.232289000
H	1.944965000	4.686960000	0.975511000
C	3.641159000	3.851506000	-0.997181000
H	4.170864000	3.822866000	-0.031686000
H	4.169011000	3.187310000	-1.702411000
H	3.721468000	4.881797000	-1.391622000
C	1.495643000	3.491068000	-2.271175000
H	1.657547000	4.481251000	-2.737036000
H	1.937897000	2.735209000	-2.944733000
H	0.407446000	3.308759000	-2.216140000
H	5.200554000	-0.337219000	0.516796000

TS-FLP5: E= -2091.301008

P	2.093303000	-0.548367000	0.717766000
C	2.214120000	-1.485794000	2.266858000
C	1.094568000	-2.128140000	2.675898000
H	1.179596000	-2.752479000	3.583158000
C	3.492878000	-1.166039000	-0.304326000
C	4.799055000	-0.625434000	-0.115556000
C	5.845571000	-1.101756000	-0.926764000
H	6.850465000	-0.685946000	-0.782377000
C	5.649611000	-2.093284000	-1.902729000
C	4.363218000	-2.645349000	-2.029968000
H	4.197905000	-3.450359000	-2.756537000

C	3.277499000	-2.211193000	-1.248583000
C	5.132660000	0.438059000	0.913833000
H	6.219306000	0.458429000	1.099885000
H	4.634938000	0.265285000	1.883510000
H	4.829367000	1.444406000	0.573797000
C	6.785615000	-2.549939000	-2.790401000
H	6.829131000	-1.938702000	-3.712171000
H	6.659970000	-3.601408000	-3.101244000
H	7.761414000	-2.449080000	-2.284855000
C	1.942536000	-2.901482000	-1.443765000
H	2.052080000	-3.770049000	-2.114433000
H	1.190289000	-2.226312000	-1.895786000
H	1.517216000	-3.262261000	-0.490285000
C	2.197672000	1.294928000	0.831936000
C	2.204977000	2.008021000	-0.407228000
C	2.129983000	3.411060000	-0.379514000
H	2.135026000	3.953106000	-1.332480000
C	2.021877000	4.134340000	0.818523000
C	2.013993000	3.409508000	2.021597000
H	1.935233000	3.954290000	2.970677000
C	2.095838000	2.005055000	2.062619000
C	2.291035000	1.337532000	-1.765262000
H	1.573485000	0.501137000	-1.872265000
H	3.295842000	0.921172000	-1.957339000
H	2.061174000	2.063841000	-2.561790000
C	1.863836000	5.637100000	0.808616000
H	0.791333000	5.909559000	0.770527000
H	2.347525000	6.091592000	-0.073098000
H	2.286775000	6.099028000	1.717325000
C	2.062496000	1.339779000	3.423831000
H	2.010174000	2.102562000	4.218271000
H	2.962749000	0.728330000	3.611960000
H	1.192144000	0.670855000	3.536169000
C	-1.072624000	-3.309728000	1.330064000
C	-2.378321000	-3.251334000	1.724604000
C	-2.659808000	-2.041191000	2.552845000
C	-1.550609000	-1.263485000	2.720056000
B	-0.345389000	-2.057349000	2.023694000
C	-2.545898000	0.643862000	-0.622454000
C	-2.149467000	-0.579946000	-0.419317000
H	-2.782384000	-1.471481000	-0.344845000
C	-2.066912000	1.981365000	-0.890547000
C	-1.322116000	2.213619000	-2.077218000
C	-0.764402000	3.475470000	-2.316983000
C	-0.952350000	4.515640000	-1.390519000
H	-1.172134000	1.387490000	-2.779315000
H	-0.177615000	3.645787000	-3.225208000
H	-0.511042000	5.499754000	-1.578499000
C	-4.704855000	0.825441000	-0.614458000
C	-4.825856000	0.219430000	-1.911658000
C	-5.075380000	-1.158032000	-1.978866000
C	-5.283088000	-1.270152000	0.457953000
C	-5.287392000	-1.917397000	-0.809434000
H	-5.120206000	-1.652061000	-2.955900000
C	-5.505915000	-3.407415000	-0.887948000
H	-5.835386000	-3.722396000	-1.891699000
H	-4.559943000	-3.937624000	-0.665153000
H	-6.247621000	-3.745614000	-0.143718000
C	-4.688391000	1.067334000	-3.147273000
H	-5.595055000	1.686646000	-3.284540000
H	-3.837757000	1.767814000	-3.059920000

H	-4.552321000	0.453751000	-4.052360000
H	-4.693674000	1.919399000	-0.558822000
C	-2.258753000	3.038178000	0.034053000
C	-1.697735000	4.294856000	-0.216484000
H	-2.833001000	2.855691000	0.947964000
H	-1.835058000	5.105079000	0.506722000
C	-5.015508000	0.091179000	0.578010000
H	-5.492918000	-1.865469000	1.353548000
C	-4.900854000	0.759558000	1.922222000
H	-5.487717000	0.231762000	2.692249000
H	-3.840254000	0.740728000	2.243463000
H	-5.225096000	1.813928000	1.889432000
Au	-0.141896000	-0.728736000	0.056396000
H	-0.651494000	-4.124613000	0.732662000
H	-3.160314000	-3.986324000	1.491446000
H	-3.655283000	-1.840508000	2.968363000
H	-1.536050000	-0.338440000	3.305071000
H	3.189586000	-1.573256000	2.760605000

