

Supporting Information for:

Rationale for the reactivity differences between main group and d^0 transition metal complexes toward olefin polymerization

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Table SI4. Cartesian coordinates and total energies for all of the calculated structures in water (page ESI2)

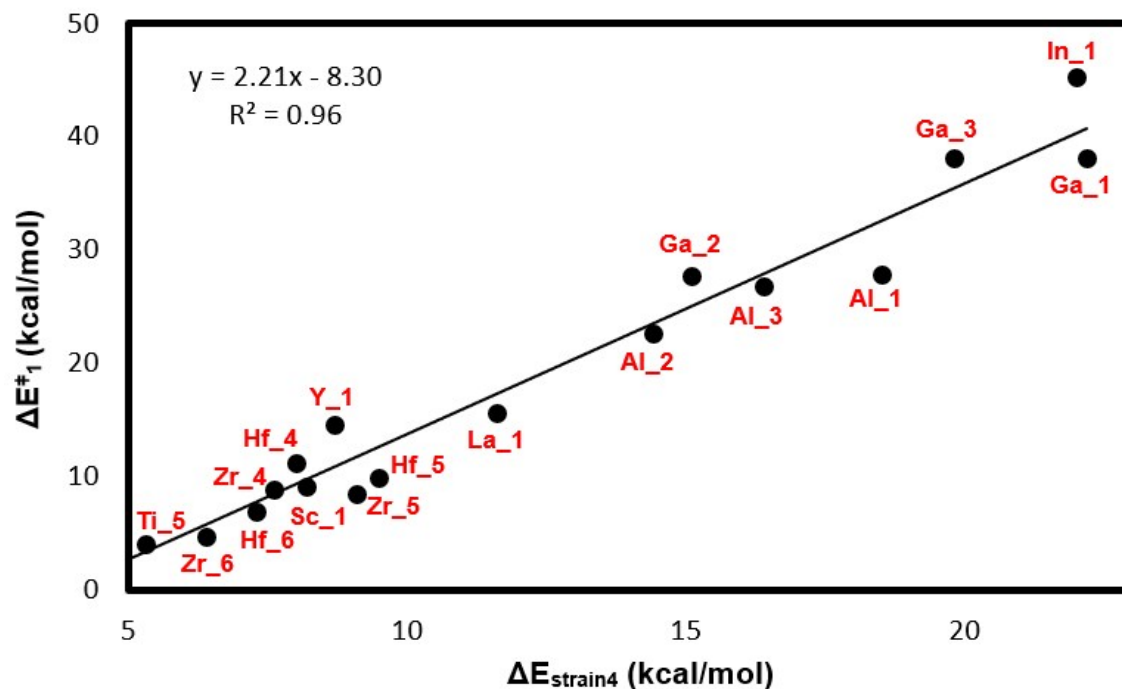


Figure ESI1. A plot of the correlation between ΔE^{\ddagger}_1 and $\Delta E_{\text{strain}4}$ (ring strain energy in M_N_V) calculated by the M06/BS2//B3LYP/BS1 method.

Table ESI1. Cartesian coordinates and total energies for all of the calculated structures

Al_1_I

E (B3LYP/BS1) = -730.691864 au

H(B3LYP/BS1) = -730.390992 au

G(B3LYP/BS1) = -730.455831 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -971.429259 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -970.821093 au

C	-1.23869900	1.93429500	-0.52104500
C	1.23868900	1.93429800	-0.52107700
C	-0.00000800	2.55871400	-0.65791100
H	2.13649500	2.53537400	-0.65725100
H	-0.00001300	3.61331100	-0.90489700
H	-2.13651000	2.53536800	-0.65719800
N	1.43799600	0.63288800	-0.24407400
N	-1.43799700	0.63288300	-0.24403800
C	2.79483400	0.16742700	-0.06495000
C	3.65524400	0.81944700	0.82649300
C	3.22979900	-0.95685800	-0.77534700
C	4.95797600	0.34858400	0.99196200
H	3.30167200	1.67093000	1.40124300
C	4.53220900	-1.42456700	-0.59658700
H	2.57036600	-1.44000000	-1.49272900
C	5.39772900	-0.77241600	0.28419800
H	5.62461200	0.85322000	1.68447400
H	4.87178500	-2.29061300	-1.15618300

H	6.41085600	-1.13759400	0.42000600
C	-2.79483800	0.16742000	-0.06492700
C	-3.22982500	-0.95680700	-0.77540300
C	-3.65522800	0.81938700	0.82657200
C	-4.53224000	-1.42451100	-0.59666200
H	-2.57040800	-1.43990200	-1.49283200
C	-4.95796400	0.34853100	0.99202300
H	-3.30163600	1.67082700	1.40137500
C	-5.39774000	-0.77241200	0.28418300
H	-4.87183600	-2.29050900	-1.15631900
H	-5.62458600	0.85312700	1.68457800
H	-6.41087100	-1.13758600	0.41997500
C	0.00003600	-2.39526300	0.57500600
H	0.00126000	-3.05609200	-0.30000100
H	0.88772200	-2.63653000	1.16933000
H	-0.88878600	-2.63714900	1.16736700
Al	0.00000400	-0.53062900	0.04974400

Ga_1_I

E(B3LYP/BS1) = -730.736241 au

H(B3LYP/BS1) = -730.435453 au

G(B3LYP/BS1) = -730.501147 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2653.843930 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2653.176980 au

C	-1.24073400	1.99191900	-0.52037700
C	1.24072700	1.99191800	-0.52041200
C	-0.00000600	2.61273700	-0.65596300
H	2.13548200	2.59705300	-0.65824900
H	-0.00000900	3.66737300	-0.90291700
H	-2.13549200	2.59705300	-0.65819200
N	1.44920200	0.69324400	-0.24523800
N	-1.44920300	0.69324400	-0.24520000
C	2.80509600	0.22983600	-0.06872200
C	3.67272200	0.89546800	0.80547800
C	3.23530700	-0.90409400	-0.76665000
C	4.97745300	0.42833400	0.96611600
H	3.32317500	1.75385600	1.37226000
C	4.53976000	-1.36749900	-0.59316900
H	2.56916900	-1.39848900	-1.46986000
C	5.41252600	-0.70182500	0.27036600
H	5.64920500	0.94316500	1.64607300
H	4.87540400	-2.24107200	-1.14339300
H	6.42726900	-1.06391300	0.40231300
C	-2.80509800	0.22983300	-0.06869900
C	-3.23532700	-0.90404500	-0.76670300
C	-3.67270900	0.89541500	0.80555200
C	-4.53978500	-1.36744700	-0.59324100
H	-2.56920100	-1.39839600	-1.46995600
C	-4.97744400	0.42828500	0.96617000
H	-3.32314800	1.75376400	1.37238400
C	-5.41253500	-0.70182200	0.27034800
H	-4.87544400	-2.24097800	-1.14352300
H	-5.64918500	0.94307900	1.64616700
H	-6.42728100	-1.06390800	0.40227900
C	0.00002200	-2.34894500	0.56523000

H	0.00156000	-2.99291200	-0.32032200
H	0.89082500	-2.57833100	1.15663100
H	-0.89223300	-2.57907200	1.15413800
Ga	0.00000200	-0.47910000	0.04759000

In_1_I

E (B3LYP/BS1) = -730.533944 au

H(B3LYP/BS1) = -730.233828 au

G(B3LYP/BS1) = -730.302243 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -919.116406 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -918.535020 au

C	-1.25478200	2.06706400	-0.48870000
C	1.25479200	2.06705600	-0.48869800
C	0.00000700	2.66785400	-0.60853000
H	2.12577000	2.70950000	-0.61870300
H	0.00001100	3.72772200	-0.83407100
H	-2.12575500	2.70951200	-0.61870900
N	1.51849800	0.77525900	-0.24624900
N	-1.51849200	0.77526800	-0.24625100
C	2.88861700	0.36400000	-0.08677200
C	3.75630500	1.06716600	0.75899900
C	3.34127100	-0.77340200	-0.76709300
C	5.07518000	0.63663100	0.90659300
H	3.39511200	1.92658600	1.31669000
C	4.65945300	-1.20117700	-0.60720700
H	2.67977500	-1.29679400	-1.45514300
C	5.52923300	-0.49613300	0.22754400
H	5.74391400	1.18220600	1.56537900
H	5.00814600	-2.07663800	-1.14632500
H	6.55492600	-0.82943900	0.35011400
C	-2.88861100	0.36400900	-0.08677500
C	-3.34125400	-0.77341200	-0.76707200
C	-3.75630900	1.06719000	0.75897400
C	-4.65943500	-1.20119000	-0.60718500
H	-2.67975000	-1.29681900	-1.45510200
C	-5.07518300	0.63665200	0.90656700
H	-3.39512500	1.92662400	1.31664900
C	-5.52922600	-0.49613000	0.22754200
H	-5.00811900	-2.07666500	-1.14628600
H	-5.74392400	1.18223800	1.56533600
H	-6.55491800	-0.82943800	0.35011100
C	-0.00004600	-2.63857000	0.57382700
H	0.00052100	-3.24552100	-0.33563900
H	0.89312200	-2.87128400	1.15806500
H	-0.89379500	-2.87147800	1.15709700
In	0.00000000	-0.59121700	0.06461100

Sc_1_I

E (B3LYP/BS1) = -775.145839 au

H(B3LYP/BS1) = -774.848457 au

G(B3LYP/BS1) = -774.915290 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1489.708029 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1489.089859 au

C	-1.22732200	2.37567700	-0.32854100
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C	1.22732900	2.37569600	-0.32857100
C	0.00000300	3.04451400	-0.32597700
H	2.14750800	2.96200700	-0.35959600
H	-0.00000600	4.12697100	-0.35433500
H	-2.14750600	2.96197600	-0.35962000
N	1.33401100	1.04860400	-0.32738900
N	-1.33399000	1.04859100	-0.32722900
C	2.53795200	0.31716300	-0.23228000
C	3.53361000	0.55988900	0.72785900
C	2.61701500	-0.84137600	-1.03890900
C	4.59502000	-0.33324100	0.85775700
H	3.45706000	1.42820100	1.37547200
C	3.67665300	-1.74458300	-0.87945100
H	1.94877000	-0.94508700	-1.90023200
C	4.66288800	-1.49147900	0.07206900
H	5.36950900	-0.13519500	1.59279900
H	3.74362200	-2.61790400	-1.52118300
H	5.48924300	-2.18376700	0.19685700
C	-2.53795000	0.31715600	-0.23219400
C	-2.61706100	-0.84128900	-1.03894400
C	-3.53358200	0.55981800	0.72798700
C	-3.67672900	-1.74447500	-0.87956700
H	-1.94881100	-0.94495000	-1.90026900
C	-4.59502300	-0.33328700	0.85780600
H	-3.45698600	1.42806200	1.37568500
C	-4.66294300	-1.49143600	0.07199200
H	-3.74373800	-2.61772600	-1.52139000
H	-5.36949500	-0.13529300	1.59288000
H	-5.48932200	-2.18370700	0.19671400
C	0.00001600	-0.98395300	2.01758500
H	0.88990600	-1.58136300	2.27480800
H	-0.00010000	-0.09804200	2.66609000
H	-0.88980000	-1.58152100	2.27470800
Sc	0.00003600	-0.52532300	-0.06375200

Y_1_I

E(B3LYP/BS1) = -766.641492 au

H(B3LYP/BS1) -766.344579 au

G(B3LYP/BS1) = -766.413694 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -767.352147 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -766.725000 au

C	-1.23529600	2.41090200	-0.30887500
C	1.23529600	2.41090000	-0.30887300
C	0.00000000	3.06542100	-0.30271800
H	2.14136200	3.02073400	-0.30341200
H	0.00000100	4.14857300	-0.30199300
H	-2.14136200	3.02073600	-0.30341400
N	1.38118400	1.08758300	-0.34738700
N	-1.38118500	1.08758500	-0.34738900
C	2.62127100	0.42364300	-0.22205300
C	3.57126800	0.71697300	0.77122900
C	2.80833800	-0.71477200	-1.04039100
C	4.68795900	-0.10216900	0.92235500
H	3.41559200	1.56688700	1.42897600
C	3.92587300	-1.54266100	-0.86387800

H	2.17520700	-0.85023600	-1.92343700
C	4.86296300	-1.23856900	0.12146800
H	5.42281500	0.13683000	1.68542500
H	4.07471500	-2.39616100	-1.51863100
H	5.73260700	-1.87254500	0.26085100
C	-2.62127100	0.42364400	-0.22205300
C	-2.80833600	-0.71477500	-1.04038800
C	-3.57127000	0.71697500	0.77122600
C	-3.92586900	-1.54266400	-0.86387400
H	-2.17520500	-0.85023800	-1.92343400
C	-4.68796000	-0.10216900	0.92235300
H	-3.41559700	1.56689200	1.42897100
C	-4.86296100	-1.23857200	0.12147000
H	-4.07470800	-2.39616700	-1.51862500
H	-5.42281800	0.13683100	1.68542100
H	-5.73260400	-1.87254900	0.26085400
C	0.00000600	-1.09509800	2.12186100
H	0.88609000	-1.68242000	2.41499700
H	-0.00004600	-0.18763700	2.74119300
H	-0.88601600	-1.68251700	2.41498800
Y	-0.00000200	-0.67423700	-0.13175500

La_1_I

E(B3LYP/BS1) = -759.934323 au

H(B3LYP/BS1) = -759.638576 au

G(B3LYP/BS1) = -759.706120 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -760.616774 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -759.992508 au

C	-1.23931800	2.47324500	-0.32474800
C	1.23940800	2.47321700	-0.32475300
C	0.00005000	3.11891900	-0.33093500
H	2.13516500	3.09825700	-0.29456000
H	0.00006300	4.20229800	-0.32543800
H	-2.13506300	3.09830100	-0.29457400
N	1.41574100	1.15399000	-0.36955800
N	-1.41567100	1.15401700	-0.36953200
C	2.68311200	0.55461100	-0.19300800
C	3.54578900	0.87693800	0.87054200
C	3.01092800	-0.53016700	-1.03735400
C	4.71341600	0.14277000	1.06517800
H	3.28280000	1.68547900	1.54630100
C	4.18005500	-1.27216000	-0.82081600
H	2.43443000	-0.69022200	-1.95243300
C	5.02902400	-0.93896000	0.23301900
H	5.37765100	0.40586800	1.88312600
H	4.43637800	-2.08345500	-1.49588000
H	5.93749600	-1.50813800	0.40202900
C	-2.68306100	0.55466100	-0.19303900
C	-3.01084100	-0.53011900	-1.03739300
C	-3.54577400	0.87698600	0.87048000
C	-4.17996500	-1.27213100	-0.82088400
H	-2.43432500	-0.69016000	-1.95246400
C	-4.71339800	0.14280800	1.06508100
H	-3.28279700	1.68551600	1.54625700
C	-5.02896800	-0.93893500	0.23292300

H	-4.43625900	-2.08343100	-1.49595300
H	-5.37766100	0.40590200	1.88300900
H	-5.93743700	-1.50812400	0.40191000
C	-0.00041900	-1.15829600	2.21428300
H	0.88340200	-1.74308900	2.51991900
H	0.00549300	-0.23145700	2.80441800
H	-0.89073000	-1.73249800	2.52110000
La	0.00001200	-0.80539300	-0.19885300

Ethylene

E (B3LYP/BS1) = -78.585824 au

H(B3LYP/BS1) = -78.530603 au

G(B3LYP/BS1) = -78.556774 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -78.617564 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -78.540923 au

C	0.00000000	0.00000000	0.66561700
C	0.00000000	0.00000000	-0.66561700
H	0.00000000	0.92372500	1.23964500
H	0.00000000	-0.92372500	1.23964500
H	0.00000000	0.92372500	-1.23964500
H	0.00000000	-0.92372500	-1.23964500

Al_1_II

E (B3LYP/BS1) = -809.295939 au

H(B3LYP/BS1) = -808.937381 au

G(B3LYP/BS1) = -809.011604 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1050.057243 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1049.383229 au

C	1.21553700	1.98459800	-0.73832600
C	-1.26468900	1.97053900	-0.72629100
C	-0.02873500	2.60481200	-0.85457300
H	-2.16168400	2.57381300	-0.86238500
H	-0.03603800	3.66065200	-1.09577100
H	2.10500500	2.59752500	-0.88108300
C	0.59097800	-1.00709400	2.42096300
C	-0.29797800	0.00360800	2.40811500
N	-1.46495600	0.66983000	-0.46642300
N	1.43006300	0.68595600	-0.48136700
C	-2.82145200	0.21588600	-0.27999300
C	-3.27624700	-0.90691300	-0.98225200
C	-3.67507500	0.87918500	0.61234900
C	-4.58317700	-1.35805600	-0.79426100
H	-2.62506800	-1.40168000	-1.69700800
C	-4.98265500	0.42431100	0.78827500
H	-3.31451600	1.73797600	1.17243900
C	-5.43837800	-0.69488600	0.08871100
H	-4.93556800	-2.22157000	-1.35014600
H	-5.64103300	0.94230200	1.47910800
H	-6.45499900	-1.04817300	0.23019300
C	2.78974600	0.24111300	-0.30536200
C	3.64532100	0.90528900	0.58496100
C	3.24606800	-0.87775200	-1.01354900
C	4.95587800	0.45546500	0.75206400
H	3.28374100	1.76011200	1.15036600

C	4.55622900	-1.32339400	-0.83482900
H	2.59324900	-1.37214600	-1.72736000
C	5.41308100	-0.65915600	0.04576500
H	5.61581700	0.97402700	1.44098100
H	4.90966900	-2.18314700	-1.39584000
H	6.43221700	-1.00788900	0.18026300
H	-1.36658700	-0.17503300	2.51079500
H	0.02140300	1.04336400	2.38218700
H	0.27465100	-2.04237500	2.51897700
H	1.66315800	-0.82477000	2.38089600
C	-0.02961400	-2.42482200	-0.51584300
H	-0.09615500	-2.61432500	-1.59485200
H	0.87756900	-2.92262500	-0.15561200
H	-0.88868500	-2.91974900	-0.04846200
Al	-0.00776300	-0.51101500	-0.14912900

Ga_1_II

E (B3LYP/BS1) = -809.336394 au

H(B3LYP/BS1) = -808.977963 au

G(B3LYP/BS1) = -809.053037 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2732.467525 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2731.734838 au

C	1.21803200	2.00818000	-0.77923100
C	-1.26739400	1.99669400	-0.76294500
C	-0.02823900	2.62334800	-0.90178600
H	-2.16078100	2.60138600	-0.91508800
H	-0.03484200	3.67441200	-1.16324100
H	2.10434700	2.62085100	-0.94079000
C	0.62289400	-0.72830500	2.60002600
C	-0.30352500	0.24225600	2.51620300
N	-1.47756300	0.70428000	-0.47903200
N	1.44209000	0.71707000	-0.49968700
C	-2.83243400	0.25102300	-0.29369300
C	-3.26992600	-0.90019900	-0.95986900
C	-3.70343100	0.94298300	0.55872900
C	-4.57733800	-1.35119400	-0.77706400
H	-2.60396400	-1.41842800	-1.64416500
C	-5.01151200	0.48770100	0.72985200
H	-3.35615100	1.82268200	1.09393500
C	-5.45043500	-0.65926300	0.06560600
H	-4.91607900	-2.23727800	-1.30521600
H	-5.68341200	1.02724600	1.39048600
H	-6.46755900	-1.01240300	0.20368200
C	2.80036900	0.27283600	-0.32602600
C	3.67460500	0.96881200	0.52036200
C	3.23812400	-0.87768400	-0.99376600
C	4.98544700	0.51820700	0.68342200
H	3.32748900	1.84745300	1.05744100
C	4.54852100	-1.32355400	-0.81943800
H	2.56969300	-1.39844100	-1.67397900
C	5.42445700	-0.62765200	0.01704200
H	5.65965700	1.06074700	1.33924600
H	4.88721300	-2.20870100	-1.34918000
H	6.44379200	-0.97678900	0.14881000
H	-1.36428900	0.03101300	2.63400600

H	-0.02543100	1.28787500	2.40390600
H	0.34680400	-1.76468700	2.77670900
H	1.68700300	-0.51021800	2.53924200
C	-0.03257400	-2.41388000	-0.26846900
H	-0.10315200	-2.71368400	-1.31992500
H	0.87971900	-2.85056800	0.14765700
H	-0.89370000	-2.83376900	0.26010200
Ga	-0.00844800	-0.47032300	-0.11891400

In_1_II

E (B3LYP/BS1) = -809.137534 au

H(B3LYP/BS1) = -808.779838 au

G(B3LYP/BS1) = -808.857590 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -997.742160 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -997.095171 au

C	1.23054000	2.09622600	-0.72903300
C	-1.28462900	2.08356400	-0.71060200
C	-0.03070900	2.68912600	-0.83625800
H	-2.15405500	2.72891600	-0.84116700
H	-0.03784800	3.74758600	-1.06832700
H	2.09224800	2.74987000	-0.86950800
C	0.66433300	-0.82044600	2.65975000
C	-0.28750000	0.12931500	2.61591800
N	-1.55030700	0.79582900	-0.46696400
N	1.51019800	0.81015500	-0.49162400
C	-2.91711100	0.39420600	-0.28305400
C	-3.38557400	-0.75563700	-0.93287800
C	-3.77505700	1.11717100	0.55798500
C	-4.70416400	-1.17198000	-0.74936300
H	-2.73344800	-1.29881400	-1.61300500
C	-5.09493700	0.69748400	0.72994100
H	-3.40705100	1.99190700	1.08719200
C	-5.56243300	-0.44652500	0.08026500
H	-5.06322200	-2.05630400	-1.26705900
H	-5.75423400	1.26228900	1.38227700
H	-6.58860100	-0.77163700	0.22008400
C	2.88033300	0.41804900	-0.32048200
C	3.74035900	1.14339100	0.51704200
C	3.35073900	-0.72858700	-0.97521700
C	5.06321400	0.72922600	0.68044100
H	3.37166100	2.01582800	1.04958300
C	4.67247900	-1.13898400	-0.80064200
H	2.69727400	-1.27255000	-1.65358700
C	5.53222500	-0.41132700	0.02559200
H	5.72379900	1.29586700	1.32988400
H	5.03273400	-2.02034700	-1.32253800
H	6.56072700	-0.73184900	0.15864700
H	-1.33989900	-0.10737200	2.76035300
H	-0.03655600	1.18193600	2.50394400
H	0.41930000	-1.86535600	2.83537100
H	1.72093400	-0.57305400	2.57522700
C	-0.03437400	-2.68300200	-0.36168900
H	-0.12832500	-2.94254500	-1.42025100
H	0.89128300	-3.11798300	0.02376300
H	-0.88194400	-3.11314100	0.17852900

In -0.00919200 -0.57944400 -0.12950200

Sc_1_II

E(B3LYP/BS1) = -853.760694 au

H(B3LYP/BS1) = -853.405333 au

G(B3LYP/BS1) = -853.485110 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1568.327945 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1567.637760 au

C	-1.23518200	2.45968600	0.27092100
C	1.23053000	2.46446500	0.26974100
C	-0.00344300	3.11711500	0.31704600
H	2.13110100	3.06980800	0.15164500
H	-0.00563400	4.20028000	0.29997800
H	-2.13768200	3.06242600	0.15421500
C	-0.03084200	-2.78286300	-0.64943700
C	0.04059600	-1.88950500	-1.65181600
N	1.38854300	1.14025800	0.33603300
N	-1.38974400	1.13493200	0.33584300
C	2.60990200	0.50990100	-0.01871200
C	3.05608600	-0.56870300	0.77082000
C	3.31245100	0.84656900	-1.19044400
C	4.18762600	-1.29805200	0.38861400
H	2.58398400	-0.77107700	1.73118000
C	4.45073600	0.12726100	-1.54649900
H	2.95349900	1.65730600	-1.81808300
C	4.88695000	-0.95098600	-0.76634200
H	4.53518700	-2.11463900	1.01447600
H	4.99553100	0.40101500	-2.44527600
H	5.77167100	-1.50874900	-1.05678600
C	-2.61167900	0.50500100	-0.01914600
C	-3.31598700	0.84644300	-1.18840300
C	-3.05848600	-0.57494800	0.76800600
C	-4.45689100	0.13104500	-1.54397200
H	-2.95660700	1.65815400	-1.81454700
C	-4.19276200	-1.30023400	0.38649700
H	-2.58411400	-0.78187200	1.72619500
C	-4.89410200	-0.94802400	-0.76577000
H	-5.00287900	0.40866200	-2.44083300
H	-4.54102000	-2.11763000	1.01093500
H	-5.78105200	-1.50260000	-1.05552000
H	0.99719100	-1.56288800	-2.05632900
H	-0.85622400	-1.49489200	-2.12657000
H	0.86603500	-3.22344600	-0.21579700
H	-0.98854300	-3.15373600	-0.28653500
C	0.01069500	-0.89477900	2.80215700
H	-0.88804200	-0.57278600	3.34756300
H	0.06296800	-1.99676300	2.88696200
H	0.86789400	-0.48826400	3.35797100
Sc	0.00323500	-0.37576200	0.72059300

Y_1_II

E(B3LYP/BS1) = -845.254832 au

H(B3LYP/BS1) = -844.900084 au

G(B3LYP/BS1) = -844.979941 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -845.969107 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -845.268910 au

C	-1.24892600	2.61877200	0.24098900
C	1.22561100	2.62306300	0.22683100
C	-0.01272700	3.27003400	0.27913500
H	2.11781100	3.24043200	0.09959400
H	-0.01466100	4.35326800	0.25598600
H	-2.14447000	3.23272400	0.12091600
C	0.02878500	-3.04432800	-0.86019600
C	-0.00426400	-2.14929000	-1.86206900
N	1.39868900	1.30353700	0.30362200
N	-1.41669900	1.29832300	0.32218300
C	2.60771600	0.67188600	-0.06383600
C	3.01795300	-0.44445000	0.69911000
C	3.32563600	1.00832700	-1.22802700
C	4.12562500	-1.20481400	0.30042200
H	2.56120700	-0.63321500	1.67244600
C	4.43707700	0.25645500	-1.59959800
H	2.99731100	1.84551100	-1.83736200
C	4.83469100	-0.85728400	-0.84748800
H	4.44839600	-2.04258800	0.91162700
H	4.99263500	0.53200700	-2.49135200
H	5.69960200	-1.43794400	-1.15218000
C	-2.62257000	0.66225600	-0.04678500
C	-3.34707900	1.00393600	-1.20548400
C	-3.02213200	-0.46487400	0.70584600
C	-4.45370800	0.24690200	-1.58084900
H	-3.02720900	1.84902900	-1.80831800
C	-4.12485200	-1.23043300	0.30339900
H	-2.56244400	-0.65824600	1.67661100
C	-4.84024600	-0.87747900	-0.83881700
H	-5.01418500	0.52684900	-2.46814600
H	-4.43881800	-2.07670000	0.90746300
H	-5.70138500	-1.46204600	-1.14665800
H	0.90906100	-1.77588800	-2.32301100
H	-0.94498100	-1.81493800	-2.29710500
H	0.97010100	-3.43195300	-0.47299700
H	-0.88400600	-3.47132300	-0.44675800
C	0.07061300	-1.07090300	2.84201800
H	-0.90578000	-1.09012300	3.34955900
H	0.48461000	-2.09249700	2.93015700
H	0.71349900	-0.41921600	3.45306200
Y	-0.00290900	-0.44853400	0.61277500

La_1_II

E(B3LYP/BS1) = -838.542156 au

H(B3LYP/BS1) = -838.187817 au

G(B3LYP/BS1) = -838.270089 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -839.233096 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -838.538730 au

C	-1.28391200	2.72574700	0.15354400
C	1.19898400	2.74859600	0.15896400
C	-0.04815600	3.37956300	0.17462600
H	2.08075400	3.38373600	0.04214700
H	-0.05791900	4.46205500	0.12623800

H	-2.17639300	3.34482000	0.03165400
C	0.18992600	-3.36328900	-1.15149200
C	0.17533500	-2.48487200	-2.16629200
N	1.40353700	1.43687000	0.26823800
N	-1.46448900	1.41094500	0.26298800
C	2.64826600	0.84864000	-0.04175400
C	3.09920900	-0.20976800	0.77947100
C	3.37761200	1.16781200	-1.20463300
C	4.25794000	-0.92289000	0.44463000
H	2.62278300	-0.38234600	1.74629800
C	4.53797200	0.46289600	-1.51525900
H	3.02161400	1.95901500	-1.85845800
C	4.97731800	-0.58953700	-0.70171100
H	4.60980000	-1.71251700	1.10227000
H	5.10040100	0.72826900	-2.40586500
H	5.88086500	-1.13401800	-0.95724500
C	-2.69573900	0.79943100	-0.05467600
C	-3.42593300	1.10748500	-1.21995500
C	-3.12968200	-0.27028200	0.76116700
C	-4.57050700	0.38055600	-1.53815500
H	-3.08257000	1.90715600	-1.87020700
C	-4.27264000	-1.00512400	0.41905900
H	-2.65642800	-0.43455400	1.73102200
C	-4.99288300	-0.68270200	-0.72981500
H	-5.13363200	0.63720300	-2.43086600
H	-4.61210800	-1.80329900	1.07284800
H	-5.88404500	-1.24439500	-0.99144200
H	1.09526700	-2.07657900	-2.58202300
H	-0.75049400	-2.20427500	-2.66583600
H	1.12253200	-3.70310300	-0.70317100
H	-0.72355800	-3.83011600	-0.78593900
C	0.02938800	-1.22283700	2.81694000
H	-0.90108800	-1.73892300	3.10633000
H	0.84963600	-1.93893200	2.99721500
H	0.16580300	-0.39412400	3.52666900
La	-0.01016800	-0.54344400	0.45161100

