

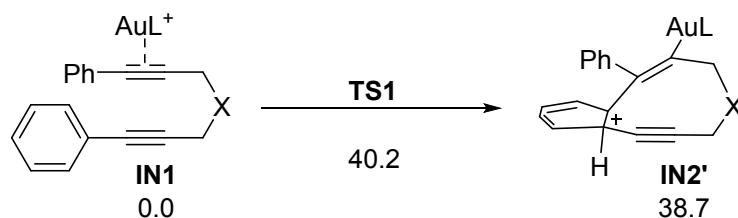
Supporting Information

Mechanism of the Gold-Catalyzed Intramolecular [3 + 2]-Cycloaddition of 1,6- Diynes: A DFT Study

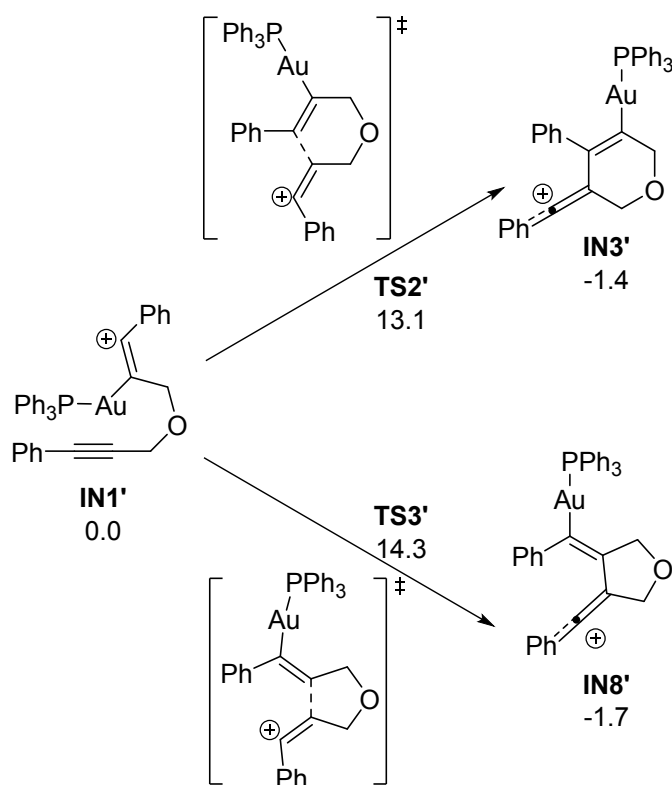
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1. Additional Computational Results
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4. Cartesian Coordinates for All Species

1. Additional Computational Results

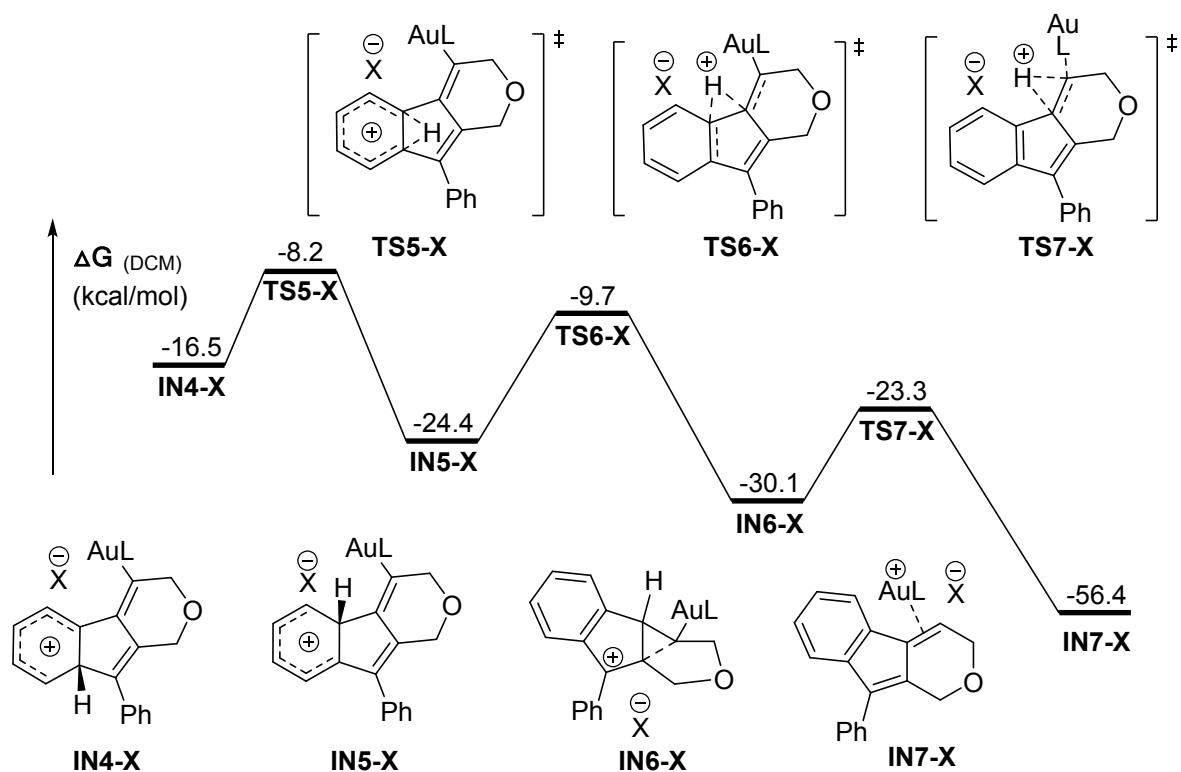


Scheme S1. Activation and Reaction Energies for Phenyl-Involved Cyclization (in kcal/mol).



Scheme S2. Activation and Reaction Energies for Cyclizations with PPh_3 -Containing Models (in kcal/mol).

The results in Scheme S2 show that when the experimental PPh_3 ligand is used in calculations, the relative activation barriers for the two pathways are higher than the calculations with PH_3 , indicating the ligand simplification may underestimate the barriers. In addition, the formation of IN3' and IN8' were found to be less exergonic in Scheme S2. However, all the energy barriers are low and suggest the easiness of the reactions with gold catalysis, corresponding well to the mild conditions used by Liu et al.



Scheme S3. Calculated Energies for H-migration When Anion is Contained (in kcal/mol; L = PH₃, X = SbF₆⁻; salvation free energies are relative to the initial reactant complex).

2. Table of Energy Values

Table S1. Energies (in Hartree) calculated at PCM-M06/6-311+G(d,p)//B3LYP/6-31G(d) level

Species	E ₀ ^a	H ₂₉₈ ^b	G ₂₉₈ ^c	E ^d	G _{Sol} ^e
IN1	-1247.560556	-1247.537157	-1247.622249	-1247.538101	-1247.820301
TS1	-1247.503123	-1247.481313	-1247.556437	-1247.482257	-1247.764496
IN2'	-1247.507105	-1247.485194	-1247.560502	-1247.486138	-1247.768318
TS2	-1247.552137	-1247.529765	-1247.611667	-1247.530709	-1247.808094
IN2	-1247.586341	-1247.564486	-1247.641172	-1247.565431	-1247.835059
TS4	-1247.575119	-1247.554141	-1247.62823	-1247.555085	-1247.82025
IN3	-1247.606144	-1247.585349	-1247.65838	-1247.586293	-1247.86382
TS5	-1247.591206	-1247.570698	-1247.643124	-1247.571642	-1247.849326
IN4	-1247.617373	-1247.596534	-1247.669943	-1247.597478	-1247.873727
TS6	-1247.585319	-1247.564722	-1247.637481	-1247.565666	-1247.845182
IN5	-1247.628304	-1247.607967	-1247.678888	-1247.608911	-1247.891184
TS7	-1247.607992	-1247.587576	-1247.659338	-1247.588520	-1247.871039
IN6	-1247.656928	-1247.636216	-1247.709432	-1247.637161	-1247.925034
TS3	-1247.543407	-1247.520714	-1247.602038	-1247.521658	-1247.805457
IN7	-1247.584342	-1247.562154	-1247.641491	-1247.563098	-1247.835738
TS8	-1247.580078	-1247.558951	-1247.633226	-1247.559895	-1247.828003
IN8	-1247.621905	-1247.600959	-1247.674618	-1247.601903	-1247.87818
TS9	-1247.607158	-1247.586531	-1247.659072	-1247.587476	-1247.864328
IN9	-1247.622653	-1247.601718	-1247.675343	-1247.602662	-1247.880202
TS10	-1247.617767	-1247.597120	-1247.670055	-1247.598065	-1247.875727
IN10	-1247.685636	-1247.665028	-1247.737547	-1247.665972	-1247.954021
SbF₆⁻	-604.638527	-604.629382	-604.671896	-604.630326	-604.7574426

IN1_{M06}	-1939.310600	-1939.273450	-1939.384513	-1939.274394	-1940.62698953
TS1_{M06}	-1939.252864	-1939.216931	-1939.325662	-1939.217875	-1940.56033278
TS2_{M06}	-1939.293174	-1939.257108	-1939.366373	-1939.258052	-1940.60171181
TS3_{M06}	-1939.286283	-1939.250062	-1939.359926	-1939.251006	-1940.59563414
IN1_{B3PW91}	-1939.929541	-1939.891687	-1940.011307	-1939.892631	-1941.22327262
TS1_{B3PW91}	-1939.870086	-1939.833927	-1939.945053	-1939.834872	-1941.15613368
TS2_{B3PW91}	-1939.918881	-1939.882226	-1939.996934	-1939.883171	-1941.20562149
TS3_{B3PW91}	-1939.913137	-1939.876145	-1939.992703	-1939.877089	-1941.20079219
IN1_{BP86}	-1940.565965	-1940.527097	-1940.648630	-1940.528041	-1941.89804758
TS1_{BP86}	-1940.515991	-1940.478732	-1940.592478	-1940.479677	-1941.8408583
TS2_{BP86}	-1940.560349	-1940.522641	-1940.639037	-1940.523585	-1941.88698061
TS3_{BP86}	-1940.553719	-1940.515719	-1940.633715	-1940.516663	-1941.88137874
IN1_{TPSSTPSS}	-1940.713473	-1940.675051	-1940.793865	-1940.675995	-1942.01117903
TS1_{TPSSTPSS}	-1940.659343	-1940.622463	-1940.734632	-1940.623407	-1941.95079084
TS2_{TPSSTPSS}	-1940.706002	-1940.668628	-1940.784434	-1940.669573	-1941.99884688
TS3_{TPSSTPSS}	-1940.699541	-1940.661876	-1940.779100	-1940.662820	-1941.99337025
IN1_{B3LYP}	-1940.490718	-1940.452875	-1940.573062	-1940.453819	-1941.82010578
TS1_{B3LYP}	-1940.426806	-1940.390703	-1940.501650	-1940.391647	-1941.74741472
TS2_{B3LYP}	-1940.477756	-1940.441139	-1940.555961	-1940.442083	-1941.79936224
TS3_{B3LYP}	-1940.472158	-1940.435228	-1940.551511	-1940.436172	-1941.79478910

^a Sum of electronic and zero-point energies

^b Sum of electronic and thermal enthalpies

^c Sum of electronic and thermal free energies

^d Electronic energies

^e Single point energies in solution

Table S2. Energies (in Hartree) calculated with dispersion-corrected DFT method (L = PPh₃)

	IN1	TS1	TS2	TS3
B3PW91-D3^a	-115.2934	-127.6941	-120.6036	-119.7437
B3LYP-D3^b	-111.477	-122.614	-116.2574	-115.7638

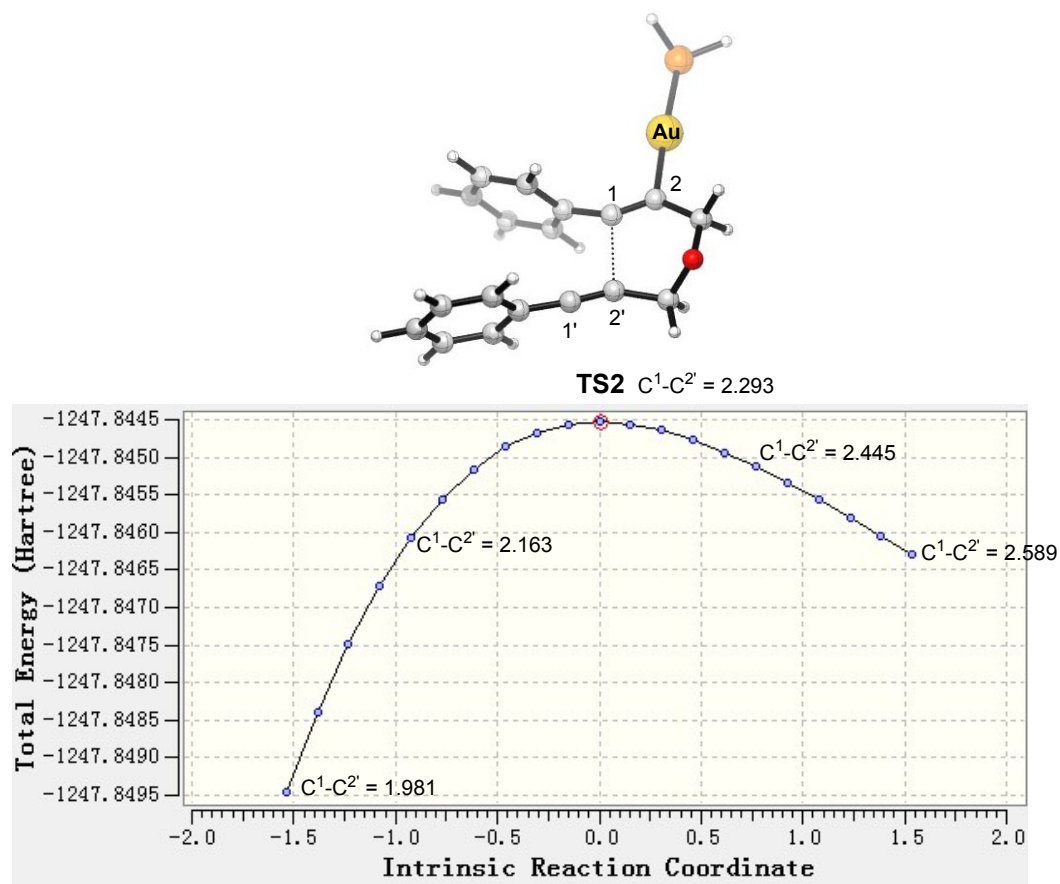
^a Calculated at (PCM)B3PW91/6-311+G(d,p)//B3PW91/6-31G(d) level^b Calculated at (PCM)B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) level**Table S3.** Energies (in Hartree) calculated at relativistic effects level with DKH2

	IN1	TS1	TS2	TS3
B3LYP-DKH2^a (L = PH₃)	-20077.3157179	-20077.2605553	-20077.3070827	-20077.2979611
B3LYP-DKH2^a (L = PPh₃)	-20770.7577909	-20770.6956389	-20770.744309	-20770.7376392

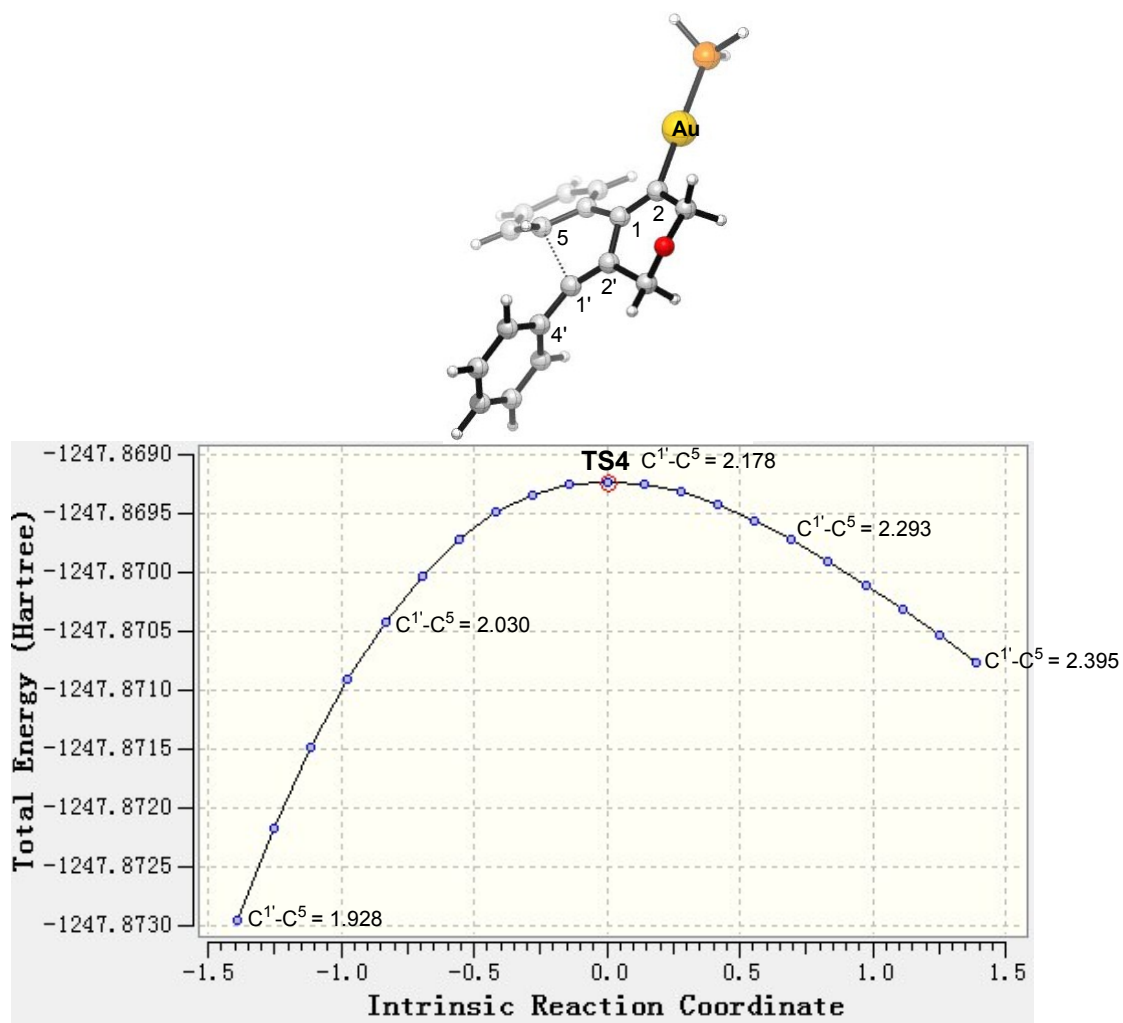
^a Calculated at (PCM)B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) level