TS-FLP6: E= -5408.619893

P	-2.937891000	0.374689000	-0.346312000
C	-2.637557000	0.268953000	-2.154759000
C	-1.306777000	0.247650000	-2.444459000
H	-1.018160000	0.174052000	-3.507732000
Si	-3.882963000	-0.124136000	-3.562346000
C	-3.356092000	-1.818379000	-4.239789000
H	-3.546916000	-2.623443000	-3.508329000
H	-2.281764000	-1.835711000	-4.497050000
H	-3.928170000	-2.053836000	-5.155836000
C	-5.681891000	-0.222616000	-2.985235000
H	-6.323684000	-0.409161000	-3.865980000
H	-6.040339000	0.704304000	-2.505059000
H	-5.827503000	-1.052476000	-2.272797000
C	-3.658652000	1.168585000	-4.930391000
H	-2.588409000	1.309610000	-5.165998000
H	-4.078739000	2.150479000	-4.654154000
H	-4.165790000	0.826134000	-5.850757000
C	-4.266750000	-0.838223000	0.066336000
C	-5.582667000	-0.465922000	0.486745000
C	-6.507340000	-1.489076000	0.772135000
H	-7.515450000	-1.199913000	1.092873000
C	-6.203978000	-2.853283000	0.641874000
C	-4.923434000	-3.192125000	0.177751000
H	-4.668643000	-4.249059000	0.033345000
C	-3.946458000	-2.223624000	-0.108356000
C	-6.101198000	0.954559000	0.605972000
H	-7.200205000	0.940428000	0.688613000
H	-5.841355000	1.574791000	-0.266277000
H	-5.706565000	1.475562000	1.495245000
C	-7.213421000	-3.919420000	0.998847000
H	-7.081696000	-4.824960000	0.382000000
H	-8.248315000	-3.557630000	0.874563000
H	-7.096264000	-4.223880000	2.056598000
C	-2.609534000	-2.727284000	-0.600000000
H	-2.592549000	-3.828645000	-0.615625000
H	-1.784477000	-2.395334000	0.057686000
H	-2.354233000	-2.363527000	-1.609343000
C	-3.324900000	2.055350000	0.320839000
C	-3.271870000	2.202309000	1.744308000
C	-3.454661000	3.476181000	2.304402000
H	-3.406902000	3.579145000	3.395434000

C	-3.694288000	4.616228000	1.519036000
C	-3.786977000	4.438943000	0.130645000
H	-3.981544000	5.310994000	-0.504699000
C	-3.605412000	3.188964000	-0.492531000
C	-3.045415000	1.055695000	2.711525000
H	-1.963599000	0.844969000	2.835366000
H	-3.532021000	0.112230000	2.411550000
H	-3.427174000	1.314222000	3.713444000
C	-3.793943000	5.983050000	2.153247000
H	-4.397787000	5.957649000	3.077229000
H	-4.233415000	6.722860000	1.464127000
H	-2.784140000	6.338877000	2.426706000
C	-3.761536000	3.137947000	-1.995655000
H	-3.991469000	4.139442000	-2.392903000
H	-4.588193000	2.467583000	-2.288794000
H	-2.854080000	2.778285000	-2.504841000
C	0.350740000	-2.588302000	-3.239463000
C	0.005267000	-4.618645000	-1.371853000
C	-0.164088000	-3.823661000	-3.652478000
C	-0.337545000	-4.850159000	-2.711058000
F	7.412980000	-2.441809000	-2.087872000
F	0.474071000	-1.614581000	-4.173568000
F	-0.510678000	-4.020608000	-4.938525000
F	-0.849084000	-6.035219000	-3.085994000
F	-0.221227000	-5.566790000	-0.438857000
C	1.002475000	-0.932679000	-1.483273000
C	2.220631000	-0.336985000	-1.273152000
C	4.004652000	1.511629000	0.595915000
C	5.055456000	2.274430000	1.110801000
C	0.700153000	-2.316299000	-1.901681000
C	0.511574000	-3.370389000	-0.988718000
C	3.561581000	-0.920901000	-1.477044000
C	4.470722000	-0.300037000	-2.360158000
C	4.013534000	-2.071816000	-0.808009000
C	5.761524000	-0.798388000	-2.576393000
C	5.296158000	-2.594322000	-1.011854000
C	6.178062000	-1.952844000	-1.893816000
F	5.796420000	1.813328000	2.140107000
F	3.746981000	0.312647000	1.176209000
F	3.225693000	-2.678794000	0.102400000
F	5.702972000	-3.681848000	-0.323600000
F	6.597327000	-0.187597000	-3.435336000
F	4.088735000	0.798475000	-3.047606000
F	0.709252000	-3.176591000	0.337870000
C	2.064754000	1.120505000	-0.927466000
C	3.186620000	1.952612000	-0.458645000
C	3.478179000	3.219127000	-1.001875000
C	4.527122000	4.007902000	-0.508302000
C	5.321053000	3.533819000	0.549993000
F	2.754014000	3.696211000	-2.033802000
F	4.789009000	5.210932000	-1.050026000
F	6.325491000	4.286071000	1.026195000
C	0.759271000	1.520121000	-1.029330000
C	0.230816000	2.851741000	-0.702742000
C	-0.375869000	3.641183000	-1.695932000
C	0.240188000	3.366265000	0.606606000
C	-0.926483000	4.895520000	-1.416030000
C	-0.326667000	4.607762000	0.920243000
C	-0.888130000	5.384427000	-0.102737000
F	-0.453087000	3.171889000	-2.963522000
F	0.755126000	2.622526000	1.616882000