TS_{Al-1}

E(B3LYP/BS1) = -809.245952 au

H(B3LYP/BS1) = -808.888712 au

G(B3LYP/BS1) = -808.959612 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1050.008640 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1049.338756 au

C	-1.24035000	2.10397900	-0.59218600
C	1.24033100	2.10400300	-0.59221400
C	-0.00001700	2.72960300	-0.72435700
H	2.13405500	2.72129900	-0.68210400
H	-0.00003000	3.79208000	-0.93359200
H	-2.13408500	2.72125900	-0.68207600
C	0.00033900	-2.64951800	0.36070800
C	0.00007600	-2.20651100	-1.01018600
Al	0.00000800	-0.39569700	-0.12480600
C	-0.00030400	-1.03595100	1.88046800
H	0.90318800	-0.46332500	2.13887300
H	-0.90532200	-0.46577300	2.13883200

H	0.00101800	-1.90670800	2.53404900
H	-0.91371200	-3.02968800	0.80678000
H	0.91471500	-3.02920600	0.80652200
N	1.45270700	0.80049900	-0.36299700
N	-1.45271000	0.80047400	-0.36295300
C	-2.80926400	0.36198700	-0.13919400
C	-3.54079500	0.86810700	0.94287700
C	-3.38423800	-0.58471100	-0.99572600
C	-4.84714900	0.42771800	1.16173600
H	-3.08480200	1.59458300	1.61008800
C	-4.68964900	-1.02266000	-0.76604400
H	-2.83017000	-0.93881800	-1.86023500
C	-5.42179700	-0.51964300	0.31186800
H	-5.41237200	0.82353100	2.00011700
H	-5.13856300	-1.74591300	-1.44022900
H	-6.43747700	-0.86118200	0.48577000
C	2.80926000	0.36202200	-0.13920600
C	3.54077800	0.86817800	0.94285700
C	3.38424600	-0.58471200	-0.99569400
C	4.84712400	0.42779000	1.16175500
H	3.08478100	1.59468400	1.61003400
C	4.68964900	-1.02266000	-0.76597300
H	2.83019400	-0.93884100	-1.86020400
C	5.42178100	-0.51960800	0.31193400
H	5.41233500	0.82363200	2.00013100
H	5.13857100	-1.74593900	-1.44012400
H	6.43745500	-0.86114600	0.48586700
H	-0.91608900	-2.39597400	-1.56732300
H	0.91610900	-2.39578300	-1.56760500

TS_{Ga-1}

E(B3LYP/BS1) = -809.275337 au

H(B3LYP/BS1) = -808.918409 au

G(B3LYP/BS1) = -808.990540 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2732.402040 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2731.674061 au

C	-1.24543700	2.13950000	-0.55572800
C	1.24452200	2.14012700	-0.55956300
C	-0.00083500	2.76126100	-0.67360300
H	2.13228500	2.76597300	-0.64935300
H	-0.00145300	3.82687100	-0.86648500
H	-2.13381000	2.76465700	-0.64410100
C	0.02177700	-2.58008900	0.51327200
C	-0.00047700	-2.21449900	-0.88569200
C	-0.01433000	-0.89473700	1.98747400
H	0.83204100	-0.23672700	2.22836800
H	-0.96887900	-0.40936200	2.22687800
H	0.07678400	-1.75566400	2.64817500
H	-0.88232600	-2.94272800	0.99231900
H	0.94863400	-2.91968600	0.96480500
N	1.47459700	0.83766200	-0.35498900
N	-1.47461100	0.83703600	-0.34951700
C	-2.83103400	0.39661200	-0.14690600
C	-3.58855800	0.91578600	0.91070400
C	-3.38319200	-0.56378100	-1.00335600

C	-4.89908100	0.47550300	1.10415700
H	-3.14950000	1.65096900	1.57964000
C	-4.69251800	-1.00133700	-0.79888000
H	-2.80693400	-0.92921300	-1.84856400
C	-5.45145800	-0.48455700	0.25404600
H	-5.48457000	0.88095900	1.92381200
H	-5.12382600	-1.73514400	-1.47315800
H	-6.47030600	-0.82603200	0.40842600
C	2.83068100	0.39806100	-0.14990800
C	3.59066900	0.92783100	0.90073500
C	3.38028800	-0.57303000	-0.99601200
C	4.90055500	0.48747100	1.09760700
H	3.15387800	1.67091700	1.56240100
C	4.68903900	-1.01063800	-0.78812800
H	2.80280500	-0.94648900	-1.83684400
C	5.45019000	-0.48329900	0.25793500
H	5.48767900	0.90103800	1.91202300
H	5.11824600	-1.75276100	-1.45460300
H	6.46857600	-0.82489700	0.41507100
H	-0.92311600	-2.44031800	-1.41701400
H	0.90882200	-2.43093900	-1.44313800
Ga	0.00033100	-0.35649800	-0.10019500

TS_{In-1}

E(B3LYP/BS1) = -809.069705 au

H(B3LYP/BS1) = -808.713784 au

G(B3LYP/BS1) = -808.788187 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -997.665471 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -997.022957 au

C	-1.26067200	2.22019100	-0.52140100
C	1.26072200	2.22019100	-0.52139000
C	0.00002600	2.81578900	-0.63022700
H	2.12254800	2.88363400	-0.60253200
H	0.00002600	3.88403400	-0.81163500
H	-2.12249600	2.88363600	-0.60254600
C	-0.00007900	-2.82936400	0.52177400
C	-0.00004700	-2.49278800	-0.88569500
C	-0.00026500	-1.16650600	2.08509400
H	0.90315900	-0.60108200	2.35331900
H	-0.90423100	-0.60195000	2.35326800
H	0.00026500	-2.06160400	2.70512400
H	-0.91524500	-3.17851500	0.98904200
H	0.91508100	-3.17852900	0.98904300
N	1.54846600	0.92716400	-0.33776500
N	-1.54842000	0.92716600	-0.33777400
C	-2.91524400	0.53878500	-0.13372000
C	-3.71327900	1.19720800	0.81167300
C	-3.44378900	-0.52808100	-0.87266700
C	-5.03646000	0.79583500	1.00124800
H	-3.29356200	2.00298600	1.40731100
C	-4.76531000	-0.92715600	-0.67122500
H	-2.83751600	-1.00936500	-1.63644500
C	-5.56463000	-0.26617100	0.26463800
H	-5.65025600	1.30894300	1.73547500

H	-5.17434000	-1.74420200	-1.25800900
H	-6.59305800	-0.57757600	0.41861600
C	2.91528500	0.53876900	-0.13370500
C	3.71334200	1.19721600	0.81165300
C	3.44380000	-0.52814200	-0.87260600
C	5.03651500	0.79581900	1.00123700
H	3.29364900	2.00302700	1.40726200
C	4.76531300	-0.92724100	-0.67115500
H	2.83751300	-1.00944500	-1.63636200
C	5.56465400	-0.26623300	0.26467300
H	5.65032700	1.30894500	1.73543800
H	5.17431900	-1.74432400	-1.25790500
H	6.59307600	-0.57765700	0.41865900
H	-0.91559900	-2.72575200	-1.42704700
H	0.91549400	-2.72584600	-1.42702600
In	0.00002500	-0.44588600	-0.12680600

TS_{Sc-1}

E(B3LYP/BS1) = -853.742519 au

H(B3LYP/BS1) = -853.387978 au

G(B3LYP/BS1) = -853.462542 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1568.311960 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1567.623237 au

C	-1.25142400	-1.97307100	1.19753400
C	1.24179800	-1.98837800	1.20293900
C	-0.00835000	-2.49659100	1.56782700
H	2.11768600	-2.59887200	1.43094900
H	-0.01574500	-3.43286000	2.11359100
H	-2.13390900	-2.57350300	1.42680600
C	0.08024500	3.18932100	0.71770200
C	0.01442900	2.32941800	1.81625700
C	-0.03800200	2.15554500	-1.30865700
H	0.62504400	1.38973400	-1.78221500
H	-1.08536600	1.94721800	-1.58787400
H	0.24634400	3.10395200	-1.76118000
H	-0.79939700	3.73270300	0.38742400
H	1.02649000	3.63240400	0.42496000
N	1.46537000	-0.82752800	0.57396200
N	-1.46477100	-0.81342400	0.56211800
C	-2.75297200	-0.54981800	0.00309100
C	-3.39182200	-1.48453100	-0.82694200
C	-3.35749700	0.69624700	0.23774000
C	-4.62386200	-1.17478900	-1.40107800
H	-2.91129500	-2.43643000	-1.03443900
C	-4.58481300	1.00339400	-0.35308000
H	-2.90060400	1.39853400	0.93328600
C	-5.22065500	0.06851500	-1.17164300
H	-5.11420400	-1.90366800	-2.03942100
H	-5.05159600	1.96372100	-0.15537900
H	-6.17753800	0.30508900	-1.62622800
C	2.74874700	-0.56457800	0.00740700
C	3.38979000	-1.50129900	-0.81919600
C	3.34484300	0.68867900	0.22738900
C	4.61576300	-1.18659200	-1.40279900
H	2.91544800	-2.45849900	-1.01619700

C	4.56587400	1.00085400	-0.37430400
H	2.88950100	1.39129500	0.92389400
C	5.20390100	0.06387900	-1.18817900
H	5.10851900	-1.91706400	-2.03746500
H	5.02628200	1.96645700	-0.18784400
H	6.15603900	0.30384000	-1.65085600
H	-0.92729700	2.22092500	2.35611000
H	0.91428200	2.14466400	2.40527000
Sc	0.01100800	0.64999000	0.27296200

TS_{Y-1}

E(B3LYP/BS1) = -845.231227 au

H(B3LYP/BS1) = -844.877508 au

G(B3LYP/BS1) = -844.953211 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -845.942979 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -845.245695 au

C	-1.24354900	2.47712600	-0.81671500
C	1.24477400	2.48077400	-0.82051200
C	-0.00031500	3.08267000	-1.02552200
H	2.12875400	3.11794300	-0.90019100
H	-0.00243200	4.13017300	-1.30316100
H	-2.12906600	3.11229000	-0.89551600
C	0.01762100	-3.29220800	-0.46981800
C	0.00014500	-2.54141100	-1.64903700
C	-0.02495000	-2.12523900	1.52684700
H	0.80858000	-1.50767100	1.93470900
H	-0.99018300	-1.68663200	1.85492500
H	0.05764700	-3.09043800	2.02480800
H	-0.88779700	-3.76882200	-0.10874700
H	0.94046400	-3.74375000	-0.12134400
N	1.44811800	1.19468400	-0.52515800
N	-1.44444500	1.19147600	-0.51853100
C	-2.71141200	0.73579000	-0.06833200
C	-3.43158700	1.38999600	0.94779200
C	-3.19486100	-0.48676900	-0.57568000
C	-4.61544600	0.83471300	1.42835600
H	-3.04874300	2.31713800	1.36486600
C	-4.37576900	-1.04451600	-0.07306600
H	-2.70607900	-0.94449600	-1.43628100
C	-5.08650800	-0.38553800	0.92909900
H	-5.16900900	1.35064000	2.20736800
H	-4.74986900	-1.97591500	-0.48762500
H	-6.00649500	-0.81253300	1.31556800
C	2.71213100	0.73752600	-0.07105600
C	3.43880700	1.39749300	0.93693900
C	3.18560500	-0.49503600	-0.56443900
C	4.61927500	0.83886600	1.42148400
H	3.06368400	2.33199700	1.34441900
C	4.36300200	-1.05621300	-0.05697600
H	2.69493900	-0.95730000	-1.42176600
C	5.08040400	-0.39086800	0.93591000
H	5.17821500	1.35965900	2.19339000
H	4.72930200	-1.99513000	-0.46139100
H	5.99789800	-0.82003900	1.32583000
H	-0.92646300	-2.47902900	-2.22125400

H	0.91487700	-2.46336700	-2.23845400
Y	0.00543200	-0.54155800	-0.21220400

TS_{La-1}

E(B3LYP/BS1) = -838.513125 au

H(B3LYP/BS1) = -838.159816 au

G(B3LYP/BS1) = -838.236413 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -839.204119 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -838.513872 au

C	-1.25305900	2.72676200	-0.62729800
C	1.24032600	2.72874000	-0.62807700
C	-0.00664400	3.34985400	-0.75515400
H	2.12146000	3.37543700	-0.65571500
H	-0.00743200	4.42157000	-0.91641700
H	-2.13531600	3.37201400	-0.65467400
C	0.04948100	-3.49171600	-0.27625700
C	0.02446800	-2.79407700	-1.48927000
C	-0.01038800	-2.31327100	1.68848000
H	0.82090200	-1.70404100	2.10895800
H	-0.97358000	-1.87682600	2.02489600
H	0.06677700	-3.28413900	2.17781300
H	-0.84897200	-3.97777000	0.08945000
H	0.97707500	-3.92753700	0.07963800
N	1.44862900	1.42098800	-0.47902300
N	-1.45787300	1.41911200	-0.47800500
C	-2.71871300	0.90261000	-0.10950500
C	-3.49153400	1.43661000	0.94024200
C	-3.14333300	-0.29595300	-0.72619300
C	-4.66317700	0.79723300	1.33935200
H	-3.15819900	2.34013500	1.44285100
C	-4.31479600	-0.93824500	-0.30513800
H	-2.63505500	-0.64666200	-1.62688100
C	-5.07423500	-0.39459500	0.72935200
H	-5.25609200	1.22510200	2.14255200
H	-4.64317900	-1.84236900	-0.80937700
H	-5.98551800	-0.88635000	1.05433400
C	2.71108100	0.90953100	-0.10792600
C	3.47953000	1.44768500	0.94300900
C	3.14266500	-0.28702500	-0.72345700
C	4.65378000	0.81445700	1.34410000
H	3.14098800	2.34980100	1.44467700
C	4.31647600	-0.92342800	-0.30011700
H	2.63718200	-0.64087900	-1.62432600
C	5.07167400	-0.37557000	0.73519200
H	5.24338100	1.24564500	2.14796000
H	4.64993600	-1.82624700	-0.80335500
H	5.98491800	-0.86265100	1.06171300
H	-0.90168800	-2.77686300	-2.06596600
H	0.93967900	-2.73689300	-2.08078600
La	-0.00095100	-0.54418900	-0.13800300

Al 1 III

E(B3LYP/BS1) = -809.3138271 au

H(B3LYP/BS1) = -808.952460 au

G(B3LYP/BS1) = -809.025035 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1050.073068 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1049.397146 au

C	1.24582500	-2.35735800	-0.57219400
C	-1.23026800	-2.36225200	-0.57085900
C	0.00890700	-2.97988700	-0.73040400
H	-2.12744000	-2.96019800	-0.72464000
H	0.01081900	-4.02565400	-1.01237200
H	2.14510500	-2.95179900	-0.72717800
C	0.00283700	1.94708000	0.68555900
H	-0.85550500	2.08004000	1.35908900
H	0.89762100	2.09589700	1.30605400
N	-1.43105300	-1.07142700	-0.25075100
N	1.44190900	-1.06585500	-0.25193300
C	2.79886000	-0.60835900	-0.05452500
C	3.65202300	-1.28370300	0.82648900
C	3.24228900	0.53004900	-0.73644000
C	4.95535800	-0.82145400	1.01073700
H	3.29215700	-2.14749600	1.37853600
C	4.54534800	0.98873000	-0.53945000
H	2.58826500	1.03137400	-1.44610300
C	5.40334700	0.31374000	0.33142100
H	5.61613700	-1.34446700	1.69521200
H	4.89149200	1.86591100	-1.07731300
H	6.41698900	0.67191900	0.48141200
C	-2.78984900	-0.61919500	-0.05318200
C	-3.63843500	-1.29416300	0.83247600
C	-3.23971800	0.51342500	-0.74039200
C	-4.94362800	-0.83698200	1.01644700
H	-3.27370600	-2.15367200	1.38800900
C	-4.54457600	0.96710100	-0.54371700
H	-2.58903100	1.01373400	-1.45370400
C	-5.39796000	0.29266300	0.33208600
H	-5.60098400	-1.35962800	1.70448600
H	-4.89570400	1.83978300	-1.08566000
H	-6.41303300	0.64686500	0.48185200
C	-0.04058300	3.03043800	-0.42352500
C	-0.03168900	4.44931700	0.15681700
H	0.87166400	4.62561500	0.75204100
H	-0.06090300	5.19949000	-0.64077100
H	-0.89894100	4.61449600	0.80642700
H	-0.93854800	2.89980700	-1.04210200
H	0.81679300	2.91243800	-1.09989100
Al	0.00324900	0.09164500	0.08548700

Ga_1_III

E(B3LYP/BS1) = -809.3590473 au

H(B3LYP/BS1) = -808.997833 au

G(B3LYP/BS1) = -809.071091 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2732.48957 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2731.755407 au

C	1.24720700	-2.36490400	-0.57504700
C	-1.23300400	-2.36947700	-0.57373400
C	0.00813300	-2.98366200	-0.73182200
H	-2.12706700	-2.97157400	-0.72928600
H	0.00990200	-4.02946100	-1.01382500

H	2.14322700	-2.96374100	-0.73185600
C	0.00347800	1.95438000	0.68352000
H	-0.85740400	2.07338600	1.35350400
H	0.90200200	2.08880100	1.29870800
N	-1.44305300	-1.08136800	-0.25558500
N	1.45283000	-1.07616900	-0.25668700
C	2.80895300	-0.62133100	-0.06232300
C	3.66965600	-1.31001400	0.80087100
C	3.24770100	0.52641500	-0.73159100
C	4.97513300	-0.85158700	0.97981800
H	3.31388700	-2.18049100	1.34491000
C	4.55293600	0.98074900	-0.54044100
H	2.58678800	1.03850000	-1.42691700
C	5.41841600	0.29246500	0.31262200
H	5.64120300	-1.38468600	1.65127400
H	4.89510400	1.86517900	-1.06894400
H	6.43380300	0.64744000	0.45835400
C	-2.80097800	-0.63163400	-0.06101800
C	-3.65687700	-1.31960500	0.80743800
C	-3.24629600	0.51005400	-0.73614700
C	-4.96414100	-0.86612900	0.98623700
H	-3.29612000	-2.18561900	1.35530700
C	-4.55324900	0.95950000	-0.54519100
H	-2.58891000	1.02076400	-1.43568900
C	-5.41389200	0.27214000	0.31348200
H	-5.62661700	-1.39857900	1.66174900
H	-4.90051900	1.83923400	-1.07819200
H	-6.43064300	0.62324600	0.45909800
C	-0.04063200	3.02628100	-0.43155700
C	-0.03035700	4.44635500	0.14707000
H	0.87389600	4.62431700	0.74024500
H	-0.06010900	5.19330500	-0.65326100
H	-0.89701400	4.61419400	0.79662800
H	-0.93969000	2.89290200	-1.04716300
H	0.81652200	2.90449400	-1.10681500
Ga	0.00278100	0.09326400	0.08080500

In 1 III

E(B3LYP/BS1) = -809.1574609 au

H(B3LYP/BS1) = -808.796877 au

G(B3LYP/BS1) = -808.871497 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -997.7635023 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -997.114257 au

C	1.28837300	-2.41362300	-0.56356700
C	-1.22014200	-2.43700400	-0.56177600
C	0.03957800	-3.02107000	-0.70866300
H	-2.08558200	-3.08089100	-0.71989300
H	0.04918500	-4.06983100	-0.98105100
H	2.16527300	-3.04140600	-0.72326000
C	-0.01210300	2.26106000	0.72335000
H	-0.83862900	2.36387300	1.43547700
H	0.91748200	2.43006800	1.27783400
N	-1.49428700	-1.15993000	-0.26254400
N	1.53952100	-1.13174600	-0.26427400
C	2.90621700	-0.71708300	-0.08969600

C	3.78049800	-1.44646100	0.72676000
C	3.35019800	0.44991600	-0.72425300
C	5.09628400	-1.01235000	0.89068700
H	3.42641900	-2.33054000	1.24939600
C	4.66549900	0.88057800	-0.54874500
H	2.68347900	0.99538800	-1.38976500
C	5.54148700	0.14962000	0.25670000
H	5.76968700	-1.57884600	1.52671500
H	5.00737800	1.77914000	-1.05320100
H	6.56494000	0.48518500	0.39137900
C	-2.86822500	-0.77004800	-0.08735000
C	-3.72813600	-1.51276900	0.73226500
C	-3.33419200	0.38653400	-0.72512400
C	-5.05144600	-1.10210900	0.89639800
H	-3.35747600	-2.38866900	1.25718600
C	-4.65692900	0.79368400	-0.54963300
H	-2.67799800	0.94161600	-1.39306300
C	-5.51850300	0.04952100	0.25926000
H	-5.71374300	-1.67880400	1.53491600
H	-5.01575400	1.68416400	-1.05666000
H	-6.54775000	0.36680800	0.39409800
C	-0.15556000	3.27036400	-0.43469400
C	-0.16476100	4.71583700	0.08072400
H	0.76380400	4.95145700	0.61278600
H	-0.26528000	5.42242300	-0.75003400
H	-1.00042400	4.88426000	0.76935900
H	-1.08238900	3.07964300	-0.99145600
H	0.66758200	3.14754600	-1.15097200
In	0.01029200	0.21493000	0.12269500

Sc_1_III

E(B3LYP/BS1) = -853.773258 au

H(B3LYP/BS1) = -853.415752 au

G(B3LYP/BS1) = -853.489188 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1568.348408 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1567.664409 au

C	-1.06545500	-2.75700000	-0.17495800
C	1.39062300	-2.65387700	-0.19148100
C	0.18829100	-3.35042700	-0.34184600
H	2.32920600	-3.19621900	-0.32086700
H	0.23106500	-4.40662200	-0.57721700
H	-1.95735000	-3.37567200	-0.29144600
C	-0.03145200	1.34239900	-1.46045000
H	0.80448100	1.27659100	-2.16264000
H	-0.97622200	1.22909100	-2.00704700
N	1.45954500	-1.36325900	0.12991900
N	-1.23688700	-1.47615100	0.14852600
C	-2.48796600	-0.82560800	0.22392900
C	-3.48142300	-0.91918600	-0.76558200
C	-2.64603300	0.09845700	1.28030700
C	-4.61669800	-0.11744500	-0.67900200
H	-3.34739900	-1.60151400	-1.59978600
C	-3.78202100	0.91645800	1.34251500
H	-1.96302900	0.06396500	2.13532300
C	-4.76560300	0.80991900	0.36133000

H	-5.38805700	-0.20318900	-1.43868200
H	-3.90639000	1.60505000	2.17277200
H	-5.65138600	1.43524800	0.40830200
C	2.65487300	-0.61253400	0.18588900
C	3.63605600	-0.62630300	-0.81997800
C	2.75725500	0.31893800	1.24225500
C	4.70665800	0.26142500	-0.74924400
H	3.54173200	-1.31546400	-1.65398300
C	3.82686900	1.22254500	1.28893700
H	2.09116700	0.23163100	2.10672400
C	4.79986600	1.19480900	0.29194000
H	5.46955900	0.23791700	-1.52182400
H	3.91055000	1.91747300	2.11903600
H	5.63462000	1.88751400	0.32661200
C	-0.00196400	2.61538300	-0.60410000
C	-1.09671000	3.64816500	-0.90248000
H	-2.09283200	3.20028700	-0.81629100
H	-1.04207900	4.50138300	-0.21802200
H	-0.98166000	4.02113600	-1.92487700
H	0.98840300	3.08242700	-0.63746000
H	-0.12228000	2.37424700	0.50547200
Sc	0.04563300	0.16732700	0.29899600

Y_1_III

E(B3LYP/BS1) = -845.266672 au

H(B3LYP/BS1) = -844.909465 au

G(B3LYP/BS1) = -844.984721 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -845.990648 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -845.296360 au

C	-1.19064300	-2.74164000	-0.41336300
C	1.28236300	-2.71047500	-0.42393300
C	0.05246800	-3.34191900	-0.63223600
H	2.19178400	-3.27654500	-0.63788000
H	0.06374100	-4.36641700	-0.98394800
H	-2.08714000	-3.33130900	-0.61766600
C	-0.05072600	1.58717900	-1.39382800
H	0.68484500	1.49698200	-2.19937300
H	-1.05562300	1.58571800	-1.84360200
N	1.42198700	-1.47051600	0.04151600
N	-1.35867000	-1.50435100	0.05137500
C	-2.61592700	-0.86850700	0.14002200
C	-3.57223100	-0.87439500	-0.89059000
C	-2.82962400	-0.04808600	1.27151100
C	-4.71928300	-0.09304200	-0.77429700
H	-3.39889000	-1.47177600	-1.78074800
C	-3.97895200	0.74890000	1.36747800
H	-2.18531700	-0.16499800	2.14946600
C	-4.92176300	0.72943900	0.34217300
H	-5.45809500	-0.11170800	-1.57013200
H	-4.14553300	1.35114800	2.25564000
H	-5.81616100	1.34005600	0.41231400
C	2.66260300	-0.80125000	0.12109300
C	3.60515600	-0.77139200	-0.92175400
C	2.86916700	0.01291600	1.25824900
C	4.73282400	0.03868200	-0.81195100

H	3.43579800	-1.36445900	-1.81556000
C	3.99848500	0.83818700	1.34825000
H	2.23669700	-0.12718700	2.14114500
C	4.92823700	0.85415700	0.31081800
H	5.46137900	0.04777800	-1.61733800
H	4.16067100	1.43562300	2.24048500
H	5.80730200	1.48717000	0.37635200
C	0.17343700	2.86061100	-0.55660700
C	-0.42644400	4.15521400	-1.12821200
H	-1.50726800	4.05032400	-1.27121800
H	-0.24665000	5.01125500	-0.46825800
H	0.02235100	4.37225400	-2.10258000
H	1.24909100	3.00851800	-0.37954800
H	-0.27378500	2.75561700	0.47493100
Y	0.01083800	0.24739900	0.44385500

La_1_III

E(B3LYP/BS1) = -838.559557 au

H(B3LYP/BS1) = -838.202259 au

G(B3LYP/BS1) = -838.279290 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -839.257787 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -838.565755 au

C	1.27188200	-2.72035500	0.64686100
C	-1.20842000	-2.74020700	0.64333900
C	0.03613700	-3.32201800	0.89995000
H	-2.09828800	-3.30783100	0.92649100
H	0.04334300	-4.30976600	1.34516300
H	2.17003200	-3.27365000	0.93222300
C	0.00410700	1.79477200	1.32383500
H	-0.82756300	1.66337600	2.02954100
H	0.94096900	1.78884800	1.89969000
N	-1.39732300	-1.55528700	0.06567400
N	1.44273000	-1.53238700	0.06987800
C	2.70832600	-0.91143800	-0.00937500
C	3.57856600	-0.78801200	1.08952500
C	3.03367600	-0.25357000	-1.21702900
C	4.75057800	-0.04533200	0.96849300
H	3.31852200	-1.25935600	2.03282100
C	4.20797400	0.50440700	-1.32166600
H	2.45167800	-0.46814800	-2.11775200
C	5.06448300	0.61258800	-0.22793600
H	5.42059600	0.03429700	1.81957500
H	4.46149200	0.97783800	-2.26571700
H	5.97707000	1.19488900	-0.30529400
C	-2.67352900	-0.95608300	-0.01646000
C	-3.54644700	-0.84507000	1.08171000
C	-3.01019700	-0.30804900	-1.22626500
C	-4.73180300	-0.12417800	0.95782700
H	-3.27864900	-1.30918200	2.02643500
C	-4.19775900	0.42820300	-1.33373300
H	-2.42253100	-0.51303500	-2.12538400
C	-5.05691100	0.52400500	-0.24082500
H	-5.40367700	-0.05416600	1.80829000
H	-4.45903600	0.89446800	-2.27923000
H	-5.97991500	1.08933800	-0.32053200

C	-0.14486100	3.10288100	0.52729500
C	-0.13638000	4.38965600	1.37074300
H	0.80159700	4.47174800	1.92981100
H	-0.24408900	5.28297700	0.74512800
H	-0.95877800	4.37437800	2.09350400
H	-1.08819000	3.09293700	-0.05525600
H	0.67231200	3.19684800	-0.21974400
La	0.00857400	0.31567900	-0.60256700

Al_1_IV

E(B3LYP/BS1) = -808.882895 au

H(B3LYP/BS1) = -808.536024 au

G(B3LYP/BS1) = -808.604462 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1049.601179 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1048.934569 au

C	1.18344600	-2.15186100	-0.53094600
C	-1.29719500	-2.12402100	-0.52887800
C	-0.06469800	-2.76512100	-0.66178500
H	-2.19131600	-2.74256000	-0.62790200
H	-0.07691900	-3.82670800	-0.87830200
H	2.06266200	-2.79068200	-0.63447400
N	-1.49796100	-0.82578200	-0.30644200
N	1.41355100	-0.86049600	-0.30509500
C	-2.84697100	-0.40075000	-0.09399200
C	-3.67964200	-1.07157400	0.81474600
C	-3.34380600	0.71143400	-0.78826200
C	-4.99384400	-0.64632700	1.00901900
H	-3.28404000	-1.90643900	1.38627300
C	-4.65677000	1.13466700	-0.58317800
H	-2.70352100	1.22530000	-1.49726100
C	-5.48813600	0.45753100	0.31170000
H	-5.62680300	-1.17188400	1.71901700
H	-5.03178900	1.99391100	-1.13242700
H	-6.50972500	0.79143000	0.46941200
C	2.77170500	-0.46384700	-0.09800200
C	3.27861200	0.65450200	-0.77494900
C	3.60315300	-1.16691800	0.78717800
C	4.60136300	1.05032700	-0.57819700
H	2.63706000	1.19455500	-1.46328400
C	4.92690300	-0.76846600	0.97312700
H	3.20028500	-2.00543200	1.34814800
C	5.43202200	0.34030200	0.29156800
H	4.98431500	1.91446100	-1.11412100
H	5.55897200	-1.31879000	1.66493500
H	6.46126500	0.65300800	0.44281900
C	0.04712200	1.74917600	1.48550600
C	0.06323600	2.27214900	-0.96752900
C	0.49654400	2.82753600	0.43677200
H	-0.95072000	1.98787000	1.87991000
H	0.71892700	1.66080800	2.34603600
H	-0.92728100	2.66479900	-1.23710900
H	0.73825700	2.55334900	-1.78468400
H	0.09488300	3.83038100	0.64471700
H	1.59069800	2.91695900	0.46459400
Al	-0.02712400	0.48824500	-0.05684100

