

Supplementary Information

Theoretical Investigation on Pt(II)- and Au(I)-Mediated Cycloisomerizations of Propargylic 3-Indoleacetate: [3+2]- versus [2+2]-Cycloaddition Products

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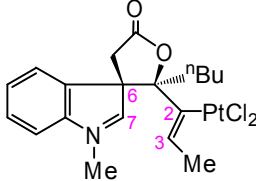
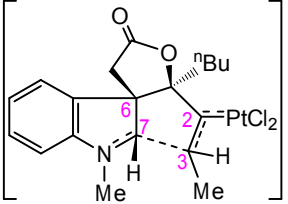
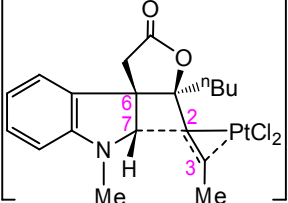
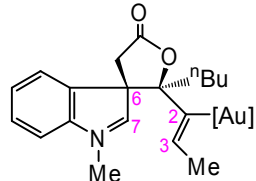
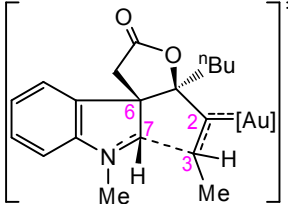
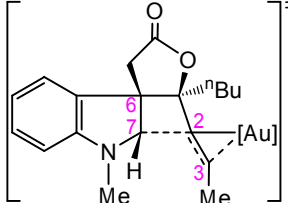
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Table S1. Comparison of the structural parameters in gas phase of the several key species calculated using B3LYP and B97D functionals. The bond lengths are given in Å.

			B3LYP	B97D
4^{Pt}		C2—C3	1.354	1.345
		C6—C7	1.501	1.495
		C7—N	1.314	1.302
		C2—C7	2.684	2.725
		C3—C7	3.283	3.274
TS9^{Pt}		C2—C3	1.377	1.378
		C6—C7	1.534	1.522
		C7—N	1.344	1.340
		C3—C7	2.239	2.417
		C2—Pt	1.912	1.911
TS11^{Pt}		C2—C3	1.394	1.408
		C6—C7	1.540	1.541
		C7—N	1.382	1.390
		C2—C7	1.862	1.851
		C2—Pt	2.037	2.014
4^{Au}		C2—C3	1.345	1.353
		C6—C7	1.499	1.498
		C7—N	1.301	1.310
		C2—C7	2.695	2.635
		C3—C7	3.403	3.312
TS9^{Au}		C2—C3	1.403	1.414
		C6—C7	1.550	1.554
		C7—N	1.382	1.389
		C3—C7	1.885	1.870
		C2—Au	2.022	2.025
TS11^{Au}		C2—C3	1.366	1.377
		C6—C7	1.549	1.548
		C7—N	1.368	1.374
		C2—C7	1.953	1.934
		C2—Au	2.144	2.134

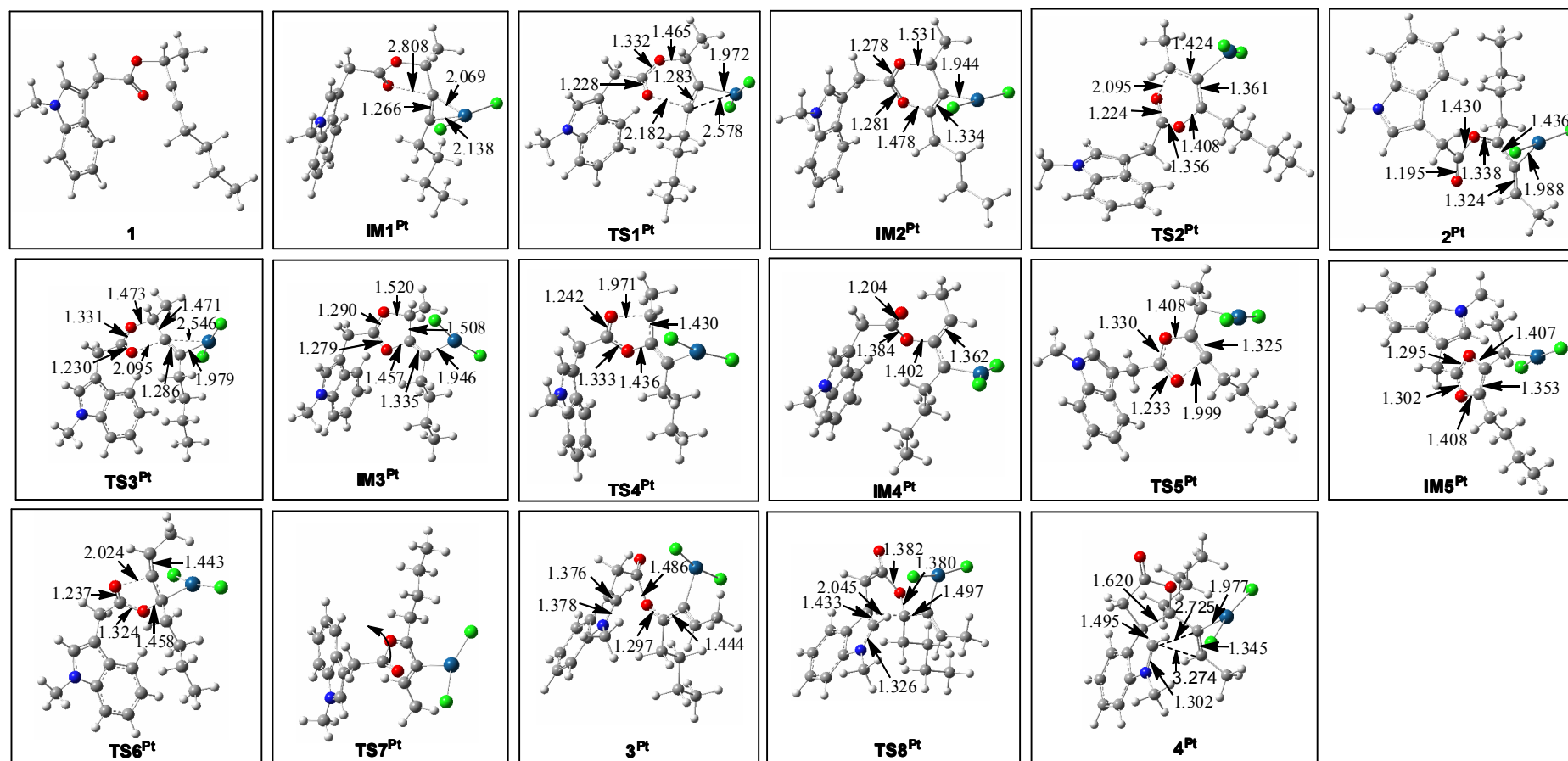


Fig. S1 Optimized geometries with selected structural parameters for the species shown in Scheme 3. The bond distances are given in Å.

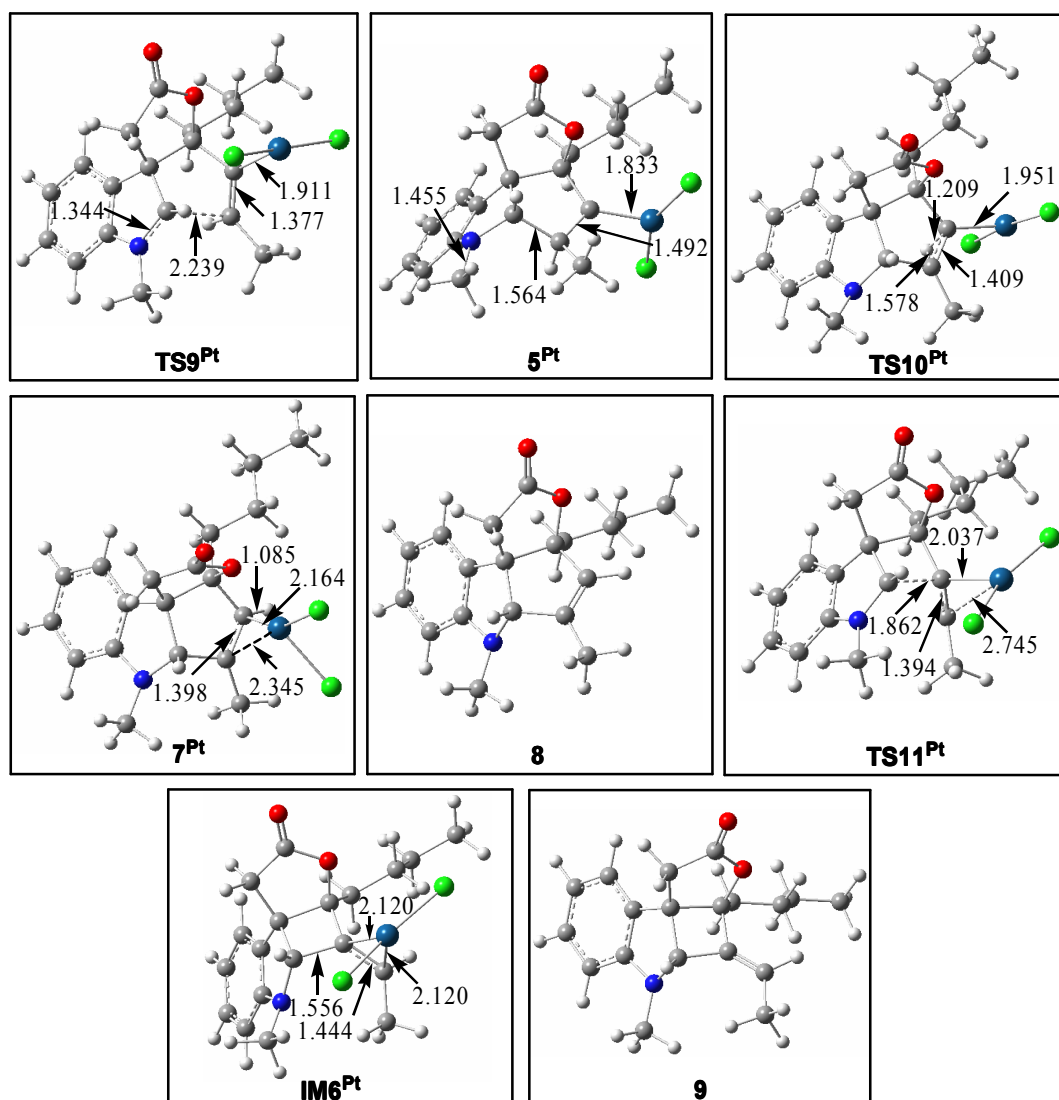


Fig. S2 Optimized geometries with selected structural parameters for the species shown in Scheme 4. The bond distances are given in Å.

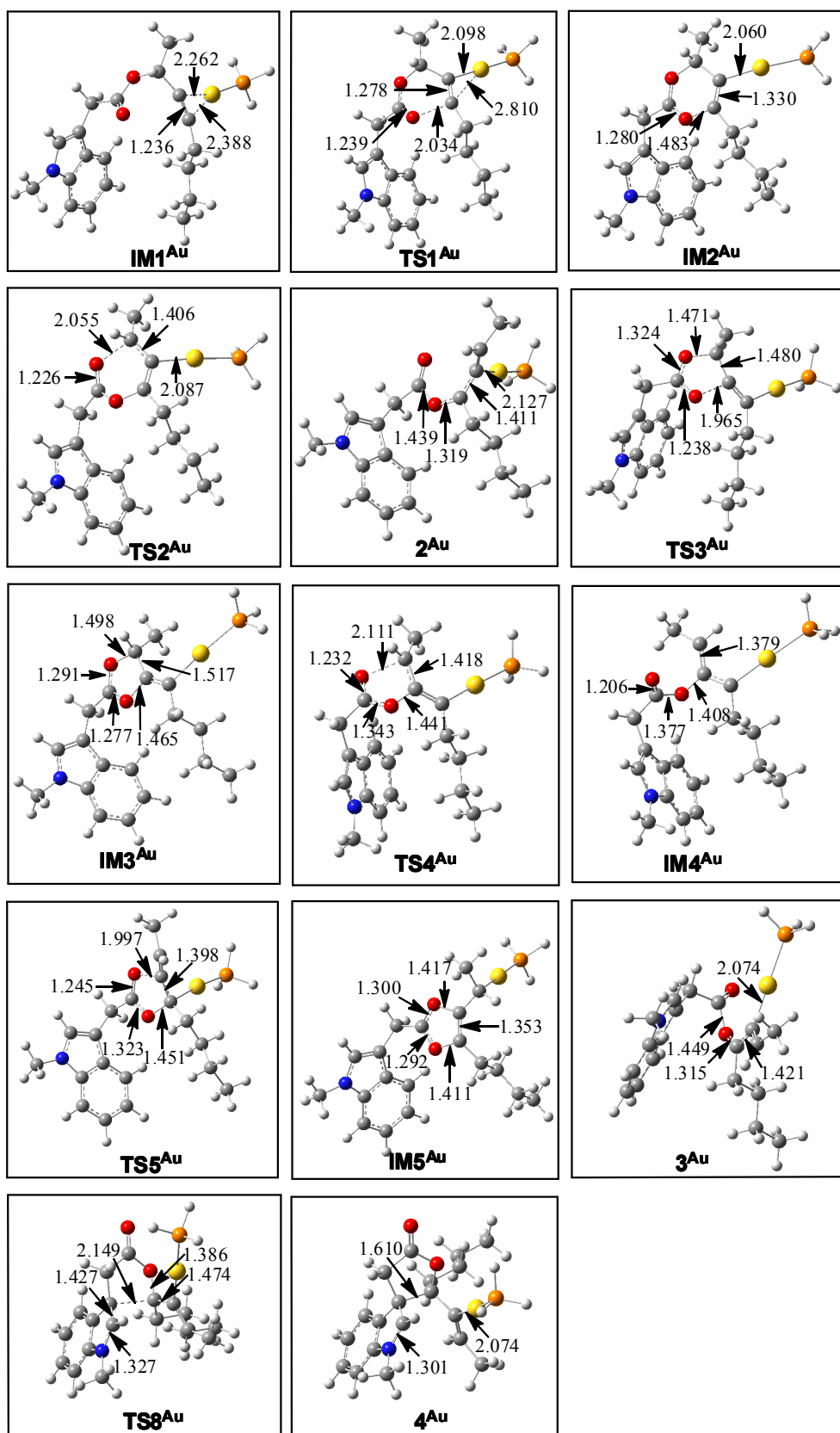


Fig. S3 Optimized geometries with selected structural parameters for the species involved in the formation of **4Au**. The counterion SbF_6^- has been omitted for clarity. The bond distances are given in Å.

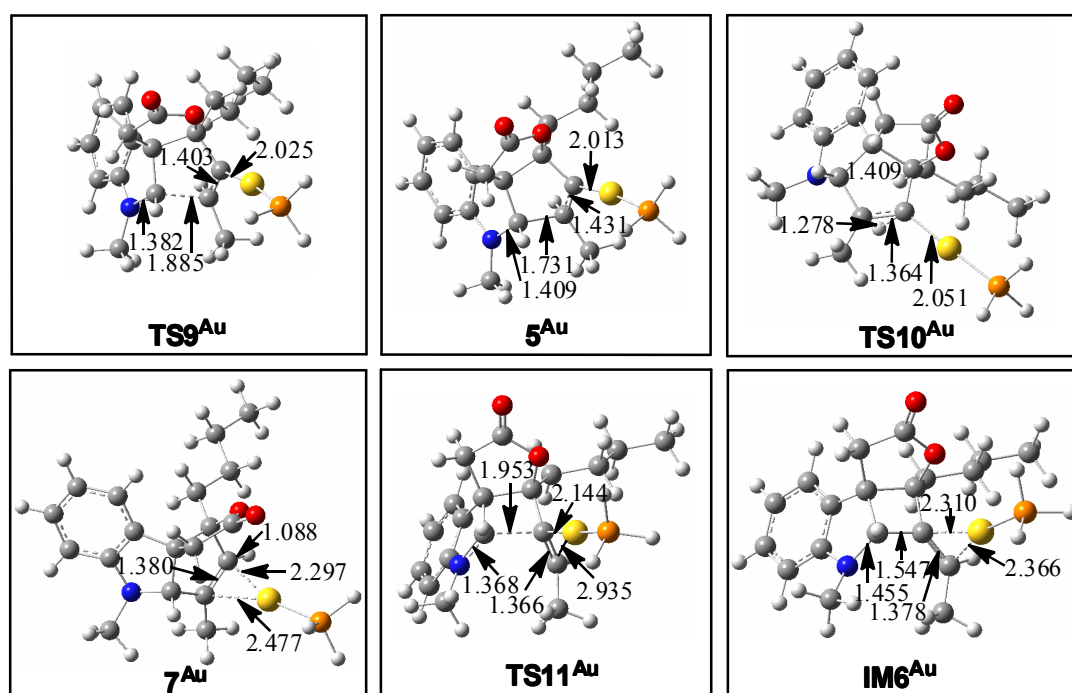


Fig. S4 Optimized geometries with selected structural parameters for the species involved in the formation of **8** and **9** from **4^{Au}**. The counterion SbF_6^- has been omitted for clarity. The bond distances are given in Å.

Cartesian Coordinates for the Stationary Points Given in Fig. S1.