F	-0.371871000	5.046301000	2.194681000
F	-1.462293000	6.566892000	0.186695000
F	-1.547933000	5.607437000	-2.376964000
B	-0.092041000	0.237757000	-1.441030000
Au	-0.893472000	-0.177003000	0.699998000
C	0.187461000	-1.443036000	2.900741000
C	0.722255000	-0.763567000	1.936749000
H	1.768179000	-0.525355000	1.735433000
C	-1.047757000	-2.010388000	3.386766000
C	-1.741266000	-1.415581000	4.470800000
C	-1.631132000	-3.101019000	2.689232000
C	-3.021567000	-1.866109000	4.808380000
C	-2.916910000	-3.536009000	3.029460000
C	-3.616294000	-2.914974000	4.079929000
H	-1.277972000	-0.584852000	5.012493000
H	-1.077923000	-3.566000000	1.870297000
H	-3.565793000	-1.390981000	5.630521000
H	-3.378672000	-4.352803000	2.467164000
H	-4.625878000	-3.252329000	4.336037000
C	1.659713000	-2.068720000	4.506265000
C	2.144924000	-3.167027000	3.731619000
C	2.418706000	-0.863334000	4.643114000
C	3.364881000	-3.017311000	3.055454000
C	3.624675000	-0.761281000	3.952384000
C	4.127079000	-1.840961000	3.176098000
H	3.742828000	-3.838645000	2.437233000
H	4.209840000	0.163896000	4.006947000
C	1.856863000	0.286054000	5.442260000
H	2.629903000	1.034982000	5.681045000
H	1.063427000	0.795038000	4.860281000
H	1.397831000	-0.060268000	6.385246000
C	5.494747000	-1.746658000	2.547129000
H	5.706996000	-0.728784000	2.185485000
H	6.266554000	-1.991449000	3.302530000
H	5.611672000	-2.460842000	1.717876000
C	1.363946000	-4.453478000	3.623452000
H	1.123164000	-4.667484000	2.565874000
H	1.960019000	-5.304922000	3.999197000
H	0.421629000	-4.415821000	4.192965000
H	0.827049000	-2.241310000	5.196143000

INT-PPh₃: E= -1830.181664

Au	-0.111969000	-0.531059000	-0.011149000
P	2.209350000	-0.294645000	0.003808000
C	2.983481000	-0.732789000	1.610196000
C	2.457140000	-1.833870000	2.320965000
C	3.045875000	-2.234858000	3.529446000
H	2.634168000	-3.088861000	4.077747000
C	4.154832000	-1.535612000	4.038072000
C	4.675699000	-0.435101000	3.336448000
H	5.537005000	0.112924000	3.733070000
C	4.093970000	-0.030942000	2.123602000
H	1.586423000	-2.371424000	1.926263000
H	4.609960000	-1.846002000	4.984698000
H	4.501410000	0.827931000	1.579689000
C	3.084087000	-1.310700000	-1.250655000
C	4.369901000	-1.841749000	-1.017040000
C	5.017368000	-2.573763000	-2.025696000
C	4.387564000	-2.778579000	-3.265155000
C	3.104118000	-2.253670000	-3.498769000
H	2.608510000	-2.418119000	-4.461478000

C	2.450281000	-1.524324000	-2.494461000
H	4.861606000	-1.686046000	-0.050656000
H	4.894692000	-3.352326000	-4.048220000
H	1.445478000	-1.121228000	-2.670523000
H	6.015133000	-2.985681000	-1.840609000
C	-2.954384000	0.451295000	0.127147000
C	-2.148957000	-0.630808000	0.008935000
H	-2.644085000	-1.616094000	-0.012870000
C	-2.511537000	1.869524000	0.060454000
C	-2.892266000	2.808797000	1.046193000
C	-1.660780000	2.297023000	-0.988265000
C	-2.401372000	4.121776000	1.010875000
C	-1.179680000	3.614373000	-1.028916000
C	-1.542825000	4.529220000	-0.026806000
H	-3.550256000	2.502021000	1.867820000
H	-1.379707000	1.580691000	-1.767559000
H	-2.687937000	4.828754000	1.796755000
H	-0.514240000	3.922323000	-1.841917000
H	-1.167289000	5.557635000	-0.057343000
C	-4.563846000	0.268496000	0.280058000
C	-4.968195000	-0.095798000	-1.103619000
C	-4.861082000	-0.712434000	1.361592000
C	-5.312973000	-1.414463000	-1.381280000
C	-5.260102000	-1.985370000	1.024542000
C	-5.453872000	-2.364388000	-0.343000000
H	-5.519806000	-1.718430000	-2.412719000
H	-5.431854000	-2.734665000	1.805036000
C	-4.604668000	-0.288478000	2.773223000
H	-4.848106000	-1.082382000	3.496127000
H	-3.535612000	-0.021214000	2.887201000
H	-5.186753000	0.617754000	3.025035000
C	-5.830115000	-3.781195000	-0.652167000
H	-4.987480000	-4.450864000	-0.390419000
H	-6.682313000	-4.101660000	-0.024994000
H	-6.079324000	-3.931088000	-1.713641000
C	-4.975454000	0.966034000	-2.157258000
H	-4.094691000	1.628166000	-2.075670000
H	-5.024970000	0.541380000	-3.172006000
H	-5.862059000	1.613667000	-2.008006000
H	-4.940911000	1.269324000	0.549857000
C	2.714323000	1.439505000	-0.334453000
C	1.859414000	2.482531000	0.083665000
C	3.935546000	1.746485000	-0.972042000
C	2.228472000	3.819535000	-0.126841000
C	4.298938000	3.086991000	-1.178655000
C	3.448073000	4.123278000	-0.755949000
H	0.897423000	2.251010000	0.555366000
H	4.597580000	0.941360000	-1.309093000
H	1.551832000	4.620226000	0.189528000
H	5.246812000	3.320966000	-1.674937000
H	3.732772000	5.167464000	-0.924208000