CH4

E(B3LYP/BS1) = -40.517663 au

H(B3LYP/BS1) = -40.468641 au

G(B3LYP/BS1) = -40.489773 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -40.535043 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -40.489214 au

C	0.00000000	0.00000000	0.00000000
H	0.63139700	0.63139700	0.63139700
H	-0.63139700	-0.63139700	0.63139700
H	-0.63139700	0.63139700	-0.63139700
H	0.63139700	-0.63139700	-0.63139700

Al_1_V

E(B3LYP/BS1) = -849.429470 au

H(B3LYP/BS1) = -849.030292 au

G(B3LYP/BS1) = -849.107931 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1090.160262 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1089.453306 au

C	1.13681200	-2.16816800	-0.87789500
C	-1.34732600	-2.11110700	-0.86657500
C	-0.12013500	-2.72001300	-1.14072400
H	-2.24306600	-2.71543600	-1.02407400
H	-0.14525500	-3.72941600	-1.53434200
H	2.00293300	-2.81283100	-1.04176600
N	-1.53763600	-0.86810300	-0.42900500
N	1.38598700	-0.93469900	-0.44588900
C	-2.85574000	-0.50051400	-0.03145500
C	-3.66282800	-1.37106300	0.71955200
C	-3.35506100	0.76810800	-0.36637900
C	-4.94961600	-0.98990800	1.09922600
H	-3.26649200	-2.33253900	1.03293300
C	-4.63907000	1.14518100	0.02400500
H	-2.74505100	1.44596100	-0.95499000
C	-5.44528600	0.26829600	0.75329400
H	-5.55865100	-1.67486800	1.68322400
H	-5.01218600	2.12800700	-0.25095100
H	-6.44489300	0.56618400	1.05646800
C	2.72394200	-0.61972500	-0.07136500
C	3.27245700	0.62059000	-0.43432500
C	3.50323300	-1.51381600	0.68090700
C	4.57751600	0.94735700	-0.06790800
H	2.68414900	1.31435400	-1.02686700
C	4.81056300	-1.18297800	1.03679700
H	3.07026200	-2.45299400	1.01294200
C	5.35499400	0.04728200	0.66431300
H	4.98907000	1.90839700	-0.36402600
H	5.39815100	-1.88475800	1.62277500
H	6.37080700	0.30589900	0.94906600
Al	-0.04413300	0.45686300	-0.24994500
C	-0.07486700	1.14225800	1.62804500
H	-1.11646800	1.40641700	1.87022300
H	0.15452300	0.29399200	2.29270900
C	-0.01336300	1.65426000	-1.86894600

H	0.76284700	1.28322900	-2.55754700
H	-0.95098700	1.50992000	-2.42939700
C	0.83291200	2.33118500	2.00524700
H	1.89247300	2.10706400	1.83028600
H	0.59489400	3.22537900	1.41599800
H	0.73519300	2.61034100	3.06435900
C	0.19958300	3.16507400	-1.64321600
H	1.15522600	3.37218800	-1.14415800
H	0.19736500	3.73739100	-2.58194300
H	-0.58189100	3.59471700	-1.00297000

Ga_1_IV

E(B3LYP/BS1) = -808.921188 au

H(B3LYP/BS1) = -808.574563 au

G(B3LYP/BS1) = -808.644000 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2732.007921 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2731.284251 au

C	-1.19359600	2.20588000	-0.52761000
C	1.29527700	2.17837900	-0.52428900
C	0.05831700	2.81274100	-0.65852200
H	2.18337500	2.80610200	-0.62290400
H	0.07050700	3.87414400	-0.87657700
H	-2.06705100	2.85269400	-0.63280200
N	1.51161100	0.88439500	-0.30372200
N	-1.43803200	0.91885100	-0.30196300
C	2.85932700	0.46691900	-0.08709300
C	3.69402300	1.15307100	0.80880000
C	3.35692700	-0.65616200	-0.76383900
C	5.00936500	0.73272400	1.00642400
H	3.29899800	1.99604400	1.36865000
C	4.67071700	-1.07434900	-0.55537800
H	2.71621300	-1.18198000	-1.46377900
C	5.50373300	-0.38161400	0.32618500
H	5.64318600	1.27052300	1.70647700
H	5.04549600	-1.94196800	-1.09154800
H	6.52610700	-0.71164900	0.48689800
C	-2.79377200	0.52707200	-0.09064800
C	-3.29546500	-0.61087700	-0.73922800
C	-3.63254100	1.25045100	0.77164400
C	-4.61802600	-1.00481000	-0.53937900
H	-2.64974500	-1.16756700	-1.41030500
C	-4.95638600	0.85363700	0.96069400
H	-3.23537900	2.10376800	1.31397000
C	-5.45562800	-0.27393600	0.30636000
H	-4.99575900	-1.88403800	-1.05413000
H	-5.59320600	1.42040000	1.63471200
H	-6.48489800	-0.58514900	0.46042800
C	-0.04443500	-1.74644400	1.48109300
C	-0.06065600	-2.25906200	-0.96346500
C	-0.47302600	-2.82996400	0.43565400
H	0.95803100	-1.95264700	1.87896800
H	-0.72223600	-1.64903900	2.33534000
H	0.93465200	-2.62167600	-1.25255700
H	-0.74183000	-2.52378300	-1.78041100
H	-0.04551500	-3.82294500	0.63835100

H	-1.56430200	-2.94575200	0.46877300
Ga	0.02139900	-0.45226300	-0.05652200

Ga_1_V

E(B3LYP/BS1) = -849.471044 au

H(B3LYP/BS1) = -849.071840 au

G(B3LYP/BS1) = -849.149065 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2772.572961 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2771.808790 au

C	1.19883100	-2.18112000	-0.88745500
C	-1.29341400	-2.16854500	-0.84383600
C	-0.05465700	-2.74651100	-1.13869700
H	-2.17433400	-2.79595300	-0.99773700
H	-0.06675100	-3.75288100	-1.54104200
H	2.06733700	-2.81888400	-1.06717800
N	-1.51378400	-0.93704000	-0.39588500
N	1.44827800	-0.95029100	-0.45098700
C	-2.83432300	-0.59779500	0.00858200
C	-3.62737800	-1.48912800	0.75071500
C	-3.35544000	0.66608800	-0.31255300
C	-4.91964100	-1.13235400	1.13562500
H	-3.21563700	-2.44760900	1.05315300
C	-4.64477000	1.01860000	0.08281000
H	-2.75751400	1.35952900	-0.89578800
C	-5.43607900	0.12131800	0.80383100
H	-5.51709000	-1.83319100	1.71280700
H	-5.03395000	1.99811100	-0.18170100
H	-6.43985800	0.39995800	1.11151900
C	2.78231400	-0.63234000	-0.07475700
C	3.31688900	0.62468900	-0.40117400
C	3.57759700	-1.53952700	0.64578600
C	4.62050600	0.95456400	-0.03321500
H	2.71688000	1.33085900	-0.96651800
C	4.88383300	-1.20570300	1.00294000
H	3.15753000	-2.49268500	0.95341700
C	5.41323300	0.04094600	0.66535700
H	5.01950700	1.92888200	-0.30213700
H	5.48232300	-1.91886500	1.56370500
H	6.42814900	0.30164600	0.95140600
C	-0.02806200	1.07764100	1.68539900
H	-1.07461500	1.26707500	1.96485300
H	0.28873800	0.23380500	2.31532200
C	-0.06745200	1.63290600	-1.84241800
H	0.86991700	1.50427800	-2.40300200
H	-0.84501500	1.23968000	-2.51407200
C	0.81811300	2.31790100	2.02935000
H	1.88007500	2.16191300	1.80376200
H	0.49444700	3.19885200	1.46161600
H	0.75067600	2.57993700	3.09485200
C	-0.31129900	3.13453600	-1.60136200
H	0.49599400	3.58692800	-1.01238200
H	-0.38298200	3.70207900	-2.53995000
H	-1.24095000	3.31623700	-1.04565600
Ga	-0.02184300	0.44466500	-0.21421600

In_1_IV

E(B3LYP/BS1) = -808.717586 au

H(B3LYP/BS1) = -808.371783 au

G(B3LYP/BS1) = -808.443318 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -997.276745 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -996.639752 au

C	1.20183800	-2.32003400	-0.46205200
C	-1.31638200	-2.28630300	-0.45841000
C	-0.06587900	-2.90343500	-0.56994500
H	-2.18237000	-2.94571000	-0.55788300
H	-0.08069100	-3.96991000	-0.76529500
H	2.04958000	-3.00202300	-0.56611000
N	-1.58146000	-0.99759000	-0.26831900
N	1.49979600	-1.03990600	-0.26949300
C	-2.94045400	-0.61281900	-0.08932700
C	-3.80828200	-1.33971000	0.74246000
C	-3.42066300	0.53806200	-0.73414300
C	-5.13314000	-0.93426100	0.90332500
H	-3.43277900	-2.20260000	1.28497800
C	-4.74430500	0.94084400	-0.56245100
H	-2.75795100	1.10001400	-1.38619200
C	-5.60840400	0.20568900	0.25237200
H	-5.79054500	-1.50449100	1.55434600
H	-5.10177900	1.82996400	-1.07467000
H	-6.63856300	0.52319700	0.38576600
C	2.86786100	-0.68678100	-0.09514100
C	3.36501700	0.46637300	-0.72307300
C	3.72836800	-1.44588500	0.71518100
C	4.69839700	0.83843100	-0.55776600
H	2.70701000	1.05472900	-1.35654900
C	5.06283400	-1.07067000	0.86971500
H	3.34086100	-2.30993300	1.24727000
C	5.55533700	0.07068500	0.23426600
H	5.06886100	1.72962300	-1.05698900
H	5.71443900	-1.66574800	1.50413300
H	6.59315200	0.36442700	0.36273000
C	0.07157200	2.06487500	1.53311100
C	0.07532800	2.49843100	-0.97126500
C	0.51753300	3.05793800	0.41639100
H	-0.93380600	2.29979500	1.90545500
H	0.74461000	2.02879700	2.39515600
H	-0.92916300	2.85174400	-1.23995800
H	0.74373700	2.76855200	-1.79601500
H	0.14003200	4.07749800	0.59187300
H	1.61377100	3.12610700	0.43141900
In	-0.01910700	0.52285500	-0.01547500

In_1_V

E(B3LYP/BS1) = -849.268267 au

H(B3LYP/BS1) = -848.869950 au

G(B3LYP/BS1) = -848.951144 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1037.842900 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1037.164086 au

C	1.14228000	-2.30664300	-0.82108300
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C	-1.37865000	-2.23843900	-0.80158700
C	-0.13547000	-2.83467600	-1.04442000
H	-2.24927500	-2.87942400	-0.96594700
H	-0.16612300	-3.85479000	-1.41139500
H	1.97478100	-2.99261500	-1.00105300
N	-1.63134000	-0.99524500	-0.40655200
N	1.46404300	-1.08000700	-0.42802100
C	-2.96853800	-0.66108600	-0.06495400
C	-3.78692500	-1.53592300	0.67110300
C	-3.48472500	0.59182800	-0.43691600
C	-5.09275600	-1.17378300	1.00084700
H	-3.38417700	-2.48521600	1.01210500
C	-4.78813200	0.95032100	-0.09666600
H	-2.86996000	1.27051900	-1.02165800
C	-5.60148900	0.06912800	0.61956700
H	-5.70820100	-1.86194700	1.57446600
H	-5.17107100	1.92067200	-0.40125000
H	-6.61621700	0.35160200	0.88483700
C	2.82065700	-0.80846200	-0.11193000
C	3.38017500	0.42696600	-0.48087100
C	3.61773400	-1.72531500	0.59563300
C	4.70439100	0.72749100	-0.16525600
H	2.78217500	1.13707900	-1.04590500
C	4.94416000	-1.42101000	0.90058700
H	3.18365700	-2.66120100	0.93515800
C	5.49569600	-0.19543600	0.52264900
H	5.12047800	1.68491200	-0.46712800
H	5.54282600	-2.14076800	1.45280900
H	6.52664500	0.04166900	0.76907200
C	-0.03152300	1.05482100	1.99858200
H	-1.07048400	1.25189200	2.29599000
H	0.27002200	0.15832700	2.55722000
C	0.01311400	1.84757700	-1.83737300
H	0.72203800	1.41472000	-2.55714800
H	-0.96421200	1.79706400	-2.33745300
C	0.85915500	2.24380300	2.40083400
H	1.91358000	2.06383500	2.15658300
H	0.56422600	3.16668800	1.88580200
H	0.81079400	2.44902700	3.48025800
C	0.37660600	3.31834200	-1.56601900
H	1.36712500	3.41869300	-1.10302900
H	0.39248600	3.92040800	-2.48617900
H	-0.33776700	3.79547600	-0.88310900
In	-0.04034300	0.52210400	-0.10566100

Sc_1_IV

E(B3LYP/BS1) = -853.345650 au

H(B3LYP/BS1) = -853.001715 au

G(B3LYP/BS1) = -853.073966 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1567.865416 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1567.182721 au

C	1.21279400	-2.24171200	-0.53945100
C	-1.30543400	-2.21204700	-0.53760200
C	-0.05303500	-2.82612400	-0.66811800
H	-2.17148600	-2.87309800	-0.63656300

H	-0.06588500	-3.88886500	-0.88449400
H	2.06414900	-2.92097700	-0.64184300
N	-1.56172600	-0.92405500	-0.32227300
N	1.49662300	-0.95958400	-0.32213600
C	-2.90759000	-0.53262900	-0.09139700
C	-3.75559000	-1.24792500	0.77219000
C	-3.39227800	0.63442800	-0.70675900
C	-5.06133600	-0.81323200	0.99514700
H	-3.37579800	-2.12505600	1.28836800
C	-4.69636900	1.06882700	-0.46907800
H	-2.75150400	1.17996100	-1.39559300
C	-5.53842500	0.34587200	0.37816500
H	-5.70376200	-1.37569300	1.66761500
H	-5.05630600	1.97008700	-0.95789800
H	-6.55391700	0.68500700	0.56129700
C	2.84860000	-0.59067600	-0.09406500
C	3.34264000	0.57973000	-0.69595800
C	3.69377900	-1.32847900	0.75331500
C	4.65351600	0.99504700	-0.46131300
H	2.70326400	1.14255200	-1.37253900
C	5.00635200	-0.91296700	0.97215900
H	3.30735100	-2.20811000	1.26021900
C	5.49302200	0.24923800	0.36842000
H	5.02088300	1.89898600	-0.93954600
H	5.64694000	-1.49296200	1.63136900
H	6.51409000	0.57296300	0.54837900
C	0.02773700	2.02754000	1.50521900
C	0.05778900	2.50787700	-1.09834000
C	0.38584600	3.04651900	0.35281400
H	-0.96492600	2.24167800	1.92740400
H	0.76125900	2.05161400	2.31654200
H	-0.91514300	2.88726900	-1.44209300
H	0.81177100	2.82126200	-1.82756200
H	-0.13900500	3.99541600	0.52051200
H	1.46056400	3.25756600	0.40589900
Sc	-0.00994800	0.61286500	-0.09193800

Sc_1_V

E(B3LYP/BS1) = -893.874594 au

H(B3LYP/BS1) = -893.479141 au

G(B3LYP/BS1) = -893.560944 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1608.408907 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1607.684971 au

C	1.10297400	-2.30109400	-0.84757100
C	-1.40917900	-2.21820300	-0.83223500
C	-0.17335800	-2.82902000	-1.07743800
H	-2.29251400	-2.84351500	-0.99082800
H	-0.20913800	-3.84775500	-1.44780000
H	1.94151500	-2.98150400	-1.02165000
N	-1.62815800	-0.96823600	-0.42939400
N	1.40789500	-1.06970300	-0.44410900
C	-2.94690800	-0.60031000	-0.05215600
C	-3.75526100	-1.43450500	0.74001000
C	-3.44308200	0.65650100	-0.43946200
C	-5.03454500	-1.02604900	1.11416500

H	-3.36347000	-2.38724000	1.08460600
C	-4.71921300	1.06283200	-0.05018800
H	-2.83948000	1.29874900	-1.07672900
C	-5.52293500	0.22298200	0.72319700
H	-5.64608500	-1.68196100	1.72817200
H	-5.08839700	2.03558500	-0.36345800
H	-6.51707600	0.54072200	1.02390300
C	2.75471700	-0.78271500	-0.09937000
C	3.31509300	0.44158700	-0.50329200
C	3.53085200	-1.66298800	0.67483500
C	4.62295900	0.77118700	-0.14724300
H	2.73564400	1.11720100	-1.12903800
C	4.84128800	-1.33139700	1.01534800
H	3.09141500	-2.59037500	1.03096700
C	5.39376200	-0.11439500	0.60832800
H	5.04178600	1.71958200	-0.47232000
H	5.42789600	-2.02186900	1.61563500
H	6.41246600	0.14331300	0.88311200
C	-0.09423800	1.48839600	1.76359300
H	-1.03103000	2.07625400	1.80699800
H	-0.22437600	0.68740900	2.51461800
C	0.01155800	1.97768200	-1.87830700
H	0.70036300	1.56944900	-2.64193300
H	-0.97506500	1.97131400	-2.37892600
C	1.08855500	2.38645500	2.16871200
H	2.03863000	1.83464500	2.16295100
H	1.20699800	3.23202300	1.47770700
H	0.98025000	2.81654300	3.17659000
C	0.40445400	3.43349500	-1.56143700
H	1.40915000	3.49795600	-1.11967200
H	0.41019700	4.08629700	-2.44818400
H	-0.28187500	3.89041200	-0.83574100
Sc	-0.05671100	0.53617600	-0.20863700

Y_1_IV

E(B3LYP/BS1) = -844.823339 au

H(B3LYP/BS1) = -844.480257 au

G(B3LYP/BS1) = -844.554416 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -845.485556 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -844.793641 au

C	1.20927100	-2.42529000	-0.47218100
C	-1.32365700	-2.38830500	-0.47029400
C	-0.06545100	-3.00024700	-0.57147600
H	-2.18044300	-3.06556300	-0.54663600
H	-0.08135800	-4.07185500	-0.74022400
H	2.04716200	-3.12541900	-0.55088500
N	-1.59705800	-1.09703300	-0.31272400
N	1.51766300	-1.14163000	-0.31417100
C	-2.93992700	-0.69873600	-0.10306300
C	-3.81250400	-1.39000700	0.75748400
C	-3.39636700	0.47814200	-0.72591200
C	-5.10883400	-0.92333400	0.96839700
H	-3.45804700	-2.27348300	1.28066400
C	-4.69137800	0.94554700	-0.49857300
H	-2.74718700	1.00326500	-1.42562400

C	-5.55504900	0.24547500	0.34555300
H	-5.76917900	-1.46786100	1.63827800
H	-5.02651200	1.85250100	-0.99413800
H	-6.56323600	0.60887100	0.52164700
C	2.86923600	-0.77391500	-0.10742000
C	3.34579500	0.39848900	-0.72411100
C	3.73148900	-1.48857700	0.74447700
C	4.65076600	0.83869000	-0.49877700
H	2.70403700	0.94174300	-1.41728700
C	5.03778400	-1.04936700	0.95211900
H	3.36196400	-2.36843600	1.26330700
C	5.50421300	0.11512200	0.33572600
H	5.00157600	1.74250400	-0.98918200
H	5.69045700	-1.61183800	1.61465900
H	6.52040600	0.45677700	0.50930600
C	0.03647300	2.30067400	1.55219700
C	0.06736600	2.72305500	-1.08745600
C	0.46441500	3.23979100	0.35480400
H	-0.97289200	2.57020500	1.90296400
H	0.72006400	2.40911300	2.40005500
H	-0.92814200	3.10703300	-1.36212200
H	0.77210700	3.08830700	-1.84189800
H	0.05091100	4.24663600	0.50924300
H	1.55812600	3.34410100	0.38544100
Y	-0.00733100	0.65130200	-0.05841700

Y_1_V

E(B3LYP/BS1) = -885.357006 au

H(B3LYP/BS1) = -884.963340 au

G(B3LYP/BS1) = -885.045068 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -886.030760 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -885.296646 au

C	1.23170000	-2.51711100	-0.67786800
C	-1.28728300	-2.51942200	-0.61947300
C	-0.03062200	-3.11334100	-0.79611100
H	-2.14750700	-3.19108300	-0.70316400
H	-0.03499500	-4.17286000	-1.02847900
H	2.08787700	-3.18870000	-0.79655300
N	-1.54920800	-1.23952900	-0.37545100
N	1.50424600	-1.23571000	-0.45167200
C	-2.87667500	-0.84841700	-0.07410900
C	-3.70309000	-1.57927000	0.79925400
C	-3.35761100	0.36198800	-0.60864600
C	-4.98005100	-1.11617400	1.11034900
H	-3.32598400	-2.49071400	1.25417600
C	-4.63241500	0.82543500	-0.27894000
H	-2.74986200	0.91367800	-1.32471900
C	-5.45046000	0.08771400	0.57787400
H	-5.60545400	-1.69118100	1.78819400
H	-4.98822300	1.75859200	-0.70675500
H	-6.44283000	0.44785400	0.83276500
C	2.84369900	-0.84864500	-0.20329300
C	3.30968000	0.35796100	-0.75884300
C	3.70099300	-1.58158500	0.63838600
C	4.59930600	0.81531900	-0.48222400

H	2.67700300	0.91222800	-1.45078700
C	4.99172600	-1.12469000	0.89700000
H	3.33760000	-2.48988200	1.11038300
C	5.44723000	0.07511200	0.34274200
H	4.94259300	1.74551300	-0.92641300
H	5.64050800	-1.70142000	1.55099100
H	6.45092100	0.43039900	0.55676500
C	0.04882200	1.41621900	2.09516700
H	-0.95749800	1.77315700	2.38391600
H	0.27852900	0.61338200	2.81903900
C	-0.13572600	2.19922600	-1.81677700
H	0.86362100	2.36465100	-2.26210100
H	-0.73595500	1.80439800	-2.65872000
C	1.05964900	2.56741100	2.28287600
H	2.08807600	2.24860000	2.05522800
H	0.83930600	3.41649200	1.61913300
H	1.08253600	2.97422200	3.30655200
C	-0.71195700	3.56587000	-1.38939600
H	-0.10543400	4.03359800	-0.60123800
H	-0.77523300	4.29728500	-2.21080000
H	-1.72917000	3.47160900	-0.97986500
Y	-0.01992700	0.53603200	-0.10424300

La_1_IV

E(B3LYP/BS1) = -838.094412 au

H(B3LYP/BS1) = -837.752221 au

G(B3LYP/BS1) = -837.827880 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -838.705372 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -838.024763 au

C	1.17158700	-2.63844900	-0.38764000
C	-1.36757600	-2.59145500	-0.38636800
C	-0.10845800	-3.21016900	-0.44332400
H	-2.22322000	-3.27576700	-0.41827900
H	-0.12798100	-4.29103800	-0.53875500
H	2.00035900	-3.35434100	-0.42641200
N	-1.63744100	-1.29485100	-0.32259500
N	1.49593800	-1.35298500	-0.31675300
C	-2.96359400	-0.86082300	-0.13108400
C	-3.85660000	-1.47557100	0.76898600
C	-3.38713500	0.30377000	-0.80511500
C	-5.13143200	-0.94919400	0.96831400
H	-3.53178900	-2.34786300	1.32896800
C	-4.66112000	0.83166600	-0.58889800
H	-2.73778800	0.75733700	-1.55506500
C	-5.54061500	0.20668400	0.29667600
H	-5.80555600	-1.43688300	1.66778100
H	-4.96820700	1.72438600	-1.12682900
H	-6.53213300	0.61628800	0.46525000
C	2.84390400	-0.98184000	-0.13326900
C	3.32105500	0.15812300	-0.81255900
C	3.70997800	-1.64027900	0.76189700
C	4.62156200	0.62064700	-0.60519900
H	2.68902800	0.64744800	-1.55450100
C	5.01158000	-1.17987500	0.95159200
H	3.34446400	-2.49373800	1.32578300

C	5.47436100	-0.04750200	0.27489500
H	4.96964500	1.49643500	-1.14594400
H	5.66463600	-1.70023500	1.64748400
H	6.48678800	0.31103700	0.43554000
C	0.11932600	2.56125900	1.58340400
C	0.15221300	2.94730700	-1.03976200
C	0.72250500	3.35272100	0.36815700
H	-0.88479500	2.95167600	1.82306200
H	0.74421700	2.67418000	2.47563800
H	-0.84435200	3.39938400	-1.18156200
H	0.79783700	3.31147200	-1.84623600
H	0.60063000	4.43642100	0.52444100
H	1.81347800	3.18279400	0.35766900
La	-0.02200000	0.69269700	-0.02854000

La_1_V

E(B3LYP/BS1) = -878.632929 au

H(B3LYP/BS1) = -878.239363 au

G(B3LYP/BS1) = -878.326147 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -879.251248 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -878.532436 au

C	-1.05136943	2.61482575	-0.48501096
C	1.46692957	2.53587675	-0.47971696
C	0.22942057	3.18787675	-0.52798396
H	2.34665857	3.18547975	-0.54459596
H	0.26381157	4.26640375	-0.64018296
H	-1.88767543	3.31840875	-0.56707396
N	1.64663621	1.18341306	-0.38614137
N	-1.35311378	1.32987090	-0.39073779
C	2.96772621	0.70955206	-0.23908437
C	3.90898921	1.30807706	0.62204863
C	3.33241121	-0.47122194	-0.91747137
C	5.17528021	0.74966706	0.77958063
H	3.62826921	2.19309706	1.18587963
C	4.59883821	-1.03271594	-0.73955637
H	2.64065021	-0.91669594	-1.63198137
C	5.52710421	-0.42428594	0.10575163
H	5.88794121	1.22528706	1.44851963
H	4.86100921	-1.93908894	-1.27859337
H	6.51287821	-0.85927694	0.24191563
C	-2.70480178	0.94008790	-0.28730179
C	-3.13379278	-0.18825010	-1.01532179
C	-3.62182878	1.57177890	0.57539721
C	-4.43906778	-0.66678110	-0.88465179
H	-2.45688778	-0.64918010	-1.73410879
C	-4.92611078	1.09430690	0.69011121
H	-3.29406178	2.41881390	1.17143121
C	-5.34168878	-0.02771310	-0.03317979
H	-4.75192878	-1.53144110	-1.46378179
H	-5.61962678	1.59402190	1.36157021
H	-6.35725578	-0.39903310	0.06775921
C	0.37696814	-1.17654521	2.43547220
H	0.90976314	-2.10122821	2.69353320
H	0.82853214	-0.36402121	3.02563220
C	0.10328214	-2.43807221	-1.60842780

H	-0.15387986	-2.22051221	-2.65726880
H	1.08318714	-2.94462421	-1.63412180
C	-1.11985886	-1.30486321	2.75926520
H	-1.75954886	-0.59271321	2.18252420
H	-1.50362786	-2.30644421	2.52092020
H	-1.39044186	-1.10235221	3.80617120
C	-0.94104686	-3.39688721	-1.00234480
H	-1.95499386	-2.96356021	-1.00949980
H	-1.02688286	-4.36546221	-1.52061780
H	-0.71515186	-3.64540721	0.04919120
La	0.05204514	-0.50523721	0.03400520

Al_2_I

E(B3LYP/BS1) = -121.750195 au

H(B3LYP/BS1) = -121.633941 au

G(B3LYP/BS1) = -121.678778 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -362.264566 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -362.115279 au

Al	-0.00013100	-0.00003400	0.00012500
C	-1.95653700	-0.34237300	-0.00043500
H	-2.25386400	-0.95577800	-0.86312600
H	-2.25866200	-0.91414000	0.88906100
H	-2.56673300	0.56837400	-0.02276200
C	0.68179400	1.86541700	0.00037200
H	1.77556200	1.93807600	0.02615200
H	0.34064500	2.41170300	-0.89099700
H	0.29648700	2.43094200	0.86095200
C	1.27486600	-1.52295900	-0.00006500
H	1.94132800	-1.48313800	-0.87380400
H	1.93486000	-1.48904700	0.87882100
H	0.79133600	-2.50706000	-0.00514800

Ga_2_I

E(B3LYP/BS1) = -121.804569 au

H(B3LYP/BS1) = -121.689047 au

G(B3LYP/BS1) = -121.731195 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2044.696478 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2044.490233 au