3. IRC Polts for Selected Transition States

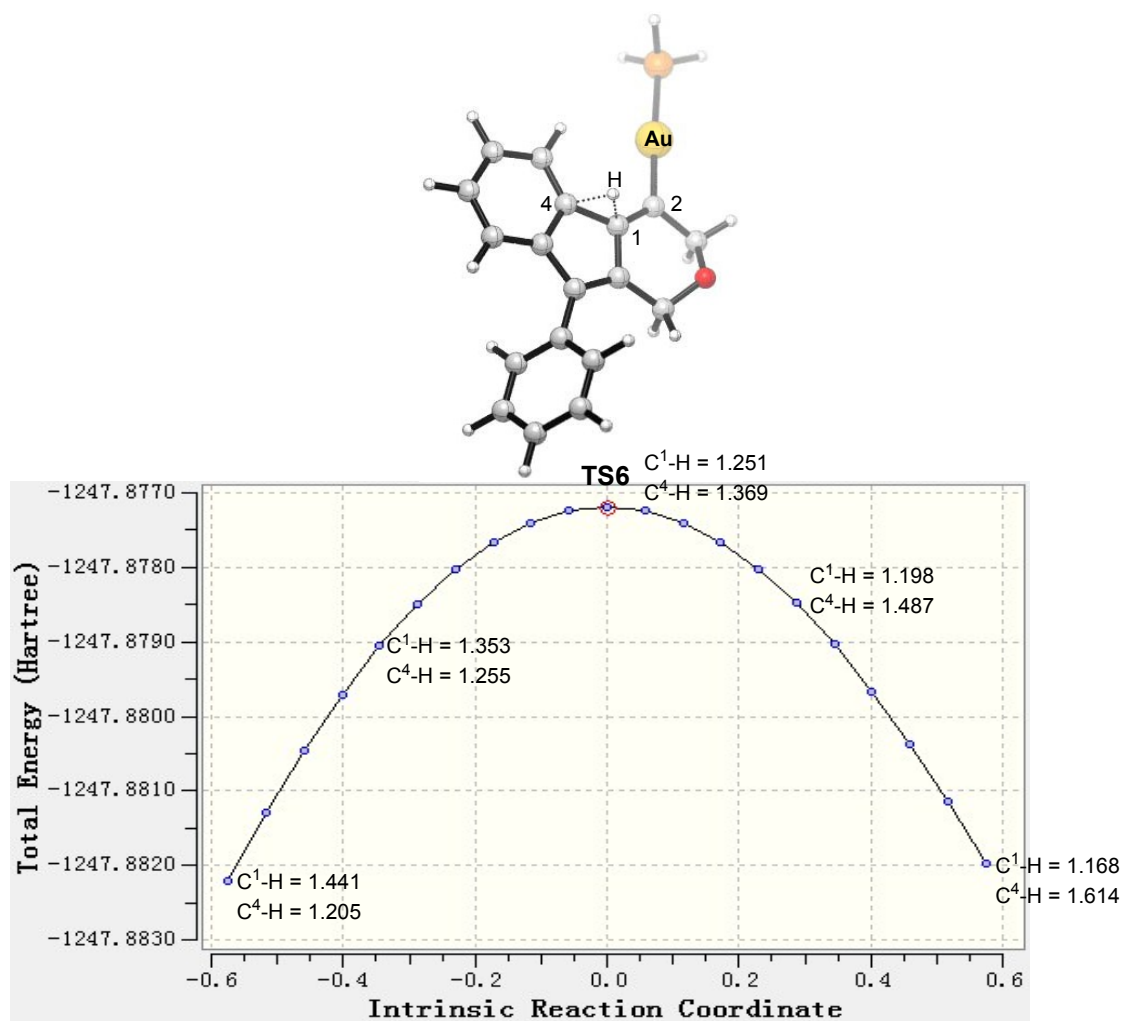
IRC Polts for **TS2**



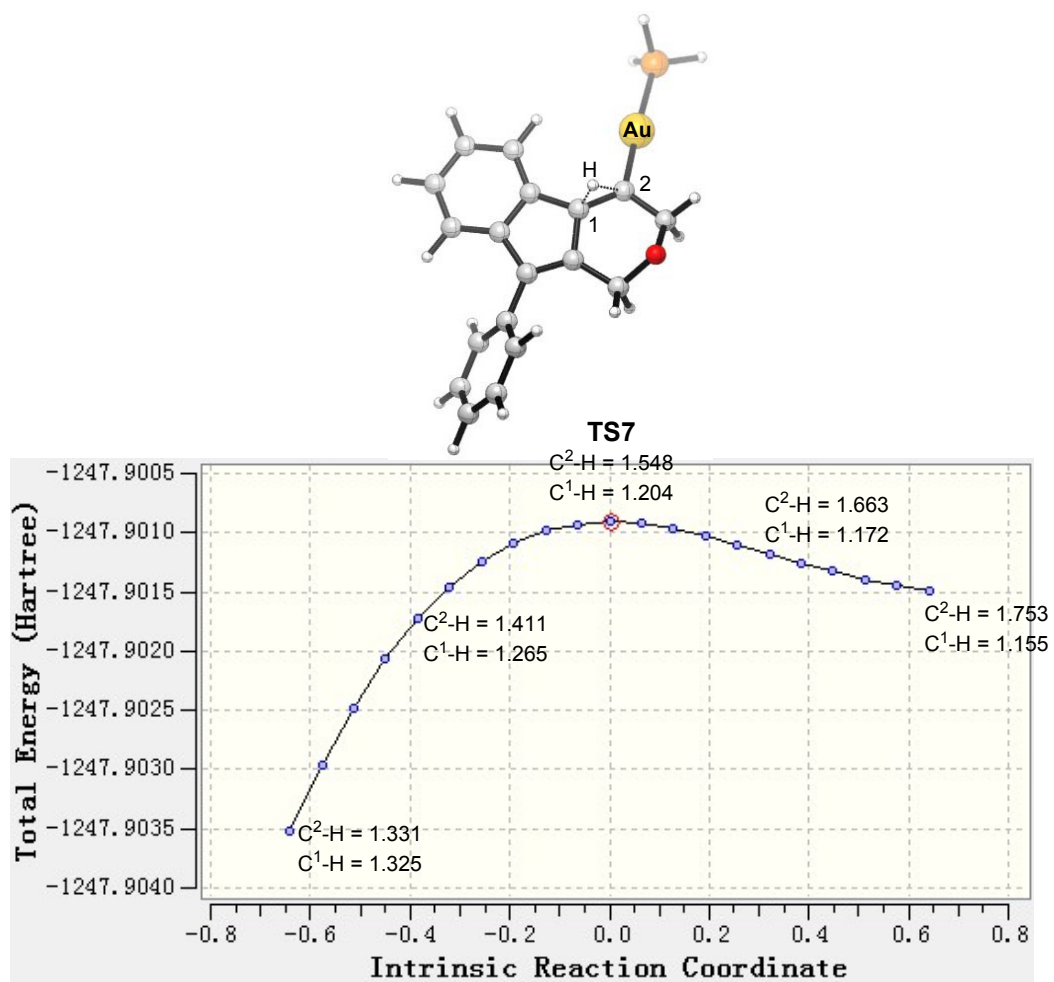
IRC Polts for **TS4**



IRC Polts for **TS6**



IRC Polts for **TS7**



4. Cartesian Coordinates for All Species

IN1

O	-0.87372600	4.54907600	1.38048600
C	-1.48598500	4.29385300	0.15174200
H	-2.36052000	3.63768800	0.25953600
H	-1.82251700	5.25851100	-0.23702200
C	-0.63175600	3.39949500	2.21067400
H	0.15749200	2.77814400	1.75774400
H	-0.22394000	3.82108400	3.13437800
C	-0.54171800	3.66838100	-0.86877500
C	-1.81830600	2.59194300	2.48111800
C	0.62864400	3.21710100	-0.95727100
C	-2.80634700	1.92332100	2.70648200
C	1.93830400	2.72763300	-1.09082600
C	2.99628200	3.61994200	-1.40065600
C	2.21290000	1.35244500	-0.87762500
C	4.29561300	3.14078300	-1.49068800
H	2.77684200	4.67116200	-1.55702200
C	3.51708700	0.88900100	-0.97319600
H	1.39737500	0.67749300	-0.63793800
C	4.55455100	1.78040400	-1.27848600
H	5.10968200	3.81980200	-1.72309100
H	3.73357600	-0.16170700	-0.80899200
H	5.57362300	1.41155900	-1.35024700
C	-3.96994000	1.14649800	2.99890100
C	-4.96686600	1.65817600	3.85262500
C	-4.13283900	-0.13710100	2.44238700
C	-6.09933400	0.90009300	4.13876200
H	-4.84047900	2.64580200	4.28498000
C	-5.26754400	-0.88892000	2.73598300
H	-3.36235300	-0.53542400	1.78902300
C	-6.25244700	-0.37279800	3.58260300
H	-6.86254100	1.30122800	4.79922100
H	-5.38374100	-1.87996200	2.30669300
H	-7.13582100	-0.96233100	3.81054100
Au	-1.22534700	3.36840200	-2.87127600
P	-2.18052700	3.14254100	-5.00965000
H	-3.46169100	2.56569300	-5.05688200
H	-1.48048500	2.35476500	-5.94077200
H	-2.37726200	4.33088300	-5.73469700

TS1

O	-1.51400200	0.64480000	-1.63967500
C	-2.06923400	1.87737200	-1.19282200
H	-3.14464300	1.68426400	-1.09840500
H	-1.69524900	2.08607600	-0.18243100
C	-0.14205500	0.42682000	-1.29452200
H	0.08289800	0.79803200	-0.28546800
H	0.00393400	-0.65859300	-1.29747000
C	-1.93694400	3.15873500	-2.01134300
C	0.66871100	1.06676300	-2.33622100
C	-1.68990500	3.56697500	-3.22989000
C	0.78010700	1.62917000	-3.40923200
C	-1.66279500	4.87669700	-3.90187200
C	-0.46591800	5.60613800	-4.00073500
C	-2.84675200	5.42405700	-4.43053600
C	-0.45820200	6.86588400	-4.60279000
H	0.44879900	5.19214200	-3.58828300
C	-2.83325100	6.68234400	-5.02826700

H	-3.77455800	4.86412400	-4.35554000
C	-1.63829000	7.40434400	-5.11892400
H	0.47016700	7.42617400	-4.66510400
H	-3.75456500	7.10137600	-5.42238600
H	-1.62955600	8.38368100	-5.58841500
C	0.22847400	2.23909100	-4.55768000
C	0.91858600	2.84672000	-5.60869700
C	-1.22589300	2.19324500	-4.57392500
C	0.20608300	3.30811400	-6.71642900
H	2.00039500	2.92115500	-5.57829100
C	-1.89406900	2.57923500	-5.78071900
H	-1.67669800	1.40382400	-3.97867900
C	-1.19378900	3.15918000	-6.81696100
H	0.74937900	3.76523900	-7.53884500
H	-2.96859100	2.43719400	-5.85061400
H	-1.70480700	3.48257400	-7.71784100
Au	-2.46478000	4.83151100	-0.81598100
P	-3.06218700	6.62455300	0.60559200
H	-2.21081300	7.74538000	0.63010700
H	-4.30463200	7.24571900	0.37715400
H	-3.16076300	6.34087000	1.98031800

IN2'

O	-1.48927000	0.70731300	-1.60993800
C	-2.12550300	1.93977700	-1.23139700
H	-3.19556600	1.69781800	-1.21803900
H	-1.83991900	2.16142300	-0.19623100
C	-0.12272000	0.58590800	-1.22566600
H	0.08525300	1.07348600	-0.26327300
H	0.08208700	-0.48506500	-1.11382200
C	-1.95592700	3.20988500	-2.06474600
C	0.67303100	1.14956500	-2.32384300
C	-1.67131100	3.41204200	-3.35741400
C	0.77080300	1.61815100	-3.44746400
C	-1.62424800	4.77931100	-3.98389100
C	-0.40150200	5.44160000	-4.16924200
C	-2.80519100	5.40411300	-4.41957200
C	-0.35943500	6.69699000	-4.78058100
H	0.51791000	4.98268900	-3.81572300
C	-2.76172200	6.65896100	-5.03067000
H	-3.76005900	4.90823100	-4.26579100
C	-1.53805200	7.30606900	-5.21681400
H	0.59436700	7.20098200	-4.90966700
H	-3.68399000	7.13068800	-5.35813800
H	-1.50356100	8.28198700	-5.69233700
C	0.15180500	2.10389800	-4.60523500
C	0.75388600	2.38687400	-5.82796100
C	-1.33537100	2.24937100	-4.41833200
C	-0.04699400	2.69367200	-6.92923000
H	1.83134600	2.32036400	-5.93400600
C	-2.08633300	2.49988000	-5.66515400
H	-1.70811300	1.34254200	-3.92271700
C	-1.46283600	2.72754300	-6.86099400
H	0.43412700	2.88641800	-7.88479000
H	-3.16987100	2.52622800	-5.59364300
H	-2.03616900	2.93087700	-7.75924600
Au	-2.37885900	4.91223700	-0.93693700

P	-2.86269600	6.82606300	0.40339700
H	-1.87332000	7.82354100	0.50719100
H	-3.97116100	7.61746400	0.04350300
H	-3.14347300	6.61568700	1.76731200

TS2

O	-1.60095900	1.06435600	-1.07820700
C	-2.05914900	1.72620800	-2.22846500
H	-1.55221200	1.34138500	-3.12909500
H	-3.11976300	1.47876300	-2.31296300
C	-0.24743900	1.32511800	-0.76615800
H	0.06918300	0.52870300	-0.08670400
H	0.38418100	1.28329100	-1.66651400
C	-1.88738800	3.23282400	-2.21982500
C	-0.08637800	2.63509300	-0.08293500
C	-1.20668800	4.04972700	-1.49840800
C	0.27910600	3.35406600	0.84710300
C	-0.78975300	5.37501800	-1.15319700
C	0.39590500	5.91345200	-1.69839400
C	-1.58224300	6.16347000	-0.29202800
C	0.75900800	7.22479200	-1.41063400
H	1.00807200	5.29996600	-2.35219800
C	-1.20921500	7.47485500	-0.01155400
H	-2.48835300	5.74195400	0.13163100
C	-0.04259300	8.00614300	-0.57020800
H	1.66341300	7.64226100	-1.84282100
H	-1.82713400	8.08390200	0.64115700
H	0.24383700	9.03044500	-0.35019500
C	0.65479800	4.27543700	1.84646100
C	-0.19001300	4.49811100	2.95976700
C	1.88840200	4.96202200	1.75742900
C	0.19329700	5.39089500	3.95290300
H	-1.12938400	3.95899500	3.02959300
C	2.26053900	5.85007400	2.75909300
H	2.53685000	4.78131600	0.90647400
C	1.41568300	6.06574700	3.85411700
H	-0.45317300	5.55864200	4.80880400
H	3.20991900	6.37270600	2.69395200
H	1.71382900	6.75768300	4.63648700
Au	-2.89322000	4.28447400	-3.74339600
P	-4.07832400	5.34335700	-5.49082200
H	-5.12538900	6.21045900	-5.12773000
H	-3.34314800	6.16222300	-6.36782000
H	-4.73510300	4.49621500	-6.40164600

IN2

O	0.09697900	1.54281100	-2.37190000
C	-0.85672300	2.35879200	-1.68520500
H	-1.77425300	1.76587100	-1.66588200
H	-0.53214200	2.50320900	-0.64085700
C	1.27027600	2.21407600	-2.66662300
H	1.73469400	2.66696500	-1.77564100
H	1.96202500	1.50395900	-3.12090400
C	-1.10334100	3.70228600	-2.32870200
C	0.94205300	3.40065200	-3.63802800
C	-0.27248800	4.18063200	-3.28175000
C	1.75240500	3.61549000	-4.61823500
C	-0.48178700	5.44607500	-4.04700700
C	0.50342700	6.44773200	-4.06058900
C	-1.66124800	5.64969200	-4.78170500
C	0.30933500	7.62740500	-4.78034900
H	1.40924300	6.31831300	-3.47333800