INT-FLP1': E= -3564.974609

Au	-0.123927000	-0.021553000	-0.919539000
B	-0.426037000	0.316642000	1.856679000
C	-2.891039000	-0.509986000	1.151535000
P	-2.410719000	-0.299577000	-0.602596000
C	-1.915972000	-0.194186000	2.045548000
H	-2.175549000	-0.297352000	3.116779000
C	-3.257056000	1.193038000	-1.249355000
C	-3.314695000	1.414673000	-2.644015000

C	-3.814022000	2.628450000	-3.139781000
H	-3.865889000	2.790920000	-4.221676000
C	-4.235928000	3.635561000	-2.252588000
C	-4.165380000	3.422678000	-0.865792000
H	-4.477738000	4.206109000	-0.167431000
C	-3.682034000	2.204019000	-0.363733000
H	-2.970406000	0.640375000	-3.339178000
H	-4.614642000	4.585781000	-2.643887000
H	-3.624024000	2.044119000	0.715176000
C	-3.047898000	-1.739772000	-1.542626000
C	-4.293148000	-1.731633000	-2.205258000
C	-4.762838000	-2.898723000	-2.828658000
C	-3.995660000	-4.076032000	-2.794391000
C	-2.746975000	-4.082803000	-2.147959000
H	-2.142460000	-4.995898000	-2.126392000
C	-2.268047000	-2.918519000	-1.530159000
H	-4.895691000	-0.818482000	-2.237490000
H	-4.367780000	-4.985716000	-3.277472000
H	-1.292607000	-2.924598000	-1.032103000
C	-0.193804000	1.876493000	1.732000000
C	-1.249964000	2.792671000	1.945636000
F	-2.396032000	2.393273000	2.549751000
C	-1.197933000	4.139562000	1.566496000
F	-2.256704000	4.949113000	1.755928000
C	-0.019846000	4.645554000	0.996389000
F	0.057242000	5.933101000	0.631417000
C	1.085661000	3.796216000	0.831041000
F	2.234001000	4.281123000	0.308498000
C	0.990125000	2.456719000	1.217976000
F	2.093823000	1.705492000	1.013242000
C	0.715524000	-0.713591000	2.223284000
C	1.859647000	-0.376322000	2.977863000
F	2.028466000	0.877579000	3.454296000
C	2.869011000	-1.298530000	3.289117000
F	3.976888000	-0.906204000	3.950089000
C	2.727267000	-2.637320000	2.894527000
F	3.691984000	-3.530502000	3.166885000
C	1.571387000	-3.038787000	2.210288000
F	1.409217000	-4.328959000	1.866270000
C	0.611055000	-2.079618000	1.875328000
F	-0.444472000	-2.524780000	1.152760000
H	-5.731719000	-2.887190000	-3.338880000
C	2.854481000	-0.575503000	-1.346048000
C	1.839952000	0.316339000	-1.358156000
H	2.112806000	1.368939000	-1.534372000
C	2.721208000	-2.048852000	-1.248320000
C	3.580541000	-2.834095000	-0.444127000
C	1.682892000	-2.703329000	-1.956815000
C	3.388683000	-4.216832000	-0.324786000
C	1.491766000	-4.087634000	-1.836276000
C	2.343015000	-4.849804000	-1.020194000
H	4.385868000	-2.360549000	0.128518000
H	1.035111000	-2.113381000	-2.613608000
H	4.043113000	-4.796833000	0.333594000
H	0.683185000	-4.570415000	-2.396021000
H	2.195250000	-5.930454000	-0.924818000
C	4.387960000	-0.039613000	-1.500766000
C	4.430144000	0.444647000	-2.903424000
C	4.639441000	0.952905000	-0.419133000
C	4.379820000	1.811749000	-3.141352000
C	4.606072000	2.295068000	-0.723154000

C	4.431474000	2.740313000	-2.070919000
H	4.307930000	2.186664000	-4.167635000
H	4.681981000	3.042424000	0.072819000
C	4.773549000	0.435515000	0.976584000
H	4.820483000	1.242818000	1.722311000
H	3.901002000	-0.202840000	1.206846000
H	5.671592000	-0.202860000	1.077048000
C	4.307039000	4.209846000	-2.331687000
H	3.391384000	4.586551000	-1.836931000
H	5.150251000	4.757556000	-1.871334000
H	4.257864000	4.449010000	-3.404618000
C	4.470177000	-0.567504000	-4.005100000
H	3.784115000	-1.409314000	-3.797981000
H	4.224686000	-0.125431000	-4.983322000
H	5.487674000	-1.001574000	-4.064866000
H	5.018393000	-0.935186000	-1.376656000
Si	-4.606103000	-1.160606000	1.677077000
C	-5.965975000	-0.170543000	0.804217000
H	-6.957665000	-0.564358000	1.092991000
H	-5.924945000	0.897316000	1.080969000
H	-5.882997000	-0.235099000	-0.293719000
C	-4.742678000	-3.002066000	1.247123000
H	-5.670661000	-3.419807000	1.679326000
H	-4.764073000	-3.168947000	0.156898000
H	-3.887234000	-3.564022000	1.662362000
C	-4.749588000	-0.925291000	3.552081000
H	-4.017276000	-1.543639000	4.101638000
H	-4.597716000	0.130233000	3.840527000
H	-5.759137000	-1.227113000	3.885679000