C	-1.49331700	-1.31468200	-0.00037900
H	-1.42043600	-1.98812500	-0.86487000
H	-1.44608000	-1.95516900	0.89080200
H	-2.48332900	-0.84666700	-0.02261800
C	-0.39231600	1.95031300	0.00039500
H	0.50739800	2.57439800	0.02627300
H	-0.96753900	2.22983100	-0.89272400
H	-1.01539600	2.22308000	0.86267800
C	1.88533500	-0.63548500	-0.00010500
H	2.42538700	-0.25033500	-0.87554500
H	2.42260500	-0.25856600	0.88063100
H	1.97556300	-1.72699800	-0.00499900
Ga	0.00011700	-0.00007500	0.00002900

Al_2_II

E(B3LYP/BS1) = -200.344050 au

H(B3LYP/BS1) = -200.170087 au
 G(B3LYP/BS1) = -200.221397 au
 E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -440.887694 au
 E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -440.668725 au

Al	0.67498400	-0.00119000	0.02091200
C	0.94861100	-1.66304300	-1.04937100
H	0.54130800	-1.59742200	-2.06701800
H	2.02693500	-1.85219200	-1.16438900
H	0.52779100	-2.56343600	-0.58347000
C	0.79640000	-0.09468000	2.00903700
H	0.31051700	0.74954400	2.51650900
H	0.37343100	-1.01680000	2.42949400
H	1.85043700	-0.07194800	2.32470100
C	0.94186000	1.75750600	-0.88434500
H	0.51800500	2.60727000	-0.33390100
H	2.01972200	1.95985900	-0.97958800
H	0.53504300	1.78880000	-1.90372600
H	-2.14563900	1.24206500	-0.98401500
H	-2.07403000	1.24304500	0.86257700
C	-2.09697900	-0.66903800	-0.05964300
C	-2.09570700	0.67057100	-0.06129300
H	-2.14763800	-1.24230200	-0.98118000
H	-2.07577600	-1.23890300	0.86583700

Ga_2_II

E(B3LYP/BS1) = -200.396580 au
 H(B3LYP/BS1) = -200.222506 au
 G(B3LYP/BS1) = -200.275899 au
 E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2123.317420 au
 E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2123.041501 au

C	0.78750200	-1.67010600	-1.05773600
H	0.36112200	-1.58865900	-2.06484600
H	1.86002200	-1.87533700	-1.18670200
H	0.35286400	-2.55354200	-0.57553100
C	0.63617200	-0.09222400	2.00747200
H	0.13836900	0.75702700	2.49112300
H	0.19751100	-1.01416100	2.40778200
H	1.68376200	-0.07208900	2.34021600
C	0.78212100	1.76250600	-0.89693300
H	0.34486300	2.59544300	-0.33404200
H	1.85413000	1.98170300	-1.00554200
H	0.35593900	1.77460400	-1.90730600
H	-2.39153000	1.24208000	-0.98338800
H	-2.33667700	1.24285300	0.86367100
C	-2.35396400	-0.66789800	-0.05887000
C	-2.35294900	0.67012200	-0.06019300
H	-2.39315900	-1.24129200	-0.98110800
H	-2.33827300	-1.23857400	0.86626100
Ga	0.55863700	-0.00078900	0.01506400

TS_{Al-2}

E(B3LYP/BS1) = -200.303110 au
 H(B3LYP/BS1) = -200.129616 au
 G(B3LYP/BS1) = -200.175170 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -440.846406 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -440.632615 au

Al	-0.47125700	0.04421900	-0.15461900
C	-1.47017500	-1.66480400	-0.32338700
H	-0.80843300	-2.52788900	-0.47244700
H	-2.07135900	-1.87136100	0.57281000
H	-2.16451200	-1.64487500	-1.17400100
C	-1.30219800	1.82144800	0.15977000
H	-0.55949100	2.61113100	0.33670600
H	-1.90948200	2.14559400	-0.69614900
H	-1.96964600	1.81201700	1.03289300
C	0.74957700	-0.38985900	1.65723100
H	1.55683200	0.09131500	2.20991900
H	-0.17751300	-0.07747600	2.16601900
H	0.83881000	-1.47485900	1.74891900
H	2.42954700	-0.84139900	0.11398400
H	2.27180100	0.95998300	0.30401700
C	1.19231200	0.15191200	-1.39296100
C	1.86522100	0.05283800	-0.13186300
H	1.25708000	-0.70691600	-2.05784100
H	1.22428300	1.12068000	-1.88752900

TS_{Ga-2}

E(B3LYP/BS1) = -200.349181 au

H(B3LYP/BS1) = -200.175508 au

G(B3LYP/BS1) = -200.222110 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2123.266754 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2122.997319 au

C	-1.30575300	-1.72339800	-0.24811600
H	-0.60208000	-2.54331000	-0.43286200
H	-1.84808900	-1.95319200	0.67743500
H	-2.03583100	-1.72543300	-1.06658600
C	-1.20511500	1.79922300	0.25920100
H	-0.44904800	2.57948700	0.40880100
H	-1.85078300	2.12416500	-0.56586500
H	-1.82486700	1.76507800	1.16418000
C	0.93541200	-0.39508100	1.69602000
H	1.77874600	0.08426000	2.19396600
H	0.04186700	-0.08940600	2.26017800
H	1.03507600	-1.48058100	1.76609400
H	2.55317900	-0.81200300	0.07006000
H	2.37953000	0.98820500	0.27784800
C	1.26787800	0.17808700	-1.39735300
C	1.97488800	0.07870400	-0.15396100
H	1.32547300	-0.67370800	-2.07125900
H	1.26912500	1.15089800	-1.88412200
Ga	-0.37987600	0.03097900	-0.12040700

Al₂ III

E(B3LYP/BS1) = -200.370117 au

H(B3LYP/BS1) = -200.195791 au

G(B3LYP/BS1) = -200.238950 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -440.907945 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -440.690131 au

Al	-1.08406700	-0.01125600	0.12417900
C	-1.86139200	1.80692000	-0.06884000
H	-1.14642500	2.61235100	0.09279900
H	-2.29850300	1.95462000	-1.06036400
H	-2.68077000	1.95931300	0.64137300
C	-2.23352400	-1.59811000	-0.20497700
H	-1.67459900	-2.45890100	-0.57411000
H	-2.70855000	-1.92273000	0.72834900
H	-3.04379200	-1.40358400	-0.90790600
C	0.82885800	-0.23471500	0.64825800
C	1.83417600	0.08370400	-0.48529300
C	3.30151900	-0.05823500	-0.05835900
H	1.05217700	0.42480800	1.50261100
H	1.01443300	-1.25747700	1.00954900
H	3.53139300	0.61463700	0.77710800
H	3.51480600	-1.08178400	0.27389900
H	1.67182200	1.10654300	-0.85595900
H	1.65387900	-0.57753200	-1.34627200
H	3.98918400	0.17868300	-0.88013500

Ga_2_III

E(B3LYP/BS1) = -200.425837 au

H(B3LYP/BS1) = -200.249062 au

G(B3LYP/BS1) = -200.300515 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2123.34199 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2123.068745 au

C	1.22877600	1.93060100	0.00604900
H	0.48854700	2.50769000	-0.56051100
H	1.20253600	2.31462100	1.03604300
H	2.22278200	2.16006800	-0.39424100
C	2.33759100	-1.32490300	-0.01596600
H	2.01321800	-2.36032200	0.13443900
H	2.86818100	-1.28200500	-0.97736500
H	3.08106700	-1.08738800	0.75591400
C	-1.05018900	-0.68648500	0.03665500
C	-2.17212300	0.36428500	-0.04343400
C	-3.58181300	-0.24014500	0.00476400
H	-1.16585700	-1.41780200	-0.77988700
H	-1.17047900	-1.28615600	0.95434800
H	-3.74003600	-0.93582400	-0.82899100
H	-3.73662000	-0.80174700	0.93474600
H	-2.06751200	0.95172800	-0.96681500
H	-2.06528800	1.08754200	0.77748000
H	-4.35798200	0.53333700	-0.05253400
Ga	0.83400000	-0.02077000	0.00125700

Al_2_IV

E(B3LYP/BS1) = -199.769475 au

H(B3LYP/BS1) = -199.608556 au

G(B3LYP/BS1) = -199.653062 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -440.385367 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -440.175152 au

Al	0.47448800	-0.01667200	-0.00038900
C	1.97999800	-1.41159100	0.00051300

H	2.63810700	-1.32543700	-0.88039500
H	2.63851400	-1.32329700	0.88090900
H	1.60276200	-2.44687200	0.00186100
C	1.27946100	1.87051300	-0.00062200
H	1.91535900	2.06028800	0.88024300
H	1.91511300	2.06148900	-0.88138300
H	0.51070900	2.65981900	0.00007000
C	-1.16544500	-0.28710200	1.23601800
C	-1.16580100	-0.28880300	-1.23558400
C	-2.03696600	0.08983600	0.00006400
H	-1.42654800	0.28269900	2.14203600
H	-1.31898100	-1.35218100	1.48249000
H	-3.06054000	-0.34499100	0.00049300
H	-2.18396500	1.18272400	-0.00067500
H	-1.42708800	0.27962200	-2.14241500
H	-1.31926700	-1.35424900	-1.48051600

Al_2_V

E(B3LYP/BS1) = -240.312225 au

H(B3LYP/BS1) = -240.099545 au

G(B3LYP/BS1) = -240.153538 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -480.939883 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -480.687327 au

Al	0.00022200	0.56836600	-0.00013200
C	0.95071700	1.75124200	-1.39212700
H	0.24730900	2.39081100	-1.95151200
H	1.68848300	2.43595700	-0.94089200
H	1.50069100	1.17118800	-2.15215300
C	-0.94977600	1.75005200	1.39318700
H	-0.24599400	2.38905200	1.95275700
H	-1.68765200	2.43522700	0.94279900
H	-1.49953100	1.16951100	2.15297900
C	1.37688500	-0.62663200	0.97377200
C	-1.37737900	-0.62549700	-0.97437000
H	0.86973700	-1.20678400	1.76568500
H	2.09686400	0.01088700	1.51805200
H	-2.09712800	0.01277200	-1.51807900
H	-0.87113300	-1.20584900	-1.76671500
C	2.16964200	-1.60680100	0.08931700
C	-2.17043100	-1.60530500	-0.08976200
H	2.73732900	-1.07581800	-0.68886400
H	2.89943700	-2.23303600	0.63797700
H	1.49982500	-2.30043300	-0.44004700
H	-1.50089600	-2.30015200	0.43836700
H	-2.73663400	-1.07420700	0.68941600
H	-2.90155300	-2.23023400	-0.63815300

Ga_2_IV

E(B3LYP/BS1) = -199.816548 au

H(B3LYP/BS1) = -199.655556 au

G(B3LYP/BS1) = -199.701175 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2122.806929 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2122.541815 au

C	-1.84195800	-1.43724800	0.00024200
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H	-2.49669500	-1.35724900	0.88267400
H	-2.49711800	-1.35753100	-0.88190100
H	-1.43749400	-2.46081400	0.00031600
C	-1.20663100	1.86468300	-0.00017300
H	-1.84389800	2.03599900	-0.88231400
H	-1.84343200	2.03575700	0.88235700
H	-0.44916100	2.66311800	-0.00023700
C	1.30064500	-0.26891600	-1.23140200
C	1.30042800	-0.26830800	1.23160800
C	2.17634800	0.09938500	0.00008900
H	1.54785500	0.30855200	-2.13635400
H	1.44127600	-1.33245100	-1.48833700
H	3.19511800	-0.34650600	0.00027600
H	2.33452700	1.19057500	-0.00017200
H	1.54745100	0.30967400	2.13628400
H	1.44107700	-1.33169200	1.48915800
Ga	-0.36491900	-0.00951600	-0.00012700

Ga_2_V

E(B3LYP/BS1) = -240.360001 au

H(B3LYP/BS1) = -240.147244 au

G(B3LYP/BS1) = -240.202460 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2163.362513 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2163.055064 au

C	-0.94696400	-1.63076200	-1.39615300
H	-0.23720200	-2.26667400	-1.94951200
H	-1.68314300	-2.31293600	-0.94104800
H	-1.49335600	-1.04704100	-2.15442500
C	0.94751500	-1.62965100	1.39672900
H	0.23799400	-2.26581300	1.95011800
H	1.68428300	-2.31153700	0.94214500
H	1.49326900	-1.04526900	2.15494600
C	-1.38534700	0.75189000	0.97428200
C	1.38514700	0.75203000	-0.97458200
H	-0.87759600	1.33034000	1.76547900
H	-2.10308800	0.10912000	1.51299300
H	2.10310200	0.10928400	-1.51304000
H	0.87752100	1.33033400	-1.76596300
C	-2.17387400	1.72834000	0.08452400
C	2.17334100	1.72868700	-0.08474300
H	-2.73517100	1.19499600	-0.69643200
H	-2.90798000	2.35144100	0.63073700
H	-1.50235100	2.42346700	-0.44032400
H	1.50159400	2.42376300	0.43988800
H	2.73454600	1.19550600	0.69638500
H	2.90746700	2.35184900	-0.63085800
Ga	0.00003900	-0.44432300	-0.00004600

Al_3_I

E(B3LYP/BS1) = -500.838036 au

H(B3LYP/BS1) = -500.599005 au

G(B3LYP/BS1) = -500.651261 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -741.509837 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -741.084232 au

C	-0.43665300	0.73760400	-0.00044900
C	-0.43639200	-0.73755300	-0.00051900
C	-1.58152100	-1.55345800	0.00049700
C	-1.58201100	1.55311700	0.00056200
C	-2.94085700	-1.24332200	0.00130300
C	-2.94127100	1.24246900	0.00110400
C	-3.56924800	-0.00051700	0.00155000
H	-1.37684000	-2.61781400	0.00076200
H	-1.37773600	2.61755700	0.00076500
H	-3.60102000	-2.10738400	0.00192700
H	-3.60172400	2.10631300	0.00142400
H	-4.65540600	-0.00067600	0.00213900
N	0.81442200	-1.29110100	-0.00158700
N	0.81396200	1.29162200	-0.00155500
Al	2.13619700	0.00050500	-0.00161000
C	1.00568300	-2.74508600	-0.00222900
C	1.00465600	2.74569700	-0.00217600
C	4.07639400	-0.00032500	0.00457800
H	0.57090800	-3.20972000	0.89036800
H	0.56696900	-3.20934800	-0.89307500
H	2.07654600	-2.96169400	-0.00435300
H	0.56613600	3.20974000	-0.89324100
H	0.56930900	3.21017500	0.89020100
H	2.07543800	2.96271400	-0.00384100
H	4.47827200	-0.88264600	-0.50580100
H	4.47945100	0.88566200	-0.49843300
H	4.46777600	-0.00485100	1.02876300

Ga 3 I

E (B3LYP/BS1) = -500.881914 au

H(B3LYP/BS1) = -500.643036 au

G(B3LYP/BS1) = -500.696366 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2423.922970 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2423.439037 au

C	-0.76289800	0.73782600	-0.00016100
C	-0.76278200	-0.73786400	-0.00017400
C	-1.90923000	-1.55277300	0.00072800
C	-1.90945000	1.55256300	0.00064000
C	-3.26842200	-1.24290700	0.00134500
C	-3.26860700	1.24249800	0.00122400
C	-3.89692500	-0.00024500	0.00146500
H	-1.70536700	-2.61723500	0.00102100
H	-1.70574400	2.61705700	0.00083800
H	-3.92837400	-2.10712100	0.00187900
H	-3.92867900	2.10662100	0.00163700
H	-4.98309700	-0.00032700	0.00197400
N	0.48384800	-1.29525700	-0.00105800
N	0.48365200	1.29543900	-0.00102400
C	0.67715700	-2.74781000	-0.00171800
C	0.67666900	2.74803500	-0.00167100
C	3.76435700	-0.00037100	0.00439000
H	0.24237500	-3.21219100	0.89100800
H	0.23843600	-3.21193000	-0.89264100
H	1.74792000	-2.96285300	-0.00376000
H	0.23793200	3.21206800	-0.89263100

H	0.24171100	3.21231500	0.89102200
H	1.74738700	2.96330300	-0.00361400
H	4.15294400	-0.88563000	-0.50765400
H	4.15376100	0.88875000	-0.50025900
H	4.14248100	-0.00483200	1.03194100
Ga	1.82369700	0.00022700	-0.00137400

Al_3_II

E(B3LYP/BS1) = -579.439211 au

H(B3LYP/BS1) = -579.141925 au

G(B3LYP/BS1) = -579.206659 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -820.136392 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -819.641657 au

C	0.83049400	-0.74246900	-0.17432200
C	0.85538200	0.73517400	-0.15795100
C	2.00621300	1.52814000	0.01041600
C	1.95627700	-1.57644900	-0.03486400
C	3.34758500	1.19287400	0.19062300
C	3.30769200	-1.28967000	0.15186900
C	3.95204400	-0.05961400	0.25766100
H	1.82266400	2.59627200	-0.00305300
H	1.73902300	-2.63726500	-0.08139100
H	4.01464300	2.04573600	0.29334400
H	3.94758000	-2.16602400	0.22569100
H	5.02799900	-0.07920800	0.40423300
N	-0.36889500	1.30744700	-0.33215500
N	-0.41335400	-1.26982900	-0.35047300
Al	-1.73662900	0.04247200	-0.49263500
C	-0.52416600	2.76153600	-0.39082200
C	-0.61670900	-2.71698400	-0.43105400
C	-3.38215700	0.11626200	-1.53421200
H	-0.23291500	3.24505600	0.55039700
H	0.06788500	3.19848800	-1.20374000
H	-1.57349100	2.99998800	-0.58229700
H	-0.05596300	-3.15959800	-1.26302100
H	-0.32249500	-3.22573200	0.49582600
H	-1.67686000	-2.91880700	-0.60479700
H	-3.15413600	0.26675600	-2.59657300
H	-3.96489800	-0.80942400	-1.45733300
H	-4.03854800	0.93784500	-1.22319300
C	-2.33399300	0.45457300	2.09642600
H	-2.65905400	1.49216100	2.05050400
H	-1.34775600	0.27238100	2.51553600
C	-3.15239500	-0.55433900	1.74895500
H	-4.16444300	-0.37426000	1.39599500
H	-2.85492200	-1.59404000	1.87017400

Ga_3_II

E(B3LYP/BS1) = -579.479243 au

H(B3LYP/BS1) = -579.182130 au

G(B3LYP/BS1) = -579.248918 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2502.545009 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2501.991775 au

C	1.06921500	-0.74353700	-0.15269600
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C	1.08911200	0.73465400	-0.13160300
C	2.23879800	1.53011800	0.03634900
C	2.19855400	-1.57364400	-0.01698400
C	3.58164900	1.19898900	0.21054200
C	3.54962200	-1.28351600	0.16574100
C	4.19044200	-0.05177300	0.27188300
H	2.05186600	2.59770300	0.02713300
H	1.98442200	-2.63506000	-0.06431700
H	4.24614900	2.05381200	0.31322300
H	4.19216500	-2.15820500	0.23564000
H	5.26698700	-0.06825500	0.41449900
N	-0.13344300	1.30798300	-0.29958300
N	-0.16920000	-1.27916900	-0.32865700
C	-0.29813800	2.76096900	-0.33974700
C	-0.37260200	-2.72590500	-0.40223300
C	-3.25092100	0.09136100	-1.32994300
H	-0.00235100	3.23322500	0.60564500
H	0.28597400	3.21051700	-1.15153700
H	-1.35001300	2.99526500	-0.51938200
H	0.18579800	-3.17062300	-1.23462700
H	-0.07323700	-3.22904400	0.52598100
H	-1.43312300	-2.92885300	-0.56911400
H	-3.12281900	0.26918900	-2.40292600
H	-3.78702000	-0.85476000	-1.20588900
H	-3.87778600	0.89191000	-0.92498500
C	-2.16628600	0.52157900	2.25837900
H	-2.68906700	1.46505500	2.11451500
H	-1.15642200	0.58110000	2.65608300
C	-2.77144700	-0.65764800	2.04371400
H	-3.80288000	-0.71746400	1.70544400
H	-2.27117600	-1.59986200	2.25490300
Ga	-1.51216000	0.03396000	-0.45364600

TS_{Al-3}

E(B3LYP/BS1) = -579.389026 au

H(B3LYP/BS1) = -579.093094 au

G(B3LYP/BS1) = -579.153018 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -820.088300 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -819.598882 au

C	0.92791200	0.74131500	-0.01674200
C	0.92969400	-0.73800000	-0.02784300
C	2.08117400	-1.54840400	-0.02317900
C	2.07762000	1.55445200	0.00074200
C	3.43975800	-1.23591600	-0.00629300
C	3.43675500	1.24518700	0.01296600
C	4.06994500	0.00523600	0.01030200
H	1.88119500	-2.61347700	-0.03488000
H	1.87477200	2.61906800	0.00519000
H	4.09934900	-2.10076900	-0.00697400
H	4.09432200	2.11149200	0.02565300
H	5.15590400	0.00645800	0.02120700
N	-0.31301400	-1.29506900	-0.04544100
N	-0.31598400	1.29480200	-0.02637100
Al	-1.65723200	-0.00246400	-0.09006900
C	-0.49266900	-2.74580700	-0.06843000

C	-0.50008300	2.74529500	-0.02895600
C	-2.82072800	-0.08639300	1.67135000
H	-0.04284700	-3.19920000	-0.96035700
H	-0.06358500	-3.22462700	0.82044700
H	-1.56186200	-2.97417000	-0.08480700
H	-0.07107800	3.21334400	0.86572400
H	-0.05316000	3.21284800	-0.91502500
H	-1.57006200	2.97073600	-0.03977100
H	-2.57178100	-1.11044500	1.97981100
H	-2.11228000	0.61972800	2.13795200
H	-3.79037300	0.15403800	2.10503000
C	-3.18069200	0.02836200	-1.40769900
H	-3.23619100	-0.88881100	-1.99435900
H	-3.18579700	0.94106700	-2.00358500
C	-3.96626900	0.05717400	-0.20017700
H	-4.50023400	-0.82951900	0.12896600
H	-4.41379400	0.99112600	0.12709500

TS_{Ga-3}

E(B3LYP/BS1) = -579.416971 au

H(B3LYP/BS1) = -579.121436 au

G(B3LYP/BS1) = -579.182830 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2502.478325 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2501.931086 au

C	1.15272800	0.74218100	-0.02045000
C	1.15260300	-0.73859300	-0.03068300
C	2.30524000	-1.54892800	-0.01723500
C	2.30569700	1.55200700	0.00551900
C	3.66381100	-1.23873100	0.01056700
C	3.66406700	1.24121000	0.02903600
C	4.29647400	0.00100600	0.03227200
H	2.10452800	-2.61378600	-0.03046400
H	2.10504500	2.61698200	0.00804100
H	4.32138200	-2.10512800	0.01543300
H	4.32188700	2.10724800	0.04691700
H	5.38225900	0.00073400	0.05242500
N	-0.08446000	-1.30165200	-0.05785100
N	-0.08424800	1.30515700	-0.04048200
C	-0.26699900	-2.75085700	-0.08351800
C	-0.26685800	2.75473200	-0.05012800
C	-2.55365200	-0.07690500	1.75747100
H	0.18978800	-3.20312300	-0.97260000
H	0.15584000	-3.23047000	0.80803600
H	-1.33592600	-2.97751000	-0.10790000
H	0.15457800	3.22468400	0.84726700
H	0.19112400	3.21730900	-0.93326200
H	-1.33582200	2.98158800	-0.07301500
H	-2.28906100	-1.09530700	2.06582400
H	-1.85757200	0.64443300	2.21164500
H	-3.53153900	0.15076100	2.18040300
C	-3.02374400	0.02289500	-1.35395400
H	-3.09793500	-0.89451600	-1.93692700
H	-3.06121500	0.93495000	-1.94852600
C	-3.75963800	0.04701700	-0.10979600
H	-4.26459000	-0.84646500	0.24479500

H	-4.19808200	0.97836200	0.23545700
Ga	-1.44490600	0.00137100	-0.09805900

Al_3_III

E(B3LYP/BS1) = -579.460290 au

H(B3LYP/BS1) = -579.159798 au

G(B3LYP/BS1) = -579.221459 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -820.154291 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -819.659640 au

C	1.22454300	0.73769900	-0.05923200
C	1.22446500	-0.73768600	-0.05925600
C	2.36139500	-1.55341300	0.07998600
C	2.36150500	1.55329700	0.08040100
C	3.71028900	-1.24305100	0.24742100
C	3.71037200	1.24279100	0.24789100
C	4.33371800	-0.00015900	0.32564600
H	2.15858800	-2.61782800	0.05419700
H	2.15878300	2.61773500	0.05497800
H	4.36559600	-2.10706000	0.32816500
H	4.36571100	2.10673700	0.32904000
H	5.41159100	-0.00022500	0.45962000
N	-0.01663500	-1.29000300	-0.21137300
N	-0.01651000	1.29013900	-0.21146700
Al	-1.33459400	0.00013700	-0.37388000
C	-0.20653200	-2.74368500	-0.23579500
C	-0.20623700	2.74384000	-0.23600500
H	0.33603300	-3.20798000	-1.06750300
H	0.11779600	-3.20899200	0.70231800
H	-1.26938300	-2.96001600	-0.36717700
H	0.11769300	3.20915400	0.70224500
H	0.33676500	3.20804400	-1.06747600
H	-1.26900400	2.96027400	-0.36789800
C	-3.27487900	0.00023000	-0.58151900
C	-4.07708000	-0.00008500	0.74762900
C	-5.59102300	-0.00017000	0.50773900
H	-6.13723500	-0.00047800	1.45704500
H	-5.90076100	0.88588200	-0.05833300
H	-5.90059400	-0.88597600	-0.05881200
H	-3.80659300	0.87736600	1.35052800
H	-3.80645400	-0.87775400	1.35014200
H	-3.56000600	0.87393900	-1.18490200
H	-3.55999800	-0.87320200	-1.18531500

Ga_3_III

E(B3LYP/BS1) = -579.505027 au

H(B3LYP/BS1) = -579.204737 au

G(B3LYP/BS1) = -579.267392 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2502.569294 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2502.016922 au

C	1.40748600	0.73794900	-0.01977500
C	1.40743900	-0.73796600	-0.01981000
C	2.54684200	-1.55291700	0.10931400
C	2.54692200	1.55282400	0.10951900
C	3.89700000	-1.24292000	0.26432100

C	3.89705900	1.24273700	0.26453100
C	4.52134100	-0.00011200	0.33664000
H	2.34410100	-2.61741100	0.08547100
H	2.34423200	2.61733200	0.08583300
H	4.55270100	-2.10715800	0.33906700
H	4.55279700	2.10693300	0.33945100
H	5.60041900	-0.00014800	0.46057400
N	0.16950000	-1.29352600	-0.16032200
N	0.16959400	1.29359600	-0.16034500
C	-0.02312100	-2.74572500	-0.18361700
C	-0.02291900	2.74580900	-0.18364800
H	0.51215900	-3.21021200	-1.02002400
H	0.30930900	-3.21141600	0.75156800
H	-1.08706000	-2.96040600	-0.30571900
H	0.30936800	3.21146000	0.75160900
H	0.51255400	3.21027000	-1.01994400
H	-1.08681900	2.96057000	-0.30595000
C	-3.11674500	0.00014400	-0.50842500
C	-3.89924900	-0.00018900	0.82812400
C	-5.41507500	-0.00007500	0.59777900
H	-5.95271000	-0.00030600	1.55176400
H	-5.72956200	0.88619300	0.03480900
H	-5.72962400	-0.88602600	0.03434500
H	-3.62251500	0.87767600	1.42668900
H	-3.62257400	-0.87838700	1.42623100
H	-3.39091700	0.87697200	-1.10894400
H	-3.39093200	-0.87637400	-1.10938700
Ga	-1.17033800	0.00008300	-0.31427400

Al 3 IV

E(B3LYP/BS1) = -579.026198 au

H(B3LYP/BS1) = -578.741024 au

G(B3LYP/BS1) = -578.800007 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -819.678123 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -819.192125 au

C	-1.01211700	0.74897000	0.00005800
C	-0.94979100	-0.73995900	-0.00005900
C	-2.07623100	-1.59922000	-0.00031500
C	-2.20548500	1.51061800	0.00024000
C	-3.44285200	-1.34057100	-0.00023900
C	-3.54674100	1.13814300	0.00029700
C	-4.12923100	-0.12726900	0.00008700
H	-1.82964700	-2.65498200	-0.00058900
H	-2.04898600	2.58343900	0.00041200
H	-4.06736100	-2.23272400	-0.00043100
H	-4.24325000	1.97529100	0.00054100
H	-5.21487500	-0.17271400	0.00016900
N	0.30068300	-1.21966600	-0.00000200
N	0.19558500	1.33125800	-0.00005800
Al	1.71337500	0.11598100	0.00012400
C	0.55731400	-2.65273500	-0.00018100
C	0.33000000	2.78097400	-0.00010100
H	0.14185400	-3.14627200	0.88942300
H	0.14233900	-3.14595900	-0.89018800
H	1.63782500	-2.81692300	0.00009800

H	-0.12553500	3.23780200	-0.88973400
H	-0.12504900	3.23782500	0.88977100
H	1.39286000	3.03630900	-0.00040700
C	3.27731500	0.11044400	1.25198800
C	3.27723900	0.11189200	-1.25173100
C	4.13292700	-0.29094900	-0.00011300
H	3.40408800	-0.55232100	-2.11407800
H	3.54689200	1.12330600	-1.59034900
H	3.40399600	-0.55495100	2.11345800
H	3.54696800	1.12136600	1.59204700
H	5.14053600	0.15181000	-0.00013900
H	4.27550600	-1.38123300	-0.00077100

Al_3_V

E(B3LYP/BS1) = -619.572039 au

H(B3LYP/BS1) = -619.234426 au

G(B3LYP/BS1) = -619.303382 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -860.236157 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -859.707478 au