C	-1.85108100	6.82755300	-5.50693300
H	-2.41611000	4.86895300	-4.80032400
C	-0.86810400	7.81965400	-5.50671600
H	1.07174700	8.40122700	-4.76414400
H	-2.76302200	6.96447200	-6.08136500
H	-1.01781400	8.73628900	-6.06980700
C	2.65162600	3.72865800	-5.65443300
C	3.83977900	4.51000000	-5.50586500
C	2.40322300	3.05178900	-6.88953000
C	4.73991300	4.59847500	-6.55194000
H	4.01804900	5.02351000	-4.56687000
C	3.31487900	3.15390600	-7.92527100
H	1.49677200	2.46458000	-6.99289200
C	4.47710100	3.92286500	-7.75527300
H	5.64566900	5.18668900	-6.44702200
H	3.13494800	2.64263400	-8.86526900
H	5.18879400	3.99795000	-8.57269100
Au	-2.72644100	4.75353500	-1.63337000
P	-4.59743900	5.94750300	-0.74981900
H	-4.33955900	7.13858000	-0.04351700
H	-5.57803800	6.40592100	-1.65128900
H	-5.41512100	5.28062900	0.18284900

TS4

O	-0.16462600	1.43030700	-2.37823200
C	-1.02215800	2.32885900	-1.68356600
H	-1.99526800	1.83160000	-1.65453800
H	-0.68245400	2.43870000	-0.63715500
C	1.08411100	1.97969100	-2.70686700
H	1.62534600	2.32139000	-1.80853200
H	1.66812700	1.19698400	-3.19434300
C	-1.14877800	3.71391500	-2.28477100
C	0.86068800	3.18682400	-3.61783800
C	-0.26190900	4.06794500	-3.24746600
C	1.66593100	3.52815200	-4.60398500
C	-0.16736800	5.31200900	-4.03326500
C	-0.35438600	6.60445900	-3.53633100
C	0.40547500	5.14939100	-5.32931300
C	0.06725500	7.70380000	-4.28557000
H	-0.74741300	6.74591800	-2.53452300
C	0.84170400	6.27594700	-6.06941200
H	0.13938000	4.25878600	-5.89804700
C	0.68124400	7.54592000	-5.54287700
H	-0.04111800	8.70150600	-3.86911700
H	1.25618500	6.13766000	-7.06373400
H	1.00821800	8.41908600	-6.09855100
C	2.73757400	3.21796100	-5.47599300
C	3.99630000	3.84691000	-5.30330300
C	2.57366600	2.26014100	-6.50987300
C	5.06341100	3.50330600	-6.12233900
H	4.11297000	4.58918700	-4.52007200
C	3.64731800	1.92849600	-7.32510200
H	1.60801700	1.78216300	-6.64491300
C	4.88915100	2.54825500	-7.13216600
H	6.03066000	3.97524100	-5.98124500
H	3.52536500	1.18703900	-8.10849000
H	5.72542300	2.28555300	-7.77352100
Au	-2.69742800	4.84787000	-1.57247500
P	-4.57647400	6.06624800	-0.71732800
H	-4.33471200	7.25555700	-0.00228000
H	-5.53514800	6.52539200	-1.64139200
H	-5.41303400	5.39584100	0.19550400

IN3

O	-0.12247300	1.51107100	-2.67466500
C	-0.87026600	2.39760200	-1.87094200
H	-1.84154700	1.91536600	-1.71842000
H	-0.41577500	2.50370600	-0.86325300
C	1.13455100	2.03349000	-3.08878000
H	1.77231300	2.23869500	-2.21106600
H	1.61827400	1.25266200	-3.67689400
C	-1.05970900	3.79462600	-2.41149300
C	0.91234200	3.29984300	-3.86629700
C	-0.19857200	4.16265800	-3.42676300
C	1.61799800	3.86593300	-4.87519400
C	-0.13737600	5.36758100	-4.20115900
C	-0.76700700	6.61051300	-4.09179400
C	0.88779800	5.15410800	-5.26409500
C	-0.27581900	7.67919300	-4.83061300
H	-1.56551000	6.76601500	-3.37350300
C	1.45734400	6.36395600	-5.89975300
H	0.25643500	4.79181800	-6.11924000
C	0.84150500	7.56666900	-5.71341200
H	-0.73584700	8.65595400	-4.70630800
H	2.27983000	6.24599400	-6.59834800
H	1.19636400	8.45306200	-6.22937100
C	2.77868600	3.33614700	-5.61570400
C	3.95897100	4.09239800	-5.73220800
C	2.72664000	2.06547700	-6.21624400
C	5.06094200	3.58551900	-6.42007500
H	4.02616000	5.06643300	-5.25392000
C	3.82838300	1.56344600	-6.90774800
H	1.81247800	1.48132600	-6.15583300
C	4.99726600	2.32122300	-7.01065100
H	5.97034500	4.17506700	-6.49084100
H	3.77205500	0.58255000	-7.37055800
H	5.85445600	1.92898000	-7.54981500
Au	-2.52723000	4.89283400	-1.51810600
P	-4.29673000	6.06163900	-0.38537200
H	-3.93498300	6.98227300	0.61652900
H	-5.16826300	6.85470800	-1.15613900
H	-5.22628700	5.27172600	0.31673700

TS5

O	-0.21080000	1.48373900	-2.73032400
C	-0.88162900	2.37663300	-1.86315500
H	-1.85216700	1.91502000	-1.65997000
H	-0.35781200	2.45737900	-0.88899300
C	1.04787100	1.95901300	-3.17999500
H	1.74853100	2.07121000	-2.33284600
H	1.45279000	1.19398100	-3.84426700
C	-1.06783900	3.78169300	-2.39743300
C	0.87774000	3.28751700	-3.86060800
C	-0.20902800	4.14877000	-3.39641400
C	1.62487100	3.89059700	-4.83542000
C	-0.10545200	5.39860200	-4.15582600
C	-0.75637500	6.66615800	-4.09604200
C	1.03631000	5.22114000	-5.07343600
C	-0.31073100	7.69087400	-4.90003200
H	-1.58278000	6.80789000	-3.40773300
C	1.46788000	6.32865500	-5.87938600
H	-0.17229000	5.02849600	-5.45017500
C	0.79186400	7.52207200	-5.78906000
H	-0.80595300	8.65602000	-4.85865800

H	2.32109800	6.20365100	-6.53707500
H	1.10498200	8.36227200	-6.40109900
C	2.78961800	3.36065900	-5.57811600
C	4.01071900	4.05702700	-5.58527700
C	2.69290900	2.15224500	-6.28878800
C	5.10883500	3.55342400	-6.28278100
H	4.11000100	4.98013000	-5.01929100
C	3.79269600	1.65124700	-6.98465700
H	1.74785600	1.61631700	-6.31129500
C	5.00199200	2.35015200	-6.98340500
H	6.04914200	4.09685600	-6.27237100
H	3.70295600	0.71796400	-7.53277000
H	5.85724400	1.95881900	-7.52626700
Au	-2.52625400	4.89044700	-1.49735500
P	-4.27884200	6.06900100	-0.34816100
H	-4.08197500	7.42858900	-0.03881500
H	-5.53928500	6.13219100	-0.97241900
H	-4.64621000	5.57306700	0.91693400

IN4

O	-0.07748800	1.51092800	-2.57997700
C	-0.70107800	2.45003100	-1.71971800
H	-1.60431200	1.95266200	-1.35805600
H	-0.07168300	2.65779200	-0.83142000
C	1.07781400	1.99482600	-3.22862800
H	1.91055200	2.15174800	-2.51435900
H	1.39874100	1.21892500	-3.92719700
C	-1.04116200	3.77423700	-2.37308200
C	0.80642500	3.30069400	-3.91172100
C	-0.26886300	4.12560500	-3.44456400
C	1.53298400	3.91457100	-4.94413200
C	-0.30339300	5.33273200	-4.36629100
C	-0.63501700	6.73935500	-3.98986700
C	0.94635100	5.17816600	-5.18023000
C	-0.09580100	7.75936500	-4.70122600
H	-1.39612100	6.91247600	-3.23487300
C	1.39614100	6.25486400	-5.97847100
H	-1.12444300	5.09461000	-5.08482600
C	0.87860300	7.50752700	-5.73541500
H	-0.38815400	8.78564600	-4.50235500
H	2.20600600	6.11211000	-6.68648600
H	1.25429800	8.35443000	-6.30340400
C	2.72587000	3.36591100	-5.63129000
C	3.95035500	4.05381800	-5.59209900
C	2.64733300	2.15052100	-6.33177600
C	5.07245000	3.53316400	-6.23723900
H	4.02947100	4.98401800	-5.03581200
C	3.77044700	1.63557000	-6.97827400
H	1.69988300	1.62115200	-6.39120100
C	4.98468200	2.32463100	-6.93095100
H	6.01577600	4.06946900	-6.19282900
H	3.69559000	0.69888300	-7.52267700
H	5.85885900	1.92094000	-7.43305300
Au	-2.56553100	4.84002300	-1.53485800
P	-4.39609200	5.98362000	-0.47232900
H	-4.27388600	7.36651100	-0.23644800
H	-5.64710200	5.94774200	-1.11729600
H	-4.75953200	5.53982500	0.81312900

TS6

O	-0.21789300	1.46467600	-2.71638700
C	-0.81520100	2.36949300	-1.81861000
H	-1.75150200	1.90390400	-1.49623800

H	-0.20285600	2.50915100	-0.90117700
C	1.02337100	1.90667000	-3.25494100
H	1.78147600	1.98132600	-2.45528100
H	1.35031400	1.12953700	-3.94721900
C	-1.07024700	3.75024700	-2.37044300
C	0.85056400	3.24353600	-3.92143100
C	-0.24897500	4.09451100	-3.43901500
C	1.60254100	3.89656300	-4.85493600
C	-0.09502000	5.42559300	-4.20698200
C	-0.78795500	6.65156100	-4.15648800
C	1.03667500	5.23124200	-5.05545100
C	-0.33519000	7.68597800	-4.96215000
H	-1.65743300	6.77650500	-3.51808000
C	1.45169400	6.28456700	-5.87551300
H	-1.01412700	4.42463800	-4.37208400
C	0.76602500	7.49762100	-5.82027700
H	-0.84006500	8.64620600	-4.93841500
H	2.30318200	6.15888800	-6.53594200
H	1.08802700	8.31905700	-6.45330700
C	2.78666400	3.37622200	-5.57468200
C	4.00510200	4.07567900	-5.54104900
C	2.71050500	2.17620100	-6.30108300
C	5.12308500	3.57876300	-6.21089400
H	4.08282300	4.99696300	-4.96994100
C	3.82879900	1.68511800	-6.97394200
H	1.76616500	1.64150000	-6.35929600
C	5.03737200	2.38379800	-6.92855900
H	6.06174000	4.12354700	-6.16916700
H	3.75440200	0.76012800	-7.53821000
H	5.90783500	1.99985800	-7.45224100
Au	-2.51753900	4.87538200	-1.48204900
P	-4.22805800	6.11126600	-0.33478300
H	-3.82415900	7.24487200	0.39467600
H	-5.26958400	6.65315300	-1.11059300
H	-4.96089900	5.41326600	0.64246900

IN5

O	-1.09192300	0.99386900	-3.73424800
C	-1.27718300	1.92416500	-2.67481000
H	-2.32294700	1.86182000	-2.35090000
H	-0.63311200	1.67662400	-1.81790300
C	0.07763100	1.39127900	-4.43284900
H	0.99074000	1.08676200	-3.89876300
H	0.05228200	0.89470800	-5.40824200
C	-0.94129700	3.31475200	-3.20074000
C	-0.01709500	2.90419600	-4.54020400
C	-1.38078900	3.53463000	-4.63020200
C	0.96196200	3.89572300	-4.89861000
C	-1.13374600	4.90507600	-5.14602100
C	-2.02637700	5.92341400	-5.45228700
C	0.27062500	5.10460000	-5.28429500
C	-1.51473300	7.13163800	-5.93903400
H	-3.09741800	5.77978800	-5.34711000
C	0.77057400	6.32353900	-5.78572000
H	-2.21406600	2.94064900	-5.00322200
C	-0.13260900	7.32843700	-6.10830400
H	-2.20085500	7.92711800	-6.21533800
H	1.83175500	6.46399800	-5.95877600
H	0.22766200	8.26798200	-6.51514800
C	2.40269000	3.70925800	-4.88009100
C	3.25642000	4.74663900	-4.43704200
C	2.98041200	2.49005000	-5.30172000

C	4.63378700	4.56175400	-4.40627500
H	2.82838300	5.67232900	-4.06770600
C	4.36135700	2.32547500	-5.30011100
H	2.35138200	1.69585500	-5.68763700
C	5.18996800	3.35574700	-4.84588900
H	5.27678700	5.35605100	-4.03985900
H	4.79281500	1.39392800	-5.65274900
H	6.26712800	3.21900100	-4.83299200
Au	-0.54919100	4.78780500	-1.81660200
P	-0.19876800	6.42025300	-0.10384400
H	0.91315700	7.27854800	-0.20924200
H	-1.22127500	7.36415300	0.11150200
H	-0.01886000	5.93999300	1.20732600

TS7

O	-0.43126400	1.38059900	-2.93544600
C	-0.98885600	2.26272200	-1.99986800
H	-1.94609400	1.83030200	-1.69332700
H	-0.37331200	2.34915600	-1.07779000
C	0.84248900	1.78934700	-3.44812100
H	1.58271500	1.81180400	-2.63037300
H	1.14409700	1.00611200	-4.14428400
C	-1.15025500	3.69018900	-2.45652500
C	0.71517600	3.14031500	-4.09028200
C	-0.40588200	4.01630300	-3.62774300
C	1.53077100	3.85248500	-4.91276000
C	-0.20164700	5.34244300	-4.29885300
C	-0.95509400	6.50553500	-4.30667600
C	0.96931700	5.22082500	-5.07585400
C	-0.51031500	7.58544100	-5.08543000
H	-1.87793100	6.58900900	-3.73778100
C	1.39761100	6.28506600	-5.86148300
H	-1.46240800	3.54941800	-3.96589600
C	0.64991000	7.47271700	-5.85169100
H	-1.08026600	8.50920200	-5.09891200
H	2.28695100	6.20048000	-6.47708200
H	0.97527200	8.31222300	-6.45873300
C	2.78804700	3.39142500	-5.52808900
C	3.95415500	4.17417100	-5.44237700
C	2.84488000	2.16072500	-6.20665600
C	5.14774100	3.72707700	-6.00677500
H	3.93051900	5.12031000	-4.90945000
C	4.03679400	1.72360500	-6.78083100
H	1.94329600	1.56448000	-6.31571400
C	5.19193300	2.50292300	-6.67818200
H	6.04371000	4.33499700	-5.92230000
H	4.06267400	0.77770200	-7.31376900
H	6.12106600	2.15967500	-7.12339800
Au	-2.38821100	4.93284700	-1.40964700
P	-3.81009700	6.32927900	-0.08161300
H	-3.25805200	7.53007500	0.40029800
H	-4.99071000	6.79696200	-0.68698400
H	-4.31705100	5.76688700	1.10364000

IN6

O	-1.02181100	1.22849000	-3.68196600
C	-2.14770400	1.90754100	-3.16543500
H	-3.02164700	1.42525200	-3.61548700
H	-2.21863800	1.75481900	-2.07600900
C	0.22106700	1.88622200	-3.43845400
H	0.36372000	2.03710200	-2.35240400
H	1.00216900	1.20802000	-3.78020500

C	-2.17402700	3.40370200	-3.52943100
C	0.21601600	3.20137500	-4.16687100
C	-1.03807800	3.92984800	-4.16201800
C	1.15573900	3.91431800	-4.87231500
C	-0.84041600	5.17632700	-4.93186700
C	-1.71431700	6.18591500	-5.30177100
C	0.50692400	5.17051700	-5.36335100
C	-1.22683600	7.22789700	-6.11351100
H	-2.75428500	6.18059600	-4.98555400
C	0.97742600	6.18106800	-6.18442300
H	-3.15019400	3.82963500	-3.76989300
C	0.09576700	7.22229100	-6.54538000
H	-1.89211100	8.03161500	-6.41260900
H	1.99351000	6.17249700	-6.56440500
H	0.45604200	8.02399000	-7.18289400
C	2.54763700	3.55039600	-5.14695500
C	3.57363900	4.50729500	-5.00685200
C	2.88882300	2.24588000	-5.55717000
C	4.90124400	4.16041000	-5.24610700
H	3.33087000	5.51207600	-4.67457400
C	4.21483700	1.91132000	-5.81672400
H	2.10636800	1.51115800	-5.71950700
C	5.22481600	2.86426500	-5.65516600
H	5.68344400	4.90240300	-5.11632500
H	4.46096300	0.90807600	-6.15134200
H	6.25903500	2.59892900	-5.85309900
Au	-1.67017100	4.65255900	-1.74560500
P	-1.38751500	5.85919400	0.25859700
H	-0.40389600	6.86454200	0.26797600
H	-2.51488900	6.56264500	0.71810700
H	-1.03784600	5.11053300	1.39632400