INT-FLP3': E= -2316.439097

B	0.424416000	-1.525999000	1.578788000
C	1.814337000	-1.136917000	2.224938000
C	2.867918000	-0.454766000	1.558944000
C	4.082448000	-0.152252000	2.205514000
H	4.862251000	0.409608000	1.678409000
C	4.281873000	-0.553642000	3.535670000
H	5.225200000	-0.322225000	4.041471000
C	3.256750000	-1.231726000	4.217553000
H	3.399539000	-1.530921000	5.261812000
C	2.037855000	-1.503770000	3.574611000
H	1.236959000	-2.006669000	4.129489000
C	0.093414000	-2.696985000	0.561520000
C	0.879217000	-3.450097000	-0.327255000
H	1.958906000	-3.273081000	-0.392812000
C	0.275564000	-4.420205000	-1.153586000
H	0.887278000	-5.001600000	-1.852243000
C	-1.111042000	-4.644640000	-1.083115000
H	-1.573075000	-5.400778000	-1.727878000
C	-1.915219000	-3.917299000	-0.178403000
H	-2.991222000	-4.119550000	-0.116286000
C	-1.314980000	-2.953664000	0.640114000
C	-1.948116000	-2.076003000	1.656581000
C	-3.285585000	-2.022529000	2.064373000
H	-4.038938000	-2.686665000	1.624724000
C	-3.657016000	-1.102763000	3.069165000
H	-4.702258000	-1.054870000	3.395747000
C	-2.705796000	-0.252093000	3.659695000
H	-3.014325000	0.450736000	4.441386000
C	-1.357101000	-0.312141000	3.247928000
H	-0.608410000	0.342601000	3.711594000

C	-0.971050000	-1.214221000	2.246422000
P	2.531747000	0.065795000	-0.162577000
Au	0.219797000	0.096148000	-0.458715000
C	-2.459275000	1.417560000	-0.700367000
C	-1.881881000	2.691238000	-0.193811000
C	-1.206331000	2.697696000	1.050817000
C	-1.941949000	3.888017000	-0.941041000
C	-0.578066000	3.862764000	1.516467000
C	-1.301315000	5.048360000	-0.480551000
C	-0.615438000	5.039255000	0.747932000
H	-2.459018000	3.903931000	-1.908042000
H	-0.057882000	3.849581000	2.480406000
H	-1.333934000	5.961477000	-1.084457000
H	-0.122378000	5.948446000	1.108356000
C	-4.024049000	1.509864000	-1.125358000
C	-4.252271000	0.765425000	-2.394113000
C	-4.700950000	1.005921000	0.097636000
C	-4.843928000	-0.475704000	-2.347286000
C	-5.274466000	-0.261293000	0.076194000
C	-5.321221000	-1.022379000	-1.112963000
H	-4.959460000	-1.066693000	-3.262458000
H	-5.709995000	-0.674037000	0.990748000
C	-4.662389000	1.831239000	1.346122000
H	-5.504925000	1.581157000	2.011358000
H	-3.732863000	1.607601000	1.906155000
H	-4.664722000	2.911324000	1.128519000
C	-5.877095000	-2.413777000	-1.103867000
H	-5.053871000	-3.131910000	-1.289183000
H	-6.354564000	-2.672615000	-0.146284000
H	-6.600710000	-2.556523000	-1.926919000
C	-3.716558000	1.365120000	-3.655642000
H	-3.909805000	0.728413000	-4.532813000
H	-4.155188000	2.364792000	-3.833920000
H	-4.214513000	2.587257000	-1.268569000
H	-1.184089000	1.777223000	1.644090000
C	-1.798438000	0.239902000	-0.748377000
H	-2.362151000	-0.668018000	-1.016517000
H	-2.623045000	1.512190000	-3.556103000
C	3.414273000	-1.097505000	-1.268424000
C	4.457847000	-1.928234000	-0.811579000
C	2.976941000	-1.187340000	-2.608312000
C	5.061625000	-2.839024000	-1.694440000
C	3.586695000	-2.095846000	-3.485119000
C	4.627620000	-2.924051000	-3.028073000
H	4.786524000	-1.877007000	0.231713000
H	2.149699000	-0.556325000	-2.955124000
H	5.868872000	-3.486391000	-1.335871000
H	3.241783000	-2.165918000	-4.522165000
H	5.095985000	-3.640855000	-3.710908000
C	3.308961000	1.708224000	-0.394607000
C	2.537233000	2.854335000	-0.100506000
C	4.645029000	1.848093000	-0.824889000
C	3.104948000	4.130560000	-0.223648000
C	5.205744000	3.130055000	-0.947278000
C	4.438973000	4.269621000	-0.646409000
H	1.493501000	2.750000000	0.219439000
H	5.240219000	0.961437000	-1.070560000
H	2.496654000	5.013192000	0.002429000
H	6.242905000	3.237930000	-1.282159000
H	4.880353000	5.266855000	-0.748451000