C	-1.09138300	-0.73800000	-0.02620000
C	-1.28144000	0.74072700	0.01083700
C	-2.53811800	1.39641800	0.02986300
C	-2.14256600	-1.68898500	-0.04875100
C	-3.84197500	0.91132600	0.02041400
C	-3.52658600	-1.54772800	-0.04242400
C	-4.31518900	-0.39906800	-0.01165100
H	-2.47424700	2.47831000	0.05686500
H	-1.80885500	-2.72011500	-0.07515100
H	-4.60732600	1.68593800	0.04154300
H	-4.07195400	-2.49023300	-0.06512400
H	-5.39296600	-0.53727700	-0.01281900
N	-0.13114200	1.42513600	0.02541500
N	0.19450200	-1.11006100	-0.03709400
Al	1.50043300	0.34779000	0.00107100
C	-0.12676000	2.88001900	0.06233600
C	0.56436400	-2.51772400	-0.07519400
H	-0.62373500	3.31861800	-0.81458400
H	-0.61820400	3.27305700	0.96362900
H	0.90871600	3.23110300	0.06785900
H	0.19281800	-3.06741600	0.80125600
H	0.18697500	-3.02070000	-0.97681700
H	1.65465100	-2.59822100	-0.08067400
C	2.49760200	0.55548300	-1.72761400
C	2.49397900	0.46535100	1.74049500
H	2.98490800	1.45083100	1.80147400
H	1.76151300	0.46538000	2.56255100
H	2.84233600	1.60031700	-1.80552600
H	1.78730800	0.43401200	-2.56009500
C	3.55404000	-0.62186700	2.01897700
C	3.70840100	-0.37227000	-1.95999900
H	4.34190300	-0.62949900	1.25501700
H	4.05294500	-0.48685400	2.98971800
H	3.11298800	-1.62800200	2.03000600
H	3.41952000	-1.43226100	-1.95330100
H	4.20460400	-0.18795200	-2.92404200

H 4.47073900 -0.24790900 -1.18048600

Ga_3_IV

E(B3LYP/BS1) = -579.063530 au

H(B3LYP/BS1) = -578.778626 au

G(B3LYP/BS1) = -578.838581 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2502.082058 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2501.539231 au

C	1.24679300	0.74104900	0.00001300
C	1.19876000	-0.74950200	-0.00005300
C	2.33628800	-1.59628100	-0.00015000
C	2.43593500	1.51225100	0.00013800
C	3.70025000	-1.32509600	-0.00011700
C	3.78034800	1.15313000	0.00015100
C	4.37631300	-0.10612500	0.00002900
H	2.10084100	-2.65451600	-0.00027800
H	2.27022800	2.58361200	0.00025900
H	4.33227400	-2.21204300	-0.00021600
H	4.46800300	1.99767700	0.00027200
H	5.46231600	-0.14118000	0.00005000
N	-0.04223700	-1.24811200	-0.00004200
N	0.03921000	1.31849700	-0.00003200
C	-0.28145400	-2.68306700	-0.00004100
C	-0.10530200	2.76608800	-0.00005100
H	0.14043600	-3.17151000	-0.88968800
H	0.14064600	-3.17154000	0.88948900
H	-1.35968000	-2.86125900	0.00008400
H	0.34749700	3.22608700	0.88959200
H	0.34782700	3.22608700	-0.88952500
H	-1.16955000	3.01500200	-0.00025200
C	-3.08528500	0.07622900	-1.24681500
C	-3.08524700	0.07559300	1.24691400
C	-3.95079900	-0.30414600	-0.00003700
H	-3.19476200	-0.60102000	2.10150000
H	-3.32707600	1.08652600	1.60371300
H	-3.19493200	-0.59982100	-2.10182700
H	-3.32704400	1.08741800	-1.60295100
H	-4.94539600	0.16628200	0.00010200
H	-4.12233900	-1.38969900	-0.00031500
Ga	-1.49508700	0.08259600	0.00002000

Ga_3_V

E(B3LYP/BS1) = -619.611974 au

H(B3LYP/BS1) = -619.274601 au

G(B3LYP/BS1) = -619.344605 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2542.645200 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2542.059980 au

C	-1.30682700	-0.76154700	-0.05854200
C	-1.46345600	0.72067100	0.02551000
C	-2.70793100	1.40123700	0.06758800
C	-2.38266700	-1.68585700	-0.10774400
C	-4.02232800	0.94658800	0.04667500
C	-3.76283800	-1.51438400	-0.09284600
C	-4.52647900	-0.35057900	-0.02434100

H	-2.62111700	2.48013900	0.12754500
H	-2.07352300	-2.72323000	-0.16647600
H	-4.76915800	1.73810700	0.09363900
H	-4.32847200	-2.44391300	-0.14287900
H	-5.60709900	-0.46437100	-0.02660700
N	-0.30361800	1.38391200	0.05919600
N	-0.03421900	-1.16891900	-0.08491000
C	-0.27195800	2.83538100	0.14304200
C	0.29821200	-2.58246000	-0.17136800
H	-0.76246700	3.31186200	-0.71792200
H	-0.75558200	3.20830100	1.05730700
H	0.76949800	3.16785400	0.15808900
H	-0.08358700	-3.15162900	0.68844600
H	-0.09730000	-3.04608000	-1.08653700
H	1.38584000	-2.69181500	-0.18612000
C	2.32089100	0.50829300	-1.73571200
C	2.30308200	0.30133700	1.76516800
H	2.83251700	1.26239900	1.85473000
H	1.54997900	0.30873600	2.56592200
H	2.52492500	1.58354100	-1.85880300
H	1.63880200	0.25088800	-2.55847100
C	3.30510100	-0.84214800	2.02023600
C	3.64134300	-0.26841100	-1.89749200
H	4.10325500	-0.86180100	1.26757900
H	3.79254100	-0.75787900	3.00210300
H	2.81642300	-1.82527200	1.99381700
H	3.48904000	-1.35412300	-1.83297500
H	4.12538400	-0.07362700	-2.86530700
H	4.36610200	-0.00315300	-1.11760200
Ga	1.33948300	0.26875500	0.00159600

Ti_4_I

E(B3LYP/BS1) = -636.783028 au

H(B3LYP/BS1) = -636.630237 au

G(B3LYP/BS1) = -636.679000 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1428.390000 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1428.085443 au

C	-0.03365200	-1.24574900	-1.13124500
C	1.30367700	-1.53251300	-0.70119800
H	2.15715700	-1.70850100	-1.34475300
C	1.31205600	-1.51869200	0.70497500
H	2.17272500	-1.68319300	1.34182000
C	-0.88510000	-1.10261800	0.00966500
C	-0.02027700	-1.22225700	1.14411600
H	-0.32436100	-1.10581500	2.18047200
Si	-2.30417000	0.14754600	0.00606300
N	-1.12135400	1.49553200	-0.00831200
Ti	0.55046400	0.67136000	-0.01260200
H	-1.38684000	2.48211000	-0.00636600
H	-3.11624500	0.09889700	-1.22693700
H	-3.10654300	0.11853100	1.24603600
H	-0.34892800	-1.14931600	-2.16629900
C	2.33082100	1.62993100	0.00583700
H	2.00593100	2.68825400	-0.04060300

H	2.91393100	1.48219900	0.92654400
H	2.98567200	1.42392700	-0.85226900

Zr_4_I

E (B3LYP/BS1) = -625.293000 au

H(B3LYP/BS1) = -625.140571 au

G(B3LYP/BS1) = -625.191309 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -626.034270 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -625.725859 au

C	0.79607000	1.27365100	-1.13914500
C	-0.31480100	2.06650000	-0.70726000
H	-1.00455500	2.60812900	-1.34547600
C	-0.31820500	2.06430300	0.70879400
H	-1.01094400	2.60391700	1.34546300
C	1.50635900	0.79109600	0.00287000
C	0.79017400	1.26944600	1.14328900
H	1.04730800	1.06921300	2.17928900
Si	2.28788900	-0.92385400	0.00181900
N	0.67446700	-1.69992100	-0.00189800
H	0.54530300	-2.71441000	-0.00232200
H	3.04921700	-1.22008800	-1.23013500
H	3.04520500	-1.22393800	1.23531800
H	1.05799000	1.07677000	-2.17457300
C	-2.85879100	-1.01838100	0.00344100
H	-2.90267600	-2.12139400	-0.00738400
H	-3.42207900	-0.68947500	0.89420600
H	-3.43580300	-0.67127900	-0.87135200
Zr	-0.78313800	-0.31409300	-0.00267800

Hf_4_I

E (B3LYP/BS1) = -627.631878 au

H(B3LYP/BS1) = -627.479015 au

G(B3LYP/BS1) = -627.527390 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -627.010824 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -626.718611 au

C	0.90286300	1.66523000	-0.78966600
C	-0.37979400	2.22578300	-0.52413700
H	-0.97695800	2.81156800	-1.21477000
C	-0.70942500	1.94016300	0.82776500
H	-1.60727900	2.25030400	1.34806500
C	1.38175500	1.00380500	0.38026100
C	0.35531400	1.17505500	1.37798900
H	0.39003900	0.78711000	2.39003200
Si	2.44796300	-0.55541100	0.31424600
N	1.03774900	-1.53781300	-0.16723200
H	1.05256900	-2.55807900	-0.13922500
H	3.49395600	-0.48151900	-0.72802900
H	2.98180500	-0.94962100	1.63552100
H	1.41736800	1.69938300	-1.74533500
C	-2.09874900	-1.10357300	0.96791200
H	-2.33136500	-2.11525700	0.58070600
H	-1.85843400	-1.23344200	2.03086500
H	-3.03077300	-0.51760700	0.92377500
Hf	-0.52470100	-0.31376600	-0.30210000

Ti_4_II

E(B3LYP/BS1) = -715.408512 au

H(B3LYP/BS1) = -715.197656 au

G(B3LYP/BS1) = -715.251513 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1507.023422 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1506.651120 au

C	0.53532500	1.09911100	-1.37694200
C	-0.48854200	1.90812700	-0.79740500
H	-1.33928100	2.33041900	-1.31797300
C	-0.15047900	2.12489000	0.56681800
H	-0.72086000	2.69945100	1.28529800
C	1.50255900	0.78674700	-0.38245800
C	1.05525300	1.43089400	0.82780200
H	1.54633100	1.36952200	1.79103400
Si	2.37761400	-0.88140600	-0.36082100
N	0.85974500	-1.63702200	0.16051900
Ti	-0.43386200	-0.27689500	0.28365200
H	0.78960400	-2.55458400	0.60333800
H	2.83185500	-1.31565200	-1.69961900
H	3.44123700	-0.98480800	0.66178000
H	0.54525900	0.73128800	-2.39756200
C	-1.11518300	-0.28292500	2.21411400
H	-1.39859900	-1.33472800	2.38387500
H	-0.46190300	0.03798700	3.02925400
H	-2.02638300	0.34134900	2.24105700
C	-2.67974400	-0.24544700	-1.21065400
H	-3.28210000	0.49503700	-0.67416100
H	-2.36666600	0.03925900	-2.22118000
C	-2.42313100	-1.47964800	-0.68400800
H	-2.82767600	-1.75082800	0.29425100
H	-1.90700600	-2.26367600	-1.23547400

Zr_4_II

E(B3LYP/BS1) = -703.924721 au

H(B3LYP/BS1) = -703.714420 au

G(B3LYP/BS1) = -703.772278 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -704.657011 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -704.280477 au

C	0.69363500	1.14489000	-1.43777000
C	-0.19799600	2.07016100	-0.82234900
H	-1.00441300	2.60412300	-1.31090100
C	0.21797800	2.24283800	0.52544800
H	-0.23621100	2.90070000	1.25599000
C	1.65834300	0.71360100	-0.48141100
C	1.34523000	1.41273500	0.73862500
H	1.87803900	1.30828600	1.67670800
Si	2.41931800	-1.01442700	-0.49675600
N	0.91092300	-1.73530500	0.09020300
H	0.85405600	-2.68205700	0.46711600
H	2.79776200	-1.44826400	-1.86100900
H	3.53980200	-1.15789600	0.45996000
H	0.63017300	0.79563900	-2.46319000
C	-1.01029000	-0.16122000	2.44067600

H	-1.46887700	-1.15300900	2.62669600
H	-0.23231000	-0.02249600	3.19936700
H	-1.78362000	0.60314200	2.62157300
C	-2.75435400	-0.02775300	-1.44945400
H	-3.32792100	0.77319000	-0.98609000
H	-2.33052800	0.17934800	-2.42908500
C	-2.65188100	-1.24661300	-0.87723600
H	-3.17709200	-1.48027200	0.05061200
H	-2.16525200	-2.07576100	-1.39072500
Zr	-0.45061300	-0.24218500	0.31467400

Hf 4 II

E(B3LYP/BS1) = -706.263444 au

H(B3LYP/BS1) = -706.053120 au

G(B3LYP/BS1) = -706.111428 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -705.615165 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -705.251056 au

C	0.91087400	1.30756800	-1.35121500
C	0.00061600	2.19973800	-0.71088700
H	-0.75409700	2.80435000	-1.19969500
C	0.32136400	2.23062400	0.67188700
H	-0.16285700	2.83525700	1.42877100
C	1.79616900	0.75878300	-0.38004700
C	1.40879700	1.34308400	0.87959800
H	1.87403600	1.13501000	1.83719500
Si	2.48485500	-0.99693400	-0.48552800
N	0.91807300	-1.70446700	-0.02407600
H	0.83552800	-2.67583800	0.27581300
H	2.91276800	-1.34958800	-1.85805200
H	3.54366900	-1.26161700	0.51392000
H	0.90870400	1.05863400	-2.40754100
C	-1.29119800	-0.34217500	2.19731000
H	-1.74203200	-1.34789100	2.28951800
H	-0.61178600	-0.23537700	3.05380300
H	-2.10315600	0.38702600	2.35419700
C	-2.44951800	0.21673700	-1.63912800
H	-3.06642800	0.91607300	-1.07631200
H	-1.99377200	0.59222300	-2.55141800
C	-2.33748900	-1.08085300	-1.27477300
H	-2.89635600	-1.47707000	-0.42449800
H	-1.80580500	-1.80160200	-1.89432300
Hf	-0.36542500	-0.18739300	0.22594500

TS_{Ti-4}

E(B3LYP/BS1) = -715.397533 au

H(B3LYP/BS1) = -715.185072 au

G(B3LYP/BS1) = -715.236433 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1507.010210 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1506.642716 au

C	-0.94316000	1.10447900	1.23896400
C	-0.01596600	2.06923900	0.75888600
H	0.68338000	2.63606100	1.36143100
C	-0.16118000	2.15710600	-0.64446500
H	0.39551000	2.81016200	-1.30613400

C	-1.69531800	0.59078700	0.13614600
C	-1.18645600	1.24677000	-1.02916800
H	-1.51332900	1.06243800	-2.04722200
Si	-2.25064100	-1.20452100	0.05896600
N	-0.56207000	-1.69179000	-0.20022800
Ti	0.48076300	-0.13051900	-0.19969500
H	-0.23005800	-2.65145300	-0.30165000
H	-2.80473200	-1.70893200	1.33478500
H	-3.12493600	-1.50731100	-1.09560400
H	-1.04540700	0.79280600	2.27193700
C	2.10184100	-0.31917000	-1.52231100
H	2.66680700	-1.15606900	-1.93219300
H	1.13076200	-0.30182200	-2.11051700
H	2.62787100	0.61864200	-1.72113900
C	1.84634800	-0.43294000	1.51686700
H	1.99703400	0.50415400	2.04499200
H	1.33908100	-1.21862000	2.07390700
C	2.76091400	-0.79859100	0.51711700
H	3.61060100	-0.16112600	0.29424700
H	2.89195300	-1.84776800	0.27030000

TS_{Zr-4}

E(B3LYP/BS1) = -703.910000 au

H(B3LYP/BS1) = -703.700007 au

G(B3LYP/BS1) = -703.752828 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -704.638643 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -704.266345 au

C	-1.18785000	1.12010800	1.22388200
C	-0.39005500	2.16279800	0.67780100
H	0.24085900	2.84471100	1.23580000
C	-0.59475800	2.18146200	-0.72498000
H	-0.16366700	2.88976900	-1.42383300
C	-1.91162400	0.48163000	0.16651600
C	-1.52674600	1.14777300	-1.03874900
H	-1.88279100	0.90375100	-2.03469700
Si	-2.31842600	-1.35771300	0.18558200
N	-0.62322800	-1.78212600	-0.11892300
H	-0.29600800	-2.74385100	-0.21363400
H	-2.80720300	-1.82739900	1.50180600
H	-3.22362300	-1.76241100	-0.91421100
H	-1.23578300	0.85011400	2.27271500
C	2.35583500	-0.44982000	-1.42115900
H	3.41373700	-0.46047900	-1.67490500
H	1.91822700	-1.40594700	-1.77099500
H	1.91436900	0.39411600	-2.01368900
C	1.88580200	-0.18234800	1.65213000
H	1.83060300	0.78227300	2.15095500
H	1.48556100	-1.02821100	2.21047300
C	2.94006900	-0.40785700	0.75413000
H	3.63960300	0.39106400	0.52893000
H	3.32248200	-1.41175100	0.59462600
Zr	0.48100400	-0.08138400	-0.24881100

TS_{Hf-4}

E(B3LYP/BS1) = -706.246000 au

H(B3LYP/BS1) = -706.036424 au
 G(B3LYP/BS1) = -706.090000 au
 E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -705.592000 au
 E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -705.233279 au

C	-1.22294200	1.22098300	1.22753900
C	-0.33975900	2.20161900	0.69767000
H	0.31335300	2.84935200	1.27048300
C	-0.49039900	2.21134300	-0.71223700
H	0.01313900	2.87777900	-1.40321600
C	-1.94942000	0.61201300	0.15180700
C	-1.47333400	1.23360400	-1.04763800
H	-1.80921200	0.99795500	-2.05262200
Si	-2.48027500	-1.19929400	0.17890600
N	-0.80710000	-1.75598200	-0.05265300
H	-0.57723800	-2.74657900	-0.11854300
H	-3.05595700	-1.60655400	1.48046100
H	-3.37013000	-1.54922500	-0.95159500
H	-1.32834600	0.97263800	2.27775000
C	2.15452900	-0.42371800	-1.40202700
H	3.14686100	-0.15991700	-1.76403800
H	1.97245600	-1.48535600	-1.64224900
H	1.45605600	0.20380900	-2.03515400
C	1.80950800	-0.27077700	1.65834900
H	1.71693000	0.63278300	2.25692400
H	1.54833200	-1.19774600	2.17021900
C	2.84389600	-0.31709900	0.69867500
H	3.43209200	0.57344500	0.49876100
H	3.34527500	-1.25372000	0.47308300
Hf	0.35524300	-0.12270100	-0.14207200

Ti_4_III

E(B3LYP/BS1) = -715.412000 au
 H(B3LYP/BS1) = -715.198745 au
 G(B3LYP/BS1) = -715.254000 au
 E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1507.040000 au
 E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1506.664862 au

C	1.21218900	1.22133100	-1.10586100
C	0.08400700	1.98492400	-0.66610900
H	-0.63844400	2.48219300	-1.30158300
C	0.07486000	1.95685400	0.74103400
H	-0.65858200	2.42613400	1.38566800
C	1.94606500	0.74634700	0.02989100
C	1.19554200	1.17544100	1.17093100
H	1.43500100	0.94321300	2.20442500
Si	2.79756400	-0.94340800	-0.00853800
N	1.20850500	-1.76672900	-0.05187900
Ti	-0.02420200	-0.35863600	-0.02114400
H	1.10891600	-2.78169700	-0.08967500
H	3.58337800	-1.16020700	-1.24157600
H	3.55730000	-1.23398800	1.22549600
H	1.46883900	1.02584300	-2.14321600
C	-1.99416000	-0.60324300	0.10174600
H	-1.94054200	-1.68484100	-0.17506300

C	-3.28504900	0.04633000	-0.36679600
C	-4.55149000	-0.64102000	0.17330400
H	-1.88849300	-0.56958700	1.22251000
H	-5.44587300	-0.13219600	-0.20018300
H	-4.60181000	-1.68816400	-0.14469600
H	-4.58042500	-0.61539600	1.26829300
H	-3.28032100	1.10125100	-0.06702700
H	-3.30370500	0.03047100	-1.46434600

Zr_4_III

E(B3LYP/BS1) = -704.564123 au

H(B3LYP/BS1) = -704.353059 au

G(B3LYP/BS1) = -704.409008 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -704.673001 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -704.299057 au

C	1.86607000	1.25519900	-0.85582600
C	0.84483800	2.20608600	-0.56280500
H	0.43438500	2.93396800	-1.24887500
C	0.49991700	2.06367800	0.79468900
H	-0.21931300	2.66201100	1.33536500
C	2.17456100	0.51546600	0.32078300
C	1.29780000	1.01230400	1.33525800
H	1.25840300	0.66221200	2.35873700
Si	2.66042100	-1.30475400	0.25232500
N	1.01914700	-1.81664700	-0.18213700
H	0.77015700	-2.80055300	-0.23668600
H	3.64350800	-1.58508600	-0.80926500
H	3.07677500	-1.83214800	1.56414200
H	2.33044700	1.11658100	-1.82404400
C	-2.25156500	-0.34612600	-0.08958900
H	-2.18765600	-1.46213900	-0.12181700
C	-3.66965500	0.12314300	-0.35515900
C	-4.73152700	-0.48348800	0.56966200
H	-1.95072500	-0.10422700	0.98603000
H	-5.72415300	-0.11156300	0.31044100
H	-4.75053700	-1.57282300	0.48939200
H	-4.54094400	-0.22575700	1.61425500
H	-3.69958100	1.21412200	-0.28807900
H	-3.90927900	-0.12333300	-1.39455500
Zr	-0.12735100	-0.14664400	-0.29836800

Hf_4_III

E(B3LYP/BS1) = -706.263000 au

H(B3LYP/BS1) = -706.050646 au

G(B3LYP/BS1) = -706.106000 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -705.641000 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -705.284803 au

C	1.69489700	1.24480100	-0.96263800
C	0.71396200	2.22407700	-0.63367700
H	0.27241600	2.94206600	-1.31584900
C	0.46805300	2.13826100	0.76259800
H	-0.21014800	2.76251000	1.33123200
C	2.06562900	0.52956600	0.21987100
C	1.27945100	1.09578800	1.28468400

H	1.29630500	0.77454300	2.32004100
Si	2.55441600	-1.29603700	0.18791900
N	0.87037900	-1.79641400	-0.10752600
H	0.58543500	-2.77341900	-0.04804600
H	3.46985700	-1.61138600	-0.93115300
H	3.07114400	-1.77595300	1.48843500
H	2.08350600	1.05257700	-1.95825800
C	-1.86637400	-0.23240300	1.17755300
H	-2.04651700	-1.28964300	1.42561200
C	-2.79724900	0.22574000	0.02833800
C	-4.05549300	-0.62094500	-0.20109500
H	-2.00272100	0.36466000	2.07922000
H	-4.63453400	-0.25752500	-1.05576400
H	-3.80293900	-1.67266200	-0.37324600
H	-4.68867800	-0.56868600	0.68966100
H	-3.04814100	1.28582900	0.13930700
H	-2.25942500	0.21795200	-0.99365400
Hf	-0.20774000	-0.11612200	-0.20457700

Ti_4_IV

E(B3LYP/BS1) = -715.037351 au

H(B3LYP/BS1) = -714.837397 au

G(B3LYP/BS1) = -714.888289 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1506.589377 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1506.226546 au

C	-0.89904300	1.27895000	1.14326700
C	0.21831900	2.02931700	0.70949700
H	0.95007400	2.50976700	1.34667400
C	0.21706100	2.02930400	-0.71068400
H	0.94746900	2.50998900	-1.34921500
C	-1.61448600	0.79547300	0.00118300
C	-0.90112800	1.27891600	-1.14229500
H	-1.13498700	1.04028600	-2.17326200
Si	-2.41811600	-0.89954300	0.00087900
N	-0.88446000	-1.72282800	-0.00235900
Ti	0.43938600	-0.31476600	-0.00120700
H	-0.74479400	-2.72879600	-0.00257600
H	-3.26145100	-1.13596700	1.20877400
H	-3.26543900	-1.13367800	-1.20466800
H	-1.13071900	1.04008900	2.17466500
C	1.96175800	-0.62187700	1.31557600
C	1.96473600	-0.62132000	-1.31436200
C	2.83247800	-0.55683700	0.00160700
H	2.31243700	0.04888100	2.09853300
H	1.88449500	-1.64695800	1.70163400
H	3.38671600	0.38519000	0.00225800
H	3.55086600	-1.38396200	0.00217500
H	2.31820200	0.04845100	-2.09691200
H	1.88730500	-1.64659500	-1.70006700

Ti_4_V

E(B3LYP/BS1) = -755.560340 au

H(B3LYP/BS1) = -755.308461 au

G(B3LYP/BS1) = -755.367536 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1547.127385 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1546.723553 au

C	-1.66145800	-1.16221500	-0.82299900
C	-1.04545500	-2.18073800	-0.06100800
H	-0.65581400	-3.11630300	-0.44203600
C	-1.01356000	-1.75028800	1.29223900
H	-0.59499300	-2.29986300	2.12612900
C	-2.02077400	-0.07775200	0.03866700
C	-1.61177000	-0.47037000	1.35248300
H	-1.67428400	0.15079300	2.23832900
Si	-1.88426800	1.70143900	-0.53673400
N	-0.14397000	1.64186300	-0.55417300
Ti	0.33416700	-0.13672000	0.01551100
H	0.48956900	2.40077600	-0.79014300
H	-2.52255400	1.92834300	-1.86531000
H	-2.47151500	2.67180600	0.43159900
H	-1.77084200	-1.16585500	-1.90116800
C	1.50953900	-1.02867200	-1.48315600
C	1.60620100	-0.01013900	1.67847100
H	1.80326700	-2.03127000	-1.13376300
H	0.90653600	-1.17538500	-2.38942000
H	2.24769800	-0.90030600	1.53485400
H	1.11088200	-0.13666800	2.64761500
C	2.75709400	-0.18737100	-1.80218100
C	2.45614200	1.27225900	1.67847900
H	3.41675800	-0.08001700	-0.93238500
H	3.36058900	-0.64327600	-2.60088900
H	2.49296300	0.82260700	-2.14233800
H	2.91986600	1.47518200	0.70381700
H	1.84455900	2.14539600	1.93297500
H	3.27742800	1.22039800	2.40839200

Zr_4_IV

E(B3LYP/BS1) = -703.540062 au

H(B3LYP/BS1) = -703.341132 au

G(B3LYP/BS1) = -703.393813 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -704.202310 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -703.835338 au

C	-1.18765400	1.29427100	1.14312900
C	-0.15765600	2.16458900	0.71161600
H	0.49758900	2.74466900	1.34983000
C	-0.15816300	2.16460700	-0.71195200
H	0.49655800	2.74476000	-1.35063700
C	-1.84219700	0.72867800	0.00046900
C	-1.18852600	1.29432900	-1.14268500
H	-1.40991600	1.04861500	-2.17552400
Si	-2.53465200	-1.02048500	0.00054800
N	-0.97876600	-1.81128600	-0.00057800
H	-0.86221300	-2.82095200	-0.00097900
H	-3.37164100	-1.28714400	1.20697500
H	-3.37312500	-1.28672400	-1.20494600
H	-1.40819000	1.04847100	2.17612700
C	2.18127700	-0.45543000	1.33872400
C	2.18298600	-0.45512700	-1.33782900
C	3.01825100	-0.28101900	0.00103600

H	2.51939900	0.22352300	2.12240300
H	2.25226500	-1.48891700	1.71207100
H	3.44418400	0.72697100	0.00141000
H	3.84817900	-0.99689100	0.00147700
H	2.52229400	0.22392700	-2.12091100
H	2.25450000	-1.48855500	-1.71126900
Zr	0.44591800	-0.27888300	-0.0006

Zr_4_V

E(B3LYP/BS1) = -744.069916 au

H(B3LYP/BS1) = -743.819094 au

G(B3LYP/BS1) = -743.881708 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -744.746901 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -744.338983 au

C	-1.78003800	-1.26422200	-0.68991200
C	-1.18706700	-2.19996400	0.19028100
H	-0.82241700	-3.18472000	-0.07541500
C	-1.17346700	-1.62343100	1.49183200
H	-0.79725200	-2.09167200	2.39324700
C	-2.13650200	-0.08455800	0.04098800
C	-1.75801900	-0.33787600	1.39983400
H	-1.84866500	0.36960300	2.21650800
Si	-2.07346100	1.63359800	-0.72093500
N	-0.33303300	1.71104800	-0.76136100
H	0.19490500	2.50833900	-1.10689200
H	-2.73928600	1.67351000	-2.05577800
H	-2.72919100	2.65483900	0.14732200
H	-1.89003700	-1.39355700	-1.76072400
C	1.58942700	-1.23013600	-1.49055300
C	1.67786500	0.22904000	1.83375900
H	1.96415800	-2.15573400	-1.01966700
H	0.99522500	-1.55472700	-2.35654000
H	2.31305100	-0.67653500	1.88509100
H	1.16199700	0.28545900	2.80091200
C	2.77995900	-0.37049300	-1.96686400
C	2.56642900	1.47588200	1.63849600
H	3.41581700	-0.03687200	-1.13411800
H	3.44139600	-0.91483800	-2.65709100
H	2.44428200	0.52989100	-2.49948100
H	3.04925700	1.50429800	0.64908000
H	1.98025100	2.39818100	1.73295800
H	3.38270700	1.53370300	2.37357700
Zr	0.35929900	-0.09655800	0.03006200