1			
C	-1.29980800	-2.56378200	-1.72475700
C	-2.03701700	-3.35284900	-0.81792300
C	-2.84361800	-2.77141000	0.15476100
C	-2.89864300	-1.37309200	0.19488300
C	-2.16710800	-0.55957700	-0.71446400
C	-1.35425100	-1.17566700	-1.68189900
C	1.22668400	2.99687400	0.66293800
C	-3.33592200	0.77247600	0.67684500
C	-2.47055800	0.81139400	-0.38731900
C	-1.95652700	2.04567500	-1.07879400
C	-0.45041700	2.20718600	-0.90535700
C	1.87249900	1.70109800	0.87300700
C	2.41340200	0.64263900	1.09695200
C	-4.48046000	-0.96344700	2.10912500
H	-3.93433000	-1.55375900	2.85392900
H	-4.89573200	-0.08352900	2.60379000
H	-5.30929800	-1.56921800	1.72474400
H	-0.67524100	-3.05305400	-2.46669200
H	-1.97204400	-4.43560200	-0.87754800
H	-3.40740800	-3.38268400	0.85331000
H	-0.76720100	-0.57065600	-2.36577800
H	-3.79605400	1.58916800	1.21696100
H	-2.14303000	1.99244300	-2.15651800
H	-2.46029500	2.93121500	-0.68123300
N	-3.60506300	-0.53594100	1.03864600
O	-0.17052900	2.85474200	0.24846100
O	0.37795700	1.79214400	-1.68647100
C	2.00374900	3.93002700	-0.27187400
H	1.45650500	4.86978800	-0.39289000
H	2.98053800	4.15018400	0.16873800
H	2.14854800	3.46471400	-1.24615000
H	1.11203400	3.48937300	1.63493000
C	3.06731300	-0.64646700	1.31824500
C	4.21370100	-0.93393900	0.32569300
H	2.31291900	-1.44158600	1.24241600
H	3.45305700	-0.69227600	2.34642700
C	4.87457500	-2.29533800	0.56920200
H	3.81807200	-0.88658600	-0.69593300
H	4.96329900	-0.13645300	0.40432000
C	6.01883700	-2.58799000	-0.40658400
H	5.25238100	-2.33673500	1.60019700

H	4.11541200	-3.08560600	0.49189900
H	6.47165500	-3.56531400	-0.21017100
H	5.66453100	-2.58736900	-1.44353200
H	6.80910800	-1.83282200	-0.32775000

IM1^{Pt}

C	-4.31456000	2.39197000	0.58336100
C	-4.91789600	2.31130000	-0.68875000
C	-5.02099200	1.09912900	-1.36257000
C	-4.50545700	-0.03791200	-0.72907300
C	-3.89642000	0.02068200	0.55541800
C	-3.80224700	1.26181500	1.21051200
C	0.90515700	-1.88572800	1.62964100
C	-3.85794500	-2.11116800	-0.17834400
C	-3.49720200	-1.32350100	0.88773100
C	-2.80131400	-1.78253700	2.14233400
C	-1.36845800	-1.27643400	2.16174200
C	1.09195500	-0.71863100	0.72412400
C	0.82866400	0.41491900	0.22480800
C	-4.97350700	-1.84006300	-2.42481300
H	-4.45115400	-1.36634900	-3.26325600
H	-4.81197600	-2.91773400	-2.48194500
H	-6.04688200	-1.64320400	-2.52290300
H	-4.25155900	3.35597600	1.07996200
H	-5.30783800	3.21279900	-1.15218300
H	-5.48363300	1.04171100	-2.34316900
H	-3.32299400	1.33203200	2.18191800
H	-3.72690500	-3.17554300	-0.32003600
H	-3.29660000	-1.37734800	3.03147100
H	-2.80590100	-2.87301900	2.20569300
N	-4.46977400	-1.35247700	-1.15640100
O	-0.50224500	-2.22954200	1.74380800
O	-1.03763700	-0.14751500	2.46242900
C	1.57501300	-1.69707900	2.99300800
H	1.42029100	-2.59594600	3.59617400
H	2.64740200	-1.54262700	2.84875800
H	1.16111400	-0.83114600	3.50907700
H	1.32476500	-2.76298400	1.13330000
Pt	2.55305200	-0.43280100	-0.71255300
Cl	1.30947400	-1.25786800	-2.51668600
Cl	4.13968400	0.33381700	0.83348900
C	0.16617800	1.68858800	-0.06300600
C	1.00050500	2.93485400	0.29548100
H	-0.76386700	1.66492500	0.52285600

H	-0.11975100	1.70380500	-1.12148700
C	0.24145800	4.23270200	-0.00513600
H	1.26948700	2.89145000	1.35700000
H	1.94278900	2.91159800	-0.26454100
C	1.04925200	5.48474300	0.34989200
H	-0.02632200	4.25748300	-1.07010000
H	-0.70745900	4.23556300	0.54758700
H	0.48758900	6.39644300	0.12287000
H	1.30141600	5.50477700	1.41592500
H	1.98860900	5.52254700	-0.21269200

TS1^{Pt}

C	-3.93571000	1.50979300	2.07465500
C	-5.12060100	1.91983900	1.42914800
C	-5.71229400	1.13886700	0.44153000
C	-5.08624900	-0.06876700	0.11236700
C	-3.89154800	-0.50232200	0.75152100
C	-3.31722500	0.30888200	1.74602800
C	0.77460800	-0.11107700	-0.94814800
C	-4.50993900	-2.04680700	-0.76870800
C	-3.54486200	-1.77300500	0.16835500
C	-2.36795700	-2.62869200	0.51614400
C	-1.03962900	-2.13003900	-0.03078600
C	1.52545900	-0.85434000	-0.22015500
C	1.34807900	-2.27991600	0.23669200
C	2.27652000	-2.71818500	1.35552000
C	-6.61193600	-0.98238900	-1.67129000
H	-6.59692800	-0.08712000	-2.30232700
H	-6.61649900	-1.86093800	-2.31861200
H	-7.53524500	-0.97932400	-1.08112000
H	-3.50145000	2.14376600	2.84160900
H	-5.58169600	2.86179200	1.71075600
H	-6.62569800	1.45815100	-0.05100500
H	-2.40425300	0.00694000	2.25254000
H	-4.60934000	-2.90343800	-1.42210100
H	-2.25011900	-2.75282500	1.59815800
H	-2.49597000	-3.64068100	0.10919400
H	1.46946000	-2.91924200	-0.64589100
H	2.04711300	-3.74832700	1.64020600
H	2.16514400	-2.06547800	2.22415500
H	3.31014700	-2.66367600	1.00719700
N	-5.44367400	-1.03086300	-0.81509300
O	-0.91565300	-1.48526700	-1.06824000
O	-0.01265300	-2.50275400	0.73084100

C	0.16622200	0.98357700	-1.68877900
C	-0.62351800	1.98763000	-0.82302300
H	-0.47630800	0.53761100	-2.45820800
H	0.98140900	1.48461200	-2.22857100
C	-1.20197500	3.13329700	-1.66160100
H	-1.43208900	1.45520900	-0.31053900
H	0.04208100	2.37959300	-0.04613100
C	-1.98452500	4.14157000	-0.81416300
H	-0.38661400	3.64878700	-2.18757300
H	-1.85709100	2.72055100	-2.44124800
H	-2.39352300	4.94630900	-1.43364500
H	-2.81884700	3.65720500	-0.29546900
H	-1.34140600	4.59898800	-0.05440900
Pt	3.09189900	0.29833600	0.10491800
Cl	4.30404100	-0.58823500	-1.69803100
Cl	2.19091600	1.37670800	1.98523400

IM2^{Pt}

C	4.70262500	2.59620000	-0.61696300
C	5.46761400	2.45240800	0.55855400
C	5.61534000	1.21624500	1.17697200
C	4.97497100	0.12034400	0.58759100
C	4.20159500	0.24280200	-0.59857900
C	4.06830000	1.50639800	-1.19996100
C	-0.28827900	0.37039000	-0.98646600
C	4.18499700	-1.91423200	0.08031200
C	3.71695100	-1.07715000	-0.90814100
C	2.81499300	-1.46866900	-2.05160300
C	1.39314900	-1.23675900	-1.63043600
C	-1.05976400	-0.60575400	-0.50589200
C	-0.73381200	-2.05470800	-0.74875500
C	-1.54114500	-2.72973600	-1.84590200
C	5.60521200	-1.75099500	2.15452900
H	5.22259000	-1.28024300	3.06596000
H	5.41027500	-2.82299800	2.20893400
H	6.68768000	-1.59392300	2.10245000
H	4.60722000	3.57793900	-1.07072400
H	5.94868300	3.32453800	0.99058400
H	6.20322400	1.11077100	2.08331900
H	3.47439500	1.63320300	-2.10052700
H	4.03389300	-2.97745100	0.21008600
H	3.01574800	-0.86078200	-2.93937700
H	2.92744200	-2.52360900	-2.31130100
H	-0.76709100	-2.61018600	0.18810800

H	-1.45456100	-2.18239500	-2.78881700
H	-2.59348100	-2.72279000	-1.55421000
H	-1.21006100	-3.76258800	-1.98619200
N	4.94748300	-1.20794700	0.97997800
O	0.93183000	-0.04443600	-1.71114000
O	0.73444600	-2.22097100	-1.15002100
Pt	-2.67406700	-0.41726900	0.56020400
Cl	-4.10891800	0.11452400	-1.22569300
Cl	-1.55963700	-0.98066100	2.56196000
C	-0.26486400	1.86880700	-0.98025800
C	-1.37729900	2.58968800	-0.21099900
H	-0.27448100	2.20190900	-2.02894400
H	0.71375700	2.17515700	-0.58263300
C	-1.19737100	4.11354700	-0.26507200
H	-2.35097800	2.31548700	-0.62783300
H	-1.38003700	2.25438700	0.83235900
C	-2.29720300	4.86231800	0.49390400
H	-0.21598200	4.38346200	0.14970600
H	-1.18714200	4.44321400	-1.31346900
H	-2.15212500	5.94638200	0.43995000
H	-3.28575000	4.63506300	0.08046900
H	-2.30922900	4.57881600	1.55212100

TS2^{Pt}

C	4.83848200	1.94266400	1.87563700
C	5.95727700	1.16265200	2.23301200
C	6.32257400	0.04445400	1.49241400
C	5.53658400	-0.27622600	0.37961300
C	4.40569900	0.49747700	0.00008900
C	4.06038600	1.62094600	0.77097900
C	-0.31489000	0.48111300	0.18784900
C	4.65838200	-1.21053600	-1.45814800
C	3.86587200	-0.11820500	-1.18608600
C	2.66095000	0.31306500	-1.98190100
C	1.40665900	-0.24599000	-1.34724800
C	-1.09100800	-0.63312100	0.09624900
C	-0.49205300	-1.87764400	-0.25131900
C	-1.19458900	-3.00686100	-0.90485000
C	6.71511300	-2.31752200	-0.50977600
H	6.70826100	-2.87135300	0.43491200
H	6.54954100	-3.02212300	-1.32632200
H	7.70048000	-1.85679400	-0.63956100
H	4.58088600	2.80764300	2.47927900
H	6.54376700	1.43980500	3.10371600

H	7.18502800	-0.55360300	1.77001000
H	3.19410800	2.22255100	0.51332400
H	4.58476400	-1.92736000	-2.26505400
H	2.58488000	1.40384800	-2.02154600
H	2.70645200	-0.07662700	-3.00099900
H	0.42982600	-2.13080500	0.27104100
H	-1.96655700	-2.65214700	-1.59075100
H	-1.68905900	-3.59100300	-0.11610200
H	-0.47728400	-3.66218800	-1.40565400
N	5.66616100	-1.31581200	-0.52622300
O	1.02210200	0.45716000	-0.25296900
O	0.84265900	-1.25814500	-1.74194100
Pt	-3.02709600	-0.58716200	0.37044100
Cl	-3.51620300	-0.25658900	-1.90987000
Cl	-2.88986000	-0.88917800	2.69444800
C	-0.72585000	1.86278300	0.56587700
C	-1.04053200	2.76216700	-0.65293300
H	0.08496800	2.31111600	1.15497400
H	-1.60974300	1.77947300	1.20423200
C	-1.46549500	4.17508100	-0.23562600
H	-0.15416500	2.82219900	-1.29961400
H	-1.83545400	2.28878800	-1.24059800
C	-1.78247800	5.07464400	-1.43457900
H	-2.34707500	4.10566000	0.41451400
H	-0.67204800	4.63333500	0.37081600
H	-2.08818500	6.07458900	-1.11046400
H	-0.90948300	5.18909600	-2.08759900
H	-2.59508700	4.65546100	-2.03747500

2^{Pt}

C	3.81380300	1.90290500	-1.64463700
C	5.10139100	2.01888000	-1.08099200
C	5.64649200	0.99686700	-0.31157500
C	4.86703600	-0.14929900	-0.11554500
C	3.56545200	-0.28648700	-0.67299700
C	3.04223500	0.76334400	-1.44780900
C	-0.72931200	-0.07057300	1.03010300
C	4.06926300	-2.15666800	0.48235400
C	3.07810900	-1.58283500	-0.27871800
C	1.73982700	-2.19702500	-0.60311300
C	0.73628100	-1.94616300	0.49528200
C	-1.93805800	-0.84087100	1.12032600
C	-2.55524300	-1.69360700	1.92333800
C	-3.91535300	-2.28793800	1.72234600

C	6.39064100	-1.58349800	1.28587100
H	6.57869900	-0.83446000	2.06284300
H	6.32153400	-2.56388900	1.76006600
H	7.23969700	-1.59021000	0.59321300
H	3.42235100	2.71799200	-2.24602800
H	5.67959500	2.92167100	-1.25409100
H	6.63987000	1.08792600	0.11727300
H	2.05159600	0.68534700	-1.88650900
H	4.09210500	-3.12612400	0.96207700
H	1.33264000	-1.79157400	-1.53385200
H	1.81344900	-3.28197800	-0.70662700
H	-1.99859000	-2.00171400	2.80881200
H	-3.84847500	-3.38165300	1.68647400
H	-4.37393900	-1.93236400	0.79805400
H	-4.57364700	-2.03137500	2.56067300
N	5.15071800	-1.30564900	0.58886000
O	0.43124900	-0.55081700	0.56804300
O	0.30646000	-2.71059600	1.30664200
Pt	-2.44732300	0.01648800	-0.59937800
Cl	-1.52476100	-1.64970100	-1.98400600
Cl	-3.67803300	1.78434700	0.31507800
C	-0.56880700	1.28508300	1.65972300
C	0.13388100	2.34182100	0.78953900
H	0.04486600	1.08820900	2.55486800
H	-1.54751500	1.63897900	1.98569800
C	0.39108500	3.64382000	1.55742500
H	1.08033600	1.94042100	0.41262200
H	-0.50313600	2.54448900	-0.07974900
C	1.08174800	4.70360100	0.69329700
H	-0.56054600	4.03872500	1.93606300
H	1.01038400	3.43020900	2.43962000
H	1.27242900	5.61831400	1.26364400
H	2.04218300	4.33772500	0.31335000
H	0.46326200	4.97298400	-0.17009300

TS3^{Pt}

C	-3.03211300	1.17206500	2.22630500
C	-4.15449100	1.93377500	1.83997000
C	-5.02901900	1.48418500	0.85605100
C	-4.75310400	0.24607800	0.26449300
C	-3.63057800	-0.54036800	0.64259100
C	-2.76310000	-0.05862000	1.63885500
C	1.18275800	0.00452100	-0.82221100
C	-4.76494400	-1.61423200	-0.98552200

C	-3.66392000	-1.72719200	-0.17327900
C	-2.69598100	-2.87102100	-0.13356600
C	-1.27676300	-2.45767900	-0.45846600
C	0.95364000	-1.23603200	-0.57304700
C	1.00574400	-2.63829200	-0.12409900
C	1.95348000	-2.93936500	1.03169500
C	-6.63979000	0.02554600	-1.38912500
H	-6.46957400	0.98024100	-1.89887000
H	-6.94566100	-0.71353800	-2.13149200
H	-7.45546800	0.15373000	-0.66898300
H	-2.36560100	1.55455200	2.99287200
H	-4.33972000	2.88985500	2.32041500
H	-5.89020500	2.07551200	0.56018600
H	-1.89018400	-0.62788400	1.94705500
H	-5.13503800	-2.29571700	-1.73996500
H	-2.67393200	-3.36974700	0.84162300
H	-2.97709800	-3.63214400	-0.87238100
H	1.23286600	-3.27936500	-0.98505900
H	1.82292600	-3.98576900	1.32040500
H	1.74751700	-2.28358500	1.87888300
H	2.98324600	-2.78074200	0.70665700
N	-5.43286200	-0.43382600	-0.73109300
O	-0.94761200	-1.66583900	-1.34021500
O	-0.34664800	-3.01722400	0.31221600
C	0.50602100	1.07650000	-1.61496100
C	-0.07033800	2.20913200	-0.74341000
H	-0.29353500	0.59964800	-2.19236200
H	1.24030100	1.47836800	-2.32211100
C	-0.78651700	3.27032800	-1.58761400
H	-0.76835900	1.78236700	-0.01406300
H	0.73888700	2.66988300	-0.16577800
C	-1.39936400	4.38544700	-0.73421300
H	-0.07896900	3.70266000	-2.30830600
H	-1.57540800	2.79044900	-2.18291100
H	-1.89729100	5.13557900	-1.35753900
H	-2.14091500	3.98235600	-0.03574300
H	-0.63191800	4.89865000	-0.14407100
Pt	2.86350200	0.26401100	0.19002100
Cl	4.23950300	-0.03239900	-1.68419600
Cl	1.82781300	0.61089400	2.27295100