TS3

O	-0.26163400	2.22353800	0.43178500
C	-0.46356000	3.42676500	1.12096400
H	-1.41765500	3.33554000	1.64836800
H	0.32369000	3.61446100	1.86981200
C	0.99924900	2.24090600	-0.23279700
H	1.80485300	2.03345800	0.48854200
H	0.96990100	1.42865000	-0.96400900
C	-0.53313700	4.57965800	0.18407100
C	1.28026200	3.53623400	-0.89489400
C	-0.98748700	5.63770700	-0.34650200
C	1.93391600	4.28750200	-1.61787000
C	-0.63724100	6.68220900	-1.30999100
C	-1.41096800	6.87807500	-2.46763100
C	0.47223300	7.50884900	-1.06364000
C	-1.05457600	7.86689200	-3.38227600
H	-2.27210500	6.24262100	-2.65367000
C	0.81291100	8.50274900	-1.97853100
H	1.05880900	7.36527100	-0.16192100
C	0.05460100	8.68169300	-3.13862300
H	-1.64633500	8.00513100	-4.28225600
H	1.67373800	9.13613100	-1.78686900
H	0.32342800	9.45865300	-3.84809400
C	2.68876000	5.14522600	-2.45394800
C	3.84704400	5.78304200	-1.95460900
C	2.32326100	5.32567300	-3.80686000
C	4.61761000	6.57988300	-2.79329000
H	4.13075700	5.63528000	-0.91731100
C	3.10264400	6.12454400	-4.63585100
H	1.43497400	4.83206400	-4.18735100

C	4.24797800	6.75060800	-4.13224800
H	5.51103200	7.06308700	-2.40957200
H	2.82337200	6.25691000	-5.67668300
H	4.85658700	7.36938700	-4.78532700
Au	-2.89097800	5.91340700	0.60975100
P	-4.99770300	6.40857800	1.52690100
H	-5.55943200	7.64237800	1.15342600
H	-6.04616100	5.52062600	1.22657900
H	-5.08126400	6.47667400	2.92915700

IN7

O	0.91586600	1.77215500	0.15530400
C	-0.13184800	2.71030500	0.39344600
H	-1.07322900	2.16036300	0.44568400
H	0.03052700	3.23717700	1.34752100
C	1.99557200	2.46928900	-0.40065600
H	2.58167400	3.01285000	0.35794400
H	2.64096400	1.76958800	-0.93452800
C	-0.06048000	3.67695300	-0.78359500
C	1.32307200	3.53257500	-1.31918400
C	-0.99116400	4.47750700	-1.32243300
C	1.90448600	4.11177300	-2.31586300
C	-0.62770500	5.31648900	-2.48299400
C	-0.90095900	4.88395900	-3.79910400
C	-0.00318500	6.56952200	-2.29664100
C	-0.53113800	5.66600300	-4.88980500
H	-1.40501400	3.93338900	-3.94989500
C	0.35243800	7.35353400	-3.39223400
H	0.18335800	6.92173000	-1.28577600
C	0.09768300	6.90139600	-4.69061900
H	-0.74548200	5.32206700	-5.89774500
H	0.82033400	8.32121600	-3.23495000
H	0.36910500	7.51618400	-5.54391200
C	2.72525000	4.58749600	-3.32178900
C	3.60633500	5.68350500	-3.07781400
C	2.73300500	3.95550900	-4.60129000
C	4.48202300	6.09898400	-4.06608500
H	3.58572200	6.16887000	-2.10786000
C	3.61628100	4.38466300	-5.57823900
H	2.05076700	3.13238300	-4.78440800
C	4.48944600	5.44899000	-5.31011400
H	5.16357900	6.92278200	-3.88011600
H	3.63526000	3.89783400	-6.54797200
H	5.18219200	5.77776500	-6.07961100
Au	-2.91483300	4.60986300	-0.61841100
P	-5.16706600	4.79597100	0.16626900
H	-6.01338000	5.71138000	-0.48866200
H	-5.97152600	3.64065000	0.12624900
H	-5.36370700	5.18865400	1.50435700

TS8

O	0.76173700	1.92771200	0.03780900
C	-0.10079500	3.02681000	0.33487000
H	-1.10419600	2.63497800	0.50997100
H	0.24129400	3.55511000	1.24054000
C	1.88781700	2.43617300	-0.63259400
H	2.64658600	2.82216400	0.06793800
H	2.32810000	1.64694800	-1.24555500
C	-0.00074400	3.90885200	-0.89584800
C	1.33955100	3.63126400	-1.45456500
C	-0.93834500	4.66136600	-1.51167100
C	1.98366800	4.20583200	-2.43454400

C	-0.57394600	5.35616600	-2.74482900
C	-1.37467400	5.28056900	-3.90442200
C	0.65155800	6.07734200	-2.81951700
C	-0.96635200	5.88612500	-5.08365900
H	-2.30628800	4.72403700	-3.86761500
C	1.02591200	6.73496400	-4.01525900
H	1.14858700	6.35788900	-1.89487000
C	0.23541000	6.62481400	-5.14270800
H	-1.58361200	5.79694600	-5.97314100
H	1.93492500	7.32872500	-4.03576500
H	0.51945100	7.12074900	-6.06577700
C	3.17901300	4.41824800	-3.15380900
C	4.29099000	5.04527400	-2.53291700
C	3.28932600	3.97108400	-4.49562200
C	5.48111300	5.19576200	-3.23122000
H	4.20131000	5.39493100	-1.50900700
C	4.48786100	4.11985000	-5.17910100
H	2.43183700	3.50356000	-4.96842700
C	5.57985500	4.73326800	-4.55033200
H	6.33518900	5.66634300	-2.75438900
H	4.57937400	3.76263700	-6.19998800
H	6.51406800	4.85143000	-5.09163100
Au	-2.86507600	4.81775000	-0.80339400
P	-5.09214200	5.03629500	0.03332500
H	-5.84603300	6.14236000	-0.40362200
H	-5.99997900	3.99305200	-0.23206000
H	-5.25213900	5.15862200	1.42692700

IN8

O	0.59014300	1.46225800	-0.95661400
C	-0.44894900	2.37845500	-0.65304800
H	-1.41378300	1.91013600	-0.87961800
H	-0.45341200	2.65318000	0.41779800
C	1.71685000	2.16760400	-1.47078300
H	2.46463900	2.36000300	-0.68359000
H	2.18587800	1.54169300	-2.23296000
C	-0.18085400	3.60129600	-1.49021600
C	1.15026000	3.47560400	-1.99074200
C	-1.03868800	4.67363900	-1.72393700
C	1.74556400	4.46939600	-2.71448800
C	-0.52566600	5.69428600	-2.55548300
C	-1.33108500	6.76987200	-3.02675000
C	0.93142600	5.71604700	-2.95472400
C	-0.89596000	7.63136100	-4.00283200
H	-2.34476200	6.84761100	-2.64627600
C	1.27426300	6.57683000	-4.13260400
H	1.33265900	6.36638400	-2.12789600
C	0.40582400	7.50853000	-4.59135900
H	-1.56367400	8.40853700	-4.36376600
H	2.27383000	6.48506600	-4.54272200
H	0.68460400	8.16123800	-5.41259300
C	3.15458600	4.40955200	-3.16362600
C	4.07399100	5.41966300	-2.82259900
C	3.59554400	3.32760000	-3.94720900
C	5.40046800	5.33955000	-3.24217800
H	3.76246700	6.25463000	-2.19944100
C	4.92015900	3.26003000	-4.37702200
H	2.89176600	2.55676600	-4.24646900
C	5.82625600	4.26139100	-4.02227600
H	6.10265000	6.11642500	-2.95490800
H	5.24241300	2.42475600	-4.99146500
H	6.85933800	4.20267900	-4.35117900

Au	-2.94709200	4.67721300	-0.94446700
P	-5.15009200	4.63257900	-0.00992000
H	-5.92827000	5.80201200	-0.10803500
H	-6.05661400	3.68529300	-0.52338100
H	-5.26657500	4.37012800	1.36846600

TS9

O	0.80678500	1.64871400	-0.61016500
C	-0.30404400	2.50514200	-0.37632000
H	-1.22458200	1.93442600	-0.53796800
H	-0.31089600	2.88056000	0.66158000
C	1.87203700	2.39843600	-1.18397100
H	2.58271400	2.74900100	-0.41568100
H	2.41892800	1.74978200	-1.87273300
C	-0.13539900	3.65180100	-1.34971400
C	1.19911400	3.57894500	-1.84822100
C	-1.04228000	4.62520800	-1.69868100
C	1.72086300	4.49347200	-2.73099000
C	-0.56944100	5.61568700	-2.64792400
C	-1.42309400	6.65458600	-3.18894800
C	0.83513100	5.55467500	-3.17803600
C	-0.98988500	7.52961600	-4.14164400
H	-2.44098300	6.69340000	-2.81594100
C	1.21352800	6.50607500	-4.20095500
H	0.45266400	6.23526800	-2.12538600
C	0.33998200	7.44983200	-4.65740500
H	-1.66478400	8.28933400	-4.52329700
H	2.21451900	6.42876700	-4.60802600
H	0.65483200	8.14438900	-5.42992300
C	3.12283300	4.41187600	-3.22951200
C	4.06316800	5.40043400	-2.89424200
C	3.52358500	3.32971100	-4.02953200
C	5.37957600	5.30267200	-3.34563400
H	3.76991700	6.23707300	-2.26471300
C	4.83993600	3.23836700	-4.48273300
H	2.79962000	2.56936800	-4.30981300
C	5.76966900	4.22248200	-4.14058900
H	6.10047500	6.06726500	-3.07164900
H	5.13702700	2.39981300	-5.10546800
H	6.79446600	4.14839600	-4.49191800
Au	-2.94802100	4.63640000	-0.92405400
P	-5.14913000	4.57151900	0.01220400
H	-6.14351100	5.36705800	-0.58816900
H	-5.80207700	3.32450100	0.03349500
H	-5.29565900	4.95722100	1.35824500

IN9

O	0.82553800	1.62649900	-0.69714200
C	-0.30841900	2.44710400	-0.43349900
H	-1.21201400	1.86529200	-0.64199300
H	-0.33515500	2.76030600	0.62369100
C	1.87561100	2.42617700	-1.22409200
H	2.57361100	2.76229100	-0.43562700
H	2.45074700	1.82886700	-1.93735000
C	-0.14258700	3.64928500	-1.34369000
C	1.19135200	3.61933000	-1.83857600
C	-1.04162700	4.63170900	-1.65970600
C	1.72105900	4.55865000	-2.71910600
C	-0.50370600	5.74015700	-2.52796200
C	-1.45581800	6.63088000	-3.25182000
C	0.84892600	5.57826800	-3.16850200
C	-1.05005100	7.42299800	-4.27417000

H	-2.47264900	6.67427000	-2.87340000
C	1.21391200	6.48226500	-4.20231100
H	-0.23321900	6.42525900	-1.67224300
C	0.30273500	7.35928200	-4.73962900
H	-1.74903600	8.09872700	-4.75676300
H	2.21730500	6.42443400	-4.60841600
H	0.60752800	8.00682200	-5.55686400
C	3.12861800	4.44655000	-3.20991300
C	4.10593900	5.35425400	-2.77269100
C	3.49279900	3.42181600	-4.09763800
C	5.42524400	5.23463600	-3.21212200
H	3.83546300	6.14729600	-2.08014400
C	4.81218700	3.30748300	-4.53723400
H	2.74034300	2.72297600	-4.45406900
C	5.78003200	4.21156000	-4.09381500
H	6.17480400	5.93868700	-2.86295800
H	5.08229000	2.51410400	-5.22786800
H	6.80685700	4.11951700	-4.43498900
Au	-2.93038600	4.66708400	-0.86429700
P	-5.13291300	4.62313400	0.08535700
H	-6.12528300	5.41985200	-0.51643400
H	-5.79011100	3.37882300	0.11934200
H	-5.26703000	5.02019300	1.42925800

TS10

O	0.84942200	1.65151900	-0.59496500
C	-0.28801800	2.47625100	-0.38420700
H	-1.19070100	1.88621100	-0.58047000
H	-0.33835500	2.83709800	0.65805900
C	1.88981100	2.40294500	-1.21443800
H	2.63316400	2.75081700	-0.47705000
H	2.40828600	1.75544500	-1.92661200
C	-0.11324800	3.63697200	-1.33740800
C	1.18948900	3.58107400	-1.85199100
C	-1.03962100	4.62640100	-1.67253500
C	1.69401000	4.52103200	-2.75305100
C	-0.52496700	5.67418200	-2.61120600
C	-1.40229000	6.70997500	-3.13069700
C	0.82627200	5.55949900	-3.18463000
C	-0.97837000	7.56543000	-4.10391500
H	-2.40279700	6.78314100	-2.71572000
C	1.20691700	6.49429000	-4.18947400
H	-0.41759900	5.89689400	-1.41796100
C	0.33829800	7.45762900	-4.63862700
H	-1.64980300	8.32902100	-4.48405400
H	2.20001600	6.41530000	-4.61536700
H	0.65322700	8.14445300	-5.41818200
C	3.09835800	4.41588100	-3.24452200
C	4.04740500	5.39378500	-2.90444800
C	3.49256400	3.32328800	-4.03365700
C	5.36733300	5.27528000	-3.34086000
H	3.75520600	6.23897000	-2.28675400
C	4.81101500	3.21425700	-4.47580200
H	2.76218400	2.57100400	-4.31954300
C	5.75075800	4.18702400	-4.12741400
H	6.09507400	6.03244100	-3.06437900
H	5.10250700	2.37057300	-5.09426200
H	6.77779500	4.09770100	-4.46855000
Au	-2.95354100	4.63545800	-0.90487300
P	-5.16509300	4.54157100	-0.01473000
H	-6.22107800	4.94391500	-0.85349300
H	-5.62910500	3.28072700	0.40361600

H	-5.43316900	5.31279500	1.13153900
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IN10

O	0.74314600	2.09045400	0.01569700
C	-0.07771600	3.17144000	0.42886500
H	-1.05724100	2.78063700	0.71777500
H	0.34869100	3.69848400	1.30169100
C	1.69392200	2.56804400	-0.93980900
H	2.64170600	2.85066600	-0.45327500
H	1.90321500	1.75438700	-1.63745900
C	-0.08421000	4.10815300	-0.75888100
C	1.02775100	3.78230100	-1.56131400
C	-0.89870000	5.22624100	-1.04114800
C	1.43890100	4.60047800	-2.60542400
C	-0.49469200	6.10722100	-2.12860100
C	-1.20982300	7.29602800	-2.40234000
C	0.65401500	5.77145600	-2.92472300
C	-0.83444600	8.11910900	-3.44531700
H	-2.06074700	7.55412700	-1.77705600
C	0.98366900	6.62241000	-4.01371800
H	-1.55229400	5.63011900	-0.26647100
C	0.25778400	7.76832500	-4.26708000
H	-1.38512800	9.03479600	-3.63849100
H	1.81965100	6.36117900	-4.65165300
H	0.53053200	8.40631500	-5.10204200
C	2.68816500	4.27687500	-3.34516000
C	3.77161700	5.17302500	-3.34960900
C	2.81502800	3.05149300	-4.02095200
C	4.95483000	4.84493400	-4.01078600
H	3.69268600	6.11673000	-2.81741500
C	3.99353500	2.73505200	-4.69564200
H	1.97933800	2.35686200	-4.03902900
C	5.06718100	3.62851200	-4.68783000
H	5.78913000	5.53992300	-3.99532000
H	4.07326900	1.79109000	-5.22664600
H	5.98752500	3.37756700	-5.20665000
Au	-2.34693100	3.88564000	-2.12330500
P	-3.98820300	2.64807800	-3.23501800
H	-4.27479600	3.02463500	-4.55901100
H	-3.75236400	1.26890700	-3.37316700
H	-5.26565000	2.66334800	-2.64881600

SbF6

Sb	3.49985200	1.61326600	-0.80370200
F	1.76198500	0.95356500	-1.00928200
F	3.37503300	2.46038800	-2.46616600
F	2.81971800	3.14412600	0.02769300
F	5.23737000	2.27283300	-0.59797400
F	3.62425600	0.76592600	0.85846400
F	4.17859900	0.08265700	-1.63652700

IN1_M06

O	-1.09594400	0.38097400	-2.78101900
C	-2.03284700	1.40814300	-2.66567200
H	-2.87623800	1.16122300	-3.32483600
H	-2.43179100	1.48361200	-1.63968100
C	-0.33929800	0.14585100	-1.60227900
H	-1.00785000	-0.21743800	-0.80126400
H	0.34284800	-0.67405200	-1.85504300
C	-1.48606100	2.72165000	-3.10361300
C	0.39267900	1.32015000	-1.14321800
C	-0.78052600	3.50101600	-3.76082400