Hf_4_IV

E(B3LYP/BS1) = -705.885459 au

H(B3LYP/BS1) = -705.686253 au

G(B3LYP/BS1) = -705.739506 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -705.167020 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -704.811782 au

C	-1.33044900	1.30088100	1.14280500
C	-0.33489600	2.21153900	0.71153200
H	0.29689200	2.81706300	1.34983900
C	-0.33475500	2.21149400	-0.71169800

H	0.29716000	2.81697700	-1.34991900
C	-1.96397100	0.71268100	-0.00019300
C	-1.33025700	1.30085100	-1.14310100
H	-1.54185400	1.04732900	-2.17611400
Si	-2.56126000	-1.07041500	-0.00026700
N	-0.95736700	-1.76805600	-0.00008600
H	-0.78733300	-2.76973700	-0.00012200
H	-3.37834600	-1.38901000	1.20616400
H	-3.37805500	-1.38897700	-1.20690500
H	-1.54222800	1.04740200	2.17579200
C	2.07682900	-0.38374300	1.32723100
C	2.07696900	-0.38374400	-1.32689300
C	2.91726800	-0.15576300	0.00021000
H	2.38198800	0.29550300	2.12562800
H	2.20487300	-1.41529900	1.68738500
H	3.29053200	0.87380900	0.00022600
H	3.78546000	-0.82409500	0.00026300
H	2.38226800	0.29541600	-2.12530600
H	2.20496400	-1.41534200	-1.68695900
Hf	0.35670100	-0.18769500	0.00007000

Hf_4_V

E(B3LYP/BS1) = -746.414015 au

H(B3LYP/BS1) = -746.162964 au

G(B3LYP/BS1) = -746.226119 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -745.712805 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -745.316102 au

C	-1.88050200	-1.20617900	-0.71957700
C	-1.30709700	-2.16156900	0.15362100
H	-0.96050900	-3.15068800	-0.11996500
C	-1.28824500	-1.59829700	1.46085200
H	-0.92620300	-2.08322000	2.35935600
C	-2.22188100	-0.02881300	0.02211200
C	-1.85087400	-0.30112000	1.37929700
H	-1.93374800	0.39929500	2.20306400
Si	-2.09265800	1.69267500	-0.72224200
N	-0.34459600	1.70646800	-0.74333100
H	0.20707200	2.49045500	-1.08126500
H	-2.73432100	1.77203900	-2.06602500
H	-2.71275400	2.73227200	0.14867600
H	-1.98851600	-1.32268300	-1.79218700
C	1.52756300	-1.15754500	-1.48159400
C	1.63421600	0.24839900	1.76075000
H	1.81359400	-2.14702800	-1.08271900
H	0.93908300	-1.37552100	-2.38711700
H	2.26217500	-0.66236200	1.82059100
H	1.11831200	0.30052900	2.73059200
C	2.80643800	-0.38650800	-1.88192500
C	2.54930000	1.48464400	1.60539900
H	3.46418100	-0.20544100	-1.02158100
H	3.40654600	-0.92907000	-2.62666100
H	2.57316000	0.59320300	-2.32147900
H	3.07520300	1.49899600	0.64003300
H	1.97078300	2.41465300	1.66749800
H	3.32609100	1.53447900	2.38192900

Hf 0.26382900 -0.09528800 0.02872700

Ti_5_I

E(B3LYP/BS1) = -657.903159 au

H(B3LYP/BS1) = -657.740961 au

G(B3LYP/BS1) = -657.794351 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1449.523643 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1449.210060 au

C	1.95579300	-1.06249000	-0.93470200
H	2.13862100	-1.36863300	-1.95956300
C	1.07971600	-1.70692500	-0.02005400
H	0.46751700	-2.57687700	-0.22352800
C	1.10596700	-0.96835200	1.19342100
H	0.54214900	-1.19744000	2.09028900
C	2.56288600	0.04104700	-0.27347000
H	3.26961100	0.73502700	-0.71231100
C	2.03752400	0.11065300	1.03704200
H	2.29258300	0.84420900	1.79029700
Ti	0.15978900	0.38229600	-0.37126300
C	0.37113800	2.35747800	0.09196800
O	-1.55310200	0.08611400	-0.19006000
Si	-3.19301500	-0.35384700	0.09112000
H	1.36660800	2.80272300	0.03885800
H	-0.27799900	2.77153300	-0.70561200
H	-0.09398600	2.60512500	1.05529600
H	-3.16688400	-1.69784900	0.70881400
H	-3.75507200	0.66831200	0.99779400
H	-3.84963200	-0.36017000	-1.23297500

Zr_5_I

E(B3LYP/BS1) = -646.418632 au

H(B3LYP/BS1) = -646.256955 au

G(B3LYP/BS1) = -646.311557 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -647.175293 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -646.860602 au

C	2.09363300	-1.18665400	-0.79378800
H	2.41663200	-1.47983600	-1.78732700
C	1.09280300	-1.83778700	-0.01931500
H	0.51085500	-2.70087600	-0.32010600
C	0.99127100	-1.15245200	1.22213000
H	0.33340900	-1.41592300	2.04205300
C	2.63134900	-0.12158700	-0.02055800
H	3.41885300	0.55592900	-0.33000500
C	1.95101500	-0.08952900	1.22140800
H	2.14272200	0.59419600	2.03737800
C	0.35913700	2.39595100	0.45947900
O	-1.69362000	0.03020800	-0.19964400
Si	-3.27096900	-0.49846800	0.20807600
H	1.35649700	2.84289900	0.35831700
H	-0.36369600	2.99458000	-0.12976400
H	0.05689800	2.48649500	1.51056000
H	-3.11606400	-1.65030000	1.12560300
H	-3.95792400	0.63526100	0.86179400
H	-3.92959200	-0.89287500	-1.05635500

Zr 0.14396700 0.41799200 -0.45110500

Hf_5_I

E(B3LYP/BS1) = -648.755179 au

H(B3LYP/BS1) = -648.593496 au

G(B3LYP/BS1) = -648.648435 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -648.132328 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -647.828185 au

C	2.01438800	-1.25421300	-0.80571900
H	2.24438200	-1.56170100	-1.82058100
C	1.11903800	-1.91497900	0.07861200
H	0.52845600	-2.79512800	-0.14640800
C	1.11851900	-1.19961200	1.31093400
H	0.55940900	-1.46639100	2.20065500
C	2.60487300	-0.16068500	-0.10716300
H	3.34295900	0.52590500	-0.50571100
C	2.05880000	-0.12395100	1.19744300
H	2.31036100	0.58443300	1.97555300
C	0.24270800	2.31073500	0.53688700
O	-1.71331800	-0.11659000	-0.10259100
Si	-3.33299400	-0.57567900	0.22439900
H	1.20742500	2.81346400	0.38799500
H	-0.53916700	2.90679100	0.03157900
H	0.01568600	2.37393100	1.61138100
H	-3.28443600	-1.92842200	0.82209500
H	-3.88800000	0.42152300	1.16332800
H	-4.03975100	-0.57281200	-1.07427000
Hf	0.09668300	0.30204000	-0.28100600

Ti_5_II

E(B3LYP/BS1) = -736.528430 au

H(B3LYP/BS1) = -736.307866 au

G(B3LYP/BS1) = -736.369000 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1528.150852 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1527.768855 au

C	1.82337400	-0.63950500	-1.33813200
H	2.11904700	-0.09610600	-2.22712200
C	0.74541700	-1.55356700	-1.25331700
H	0.06154400	-1.81342400	-2.05144800
C	0.69847900	-2.04159700	0.08035100
H	-0.01565100	-2.75711700	0.47025700
C	2.46088700	-0.57987800	-0.06602100
H	3.31853700	0.03065900	0.18828400
C	1.77208200	-1.44579300	0.81079900
H	2.01535000	-1.63321700	1.84726000
Ti	0.14195200	0.17753300	0.20424500
C	0.30347000	0.58360500	2.21874800
O	-1.59646600	0.04211400	0.01299800
Si	-3.23794400	-0.37947900	-0.21127700
H	1.31195900	0.84268000	2.55756100
H	-0.37185500	1.44369000	2.34771600
H	-0.07800700	-0.23823300	2.83660800
H	-3.25862000	-1.69966400	-0.88175300
H	-3.86495800	-0.43053100	1.12648800

H	-3.83268900	0.67464300	-1.06265000
C	-0.00137300	2.59556300	-0.60255300
H	-0.56791500	2.48273500	-1.52518000
H	-0.55868700	2.91430900	0.27613100
C	1.34372200	2.48147400	-0.58079600
H	1.91165800	2.27586300	-1.48275500
H	1.91391200	2.67196700	0.32662100

Zr_5_II

E(B3LYP/BS1) = -725.046000 au

H(B3LYP/BS1) = -724.826628 au

G(B3LYP/BS1) = -724.891000 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -725.782000 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -725.395011 au

C	2.09226500	-0.54184200	-1.21924900
H	2.59422400	0.11010900	-1.92282700
C	0.97007200	-1.36858500	-1.50801100
H	0.44170400	-1.42443000	-2.45223500
C	0.67934200	-2.12521800	-0.34399200
H	-0.10447700	-2.86725500	-0.24706400
C	2.50291200	-0.80302600	0.11822800
H	3.33743000	-0.33971200	0.63112500
C	1.63312700	-1.77272000	0.66488700
H	1.69437400	-2.19779400	1.65767600
C	0.21819100	0.28940700	2.44442200
O	-1.78120100	0.01543000	-0.06022900
Si	-3.39802400	-0.41038900	-0.38002500
H	1.22327400	0.50623200	2.83034500
H	-0.45378300	1.12379400	2.71557700
H	-0.15363400	-0.59839400	2.97226800
H	-3.38585300	-1.70456800	-1.10162400
H	-4.10303200	-0.52272900	0.91560400
H	-3.97567400	0.66370600	-1.22023800
C	0.23533600	2.80673200	-0.23544100
H	-0.75482300	2.90189300	-0.68060700
H	0.33141800	3.08536300	0.81508700
C	1.32414300	2.54066600	-0.99008800
H	1.24556500	2.37633700	-2.06218300
H	2.32732000	2.55814200	-0.57013500
Zr	0.09064000	0.19497100	0.24842200

Hf_5_II

E(B3LYP/BS1) = -727.387000 au

H(B3LYP/BS1) = -727.167879 au

G(B3LYP/BS1) = -727.232000 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -726.742101 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -726.368097 au

C	1.83630200	-0.78150100	-1.44593400
H	2.06613600	-0.30831600	-2.39321000
C	0.84236800	-1.76984000	-1.23764900
H	0.16151700	-2.16121900	-1.98364000
C	0.89554900	-2.15564300	0.13279900
H	0.27948500	-2.91350900	0.60362200
C	2.52587300	-0.57571200	-0.21242300

H	3.36364400	0.09297100	-0.05531200
C	1.95184500	-1.42545600	0.75939000
H	2.26060000	-1.51767600	1.79182900
C	0.17441300	0.58888700	2.29641000
O	-1.77555500	-0.08518500	-0.12695100
Si	-3.41362900	-0.50391800	-0.33093400
H	1.15262100	0.93997500	2.65354900
H	-0.56941600	1.37295800	2.51728800
H	-0.09736300	-0.27044900	2.92693200
H	-3.45662800	-1.82941300	-0.99013500
H	-4.04125800	-0.54410100	1.00773800
H	-4.02405600	0.53973000	-1.18563800
C	0.00154100	2.62039100	-0.69309800
H	-0.68806300	2.53072800	-1.53196900
H	-0.41704600	2.97677700	0.24926800
C	1.33560700	2.47234900	-0.85560100
H	1.76969300	2.23666500	-1.82326700
H	2.03167200	2.65790000	-0.03904500
Hf	0.06698200	0.14017300	0.15885100

TS_{Ti-5}

E(B3LYP/BS1) = -736.519000 au

H(B3LYP/BS1) = -736.298627 au

G(B3LYP/BS1) = -736.356000 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1528.139130 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1527.762338 au

C	1.63661800	-1.05673800	-1.26617300
H	1.66181500	-0.91915200	-2.33961400
C	0.79131200	-1.95525200	-0.56246800
H	0.03199400	-2.59140800	-0.99981300
C	1.07473000	-1.82561400	0.82085900
H	0.59185800	-2.36948100	1.62411600
C	2.48788500	-0.41664500	-0.31694900
H	3.24703000	0.32238100	-0.54213100
C	2.14381100	-0.88526000	0.96451800
H	2.59774800	-0.58207700	1.89985900
Ti	0.14715300	0.17841300	0.11481300
C	0.32678800	1.65973500	1.60966000
O	-1.58871000	-0.08039500	0.03007800
Si	-3.21385200	-0.60341400	-0.04522200
H	1.28178100	2.02404000	1.98768300
H	-0.49441600	2.28635900	1.95631700
H	0.15084800	0.64423700	2.08381300
H	-3.19103700	-2.06579800	-0.27409900
H	-3.84084600	-0.25957800	1.24976300
H	-3.84534000	0.11786800	-1.17202100
C	0.40024500	1.72458800	-1.44957000
H	1.35397100	1.63343100	-1.95721100
H	-0.48534000	1.54024000	-2.05768200
C	0.29197400	2.61352000	-0.36831600
H	1.15785600	3.18137800	-0.04464500
H	-0.67184600	3.05343500	-0.13710400

TS_{Zr-5}

E(B3LYP/BS1) = -725.032000 au

H(B3LYP/BS1) = -724.812661 au
 G(B3LYP/BS1) = -724.872000 au
 E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -725.782000 au
 E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -725.381416 au

C	1.60867200	-1.33673600	-1.26357600
H	1.56259200	-1.31937400	-2.34597000
C	0.83547200	-2.17289800	-0.40887700
H	0.08209200	-2.88545900	-0.72316100
C	1.22295100	-1.90311100	0.93080600
H	0.83556200	-2.39440700	1.81627100
C	2.50776300	-0.58832500	-0.45091000
H	3.24548800	0.11959400	-0.80883000
C	2.27007500	-0.92812100	0.89860600
H	2.80584400	-0.54509600	1.75882000
C	0.35580000	1.85570100	1.56811400
O	-1.82327000	-0.11904100	0.01002300
Si	-3.46970100	-0.54545400	-0.07185800
H	1.10116000	2.51095100	2.01664900
H	-0.64776900	2.24440200	1.77159300
H	0.47245800	0.88226600	2.13552600
H	-3.54587600	-2.00022100	-0.33891800
H	-4.08427000	-0.20583600	1.23162600
H	-4.07621100	0.23598300	-1.17316300
C	0.45904500	1.79916000	-1.50379000
H	1.27527900	1.48120600	-2.14606100
H	-0.50486600	1.93308700	-1.99762800
C	0.76432000	2.65014600	-0.41653700
H	1.80400200	2.86056600	-0.18716200
H	0.06560000	3.42761900	-0.12433000
Zr	0.06565700	0.14971300	0.09793900

TS_{Hf-5}

E(B3LYP/BS1) = -727.387000 au
 H(B3LYP/BS1) = -727.152680 au
 G(B3LYP/BS1) = -727.232000 au
 E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -726.742000 au
 E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -726.352289 au

C	-1.65864800	-1.28114900	1.27853700
H	-1.64461800	-1.24131100	2.36104300
C	-0.87911300	-2.15296500	0.46565800
H	-0.15510500	-2.87811000	0.81790800
C	-1.22101900	-1.90503400	-0.89270000
H	-0.82235500	-2.42852800	-1.75424200
C	-2.51178400	-0.52746300	0.42257600
H	-3.24140100	0.20689900	0.74186800
C	-2.24399300	-0.90618000	-0.91233600
H	-2.74332300	-0.52799600	-1.79628200
C	-0.25241200	1.77183600	-1.56015200
O	1.79381300	-0.20193000	0.00294700
Si	3.43976200	-0.62659600	0.08063400
H	-1.01119200	2.39256900	-2.03560000
H	0.74322100	2.16324700	-1.79093300
H	-0.34971300	0.77678000	-2.10352500
H	3.51939600	-2.09314600	0.26806300

H	4.06625700	-0.21195200	-1.19493100
H	4.03040500	0.09586900	1.22971500
C	-0.35369600	1.76485400	1.50662700
H	-1.19149400	1.52031100	2.15420000
H	0.60999300	1.86864500	2.00851000
C	-0.60857400	2.62761300	0.41100700
H	-1.63386100	2.89392700	0.17440500
H	0.13330500	3.35976200	0.10883100
Hf	-0.06168400	0.11308000	-0.06467700

Ti_5_III

E(B3LYP/BS1) = -736.545000 au

H(B3LYP/BS1) = -736.322998 au

G(B3LYP/BS1) = -736.382000 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1528.170000 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1527.792413 au

C	1.39011500	-1.52146100	-1.21298100
H	1.65960300	-1.31141800	-2.24192800
C	0.22695200	-2.21633300	-0.78028300
H	-0.55855900	-2.60836300	-1.41494600
C	0.25556100	-2.26253000	0.64111200
H	-0.49196200	-2.72228400	1.27758900
C	2.15951700	-1.18462300	-0.06298600
H	3.09774300	-0.64438300	-0.06540800
C	1.46253300	-1.63144000	1.08051600
H	1.77898900	-1.51334100	2.10897300
Ti	-0.02675800	-0.08855100	0.03533100
C	0.80614800	1.42753000	1.14584700
O	-1.74525000	0.26154900	-0.02500700
Si	-3.44546200	0.46909500	-0.08966100
H	-4.01417400	-0.78602000	-0.62767300
H	-3.90058000	0.73509900	1.29186600
H	-3.69453600	1.61847600	-0.98665100
C	2.37059800	2.71902300	-0.46190100
C	0.98953100	2.10219200	-0.20051600
H	1.72840300	1.26158800	1.69970900
H	0.02397800	1.86884800	1.76943100
H	3.17110300	1.99308200	-0.28954200
H	2.44931900	3.09001800	-1.48774300
H	2.52152600	3.56028100	0.22051600
H	0.86624400	1.33905400	-1.06132200
H	0.18433500	2.81361600	-0.40766400

Zr_5_III

E(B3LYP/BS1) = -725.712723 au

H(B3LYP/BS1) = -725.492454 au

G(B3LYP/BS1) = -725.554253 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -725.804099 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -725.422441 au

C	1.47343700	-1.71489100	-1.16421100
H	1.76114300	-1.60447500	-2.20055700
C	0.31742500	-2.38884800	-0.68907000
H	-0.43881000	-2.86548600	-1.29623600
C	0.33756200	-2.33519500	0.72762300

H	-0.39127100	-2.78184200	1.38953600
C	2.22142300	-1.27928700	-0.04109500
H	3.16252400	-0.75093500	-0.07498500
C	1.52248400	-1.64839400	1.12501800
H	1.83975000	-1.46920400	2.14100300
C	0.87279300	1.59652200	1.12969600
O	-1.94964600	0.29809700	-0.06906200
Si	-3.63085500	0.48068500	-0.06324800
H	-4.20389600	-0.65445700	-0.81004200
H	-4.07124200	0.47744200	1.34352800
H	-3.92901500	1.76545100	-0.72205900
C	2.58474200	2.75527800	-0.44078300
C	1.16185500	2.23713400	-0.21913100
H	1.76728600	1.41052600	1.71704700
H	0.13115900	2.14440200	1.71214400
H	3.32641400	1.98835900	-0.21375100
H	2.73436600	3.09335400	-1.46692800
H	2.75999900	3.60009100	0.22637200
H	1.01647400	1.47845100	-1.08985600
H	0.42339500	3.00076200	-0.47181900
Zr	-0.06023700	-0.03201800	-0.03284300

Hf_5_III

E(B3LYP/BS1) = -727.391000 au

H(B3LYP/BS1) = -727.169257 au

G(B3LYP/BS1) = -727.232000 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -726.759000 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -726.392547 au

C	1.53071200	-1.62700600	-1.18275600
H	1.80753800	-1.49754200	-2.22329800
C	0.40424300	-2.35507800	-0.70389300
H	-0.33799400	-2.86037100	-1.31100900
C	0.43075900	-2.30890500	0.72171900
H	-0.27073800	-2.80139900	1.38619700
C	2.27351900	-1.17002100	-0.05597200
H	3.19217100	-0.59750800	-0.09220800
C	1.59913800	-1.58272100	1.11686100
H	1.91734600	-1.39705800	2.13476900
C	0.78296800	1.60009600	1.13730500
O	-1.89831800	0.22640200	-0.07051300
Si	-3.59560200	0.41878500	-0.06915400
H	-4.18233700	-0.82063600	-0.62523300
H	-4.01600900	0.63868600	1.33189300
H	-3.89634700	1.59180600	-0.91947100
C	2.42885700	2.87664000	-0.43870900
C	1.04238200	2.25712100	-0.23341100
H	1.70124400	1.48487900	1.71530600
H	0.04515400	2.16328000	1.71717300
H	3.22171900	2.15478200	-0.22003000
H	2.55911000	3.24317100	-1.46135500
H	2.54167900	3.72232600	0.24619800
H	0.96550000	1.48311800	-1.10242400
H	0.25038500	2.96781800	-0.49361200
Hf	-0.04067900	-0.04569900	-0.00996500

Ti_5_IV

E(B3LYP/BS1) = -736.161256 au

H(B3LYP/BS1) = -735.951737 au

G(B3LYP/BS1) = -736.010579 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1527.721479 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1527.34894042 au

C	-0.77354900	-1.95496100	0.70959400
H	-0.07609200	-2.48718700	1.34448200
C	-0.77393500	-1.95468800	-0.71019900
H	-0.07682800	-2.48667400	-1.34567300
C	-1.82011700	-1.10258500	-1.14868200
H	-2.06724400	-0.87723700	-2.17709600
C	-1.81948300	-1.10301900	1.14898000
H	-2.06601500	-0.87804000	2.17761700
C	-2.46239100	-0.57850700	0.00042500
H	-3.27709200	0.13520400	0.00076600
Ti	-0.15283900	0.21977000	-0.00004000
O	1.65191800	0.04730400	-0.00011200
Si	3.22018000	-0.48210400	0.00000700
H	3.26681100	-1.97205200	0.00045500
H	3.93419200	0.01247300	-1.20904000
H	3.93424700	0.01319900	1.20872400
C	-0.51551800	1.72754200	-1.32446500
C	-0.51537300	1.72745700	1.32451300
C	-0.52273300	2.59137200	0.00003600
H	-1.43321500	3.19506400	0.00011000
H	0.34502100	3.25512300	0.00002200
H	-1.44483300	1.80903400	-1.88742900
H	0.34435100	1.94633600	-1.96182700
H	-1.44464200	1.80890500	1.88755700
H	0.34453700	1.94626500	1.96181400

Ti_5_V

E(B3LYP/BS1) = -776.683093 au

H(B3LYP/BS1) = -776.422165 au

G(B3LYP/BS1) = -776.488012 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1568.259128 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1567.846656 au

C	-1.14001700	1.65831700	-1.14645700
H	-1.44839300	1.52411400	-2.17418900
C	0.12509500	2.13526300	-0.71221700
H	0.95315200	2.41692400	-1.35070000
C	0.12866300	2.13703100	0.70534700
H	0.95995500	2.42016000	1.33894600
C	-1.91608600	1.37153500	0.00263900
H	-2.91155000	0.94646800	0.00574900
C	-1.13415200	1.66105500	1.14709900
H	-1.43726600	1.52912200	2.17670100
Ti	0.02455900	-0.12335800	-0.00061400
O	1.80308700	-0.46957800	-0.00090900
Si	3.45839300	-0.43102800	0.00043200
H	3.94509700	0.97802900	-0.00056600
H	3.98887800	-1.11451100	1.21133000
H	3.99088500	-1.11696100	-1.20818700

C	-0.61960700	-1.27620900	1.63164000
C	-0.62079700	-1.27723500	-1.63169800
H	-0.04797000	-0.90275200	2.49616200
H	-0.15307400	-2.23665900	1.35104200
H	-0.05244600	-0.90229500	-2.49773500
H	-0.15137900	-2.23671200	-1.35264200
C	-2.08824100	-1.49201800	2.00002200
C	-2.09001800	-1.49628700	-1.99587400
H	-2.56160100	-0.56861400	2.35520100
H	-2.67502700	-1.84807800	1.14430800
H	-2.20418300	-2.23994000	2.79796600
H	-2.56657400	-0.57391800	-2.34945500
H	-2.20655000	-2.24429400	-2.79365400
H	-2.67349500	-1.85390400	-1.13854800

Zr_5_IV

E(B3LYP/BS1) = -724.666783 au

H(B3LYP/BS1) = -724.460466 au

G(B3LYP/BS1) = -724.514269 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -725.336792 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -724.960585 au

C	-0.98449500	-2.09225400	0.71009500
H	-0.35454200	-2.70301700	1.34613000
C	-0.98479500	-2.09194400	-0.71072800
H	-0.35511900	-2.70243800	-1.34729500
C	-1.95996800	-1.15421700	-1.14898900
H	-2.20167700	-0.92169300	-2.17768400
C	-1.95947300	-1.15470900	1.14917200
H	-2.20073200	-0.92260800	2.17807000
C	-2.56187900	-0.58384800	0.00034300
H	-3.33139000	0.17846400	0.00067700
O	1.90656200	-0.10908900	-0.00008400
Si	3.52429500	-0.45579000	-0.00003400
H	3.74469200	-1.93002700	0.00119300
H	4.18235100	0.11427800	-1.20836600
H	4.18270300	0.11634200	1.20713000
C	-0.50696900	1.83833500	-1.33763700
C	-0.50685600	1.83818000	1.33782200
C	-0.91910600	2.58528500	0.00015300
H	-2.00618900	2.70002800	0.00020500
H	-0.47203000	3.58526800	0.00019200
H	-1.29531900	1.88209500	-2.08902100
H	0.41760800	2.25770800	-1.75500800
H	-1.29514200	1.88185100	2.08927900
H	0.41775900	2.25750200	1.75516100
Zr	-0.04310900	0.15877600	-0.00002200

Zr_5_V

E(B3LYP/BS1) = -765.194329 au

H(B3LYP/BS1) = -764.935580 au

G(B3LYP/BS1) = -765.001351 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -765.878921 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -765.461948 au

C	-1.35073000	1.70694600	-1.14880400
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H	-1.65406900	1.55992900	-2.17689700
C	-0.13146500	2.29640800	-0.71349400
H	0.65684500	2.67691800	-1.35204200
C	-0.12872500	2.29863100	0.70614100
H	0.66208000	2.68105500	1.34043600
C	-2.09870300	1.35267000	0.00158900
H	-3.06317900	0.85972800	0.00429900
C	-1.34624200	1.71045600	1.14796700
H	-1.64558300	1.56651600	2.17767600
O	2.00806900	-0.31811500	-0.00021000
Si	3.66318200	-0.27823000	0.00062100
H	4.15178700	1.12997500	-0.00206900
H	4.19974800	-0.95908800	1.21099700
H	4.20106300	-0.96418800	-1.20628000
C	-0.58254000	-1.35798700	1.77777400
C	-0.58295400	-1.36068100	-1.77655300
H	-0.07125800	-0.96017700	2.67023800
H	-0.06128200	-2.30911100	1.54940700
H	-0.07422000	-0.96274300	-2.67040200
H	-0.05947300	-2.31060200	-1.54831500
C	-2.05537300	-1.64966200	2.09847100
C	-2.05589100	-1.65548000	-2.09400400
H	-2.58491000	-0.74365700	2.41840300
H	-2.59364700	-2.04434800	1.22659600
H	-2.17163700	-2.39051000	2.90293000
H	-2.58776900	-0.75086700	-2.41397500
H	-2.17234100	-2.39750200	-2.89735500
H	-2.59172100	-2.05015000	-1.22061500
Zr	0.05265500	-0.13097100	-0.00036400

Hf_5_IV

E(B3LYP/BS1) = -727.013356 au

H(B3LYP/BS1) = -726.805764 au

G(B3LYP/BS1) = -726.862334 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -726.302480 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -725.937969 au

C	-1.04713500	-2.09044700	0.70827600
H	-0.44225000	-2.72672900	1.34347700
C	-1.04812100	-2.08815900	-0.71295400
H	-0.44407500	-2.72233300	-1.35106000
C	-1.98573700	-1.11239800	-1.14899700
H	-2.21690100	-0.86758200	-2.17727600
C	-1.98404100	-1.11597200	1.14877600
H	-2.21365700	-0.87427200	2.17815500
C	-2.56394900	-0.51878300	0.00123900
H	-3.30235700	0.27363700	0.00306100
O	1.85559800	-0.23959900	0.00172800
Si	3.47964500	-0.56169700	-0.00025300
H	3.82660400	-1.47914700	-1.12080200
H	4.25514700	0.69832400	-0.16152300
H	3.88430700	-1.20771100	1.27884400
C	-0.36351700	1.81315800	-1.32804600
C	-0.36700200	1.81402200	1.32734000
C	-0.75657800	2.58794800	-0.00112600
H	-1.83877300	2.74494800	-0.00267000

H	-0.27351500	3.57081400	-0.00081600
H	-1.13524400	1.90051200	-2.09417500
H	0.58062700	2.19785000	-1.73489000
H	-1.14130500	1.90089100	2.09095000
H	0.57534000	2.19984000	1.73718500
Hf	-0.04135100	0.11715700	0.00047500

Hf_5_V

E(B3LYP/BS1) = -767.540519 au

H(B3LYP/BS1) = -767.280563 au

G(B3LYP/BS1) = -767.349161 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -766.845313 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -766.439979 au