IM3^{Pt}

C	-4.86741100	0.89717500	2.38464400
C	-5.75034100	1.57337600	1.51796900

C	-5.90980800	1.17570000	0.19562500
C	-5.15882100	0.07893100	-0.24265200
C	-4.26232500	-0.61635200	0.61371200
C	-4.12341100	-0.19050900	1.94603800
C	1.20691300	0.11231200	-0.37867500
C	-4.22371400	-1.57318000	-1.43217300
C	-3.67721800	-1.66966300	-0.17421500
C	-2.67389900	-2.68278500	0.27701600
C	-1.27141800	-2.17507300	0.40852200
C	0.53484400	-0.89873700	0.17608000
C	0.94557400	-2.11275800	0.97007000
C	1.33661400	-1.89102900	2.41886500
C	-5.88686300	-0.12030700	-2.64722800
H	-5.64399900	0.90792400	-2.93499800
H	-5.64945800	-0.78025800	-3.48298200
H	-6.96104900	-0.18544200	-2.44451600
H	-4.76770800	1.23665500	3.41100500
H	-6.31598800	2.42172900	1.89077600
H	-6.59025800	1.69990700	-0.46809500
H	-3.44654000	-0.69934600	2.62774400
H	-4.04403800	-2.18148100	-2.30871000
H	-2.93243200	-3.12733300	1.24749400
H	-2.61803600	-3.52934500	-0.42131200
H	1.67206500	-2.72593900	0.43171200
H	1.51853100	-2.84488400	2.92157100
H	0.56601600	-1.33092200	2.95599000
H	2.25606300	-1.29883300	2.42694100
N	-5.11650000	-0.52744500	-1.48676900
O	-0.90257000	-1.02861300	-0.02320700
O	-0.35303600	-2.90234200	0.94932000
C	0.55011100	1.22669500	-1.15674400
C	0.11255700	2.41334900	-0.27396600
H	-0.32481500	0.82260000	-1.68447400
H	1.24966300	1.57645100	-1.92133800
C	-0.49235300	3.55769400	-1.09640400
H	-0.62214900	2.06065000	0.46238000
H	0.97664000	2.77394500	0.29392100
C	-0.94164000	4.73816900	-0.22944000
H	0.24820200	3.90420100	-1.82977300
H	-1.34646800	3.18324400	-1.67857600
H	-1.35963800	5.54577800	-0.83972200
H	-1.70984400	4.43211800	0.49001200
H	-0.10131600	5.14998000	0.33976700
Pt	3.14034500	0.08087100	-0.16233200

C1	3.39058100	-1.73569400	-1.65247100
C1	3.32563500	1.78053800	1.44737100

TS4^{Pt}

C	-4.45616200	2.39174800	0.07152100
C	-4.99718000	2.09185000	-1.19590900
C	-5.00256900	0.79212500	-1.68860700
C	-4.45006600	-0.20729600	-0.87923000
C	-3.90082900	0.07249400	0.40256600
C	-3.90778200	1.39740300	0.87265300
C	0.99225300	0.21567600	0.15714700
C	-3.71862100	-2.14073200	-0.01510100
C	-3.44965900	-1.18477700	0.93868500
C	-2.75530400	-1.41633900	2.25701000
C	-1.26977500	-1.46098100	2.02777700
C	0.61092000	-0.52948400	1.23133800
C	1.19117500	-1.73223100	1.74254900
C	1.58867000	-1.92380100	3.16957100
C	-4.74250100	-2.25808900	-2.31435400
H	-4.21025100	-1.87068500	-3.18924900
H	-4.51544100	-3.32026600	-2.21275200
H	-5.81964200	-2.14370000	-2.47550100
H	-4.46984700	3.41827600	0.42501300
H	-5.41630500	2.89167900	-1.79869400
H	-5.41839100	0.56579600	-2.66543600
H	-3.48951200	1.64511800	1.84440800
H	-3.51888900	-3.20370700	0.00127000
H	-2.97470000	-0.60345100	2.95613800
H	-3.05232200	-2.36191000	2.71586900
H	1.71308800	-2.33997200	1.00455300
H	1.53733800	-2.97639100	3.45850500
H	1.00469200	-1.31309400	3.86104900
H	2.63902000	-1.60978100	3.23918800
N	-4.32413700	-1.56640200	-1.10887400
O	-0.66372900	-0.28778700	1.84756300
O	-0.60850700	-2.50912000	1.94757500
C	0.20843700	1.41266600	-0.31194800
C	0.40091200	2.66309800	0.57600200
H	-0.85538200	1.13826400	-0.32470700
H	0.49887900	1.64746200	-1.33877100
C	-0.36558000	3.87471200	0.03071600
H	0.05946400	2.43751200	1.59444900
H	1.46959600	2.89256300	0.64047500
C	-0.20092600	5.12116500	0.90612500

H	-0.01365500	4.09350200	-0.98611600
H	-1.43108300	3.62350600	-0.06057000
H	-0.75111400	5.97338900	0.49359900
H	-0.57297000	4.94555700	1.92230800
H	0.85237900	5.41121500	0.98606600
Pt	2.66301700	-0.22792400	-0.68985800
Cl	1.88984400	-2.23038200	-1.66733100
Cl	3.92275200	1.58932200	0.09367100

IM4^{Pt}

C	-4.04453700	-1.08222500	-2.35202100
C	-4.86640600	-1.88383500	-1.53242000
C	-5.16681600	-1.51030200	-0.22687000
C	-4.62523000	-0.30672800	0.24165800
C	-3.79785600	0.51924200	-0.56988600
C	-3.50673000	0.11032400	-1.88301900
C	1.09647000	0.17571500	0.06492200
C	-4.05467600	1.49405700	1.44719900
C	-3.45075800	1.66984600	0.22439700
C	-2.62291000	2.85640600	-0.19270300
C	-1.13869600	2.69397800	0.08348200
C	0.76636800	1.42313600	-0.56595100
C	1.68326900	2.29549400	-1.07035300
C	1.37987700	3.57895000	-1.75087100
C	-5.53670000	-0.20001700	2.58726700
H	-5.16992300	-1.18289900	2.90224400
H	-5.44539100	0.48868100	3.42863900
H	-6.59622200	-0.28930700	2.32271600
H	-3.83092100	-1.40517600	-3.36661100
H	-5.27242100	-2.80986500	-1.92822100
H	-5.80076900	-2.12970600	0.40018900
H	-2.86539600	0.71389900	-2.51864000
H	-4.04322700	2.13775000	2.31665900
H	-2.75122500	3.04006900	-1.26617200
H	-2.93271400	3.75685600	0.34206700
H	2.72541900	2.02149500	-0.95153300
H	1.52954100	4.40406200	-1.04049300
H	0.35258200	3.62885100	-2.11631000
H	2.07431200	3.73929800	-2.58108100
N	-4.76195900	0.30884700	1.47229800
O	-0.60116900	1.69564500	-0.70932600
O	-0.48514000	3.33214700	0.86778700
C	0.02609400	-0.74105100	0.55562000
C	-0.24293900	-1.90459700	-0.44418800

H	-0.90457000	-0.18608900	0.70868600
H	0.35062800	-1.16596900	1.51061400
C	-1.26364400	-2.90039200	0.11892200
H	-0.61015900	-1.48857400	-1.38914900
H	0.70192000	-2.41491300	-0.65966100
C	-1.54214500	-4.05539800	-0.84823900
H	-0.88886800	-3.29809800	1.07141900
H	-2.20122900	-2.37669500	0.34151700
H	-2.25901100	-4.76320000	-0.41939300
H	-1.96237900	-3.68641000	-1.78977500
H	-0.62592300	-4.60885500	-1.08213500
Pt	2.87885100	-0.39596600	0.26471900
Cl	2.95488800	-0.54470500	2.59657200
Cl	3.47732300	-0.45645700	-1.99534300

TS5^{Pt}

C	5.23620400	2.44664900	1.05452300
C	6.19691200	1.64405100	1.70343700
C	6.36398800	0.30497700	1.36918200
C	5.54258000	-0.21457300	0.36196300
C	4.57111400	0.57864900	-0.30728400
C	4.42169000	1.92843200	0.05577300
C	-0.60905900	0.58365500	-0.15840200
C	4.51908700	-1.51832700	-1.14701400
C	3.93594600	-0.27942000	-1.27403100
C	2.83354100	0.09509100	-2.22954400
C	1.52648400	0.22579800	-1.49270600
C	-0.35486900	-0.63962000	-0.60041600
C	-1.25695300	-1.80185000	-0.37217300
C	-1.58976800	-2.63279900	-1.60626000
C	6.32387100	-2.60679800	0.23641300
H	6.17716600	-2.83741500	1.29688900
H	6.05506900	-3.48654000	-0.35038300
H	7.38302400	-2.38445400	0.06779000
H	5.13126300	3.48738700	1.34583400
H	6.81655800	2.07963900	2.48140700
H	7.10332100	-0.30966400	1.87321000
H	3.67526500	2.55196600	-0.42754000
H	4.31909600	-2.43143700	-1.69146400
H	3.03307000	1.05699900	-2.71154400
H	2.71652600	-0.66708900	-3.00457700
H	-0.84510100	-2.42117100	0.43207700
H	-0.68142700	-3.14257200	-1.95528100
H	-1.99478900	-2.02241300	-2.41379900

H	-2.32769500	-3.39665300	-1.35270000
N	5.48910700	-1.49209900	-0.16942000
O	1.07589800	1.25987900	-0.99391600
O	0.82172700	-0.89069500	-1.33148100
Pt	-2.80510600	-0.78051900	0.45631200
Cl	-3.95751300	-0.16763100	-1.50290300
Cl	-1.96639800	-1.19035100	2.61584800
C	-0.99884200	1.85471500	0.48506200
C	-1.78611300	2.81242200	-0.43062300
H	-0.07194900	2.33108900	0.82747200
H	-1.56629600	1.61206300	1.38830500
C	-2.18638100	4.09721600	0.30489500
H	-1.16541800	3.05757300	-1.30115200
H	-2.67498900	2.29605900	-0.80782400
C	-2.95921600	5.07027700	-0.59066700
H	-2.79981800	3.83769700	1.17811600
H	-1.28782500	4.59267200	0.69832600
H	-3.23898200	5.97607200	-0.04334200
H	-2.35919400	5.37531000	-1.45554900
H	-3.87816200	4.61102000	-0.97034500

IM5^{Pt}

C	-6.99918800	0.98704400	-0.95861100
C	-7.37183100	-0.19648700	-0.28942300
C	-6.44818200	-0.92839500	0.44852700
C	-5.13528600	-0.44710900	0.50205100
C	-4.73708200	0.74256100	-0.16945800
C	-5.69498900	1.46299000	-0.90350200
C	1.05806300	1.89111000	-1.09360300
C	-2.94997100	-0.13772900	0.90662400
C	-3.33523600	0.91305900	0.10428400
C	-2.48879300	2.06121000	-0.36794800
C	-1.08718100	1.70295400	-0.70212500
C	0.70088000	0.60657300	-1.32494300
C	1.42618600	-0.64505900	-1.59304600
C	0.60355100	-1.71525800	-2.31202100
C	-3.98769000	-2.18859900	1.92195700
H	-4.24202500	-3.05147300	1.29719400
H	-2.98014600	-2.32661400	2.31619900
H	-4.69043600	-2.14013900	2.76025700
H	-7.74697700	1.53525500	-1.52384200
H	-8.39936900	-0.54204900	-0.35040000
H	-6.73858900	-1.83897300	0.96334500
H	-5.42757300	2.38137300	-1.42084500

H	-1.97342700	-0.37352300	1.31409800
H	-2.92718800	2.49178700	-1.28184200
H	-2.42925700	2.89293800	0.34760300
H	2.32992000	-0.40817500	-2.16218600
H	0.25735600	-1.34524600	-3.28785500
H	-0.26935800	-2.01752400	-1.72921800
H	1.23116300	-2.59141500	-2.47578700
N	-4.02512200	-0.96033700	1.14788800
O	-0.68732000	0.54009400	-1.10685600
O	-0.10911300	2.56199000	-0.68178400
C	2.34698600	2.62001700	-1.03212900
C	2.76063100	2.99318000	0.40993600
H	2.29423700	3.51978800	-1.65906200
H	3.10202200	1.96307400	-1.47641800
C	4.13993500	3.66048600	0.45866000
H	2.00698500	3.66670200	0.83762100
H	2.75585200	2.08472200	1.02230000
C	4.55878300	4.04093900	1.88213000
H	4.88484400	2.97883500	0.02779300
H	4.13784900	4.55680800	-0.17743000
H	5.54666900	4.51199300	1.89051800
H	3.84928900	4.74558200	2.33051200
H	4.60383200	3.15822800	2.52876500
Pt	2.12556600	-1.29590300	0.21444300
Cl	3.84192900	-2.43202500	-0.90322900
Cl	0.59454000	-0.23895900	1.73451300

TS6^{Pt}

C	-3.73346800	1.55235400	2.07022900
C	-4.95340800	1.87267800	1.43928600
C	-5.49894400	1.04745600	0.46214800
C	-4.78904500	-0.11183300	0.12801700
C	-3.55797500	-0.45371900	0.75216000
C	-3.03064100	0.40048100	1.73703300
C	0.86769200	-0.26143100	-0.57094000
C	-4.08806700	-2.04858100	-0.75582200
C	-3.13302800	-1.70137900	0.17040400
C	-1.88877500	-2.48634700	0.49258900
C	-0.67721800	-1.93856500	-0.22043600
C	1.56743900	-1.36141000	-1.18843900
C	2.44206800	-2.08465100	-1.84383000
C	3.93499900	-1.91367300	-1.90947000
C	-6.27730400	-1.14450700	-1.62227800
H	-6.34683500	-0.24890700	-2.24891000

H	-6.22641800	-2.01897000	-2.27315300
H	-7.18423200	-1.21582800	-1.01145500
H	-3.33764500	2.21933800	2.83007400
H	-5.47768000	2.78028900	1.72317800
H	-6.43965600	1.29675300	-0.01929300
H	-2.08694900	0.16997500	2.22203600
H	-4.13775300	-2.91711200	-1.39900500
H	-1.67243400	-2.45241900	1.56679400
H	-1.99273500	-3.53149800	0.19438000
H	2.01326800	-2.93142900	-2.37804500
H	4.41766000	-2.74381000	-1.38049800
H	4.25313000	-0.96786800	-1.47320300
H	4.25729100	-1.95568400	-2.95523100
N	-5.08982100	-1.10130900	-0.79210400
O	-0.23625400	-0.77449200	0.23071800
O	-0.11059300	-2.49322800	-1.17020700
Pt	2.47426000	0.21089400	0.54772500
Cl	2.00067600	-1.21693500	2.35723000
Cl	3.46410900	1.76263800	-0.92211400
C	0.31035100	0.82108400	-1.49943700
C	-0.25499900	2.04991300	-0.77606200
H	-0.48318000	0.33919300	-2.09051000
H	1.10663400	1.11775600	-2.18548300
C	-0.90172500	3.04302900	-1.75072600
H	-0.99587200	1.73369300	-0.03309900
H	0.55840100	2.54355300	-0.23267400
C	-1.49334600	4.26385900	-1.03906600
H	-0.15472400	3.37039000	-2.48595800
H	-1.69213200	2.53381300	-2.31976300
H	-1.95122100	4.95772000	-1.75176600
H	-2.26397600	3.96398900	-0.32007900
H	-0.72071500	4.81271100	-0.48939400

TS7^{Pt}

C	-4.05173400	2.67312400	-0.63885800
C	-4.83370600	1.99158600	-1.59469200
C	-5.00140200	0.61288100	-1.53853300
C	-4.36174200	-0.07437200	-0.49950500
C	-3.56772500	0.59236700	0.47540200
C	-3.41856200	1.98910300	0.39165100
C	0.23329600	0.71944700	0.22541700
C	-3.59480600	-1.61718700	0.93371000
C	-3.08960200	-0.41881000	1.38201600
C	-2.20864800	-0.22938400	2.58559000

C	-0.72846900	-0.30122700	2.28599700
C	0.39200500	-0.51769200	-0.50038300
C	-0.53682000	-1.21119000	-1.16671400
C	-0.32764700	-2.47440300	-1.94391300
C	-5.08329200	-2.45199100	-0.92319200
H	-4.77418800	-2.47806300	-1.97320400
H	-4.86883200	-3.42327100	-0.47495700
H	-6.16365500	-2.27638100	-0.87877800
H	-3.94761700	3.75158500	-0.71087400
H	-5.31522300	2.55491200	-2.38810100
H	-5.60739000	0.09281100	-2.27394200
H	-2.82115500	2.52669000	1.12288900
H	-3.46559800	-2.61088100	1.34125400
H	-2.39772600	0.74922400	3.04538400
H	-2.39503800	-0.99345500	3.34385900
H	-1.54328000	-0.78966300	-1.17840700
H	-1.06900600	-3.22778300	-1.65207700
H	0.66965800	-2.88262300	-1.77673200
H	-0.46209400	-2.29087900	-3.01767200
N	-4.35843900	-1.42498200	-0.19781700
O	-0.34446100	0.80136900	1.40485000
O	0.10123600	-1.00666900	2.74966300
Pt	2.31981600	-0.83353300	-0.23492600
Cl	3.35798200	0.86844400	-1.48743300
Cl	1.99159700	-2.85151900	0.90107000
C	0.50460600	2.06903500	-0.35984500
C	1.27964900	3.04507000	0.54558000
H	-0.50402500	2.47123800	-0.55640200
H	1.01297100	1.94181100	-1.31445300
C	1.43122800	4.42487800	-0.10572100
H	0.76971400	3.13980900	1.51147500
H	2.26962600	2.61686900	0.73578700
C	2.21918700	5.40417000	0.76972600
H	1.93603700	4.30977800	-1.07296100
H	0.43717400	4.84089200	-0.32167200
H	2.31515200	6.38032900	0.28384100
H	1.72669900	5.55988400	1.73646800
H	3.22926700	5.02985600	0.96790500
3rd			
C	4.96594400	0.64199600	-1.42561000
C	5.65428800	0.20892100	-0.27466500
C	5.08721900	-0.71280300	0.60006700
C	3.80859100	-1.19151600	0.29456100