INT-FLP4: E= -1978.255149

Au	-0.104790000	-1.068389000	-0.059936000
B	2.644038000	0.857267000	1.052224000
C	3.308655000	-0.561636000	0.730568000
P	2.142034000	-1.744270000	-0.140242000
H	4.258946000	-0.512895000	0.176047000
C	1.490508000	0.907732000	2.118251000
C	1.471410000	0.067276000	3.262140000
C	0.402701000	0.079270000	4.169742000
C	-0.694038000	0.934102000	3.952629000
C	-0.699463000	1.784403000	2.834368000
C	0.378621000	1.772803000	1.938155000
C	3.132073000	2.166096000	0.345118000
C	2.835411000	3.451202000	0.877137000
C	3.224135000	4.629867000	0.225801000
C	3.917308000	4.560725000	-0.995326000
C	4.254228000	3.306510000	-1.535882000
C	3.884047000	2.135861000	-0.860169000
C	-2.552270000	0.747481000	-0.371403000
C	-2.064661000	-0.500907000	-0.169659000
H	-2.823296000	-1.293828000	-0.050647000
C	-1.758440000	1.968906000	-0.657761000
C	-2.053453000	3.210961000	-0.048867000
C	-0.621940000	1.895618000	-1.501971000
C	-1.206778000	4.316356000	-0.218717000
C	0.230751000	2.996113000	-1.664852000
C	-0.054432000	4.210592000	-1.017976000
H	-2.923655000	3.307577000	0.611149000
H	-0.406642000	0.953239000	-2.012688000
H	-1.439282000	5.258132000	0.289604000
H	1.126694000	2.904085000	-2.287950000
H	0.620048000	5.064360000	-1.133125000
C	-4.163437000	0.985255000	-0.370250000
C	-4.570096000	0.414674000	-1.680084000
C	-4.764429000	0.390718000	0.855251000
C	-5.242246000	-0.802513000	-1.706871000
C	-5.478348000	-0.781886000	0.754872000
C	-5.691505000	-1.413071000	-0.512384000
H	-5.463226000	-1.282746000	-2.665896000
H	-5.884654000	-1.258691000	1.653755000
C	-4.448665000	1.036512000	2.166639000
H	-5.005870000	0.580450000	2.999606000
H	-3.363574000	0.924568000	2.366290000
H	-4.655495000	2.122423000	2.141438000
C	-6.415425000	-2.724852000	-0.553354000
H	-6.609957000	-3.068367000	-1.580773000
H	-5.814133000	-3.494996000	-0.032044000
H	-7.371765000	-2.657296000	-0.002317000
C	-4.222211000	1.160381000	-2.930305000
H	-3.186628000	1.545427000	-2.895641000
H	-4.354057000	0.540446000	-3.830786000
H	-4.879477000	2.047663000	-3.018997000
H	-4.293294000	2.079965000	-0.366855000
H	3.538492000	-1.047651000	1.696634000
H	2.317481000	-0.599097000	3.459628000
H	0.423562000	-0.575335000	5.048421000
H	-1.533509000	0.942493000	4.657275000
H	-1.540018000	2.463822000	2.656087000
H	0.346921000	2.422945000	1.060881000
H	2.293665000	3.524808000	1.825724000
H	2.980104000	5.603892000	0.664153000

H	4.208731000	5.479803000	-1.516023000
H	4.813213000	3.244423000	-2.476100000
C	2.382577000	-3.443731000	0.706316000
C	2.714940000	-1.750283000	-1.970582000
C	2.111159000	-0.476711000	-2.617864000
H	2.269721000	0.433521000	-2.016523000
H	2.579417000	-0.316008000	-3.607402000
H	1.024126000	-0.593612000	-2.768952000
C	2.124151000	-2.976045000	-2.701299000
H	2.271336000	-2.842643000	-3.789714000
H	2.624499000	-3.916243000	-2.415174000
H	1.039004000	-3.076128000	-2.518392000
C	4.249868000	-1.743307000	-2.143068000
H	4.483156000	-1.848942000	-3.218994000
H	4.710642000	-0.798913000	-1.808525000
H	4.744135000	-2.571493000	-1.611162000
C	1.305075000	-4.432657000	0.199276000
H	1.386516000	-5.370514000	0.780489000
H	0.287783000	-4.026645000	0.346186000
H	1.422599000	-4.692292000	-0.862650000
C	3.795548000	-4.021606000	0.495489000
H	3.968052000	-4.321275000	-0.551880000
H	4.582857000	-3.304752000	0.790481000
H	3.916378000	-4.925842000	1.121593000
C	2.131372000	-3.226961000	2.218966000
H	2.057475000	-4.215388000	2.709155000
H	2.957207000	-2.686472000	2.712037000
H	1.191011000	-2.677956000	2.407495000
H	4.176212000	1.172929000	-1.289928000

INT-FLP5: E= -2091.309350

P	2.004222000	-0.549181000	0.654593000
C	2.003695000	-1.391165000	2.266091000
C	0.848642000	-1.989826000	2.641561000
H	0.872672000	-2.571935000	3.580500000
C	3.427900000	-1.351525000	-0.201289000
C	4.759500000	-0.979330000	0.146272000
C	5.829048000	-1.616951000	-0.511329000
H	6.853662000	-1.329715000	-0.243910000
C	5.629459000	-2.604542000	-1.489352000
C	4.306550000	-2.975797000	-1.788213000
H	4.128837000	-3.764679000	-2.529661000
C	3.198539000	-2.375891000	-1.164250000
C	5.103205000	0.088695000	1.168645000
H	6.142224000	-0.037509000	1.516141000
H	4.450081000	0.068134000	2.056907000
H	5.012332000	1.101027000	0.734772000
C	6.796619000	-3.243914000	-2.208479000
H	6.958570000	-2.765614000	-3.193359000
H	6.617238000	-4.317208000	-2.395495000
H	7.733217000	-3.142390000	-1.634209000
C	1.816191000	-2.861943000	-1.551079000
H	1.886868000	-3.724507000	-2.234805000
H	1.232857000	-2.075815000	-2.067372000
H	1.224167000	-3.174811000	-0.672879000
C	2.318048000	1.274688000	0.673315000
C	2.633053000	1.892149000	-0.573373000
C	2.828614000	3.284250000	-0.608890000
H	3.071804000	3.753513000	-1.570360000
C	2.681421000	4.092620000	0.528802000
C	2.306060000	3.467405000	1.729662000