C	-1.40817800	1.69533900	-1.14869300
H	-1.70452100	1.53387500	-2.17674500
C	-0.21036400	2.32688000	-0.71405500
H	0.56317300	2.73619900	-1.35277900
C	-0.20768300	2.32933400	0.70644500
H	0.56833700	2.74072000	1.34080600
C	-2.14314800	1.31317600	0.00158100
H	-3.08933300	0.78595700	0.00433200
C	-1.40375800	1.69919200	1.14775400
H	-1.69617100	1.54112300	2.17746600
O	1.96324600	-0.21601200	0.00015000
Si	3.61980000	-0.22811700	0.00102200
H	4.14608800	1.16552000	-0.00059700
H	4.13067400	-0.92584100	1.21186100
H	4.13193200	-0.92914800	-1.20736800
C	-0.51694600	-1.35767700	1.73848400
C	-0.51666400	-1.36009600	-1.73757600
H	-0.01866400	-0.94813600	2.63470600
H	0.03742100	-2.29069400	1.51792000
H	-0.02211100	-0.94935200	-2.63530200
H	0.04102500	-2.29139000	-1.51823100
C	-1.97529900	-1.71142100	2.07643300
C	-1.97492700	-1.71832600	-2.07130700
H	-2.54018500	-0.82889400	2.40163300
H	-2.50458700	-2.12819200	1.20981700
H	-2.05160600	-2.45560500	2.88211300
H	-2.54350300	-0.83759400	-2.39492800
H	-2.05126100	-2.46281300	-2.87670600
H	-2.50038000	-2.13668200	-1.20312300
Hf	0.03975400	-0.07910700	-0.00034400

Zr_6_I

E(B3LYP/BS1) = -473.378000 au

H(B3LYP/BS1) = -473.160874 au

G(B3LYP/BS1) = -473.214000 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -474.101000 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -473.706343 au

Zr	0.00007400	0.24145800	-0.25695000
C	-2.20701700	-0.72366500	-1.03555900
C	-1.68782300	-1.60527000	-0.05612600
C	-2.51402100	0.51580900	-0.40062700

H	-2.36323000	-0.95683500	-2.08379300
C	-1.66447900	-0.90805200	1.19061300
H	-1.39029800	-2.63357700	-0.21657300
C	-2.20005900	0.39433300	0.97674800
H	-2.94136800	1.38807700	-0.88056500
H	-1.37135300	-1.32535600	2.14554500
H	-2.34166700	1.15593400	1.73188700
C	2.20371900	0.40245900	0.96890100
C	1.66743000	-0.89743200	1.19568100
C	2.51334400	0.51162400	-0.41052900
H	2.34847000	1.17031200	1.71701600
C	1.68678200	-1.60572700	-0.04491300
H	1.37664800	-1.30598500	2.15512400
C	2.20375100	-0.73332900	-1.03354900
H	2.94011500	1.37922900	-0.89942400
H	1.38771700	-2.63508600	-0.19535300
H	2.35653300	-0.97585700	-2.08016000
C	-0.00109400	2.42257700	0.12453300
H	-0.88685600	2.92488900	0.51827800
H	0.89021800	2.92639100	0.50346800
H	-0.01107100	2.58958500	-0.98848400

Hf_6_I

E(B3LYP/BS1) = -475.708000 au

H(B3LYP/BS1) = -475.491438 au

G(B3LYP/BS1) = -475.540000 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -475.052000 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -474.667520 au

C	1.87916700	-0.75387800	1.23473000
C	1.63409400	-1.67793900	0.18087400
C	2.37369600	0.45435700	0.65392200
H	1.78193600	-0.95816500	2.29501000
C	1.92367600	-1.03004200	-1.04921600
H	1.29025300	-2.69719100	0.29682200
C	2.39417900	0.28616800	-0.75208400
H	2.67655000	1.34407300	1.19119200
H	1.85948300	-1.47788800	-2.03466800
H	2.71921300	1.02602100	-1.47394500
C	-2.39825800	0.29881800	-0.73706100
C	-1.93058400	-1.01304300	-1.05701000
C	-2.36926700	0.44528400	0.67118100
H	-2.72692400	1.04981600	-1.44553500
C	-1.63444900	-1.68005300	0.16118200
H	-1.87244100	-1.44567700	-2.04963700
C	-1.87243000	-0.77206400	1.23061800
H	-2.66798300	1.32713800	1.22364200
H	-1.29094100	-2.70132200	0.25910700
H	-1.76949500	-0.99284700	2.28701600
C	0.00014500	2.41312000	0.04881300
H	0.88557900	2.91173800	-0.36418500
H	-0.88785500	2.91150200	-0.35882900
H	0.00342800	2.66150000	1.13002700
Hf	-0.00000900	0.21134600	-0.06210700

Zr_6_II

E(B3LYP/BS1) = -551.994000 au
 H(B3LYP/BS1) = -551.719249 au
 G(B3LYP/BS1) = -551.778000 au
 E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -552.712000 au
 E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -552.252377 au

Zr	0.00002700	0.04166000	0.15037800
C	1.65379700	-1.82338000	-0.04263600
C	1.62935900	-1.21382500	-1.33223100
C	2.24804400	-0.90540700	0.86737300
H	1.34893100	-2.83661900	0.18640300
C	2.17589400	0.08374100	-1.20872300
H	1.28250700	-1.67357200	-2.24803700
C	2.54730800	0.28074600	0.15368500
H	2.43844100	-1.08328500	1.91667900
H	2.31996800	0.78823800	-2.01882000
H	3.02032000	1.16490000	0.56383800
C	-2.54713400	0.28117500	0.15270000
C	-2.17541000	0.08239100	-1.20939100
C	-2.24833600	-0.90416800	0.86792500
H	-3.02010900	1.16592400	0.56162000
C	-1.62917500	-1.21545000	-1.33113900
H	-2.31909600	0.78590600	-2.02040900
C	-1.65402200	-1.82337900	-0.04078900
H	-2.43907300	-1.08073900	1.91738700
H	-1.28214500	-1.67640500	-2.24626800
H	-1.34940000	-2.83638400	0.18960300
C	0.00024400	0.32124000	2.38263900
H	0.89217100	0.88456300	2.68909200
H	-0.89150100	0.88478500	2.68922000
H	0.00016200	-0.61028700	2.96450600
C	0.00066800	2.86555500	0.25317800
H	-0.92420600	2.94869200	0.81959900
H	0.92729000	2.94823900	0.81680500
C	-0.00137900	2.79599300	-1.09115600
H	0.92218000	2.80383800	-1.66388200
H	-0.92666000	2.80440000	-1.66107200

Hf_6_II

E(B3LYP/BS1) = -554.325000 au
 H(B3LYP/BS1) = -554.049826 au
 G(B3LYP/BS1) = -554.111000au
 E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -553.670000 au
 E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -553.224133 au

C	1.51485800	-1.88494300	-0.28678600
C	1.59672400	-1.06639200	-1.45172000
C	2.10657000	-1.17377100	0.79241300
H	1.12635800	-2.89405100	-0.24665800
C	2.23319200	0.14645700	-1.08363500
H	1.27410400	-1.33956800	-2.44816700
C	2.53963600	0.08399100	0.30314700
H	2.20877800	-1.52744400	1.81009100
H	2.47410800	0.96326600	-1.75400100
H	3.03719900	0.84913000	0.88502700
C	-2.50503200	0.37784500	0.03806600

C	-2.12479300	-0.06310100	-1.26762500
C	-2.26471000	-0.67963600	0.94568700
H	-2.94254100	1.33659900	0.28854400
C	-1.64098100	-1.38521700	-1.15855400
H	-2.22691300	0.49849600	-2.18835700
C	-1.69668700	-1.76232300	0.21533400
H	-2.46759200	-0.66641000	2.00754300
H	-1.29565800	-2.00612000	-1.97456800
H	-1.43282600	-2.73093000	0.62133500
C	0.07123800	0.59784300	2.27422100
H	1.00072400	1.11036300	2.55517200
H	-0.77150300	1.24532200	2.55619500
H	0.00319800	-0.28272600	2.93250100
C	0.41043700	2.84815300	-0.05385600
H	-0.06458600	3.21645200	0.85170200
H	1.49502100	2.79167800	-0.04451300
C	-0.30592400	2.57808500	-1.16351300
H	0.17287500	2.28820100	-2.09798800
H	-1.37639100	2.75188300	-1.19974800
Hf	0.00247900	0.03741500	0.12259500

TS_{Zr-6}

E(B3LYP/BS1) = -551.983000 au

H(B3LYP/BS1) = -551.707735 au

G(B3LYP/BS1) = -551.764000 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -552.700000 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -552.244892 au

Zr	0.00000600	0.06347700	0.05983400
C	1.69499700	-1.70172800	0.66921600
C	1.63435700	-1.68235600	-0.75547900
C	2.27973200	-0.47952100	1.09444700
H	1.40712100	-2.52686100	1.30822800
C	2.16127300	-0.44389600	-1.20114700
H	1.28951100	-2.48978100	-1.38809400
C	2.54677700	0.30665400	-0.05515000
H	2.48808200	-0.19957600	2.11999400
H	2.28006900	-0.14132600	-2.23339500
H	3.00865500	1.28611300	-0.06171700
C	-2.54681500	0.30633800	-0.05658300
C	-2.16063200	-0.44546700	-1.20153000
C	-2.28020400	-0.47842600	1.09404600
H	-3.00878700	1.28574500	-0.06456700
C	-1.63386000	-1.68338300	-0.75416900
H	-2.27890300	-0.14408800	-2.23419100
C	-1.69510400	-1.70107700	0.67052200
H	-2.48908000	-0.19728400	2.11915700
H	-1.28862100	-2.49152700	-1.38565100
H	-1.40745800	-2.52541200	1.31066700
C	0.00007100	1.76670200	1.63300400
H	0.89273800	2.26670600	2.00767600
H	-0.89239300	2.26685300	2.00796400
H	0.00004200	0.74625500	2.12781100
C	-0.00034800	2.70461000	-0.31110100
H	-0.91280100	3.21599600	-0.02540800
H	0.91190800	3.21639600	-0.02549100

C	-0.00022000	1.89443300	-1.47109900
H	0.91505600	1.85789900	-2.05313000
H	-0.91552000	1.85751400	-2.05307400

TS_{Hf-6}

E(B3LYP/BS1) = -554.313000 au

H(B3LYP/BS1) = -554.038043 au

G(B3LYP/BS1) = -554.095000 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -553.654000 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -553.213090 au

C	1.67917800	-1.62573500	0.79356800
C	1.55003300	-1.79108000	-0.61648100
C	2.30211000	-0.36850700	1.02645300
H	1.41939600	-2.35770600	1.54787000
C	2.05811100	-0.62565900	-1.24463400
H	1.16307900	-2.66704100	-1.11968000
C	2.51877900	0.25562400	-0.22565000
H	2.56785100	0.03659100	1.99491400
H	2.11631400	-0.45334800	-2.31199200
H	2.98561800	1.21996900	-0.38283700
C	-2.51494100	0.33941700	0.01188000
C	-2.17104400	-0.34416800	-1.18768700
C	-2.23205700	-0.52298100	1.10321700
H	-2.96223400	1.32330900	0.07788500
C	-1.64566500	-1.61273400	-0.83445000
H	-2.31317800	0.02191900	-2.19578500
C	-1.67620100	-1.72237500	0.58769600
H	-2.41075700	-0.30620800	2.14936700
H	-1.32672200	-2.38083400	-1.52664600
H	-1.38210100	-2.58858900	1.16640000
C	0.00642600	1.69684200	1.62902700
H	0.88454600	2.19408800	2.03997800
H	-0.89979400	2.17895700	1.99549200
H	0.00587700	0.66717900	2.10973600
C	0.08727800	2.67127400	-0.30366000
H	-0.79476000	3.22562600	-0.00267500
H	1.02668800	3.12581500	-0.00959600
C	0.03796300	1.86573700	-1.46766800
H	0.94321100	1.80739300	-2.06470000
H	-0.88281100	1.89267400	-2.04143300
Hf	-0.00194500	0.05230900	0.04088900

Zr_6_III

E(B3LYP/BS1) = -552.014000 au

H(B3LYP/BS1) = -551.737353 au

G(B3LYP/BS1) = -551.798000 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -552.739000 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -552.281219 au

Zr	-0.11269900	0.03823400	0.02890000
C	0.75217200	2.06832200	-1.22698300
C	-0.28026800	2.52820200	-0.37340100
C	1.82787600	1.61120000	-0.40854600
H	0.74260200	2.09133100	-2.31092200
C	0.14278000	2.33435800	0.97462000

H	-1.22258800	2.95835400	-0.68740100
C	1.45947900	1.79000800	0.94926600
H	2.77677900	1.23201700	-0.76713500
H	-0.41170400	2.61899200	1.86127000
H	2.07445200	1.57311100	1.81219500
C	-1.70268600	-1.95558300	0.08170600
C	-2.14772600	-1.06271200	1.08627000
C	-1.86941400	-1.31978500	-1.18310600
H	-1.32576600	-2.95684700	0.24499800
C	-2.57610100	0.13779400	0.45148800
H	-2.15713700	-1.25870500	2.15192500
C	-2.41499400	-0.02886700	-0.95661600
H	-1.65390800	-1.76039900	-2.14999800
H	-3.00859600	0.99952700	0.94453700
H	-2.68965800	0.69003800	-1.71845200
C	1.66155200	-1.89726200	-0.21182700
H	1.23959500	-1.23417600	-1.07115900
H	1.19754700	-2.86051000	-0.44283800
C	3.17131000	-1.94185200	-0.47837600
H	3.38971500	-2.21158200	-1.51626800
H	3.62599200	-2.69399000	0.17346000
C	1.22744000	-1.37763700	1.14806500
H	2.04852700	-0.92411700	1.70486700
H	0.72675400	-2.12891200	1.75924400
H	3.64682600	-0.98063000	-0.25969600

Hf_6_III

E(B3LYP/BS1) = -554.343000 au

H(B3LYP/BS1) = -554.066370 au

G(B3LYP/BS1) = -554.125000 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -553.692000 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -553.250883 au

C	-0.40143500	2.13228200	1.15685300
C	0.18810300	2.52326800	-0.07738800
C	-1.65849300	1.52662900	0.86864500
H	0.01116500	2.30584200	2.14337000
C	-0.69428600	2.14399200	-1.12596800
H	1.13366800	3.03642000	-0.19629200
C	-1.83964600	1.53531200	-0.54302100
H	-2.37121400	1.16374900	1.59964800
H	-0.53565800	2.31352800	-2.18508500
H	-2.70788500	1.17717400	-1.07824700
C	1.72144700	-1.89059200	0.12813600
C	2.11686600	-1.13101700	-0.99901400
C	1.88785700	-1.08193000	1.29162100
H	1.37246300	-2.91498800	0.11073800
C	2.51310300	0.16017100	-0.54367800
H	2.11339900	-1.47132300	-2.02729900
C	2.38948700	0.17933600	0.87868200
H	1.70499000	-1.39254700	2.31407300
H	2.91167200	0.95777100	-1.15857000
H	2.64957900	1.00557100	1.52791400
C	-1.60013100	-1.91650500	0.23469200
H	-1.14294700	-1.25000900	1.08157100
H	-1.16350100	-2.88538500	0.49246400

C	-3.10484200	-1.89940600	0.51892000
H	-3.32374600	-2.15064700	1.56152500
H	-3.59427100	-2.64073400	-0.12031400
C	-1.15958300	-1.44146300	-1.15005000
H	-1.99961800	-1.07679200	-1.74298500
H	-0.63798900	-2.22211500	-1.70627200
H	-3.54563300	-0.92293700	0.29526300
Hf	0.09687300	0.02676300	-0.06586200

Zr_6_IV

E(B3LYP/BS1) = -551.604204 au

H(B3LYP/BS1) = -551.340039 au

G(B3LYP/BS1) = -551.396383 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -552.266046 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -551.815648 au

Zr	-0.00021100	0.07422100	-0.00002300
C	1.71545700	-1.69512800	0.71420100
C	1.71427600	-1.69790200	-0.71007600
C	2.25503000	-0.45933900	1.14949600
H	1.38148000	-2.50380600	1.35216600
C	2.25296800	-0.46375800	-1.15108800
H	1.37868400	-2.50882300	-1.34433100
C	2.57394300	0.30524900	-0.00253500
H	2.38807500	-0.14936600	2.17724400
H	2.38418000	-0.15758200	-2.18022900
H	2.98757200	1.30595800	-0.00486700
C	-2.57358800	0.31329100	0.00474400
C	-2.25784000	-0.45031700	-1.14882800
C	-2.25468500	-0.45888700	1.15173000
H	-2.98414200	1.31526500	0.00901800
C	-1.72215600	-1.68866100	-0.71602900
H	-2.39063100	-0.13815200	-2.17594200
C	-1.72028700	-1.69397000	0.70822500
H	-2.38403000	-0.15391700	2.18147800
H	-1.39075600	-2.49714900	-1.35557500
H	-1.38734600	-2.50728400	1.34079900
C	0.00300500	1.83789800	1.35621100
H	0.88927600	2.05764100	1.95429000
C	0.00291700	1.83801400	-1.35615300
H	0.88936800	2.05751000	-1.95411000
C	0.00932300	2.67267200	0.00018100
H	-0.88580700	2.06287500	-1.94878100
H	-0.88598300	2.06164300	1.94883000
H	0.89853900	3.30902300	0.00023800
H	-0.87022300	3.32236000	0.00021100

Zr_6_V

E(B3LYP/BS1) = -592.128363 au

H(B3LYP/BS1) = -591.812914 au

G(B3LYP/BS1) = -591.876608 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -592.804207 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -592.314984 au

Zr	-0.00013300	-0.04775500	-0.00005000
C	1.78944100	-1.83330100	0.39909300

C	1.48839900	-1.88149600	-0.99120700
C	2.44179300	-0.60211700	0.66290800
H	1.58142300	-2.61043300	1.12342700
C	1.95263000	-0.67919000	-1.58051600
H	1.00994700	-2.70190200	-1.51054700
C	2.53304600	0.11282200	-0.55770300
H	2.79702100	-0.26536400	1.62743000
H	1.86522500	-0.40558800	-2.62375900
H	2.95957200	1.09945100	-0.68378700
C	-2.53258300	0.11272400	0.55841000
C	-2.44203500	-0.60114200	-0.66287900
C	-1.95211600	-0.68048800	1.58031000
H	-2.95870000	1.09939200	0.68560000
C	-1.78987600	-1.83273700	-0.40045400
H	-2.79752100	-0.26343000	-1.62697000
C	-1.48848200	-1.88238100	0.98972000
H	-1.86425400	-0.40785200	2.62377000
H	-1.58265400	-2.60938600	-1.12553600
H	-1.01031500	-2.70353200	1.50813800
C	0.30748500	1.44123300	1.72597900
H	-0.67292400	1.93457100	1.82750700
C	-0.30651000	1.44326300	-1.72423700
H	-0.45398000	0.91330500	-2.67889100
H	0.67377300	1.93775600	-1.82184800
H	0.45852800	0.90965700	2.67917800
C	-1.38526300	2.52899500	-1.56598700
C	1.38465100	2.52842900	1.56628800
H	2.40023900	2.11625800	1.60550400
H	1.29179100	3.06104700	0.61042100
H	1.32197400	3.29032200	2.35806200
H	-1.32166400	3.29184500	-2.35676800
H	-2.40029700	2.11566500	-1.60796400
H	-1.29534900	3.06071100	-0.60931300

Hf_6_IV

E(B3LYP/BS1) = -553.940072 au

H(B3LYP/BS1) = -553.675710 au

G(B3LYP/BS1) = -553.733093 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -553.226081 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -552.788026 au

C	1.68132000	-1.71063200	0.71346600
C	1.68071300	-1.71240700	-0.71072700
C	2.22589900	-0.47724700	1.14912400
H	1.34496700	-2.51821100	1.35111900
C	2.22482600	-0.48008400	-1.14991900
H	1.34378600	-2.52158000	-1.34605700
C	2.55012200	0.28680500	-0.00147600
H	2.35558700	-0.16671600	2.17705100
H	2.35356000	-0.17202300	-2.17872200
H	2.96326200	1.28749900	-0.00291600
C	-2.54990900	0.29353100	0.00270800
C	-2.22828200	-0.47043200	-1.14866300
C	-2.22613600	-0.47518100	1.15036700
H	-2.96019400	1.29540500	0.00517400
C	-1.68674000	-1.70561400	-0.71428800

H	-2.35766100	-0.15871200	-2.17627200
C	-1.68557300	-1.70860000	0.70990100
H	-2.35356500	-0.16760700	2.17948600
H	-1.35289800	-2.51358000	-1.35277300
H	-1.35060800	-2.51923000	1.34440600
C	0.00226300	1.81178100	1.34471400
H	0.88543900	2.03599000	1.94746200
C	0.00265200	1.81196900	-1.34460300
H	0.88617800	2.03597900	-1.94692200
C	0.00789700	2.66368200	0.00011500
H	-0.88274800	2.04015600	-1.94262700
H	-0.88349100	2.03958800	1.94236900
H	0.89548300	3.30261500	0.00030800
H	-0.87130400	3.31413700	0.00001900
Hf	-0.00014000	0.06417900	-0.00007500

Hf_6_V

E(B3LYP/BS1) = -594.464484 au

H(B3LYP/BS1) = -594.148864 au

G(B3LYP/BS1) = -594.213016 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -593.765821 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -593.288949 au

C	1.77450600	-1.81560000	0.42192500
C	1.46537200	-1.88814600	-0.96530500
C	2.42338100	-0.57731700	0.66058700
H	1.57641800	-2.58149100	1.16062400
C	1.91907600	-0.69280500	-1.57641800
H	0.98797300	-2.71886200	-1.46852000
C	2.50390500	0.11858400	-0.57119000
H	2.78047500	-0.22195900	1.61767700
H	1.82131000	-0.43532600	-2.62290500
H	2.92213900	1.10598800	-0.71561000
C	-2.50391900	0.11835100	0.57106900
C	-2.42329600	-0.57767600	-0.66063000
C	-1.91904300	-0.69287400	1.57639900
H	-2.92225700	1.10572900	0.71536700
C	-1.77426800	-1.81585200	-0.42182500
H	-2.78040300	-0.22245600	-1.61776800
C	-1.46516500	-1.88821700	0.96542100
H	-1.82133600	-0.43527500	2.62286200
H	-1.57607500	-2.58179900	-1.16043700
H	-0.98767800	-2.71882300	1.46873400
C	0.29583400	1.46369100	1.67443900
H	-0.68088100	1.96438500	1.77916900
C	-0.29593700	1.46380400	-1.67433900
H	-0.43896700	0.94103500	-2.63560700
H	0.68070300	1.96470700	-1.77879600
H	0.43917600	0.94081900	2.63560400
C	-1.37585400	2.55319500	-1.53131700
C	1.37549700	2.55333100	1.53134700
H	2.39121200	2.14030800	1.56522600
H	1.28337000	3.09615400	0.58158800
H	1.31405400	3.30486300	2.33250500
H	-1.31439300	3.30486700	-2.33234100
H	-2.39147200	2.13995500	-1.56548900

H	-1.28405400	3.09588500	-0.58145000
Hf	0.00000200	-0.04338200	-0.00002000

Al_7_II

E(B3LYP/BS1) = -886.683824 au

H(B3LYP/BS1) = -886.289166 au

G(B3LYP/BS1) = -886.368359 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1127.468763 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1126.732319 au

C	-1.36243800	-2.35847900	-0.34662500
C	1.11473400	-2.42390000	-0.31861300
C	-0.14061100	-3.03174900	-0.31986800
H	1.99240100	-3.06925400	-0.34409400
H	-0.16863400	-4.11398900	-0.35005100
H	-2.27231300	-2.95658300	-0.38920100
C	-0.72478600	1.02994700	2.24816000
C	0.26183800	0.12407300	2.38983800
N	1.35706500	-1.10455600	-0.31274500
N	-1.53158300	-1.02873700	-0.34579300
C	2.73584000	-0.67705100	-0.26504100
C	3.22774800	0.17924900	-1.25719300
C	3.57445900	-1.10783500	0.77112700
C	4.55696400	0.60223200	-1.20904800
H	2.58477600	0.48396900	-2.07812600
C	4.90394600	-0.68384800	0.80809200
H	3.18657200	-1.76445400	1.54553300
C	5.39625800	0.17318900	-0.17798200
H	4.93875100	1.25645400	-1.98697300
H	5.55139700	-1.02110900	1.61186800
H	6.42998600	0.50290700	-0.14556400
C	-2.87785200	-0.51521400	-0.29914000
C	-3.77021800	-0.95080900	0.69056600
C	-3.28379800	0.44243400	-1.23686100
C	-5.06631000	-0.43444300	0.73091000
H	-3.44830100	-1.68080200	1.42869000
C	-4.57986500	0.95702700	-1.18472100
H	-2.60318800	0.75316000	-2.02463700
C	-5.47266000	0.52092800	-0.20303500
H	-5.75487600	-0.77611800	1.49783100
H	-4.89435700	1.68973200	-1.92165800
H	-6.48054500	0.92243800	-0.16719700
H	1.30827000	0.42553000	2.39664500
H	0.05309300	-0.92360000	2.59617100
H	-0.49718000	2.08398800	2.10409300
H	-1.77312500	0.74425000	2.30516400
C	0.02508900	2.00768700	-0.87160400
H	-0.98402900	2.43714400	-0.82395400
H	0.27335400	1.92446600	-1.94132200
C	1.01050100	2.90853500	-0.17862900
C	0.69392000	3.96651200	0.57657300
H	1.45900700	4.57563600	1.04881000
H	-0.33729400	4.28613100	0.71892900
H	2.06372200	2.66119800	-0.31308800
Al	-0.05710900	0.16315700	-0.17227200

Ga_7_II

E(B3LYP/BS1) = -886.724246 au

H(B3LYP/BS1) = -886.329833 au

G(B3LYP/BS1) = -886.410510 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2809.879479 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2809.084915 au

C	-1.35899200	-2.37442300	-0.27403800
C	1.12420500	-2.44011100	-0.25054400
C	-0.13431800	-3.04173900	-0.22506200
H	1.99740100	-3.09192800	-0.25790800
H	-0.16290600	-4.12440900	-0.21632200
H	-2.26508500	-2.97928000	-0.29586300
C	-0.73167400	0.97448100	2.35924300
C	0.27930500	0.09553400	2.48296800
N	1.37760500	-1.12528200	-0.29405200
N	-1.53935200	-1.04846000	-0.32195200
C	2.75364500	-0.69571500	-0.26803400
C	3.22593300	0.16251300	-1.26824200
C	3.61121300	-1.12399800	0.75339900
C	4.55444100	0.58886800	-1.24390100
H	2.56801200	0.46512300	-2.07832700
C	4.94013300	-0.69691800	0.76629900
H	3.23796100	-1.77775400	1.53716900
C	5.41313500	0.16114300	-0.22819900
H	4.92072800	1.24427600	-2.02825900
H	5.60206300	-1.03157200	1.55929400
H	6.44645100	0.49339800	-0.21395300
C	-2.88360000	-0.53428500	-0.29635200
C	-3.79070300	-0.96080000	0.68351100
C	-3.27488900	0.41568400	-1.24801000
C	-5.08701500	-0.44360300	0.69936500
H	-3.48008300	-1.68216500	1.43467700
C	-4.57094100	0.93144500	-1.22017600
H	-2.58201500	0.71934700	-2.02812100
C	-5.47894500	0.50368600	-0.24864700
H	-5.78682000	-0.77763300	1.45944100
H	-4.87374600	1.65814300	-1.96788700
H	-6.48699400	0.90598200	-0.23136900
H	1.31698700	0.42418100	2.48648000
H	0.10025000	-0.96165600	2.66635100
H	-0.53577200	2.03645100	2.23227500
H	-1.77162600	0.66035600	2.41323700
C	0.02278300	2.02908600	-0.81319000
H	-0.98950900	2.44138200	-0.73326300
H	0.26080700	1.97403100	-1.88537100
C	1.01521800	2.89877400	-0.09419500
C	0.69887100	3.94592500	0.67464500
H	1.46412900	4.54412600	1.16028100
H	-0.33196700	4.26510500	0.81921700
H	2.06616700	2.64446700	-0.23027100
Ga	-0.04996900	0.15461100	-0.18498400

In_7_II

E(B3LYP/BS1) = -886.526989 au

H(B3LYP/BS1) = -886.133298 au

G(B3LYP/BS1) = -886.216688 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1075.156432 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1074.446516 au