C	3.09590800	-0.77031000	-0.86319300
C	3.69576100	0.16212300	-1.72762200
C	0.21166600	1.00832800	0.12016700
C	1.83125800	-2.24885000	0.28230100
C	1.82841500	-1.45984900	-0.84556100
C	0.74337400	-1.43344700	-1.87449400
C	-0.00952000	-0.13217800	-2.11140500
C	-0.76586400	0.23755100	0.85136400
C	-0.63181300	0.14531700	2.20671800
C	-1.53768600	-0.56185500	3.15179700
C	3.38051500	-2.79431900	2.19257500
H	3.61624000	-2.08602500	2.99446300
H	2.54378900	-3.41708700	2.51250200
H	4.25208400	-3.43736700	2.02777100
H	5.43984400	1.35922300	-2.08914900
H	6.64613100	0.59953100	-0.06777400
H	5.62199100	-1.04634100	1.48422600
H	3.18052200	0.50134800	-2.62223400
H	1.05184400	-2.90702700	0.64213700
H	1.12392000	-1.68905900	-2.87194800
H	-0.02441700	-2.17613700	-1.63032300
H	0.23109300	0.61994600	2.67063000
H	-0.95716700	-1.16623000	3.85918500
H	-2.26413900	-1.18938700	2.63697700
H	-2.07713100	0.18479500	3.75322400
N	3.01111600	-2.09573300	0.97658700
O	0.35730100	0.95457600	-1.16723000
O	-0.63828200	0.18357500	-3.06329100
Pt	-2.28751900	-0.52989100	-0.11395400
Cl	-3.15971100	1.60844700	-0.53001500
Cl	-1.78429900	-2.81867300	0.21187200
C	1.05441800	2.10648800	0.69987500
C	0.38720400	3.48635700	0.43968600
H	2.03213800	2.07110600	0.20911000
H	1.19818900	1.97708100	1.77303400
C	1.21798000	4.63627900	1.02133600
H	0.26274900	3.61762200	-0.64050900
H	-0.61994400	3.48600400	0.87145900
C	0.57848100	6.00464100	0.76385800
H	1.34350600	4.48635600	2.10232300
H	2.22695000	4.61248000	0.58860000
H	1.18680100	6.80958100	1.18814200
H	0.47192500	6.19595900	-0.30929300
H	-0.41906600	6.06667900	1.21181000

TS8 ^{Pt}			
C	-5.07963000	-0.12883900	1.46708000
C	-5.64322900	-0.62907600	0.28429400
C	-4.85062200	-1.24972800	-0.68477600
C	-3.48972200	-1.33789300	-0.41596800
C	-2.89527200	-0.82514700	0.75226500
C	-3.70669500	-0.21884500	1.71288600
C	-0.47565800	0.66545800	0.16920800
C	-1.30727400	-1.85001200	-0.53569300
C	-1.44197400	-1.06916300	0.65791500
C	-0.59298500	-1.33566800	1.87808100
C	-0.04885300	-0.02033800	2.41957700
C	0.66964700	0.32121700	-0.73115400
C	0.56850800	0.53298400	-2.06139100
C	1.62215400	0.29066700	-3.09901600
C	-2.66810500	-2.60381100	-2.46803000
H	-3.03857900	-1.87914200	-3.19793600
H	-1.71839800	-3.01273200	-2.81207000
H	-3.39651300	-3.41190900	-2.36137500
H	-5.72363900	0.33685600	2.20638900
H	-6.71239800	-0.54122100	0.12072800
H	-5.28661000	-1.64855100	-1.59487800
H	-3.28458600	0.17588900	2.63220100
H	-0.38196400	-2.27511600	-0.91754900
H	-1.15779400	-1.82103000	2.67840700
H	0.26440700	-1.97008600	1.62945900
H	-0.36322300	0.94606400	-2.44910800
H	1.98295400	1.24605800	-3.50270400
H	1.21066300	-0.27409000	-3.94584500
H	2.47515600	-0.25055300	-2.68780300
N	-2.46277900	-1.95238200	-1.17843600
O	-0.14118200	0.97983700	1.47093500
O	0.34177500	0.19933600	3.52637900
Pt	2.32883400	-0.37801700	0.07139400
Cl	3.14434700	1.73597200	0.62125800
Cl	1.91995100	-2.68530000	-0.40996800
C	-1.52684300	1.65519000	-0.31162800
C	-0.96775100	3.08778800	-0.46024100
H	-2.33451100	1.67409800	0.42328400
H	-1.96383100	1.31808100	-1.25681500
C	-2.05542500	4.08255900	-0.88612400
H	-0.53303400	3.39634600	0.49654200
H	-0.14825700	3.09481700	-1.18559500
C	-1.52335200	5.51309100	-1.02094100

H	-2.49164200	3.76157000	-1.84267300
H	-2.87602100	4.06325300	-0.15586200
H	-2.31512400	6.20490300	-1.32607400
H	-1.11227900	5.87207200	-0.07130100
H	-0.72370300	5.56902600	-1.76760500
4^{Pt}			
C	-4.92936900	1.41248700	-0.90059400
C	-5.33258800	0.15354900	-1.35785000
C	-4.59137800	-0.99113600	-1.04887200
C	-3.44700200	-0.80410700	-0.28704400
C	-3.00835500	0.44515400	0.17104400
C	-3.77058400	1.57017100	-0.12998200
C	-0.36189900	0.89377100	0.47339900
C	-1.59387200	-1.24692000	0.90259000
C	-1.75082000	0.23727400	0.98701900
C	-1.79187500	0.70844100	2.45658800
C	-0.32139500	0.91293500	2.81723100
C	0.30336500	0.00715900	-0.59936100
C	-0.24284500	-0.04577300	-1.82692400
C	0.24164700	-0.83972600	-3.00644800
C	-2.62027300	-3.22088400	-0.14160500
H	-2.74720000	-3.31586400	-1.22189100
H	-1.68431300	-3.69554600	0.15476600
H	-3.47350500	-3.67096400	0.37157500
H	-5.52641100	2.28505900	-1.14567700
H	-6.23476900	0.05985500	-1.95331400
H	-4.90493900	-1.97268200	-1.38716200
H	-3.47954400	2.55496000	0.21783500
H	-0.78250500	-1.84684300	1.31388600
H	-2.32449100	1.65997100	2.54380700
H	-2.25791300	0.00648200	3.15144300
H	-1.12485600	0.56978500	-2.02088800
H	0.57006500	-0.16891800	-3.81085500
H	-0.56172900	-1.46237900	-3.42269300
H	1.08115900	-1.48123800	-2.73339800
N	-2.53850100	-1.79626100	0.19445700
O	0.42738900	0.90300300	1.68576300
O	0.13521800	1.05470900	3.91836200
Pt	1.93995200	-0.99558300	-0.12349500
Cl	3.39926000	0.71422400	-0.74711800
Cl	0.95358500	-3.08975700	0.52772100
C	-0.56619300	2.35864600	0.03899800
C	0.73622000	3.13869600	-0.18885400

H	-1.15571200	2.87374200	0.81208900
H	-1.16713100	2.37108600	-0.87534000
C	0.46694200	4.58862700	-0.61331200
H	1.33335000	3.12394500	0.72891800
H	1.34008900	2.63032500	-0.94583600
C	1.75649700	5.38508000	-0.83659700
H	-0.13077500	4.59614600	-1.53615100
H	-0.14570200	5.09072200	0.14974200
H	1.54176300	6.41454300	-1.14212900
H	2.35828700	5.42496300	0.07775800
H	2.37346300	4.92386600	-1.61484200

Cartesian Coordinates for the Stationary Points Given in Fig. S2.

TS9^{Pt}

C	-5.18782000	1.31408300	0.26880000
C	-5.67154000	0.43016600	-0.69635100
C	-4.88171800	-0.63047100	-1.15919100
C	-3.60433800	-0.74953600	-0.62798400
C	-3.08612900	0.14171700	0.32379000
C	-3.89384500	1.16961900	0.79259300
C	-0.46637100	0.69206700	0.52524000
C	-1.48608200	-1.48261700	-0.26345600
C	-1.68704900	-0.32009800	0.71659100
C	-1.56363000	-0.76787900	2.19277500
C	-0.42579000	0.05676000	2.78187400
C	0.42157500	-0.02216400	-0.51881000
C	-0.21091500	-0.33414600	-1.70152900
C	0.38873700	-1.13096800	-2.82866500
C	-2.87677600	-2.89192400	-1.76883400
H	-2.97616200	-2.55492500	-2.80612500
H	-2.03397800	-3.57994000	-1.69691200
H	-3.79265000	-3.41331600	-1.47560300
H	-5.81888500	2.12300500	0.62247400
H	-6.67470100	0.55730200	-1.09074300
H	-5.26267200	-1.33062600	-1.89507900
H	-3.54119200	1.85538200	1.55588900
H	-0.76239400	-2.27196000	-0.09222000
H	-2.47658300	-0.60014400	2.76784300
H	-1.28419200	-1.82034200	2.29444300
H	-1.09322800	0.25474300	-1.95879800
H	1.00411400	-0.48120700	-3.46259400
H	-0.39051600	-1.56759800	-3.46276400
H	1.03977800	-1.92389100	-2.45368600

N	-2.64688000	-1.76467100	-0.87890000
O	0.17232000	0.79077000	1.80295600
O	-0.08232600	0.09798400	3.92979300
Pt	2.15956000	-0.66593400	-0.05220400
Cl	3.38990600	0.94913500	-1.21628200
Cl	1.43216500	-2.58438700	1.15060100
C	-0.82500200	2.12710500	0.09905200
C	0.39242200	3.04605800	-0.07413700
H	-1.48543600	2.54609500	0.86734800
H	-1.40896000	2.09366800	-0.82724900
C	-0.01270000	4.47076300	-0.47424600
H	0.95814500	3.07086200	0.86360400
H	1.07372200	2.63112700	-0.82576600
C	1.19054700	5.40513300	-0.63488400
H	-0.57973300	4.43914100	-1.41549500
H	-0.69877000	4.88260300	0.27960200
H	0.87663200	6.41330200	-0.92480300
H	1.75445500	5.48614900	0.30079700
H	1.87906000	5.03333700	-1.40118400

5^{pt}

C	-4.21681200	1.94548500	-1.86637000
C	-5.00092100	0.80657100	-2.05078900
C	-4.76443500	-0.36268700	-1.31999300
C	-3.71796600	-0.36209700	-0.39551500
C	-2.89501500	0.77155200	-0.22413300
C	-3.16315500	1.93190900	-0.94125600
C	-0.35894600	0.74242800	0.70198900
C	-2.01296000	-1.08974200	0.98468300
C	-1.89900500	0.46797100	0.88577800
C	-2.18668400	1.16393200	2.22351400
C	-0.87012100	1.06379400	2.97261900
C	0.20260900	-0.56891000	0.14105400
C	-0.83979100	-1.63623000	0.10729300
C	-0.37213500	-3.06771500	0.40665100
C	-3.85771900	-2.72844400	0.37344500
H	-3.51673800	-3.25808500	-0.53035800
H	-3.54975200	-3.30389900	1.25047300
H	-4.95174500	-2.70688400	0.35949300
H	-4.41672100	2.84383900	-2.44110100
H	-5.81016100	0.82198000	-2.77513500
H	-5.38143700	-1.24185100	-1.47157900
H	-2.56477300	2.82606900	-0.80454400
H	-1.89870400	-1.46169100	2.00979400

H	-2.44070300	2.22086000	2.08534400
H	-2.99603900	0.70206100	2.79261700
H	-1.18601200	-1.58233400	-0.94436400
H	0.38959500	-3.38780500	-0.30688900
H	-1.21433700	-3.76084000	0.34555000
H	0.05911900	-3.12729500	1.40963600
N	-3.34816700	-1.37809000	0.48481500
O	0.13345100	0.77233300	2.07251800
O	-0.64472900	1.20003000	4.14208000
Pt	1.91224100	-0.81942400	-0.47114900
Cl	1.60446600	-0.37461300	-2.74081500
Cl	3.13284500	-1.46935300	1.38823200
C	0.01763600	2.03697400	-0.02744600
C	1.44492800	2.56089800	0.18843600
H	-0.68306400	2.80886600	0.31551500
H	-0.17634700	1.89206600	-1.09664600
C	1.67149100	3.89984400	-0.52677400
H	1.63385000	2.67361800	1.26155000
H	2.17357200	1.82909000	-0.17885800
C	3.08508800	4.45092800	-0.31559900
H	1.48356600	3.77393500	-1.60133000
H	0.93536100	4.63424000	-0.17004500
H	3.21991600	5.40727300	-0.83094500
H	3.29272200	4.61188900	0.74809800
H	3.84062900	3.75633200	-0.69878300

TS10^{Pt}

C	-4.25284500	1.82468100	-1.91174300
C	-4.95166300	0.63723500	-2.14475300
C	-4.63927900	-0.53038600	-1.44589700
C	-3.60680600	-0.48589000	-0.50719700
C	-2.89329300	0.70173400	-0.26536000
C	-3.22596000	1.86160500	-0.96392400
C	-0.37418500	0.77969900	0.69123400
C	-1.98991100	-1.07739000	1.03693900
C	-1.91630600	0.48345300	0.87577000
C	-2.22886800	1.24926700	2.16699300
C	-0.90920100	1.23683600	2.92539400
C	0.20388900	-0.55217900	0.15793100
C	-0.68831900	-1.60107500	0.45526700
C	-0.44773700	-3.03773900	0.19661100
C	-4.10387700	-2.43390700	0.95255300
H	-4.79714300	-2.85003300	0.21895800
H	-3.57710200	-3.27227100	1.41507700

H	-4.68948500	-1.91384800	1.72705000
H	-4.50850200	2.72306500	-2.46397500
H	-5.74955900	0.61730300	-2.88107600
H	-5.18372100	-1.44926700	-1.63653900
H	-2.70433700	2.79349000	-0.77533900
H	-2.02487900	-1.39371900	2.08938500
H	-2.50843800	2.28707200	1.95402800
H	-3.02901900	0.81470700	2.76997400
H	-0.41798200	-0.76742700	-0.85668400
H	-1.37828700	-3.58185700	0.02702300
H	0.05895200	-3.43814300	1.08676200
H	0.25089300	-3.17228800	-0.63352400
N	-3.14473500	-1.56026000	0.28311000
O	0.09828000	0.91820600	2.05590700
O	-0.71415100	1.45215700	4.08980700
Pt	2.03090100	-0.84686700	-0.45964700
Cl	3.05381100	-1.30448400	1.57930100
Cl	1.23248300	-0.57671700	-2.68347800
C	-0.02258900	2.03878800	-0.10679300
C	1.40934900	2.56630100	0.06774400
H	-0.71641200	2.83090400	0.20366900
H	-0.22197300	1.83767300	-1.16553800
C	1.64865500	3.84866500	-0.73962100
H	1.60186200	2.75176100	1.13011200
H	2.12527100	1.79730800	-0.24599200
C	3.06483700	4.40413100	-0.55909000
H	1.46661100	3.64793600	-1.80379200
H	0.91581200	4.61234700	-0.44139900
H	3.21067600	5.31999500	-1.14095200
H	3.26685000	4.63923500	0.49186200
H	3.81740400	3.67806400	-0.88544200

7Pt

C	-5.34986600	0.84117700	0.06064100
C	-5.74205000	-0.42486300	-0.38134600
C	-4.82458700	-1.47273300	-0.48610600
C	-3.48960800	-1.22602000	-0.14796300
C	-3.08521600	0.04365200	0.30230100
C	-4.01584600	1.07274500	0.41553400
C	-0.60687900	0.95373000	0.02476600
C	-1.19445000	-1.45160100	0.23977500
C	-1.62822200	-0.01129600	0.72308000
C	-1.40378600	0.25696400	2.21947900
C	0.03430300	0.71021200	2.34414000

C	0.00303800	0.15650500	-1.12289500
C	-0.25202300	-1.20772700	-0.95488400
C	-0.12011300	-2.24937700	-2.02628900
C	-2.61006700	-3.54086000	0.07473700
H	-3.36477700	-3.95638600	-0.59811800
H	-1.67608600	-4.07260700	-0.11742300
H	-2.92180100	-3.74216600	1.11199600
H	-6.07834700	1.64128700	0.14108600
H	-6.78030500	-0.60386700	-0.64564800
H	-5.14518700	-2.45242800	-0.82398300
H	-3.72324400	2.04937100	0.78956700
H	-0.69955900	-2.03732600	1.02387500
H	-2.05285100	1.06160000	2.58359800
H	-1.57950700	-0.60901200	2.86172800
H	0.27420800	0.61733000	-2.06653300
H	-1.12013700	-2.45798400	-2.42202100
H	0.29693000	-3.18066600	-1.63432400
H	0.52771400	-1.91088100	-2.83393100
N	-2.42526900	-2.12374200	-0.19264900
O	0.50548700	1.01059300	1.04160300
O	0.72576500	0.84769400	3.30265400
Pt	1.78033700	-0.46042700	-0.05420000
Cl	3.66305800	-0.23782200	1.30066800
Cl	3.00144000	-1.79065900	-1.49512200
C	-1.04371400	2.37848400	-0.27892500
C	0.07498000	3.30094000	-0.78860600
H	-1.47981100	2.81394400	0.62982600
H	-1.85494100	2.32173200	-1.01467700
C	-0.41756400	4.73345300	-1.03490000
H	0.89539800	3.31225500	-0.06241300
H	0.49571200	2.90152000	-1.72022400
C	0.68879700	5.66120500	-1.54601900
H	-1.24614500	4.71600300	-1.75627600
H	-0.83398200	5.13815900	-0.10228600
H	0.31229400	6.67596800	-1.70848400
H	1.51605900	5.72197300	-0.83060500
H	1.09972200	5.30204700	-2.49609300