C	0.93615600	2.35331700	-0.81737900
C	0.02300100	4.43301600	-4.47887300
C	1.10473000	5.05865500	-3.83457700
C	-0.26836000	4.73351400	-5.81874500
C	1.87528200	5.98013200	-4.52547200
H	1.32692300	4.80837200	-2.79736500
C	0.51719400	5.64990400	-6.50200600
H	-1.10443600	4.23926700	-6.30986700
C	1.58250100	6.27537000	-5.85630100
H	2.71364200	6.46286500	-4.02600600
H	0.29814000	5.88058000	-7.54211200
H	2.19276000	6.99520100	-6.39831300
C	1.53960700	3.60366300	-0.49282700
C	0.77080800	4.61260600	0.10843300
C	2.87445500	3.87087400	-0.83104100
C	1.31980200	5.86555200	0.35030900
H	-0.26041000	4.39859400	0.39183700
C	3.41777800	5.12611400	-0.58640500
H	3.47069500	3.08708100	-1.29459800
C	2.64216100	6.12689800	-0.00291400
H	0.71265700	6.63598300	0.82683500
H	4.45520700	5.32471900	-0.84898100
H	3.07474900	7.10705900	0.18902500
P	-2.83629400	6.47277700	-0.79290300
C	-4.64528900	6.58871700	-0.79537500
C	-5.32958500	6.32604700	-1.98742500
C	-5.35052900	6.98388400	0.34436900
C	-6.71033900	6.46290100	-2.03795500
H	-4.77672200	6.01969900	-2.87758700
C	-6.73479900	7.11264000	0.28781000
H	-4.82233400	7.18967400	1.27510000
C	-7.41223700	6.85304600	-0.89921900
H	-7.24197000	6.25865300	-2.96497500
H	-7.28545400	7.41503800	1.17612100
H	-8.49505600	6.95236900	-0.93835500
C	-2.19491300	7.99772400	-1.54061700
C	-0.88755200	8.00757700	-2.04008200
C	-2.96716500	9.16186300	-1.57753900
C	-0.35818800	9.17681300	-2.57092500
H	-0.28050400	7.09990400	-2.00913800
C	-2.43030400	10.32863100	-2.11222700
H	-3.98618100	9.15663500	-1.19066300
C	-1.13001500	10.33543400	-2.60867700
H	0.65708700	9.18122500	-2.96279400
H	-3.03206100	11.23453400	-2.14325800
H	-0.71665000	11.24978700	-3.02987600
C	-2.30707200	6.47007500	0.94172900
C	-2.39943400	5.27893400	1.67022800
C	-1.83768300	7.63188500	1.56037400
C	-2.01160000	5.24711200	3.00373900
H	-2.77232200	4.37233500	1.18788400
C	-1.45186300	7.59369200	2.89748200
H	-1.76884600	8.56335100	0.99853300
C	-1.53252300	6.40411200	3.61476400
H	-2.07730200	4.31835800	3.56637600
H	-1.08365100	8.49765700	3.37836500
H	-1.22169400	6.37744900	4.65708800
Au	-2.04638800	4.62431500	-2.01231900

TS1_{M06}

O	-0.29884600	0.95175000	-1.37596900
C	-0.99022700	2.07582800	-0.86675500

H	-1.88212400	1.66916100	-0.36761000
H	-0.38157300	2.53952600	-0.07117800
C	1.10055400	1.12341200	-1.48720000
H	1.51834800	1.61908600	-0.59542300
H	1.53613000	0.11731600	-1.54217800
C	-1.47575500	3.17399000	-1.77031200
C	1.34571100	1.86416000	-2.72170000
C	-1.71451400	3.49152900	-3.01101800
C	1.01314200	2.35173900	-3.78309500
C	-2.22944100	4.70647100	-3.66699100
C	-1.35094800	5.73313700	-4.02572600
C	-3.59674000	4.84707500	-3.93184100
C	-1.83156900	6.87894300	-4.65437100
H	-0.29004200	5.62741000	-3.79871000
C	-4.07370600	5.99222800	-4.55689500
H	-4.28187000	4.05386600	-3.63152500
C	-3.19019000	7.00505300	-4.92870900
H	-1.14201500	7.67474500	-4.92910000
H	-5.13997700	6.09844800	-4.74949300
H	3.56361000	7.89782200	-5.42803500
C	0.04830300	2.71198500	-4.74710400
C	0.23506600	3.45687300	-5.90636900
C	-1.27580400	2.24801000	-4.38707300
C	-0.83738700	3.64629700	-6.77258600
H	1.21921700	3.85158900	-6.14706100
C	-2.30818700	2.36762300	-5.36632600
H	-1.30693800	1.38262300	-3.72276400
C	-2.10240300	3.08973100	-6.51844100
H	-0.68276100	4.21677400	-7.68678000
H	-3.27673300	1.91310900	-5.16267500
H	-2.90269000	3.21725900	-7.24331400
Au	-2.15580900	4.85445800	-0.59529600
P	-2.83758700	6.69381900	0.72699100
C	-1.49495200	7.89363100	0.96612100
C	-1.73050400	9.27069200	0.96199400
C	-0.20633700	7.40726800	1.21020300
C	-0.68021700	10.15188700	1.19937800
H	-2.73253700	9.65577300	0.77300100
C	0.83701000	8.29149400	1.45324300
H	-0.02476700	6.33084500	1.21027100
C	0.59981400	9.66393500	1.44444600
H	-0.86369500	11.22443500	1.19252000
H	1.83829100	7.91027500	1.64331800
H	1.41803900	10.35757200	1.62783000
C	-4.20770600	7.59917900	-0.04771200
C	-5.24203000	8.15403300	0.71081000
C	-4.18826400	7.77287700	-1.43550700
C	-6.24831800	8.88024100	0.08172900
H	-5.26262700	8.01782100	1.79211100
C	-5.19371600	8.50380700	-2.05598000
H	-3.38418500	7.33562100	-2.03304500
C	-6.22420900	9.05533900	-1.29863400
H	-7.05474100	9.30960800	0.67273200
H	-5.17415700	8.63706500	-3.13659600
H	-7.01511100	9.62092500	-1.78757600
C	-3.40598100	6.21571500	2.38395700
C	-3.07639900	6.96051300	3.51893400
C	-4.23066600	5.09177600	2.50072400
C	-3.57029400	6.57805800	4.76254100
H	-2.43331100	7.83636100	3.43418800
C	-4.72651900	4.71975600	3.74346400
H	-4.48408600	4.51024500	1.61208500

C	-4.39309200	5.46194900	4.87446900
H	-3.30949200	7.15549200	5.64723100
H	-5.36875100	3.84590500	3.83178800
H	-4.77496500	5.16471200	5.84918900

TS2_{M06}

O	0.84672800	1.79727000	-1.21134500
C	-0.21419700	2.48483100	-0.60926500
H	-1.01747200	1.75269000	-0.46964500
H	0.07550400	2.84809500	0.39516000
C	1.91476300	2.62707300	-1.57025200
H	2.16682300	3.32910400	-0.75513200
H	2.77985800	1.97604200	-1.73913200
C	-0.70657000	3.65362500	-1.39574700
C	1.62829900	3.38153000	-2.81349200
C	-0.24472400	4.30821900	-2.39868000
C	1.83697000	3.73461900	-3.97525100
C	-0.43735200	5.38660900	-3.33562300
C	0.08124700	6.66019100	-3.06051000
C	-1.17335100	5.17104900	-4.50844800
C	-0.16534600	7.71113300	-3.93383700
H	0.65584600	6.81464200	-2.14793300
C	-1.40549800	6.22436400	-5.38423700
H	-1.56855900	4.17595100	-4.71061700
C	-0.90561200	7.49258500	-5.09576900
H	0.22206200	8.70330800	-3.71170200
H	-1.98246200	6.05588400	-6.29158000
H	-1.08997500	8.31702800	-5.78270900
C	1.87661500	4.26585500	-5.27918100
C	2.46538600	5.52184000	-5.51620400
C	1.27701600	3.56041300	-6.34011300
C	2.43204200	6.06638800	-6.78933700
H	2.93416900	6.05383300	-4.69034900
C	1.25242000	4.11403300	-7.60903600
H	0.83362400	2.58543500	-6.14462100
C	1.82479300	5.36660500	-7.83172200
H	2.88475100	7.03784500	-6.97589500
H	0.78903500	3.57192900	-8.43035700
H	1.80416900	5.79865200	-8.83044500
P	-4.50830100	5.87788300	-0.48240800
C	-5.84022600	4.87898000	0.23813900
C	-6.00338800	3.56213200	-0.20431700
C	-6.72945700	5.41687100	1.17237200
C	-7.05393300	2.79222600	0.27894900
H	-5.30478000	3.14306200	-0.93096500
C	-7.77681900	4.63933900	1.65554400
H	-6.60346200	6.44067700	1.52446800
C	-7.93919400	3.33124900	1.20935500
H	-7.17952700	1.76817000	-0.06654800
H	-8.46794100	5.05689600	2.38495100
H	-8.75869100	2.72575900	1.59138200
C	-5.15040700	6.55915800	-2.04030300
C	-4.24003000	7.06740900	-2.97392900
C	-6.52200100	6.62208600	-2.30073800
C	-4.70182100	7.64316000	-4.15068100
H	-3.16468800	7.01334400	-2.78343000
C	-6.97665400	7.19414300	-3.48472600
H	-7.23518100	6.22106200	-1.58035200
C	-6.06908500	7.70576500	-4.40702600
H	-3.98884600	8.03829200	-4.87242300
H	-8.04483300	7.23839700	-3.68719000
H	-6.42954500	8.15057300	-5.33260800

C	-4.25479800	7.28659000	0.63406900
C	-3.45326600	7.10082200	1.76538800
C	-4.88196700	8.51615900	0.41779700
C	-3.28855700	8.13494900	2.67795400
H	-2.96156400	6.14018600	1.93085600
C	-4.70856400	9.54995800	1.33260300
H	-5.50487200	8.66646500	-0.46391100
C	-3.91553300	9.35962700	2.46026300
H	-2.66673600	7.98748100	3.55848500
H	-5.19524200	10.50847600	1.16340000
H	-3.78271000	10.17039400	3.17385500
Au	-2.51415200	4.68239600	-0.89810000

TS3_{M06}

O	1.09602200	2.15433200	0.94214400
C	0.51738100	3.40307300	1.15156100
H	-0.43136000	3.24957900	1.68224100
H	1.16064300	4.04853600	1.77982400
C	2.29132700	2.32390700	0.21945300
H	3.09291200	2.68910700	0.88680800
H	2.58157700	1.33858500	-0.16067300
C	0.25050200	4.07541600	-0.14340000
C	2.13756000	3.29697100	-0.88804100
C	-0.46483600	4.74985700	-0.94775300
C	2.55984900	3.81490500	-1.92518300
C	-0.32664000	5.42108700	-2.22683800
C	0.65782800	6.40471400	-2.38390400
C	-1.14781700	5.07955300	-3.31015800
C	0.84011100	7.01228300	-3.61886700
H	1.28205800	6.67454000	-1.53256200
C	-0.94509400	5.67666400	-4.54642600
H	-1.92280800	4.32373200	-3.17800200
C	0.05116800	6.63923200	-4.70321900
H	1.61948500	7.76220000	-3.74344000
H	-1.56717300	5.39283300	-5.39301600
H	0.20682100	7.10599400	-5.67418400
C	3.02698400	4.41607300	-3.11496600
C	4.00293400	5.42811300	-3.05576100
C	2.53216500	3.99705600	-4.36288400
C	4.47227400	6.00471700	-4.22434500
H	4.38126200	5.74564000	-2.08545300
C	3.00458800	4.58518600	-5.52568200
H	1.77785800	3.21329600	-4.39794900
C	3.97373700	5.58467800	-5.45799400
H	5.23280100	6.78127200	-4.17873200
H	2.62226200	4.25962600	-6.49079600
H	4.34789000	6.03747900	-6.37427800
P	-4.60144000	4.96096400	0.83763700
C	-4.82638100	3.85614200	2.25947300
C	-4.25959500	2.57756800	2.20731600
C	-5.59218600	4.23625000	3.36419900
C	-4.46738900	1.68346200	3.24958900
H	-3.66198300	2.28186800	1.34212300
C	-5.79116300	3.33771700	4.40793600
H	-6.03163300	5.23261800	3.41090700
C	-5.23190800	2.06491400	4.35006100
H	-4.02933700	0.68843200	3.20576600
H	-6.38545300	3.63422700	5.26983200
H	-5.38969300	1.36483700	5.16802500
C	-5.83488100	4.48102800	-0.40277400
C	-5.68256800	4.95238300	-1.71137300
C	-6.94447300	3.70270300	-0.06474500

C	-6.63974500	4.65257200	-2.67212700
H	-4.81365700	5.56028100	-1.97445000
C	-7.89580800	3.40020900	-1.03403300
H	-7.06531700	3.33128300	0.95270100
C	-7.74465800	3.87467700	-2.33305000
H	-6.52296600	5.02312600	-3.68847200
H	-8.75863100	2.79138800	-0.77165000
H	-8.49117000	3.63605600	-3.08797300
C	-5.02757800	6.63418600	1.39118800
C	-4.04680400	7.38937700	2.04256900
C	-6.31513000	7.15310100	1.22920400
C	-4.35420600	8.65124500	2.53475700
H	-3.04037800	6.98411000	2.16365600
C	-6.61515800	8.41971700	1.72018100
H	-7.08273700	6.57153000	0.71864600
C	-5.63789700	9.16620200	2.37174000
H	-3.58969700	9.23698100	3.04085800
H	-7.61620000	8.82602300	1.59053000
H	-5.87637300	10.15776300	2.75127400
Au	-2.41244200	4.82678300	-0.02130500

IN1_{B3PW91}

O	-0.84124700	0.82837500	-2.04825300
C	-1.59748300	1.87795800	-1.51619700
H	-2.65470400	1.62130600	-1.65254200
H	-1.42221900	2.00592900	-0.43870300
C	0.36846400	0.53852900	-1.34988100
H	0.14020800	0.31670400	-0.29499600
H	0.73406500	-0.38614300	-1.80811900
C	-1.35499700	3.17697200	-2.22310200
C	1.39694300	1.57397600	-1.42264600
C	-0.87358900	3.78905800	-3.19788000
C	2.29531200	2.39069700	-1.44705900
C	-0.31058300	4.48980700	-4.29058000
C	0.99788700	5.00791300	-4.19431300
C	-1.04221400	4.63520900	-5.48818900
C	1.55863600	5.65932200	-5.28427400
H	1.55816100	4.87974700	-3.27379700
C	-0.46898000	5.29110400	-6.56827000
H	-2.04525300	4.22461500	-5.55447200
C	0.82779000	5.80268900	-6.46629800
H	2.56845200	6.05253600	-5.21543700
H	-1.02723300	5.40181800	-7.49309900
H	1.27243100	6.31343000	-7.31609200
C	3.36097500	3.33860500	-1.50115100
C	3.49350600	4.33035400	-0.51195900
C	4.30095000	3.28467400	-2.54737800
C	4.54162700	5.24330000	-0.57151900
H	2.77686400	4.36543400	0.30372400
C	5.34636000	4.20084600	-2.59768400
H	4.20515600	2.51433700	-3.30689400
C	5.46945200	5.18143000	-1.61222200
H	4.64120200	6.00007400	0.20201500
H	6.07268900	4.14472300	-3.40401400
H	6.29119300	5.89136300	-1.65097400
P	-3.41013900	6.74347300	-0.42877000
C	-5.15546100	6.82666800	-0.93490400
C	-5.49007600	6.57733300	-2.27372000
C	-6.15847700	7.16489300	-0.01689100
C	-6.81481000	6.67406900	-2.68989700
H	-4.71496600	6.30729500	-2.98782000
C	-7.48335400	7.25514900	-0.44028100

H	-5.90908400	7.35021000	1.02402500
C	-7.81164600	7.01127300	-1.77324800
H	-7.07051000	6.47889500	-3.72749700
H	-8.25957100	7.51307700	0.27460800
H	-8.84616700	7.07873300	-2.09811400
C	-2.65138000	8.35875000	-0.78819400
C	-1.25253100	8.46282600	-0.78994000
C	-3.43545600	9.49206200	-1.03752000
C	-0.64680000	9.69290400	-1.02792000
H	-0.64001100	7.58309200	-0.60340900
C	-2.82069500	10.71940900	-1.28135700
H	-4.51910100	9.41870500	-1.04601300
C	-1.43050200	10.82110600	-1.27578700
H	0.43680300	9.77015800	-1.02666600
H	-3.43144000	11.59615900	-1.47742400
H	-0.95588900	11.77924200	-1.46836700
C	-3.38237900	6.51815800	1.37746800
C	-3.64058900	5.24290000	1.90158900
C	-3.13884200	7.59103400	2.24349800
C	-3.66114500	5.04697000	3.27907000
H	-3.83017100	4.40634600	1.23203300
C	-3.15493100	7.38555800	3.62267600
H	-2.93340200	8.58066700	1.84594200
C	-3.41578900	6.11798400	4.14016200
H	-3.86351400	4.05827700	3.68120300
H	-2.96219800	8.21922300	4.29201100
H	-3.42578500	5.96214800	5.21529500
Au	-2.27723000	5.01387500	-1.50032300

TS1_{B3PW91}

O	-1.23476700	0.78408300	-1.38766300
C	-1.85606700	1.95002800	-0.86185800
H	-2.88636000	1.64440500	-0.64064100
H	-1.38832000	2.19513100	0.10148500
C	0.17145600	0.71565400	-1.18969400
H	0.45747600	1.06468000	-0.18732700
H	0.44177000	-0.34334400	-1.26868800
C	-1.96003200	3.23080300	-1.66416100
C	0.79631000	1.49016000	-2.26292400
C	-1.88360000	3.68217300	-2.88869300
C	0.75076000	2.10382700	-3.31344800
C	-2.07982200	5.01237500	-3.49353400
C	-1.00359500	5.90074400	-3.62198800
C	-3.35203000	5.40906700	-3.93542400
C	-1.19863000	7.16727100	-4.17228900
H	-0.02029300	5.60237300	-3.27028500
C	-3.54167200	6.67396500	-4.48461500
H	-4.19073300	4.72573200	-3.83118400
C	-2.46466300	7.55482400	-4.60713800
H	-0.35922200	7.85197800	-4.25732200
H	-4.53177400	6.97363100	-4.81795200
H	-2.61435900	8.54104900	-5.03793200
C	0.03925800	2.68773100	-4.38135200
C	0.55530600	3.42319100	-5.44751900
C	-1.39256500	2.46014000	-4.27861500
C	-0.29928800	3.83023300	-6.47017200
H	1.61819900	3.63630200	-5.49808500
C	-2.19941800	2.79467200	-5.41312800
H	-1.68340100	1.58562900	-3.70011600
C	-1.66845600	3.50013700	-6.46985800
H	0.11017200	4.38841800	-7.30807600
H	-3.24865400	2.51240700	-5.40726100