H	2.144192000	4.083556000	2.623008000
C	2.114249000	2.077288000	1.831850000
C	2.726380000	1.130964000	-1.881789000
H	1.877956000	0.431375000	-2.009842000
H	3.651906000	0.534364000	-1.958149000
H	2.705816000	1.832220000	-2.732723000
C	2.899338000	5.587570000	0.461756000
H	3.935492000	5.850403000	0.748914000
H	2.224293000	6.124662000	1.150700000
H	2.733727000	5.975134000	-0.558465000
C	1.663509000	1.519889000	3.166992000
H	1.495156000	2.339877000	3.885078000
H	2.409415000	0.836439000	3.609792000
H	0.723331000	0.947981000	3.074144000
C	-1.211168000	-3.227077000	1.204712000
C	-2.527700000	-3.238858000	1.570513000
C	-2.885120000	-2.058991000	2.405611000
C	-1.818782000	-1.226190000	2.597515000
B	-0.557192000	-1.943288000	1.911927000
C	-2.834848000	0.789912000	-0.575953000
C	-2.250849000	-0.413396000	-0.373467000
H	-2.882342000	-1.304613000	-0.249407000
C	-2.091473000	2.048505000	-0.824954000
C	-1.037881000	2.064863000	-1.774374000
C	-0.238486000	3.205499000	-1.934964000
C	-0.480876000	4.350759000	-1.160430000
H	-0.864333000	1.175780000	-2.391376000
H	0.576024000	3.196581000	-2.665605000
H	0.153683000	5.235452000	-1.274800000
C	-4.445610000	0.911562000	-0.587173000
C	-4.771414000	0.282635000	-1.894725000
C	-5.297258000	-1.006285000	-1.910018000
C	-5.572097000	-0.973801000	0.547508000
C	-5.687734000	-1.646585000	-0.712005000
H	-5.445143000	-1.523340000	-2.863905000
C	-6.243503000	-3.037663000	-0.733014000
H	-5.551992000	-3.715131000	-0.194958000
H	-7.203617000	-3.080375000	-0.185931000
H	-6.386895000	-3.421243000	-1.754437000
C	-4.500962000	1.050740000	-3.150042000
H	-5.309565000	1.794876000	-3.294287000
H	-3.559224000	1.624526000	-3.082496000
H	-4.473298000	0.398202000	-4.036860000
H	-4.658618000	1.993909000	-0.599589000
C	-2.351249000	3.222656000	-0.082134000
C	-1.543996000	4.358232000	-0.239240000
H	-3.161220000	3.233778000	0.656208000
H	-1.739129000	5.249665000	0.366389000
C	-5.000203000	0.273385000	0.640597000
H	-5.939640000	-1.480372000	1.446020000
C	-4.782030000	0.970794000	1.944527000
H	-5.263744000	0.442842000	2.782089000
H	-3.692866000	1.016456000	2.141798000
H	-5.151927000	2.012020000	1.911776000
Au	-0.251776000	-0.613751000	-0.020022000
H	-0.740913000	-4.016260000	0.608742000
H	-3.264845000	-4.010575000	1.309240000
H	-3.896336000	-1.915279000	2.807593000
H	-1.862621000	-0.309004000	3.193860000
H	2.944991000	-1.483913000	2.822098000

INT-FLP6: E= -5408.633321

P	-3.070619000	0.284356000	-0.233732000
C	-2.755123000	0.052389000	-2.030641000
C	-1.422913000	-0.019380000	-2.308289000
H	-1.132551000	-0.174532000	-3.363516000
Si	-3.974481000	-0.393685000	-3.439250000
C	-3.431221000	-2.105844000	-4.060672000
H	-3.583961000	-2.884398000	-3.292503000
H	-2.363326000	-2.113236000	-4.343845000
H	-4.019893000	-2.391753000	-4.951563000
C	-5.781608000	-0.480509000	-2.884656000
H	-6.412032000	-0.720019000	-3.760857000
H	-6.149666000	0.469854000	-2.460062000
H	-5.929771000	-1.269034000	-2.127322000
C	-3.748569000	0.847659000	-4.857485000
H	-4.148348000	0.421099000	-5.795460000
H	-2.678232000	1.072738000	-5.014022000
H	-4.271172000	1.800449000	-4.667294000
C	-4.473736000	-0.826004000	0.225813000
C	-5.779269000	-0.365681000	0.578891000
C	-6.754732000	-1.318015000	0.933326000
H	-7.756326000	-0.958966000	1.200342000
C	-6.507327000	-2.699559000	0.936845000
C	-5.231714000	-3.131984000	0.539298000
H	-5.018977000	-4.207344000	0.497099000
C	-4.210971000	-2.232150000	0.184900000
C	-6.229670000	1.082763000	0.557538000
H	-7.328957000	1.130673000	0.626202000
H	-5.930967000	1.602327000	-0.366877000
H	-5.815932000	1.668076000	1.397013000
C	-7.572839000	-3.685386000	1.359132000
H	-7.454335000	-4.655135000	0.845795000
H	-8.586114000	-3.300968000	1.150800000
H	-7.513574000	-3.880962000	2.446977000
C	-2.891446000	-2.825069000	-0.253780000
H	-2.902687000	-3.922510000	-0.156225000
H	-2.050834000	-2.444641000	0.352793000
H	-2.639764000	-2.575030000	-1.298434000
C	-3.393174000	2.032984000	0.291186000
C	-3.323238000	2.288822000	1.697542000
C	-3.406265000	3.613089000	2.156356000
H	-3.350344000	3.796949000	3.236588000
C	-3.559675000	4.702835000	1.282854000
C	-3.688216000	4.422043000	-0.085440000
H	-3.829648000	5.251842000	-0.788316000
C	-3.613812000	3.114413000	-0.605093000
C	-3.201282000	1.199222000	2.743367000
H	-2.157624000	0.838173000	2.844058000
H	-3.825265000	0.314917000	2.532825000
H	-3.489709000	1.580635000	3.736446000
C	-3.545416000	6.120513000	1.804957000
H	-4.108121000	6.209540000	2.750790000
H	-3.969483000	6.829037000	1.074172000
H	-2.505076000	6.434014000	2.006663000
C	-3.822137000	2.947047000	-2.092932000
H	-4.093967000	3.909411000	-2.555634000
H	-4.639152000	2.234931000	-2.302392000
H	-2.924939000	2.570879000	-2.608860000
C	0.174331000	-2.930850000	-3.005100000
C	-0.359747000	-4.799769000	-1.018502000
C	-0.398280000	-4.160498000	-3.353573000