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C	-1.89896300	3.00943700	1.30614900
C	-2.73660500	3.07777800	0.19113900
C	-2.85671000	2.00342600	-0.69710800
C	-2.10732200	0.84912600	-0.45016100
C	-1.26485300	0.77196400	0.67364700

C	-1.15821700	1.84493800	1.54966100
C	0.92181100	-0.64550700	0.23470000
C	-1.37783800	-1.36702300	-0.40552100
C	-0.59928400	-0.58306100	0.69877900
C	-0.55141500	-1.27874100	2.06991300
C	0.91523100	-1.37207700	2.46285000
C	0.91556900	-1.77940600	-0.75976400
C	-0.30886600	-2.15415400	-1.14554800
C	-0.63832600	-3.21418900	-2.15327800
C	-3.23980000	-0.72620600	-1.96195600
H	-3.52135800	0.06321900	-2.66361600
H	-3.01880900	-1.61886000	-2.55042200
H	-4.10814000	-0.94149200	-1.31583600
H	-1.82611700	3.85200300	1.98642100
H	-3.31701900	3.97824400	0.00994100
H	-3.52279700	2.07242500	-1.55071700
H	-0.51427200	1.78165300	2.42362500
H	-2.13612400	-2.04035500	0.03310000
H	-1.10869800	-0.74936500	2.84622000
H	-0.94845900	-2.29929700	2.03031300
H	1.83978200	-2.20655000	-1.13645800
H	-1.08401400	-2.78019800	-3.05674000
H	-1.36525200	-3.93159500	-1.75207900
H	0.25522000	-3.76582500	-2.45782100
N	-2.06251800	-0.32805800	-1.20907100
O	1.69743100	-1.00673200	1.41526300
O	1.37093200	-1.71661100	3.52322900
C	1.52116200	0.65613700	-0.31008500
C	2.98590400	0.54749300	-0.75714600
H	1.43446400	1.42177100	0.46951900
H	0.89691700	0.99002000	-1.14706700
C	3.56429800	1.89705700	-1.20335400
H	3.58645500	0.14497600	0.06733000
H	3.07272200	-0.16812800	-1.58583400
C	5.02118000	1.80202600	-1.66704600
H	2.94690700	2.30719900	-2.01431200
H	3.48991000	2.61344000	-0.37413100
H	5.40826200	2.77958600	-1.97269800
H	5.66718900	1.42335300	-0.86694800
H	5.12220900	1.12282400	-2.52145100

TS11^{Pt}

C	-5.04249400	0.96766700	-0.73356300
C	-5.24363300	-0.32154400	-1.23811100

C	-4.32107300	-1.34405500	-1.00136100
C	-3.18893700	-1.03187700	-0.24694300
C	-2.96523500	0.26546600	0.25884100
C	-3.90244200	1.26575200	0.02341800
C	-0.44753900	1.04405000	0.54083700
C	-1.13711300	-1.14369700	0.72668000
C	-1.69124600	0.25057800	1.07310500
C	-1.75644900	0.59706300	2.55918400
C	-0.33259300	1.05117600	2.87999200
C	0.05761200	-0.15712900	-0.30662700
C	-0.21185800	-0.17815900	-1.67435600
C	-0.19451900	-1.36640000	-2.56882000
C	-2.14122800	-3.31630000	-0.09425700
H	-2.21743000	-3.53258100	-1.16542000
H	-1.20080100	-3.72638100	0.27196600
H	-2.98295100	-3.79265900	0.42043700
H	-5.77729700	1.74263500	-0.92643100
H	-6.13415400	-0.53588900	-1.82119100
H	-4.48783700	-2.34535500	-1.38366300
H	-3.76000200	2.26567100	0.42151800
H	-0.49370000	-1.68503600	1.40993000
H	-2.44826300	1.42352700	2.75606300
H	-2.04328000	-0.23404600	3.20767700
H	-0.54881000	0.74648900	-2.14813400
H	0.51473500	-1.20132800	-3.39025100
H	-1.18143600	-1.47387000	-3.04154200
H	0.09040000	-2.28082000	-2.04763000
N	-2.15428000	-1.88207600	0.15109000
O	0.36452000	1.23120900	1.71546500
O	0.15320700	1.23893700	3.96076600
Pt	1.94950000	-0.89231300	-0.13974200
Cl	3.12939000	1.07591700	-0.54646300
Cl	1.40195200	-3.16230300	0.26745900
C	-0.73159700	2.41128800	-0.08677200
C	0.48030400	3.25795600	-0.49502700
H	-1.31104000	2.96939100	0.66349400
H	-1.40748100	2.28218300	-0.93981000
C	0.07069900	4.67318500	-0.92416400
H	1.18346500	3.30789300	0.34203100
H	1.02535300	2.76813000	-1.30795800
C	1.26633700	5.53279900	-1.34694900
H	-0.64940700	4.61379300	-1.75312700
H	-0.45996700	5.16611100	-0.09732900
H	0.95007400	6.53777800	-1.64510000

H	1.98545400	5.63677100	-0.52741000
H	1.79674700	5.08302400	-2.19331500

IM6^{Pt}

C	-5.37222600	0.36179000	-0.29081200
C	-5.37746700	-0.76715000	-1.11372600
C	-4.25451200	-1.59355700	-1.22383600
C	-3.11334500	-1.26076800	-0.48874000
C	-3.10128700	-0.12832300	0.34982300
C	-4.22792200	0.67913900	0.45229600
C	-0.65049800	0.92865600	0.55126900
C	-0.99642800	-1.28422800	0.47489100
C	-1.78115200	-0.06075500	1.06749900
C	-1.78497700	0.13168200	2.57957300
C	-0.49789700	0.88618000	2.89091400
C	0.00475000	-0.28467200	-0.17192700
C	0.55928100	-0.28880700	-1.50549300
C	0.41115800	-1.37389500	-2.53531500
C	-1.84357500	-3.39079600	-0.65389600
H	-2.08028800	-3.64525800	-1.69256900
H	-0.83174800	-3.74117900	-0.44435700
H	-2.54749600	-3.92546100	0.00089000
H	-6.25569500	0.98788800	-0.21965900
H	-6.27167800	-1.01473400	-1.67863600
H	-4.27528400	-2.47169300	-1.86068700
H	-4.23047000	1.54380200	1.11110400
H	-0.54313600	-1.97119900	1.19054700
H	-2.63281300	0.74131100	2.91202500
H	-1.81658800	-0.80187700	3.14719900
H	0.75194100	0.69834600	-1.92438400
H	0.35330400	-2.36924900	-2.10094200
H	1.25060800	-1.34001800	-3.23510700
H	-0.50651600	-1.17921400	-3.10700700
N	-1.89805900	-1.94977400	-0.45090800
O	0.08059100	1.31560300	1.72139600
O	-0.01296400	1.11920100	3.96295200
Pt	2.09611800	-0.62022700	-0.08370100
Cl	3.03529700	1.48685900	-0.38767500
Cl	1.86592100	-2.92885500	0.34365500
C	-1.10101700	2.15812500	-0.23236500
C	-0.05645800	3.24379900	-0.52503000
H	-1.91255200	2.60970700	0.35533800
H	-1.57341900	1.81639300	-1.16188800
C	-0.68956300	4.47951700	-1.17955300

H	0.43682500	3.52909000	0.41028400
H	0.73766300	2.85642100	-1.17098300
C	0.33177400	5.57904500	-1.48700900
H	-1.19886000	4.18270800	-2.10725400
H	-1.47226700	4.87953200	-0.52006100
H	-0.14591800	6.44914000	-1.94896000
H	0.83382100	5.91809400	-0.57425400
H	1.10620400	5.21915300	-2.17340600

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C	-3.32770900	2.13541400	1.14685500
C	-3.82224000	2.06139100	-0.15590500
C	-3.30260500	1.15259400	-1.08618600
C	-2.25989500	0.31348600	-0.68309300
C	-1.76375800	0.37507500	0.63662400
C	-2.28936000	1.28057200	1.54619700
C	0.83069600	-0.27791500	0.43943000
C	-0.73844500	-1.46781800	-0.55705300
C	-0.67955400	-0.65525300	0.78345100
C	-0.55732300	-1.42852300	2.09375900
C	0.92402300	-1.41725800	2.47070100
C	0.77063900	-1.30768000	-0.69202700
C	1.72211600	-1.97717400	-1.34278100
C	1.50047500	-3.09452000	-2.32100200
C	-2.10744000	-1.19959400	-2.65432800
H	-2.47346400	-0.40643600	-3.31191300
H	-1.31606200	-1.72833500	-3.19236200
H	-2.93538800	-1.90495200	-2.46898200
H	-3.74695700	2.84739500	1.85054100
H	-4.63402500	2.71682200	-0.45943600
H	-3.71033000	1.10538600	-2.09060700
H	-1.90658600	1.32636300	2.56298400
H	-1.12349800	-2.49868200	-0.51219600
H	-1.12238600	-0.96536300	2.90860500
H	-0.89933200	-2.46596300	2.02563200
H	2.76003300	-1.71411400	-1.14021800
H	0.44243700	-3.35279700	-2.42055800
H	2.04482600	-3.99603800	-2.01419000
H	1.87791500	-2.82520100	-3.31555800
N	-1.56490100	-0.62905300	-1.44121100
O	1.64170500	-0.70621700	1.55489500
O	1.43487900	-1.92737000	3.43320100
C	1.16947500	1.16762600	0.10621000
C	2.62726900	1.39053100	-0.31805000

H	0.93998800	1.77907500	0.98874400
H	0.49319900	1.49887300	-0.68992000
C	2.94275200	2.86529200	-0.60023600
H	3.29413600	1.01603000	0.46800700
H	2.83829600	0.79755600	-1.21797300
C	4.39547200	3.09693100	-1.02746000
H	2.26621900	3.23899900	-1.38102600
H	2.72649300	3.45944300	0.29796800
H	4.59197600	4.15699300	-1.21851600
H	5.09410000	2.76336300	-0.25184400
H	4.63251800	2.54459600	-1.94411100

Cartesian Coordinates for the Stationary Points Given in Fig. 3S.

IM1 ^{Au}			
C	3.52795000	1.57272300	1.95030100
C	4.84191700	1.22650000	2.32876200
C	5.68793100	0.54684600	1.45755400
C	5.18123900	0.21507900	0.19533500
C	3.85692400	0.55014100	-0.20194300
C	3.02747800	1.24379600	0.69558700
C	-0.64440700	-2.65232500	-0.02919800
C	4.87505100	-0.52284400	-1.90031300
C	3.68677400	0.06538900	-1.54883700
C	2.44181000	0.14986000	-2.37815500
C	1.54675000	-1.07417600	-2.26158800
C	-0.92586800	-2.18512500	-1.13786100
C	-0.69735800	-1.82176900	-2.56846600
C	-1.93021100	-1.33374900	-3.31696400
C	7.14891900	-0.92494900	-0.88155400
H	7.33133400	-1.62190700	-0.05564100
H	7.32762300	-1.45151000	-1.82096400
H	7.86642000	-0.09916200	-0.80336600
H	2.89385700	2.11884400	2.64221800
H	5.20464500	1.50299500	3.31491000
H	6.70212100	0.28878700	1.74851700
H	2.01926700	1.52545100	0.42416300
H	5.15405700	-1.01165100	-2.82428600
H	1.83935700	1.02676800	-2.12454000
H	2.68509100	0.24718900	-3.44528100
H	-0.27248800	-2.72089000	-3.03030900
H	-1.67543900	-1.17044100	-4.36685500
H	-2.27047500	-0.38822000	-2.88777400
H	-2.73042300	-2.07738200	-3.25909700

N	5.78468700	-0.44405500	-0.86014100
O	1.87119000	-2.18954100	-1.92164800
O	0.27075300	-0.76289000	-2.64073200
Au	-2.49707600	-1.15236100	0.12011100
P	-4.31344500	0.05292700	0.96301200
H	-4.21993900	0.50326700	2.28657400
H	-4.60333200	1.22075100	0.24609600
H	-5.56515200	-0.59598400	0.97789900
Sb	-0.96016200	2.21206800	-0.04551500
F	0.18892400	2.90442900	1.23747100
F	-0.18722700	0.50560600	0.21440400
F	-2.20398400	1.77245600	1.31973400
F	-2.16888600	1.39296700	-1.25863300
F	0.25813900	2.51758500	-1.41832100
F	-1.80604200	3.83639400	-0.31056400
C	-0.06852500	-3.20412800	1.19929500
C	0.43506100	-2.12183900	2.18168700
H	0.77635400	-3.82267700	0.86414500
H	-0.78164900	-3.87837000	1.68809400
C	1.24583600	-2.72559000	3.33323200
H	1.03792900	-1.39274300	1.63229200
H	-0.42692500	-1.56983700	2.57713100
C	1.74944500	-1.66096800	4.31338200
H	0.63426600	-3.46548300	3.86894400
H	2.10163900	-3.27593600	2.91952100
H	2.33642800	-2.11323000	5.11918800
H	2.38256600	-0.92655900	3.80485600
H	0.91488100	-1.11922100	4.77251000

TS1^{Au}

C	3.71120600	2.10254500	1.35335300
C	5.02509100	1.78933700	1.76016400
C	5.77393900	0.81907800	1.10075000
C	5.17024100	0.16741600	0.01826900
C	3.84668600	0.46935300	-0.40409600
C	3.11314400	1.45457500	0.28010500
C	-0.19446400	-2.45511200	0.13733200
C	4.69675200	-1.12546000	-1.75270800
C	3.56767800	-0.37410300	-1.53938900
C	2.29898700	-0.40481400	-2.33197300
C	1.27222200	-1.42385200	-1.88461300
C	-1.15661400	-2.19291400	-0.66236200
C	-0.98442000	-2.15964300	-2.16876200
C	-2.17602100	-1.67582700	-2.97378300

C	6.99836800	-1.38227400	-0.75064300
H	7.17944100	-1.83848500	0.22914200
H	7.09783100	-2.15570500	-1.51455400
H	7.76598600	-0.61929000	-0.92566100
H	3.14938000	2.86487600	1.88402000
H	5.46394400	2.31828400	2.60151700
H	6.78736800	0.58479600	1.41312400
H	2.10077700	1.70457500	-0.00729000
H	4.89551100	-1.87313900	-2.50927100
H	1.77999000	0.56144100	-2.30045200
H	2.48802900	-0.60487500	-3.39482300
H	-0.68343100	-3.16768400	-2.47805200
H	-1.95500200	-1.73816000	-4.04282700
H	-2.40414100	-0.63988600	-2.71516900
H	-3.04219900	-2.30714000	-2.75610700
N	5.66843100	-0.81511100	-0.81952300
O	1.45753000	-2.31224300	-1.04114800
O	0.11794300	-1.27162100	-2.51664900
Au	-2.69283000	-1.18600800	0.35171500
P	-4.31887300	0.18834600	1.33320200
H	-3.99483600	0.79360500	2.55663700
H	-4.69841200	1.29082500	0.55387700
H	-5.57658800	-0.37251900	1.64012300
Sb	-0.93078300	2.17820000	-0.34654000
F	0.28163200	3.06676700	0.74795900
F	-0.10489600	0.54452500	0.11317400
F	-2.09525800	1.93830000	1.12461900
F	-2.18648100	1.20698200	-1.37221300
F	0.23130700	2.25266000	-1.80774100
F	-1.77428600	3.75731200	-0.81678000
C	0.47460000	-2.73580400	1.40543100
C	1.23187100	-1.55760900	2.05124300
H	1.14999200	-3.58612900	1.24621700
H	-0.31585000	-3.10088000	2.07720300
C	1.80722200	-1.94005000	3.41990800
H	2.03492000	-1.24133000	1.37980600
H	0.55398300	-0.70358900	2.14040500
C	2.53891200	-0.77602800	4.09597700
H	0.99716100	-2.29337900	4.07432200
H	2.49503400	-2.78940200	3.30285700
H	2.95026600	-1.07732400	5.06511100
H	3.36325200	-0.41046300	3.47539100
H	1.86087600	0.06708700	4.26713800

IM2 ^{Au}			
C	3.61070000	2.30595900	0.08336400
C	4.86854200	2.40350700	0.71247500
C	5.74476100	1.32372400	0.75074700
C	5.33048500	0.13940200	0.13027600
C	4.07260200	0.02514700	-0.52160400
C	3.20254200	1.12999300	-0.53395500
C	0.16712400	-2.05348200	0.68274600
C	5.17590800	-1.94153000	-0.68926200
C	4.00095500	-1.32009800	-1.03811200
C	2.92286300	-1.91276000	-1.88702200
C	1.59024800	-2.16740600	-1.23182700
C	-0.92544900	-2.20165700	-0.06032300
C	-0.79003400	-2.67940200	-1.47365400
C	-1.72876300	-2.07871900	-2.50476000
C	7.30130100	-1.37389700	0.54241900
H	7.32412200	-1.25498000	1.63139200
H	7.55981500	-2.40644300	0.30083700
H	8.05760100	-0.71358800	0.10353600
H	2.93007200	3.14999800	0.09273500
H	5.15653900	3.33824800	1.18482000
H	6.70919200	1.39985000	1.24390000
H	2.21341100	1.07260300	-0.97493300
H	5.51197900	-2.94794500	-0.90233800
H	2.68985000	-1.28507700	-2.75740800
H	3.24093800	-2.87872900	-2.30285000
H	-0.81212100	-3.77475500	-1.52207100
H	-1.43968700	-2.39947200	-3.50962500
H	-1.72288000	-0.98955300	-2.44229000
H	-2.74279200	-2.43631500	-2.30673500
N	5.98497900	-1.07713200	0.01564000
O	1.49529400	-2.21435100	0.04407900
O	0.60521000	-2.36352300	-2.02012100
Au	-2.67909300	-1.30869100	0.54842500
P	-4.45514300	0.15517100	1.07414900
H	-4.29264900	0.94288400	2.22780900
H	-4.63686700	1.14763800	0.09689500
H	-5.78429900	-0.28023800	1.26366800
Sb	-1.04668800	2.03209700	-0.85436800
F	0.43470000	2.80224400	-0.01913600
F	-0.04214800	0.43465300	-1.03823400
F	-1.64838200	1.47930700	0.85579000
F	-2.51595900	1.09748600	-1.57741900
F	-0.46412600	2.52839600	-2.54183000