H	-2.29053100	3.78638900	-7.31201300
Au	-2.56712000	4.80508600	-0.36905900
P	-3.20953000	6.40612200	1.21892800
C	-2.04471700	7.80596000	1.31162600
C	-2.48707700	9.11061700	1.56658100
C	-0.67425500	7.55653000	1.15040200
C	-1.56423400	10.15076500	1.66544900
H	-3.54755400	9.31576100	1.68290700
C	0.24255600	8.59894100	1.25611000
H	-0.32744000	6.54688200	0.94106200
C	-0.20191800	9.89663600	1.51225900
H	-1.91230200	11.16127500	1.86084900
H	1.30348800	8.39950800	1.13294600
H	0.51402500	10.71039000	1.58881400
C	-4.85345300	7.11244100	0.86955800
C	-5.77469300	7.37360200	1.89176300
C	-5.18253900	7.41737900	-0.45910300
C	-7.01087000	7.94074200	1.58479900
H	-5.53165400	7.13081900	2.92230400
C	-6.41635700	7.98893100	-0.75689200
H	-4.47419400	7.20607100	-1.25730400
C	-7.33166100	8.24959500	0.26386100
H	-7.72388500	8.13854800	2.38034000
H	-6.66745100	8.22527100	-1.78724600
H	-8.29698700	8.68922300	0.02836600
C	-3.29524100	5.67985000	2.88979400
C	-2.81795400	6.36175000	4.01576600
C	-3.87287900	4.41029000	3.03947500
C	-2.92219700	5.77789600	5.27787900
H	-2.36193800	7.34176600	3.90935600
C	-3.98056900	3.83651600	4.30296400
H	-4.23877700	3.87413000	2.16628600
C	-3.50286500	4.51912500	5.42285300
H	-2.54682800	6.30914300	6.14810700
H	-4.43153700	2.85421900	4.41347300
H	-3.58067700	4.06714100	6.40783500

TS2_{B3PW91}

O	0.29496300	1.93336300	-1.38293500
C	-0.75467500	2.72835600	-0.90244000
H	-1.63414100	2.08031400	-0.86881800
H	-0.54893700	3.06284300	0.12849600
C	1.48618400	2.64926700	-1.59782800
H	1.69599900	3.33674700	-0.76342200
H	2.28893800	1.90732300	-1.64251900
C	-1.05090400	3.95163500	-1.72727400
C	1.45565900	3.39456900	-2.88056800
C	-0.44218000	4.57097800	-2.66910500
C	1.88473600	3.67009000	-4.00157600
C	-0.36741700	5.63892100	-3.62434600
C	0.31095100	6.83029600	-3.30591800
C	-1.00348900	5.51174000	-4.87272300
C	0.32700400	7.88297800	-4.21295900
H	0.80462200	6.92135100	-2.34287300
C	-0.98144900	6.57125100	-5.77339600
H	-1.52140600	4.58840600	-5.11401500
C	-0.31859500	7.75499200	-5.44541000
H	0.83952900	8.80667900	-3.95956200
H	-1.48085300	6.47366600	-6.73312100
H	-0.30334900	8.58040500	-6.15197400
C	2.28283100	4.06378800	-5.29545200
C	3.11392700	5.19004300	-5.47499400

C	1.87404600	3.31259900	-6.41886600
C	3.51974600	5.55376800	-6.75146400
H	3.43257300	5.75954700	-4.60763900
C	2.28552100	3.68843800	-7.68987600
H	1.24511300	2.43946300	-6.27374700
C	3.10685800	4.80635300	-7.85743600
H	4.16323900	6.41796900	-6.88857100
H	1.97354000	3.10771300	-8.55308800
H	3.43156700	5.09289100	-8.85399500
P	-4.79704100	6.02419300	-0.52111600
C	-5.87064800	4.83280300	0.34410500
C	-6.00262700	3.54075900	-0.18609300
C	-6.57517100	5.18363500	1.50234000
C	-6.83776300	2.61479200	0.43216700
H	-5.45261600	3.26126200	-1.08234500
C	-7.40532000	4.24881000	2.11988700
H	-6.47338500	6.17883100	1.92535500
C	-7.53795100	2.96774900	1.58680000
H	-6.93716500	1.61578400	0.01692200
H	-7.94676100	4.52382000	3.02074200
H	-8.18377500	2.24166800	2.07275600
C	-5.76465900	6.70041500	-1.90928900
C	-5.08641500	7.33279600	-2.96126600
C	-7.16291300	6.61889900	-1.93283900
C	-5.80256500	7.88788700	-4.01804500
H	-3.99993000	7.38784600	-2.95377800
C	-7.87294300	7.17219400	-2.99735300
H	-7.69582900	6.12056600	-1.12809600
C	-7.19556900	7.80678200	-4.03749500
H	-5.27286200	8.37776300	-4.83032700
H	-8.95708800	7.10369300	-3.01353100
H	-7.75267100	8.23426500	-4.86661300
C	-4.48239000	7.39932600	0.63227300
C	-3.46690700	7.25816600	1.58913400
C	-5.24784500	8.57182800	0.59891300
C	-3.22965600	8.27504500	2.50956900
H	-2.86406300	6.35286500	1.61258700
C	-5.00067300	9.58881600	1.51993100
H	-6.03007600	8.69344600	-0.14495600
C	-3.99540800	9.44128300	2.47453000
H	-2.44321500	8.16013600	3.25027300
H	-5.59481300	10.49788200	1.48889000
H	-3.80490600	10.23685200	3.18957000
Au	-2.81230300	5.00720500	-1.22702300

TS3_{B3PW91}

O	1.13199300	2.40750100	1.11833500
C	0.53069500	3.66659800	1.20838000
H	-0.37862100	3.54806400	1.80467300
H	1.18179400	4.39975700	1.71397200
C	2.32894400	2.50634100	0.36817700
H	3.14464300	2.88115000	1.00699800
H	2.58037300	1.49285200	0.04291600
C	0.17297800	4.17206400	-0.14252500
C	2.20063600	3.41358100	-0.79608200
C	-0.58848300	4.66693800	-1.02619300
C	2.65245300	3.94237000	-1.81357100
C	-0.59275300	5.17304500	-2.39121900
C	0.13325400	6.33136100	-2.70824100
C	-1.33259300	4.52002900	-3.39052300
C	0.13405300	6.81389000	-4.01324300
H	0.69157900	6.84251000	-1.92997200

C	-1.31424100	5.00270900	-4.69502200
H	-1.90248400	3.62943900	-3.13984500
C	-0.58450600	6.15064700	-5.00846000
H	0.70079400	7.70864700	-4.25443900
H	-1.87527400	4.48471500	-5.46801000
H	-0.58085200	6.53114000	-6.02611500
C	3.17821900	4.54929000	-2.97687300
C	4.03337800	5.66593200	-2.86498500
C	2.90299400	4.00930100	-4.25032200
C	4.59758200	6.22468300	-4.00356700
H	4.25025500	6.07369700	-1.88214200
C	3.47494400	4.57598900	-5.38136700
H	2.24536700	3.14958800	-4.33159200
C	4.32100600	5.68085900	-5.26052700
H	5.26038800	7.08061700	-3.91437500
H	3.26616400	4.15498900	-6.36062100
H	4.76991000	6.11753700	-6.14850700
P	-4.63925000	4.97893800	0.85710000
C	-4.91133100	3.80054700	2.21944600
C	-4.40992900	2.49637100	2.09426800
C	-5.62316200	4.16544700	3.36916100
C	-4.62811400	1.56591100	3.10614100
H	-3.85160100	2.20962600	1.20544700
C	-5.83302400	3.22925000	4.38080700
H	-6.00756400	5.17545700	3.47831800
C	-5.33787900	1.93264500	4.25068400
H	-4.23888000	0.55678100	3.00433100
H	-6.38261300	3.51671000	5.27276200
H	-5.50126400	1.20735500	5.04294500
C	-5.90857900	4.65045700	-0.40636800
C	-5.74204300	5.19956300	-1.68630900
C	-7.04717500	3.88834600	-0.11740700
C	-6.71221100	4.99443700	-2.66284900
H	-4.85555400	5.78671300	-1.91728900
C	-8.01139400	3.68185000	-1.10321100
H	-7.17943200	3.45350900	0.86904800
C	-7.84611700	4.23398300	-2.37236700
H	-6.58070600	5.42315200	-3.65238200
H	-8.89180200	3.08682800	-0.87719100
H	-8.59916100	4.06904100	-3.13799400
C	-4.95041800	6.64950500	1.51038900
C	-3.91653600	7.32034900	2.17922300
C	-6.20564000	7.25799700	1.38045500
C	-4.14064400	8.58278500	2.72087100
H	-2.93767200	6.85496800	2.27341400
C	-6.42129500	8.52453400	1.92131900
H	-7.00882100	6.74950300	0.85477200
C	-5.39244200	9.18574100	2.59070800
H	-3.33670800	9.09926800	3.23769600
H	-7.39462800	8.99538500	1.81562400
H	-5.56397500	10.17438100	3.00736500
Au	-2.49339000	4.77601100	-0.02464500

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O	-0.85801700	0.83934500	-2.09959200
C	-1.65350600	1.88728400	-1.58491200
H	-2.70844400	1.61915100	-1.77965100
H	-1.53055900	2.00150700	-0.48888300
C	0.35023500	0.57577300	-1.34702900
H	0.08439900	0.38088900	-0.28532400
H	0.72771400	-0.36984700	-1.77470300
C	-1.39372600	3.21276300	-2.26604300

C	1.37852900	1.61562900	-1.42204600
C	-0.86620400	3.77723200	-3.26637100
C	2.28638700	2.44090100	-1.44426000
C	-0.26532900	4.43400800	-4.36500600
C	1.07514600	4.90478200	-4.26697900
C	-0.98472000	4.58830500	-5.58468000
C	1.67464900	5.51466500	-5.37174100
H	1.62516000	4.76953500	-3.33106500
C	-0.37079600	5.20389000	-6.67761000
H	-2.01164600	4.21590200	-5.65152600
C	0.95515800	5.66675700	-6.57214300
H	2.70737100	5.87017600	-5.30037100
H	-0.92022000	5.32182900	-7.61696600
H	1.43148800	6.14681400	-7.43375000
C	3.35481700	3.38932000	-1.49628700
C	3.47574800	4.40393800	-0.51126200
C	4.32026800	3.31987100	-2.53529200
C	4.53415300	5.31962500	-0.56796400
H	2.74010000	4.45126700	0.29841700
C	5.37490600	4.24025400	-2.58122300
H	4.23461900	2.53165900	-3.29013900
C	5.48528600	5.24139900	-1.60034500
H	4.62359800	6.09309800	0.20261700
H	6.12019800	4.17081500	-3.38103700
H	6.31556100	5.95488200	-1.63599500
P	-3.43704100	6.74836400	-0.40675500
C	-5.19672200	6.84314100	-0.90313200
C	-5.55140900	6.54941000	-2.23822700
C	-6.19030200	7.23549100	0.01991900
C	-6.88825200	6.65767200	-2.64711300
H	-4.78103800	6.23347500	-2.95216100
C	-7.52657700	7.33805500	-0.39749800
H	-5.92318500	7.45212800	1.05973200
C	-7.87565700	7.05096200	-1.72743200
H	-7.16059700	6.42669700	-3.68227700
H	-8.29642500	7.63839900	0.32102800
H	-8.92035100	7.12723400	-2.04686800
C	-2.66724200	8.37385200	-0.75877600
C	-1.25759200	8.46722900	-0.78065000
C	-3.45347900	9.52359900	-0.98361500
C	-0.64270300	9.70529400	-1.01297400
H	-0.64637400	7.57146000	-0.61567700
C	-2.82840300	10.75844500	-1.22059100
H	-4.54627200	9.45531000	-0.97759800
C	-1.42734100	10.85066200	-1.23463600
H	0.45005200	9.77497100	-1.02817100
H	-3.44058800	11.64911200	-1.39703700
H	-0.94482900	11.81551800	-1.42315900
C	-3.39486100	6.50415000	1.40861000
C	-3.61600600	5.20789600	1.92483300
C	-3.17849100	7.58516000	2.28884600
C	-3.62815400	4.99903100	3.31080400
H	-3.78046400	4.36627300	1.24083300
C	-3.18711300	7.36575900	3.67599200
H	-2.99931300	8.59063500	1.89402800
C	-3.41186500	6.07730600	4.18670600
H	-3.80060400	3.99316400	3.70785500
H	-3.01558100	8.20567800	4.35740100
H	-3.41498700	5.91084300	5.26906400
Au	-2.30997700	5.01951600	-1.50887800

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O	-1.21985600	0.81722900	-1.40126900
C	-1.82973900	2.04886800	-0.97357000
H	-2.88193900	1.77827500	-0.76405800
H	-1.37937800	2.35354200	-0.00790600
C	0.19757200	0.74020000	-1.15461400
H	0.46173200	1.16867300	-0.16655000
H	0.44030900	-0.33801600	-1.13477600
C	-1.86963000	3.27318200	-1.87913000
C	0.87620200	1.40767200	-2.27279500
C	-1.75215000	3.63207700	-3.14103400
C	0.87587400	1.92660200	-3.38944700
C	-1.88574600	4.91726900	-3.85913200
C	-0.76216800	5.75436900	-4.04302700
C	-3.14240300	5.32756900	-4.36388200
C	-0.89783900	6.98681200	-4.70182800
H	0.20979900	5.44179100	-3.64811100
C	-3.27092100	6.55900200	-5.02189400
H	-4.01596900	4.68229300	-4.22099000
C	-2.14909000	7.39009300	-5.19467300
H	-0.02255400	7.63311600	-4.82750600
H	-4.24968800	6.87064100	-5.40285300
H	-2.25196800	8.34991600	-5.71210600
C	0.20372900	2.43731000	-4.52363500
C	0.77248500	3.06097400	-5.64783300
C	-1.25015900	2.26861000	-4.43735500
C	-0.04788400	3.40887700	-6.73179000
H	1.85246600	3.23038400	-5.69018200
C	-2.02289900	2.53434100	-5.62354800
H	-1.58714700	1.45272500	-3.78610800
C	-1.43779800	3.12914800	-6.73298100
H	0.40449900	3.87736200	-7.61270500
H	-3.09098800	2.29161900	-5.61912100
H	-2.03616700	3.36259600	-7.61887500
Au	-2.44728300	4.97184000	-0.72438500
P	-3.04330300	6.74496300	0.70299100
C	-1.77563500	8.07192400	0.69896700
C	-2.13280000	9.43603900	0.74457000
C	-0.41210700	7.70330200	0.67424500
C	-1.13080100	10.41956400	0.77348700
H	-3.18784200	9.72923200	0.75287900
C	0.58213200	8.69118100	0.70989200
H	-0.13377400	6.64347100	0.62405300
C	0.22368700	10.04963200	0.75831300
H	-1.41217500	11.47750500	0.80663000
H	1.63798900	8.40060600	0.69327000
H	1.00166800	10.82021400	0.77975100
C	-4.63657000	7.52124800	0.22840900
C	-5.56412200	7.95002000	1.20159300
C	-4.92104700	7.70294400	-1.14337900
C	-6.76254300	8.56288500	0.80201400
H	-5.35424000	7.80057400	2.26582500
C	-6.11813100	8.32081200	-1.53264100
H	-4.20811800	7.35784600	-1.90209900
C	-7.03968900	8.74963500	-0.56178600
H	-7.48152800	8.89122200	1.56006200
H	-6.33642400	8.46085400	-2.59671200
H	-7.97739600	9.22453700	-0.86948200
C	-3.22188200	6.18192200	2.44006900
C	-2.81429200	6.99051300	3.52237200
C	-3.80679600	4.92011500	2.68740700
C	-2.99648000	6.53821200	4.83917400
H	-2.35201300	7.96603300	3.33795700

C	-3.99019600	4.47807000	4.00539900
H	-4.11556800	4.28784100	1.84603400
C	-3.58357400	5.28576700	5.08161200
H	-2.67547300	7.16679800	5.67657600
H	-4.44494300	3.49946300	4.19254500
H	-3.72077000	4.93575400	6.11025800