C	-0.666980000	-5.104997000	-2.351510000
F	7.286136000	-2.932705000	-1.299118000
F	0.378800000	-2.030230000	-3.996310000
F	-0.712932000	-4.426911000	-4.635529000
F	-1.232532000	-6.284309000	-2.663854000
F	-0.671857000	-5.672969000	-0.038527000
C	0.868019000	-1.191904000	-1.362616000
C	2.118133000	-0.635743000	-1.278752000
C	4.158218000	1.447009000	0.105296000
C	5.256357000	2.271394000	0.363390000
C	0.491864000	-2.585462000	-1.675945000
C	0.204407000	-3.557221000	-0.701751000
C	3.424868000	-1.320525000	-1.356942000
C	4.414986000	-0.893689000	-2.264207000
C	3.788324000	-2.331592000	-0.448496000
C	5.711102000	-1.427070000	-2.260497000
C	5.076609000	-2.876265000	-0.419418000
C	6.045646000	-2.419315000	-1.325212000
F	6.117416000	1.976176000	1.363446000
F	3.983114000	0.357599000	0.894505000
F	2.904220000	-2.753995000	0.480068000
F	5.409199000	-3.804224000	0.507531000
F	6.632257000	-0.998330000	-3.142231000
F	4.120519000	0.062866000	-3.170901000
F	0.372080000	-3.278442000	0.615797000
C	2.037126000	0.855081000	-1.101567000
C	3.213540000	1.723158000	-0.896903000
C	3.436245000	2.880856000	-1.669295000
C	4.531188000	3.725951000	-1.438367000
C	5.447900000	3.420573000	-0.418532000
F	2.596219000	3.197205000	-2.675267000
F	4.718976000	4.821094000	-2.196794000
F	6.497210000	4.226518000	-0.190645000
C	0.737386000	1.286663000	-1.115012000
C	0.275125000	2.664312000	-0.897817000
C	-0.387065000	3.364804000	-1.921563000
C	0.398087000	3.312828000	0.344233000
C	-0.897593000	4.652395000	-1.732681000
C	-0.127847000	4.591520000	0.569571000
C	-0.755685000	5.271005000	-0.483037000
F	-0.555948000	2.776563000	-3.129739000
F	0.996280000	2.672812000	1.380189000
F	-0.060882000	5.163931000	1.789789000
F	-1.284733000	6.492178000	-0.277603000
F	-1.577276000	5.277821000	-2.714935000
B	-0.191897000	0.008639000	-1.318041000
Au	-0.980225000	-0.203349000	0.821440000
C	0.677257000	-0.927467000	3.153129000
C	0.768006000	-0.518174000	1.866168000
H	1.748853000	-0.307523000	1.420760000
C	-0.633146000	-1.270838000	3.774544000
C	-1.075378000	-0.658308000	4.967011000
C	-1.514024000	-2.153804000	3.099933000
C	-2.380471000	-0.872543000	5.435321000
C	-2.825487000	-2.355644000	3.560602000
C	-3.265153000	-1.705815000	4.724421000
H	-0.412066000	0.026889000	5.507694000
H	-1.140205000	-2.711413000	2.237996000
H	-2.715909000	-0.371177000	6.349425000
H	-3.497283000	-3.018570000	3.004789000
H	-4.287757000	-1.854968000	5.086238000

C	1.962711000	-1.091064000	4.062082000
C	2.603185000	-2.381338000	3.663332000
C	2.828295000	0.130549000	4.056151000
C	3.906863000	-2.384102000	3.194889000
C	4.134565000	0.038732000	3.634106000
C	4.679220000	-1.197885000	3.168760000
H	4.350274000	-3.312315000	2.822056000
H	4.763676000	0.933836000	3.587914000
C	2.205591000	1.431297000	4.455010000
H	2.953222000	2.234382000	4.545948000
H	1.459613000	1.726228000	3.692086000
H	1.657819000	1.338011000	5.410712000
C	6.084272000	-1.225926000	2.653969000
H	6.277898000	-0.344736000	2.020125000
H	6.788046000	-1.161009000	3.507738000
H	6.303622000	-2.148490000	2.096356000
C	1.787807000	-3.637734000	3.696791000
H	1.303217000	-3.773511000	2.710976000
H	2.424796000	-4.520075000	3.873143000
H	0.988047000	-3.597613000	4.453172000
H	1.571610000	-1.211912000	5.093997000