F	-2.07102200	3.56723300	-0.67559700
C	0.39035300	-1.56297300	2.07588700
C	0.99440500	-0.14383100	2.14427800
H	1.03653100	-2.27286000	2.61168700
H	-0.58489600	-1.58299600	2.57272800
C	0.95954700	0.44963200	3.55606400
H	2.02795200	-0.17328800	1.78232200
H	0.44606700	0.51127100	1.46557200
C	1.53635000	1.86925200	3.59368600
H	-0.08034800	0.46896900	3.91094000
H	1.51014500	-0.19881800	4.25291700
H	1.45626300	2.30865800	4.59388900
H	2.59364100	1.87283100	3.30678800
H	1.00592900	2.51807500	2.88890000

TS2^{Au}

C	3.93509700	2.14042800	1.25050400
C	5.21300200	1.77803400	1.72490600
C	5.89341800	0.68394900	1.20099000
C	5.25986500	-0.03890100	0.18305900
C	3.97154300	0.31009400	-0.30732500
C	3.30382200	1.41901600	0.24362500
C	0.14406600	-2.20741100	0.17749100
C	4.73023000	-1.48166300	-1.44963200
C	3.65544900	-0.63059800	-1.35328900
C	2.43204600	-0.64012300	-2.21607700
C	1.29380800	-1.56325000	-1.83527700
C	-1.07828100	-2.29172000	-0.41221900
C	-1.24775300	-2.66058400	-1.75856800
C	-2.31108400	-2.12010100	-2.65596300
C	6.97887700	-1.79850300	-0.35062900
H	7.08247800	-2.19407900	0.66612700
H	7.05508000	-2.62935500	-1.05441700
H	7.80626700	-1.10522300	-0.54026300
H	3.42966600	3.00097600	1.67806300
H	5.67601700	2.36482300	2.51311000
H	6.87783700	0.40792500	1.56706900
H	2.31064400	1.70336300	-0.08600900
H	4.89276000	-2.31502000	-2.12067600
H	1.95284900	0.34794700	-2.22505000
H	2.66709600	-0.86947900	-3.26026700
H	-0.82868600	-3.62075200	-2.05696800
H	-2.03703300	-2.27467100	-3.70219200
H	-2.48338600	-1.05882100	-2.46140700

H	-3.24260700	-2.67070500	-2.47055300
N	5.69978500	-1.14291700	-0.52630400
O	1.31615100	-2.03937500	-0.56685100
O	0.42080100	-1.85343000	-2.64517500
Au	-2.59439600	-1.22572400	0.54711900
P	-4.14892300	0.28992700	1.45870900
H	-3.74483400	1.00017900	2.60107000
H	-4.49296200	1.33747700	0.58936400
H	-5.42825900	-0.14274700	1.86883500
Sb	-0.95094100	2.10473700	-0.78379900
F	0.41832900	3.07554200	0.02047100
F	0.11660500	0.54912900	-0.63497300
F	-1.65284100	1.71423900	0.93384400
F	-2.33049300	1.03531600	-1.50282000
F	-0.22484000	2.34612700	-2.47502400
F	-2.04811800	3.59124300	-0.90418900
C	0.45058900	-2.12277300	1.63987100
C	0.84382200	-0.72707400	2.17036700
H	1.27741800	-2.82038600	1.83611100
H	-0.42734100	-2.49692900	2.17690200
C	1.10380400	-0.75005300	3.68143400
H	1.73941100	-0.38284400	1.64491400
H	0.05251500	-0.00820200	1.93361500
C	1.49042100	0.62620300	4.23277900
H	0.20724900	-1.11655000	4.20199500
H	1.90133800	-1.47256000	3.90503200
H	1.67458900	0.58543300	5.31168500
H	2.39736400	1.00193700	3.74803200
H	0.69534500	1.35862900	4.05487100

2^{Au}

C	4.04030500	1.56234100	1.36563600
C	5.35587500	1.11901800	1.61534500
C	5.92472300	0.08943100	0.87295900
C	5.13598100	-0.49314300	-0.12687000
C	3.80724500	-0.06257300	-0.38792300
C	3.25876700	0.98486900	0.37225800
C	0.15398100	-2.04881100	0.85145700
C	4.32814500	-1.73243700	-1.81346800
C	3.31203900	-0.87250300	-1.47140100
C	1.94803500	-0.80426500	-2.09859900
C	0.91442200	-1.69545800	-1.45035400
C	-1.04892700	-2.72488100	0.55754000
C	-1.37551500	-4.00513300	0.77149100

C	-2.72320800	-4.63502500	0.58835000
C	6.70574400	-2.19930300	-1.10952700
H	6.96314800	-2.68770500	-0.16291100
H	6.64345300	-2.96320600	-1.88664900
H	7.50976600	-1.50167500	-1.37085900
H	3.62901000	2.37743100	1.95331300
H	5.93982000	1.59505700	2.39792900
H	6.94063600	-0.24394900	1.06315900
H	2.25688500	1.34981100	0.18510300
H	4.35942200	-2.49082800	-2.58479100
H	1.54729800	0.21520500	-2.03632300
H	1.96582700	-1.08795400	-3.15394500
H	-0.58123300	-4.69460600	1.06818400
H	-2.69664400	-5.37427100	-0.22236400
H	-3.48799300	-3.89181600	0.34890300
H	-3.02496400	-5.17245800	1.49600400
N	5.43244100	-1.51664600	-1.01143700
O	1.03838800	-1.60214600	-0.01944500
O	0.09694600	-2.39706900	-1.96419000
Au	-2.41517900	-1.22469400	-0.07979500
P	-4.02353700	0.34826700	-0.79032800
H	-4.63530800	1.13012900	0.20140100
H	-3.55266700	1.30834600	-1.69929200
H	-5.15549900	-0.17377700	-1.44886800
Sb	-0.60548200	2.51449100	-0.53146500
F	0.41807000	2.56877800	1.03782400
F	-0.27199300	0.64458400	-0.60888200
F	-2.12150200	2.08678700	0.50743000
F	-1.67657800	2.32355600	-2.05656200
F	0.91885300	2.71735300	-1.57856700
F	-0.95246900	4.32681600	-0.43849900
C	0.51584000	-1.64022900	2.24595300
C	-0.15150100	-0.29701900	2.66303700
H	1.60315700	-1.52043500	2.28289600
H	0.20706000	-2.43541900	2.93244900
C	0.45653600	0.26835100	3.95070700
H	-0.03728800	0.43117400	1.85827400
H	-1.22714200	-0.46922700	2.79172100
C	-0.20147600	1.59245000	4.35483100
H	0.36435100	-0.46505600	4.76400000
H	1.53100500	0.42821400	3.79334200
H	0.26629900	2.00715200	5.25370500
H	-0.10955000	2.32575300	3.54834500
H	-1.26834800	1.45722700	4.56657100

TS3 ^{Au}			
C	2.19243900	2.31724400	0.61804700
C	3.17972100	2.58562300	1.58861000
C	4.45275100	2.02852800	1.50632300
C	4.71657400	1.18398400	0.42102300
C	3.73953700	0.90483400	-0.57208200
C	2.46355900	1.48717100	-0.46320200
C	0.07817300	-2.37183300	-0.04710100
C	5.63140500	-0.23169100	-1.05946800
C	4.35385900	-0.00354300	-1.50783600
C	3.71857000	-0.59568200	-2.73315400
C	2.45281500	-1.34947700	-2.40103700
C	0.40977500	-2.15692900	-1.26138000
C	0.20913800	-1.78769600	-2.68014700
C	-1.04024100	-0.97448800	-2.98668000
C	7.10419200	0.50576000	0.85054700
H	6.94264800	0.16672100	1.87989200
H	7.82522800	-0.16186300	0.37542100
H	7.53009300	1.51509800	0.87898100
H	1.20418000	2.75297100	0.71362300
H	2.94049600	3.24307100	2.41928000
H	5.20821400	2.24259600	2.25657200
H	1.68456900	1.30649100	-1.19689700
H	6.40802800	-0.85606900	-1.48099500
H	3.45978100	0.16067600	-3.48172500
H	4.40356900	-1.30968000	-3.20563700
H	0.25487700	-2.69026500	-3.30278600
H	-1.04296600	-0.72932400	-4.05219600
H	-1.06808400	-0.05573200	-2.40128600
H	-1.92825000	-1.57035200	-2.76408800
N	5.86685100	0.48183300	0.09794300
O	2.35346600	-2.23389900	-1.54075000
O	1.37470200	-0.98311600	-3.07687400
C	0.91768300	-2.78435000	1.13784700
C	1.20573000	-1.59687300	2.07855900
H	1.86009200	-3.20367600	0.77057900
H	0.39407600	-3.57254200	1.68987300
C	2.06742400	-2.00655600	3.27927400
H	1.70822500	-0.80558700	1.51162300
H	0.25995900	-1.16326500	2.42579800
C	2.37131000	-0.82985200	4.21254100
H	1.55896500	-2.80246700	3.84134600
H	3.00963900	-2.44177800	2.91862300
H	2.99614500	-1.14178500	5.05622100

H	2.89589700	-0.03043100	3.67841000
H	1.44886800	-0.40178400	4.62039800
Au	-1.92262600	-1.79516600	0.30192700
P	-4.07764200	-1.02761700	0.86118700
H	-4.10274200	0.26848600	1.40363800
H	-4.99809200	-0.92573200	-0.19449600
H	-4.83479500	-1.76951500	1.79105900
Sb	-1.95245100	2.19670800	-0.15818000
F	-2.79880000	3.41749600	-1.26265400
F	-3.33889900	2.26483200	1.10184300
F	-0.98935700	3.53416800	0.70190100
F	-0.58519700	1.92617300	-1.41622000
F	-2.90996300	0.78755300	-1.00340100
F	-1.11459800	0.91358800	0.93599600

IM3^{Au}

C	3.93784900	0.45565100	2.02755200
C	5.00795700	-0.33214000	2.50052400
C	5.61747900	-1.28503100	1.69147900
C	5.12520600	-1.42882400	0.38858400
C	4.04967800	-0.64232500	-0.10419500
C	3.44908300	0.31278900	0.73498700
C	-1.13685800	-1.63525900	0.03586100
C	4.74480500	-2.04811900	-1.73337700
C	3.82727700	-1.06098700	-1.46558600
C	2.82914400	-0.50447900	-2.43256700
C	1.40631300	-0.87021200	-2.17541100
C	-0.47436100	-1.37268500	-1.08253900
C	-0.83760500	-0.99795100	-2.50716400
C	-1.72892300	0.20913500	-2.73302500
C	6.61996500	-3.23363100	-0.53572600
H	6.43815500	-3.96243600	0.26197400
H	6.70536800	-3.77045900	-1.48225100
H	7.57099500	-2.72745300	-0.33526400
H	3.47939400	1.19131600	2.68062600
H	5.36431900	-0.19243100	3.51708100
H	6.44106700	-1.88985400	2.05888700
H	2.61864900	0.92145800	0.39934400
H	4.91111400	-2.60668200	-2.64519300
H	2.80637500	0.59568900	-2.39967200
H	3.05229200	-0.77853300	-3.46899200
H	-1.18681400	-1.86265500	-3.08204300
H	-1.83084800	0.39346500	-3.80637600
H	-1.33520600	1.09368900	-2.23757700

H	-2.71997800	-0.00916600	-2.32488500
N	5.53212700	-2.28151600	-0.62555500
O	0.99088500	-1.35154400	-1.06830300
O	0.50934100	-0.69507500	-3.08787800
C	-0.40882500	-1.90810300	1.33674900
C	-0.55037200	-0.73063700	2.32404100
H	0.65597400	-2.08721700	1.15028000
H	-0.81168200	-2.82176400	1.79212400
C	0.32567100	-0.88135600	3.57285900
H	-0.29067200	0.19722200	1.81012900
H	-1.60473000	-0.63184700	2.62120900
C	0.20909800	0.33119200	4.50276800
H	0.05870000	-1.80037500	4.11480300
H	1.37218800	-0.99656200	3.26167500
H	0.86309400	0.23254100	5.37601600
H	0.48382600	1.24687800	3.96930900
H	-0.81719800	0.45510500	4.86854800
Au	-3.17562800	-1.43735400	0.11052100
P	-5.52747800	-1.10949900	0.33432800
H	-6.41099700	-1.80211600	-0.51970200
H	-6.11949300	-1.41913500	1.57589100
H	-6.01791300	0.20083100	0.16289000
Sb	0.06379000	2.80412900	-0.17270200
F	0.90400300	2.16408000	1.38018300
F	-1.36976700	1.63465400	0.15274500
F	0.89443500	1.37482700	-1.13522500
F	1.55241700	3.83553000	-0.56802100
F	-0.75962400	3.27838200	-1.78054000
F	-0.77086700	4.16750200	0.76156100

TS4^{Au}

C	1.92961600	2.41758500	0.47902200
C	2.82633300	2.66836300	1.53845100
C	4.10048900	2.10974100	1.56061500
C	4.46001600	1.28429000	0.48804600
C	3.57954600	1.02917100	-0.59894900
C	2.29719500	1.61048900	-0.59101600
C	0.37720200	-2.06114600	-0.23207400
C	5.50640300	-0.10877700	-0.92426200
C	4.27874500	0.13472000	-1.49006200
C	3.79684100	-0.40416000	-2.80989900
C	2.38369800	-0.92561200	-2.74596400
C	0.76035700	-1.97430500	-1.53960200
C	0.00580500	-1.85206100	-2.73334000

C	-1.35832700	-1.29950200	-2.88707900
C	6.79126500	0.58209500	1.13328100
H	6.53186300	0.21458600	2.13246800
H	7.55593100	-0.07247100	0.71120900
H	7.21079300	1.58967800	1.23083500
H	0.93329400	2.84441000	0.50246700
H	2.51289900	3.31092000	2.35599500
H	4.78494200	2.30577400	2.38056300
H	1.58300500	1.43923900	-1.38968700
H	6.31931900	-0.72596200	-1.28340800
H	3.80572000	0.35095300	-3.60278400
H	4.43848000	-1.23416100	-3.13012500
H	0.38274200	-2.42014600	-3.58068700
H	-1.51628500	-1.01133000	-3.92994100
H	-1.55611900	-0.45452400	-2.22877800
H	-2.08312900	-2.09499600	-2.66059100
N	5.63289500	0.58203300	0.26350800
O	2.16381100	-1.91207600	-1.86133600
O	1.45677000	-0.48417500	-3.42710500
C	1.42994400	-2.28156700	0.82267700
C	1.28203100	-1.35748700	2.05133100
H	2.43688000	-2.18022900	0.40612900
H	1.32606800	-3.32521200	1.15841000
C	2.43190700	-1.54158300	3.04917600
H	1.23806800	-0.31509800	1.71899200
H	0.32495000	-1.56173700	2.54844200
C	2.31014200	-0.61730200	4.26485300
H	2.46656100	-2.58920900	3.38056700
H	3.38509000	-1.34790300	2.53935600
H	3.13766200	-0.76945400	4.96620200
H	2.31827300	0.43319200	3.95616600
H	1.37605200	-0.79716500	4.80902900
Au	-1.56415200	-1.85459700	0.39720600
P	-3.75967100	-1.37511000	1.20086500
H	-3.92012300	-0.05784200	1.66443100
H	-4.82203300	-1.48018800	0.28652800
H	-4.28947300	-2.12683300	2.27136900
Sb	-2.18559900	2.02865200	-0.18462200
F	-3.12798500	3.06238700	-1.39774300
F	-3.54586200	2.13048900	1.09552700
F	-1.29069900	3.51747400	0.47946300
F	-0.83482100	1.68206300	-1.43986300
F	-3.07115900	0.47899000	-0.85368000
F	-1.23869500	0.94774400	1.03430700