TS2_{BP86}

O	0.20711900	1.90370500	-1.43624000
C	-0.81198500	2.74466900	-0.92882100
H	-1.71621100	2.11752800	-0.87000500
H	-0.56809800	3.08207800	0.10369600
C	1.44724600	2.58264500	-1.62923600
H	1.66673500	3.25989400	-0.77623800
H	2.22134300	1.79629000	-1.65512100
C	-1.09506000	3.98150800	-1.75898300
C	1.48040200	3.33175700	-2.91231900
C	-0.48526000	4.60908400	-2.70622400
C	1.92948900	3.61656200	-4.03426900
C	-0.35654900	5.65169100	-3.68049400
C	0.36096800	6.83794700	-3.37177500
C	-0.97374300	5.51724100	-4.95220000
C	0.42867200	7.87633400	-4.30656900
H	0.84111400	6.93295000	-2.39272500
C	-0.89833200	6.56356400	-5.87889700
H	-1.51980600	4.59804000	-5.18572800
C	-0.20041400	7.74168700	-5.55855300
H	0.96959300	8.79591800	-4.05991300
H	-1.38452600	6.46104000	-6.85462000
H	-0.14443500	8.55769300	-6.28702600
C	2.35127300	4.02548000	-5.32139900
C	3.21896800	5.14274700	-5.47510900
C	1.93527600	3.29945600	-6.47320100
C	3.65175600	5.51994100	-6.74940300
H	3.54440100	5.69250500	-4.58685500
C	2.37393700	3.69064100	-7.74120300
H	1.27894100	2.43248100	-6.34925000
C	3.23113200	4.79790100	-7.88191700
H	4.32397600	6.37661400	-6.86416500
H	2.05502500	3.12793700	-8.62468200
H	3.57797700	5.09536100	-8.87730300
P	-4.83864700	6.05111500	-0.49463600
C	-5.89070800	4.82849100	0.37754100
C	-5.99927200	3.52547700	-0.15817700
C	-6.60258900	5.16851400	1.54710600
C	-6.82109800	2.57707400	0.46679400
H	-5.43947200	3.25679100	-1.06243300
C	-7.41933000	4.21071500	2.16973700
H	-6.51537300	6.17324100	1.97342000
C	-7.53004300	2.91850600	1.63171400
H	-6.90258700	1.56842400	0.04810300
H	-7.96731700	4.47685600	3.07979100
H	-8.16550300	2.17395300	2.12281200
C	-5.83618400	6.73490400	-1.87326200
C	-5.17135400	7.38806300	-2.93465400
C	-7.24405200	6.63819100	-1.87850600
C	-5.91221500	7.95121800	-3.98330900
H	-4.07636100	7.45004600	-2.93914500
C	-7.97763400	7.20100200	-2.93521400
H	-7.76393000	6.12043500	-1.06560000
C	-7.31474700	7.85744800	-3.98476900
H	-5.39365400	8.45734000	-4.80447900

H	-9.06990800	7.12187500	-2.93806700
H	-7.89105100	8.29172900	-4.80861500
C	-4.51627200	7.42691000	0.67365400
C	-3.44674500	7.30765300	1.58852300
C	-5.33292700	8.57774700	0.69303800
C	-3.20663700	8.32584100	2.52212200
H	-2.80469400	6.41873200	1.56598900
C	-5.08280300	9.59452400	1.62830500
H	-6.15602300	8.68114900	-0.02192100
C	-4.02364400	9.46943700	2.54211200
H	-2.37674500	8.22940600	3.23013100
H	-5.71676700	10.48746300	1.63938800
H	-3.83049000	10.26658200	3.26782800
Au	-2.84991800	5.05106700	-1.24141000

TS3_{BP86}

O	1.21262600	2.71843000	1.30775000
C	0.58015400	3.98460200	1.32112100
H	-0.32098400	3.87990400	1.94970400
H	1.22827100	4.76739700	1.77733200
C	2.44319600	2.81164000	0.57760600
H	3.21706300	3.30707600	1.20463200
H	2.76149400	1.77272100	0.38714100
C	0.18380900	4.41058800	-0.04817500
C	2.31815700	3.56624900	-0.69438000
C	-0.57113500	4.85221000	-0.97954200
C	2.74527200	3.96717700	-1.79022800
C	-0.57759400	5.34035600	-2.35331000
C	0.32950600	6.35709300	-2.73661800
C	-1.48846000	4.82114800	-3.30495600
C	0.33258100	6.82928700	-4.05531000
H	1.02177500	6.76664100	-1.99498600
C	-1.46874500	5.29248100	-4.62355300
H	-2.19195200	4.03698200	-3.00416100
C	-0.56218400	6.29869200	-5.00063200
H	1.03891200	7.61350000	-4.34652600
H	-2.16531700	4.87582900	-5.35879000
H	-0.55608700	6.67258800	-6.02996100
C	3.23267300	4.42120300	-3.04258300
C	4.14211200	5.51362300	-3.10062600
C	2.86565700	3.75469100	-4.24396300
C	4.66735200	5.92245400	-4.33012800
H	4.43156900	6.01819100	-2.17330500
C	3.39706400	4.17543300	-5.46672000
H	2.16944500	2.91196500	-4.19518700
C	4.29723600	5.25584300	-5.51299500
H	5.37329300	6.75862700	-4.36921300
H	3.11516600	3.65683100	-6.38896900
H	4.71545100	5.57667400	-6.47310000
P	-4.66185900	4.97529200	0.88567200
C	-4.93825600	3.72492400	2.19702400
C	-4.32585400	2.45764500	2.07414300
C	-5.76584500	4.00324400	3.30591000
C	-4.55115500	1.47437800	3.04811700
H	-3.67284900	2.24492800	1.21866700
C	-5.98292400	3.01363600	4.27772500
H	-6.23178000	4.98839000	3.41330300
C	-5.37843600	1.75227700	4.15000400
H	-4.07437400	0.49345400	2.95022800
H	-6.62288100	3.23255000	5.13897900
H	-5.54734800	0.98555900	4.91351000
C	-5.89703900	4.67854500	-0.43475400

C	-5.72329700	5.32228600	-1.68051300
C	-7.01520900	3.84606000	-0.22089400
C	-6.66987700	5.14047200	-2.69836100
H	-4.84914100	5.96276900	-1.85031800
C	-7.95497800	3.66519900	-1.24876700
H	-7.14890600	3.33843200	0.73989500
C	-7.78470500	4.31093600	-2.48376900
H	-6.53448700	5.64253400	-3.66216800
H	-8.82075100	3.01576500	-1.08181400
H	-8.51920300	4.16518300	-3.28290200
C	-5.02045400	6.62218300	1.60327000
C	-4.00361200	7.29153700	2.31919500
C	-6.29690900	7.21095100	1.47598500
C	-4.26632600	8.53510200	2.91076600
H	-3.00833000	6.83920700	2.40734700
C	-6.55037800	8.45784800	2.06944600
H	-7.08475900	6.70234100	0.91051400
C	-5.53891800	9.11873900	2.78533300
H	-3.47503300	9.05260600	3.46316900
H	-7.54033900	8.91468000	1.96686200
H	-5.74024800	10.09367200	3.24171100
Au	-2.48727600	4.85972300	0.03951200

IN1_{TPSSTPSS}

O	-0.95410600	0.58852400	-2.65121000
C	-1.97205600	1.55561900	-2.46641300
H	-2.82700800	1.23641200	-3.07596200
H	-2.29257300	1.61345400	-1.41651500
C	-0.09033900	0.41812800	-1.49823600
H	-0.69407000	0.05419100	-0.64905800
H	0.59662300	-0.38145300	-1.79786800
C	-1.54652700	2.91840100	-2.96615800
C	0.64393200	1.62537100	-1.11296500
C	-0.90682300	3.56859100	-3.83288600
C	1.23472800	2.64382600	-0.78319000
C	-0.15462800	4.30007400	-4.78682500
C	1.19605900	4.64165900	-4.51125900
C	-0.73573700	4.65293200	-6.03316600
C	1.94469200	5.31846500	-5.47390600
H	1.63113000	4.36531100	-3.55364000
C	0.02701900	5.33113800	-6.98355100
H	-1.76987800	4.38304800	-6.23577600
C	1.36364700	5.66308600	-6.70578400
H	2.98175400	5.57675300	-5.26904900
H	-0.41406600	5.59904100	-7.94141400
H	1.95452200	6.19031800	-7.45278500
C	1.94227900	3.82990100	-0.41852200
C	1.30855200	4.83785300	0.34813600
C	3.28784600	4.01506100	-0.81973400
C	2.00470600	5.99922200	0.69819500
H	0.27991600	4.69095700	0.67140300
C	3.97482100	5.17946600	-0.46259700
H	3.78228600	3.23561200	-1.39639400
C	3.33729600	6.17419200	0.29428300
H	1.50909000	6.76233800	1.29693500
H	5.01192900	5.30766900	-0.76845000
H	3.87938000	7.07545700	0.57615600
P	-2.96034900	6.55989300	-0.74230100
C	-4.77839600	6.69422300	-0.87513200
C	-5.39620600	6.41678100	-2.11254400
C	-5.56129000	7.09225800	0.22675300
C	-6.78304900	6.54687900	-2.24573400

H	-4.79340800	6.10083400	-2.96428800
C	-6.94987100	7.21443600	0.08538100
H	-5.09213200	7.29791400	1.18719100
C	-7.56004300	6.94346000	-1.14705900
H	-7.25654000	6.33125100	-3.20185400
H	-7.55273800	7.51743300	0.93954000
H	-8.63972700	7.03562100	-1.25069200
C	-2.23896900	8.14019900	-1.31551900
C	-0.84865300	8.20224100	-1.54926300
C	-3.03773900	9.28328300	-1.51169700
C	-0.26567600	9.40419300	-1.96453500
H	-0.22908800	7.31703500	-1.40294500
C	-2.44449800	10.48083500	-1.93448800
H	-4.11149800	9.23845000	-1.33955500
C	-1.06292500	10.54270200	-2.15988400
H	0.80740100	9.45004500	-2.14209200
H	-3.06415400	11.36250700	-2.08807100
H	-0.60756800	11.47455600	-2.49057500
C	-2.55590400	6.39414000	1.03396300
C	-2.65897900	5.12565700	1.64278800
C	-2.17035900	7.51101600	1.80130300
C	-2.38679600	4.98072300	3.00795700
H	-2.95055700	4.25899300	1.04875400
C	-1.89590600	7.35597100	3.16714200
H	-2.08146500	8.49104300	1.33578600
C	-2.00397600	6.09512700	3.76996200
H	-2.46748100	4.00047000	3.47427100
H	-1.59778800	8.22065300	3.75750300
H	-1.78692100	5.97883900	4.83024300
Au	-2.12856700	4.77503500	-1.99884200

TS1_{TPSSTPSS}

O	-1.17610900	0.79613900	-1.42070900
C	-1.80217100	2.02012400	-0.97951100
H	-2.84275300	1.73234700	-0.77667400
H	-1.35107200	2.31666800	-0.02077200
C	0.24501100	0.74014000	-1.18322100
H	0.50593600	1.17094800	-0.20437000
H	0.50265800	-0.32652700	-1.17662600
C	-1.85550300	3.25211000	-1.87431200
C	0.89080100	1.42876000	-2.30902700
C	-1.74882500	3.59707800	-3.14254100
C	0.87180700	1.95333000	-3.41826500
C	-1.88568500	4.90537700	-3.82694900
C	-0.76974800	5.75557400	-3.96703700
C	-3.13398200	5.31723500	-4.34146200
C	-0.90439700	7.00152000	-4.59500400
H	0.19279900	5.44371500	-3.56579400
C	-3.26259000	6.56260400	-4.96774800
H	-3.99984100	4.66603100	-4.23111500
C	-2.14797200	7.40612800	-5.09828400
H	-0.03801900	7.65443600	-4.68765900
H	-4.23222500	6.87424700	-5.35375400
H	-2.25006000	8.37290700	-5.58852700
C	0.17206100	2.46521800	-4.53250200
C	0.69927400	3.10927800	-5.66040900
C	-1.27894000	2.27752800	-4.40439400
C	-0.15450000	3.45184000	-6.71709000
H	1.76784200	3.29799400	-5.73010600
C	-2.08335700	2.53217000	-5.57538300
H	-1.57519900	1.44042300	-3.77093600
C	-1.53715300	3.14647800	-6.68870300

H	0.26379600	3.93539700	-7.59844700
H	-3.13984200	2.27056800	-5.54674100
H	-2.15558400	3.37597200	-7.55345700
Au	-2.42533000	4.94331100	-0.71611400
P	-3.02329000	6.72833900	0.69305900
C	-1.75929600	8.05402700	0.69267400
C	-2.11740400	9.41581900	0.73254600
C	-0.39723700	7.68877500	0.67653800
C	-1.11901100	10.39895600	0.76475100
H	-3.16675300	9.70576800	0.73415300
C	0.59348900	8.67625000	0.71518700
H	-0.11877800	6.63549100	0.63226400
C	0.23344800	10.03161000	0.75823200
H	-1.40024900	11.45033400	0.79383000
H	1.64365500	8.38908800	0.70560100
H	1.00555100	10.79878500	0.78232800
C	-4.60466300	7.50588800	0.19339400
C	-5.56724000	7.89890600	1.14365200
C	-4.84607700	7.71995700	-1.17992700
C	-6.75713300	8.50677400	0.72058400
H	-5.39129200	7.72749500	2.20410500
C	-6.03431500	8.33321400	-1.59225900
H	-4.10821200	7.40633100	-1.91865800
C	-6.99107200	8.72500100	-0.64373000
H	-7.49997100	8.80631900	1.45792200
H	-6.21707000	8.49823300	-2.65293000
H	-7.91820200	9.19442400	-0.96826900
C	-3.22326300	6.18899600	2.43139000
C	-2.83068100	7.01024600	3.50680100
C	-3.80659100	4.93093900	2.68821000
C	-3.02634300	6.57492400	4.82435400
H	-2.37160500	7.97895500	3.31659300
C	-4.00410000	4.50608500	4.00693000
H	-4.10234000	4.29106400	1.85643000
C	-3.61241400	5.32672900	5.07530200
H	-2.71822900	7.21081900	5.65254300
H	-4.45608300	3.53464800	4.20014600
H	-3.75981100	4.99140200	6.10048000

TS2_{TPSSTPSS}

O	0.29950900	1.90412000	-1.39838400
C	-0.74282400	2.71679300	-0.88374600
H	-1.62596300	2.07198700	-0.84152600
H	-0.50591400	3.04489200	0.14432500
C	1.51552400	2.62370800	-1.60252100
H	1.71378300	3.30801500	-0.76063400
H	2.30766200	1.86754300	-1.63958300
C	-1.04332000	3.95435600	-1.70517900
C	1.49596700	3.36810200	-2.89084500
C	-0.44088800	4.58632800	-2.65165100
C	1.91418900	3.63540200	-4.02591900
C	-0.34868800	5.64957000	-3.61133900
C	0.37093100	6.83055300	-3.30355700
C	-1.00065900	5.53403700	-4.86357400
C	0.40832700	7.88307000	-4.22035100
H	0.87670900	6.91089400	-2.34356800
C	-0.95621500	6.59455100	-5.77259400
H	-1.54552600	4.62187300	-5.09702800
C	-0.25443300	7.76735700	-5.45363600
H	0.94992200	8.79488700	-3.97517700
H	-1.46649800	6.50652000	-6.73001800
H	-0.22201200	8.59055200	-6.16543000

C	2.28434800	4.03776700	-5.32906100
C	3.11667500	5.17199400	-5.52326500
C	1.84429700	3.29232300	-6.45582500
C	3.49038700	5.54790900	-6.81344600
H	3.45750600	5.73557700	-4.65777000
C	2.22467000	3.68171400	-7.73997400
H	1.21686800	2.41716500	-6.30120900
C	3.04614100	4.80675000	-7.92108300
H	4.13171100	6.41499100	-6.96002000
H	1.88884300	3.10738900	-8.60130800
H	3.34522100	5.10244900	-8.92523100
P	-4.79736200	6.03358900	-0.49676100
C	-5.88180700	4.83077500	0.35562800
C	-5.99437000	3.52958600	-0.17771800
C	-6.61285700	5.18104500	1.50738100
C	-6.83883600	2.59439300	0.43034600
H	-5.42228900	3.25394800	-1.06415200
C	-7.45235200	4.23626700	2.11329700
H	-6.52307800	6.17973700	1.93089800
C	-7.56696600	2.94674800	1.57676400
H	-6.92306800	1.59169400	0.01490300
H	-8.01308200	4.50931600	3.00556000
H	-8.21782700	2.21556700	2.05301000
C	-5.75414800	6.71366200	-1.90130200
C	-5.05936000	7.34356400	-2.95467600
C	-7.16044600	6.63493300	-1.93782400
C	-5.76791800	7.90062400	-4.02495500
H	-3.97028800	7.39276900	-2.93576200
C	-7.86156200	7.19164400	-3.01594200
H	-7.70205900	6.13747200	-1.13513000
C	-7.16841500	7.82443900	-4.05677600
H	-5.22779700	8.38653100	-4.83580900
H	-8.94791900	7.12654600	-3.04232200
H	-7.71732300	8.25222900	-4.89396000
C	-4.49718300	7.41223000	0.66835300
C	-3.45152100	7.29256000	1.60680800
C	-5.30681200	8.56540400	0.66430900
C	-3.22891900	8.31112600	2.54013700
H	-2.81765800	6.40551200	1.60283400
C	-5.07423100	9.58257500	1.59953000
H	-6.10786300	8.66908700	-0.06571100
C	-4.03952700	9.45607500	2.53673200
H	-2.42141700	8.21433600	3.26377400
H	-5.70018100	10.47324500	1.59262000
H	-3.86112600	10.25012800	3.25976800
Au	-2.80445100	5.01831200	-1.19655600

TS3_{TPSSTPSS}

O	1.14390300	2.57243100	1.22044600
C	0.54082000	3.85390300	1.26806400
H	-0.36334500	3.74928500	1.87792700
H	1.20320000	4.60046300	1.74287400
C	2.37766100	2.66063900	0.49246500
H	3.16015700	3.09434200	1.13910900
H	2.65266500	1.63070800	0.24110500
C	0.17270500	4.31353900	-0.10198500
C	2.26503400	3.49356800	-0.73341300
C	-0.58416400	4.77222200	-1.01972300
C	2.72254600	3.95024400	-1.79107600
C	-0.59602700	5.25660900	-2.39493900
C	0.27793300	6.29778500	-2.77740700
C	-1.48399700	4.70502300	-3.34562500