IM4 ^{Au}			
C	-4.93360400	-0.17729800	2.89664800
C	-6.03857300	0.66248400	2.64425100
C	-6.66873000	0.67225200	1.40426300
C	-6.16684300	-0.18609100	0.41795300
C	-5.05539800	-1.04359500	0.65241300
C	-4.43525200	-1.02478800	1.91413700
C	-0.53635400	0.40375800	-0.72931800
C	-5.79415000	-1.36051000	-1.45396400
C	-4.84050100	-1.78916600	-0.56172600
C	-3.80370800	-2.85150400	-0.81644500
C	-2.47947200	-2.29283200	-1.30675500
C	-0.61031600	-0.99526100	-0.62759000
C	0.50155800	-1.80341400	-0.73649400
C	0.56292600	-3.25912000	-0.52730500
C	-7.72120700	0.26779700	-1.51070500
H	-7.57701000	1.35364200	-1.52721600
H	-7.81088600	-0.08453100	-2.53957400
H	-8.65628800	0.04698000	-0.98383600
H	-4.46765000	-0.16044300	3.87744000
H	-6.40523400	1.31228900	3.43323000
H	-7.52073200	1.31815900	1.21505100
H	-3.57646300	-1.65814400	2.11520600
H	-5.97397900	-1.68052400	-2.47163200
H	-3.61745300	-3.41963000	0.10258900
H	-4.14391100	-3.55030400	-1.58362900
H	1.43911800	-1.32291900	-0.99337900
H	0.76837300	-3.74434600	-1.49267800
H	-0.34367100	-3.68297900	-0.09577300
H	1.44076300	-3.45997000	0.09971400
N	-6.59700300	-0.39446400	-0.87948800
O	-1.84615100	-1.58867600	-0.30741500
O	-2.01546500	-2.42731400	-2.41175600
C	-1.78049100	1.20963800	-0.57153700
C	-1.83107900	1.87153500	0.83869300
H	-2.68711100	0.61294200	-0.70795900
H	-1.76622700	2.01459400	-1.31601000
C	-3.02496700	2.82550600	0.97430100
H	-1.89652300	1.08388400	1.59722100
H	-0.89562300	2.41432800	1.02040600
C	-3.09457200	3.47734000	2.35861800
H	-2.95274900	3.60337100	0.20197000
H	-3.95399400	2.27536900	0.78290700
H	-3.94376600	4.16499400	2.42757900

H	-3.21461700	2.72190400	3.14218000
H	-2.18473100	4.04722200	2.57847500
Au	1.24481200	1.39223700	-0.93359800
P	3.27575400	2.61777600	-1.22084300
H	3.24895600	3.64588800	-2.18787900
H	3.78268700	3.32210600	-0.11864900
H	4.39317000	1.88477400	-1.64395200
Sb	3.87842900	-0.91792400	0.81781700
F	4.07264900	0.95676000	0.88532400
F	3.40977900	-0.70077500	-1.01435200
F	2.05264200	-0.67718700	1.22978900
F	4.27695200	-1.08653700	2.61444600
F	3.52027600	-2.74154500	0.61747300
F	5.64720700	-1.11173000	0.30949300

TS5^{Au}

C	-3.66040900	-2.32949500	0.81439600
C	-5.02600500	-2.16866900	1.12703900
C	-5.75309900	-1.08074900	0.65503300
C	-5.07172800	-0.15000300	-0.13872700
C	-3.69594600	-0.29602800	-0.46140900
C	-2.98658000	-1.40720800	0.02451000
C	0.16055000	2.06520300	0.93791000
C	-4.48133600	1.58738300	-1.43004900
C	-3.34368100	0.82836800	-1.28998700
C	-1.99598000	1.12944500	-1.88469500
C	-1.09152200	1.89945900	-0.95870400
C	0.26220400	3.39382900	0.51498700
C	0.50081600	4.67672400	0.63134700
C	1.03507500	5.60331100	-0.42585100
C	-6.89077900	1.50222700	-0.68934100
H	-7.20165000	1.68599700	0.34528200
H	-6.95362100	2.44172900	-1.24148700
H	-7.58779100	0.78618300	-1.13979900
H	-3.11743600	-3.18785500	1.19708800
H	-5.52227800	-2.91030200	1.74655400
H	-6.80595800	-0.96293900	0.89382800
H	-1.93928800	-1.55208900	-0.20491000
H	-4.63513300	2.50444000	-1.98353900
H	-1.45496400	0.20047000	-2.10748900
H	-2.07658000	1.70946000	-2.80663800
H	0.28264100	5.08060100	1.62266900
H	0.40633000	6.49579700	-0.50820000
H	1.06718200	5.10526700	-1.39585100

H	2.04791700	5.93614400	-0.16894000
N	-5.52986100	1.01072000	-0.74125600
O	-0.96317300	1.43257000	0.27242600
O	-0.44401500	2.91005900	-1.28958900
Au	2.00916200	1.31044100	-0.00976000
P	3.90903400	0.28143000	-0.93641100
H	4.77435000	-0.33449500	-0.01827600
H	3.60134600	-0.76817100	-1.81812800
H	4.82162000	1.06204500	-1.67536200
Sb	1.01213900	-2.53351300	-0.58813900
F	2.32906200	-1.66898300	0.47128800
F	0.33141800	-0.80876300	-1.02054300
F	2.18016400	-2.33808200	-2.04420600
F	-0.31304100	-3.25649300	-1.65873900
F	-0.11652200	-2.55145500	0.90546900
F	1.72413500	-4.18487800	-0.15839700
C	0.16303600	1.70080400	2.42522800
C	0.42746700	0.21133300	2.69632700
H	-0.82001500	1.98850000	2.82399200
H	0.90946900	2.32771000	2.92522000
C	0.02772900	-0.21935200	4.11201300
H	-0.10950800	-0.40109900	1.96715400
H	1.49205100	0.00059800	2.53300300
C	0.37378800	-1.68802100	4.38301100
H	0.52122100	0.42384300	4.85504600
H	-1.05216600	-0.06502100	4.24168500
H	0.00825500	-2.01027400	5.36351100
H	-0.06424700	-2.33702700	3.61853200
H	1.45786600	-1.84615300	4.36136500

IM5^{Au}

C	4.58665200	1.89831700	0.70336700
C	5.94848500	1.57047900	0.86883000
C	6.46766300	0.37123500	0.39321700
C	5.58106700	-0.49918000	-0.25271800
C	4.20674100	-0.18471100	-0.42417800
C	3.70749000	1.03611700	0.06152700
C	0.28606700	-1.89051800	1.52279000
C	4.61902800	-2.20817600	-1.34282300
C	3.61506800	-1.29622900	-1.12285500
C	2.17895400	-1.42993500	-1.53432100
C	1.25497500	-1.80221800	-0.43046000
C	-0.58467100	-2.38958600	0.61474200
C	-1.99758000	-2.77282200	0.60796500

C	-2.29234300	-4.08111600	-0.14733700
C	7.09262800	-2.40871600	-0.89477000
H	7.50117800	-2.57879900	0.10746500
H	6.96750700	-3.37537400	-1.38594200
H	7.81346300	-1.81632900	-1.46954400
H	4.21428400	2.84518600	1.08184700
H	6.60723800	2.27027100	1.37499700
H	7.51780000	0.12518900	0.51865800
H	2.66742300	1.31098800	-0.06556400
H	4.58487500	-3.16606100	-1.84499700
H	1.78446700	-0.46506200	-1.89784700
H	2.03714200	-2.15421900	-2.34250600
H	-2.30706200	-2.86783300	1.65431000
H	-1.75033300	-4.93336200	0.28624000
H	-2.01832300	-4.00980700	-1.20349400
H	-3.36068600	-4.30550600	-0.10242800
N	5.80884100	-1.74123300	-0.82335600
O	1.45670800	-1.53892900	0.81783700
O	0.10151300	-2.36896100	-0.62493200
Au	-3.06396900	-1.08875800	-0.15335100
P	-4.27923500	0.77898300	-0.98882100
H	-3.93743300	2.03211600	-0.45879700
H	-4.24433100	1.03317100	-2.37011100
H	-5.67614100	0.76807300	-0.78112600
Sb	-0.37049200	2.11585300	-0.72165400
F	-1.75944700	2.29016900	0.52177200
F	-0.18260800	0.31541300	-0.17137400
F	-1.63972300	1.52554400	-1.97691400
F	1.00704500	1.74132100	-1.93591400
F	0.87296100	2.57968300	0.59428600
F	-0.53734400	3.86425700	-1.29943500
C	0.18515500	-1.40537600	2.92254700
C	-0.09642200	0.11603000	2.98083300
H	1.11307700	-1.64118900	3.45850500
H	-0.61756500	-1.96185200	3.41932900
C	-0.13205100	0.66112100	4.41156300
H	0.66155100	0.64976400	2.39869500
H	-1.04674600	0.32322000	2.47644300
C	-0.42450900	2.16515000	4.44358800
H	-0.89215600	0.12271200	4.99538300
H	0.82973900	0.46109800	4.90444000
H	-0.42637400	2.55029300	5.46854800
H	0.32474300	2.72180300	3.87105600
H	-1.40022000	2.38518100	3.99722600

3Au			
C	-4.76089000	3.20681500	-0.98450200
C	-4.38958200	4.16969700	-0.02502200
C	-3.07246500	4.27925700	0.41139900
C	-2.13191800	3.39859300	-0.13253300
C	-2.48614100	2.40978200	-1.09836000
C	-3.82396300	2.32972100	-1.52383900
C	-2.46750100	-0.75410300	0.18305800
C	-0.27390600	2.27387700	-0.66700100
C	-1.27477200	1.69233200	-1.41180600
C	-1.03687400	0.60199700	-2.40534800
C	-1.63881200	-0.77347000	-2.16649200
C	-1.23123000	-1.01491100	0.83429500
C	-1.12283900	-0.61969000	2.14423400
C	0.03074700	-0.88336700	3.04051000
C	0.01883500	4.09676000	1.01927800
H	-0.34547700	3.99135800	2.04679400
H	1.05211200	3.75229600	0.97264200
H	-0.02219600	5.15401600	0.73705400
H	-5.79491600	3.15559900	-1.31336400
H	-5.14243800	4.84174000	0.37604200
H	-2.78676300	5.02693900	1.14512800
H	-4.12477800	1.59743800	-2.26868900
H	0.77151100	2.02706300	-0.62970400
H	-1.40260300	0.87025600	-3.40801900
H	0.03986700	0.42969200	-2.51067300
H	-1.90112500	0.00853100	2.58133300
H	-0.27573500	-0.90499400	4.09072100
H	0.75985600	-0.07026500	2.90939700
H	0.54907700	-1.80845900	2.77276100
N	-0.77321000	3.28928500	0.10570000
O	-2.63820900	-0.83138600	-1.11899200
O	-1.51937900	-1.73570800	-2.85870000
Au	0.39533800	-1.90333000	-0.09561300
P	2.31419000	-2.89429300	-1.09005500
H	3.15779200	-2.01776300	-1.78872500
H	3.22366100	-3.53517200	-0.23251100
H	2.12490600	-3.90949100	-2.05161400
Sb	3.25764600	0.83125600	0.29223200
F	4.71081900	0.53759400	-0.82103300
F	3.27232500	-0.98821100	0.80159900
F	2.13524900	0.34708700	-1.16404800
F	1.70823500	1.05237000	1.34423900
F	3.06139000	2.61544800	-0.22530600

F	4.32334200	1.27996300	1.73644300
C	-3.79915600	-0.56755400	0.85223200
C	-4.63322900	-1.87439600	0.81612800
H	-4.33280900	0.22426900	0.31561100
H	-3.67110600	-0.25632000	1.89004300
C	-6.01366800	-1.69563800	1.45887600
H	-4.74460800	-2.19471800	-0.22597600
H	-4.08023800	-2.66769100	1.33469800
C	-6.84809400	-2.98004800	1.42324200
H	-5.89189600	-1.36421200	2.49876900
H	-6.55177400	-0.89060100	0.94163600
H	-7.82712500	-2.82726700	1.88774200
H	-7.01617100	-3.31540800	0.39397100
H	-6.34780000	-3.79382900	1.95976300

TS8^{Au}

C	-4.90289000	3.00198400	-1.58364100
C	-4.67858900	3.96300200	-0.58725200
C	-3.50690200	3.95124300	0.17440400
C	-2.58743600	2.94590300	-0.10090500
C	-2.79883500	1.95369600	-1.08187000
C	-3.97168200	1.99170200	-1.83922500
C	-2.17618700	-0.76229100	-0.03422800
C	-0.74788100	1.66976700	-0.12128900
C	-1.63732900	1.05227900	-1.05117300
C	-1.10735100	0.31989100	-2.25381500
C	-1.69695800	-1.07792600	-2.37126900
C	-1.01417000	-1.16646700	0.77785200
C	-1.07072000	-0.96599800	2.11715000
C	-0.00935700	-1.30675100	3.11601700
C	-0.66594300	3.55155400	1.47961500
H	-1.17467800	3.42939400	2.43980500
H	0.37832300	3.25005100	1.55579800
H	-0.71638300	4.59927200	1.17343800
H	-5.81633200	3.04605600	-2.16861900
H	-5.42130800	4.73405900	-0.40909300
H	-3.32507200	4.70120300	0.93713900
H	-4.15904900	1.25471000	-2.61482000
H	0.24903600	1.36001800	0.14462100
H	-1.32674600	0.84394800	-3.18881400
H	-0.01879700	0.21895600	-2.18560700
H	-1.95138000	-0.49202600	2.55786100
H	-0.44227100	-1.80039700	3.99460900
H	0.48417300	-0.39012400	3.46394600

H	0.76313100	-1.94904500	2.68772100
N	-1.30787900	2.72237100	0.46026400
O	-2.33751400	-1.46806900	-1.21581600
O	-1.68189700	-1.78345800	-3.33894200
Au	0.68217000	-1.95165100	-0.11753000
P	2.67248800	-2.77291100	-1.12969500
H	3.30568000	-1.93071900	-2.05886400
H	3.75313500	-3.10002700	-0.29331700
H	2.58569300	-3.95838800	-1.89172100
Sb	3.08067700	1.24697000	0.27508000
F	4.34574000	1.76208100	-0.97240400
F	3.75115400	-0.50536300	0.33606300
F	1.94852800	0.69315600	-1.14557800
F	1.70696300	0.73915800	1.47316800
F	2.20570200	2.90832800	0.20679500
F	4.13614800	1.77066700	1.70116300
C	-3.54086500	-0.50505300	0.57419900
C	-4.20070700	-1.79588300	1.11168900
H	-4.19039600	-0.07840700	-0.19311300
H	-3.46251500	0.23780200	1.37372800
C	-5.60882700	-1.53531300	1.66163000
H	-4.24956600	-2.53138700	0.30046200
H	-3.57011100	-2.23458100	1.89230200
C	-6.27614400	-2.80369500	2.20350900
H	-5.55573900	-0.78002100	2.45789700
H	-6.23444200	-1.10017100	0.87071700
H	-7.27907300	-2.59190600	2.58776400
H	-6.37226200	-3.56527900	1.42183000
H	-5.69140900	-3.24086400	3.02048500

4Au

C	3.78685400	4.33616900	-0.12603600
C	3.05801400	4.86963900	-1.19328200
C	1.86846100	4.26876000	-1.61718000
C	1.47073000	3.12606600	-0.93873200
C	2.18841400	2.55646200	0.12012000
C	3.35798700	3.18207700	0.54204700
C	2.14099600	-0.09055200	0.53524900
C	0.23673200	1.36464000	-0.29894100
C	1.42158600	1.34733600	0.61946200
C	0.92015400	1.40343300	2.08607100
C	0.91751700	-0.04974100	2.54943300
C	1.82754900	-0.75058300	-0.80747200
C	2.61113200	-0.49801200	-1.87070300

C	2.40968400	-1.01016900	-3.26911500
C	-0.77256300	2.71598500	-2.08893200
H	-0.35541900	2.70310600	-3.09863200
H	-1.58082700	1.99350300	-1.99333100
H	-1.13685700	3.71768900	-1.85032400
H	4.69998800	4.82711700	0.19531200
H	3.41099500	5.76563400	-1.69342700
H	1.28581800	4.68559900	-2.43129100
H	3.93307600	2.79398000	1.37499100
H	-0.61530900	0.70766100	-0.24866500
H	1.59220900	1.98995700	2.71856700
H	-0.08736500	1.81465200	2.18426700
H	3.49983300	0.13000600	-1.75389200
H	3.26583000	-1.61872000	-3.58915800
H	2.33061900	-0.18399900	-3.98853900
H	1.50643600	-1.62171400	-3.34438200
N	0.28030300	2.36147400	-1.13322600
O	1.48129800	-0.83819100	1.59398700
O	0.50668500	-0.47455800	3.59340300
Au	0.12472900	-1.93514900	-0.82974100
P	-1.90976100	-3.16399800	-0.66540500
H	-2.07063200	-4.36027900	-1.39634000
H	-3.09794400	-2.48570800	-0.98252100
H	-2.22386300	-3.62714800	0.62552000
Sb	-3.33897600	0.60157800	0.52309600
F	-2.52674200	0.32426000	-1.17802700
F	-4.25652300	-1.00494300	0.28477700
F	-4.66484800	1.59550900	-0.29880900
F	-2.24185800	2.13401900	0.66791600
F	-4.02252300	0.86340500	2.21706400
F	-1.86637100	-0.36507900	1.21427600
C	3.63108900	-0.03045100	0.92096400
C	4.28571500	-1.41127100	1.07838200
H	3.72300300	0.51356200	1.87158800
H	4.17734400	0.55381700	0.17409100
C	5.76315000	-1.31481200	1.48088800
H	3.73374800	-1.98686600	1.82930600
H	4.19477800	-1.96224900	0.13584200
C	6.42571200	-2.68688000	1.64171100
H	6.31080900	-0.73037700	0.72818700
H	5.84981300	-0.75501700	2.42255900
H	7.47793200	-2.59165800	1.92887900
H	5.92173000	-3.28056000	2.41230800
H	6.38521300	-3.25717500	0.70693100

Cartesian Coordinates for the Stationary Points Given in Fig. S4.

	TS9^{Au}		
C	5.65542300	2.18720500	0.72525900
C	5.40066400	3.17874200	-0.22247900
C	4.11955000	3.34864200	-0.76305200
C	3.11550700	2.48783400	-0.32845300
C	3.36035500	1.46545200	0.60869500
C	4.62804500	1.33215400	1.15689100
C	1.90628200	-0.80483700	0.76194200
C	1.12907700	1.37019200	-0.18485100
C	2.03828000	0.77055600	0.91786700
C	1.50861700	1.06156300	2.33888100
C	0.97858800	-0.26197100	2.86373900
C	0.98165400	-0.96650500	-0.43626700
C	1.26306700	-0.02914900	-1.44092300
C	0.39146000	0.13729600	-2.66923500
C	1.14288500	3.48194100	-1.55338700
H	1.51627600	3.38286200	-2.58042400
H	0.06293100	3.33422500	-1.54430400
H	1.37339300	4.49082700	-1.19606500
H	6.65323300	2.07675000	1.13756300
H	6.20332600	3.83513300	-0.54447000
H	3.91822700	4.13286900	-1.48502500
H	4.83490500	0.58039300	1.91228800
H	0.06195700	1.46031800	-0.02009800
H	2.29089200	1.42170000	3.01289600
H	0.69621700	1.79263500	2.35234800
H	2.32579100	0.17539200	-1.60529800
H	0.44712800	-0.75595200	-3.30090800
H	0.72271400	0.98772800	-3.27213900
H	-0.65271100	0.29752900	-2.39166800
N	1.75501600	2.50282100	-0.66905800
O	1.22341600	-1.25223300	1.95826100
O	0.44681800	-0.47448900	3.91871500
Au	-0.76864400	-1.96875900	-0.25539800
P	-2.98542300	-2.81674000	0.00865000
H	-3.73853900	-2.98208900	-1.16665500
H	-3.80527200	-1.94415100	0.74533800
H	-3.22079200	-4.05511400	0.63979900
Sb	-3.07148600	1.32505700	-0.03313600
F	-1.62000800	0.63976300	0.98393500
F	-3.18925200	2.73396600	1.15894300
F	-4.21612900	0.23362600	0.96005300

F	-2.87249200	-0.11941100	-1.24637300
F	-4.44248800	1.99290900	-1.07737200
F	-1.77228900	2.23731100	-1.05656500
C	3.16987900	-1.69639900	0.68630300
C	3.98299000	-1.72848400	-0.61408500
H	2.81392900	-2.70920000	0.90501200
H	3.81472300	-1.42073200	1.52899300
C	5.21054900	-2.64400900	-0.49686100
H	3.35115200	-2.08552800	-1.43678800
H	4.31881200	-0.72117900	-0.88751700
C	6.02928200	-2.71167400	-1.78947400
H	5.84908100	-2.29018700	0.32385400
H	4.88423700	-3.65375100	-0.21434600
H	6.89896200	-3.36623100	-1.67496300
H	5.42874100	-3.09965700	-2.61990900
H	6.39472600	-1.72016700	-2.07996200

5^{Au}

C	5.38383700	2.94332000	0.74520700
C	5.05050500	3.90255500	-0.21041100
C	3.79033000	3.90881000	-0.82312000
C	2.88034200	2.91995100	-0.45162900
C	3.21293600	1.92891700	0.49393500
C	4.45436700	1.95431800	1.11023700
C	2.14428800	-0.51870700	0.45900000
C	1.02981700	1.54702300	-0.40480300
C	1.99265000	1.04315000	0.72014600
C	1.40089800	1.11282200	2.14319000
C	1.42462900	-0.30874100	2.67985200
C	1.08965400	-0.75006200	-0.60618500
C	1.17194500	0.28969500	-1.58632400
C	0.17373400	0.36366700	-2.73071200
C	0.84710000	3.69547900	-1.72557100
H	1.18883000	3.63012800	-2.76771800
H	-0.21927100	3.46872100	-1.68189500
H	1.00477800	4.72188600	-1.37718800
H	6.36345400	2.95901600	1.21181300
H	5.77515900	4.66358800	-0.48425000
H	3.52933100	4.66980200	-1.55089400
H	4.71394800	1.22416200	1.87147100
H	-0.02708400	1.60037400	-0.16491300
H	1.95975100	1.76776000	2.81493200
H	0.35549800	1.43622000	2.13923100
H	2.20463800	0.48772800	-1.90210700

H	0.27175600	-0.51296200	-3.37896600
H	0.35275000	1.25141200	-3.34328400
H	-0.85096500	0.40690400	-2.35630500
N	1.55413200	2.77410800	-0.85639500
O	1.80477300	-1.17824800	1.69016200
O	1.15887700	-0.68756600	3.78708400
Au	-0.53165500	-1.89948600	-0.28356800
P	-2.63441400	-2.95567500	0.16116700
H	-3.45355900	-3.20008300	-0.95417200
H	-3.47214100	-2.15857200	0.96057800
H	-2.68940200	-4.20677800	0.80715100
Sb	-3.15198100	1.14420100	0.10998100
F	-1.57182500	0.58939000	1.01495600
F	-3.33184900	2.51304900	1.33883800
F	-4.10392500	-0.06977400	1.16618700
F	-2.88013100	-0.27274200	-1.12406300
F	-4.65752000	1.66081500	-0.82780100
F	-2.03407900	2.19875700	-0.98092200
C	3.52728200	-1.04697700	0.02418500
C	3.53290400	-2.54247300	-0.32639900
H	4.22260600	-0.86125000	0.84975300
H	3.88836800	-0.45565500	-0.82378900
C	4.93486700	-3.05524300	-0.67845900
H	3.13060600	-3.11191400	0.51926300
H	2.85550900	-2.72884000	-1.17215600
C	4.95354500	-4.54481600	-1.03533500
H	5.33747100	-2.47105500	-1.51737100
H	5.60834200	-2.87248800	0.16995200
H	5.96569300	-4.88379000	-1.27762400
H	4.58759300	-5.15530900	-0.20242400
H	4.31641900	-4.75256200	-1.90253200

TS10^{Au}

C	-6.12201600	-1.60222200	1.32039300
C	-6.51610500	-1.96699000	0.03125600
C	-5.59140400	-2.05987900	-1.01523500
C	-4.25321900	-1.77271500	-0.74112300
C	-3.84927300	-1.40663100	0.55376600
C	-4.77617400	-1.31868600	1.58554900
C	-1.90297200	0.36956600	0.46463600
C	-1.93372000	-1.75183700	-0.82308500
C	-2.36381000	-1.15301100	0.54546200
C	-1.56834900	-1.65038000	1.76387900
C	-1.21109600	-0.40728600	2.55655200

C	-0.74020600	0.35108000	-0.54738800
C	-0.83312100	-0.81297700	-1.33624000
C	0.17780600	-1.27084700	-2.34751800
C	-3.19740400	-2.70660300	-2.76469900
H	-4.10152500	-2.53511600	-3.35266000
H	-2.34587700	-2.52475100	-3.42287600
H	-3.17865200	-3.76196400	-2.44876600
H	-6.85551300	-1.54505000	2.11806100
H	-7.55946600	-2.19479500	-0.16688000
H	-5.91690600	-2.35734500	-2.00627600
H	-4.46216500	-1.04403400	2.58935100
H	-1.50432800	-2.76122200	-0.71906000
H	-2.11415800	-2.36038900	2.38719000
H	-0.61623200	-2.10628700	1.47031500
H	-1.36575700	0.26989600	-1.75724400
H	-0.29228200	-1.79479000	-3.18279100
H	0.85697600	-1.96222200	-1.83710900
H	0.78766600	-0.44571300	-2.71460100
N	-3.16242800	-1.78308100	-1.63726800
O	-1.37059900	0.70222100	1.75464700
O	-0.84253000	-0.31360400	3.69270200
Au	0.87705600	1.60640000	-0.42804800
P	2.87820400	2.82766300	-0.10546800
H	2.93902800	4.17281400	-0.52627900
H	4.00687600	2.29377200	-0.74434900
H	3.32096900	2.94840000	1.22035100
Sb	3.16194200	-1.35542600	0.20821200
F	3.39384300	-2.33266100	1.75992100
F	2.77191100	-2.86441500	-0.82010900
F	1.29778400	-1.26587900	0.58098000
F	2.87471100	-0.30837300	-1.34205600
F	3.35208400	0.27951400	1.13350700
F	4.96872800	-1.39759500	-0.18915400
C	-3.00139900	1.38827600	0.12495900
C	-2.56396600	2.86008300	0.11690600
H	-3.79518300	1.25119100	0.86738200
H	-3.44151200	1.11556200	-0.84307100
C	-3.74756700	3.81684700	-0.08018700
H	-2.05980000	3.08841200	1.06311500
H	-1.82535900	3.03351300	-0.67592500
C	-3.32347000	5.28865200	-0.10007000
H	-4.26496600	3.57160900	-1.01810500
H	-4.48097300	3.65694300	0.72161100
H	-4.18427400	5.95031000	-0.23954000

H	-2.83430200	5.57166200	0.83868600
H	-2.61652400	5.48644300	-0.91413600
7Au			
C	4.69825200	3.35839500	1.55107500
C	4.38756200	4.29288300	0.56013700
C	3.31941600	4.09146800	-0.31930100
C	2.56694300	2.91966600	-0.19213900
C	2.87338000	1.97429000	0.79979400
C	3.93232200	2.19217800	1.67405100
C	2.45618900	-0.54635800	0.14546200
C	0.85157900	1.34568700	-0.33585200
C	1.88572900	0.83009900	0.73051600
C	1.28273500	0.40519700	2.08352200
C	1.60716800	-1.06565800	2.26953700
C	1.53499900	-0.84814900	-1.03216900
C	0.72901000	0.22161300	-1.36566900
C	-0.01453200	0.41962300	-2.65026000
C	0.55971900	3.59781900	-1.44110500
H	0.99237700	4.08669700	-2.32007200
H	-0.40077700	3.16591900	-1.72056000
H	0.37377400	4.36319900	-0.67365300
H	5.52528400	3.53834200	2.23031300
H	4.97850900	5.20030400	0.47362100
H	3.07812500	4.83174800	-1.07468000
H	4.15966800	1.47423000	2.45855500
H	-0.13043100	1.57693000	0.08768200
H	1.69979400	0.96738000	2.92386600
H	0.19668800	0.53142400	2.12128200
H	1.77190600	-1.64427500	-1.73415900
H	0.48271300	1.22263500	-3.20696700
H	-1.04386500	0.72840500	-2.45558600
H	-0.01545400	-0.48376400	-3.26473700
N	1.45162500	2.54660100	-0.94831700
O	2.31148200	-1.53274000	1.19427300
O	1.31797000	-1.78051300	3.19379000
Au	-0.47735200	-1.63238400	-0.25110700
P	-2.14344600	-2.90024400	0.81387200
H	-1.77685900	-4.20277700	1.19904900
H	-3.32014600	-3.12408000	0.08588200
H	-2.61949800	-2.35279700	2.01185500
Sb	-3.40498800	0.83947300	-0.01405400
F	-3.95863700	2.03876500	1.27655900
F	-2.35719400	2.12619000	-0.89158700

F	-1.86660400	0.45731000	1.04948800
F	-2.76290600	-0.40619200	-1.29591700
F	-4.20937500	-0.62110400	0.84168400
F	-4.87499100	1.16387500	-1.08299600
C	3.93118800	-0.54852400	-0.28065200
C	4.45939000	-1.90312200	-0.77761800
H	4.52382300	-0.22731600	0.58216100
H	4.06983600	0.22055700	-1.04982000
C	5.96946500	-1.87541300	-1.05106300
H	4.23556100	-2.67345200	-0.03068000
H	3.94142300	-2.20245300	-1.69901400
C	6.50854900	-3.21590000	-1.56007000
H	6.19335500	-1.08712900	-1.78256600
H	6.49674900	-1.59352200	-0.12997700
H	7.58703500	-3.16879800	-1.74101400
H	6.32701900	-4.01685900	-0.83468300
H	6.02631900	-3.50621700	-2.50050600

TS11^{Au}

C	4.60394300	3.86100000	-0.10439000
C	3.76074500	4.56081300	-0.97227500
C	2.43018800	4.17238000	-1.15969500
C	1.97605400	3.06249700	-0.44915700
C	2.81545400	2.33903700	0.41756200
C	4.13260800	2.74410100	0.59860700
C	2.38696900	-0.24282000	0.61070300
C	0.67991400	1.33540100	0.26262800
C	2.01547900	1.21824000	1.03793800
C	1.87700100	1.14762100	2.56018500
C	1.61064100	-0.33191100	2.82953600
C	1.44759500	-0.24375000	-0.59157400
C	1.92141900	-0.06895100	-1.86097400
C	1.07977700	0.30871400	-3.03869500
C	-0.45925200	3.14295400	-1.08132800
H	-0.37017300	3.07063100	-2.17043900
H	-1.37156100	2.65041000	-0.76394700
H	-0.49951200	4.19872000	-0.79725800
H	5.63091000	4.18580300	0.02872400
H	4.14112100	5.42422700	-1.50968800
H	1.77647300	4.72366200	-1.82684900
H	4.79111800	2.21041800	1.27750600
H	-0.27464500	1.03845800	0.67505100
H	2.80279000	1.44169100	3.06706100
H	1.06669400	1.75574800	2.96836800

H	2.99165500	-0.16187000	-2.06332000
H	1.15832700	-0.45284600	-3.82527100
H	1.45035500	1.24286100	-3.48125100
H	0.02822200	0.42377500	-2.76642900
N	0.68386400	2.51910700	-0.42283800
O	1.83908600	-1.05303200	1.68641300
O	1.25937100	-0.84691800	3.85482100
Au	-0.19815700	-1.61681600	-0.54715100
P	-2.00794500	-3.09823700	-0.43991700
H	-1.96036000	-4.30730700	-1.16370300
H	-3.22737200	-2.54288100	-0.86181300
H	-2.32730600	-3.57338800	0.84210600
Sb	-3.40955700	0.63671500	0.25449800
F	-2.07043800	0.50250600	-1.08922400
F	-4.38828800	-0.64190200	-0.69524400
F	-4.11111400	2.06125100	-0.70114900
F	-2.23889400	1.80044800	1.16110800
F	-4.68974300	0.76657400	1.57974400
F	-2.55318000	-0.77868700	1.17373600
C	3.85535700	-0.62523000	0.44335400
C	4.07461600	-2.10736100	0.09861000
H	4.37599300	-0.39568600	1.38326600
H	4.31045100	0.01442700	-0.32079800
C	5.55882600	-2.47294900	-0.03068100
H	3.60671600	-2.72489800	0.87349800
H	3.55648300	-2.34974900	-0.83821300
C	5.78060500	-3.94903600	-0.37525400
H	6.02605100	-1.84253100	-0.80011400
H	6.07407100	-2.23538100	0.91000400
H	6.84643700	-4.18393700	-0.45945900
H	5.35470400	-4.60237200	0.39425800
H	5.30592100	-4.20880500	-1.32835100

IM6^{Au}

C	4.76492600	3.83496300	0.44784800
C	4.16759600	4.50111900	-0.62550900
C	2.94031600	4.08549100	-1.15071100
C	2.31426900	2.97272500	-0.57943400
C	2.90582400	2.30187600	0.51188600
C	4.12382800	2.73174600	1.02568900
C	2.28446300	-0.28813500	0.55069800
C	0.81344800	1.27724400	-0.07619800
C	1.98552600	1.20637100	0.97637300
C	1.61617200	1.12062700	2.45360000

C	1.33874700	-0.35462500	2.70775800
C	1.28391700	-0.09657700	-0.60913200
C	1.27557600	-0.63720500	-1.87649700
C	0.58222600	-0.03978000	-3.07232600
C	0.01855300	3.22921100	-1.49829500
H	0.26170500	3.54598200	-2.51851900
H	-0.89692500	2.64133700	-1.52679900
H	-0.16493400	4.12403400	-0.88824000
H	5.71726000	4.17685700	0.84017800
H	4.66204800	5.36451800	-1.06196200
H	2.48477700	4.61849700	-1.97863400
H	4.57199300	2.22772100	1.87866200
H	-0.19970400	1.30208900	0.32060100
H	2.43692300	1.43941100	3.10642400
H	0.73606300	1.71146200	2.72016000
H	1.98390900	-1.43973300	-2.08045700
H	0.31185900	-0.81715100	-3.79206600
H	1.27880100	0.64738700	-3.57017900
H	-0.31409500	0.51307400	-2.79358600
N	1.09360000	2.40785000	-0.94886000
O	1.72412600	-1.09536600	1.60931800
O	0.87490800	-0.87965900	3.68126100
Au	-0.34960600	-1.72908500	-0.54803500
P	-2.08372300	-3.08790600	0.25065800
H	-2.12962700	-4.44403100	-0.12374900
H	-3.36374300	-2.60766800	-0.06449800
H	-2.10988200	-3.17671900	1.65092800
Sb	-3.21434400	0.87447800	0.21130800
F	-2.02006000	0.57625000	-1.24281300
F	-4.15387800	-0.64970500	-0.34436100
F	-4.21846200	1.98256200	-0.87372700
F	-2.09368800	2.27992700	0.73600400
F	-4.31679200	1.09949800	1.67576000
F	-2.09915900	-0.28777600	1.22967900
C	3.71105500	-0.73989000	0.26806500
C	3.89063200	-2.25092800	0.04915000
H	4.32711100	-0.43222000	1.12379800
H	4.08746100	-0.17599100	-0.59321500
C	5.35519000	-2.63929700	-0.19333600
H	3.50611900	-2.78551200	0.92480700
H	3.28470700	-2.59163500	-0.80156700
C	5.54757900	-4.14465000	-0.40114700
H	5.73800300	-2.09503300	-1.06741100
H	5.96120000	-2.30654200	0.66010500

H	6.60082300	-4.39311400	-0.56539000
H	5.20327900	-4.71149700	0.47103200
H	4.98296300	-4.50082800	-1.27057300