C	0.27663200	6.75856200	-4.09749900
H	0.94862500	6.73138900	-2.03910800
C	-1.46953100	5.16621100	-4.66516100
H	-2.16180900	3.90716900	-3.04546600
C	-0.59241100	6.19424700	-5.04327600
H	0.95795800	7.55601400	-4.38844700
H	-2.14442900	4.72614500	-5.39733200
H	-0.58973100	6.55757600	-6.06947400
C	3.23298400	4.48138700	-3.00126800
C	4.10007200	5.60541000	-2.97503200
C	2.92494200	3.86723500	-4.24315300
C	4.63966400	6.09856000	-4.16344600
H	4.34209800	6.06813600	-2.02041500
C	3.47276300	4.37001100	-5.42375800
H	2.26220800	3.00495500	-4.25898600
C	4.32833200	5.48321700	-5.38725200
H	5.30841700	6.95699400	-4.13901400
H	3.23812200	3.89403700	-6.37402800
H	4.75618000	5.86836400	-6.31132600
P	-4.64852500	4.97935600	0.87810000
C	-4.92554700	3.75680600	2.21056000
C	-4.34456200	2.47686200	2.09213400
C	-5.71989100	4.06649300	3.33242100
C	-4.56787700	1.51353600	3.08212000
H	-3.72117200	2.23946700	1.22946000
C	-5.93482500	3.09661900	4.32058200
H	-6.16040600	5.05661100	3.43600800
C	-5.36167700	1.82341100	4.19665900
H	-4.11782600	0.52695200	2.98718400
H	-6.54645300	3.33907100	5.18784100
H	-5.52835500	1.07515200	4.96954000
C	-5.90049400	4.67236700	-0.41923300
C	-5.72606100	5.27303600	-1.68370400
C	-7.03283000	3.87299700	-0.17092700
C	-6.68480700	5.08251400	-2.68464600
H	-4.84491300	5.88480500	-1.87991600
C	-7.98485300	3.68303400	-1.18187000
H	-7.16697800	3.39970300	0.80001500
C	-7.81329500	4.28667800	-2.43479000
H	-6.54892500	5.54927700	-3.65871400
H	-8.85787800	3.06217700	-0.98861400
H	-8.55458900	4.13458600	-3.21735600
C	-4.98582300	6.63668800	1.57246800
C	-3.96008800	7.30230000	2.27473700
C	-6.25240800	7.23993300	1.44059000
C	-4.20415900	8.55484900	2.84821000
H	-2.97669100	6.84054100	2.36693200
C	-6.48691200	8.49627800	2.01510300
H	-7.04433300	6.73587900	0.88932100
C	-5.46678900	9.15239100	2.71759700
H	-3.40954400	9.06652000	3.38829800
H	-7.46513100	8.96203200	1.90937700
H	-5.65277000	10.13043400	3.15792200
Au	-2.48915200	4.82543500	0.01161000

IN1_{B3LYP}

O	-0.83447200	0.81734300	-2.12008900
C	-1.61067800	1.86123300	-1.58868800
H	-2.66258000	1.59650500	-1.74553200
H	-1.45317100	1.97798000	-0.50792400
C	0.37198000	0.51965100	-1.40433900
H	0.12729000	0.28989900	-0.35550300

H	0.74041000	-0.40157900	-1.86628300	TS1 _{B3LYP}			
C	-1.36580800	3.17544900	-2.28177100	O	-1.10175900	0.83696100	-1.43056000
C	1.40111200	1.56001600	-1.45672700	C	-1.73555800	2.04426800	-0.99586800
C	-0.85410000	3.75304900	-3.26227200	H	-2.76817400	1.75003900	-0.77253500
C	2.28503800	2.39139100	-1.46813000	H	-1.28201100	2.35070300	-0.04470300
C	-0.26221100	4.42889900	-4.35378900	C	0.30853000	0.77787500	-1.21379400
C	1.05631900	4.92819900	-4.24430800	H	0.58876800	1.21925100	-0.24756100
C	-0.97072300	4.56823500	-5.56994300	H	0.57088600	-0.28549100	-1.18968100
C	1.64723800	5.55365700	-5.33554600	C	-1.82099900	3.27099200	-1.89113100
H	1.59891000	4.80597400	-3.31312500	C	0.95048900	1.44474400	-2.35353300
C	-0.36757000	5.19842200	-6.65103800	C	-1.72435600	3.59545700	-3.15894700
H	-1.97900200	4.17399300	-5.64751300	C	0.90704800	1.95800600	-3.45675900
C	0.93796300	5.69053600	-6.53415500	C	-1.89263400	4.89311800	-3.85646200
H	2.66196600	5.93073200	-5.25521200	C	-0.79604200	5.74815200	-4.04625000
H	-0.90768800	5.30446400	-7.58663800	C	-3.15696800	5.29041400	-4.32472900
H	1.40539500	6.18030200	-7.38358300	C	-0.96212600	6.98069700	-4.68198100
C	3.33257700	3.36402300	-1.50312900	H	0.18154900	5.45243700	-3.67782000
C	3.43824900	4.34406900	-0.49578200	C	-3.31930500	6.52162200	-4.95926300
C	4.27910500	3.35138800	-2.54805600	H	-4.01189300	4.63702600	-4.17489600
C	4.46517200	5.28475300	-0.53601800	C	-2.22152500	7.36868800	-5.14193900
H	2.71816000	4.34865600	0.31703100	H	-0.10695800	7.63736800	-4.81380300
C	5.30294900	4.29564000	-2.57948300	H	-4.30280900	6.81978300	-5.31197600
H	4.20541800	2.59212300	-3.32049200	H	-2.34908800	8.32616000	-5.63875000
C	5.39889900	5.26363000	-1.57578600	C	0.18520000	2.44682900	-4.56575600
H	4.54288600	6.03074200	0.24988400	C	0.70102100	3.04027200	-5.71871400
H	6.03277800	4.27109600	-3.38375000	C	-1.26038700	2.27920500	-4.40816000
H	6.20225900	5.99435500	-1.60005000	C	-0.16080100	3.34833500	-6.77208000
P	-3.42866000	6.75268000	-0.39919700	H	1.76776900	3.21481600	-5.81027300
C	-5.18310900	6.84933900	-0.89686000	C	-2.07539900	2.50277400	-5.57537300
C	-5.53203100	6.58060500	-2.23068600	H	-1.54960600	1.44608400	-3.77137700
C	-6.17951100	7.21560300	0.02155000	C	-1.54227200	3.06116700	-6.71504100
C	-6.85996900	6.68649800	-2.64130900	H	0.24980500	3.79055800	-7.67565900
H	-4.76689300	6.28751200	-2.94528100	H	-3.13225600	2.25764200	-5.52222600
C	-7.50775000	7.31592800	-0.39580200	H	-2.16833900	3.26389700	-7.57775600
H	-5.02377300	7.41601000	1.05733700	Au	-2.40590300	4.95697900	-0.70585200
C	-7.84849000	7.05299400	-1.72406100	P	-3.02292600	6.75191100	0.71935000
H	-7.12390800	6.47606300	-3.67346900	C	-1.75191600	8.06976400	0.75024400
H	-8.27552900	7.59587300	0.31936700	C	-2.09738000	9.42803400	0.81678000
H	-8.88372000	7.12801500	-2.04367100	C	-0.39650000	7.70118400	0.72982300
C	-2.65815500	8.36944500	-0.76399900	C	-1.09776600	10.40153700	0.86964200
C	-1.25640200	8.46115600	-0.79622400	H	-3.14076800	9.72738900	0.82347700
C	-3.43478000	9.51601700	-0.98916000	C	0.59707200	8.67737700	0.78907800
C	-0.64163900	9.68800800	-1.03951900	H	-0.12050900	6.65153700	0.66533100
H	-0.64828000	7.57512900	-0.63031400	C	0.24741200	10.02863800	0.85780300
C	-2.81174200	10.74068700	-1.23743700	H	-1.37271000	11.45116300	0.91883100
H	-4.51839200	9.45641700	-0.97486300	H	1.64283700	8.38414800	0.77556600
C	-1.41887500	10.82829000	-1.26204700	H	1.02223900	10.78877200	0.89806900
H	0.44218900	9.75313200	-1.06163100	C	-4.59137800	7.54384300	0.20378400
H	-3.41743800	11.62471500	-1.41344800	C	-5.54921500	7.96280200	1.13950200
H	-0.93846600	11.78240500	-1.45803300	C	-4.82633700	7.74604500	-1.16668200
C	-3.38881200	6.52567800	1.41354200	C	-6.72399400	8.58183200	0.70765100
C	-3.60395800	5.24155600	1.94145800	H	-5.38391600	7.80373700	2.20035200
C	-3.17706200	7.60678500	2.28212200	C	-5.99881400	8.37023300	-1.59005300
C	-3.61464100	5.04485800	3.32106400	H	-4.09603900	7.41492200	-1.90082000
H	-3.76544800	4.39800300	1.27454100	C	-6.94945600	8.78714000	-0.65440200
C	-3.18376000	7.40151000	3.66340200	H	-7.46252900	8.90059300	1.43743500
H	-3.00404900	8.60237600	1.88603700	H	-6.17405900	8.52505700	-2.65082700
C	-3.40245100	6.12464100	4.18301500	H	-7.86548100	9.26666100	-0.98718400
H	-3.78275900	4.05015700	3.72315300	C	-3.25424300	6.20007000	2.44960700
H	-3.01625000	8.24116400	4.33145100	C	-2.86376700	6.99575000	3.53738500
H	-3.40462100	5.96892100	5.25782300	C	-3.86057700	4.95493700	2.68584800
Au	-2.30235200	5.00231500	-1.49784800	C	-3.08227000	6.55044700	4.84261600

H	-2.38754300	7.95666400	3.36959200
C	-4.08160100	4.51839000	3.99134000
H	-4.15866600	4.32901300	1.84835900
C	-3.69079600	5.31501900	5.07096000
H	-2.77421700	7.16991900	5.67987800
H	-4.55252400	3.55530300	4.16576600
H	-3.85701300	4.97099900	6.08769300

TS2_{B3LYP}

O	0.31376600	1.88720400	-1.42144300
C	-0.73435800	2.68702100	-0.92363100
H	-1.61302900	2.03903300	-0.88577700
H	-0.51487900	3.01241200	0.10685500
C	1.50917100	2.59918500	-1.65195500
H	1.74658700	3.26485000	-0.80789800
H	2.30190900	1.85109900	-1.73717100
C	-1.03642600	3.91960700	-1.74198900
C	1.44656600	3.38409800	-2.91921900
C	-0.41162500	4.52918700	-2.68392500
C	1.90002500	3.66271900	-4.03245900
C	-0.36686100	5.61264200	-3.63296900
C	0.31523000	6.80591300	-3.32172900
C	-1.02967100	5.49409300	-4.87033500
C	0.30917400	7.86724700	-4.22245700
H	0.83014000	6.89229600	-2.36979900
C	-1.03024600	6.56170300	-5.76543800
H	-1.54951700	4.57143200	-5.10866700
C	-0.36272900	7.74682800	-5.44368600
H	0.82433600	8.79010000	-3.97281500
H	-1.55041800	6.46916400	-6.71424300
H	-0.36485600	8.57705500	-6.14414900
C	2.31348200	4.07475300	-5.31529500
C	3.14663700	5.20768700	-5.46907100
C	1.91541000	3.34117700	-6.45826600
C	3.56382100	5.59420400	-6.73673000
H	3.45474100	5.76347100	-4.58965900
C	2.33863600	3.73973600	-7.72008300
H	1.28501200	2.46648600	-6.33407400
C	3.16121800	4.86346000	-7.86055400
H	4.20604900	6.46172400	-6.85389500
H	2.03505900	3.17478300	-8.59610000
H	3.49376300	5.16782800	-8.84878000
P	-4.81506800	6.01530800	-0.50244900
C	-5.90619000	4.83769300	0.37471400
C	-6.03177000	3.53176200	-0.12846900
C	-6.62919300	5.21181700	1.51729700
C	-6.87677900	2.61750000	0.49847000
H	-5.46885000	3.23131000	-1.00888700
C	-7.46988500	4.28941600	2.14371300
H	-6.53469700	6.21462300	1.92160800
C	-7.59521000	2.99515200	1.63626500
H	-6.96927400	1.60996000	0.10367800
H	-8.02389700	4.58398300	3.03019700
H	-8.24774000	2.27972800	2.12820000
C	-5.77842600	6.69521900	-1.90139300
C	-5.09213700	7.28469100	-2.97597000
C	-7.18124800	6.65739100	-1.91278600
C	-5.80192300	7.83944000	-4.03998700
H	-4.00517600	7.30645200	-2.98188900
C	-7.88562900	7.21041500	-2.98380000
H	-7.72291000	6.19404100	-1.09417700
C	-7.19873200	7.80187300	-4.04554300

H	-5.26489700	8.29424200	-4.86727400
H	-8.97111100	7.17508700	-2.98808100
H	-7.75022100	8.22828800	-4.87846100
C	-4.48379700	7.40033800	0.64620000
C	-3.46627500	7.25563400	1.60403600
C	-5.23336000	8.58573400	0.60611400
C	-3.21224600	8.27848500	2.51637000
H	-2.87416000	6.34437100	1.63477700
C	-4.97005500	9.60883700	1.51907800
H	-6.01583600	8.71377400	-0.13521600
C	-3.96303800	9.45648900	2.47378600
H	-2.42537600	8.15890200	3.25536400
H	-5.55221200	10.52495000	1.48128800
H	-3.75994900	10.25528100	3.18115200
Au	-2.81461700	4.97042200	-1.21335700

TS3_{B3LYP}

O	1.19660500	2.33466400	1.08555600
C	0.56086000	3.58117100	1.20807800
H	-0.35744100	3.42058100	1.77897100
H	1.18696000	4.30727800	1.75291600
C	2.38959600	2.47862700	0.32664700
H	3.19846800	2.86872600	0.96431300
H	2.66634200	1.47745300	-0.01440800
C	0.22031600	4.12524300	-0.13769100
C	2.21775400	3.40341700	-0.82666400
C	-0.55609700	4.65489400	-0.99040500
C	2.65839900	3.92861700	-1.85258700
C	-0.53264100	5.19701800	-2.34698900
C	0.16690000	6.38697500	-2.61246300
C	-1.21163500	4.54278300	-3.39057400
C	0.20458600	6.89866500	-3.90803600
H	0.67816900	6.89846400	-1.80297300
C	-1.15644300	5.05446300	-4.68528600
H	-1.76275700	3.63038200	-3.18220600
C	-0.45094400	6.23275600	-4.94683500
H	0.75101300	7.81576000	-4.10740200
H	-1.66943600	4.53607400	-5.49027900
H	-0.41859400	6.63423200	-5.95548100
C	3.16567400	4.53507100	-3.02488500
C	4.04141900	5.64093100	-2.92731600
C	2.84960900	4.00893700	-4.29809800
C	4.58628700	6.19993400	-4.07703100
H	4.28752500	6.03893200	-1.94791000
C	3.40177700	4.57675000	-5.44050800
H	2.17589200	3.16144200	-4.36926000
C	4.26934400	5.66894500	-5.33254400
H	5.26336600	7.04517700	-3.99881100
H	3.16136900	4.16757400	-6.41707900
H	4.70187300	6.10577900	-6.22805800
P	-4.66823600	4.97786500	0.86928700
C	-4.94668700	3.80527500	2.24499000
C	-4.43446000	2.50109500	2.13792200
C	-5.67222000	4.17373400	3.38798800
C	-4.65531100	1.57649000	3.15737200
H	-3.86551700	2.20927400	1.25842600
C	-5.88548700	3.24372000	4.40750200
H	-6.06567500	5.18045300	3.48668400
C	-5.37946200	1.94776500	4.29377000
H	-4.25774500	0.56983700	3.06766800
H	-6.44527600	3.53544800	5.29124800
H	-5.54503100	1.22842900	5.09046800

C	-5.93785900	4.63599700	-0.40072600
C	-5.75261100	5.14415500	-1.69743200
C	-7.09473700	3.90093300	-0.10165100
C	-6.71916100	4.92696900	-2.67790800
H	-4.85495400	5.70809000	-1.93946700
C	-8.05609800	3.68250700	-1.09051300
H	-7.24448700	3.49641800	0.89430900
C	-7.87062400	4.19453800	-2.37572700
H	-6.57108200	5.32364300	-3.67801000
H	-8.94823000	3.10986400	-0.85460400
H	-8.61962100	4.02027500	-3.14270800
C	-4.98366400	6.66003800	1.51052200
C	-3.94303300	7.35241400	2.15141500
C	-6.24824400	7.25833500	1.39698100
C	-4.16913500	8.62169800	2.68167800
H	-2.95762000	6.90019600	2.23226900
C	-6.46665300	8.53128200	1.92666600
H	-7.05708000	6.73797100	0.89362100
C	-5.43059700	9.21214400	2.56881200
H	-3.36021800	9.15203500	3.17545500
H	-7.44618000	8.99093200	1.83335900
H	-5.60369300	10.20398700	2.97611100
Au	-2.49378600	4.76965300	-0.01108300