C	-1.38260200	-2.43496200	-0.29080300
C	1.13125200	-2.50995700	-0.27772300
C	-0.14401500	-3.08254400	-0.26790300
H	1.97627300	-3.19967500	-0.27392000
H	-0.17620700	-4.16567800	-0.26990300
H	-2.26762500	-3.07252800	-0.29441000
C	-0.67902600	1.08560500	2.38296700
C	0.31255300	0.19241100	2.55873900
N	1.44479600	-1.21062200	-0.31287200
N	-1.61536100	-1.11904400	-0.32891300
C	2.82854500	-0.83317300	-0.23582900
C	3.33409400	0.10570200	-1.14539100
C	3.66801900	-1.36780700	0.75141800
C	4.67006100	0.50062200	-1.07005700
H	2.69534500	0.49186100	-1.93636200
C	5.00520200	-0.97239100	0.81524100
H	3.27263300	-2.07623200	1.47426800
C	5.50882400	-0.03725700	-0.09079200
H	5.05822700	1.21705400	-1.78780900
H	5.64995200	-1.39096600	1.58225400
H	6.54837000	0.27023200	-0.03538600
C	-2.96961000	-0.65061800	-0.25381600
C	-3.85409300	-1.14816800	0.71421900
C	-3.39885400	0.34615800	-1.14107000
C	-5.16014500	-0.65988300	0.77826200
H	-3.51679200	-1.90010700	1.42237900
C	-4.70379500	0.83337600	-1.06522000
H	-2.72755100	0.70592300	-1.91775900
C	-5.58782500	0.33146100	-0.10713200
H	-5.83988600	-1.05022400	1.52980400
H	-5.03261700	1.59521600	-1.76556700
H	-6.60327600	0.71091600	-0.05115400
H	1.35704600	0.49892500	2.57545100
H	0.10894400	-0.85763800	2.75698400
H	-0.46235300	2.14240400	2.23909600
H	-1.72540500	0.78933600	2.42577800
C	0.08167200	2.30358700	-0.93615600
H	-0.93153800	2.71710700	-0.90577600
H	0.38442400	2.23751600	-1.98837100
C	1.04198600	3.13029900	-0.13877300
C	0.69816200	4.12920900	0.68282000
H	1.44650700	4.70177500	1.22246500
H	-0.33811900	4.43582800	0.81473100
H	2.09844700	2.88707400	-0.25709900
In	-0.04455700	0.26631700	-0.24582000

Sc 8 II

E(B3LYP/BS1) = -931.179234 au

H(B3LYP/BS1) = -930.786473 au

G(B3LYP/BS1) = -930.865676 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1645.766874 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1645.019816 au

C	-1.25016200	-2.04188400	-1.31007200
C	1.23389700	-2.06368800	-1.30891600
C	-0.01255700	-2.57727500	-1.67475200
H	2.11310300	-2.67153200	-1.53064500
H	-0.02116100	-3.51883500	-2.21114300
H	-2.13800400	-2.63677200	-1.53248300
C	0.05906200	1.48643400	2.33511500
C	0.03108700	0.14120400	2.21735800
N	1.44864600	-0.89995700	-0.68589800
N	-1.45237500	-0.87542500	-0.68459700
C	2.73437900	-0.63148100	-0.13047100
C	3.33364000	0.61727400	-0.36593300
C	3.37539900	-1.55967100	0.70805400
C	4.55722700	0.93273500	0.23093700
H	2.88137200	1.30633800	-1.07532900
C	4.60250800	-1.24095900	1.28710800
H	2.90269000	-2.51669900	0.91119100
C	5.19364900	0.00571600	1.05666700
H	5.02105400	1.89376500	0.02946700
H	5.09558400	-1.96596500	1.92789700
H	6.14749200	0.24836500	1.51444500
C	-2.74367100	-0.61008900	-0.13125700
C	-3.34688700	-1.51942300	0.75422600
C	-3.39146700	0.60101100	-0.42436900
C	-4.58204300	-1.21924400	1.32676600
H	-2.83902500	-2.44924300	0.99569400
C	-4.62383800	0.89843900	0.16306800
H	-2.97008200	1.27729200	-1.16419800
C	-5.22074700	-0.00906500	1.03891300
H	-5.04416200	-1.93039100	2.00505700
H	-5.12452300	1.82998600	-0.08350000
H	-6.18088200	0.22055300	1.49023000
H	0.94901500	-0.44368400	2.20608900
H	-0.90564100	-0.41068800	2.26717500
H	0.99658600	2.03259300	2.39835400
H	-0.85010700	2.06498300	2.47000900
C	0.02030000	1.89524500	-2.25912200
H	-1.04276900	1.73151400	-2.46309700
H	0.66997500	1.70578800	-3.10865500
C	0.38724900	2.84538700	-1.28680800
C	-0.34195500	3.08119800	-0.12794100
H	0.03134100	3.76954500	0.62169600
H	-1.42366800	2.92737500	-0.11878500
H	1.41413200	3.21377300	-1.30648100
Sc	0.01206500	0.59802000	-0.34480800

La_8_II

E(B3LYP/BS1) = -915.958521 au

H(B3LYP/BS1) = -915.567409 au

G(B3LYP/BS1) = -915.651026 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -916.661181 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -915.901832 au

C	-1.30058100	-2.73596000	-0.88230400
C	1.18797600	-2.76272100	-0.87812500
C	-0.06169100	-3.35798500	-1.07143000

H	2.06393000	-3.41343400	-0.94287800
H	-0.07216900	-4.41243100	-1.32167100
H	-2.18974000	-3.36920600	-0.94294300
C	0.15730300	1.81965900	2.68183900
C	0.06084300	0.47616200	2.71910500
N	1.40582000	-1.47348700	-0.61680400
N	-1.48833700	-1.44223000	-0.62862900
C	2.66657500	-1.01784600	-0.17241900
C	3.13758900	0.21561000	-0.67394500
C	3.39815500	-1.66310700	0.84462100
C	4.31544600	0.78401900	-0.17122300
H	2.65754200	0.66000600	-1.54795800
C	4.57647900	-1.09597800	1.32359200
H	3.02960700	-2.59828600	1.25685700
C	5.03470300	0.13171800	0.82801500
H	4.68015100	1.71868500	-0.58718700
H	5.13893300	-1.60969200	2.09796500
H	5.95178000	0.56602400	1.21320900
C	-2.73505200	-0.95481000	-0.17996500
C	-3.46977700	-1.57069800	0.85279100
C	-3.18661600	0.28141700	-0.69274600
C	-4.63022600	-0.97172300	1.33718700
H	-3.11663900	-2.50807100	1.27341800
C	-4.34700900	0.88155900	-0.18651800
H	-2.71164300	0.70010500	-1.58150100
C	-5.06793300	0.25869300	0.83040000
H	-5.19464100	-1.46302400	2.12457300
H	-4.69729400	1.81694900	-0.61311700
H	-5.97098200	0.71778700	1.21989800
H	0.94728500	-0.15670200	2.76070300
H	-0.89947000	-0.02298300	2.84605100
H	1.12047900	2.32273700	2.65779400
H	-0.71927800	2.45846300	2.74680900
C	0.05495900	2.22331500	-2.24156000
H	-1.02289500	2.22395300	-2.44383500
H	0.65337300	2.08430300	-3.13946900
C	0.52499400	3.12259800	-1.24268600
C	-0.15722600	3.46322800	-0.09317900
H	0.28969200	4.12174400	0.64365600
H	-1.24530400	3.37159600	-0.04518500
H	1.58151900	3.39696800	-1.28538600
La	-0.01140500	0.50248500	-0.26772800

Y_8_II

E(B3LYP/BS1) = -922.673905 au

H(B3LYP/BS1) = -922.283069 au

G(B3LYP/BS1) = -922.282125 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -923.3956704 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -922.6376597 au

C	-1.26417600	-2.44494400	-1.07717400
C	1.22124600	-2.47021600	-1.06710000
C	-0.02606100	-3.03904800	-1.33830100
H	2.10043200	-3.10693700	-1.18995600
H	-0.03521700	-4.05794100	-1.70739700
H	-2.15347100	-3.06682700	-1.20348000

C	0.06961000	1.56641200	2.49315900
C	0.02297200	0.21931900	2.41677600
N	1.43089900	-1.21759300	-0.65634200
N	-1.45728000	-1.18797600	-0.66944400
C	2.69437200	-0.82031700	-0.14985100
C	3.18570300	0.44825300	-0.51697700
C	3.40581300	-1.58582700	0.79302300
C	4.36629000	0.94131800	0.05129800
H	2.70675700	0.99524200	-1.32917000
C	4.58907900	-1.09244500	1.33781000
H	3.01893100	-2.55315500	1.10115700
C	5.06838000	0.17355600	0.97879700
H	4.74733900	1.91034800	-0.25730400
H	5.13712000	-1.69444100	2.05677300
H	5.98855300	0.55014100	1.41416900
C	-2.72132700	-0.78578100	-0.16299700
C	-3.41741800	-1.54072000	0.79960700
C	-3.23378700	0.46673300	-0.55294700
C	-4.60388500	-1.05266900	1.34274300
H	-3.01549300	-2.49659000	1.12392600
C	-4.41768700	0.95526500	0.01137200
H	-2.76914600	1.00720000	-1.37669700
C	-5.10315000	0.19819700	0.96018600
H	-5.13852800	-1.64723500	2.07779200
H	-4.81367700	1.91204700	-0.31599400
H	-6.02565900	0.57160200	1.39333700
H	0.93260400	-0.38069900	2.42420100
H	-0.92070700	-0.32068100	2.48567900
H	1.01389600	2.10301400	2.53443200
H	-0.83108800	2.16369400	2.60287400
C	0.05331000	2.05585500	-2.26517100
H	-1.01282500	1.96090100	-2.49882400
H	0.69729800	1.92601800	-3.13103600
C	0.43102300	2.96844000	-1.25045300
C	-0.30002200	3.21612800	-0.09819400
H	0.07937600	3.89584600	0.65665700
H	-1.38404900	3.07382600	-0.09476700
H	1.46639200	3.31554000	-1.25658200
Y	0.00702900	0.52597500	-0.31956200

TS_{Al-7}

E(B3LYP/BS1) = -886.636160 au

H(B3LYP/BS1) = -886.242976 au

G(B3LYP/BS1) = -886.319403 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1127.423532 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1126.689799 au

C	-1.14209700	-2.34373600	-0.74889300
C	1.33963500	-2.27066200	-0.77433000
C	0.11190000	-2.86406800	-1.07356600
H	2.24471500	-2.78533900	-1.09639800
H	0.13483100	-3.81156000	-1.59738200
H	-2.02306500	-2.90596300	-1.05835700
C	-0.15035900	2.00415000	1.29703400
C	0.02878300	0.89318000	2.20342900
C	0.08443500	1.63079700	-0.90739400

H	1.15143400	1.84722100	-1.01759100
H	-0.15936300	0.77740200	-1.57179400
H	-1.14551400	2.40402900	1.12619900
H	0.64392500	2.72406900	1.12595000
N	1.52863800	-1.11856800	-0.11523100
N	-1.37957400	-1.20747600	-0.07900800
C	-2.74660300	-0.76864000	0.06312000
C	-3.52503000	-0.51490300	-1.07389800
C	-3.28515400	-0.57656700	1.34135200
C	-4.84131000	-0.07403000	-0.92714600
H	-3.09817700	-0.65413600	-2.06349700
C	-4.60070100	-0.13025300	1.47778400
H	-2.69308100	-0.81821600	2.21929200
C	-5.37961100	0.12281000	0.34632300
H	-5.44300900	0.11871600	-1.81025700
H	-5.02036500	0.00430800	2.47017400
H	-6.40312700	0.46729600	0.45681500
C	2.87861000	-0.62410300	0.01877300
C	3.63779700	-0.33585300	-1.12241900
C	3.41908900	-0.42103400	1.29424000
C	4.93871200	0.15042600	-0.98270200
H	3.20724500	-0.48200200	-2.10930900
C	4.71892500	0.07107900	1.42355100
H	2.84159900	-0.68668800	2.17494800
C	5.47966300	0.35807200	0.28783100
H	5.52575100	0.37115100	-1.86910100
H	5.14100700	0.21508300	2.41358900
H	6.49109600	0.73817600	0.39279100
H	-0.83855100	0.63163100	2.80827400
H	0.97861000	0.85305300	2.73461700
Al	0.04911400	-0.08006000	0.44595800
C	-0.78132900	2.77027500	-1.29958000
H	-1.83637600	2.53960100	-1.44665500
C	-0.35709600	4.03014400	-1.45315800
H	-1.04017200	4.82788200	-1.72776900
H	0.68909300	4.30487300	-1.33442800

TS_{Al-7a}

E(B3LYP/BS1) = -886.676961 au

H(B3LYP/BS1) = -886.283549 au

G(B3LYP/BS1) = -886.358583 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1127.460388 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1126.724517 au

C	1.28516800	-2.48916000	-0.05184500
C	-1.18550200	-2.50418300	-0.21797800
C	0.05813500	-3.13523500	-0.19932000
H	-2.07162100	-3.13277700	-0.30511600
H	0.07085600	-4.21420400	-0.29182300
H	2.18570000	-3.10316800	-0.04782800
C	0.26144800	2.57780100	-1.73742100
C	0.41079900	1.19582400	-1.79108700
Al	0.02273300	0.08705400	0.04117800
C	-0.33323400	1.46028500	1.48396800
H	-1.41211300	1.33978300	1.64582200
H	0.19646900	1.13389400	2.38494400

H	1.10890700	3.22437900	-1.54217700
H	-0.62539500	3.06592600	-2.12646400
N	-1.40413000	-1.18399700	-0.14513000
N	1.46888500	-1.17152500	0.10490300
C	2.82101400	-0.67958600	0.15477200
C	3.21968000	0.14727400	1.21326800
C	3.72930900	-0.99398800	-0.86615100
C	4.52165500	0.64883800	1.25096700
H	2.52891400	0.35834800	2.02450900
C	5.03107100	-0.49306100	-0.81655600
H	3.41290700	-1.61699000	-1.69843200
C	5.42950500	0.33039800	0.23848000
H	4.83004000	1.27551300	2.08251500
H	5.73066900	-0.74278700	-1.60861300
H	6.44233200	0.71955000	0.27306600
C	-2.77061400	-0.73669800	-0.06170600
C	-3.62631400	-1.25461800	0.91990700
C	-3.23894700	0.24405100	-0.94546200
C	-4.94359600	-0.80221400	1.00325200
H	-3.25420200	-1.99177400	1.62585400
C	-4.55626000	0.69617200	-0.85112100
H	-2.59182100	0.61901500	-1.73343800
C	-5.41143800	0.17441100	0.12156700
H	-5.60066800	-1.20833100	1.76639600
H	-4.91773000	1.44469500	-1.55003700
H	-6.43603900	0.52607600	0.19141200
H	1.44164400	0.83407100	-1.84540100
H	-0.29632200	0.65102000	-2.42077800
C	0.01577200	2.82134900	1.08032800
C	-0.76146400	3.62669900	0.31249700
H	-1.78771700	3.35557200	0.07394700
H	-0.45357200	4.63705300	0.06133200
H	1.01283800	3.17592200	1.34441400

TS_{Ga-7}

E(B3LYP/BS1) = -886.664687 au

H(B3LYP/BS1) = -886.271819 au

G(B3LYP/BS1) = -886.349139 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2809.816183 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2809.024876 au

C	-1.39630500	-2.19816300	-0.81824800
C	1.09139800	-2.30525600	-0.75413000
C	-0.16789300	-2.79986700	-1.09928800
H	1.96271100	-2.88612800	-1.05590000
H	-0.19483200	-3.74333900	-1.63021800
H	-2.29795300	-2.70453600	-1.16207900
C	0.01041300	2.08075000	1.21166400
C	-0.08892300	0.99577700	2.16692500
C	-0.10456900	1.63709800	-1.06611900
H	0.42589800	0.88378700	-1.66786900
H	-1.17794400	1.58720000	-1.27592800
H	-0.85124900	2.71166600	1.01613700
H	0.97082800	2.54507600	1.00988400
N	1.35326700	-1.18254200	-0.07342800
N	-1.59501300	-1.05468300	-0.15169600

C	-2.93734500	-0.54397100	-0.03780300
C	-3.69089000	-0.28121900	-1.18907500
C	-3.48024400	-0.30044200	1.22973200
C	-4.98864000	0.21845700	-1.06698500
H	-3.25824700	-0.45649000	-2.17027600
C	-4.77626800	0.20490400	1.34114900
H	-2.90785400	-0.54665500	2.11942500
C	-5.53175600	0.46558300	0.19530500
H	-5.57077900	0.41980700	-1.96117400
H	-5.20026900	0.37973800	2.32539500
H	-6.54038600	0.85649700	0.28646500
C	2.72508200	-0.77621200	0.08865200
C	3.54730900	-0.60934600	-1.03361700
C	3.23094000	-0.53615200	1.37207900
C	4.87379700	-0.20805300	-0.86646400
H	3.14684300	-0.78369000	-2.02867200
C	4.55644200	-0.12884200	1.52850800
H	2.60483700	-0.71264200	2.24188900
C	5.37918800	0.03699500	0.41190000
H	5.50897900	-0.08266500	-1.73820600
H	4.94965500	0.04301900	2.52595400
H	6.41048000	0.35148300	0.53817800
H	-1.02266900	0.91936900	2.72044200
H	0.80663400	0.79681600	2.75259900
Ga	-0.08959500	-0.03451800	0.43696600
C	0.46612800	2.97469600	-1.35667000
H	-0.17623600	3.82872000	-1.14255100
C	1.69170400	3.19633400	-1.84880600
H	2.04995700	4.20290900	-2.04042800
H	2.37386500	2.38225600	-2.08539500

TS_{Ga-7a}

E(B3LYP/BS1) = -886.715075 au

H(B3LYP/BS1) = -886.321796 au

G(B3LYP/BS1) = -886.397925 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2809.868113 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2809.074171 au

C	-1.25871600	-2.50438700	0.07442300
C	1.21856900	-2.50200800	0.24486000
C	-0.02446100	-3.13522300	0.23179800
H	2.10310900	-3.13117300	0.34359000
H	-0.03062200	-4.21309000	0.33760300
H	-2.15015100	-3.13167000	0.07206600
C	-0.33290800	2.61644700	1.71986700
C	-0.41751300	1.22504200	1.79885000
C	0.34126000	1.47767800	-1.48375100
H	1.42743600	1.39663400	-1.60326300
H	-0.15589800	1.10795400	-2.38510600
H	-1.21724300	3.21488500	1.53417500
H	0.51891400	3.14930400	2.12807000
N	1.44294100	-1.18561100	0.15449300
N	-1.46416000	-1.19334700	-0.09445300
C	-2.81892500	-0.71655200	-0.15173100
C	-3.21733200	0.11406200	-1.20755100
C	-3.73373000	-1.05007000	0.85716000

C	-4.52475900	0.59930200	-1.25538000
H	-2.52046500	0.34045900	-2.00960600
C	-5.04115200	-0.56487000	0.79779900
H	-3.41803400	-1.67439100	1.68861700
C	-5.43922100	0.26146800	-0.25486900
H	-4.83257900	1.22843000	-2.08532800
H	-5.74535400	-0.82889000	1.58109900
H	-6.45643500	0.63823100	-0.29703100
C	2.80515900	-0.73621000	0.06224700
C	3.67726600	-1.30146500	-0.87838100
C	3.25743900	0.29384800	0.89741800
C	4.99395700	-0.84839900	-0.96670200
H	3.31846100	-2.07517700	-1.55120000
C	4.57398200	0.74600700	0.79788400
H	2.59625500	0.70971500	1.65253900
C	5.44576900	0.17585400	-0.13213900
H	5.66300000	-1.29128700	-1.69836000
H	4.92201100	1.53354300	1.45980100
H	6.46996200	0.52783400	-0.20616000
H	-1.43158100	0.82474200	1.87864900
H	0.31415900	0.73066900	2.44075600
C	-0.08805500	2.81128300	-1.08806400
C	0.62738100	3.64233000	-0.28400700
H	1.66164900	3.42034500	-0.03090100
H	0.27174600	4.63975500	-0.04516000
H	-1.09416100	3.11730000	-1.37607800
Ga	-0.01063600	0.09012200	-0.02991700

TS_{In-7}

E(B3LYP/BS1) = -886.4617281 au

H(B3LYP/BS1) = -886.069859 au

G(B3LYP/BS1) = -886.150053 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1075.084103 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1074.376176 au

C	-1.20111000	-2.40018300	-0.70389900
C	1.32074800	-2.35498300	-0.72365500
C	0.06724800	-2.91909100	-0.98341700
H	2.19046700	-2.93415200	-1.03599400
H	0.08108300	-3.89270200	-1.45874000
H	-2.05472100	-3.00909800	-1.00387300
C	-0.08009400	2.39196800	1.00967200
C	0.02064900	1.45773900	2.11776800
C	0.13381100	1.77981100	-1.24834800
H	1.21117700	1.94069500	-1.33526800
H	-0.14622200	0.88486300	-1.82839000
H	-1.04446900	2.81563400	0.74977800
H	0.76469400	3.01416300	0.73312300
N	1.59267900	-1.19208100	-0.12229000
N	-1.50358100	-1.24755400	-0.09684400
C	-2.87886600	-0.84890200	0.00528300
C	-3.72038100	-0.87923800	-1.11512000
C	-3.37253600	-0.39945800	1.23737100
C	-5.05074900	-0.47548800	-0.99342700
H	-3.33018700	-1.19653200	-2.07808800
C	-4.70180600	0.00933100	1.34777600

H	-2.73168900	-0.41680700	2.11595600
C	-5.54409800	-0.02873400	0.23403100
H	-5.69808400	-0.50087200	-1.86490000
H	-5.08229300	0.34224700	2.30877700
H	-6.57852500	0.28814500	0.32267000
C	2.95691100	-0.75184800	-0.03495000
C	3.78127400	-0.74346200	-1.16820400
C	3.45554600	-0.30394500	1.19555600
C	5.10101900	-0.30225800	-1.06123900
H	3.38511800	-1.05964200	-2.12906800
C	4.77394000	0.14216400	1.29123100
H	2.82823300	-0.34939100	2.08273800
C	5.59978100	0.14300700	0.16452900
H	5.73521700	-0.29712200	-1.94265100
H	5.15926500	0.47408500	2.25065400
H	6.62572300	0.48912000	0.24186200
H	-0.87167200	1.35237900	2.73347400
H	0.95520300	1.46408500	2.67636000
In	0.02700600	0.03643100	0.47472200
C	-0.68311500	2.92466200	-1.68635200
H	-1.73317500	2.71533900	-1.89104900
C	-0.23373500	4.18201700	-1.81692200
H	-0.88821000	4.98801100	-2.13368600
H	0.80946500	4.44121100	-1.64723200

TS_{In-7a}

E(B3LYP/BS1) = -886.516791 au

H(B3LYP/BS1) = -886.124134 au

G(B3LYP/BS1) = -886.202128 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1075.142695 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1074.43278 au

C	-1.22906600	-2.58712100	0.05711400
C	1.27887200	-2.56202500	0.21896900
C	0.02714100	-3.18320000	0.19595900
H	2.14541900	-3.21750100	0.31718800
H	0.03203800	-4.26278800	0.28928000
H	-2.09017600	-3.25708400	0.05887700
C	-0.52168700	2.86249600	1.68301700
C	-0.49892800	1.47191900	1.84098100
C	0.40439700	1.75447700	-1.58935600
H	1.49827300	1.73604100	-1.61364900
H	-0.01299700	1.36010300	-2.51865100
H	-1.45375900	3.36891800	1.45964100
H	0.25129500	3.47749700	2.13011900
N	1.54432600	-1.25396500	0.14817600
N	-1.50257500	-1.28828000	-0.09684500
C	-2.87376000	-0.87359500	-0.13442400
C	-3.29590400	0.01299100	-1.13557400
C	-3.78786400	-1.30809200	0.83675800
C	-4.62014500	0.45100400	-1.16970100
H	-2.60079900	0.31728200	-1.91502200
C	-5.11224000	-0.87014600	0.79140000
H	-3.45747700	-1.96970300	1.63263800
C	-5.53209500	0.01025600	-0.20777800
H	-4.94253400	1.12338500	-1.95929400

H	-5.81354600	-1.21207600	1.54676400
H	-6.56268700	0.34992600	-0.23758800
C	2.91325000	-0.83565800	0.08096200
C	3.81570400	-1.45105100	-0.79881300
C	3.34709400	0.23146000	0.88034400
C	5.13845100	-1.01172200	-0.85959800
H	3.47587700	-2.25145500	-1.44974600
C	4.66977000	0.66991100	0.80835200
H	2.66303300	0.68551000	1.59403700
C	5.56988000	0.04862600	-0.05982500
H	5.82930000	-1.49346600	-1.54509300
H	4.99975900	1.48684100	1.44335400
H	6.59909500	0.38935000	-0.11382900
H	-1.47854600	0.99412000	1.92949200
H	0.25859800	1.07067700	2.51670700
C	-0.16121000	3.01144300	-1.15924800
C	0.41373300	3.85190100	-0.24841800
H	1.44850800	3.71218000	0.05571000
H	-0.02607300	4.81974900	-0.03041800
H	-1.16648900	3.24952200	-1.50839500
In	0.00896500	0.18684600	-0.05363600

TS_{La-8}

E(B3LYP/BS1) = -915.907267 au

H(B3LYP/BS1) = -915.517794 au

G(B3LYP/BS1) = -915.599578 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -916.624268 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -915.862559 au

C	1.38054000	-3.03559100	-0.35279000
C	-1.10790800	-3.13634200	-0.35868800
C	0.16295900	-3.71730100	-0.43569900
H	-1.96300600	-3.81577600	-0.30759500
H	0.20726400	-4.79864900	-0.49401300
H	2.28757300	-3.64334400	-0.29797700
C	0.00287400	2.84903700	-1.56253500
C	-0.01317100	1.72896600	-2.40603000
C	-0.05727600	2.61972800	0.77349200
H	-1.05039100	2.24713700	1.09442400
H	0.74637900	2.06793300	1.31197000
H	0.92021800	3.41112400	-1.42202400
H	-0.89928300	3.42394100	-1.38259500
N	-1.36284600	-1.82928400	-0.33666700
N	1.53253800	-1.71070800	-0.32836300
C	2.75828400	-1.11748200	0.04544200
C	3.49909800	-1.53391500	1.16938300
C	3.17364700	0.03803400	-0.65388700
C	4.63212300	-0.82474700	1.56037100
H	3.17043600	-2.40161300	1.73427900
C	4.30608000	0.75213800	-0.24067300
H	2.69456600	0.29594800	-1.60014400
C	5.03473200	0.32398500	0.86708700
H	5.20103300	-1.16282200	2.42163300
H	4.62913100	1.62085400	-0.80681600
H	5.91585000	0.87148300	1.18610000
C	-2.63511400	-1.33063200	0.01793100

C	-3.35682600	-1.79584500	1.13482500
C	-3.12789100	-0.21415700	-0.69455800
C	-4.54498600	-1.17172200	1.50735500
H	-2.97076600	-2.63293600	1.70951800
C	-4.31658300	0.41421400	-0.30085500
H	-2.65807800	0.07220300	-1.63741700
C	-5.02448400	-0.06100600	0.80138900
H	-5.09752200	-1.54666000	2.36400900
H	-4.69772000	1.25200900	-0.87742800
H	-5.94840400	0.42016100	1.10594100
H	0.89136800	1.46771700	-2.95765200
H	-0.94378700	1.46481900	-2.91165600
La	0.01282600	0.22072200	-0.27574500
C	0.07107300	4.05863800	1.03665700
H	1.08915700	4.44832400	1.05721200
C	-0.94977400	4.91645200	1.18623200
H	-0.78137900	5.97908800	1.32864600
H	-1.98592300	4.58312100	1.18755900

TS_{La-8a}

E(B3LYP/BS1) = -915.937632 au

H(B3LYP/BS1) = -915.546732 au

G(B3LYP/BS1) = -915.625353 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -916.635252 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -915.877242 au

C	1.37763700	-2.82507000	-0.66968400
C	-1.10884000	-2.89209200	-0.66923700
C	0.15031400	-3.48049300	-0.81484800
H	-1.97483800	-3.55864600	-0.69512100
H	0.17819800	-4.54968800	-0.98953700
H	2.27842100	-3.44448900	-0.68578800
C	-0.23887500	3.19800600	-1.42560000
C	-0.03364800	2.02418000	-2.22032600
C	-0.25282800	1.43531500	2.35018100
H	-1.27024400	1.03691100	2.37424500
H	0.41809100	1.07197800	3.12326300
H	0.62077600	3.84316500	-1.26224800
H	-1.15813400	3.75307400	-1.59039900
N	-1.34963100	-1.59198400	-0.49759700
N	1.54073900	-1.51368400	-0.50933500
C	2.77871500	-0.97214400	-0.09982800
C	3.53066600	-1.50324500	0.96658900
C	3.20158600	0.23709700	-0.69503800
C	4.68056500	-0.85025900	1.40362200
H	3.19693900	-2.41556100	1.45270400
C	4.35109800	0.89312600	-0.23588100
H	2.71057100	0.58808000	-1.60395000
C	5.09013300	0.35283300	0.81482000
H	5.25778200	-1.27639600	2.21913800
H	4.68003400	1.80570000	-0.72458100
H	5.98508800	0.85503400	1.16821500
C	-2.62751300	-1.13261700	-0.10458500
C	-3.34534400	-1.70218600	0.96542600
C	-3.13463100	0.03030800	-0.72350900
C	-4.54425600	-1.13051900	1.38483900

H	-2.94810200	-2.58008500	1.46704300
C	-4.33366600	0.60494800	-0.28294800
H	-2.65612300	0.41056900	-1.62714100
C	-5.03830600	0.02810500	0.77222100
H	-5.09388800	-1.58508200	2.20402500
H	-4.72641100	1.48248700	-0.78843000
H	-5.97112100	0.46757400	1.11102400
H	0.95819600	1.90046700	-2.66218600
H	-0.83987400	1.73131300	-2.89490100
C	0.03877000	2.57701400	1.64169100
C	-0.76632100	3.15669500	0.58834300
H	-1.81182900	2.83152500	0.58175600
H	-0.69576700	4.23964700	0.54685900
H	1.01688900	3.03331500	1.81049700
La	0.03256200	0.41762800	-0.23093800

TS_{Sc-8}

E(B3LYP/BS1) = -931.137434 au

H(B3LYP/BS1) = -930.746488 au

G(B3LYP/BS1) = -930.825517 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1645.730648 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1644.978507 au

C	-1.36635200	-2.60391800	0.50405200
C	1.12372900	-2.67115400	0.51698200
C	-0.13912400	-3.25367000	0.66065800
H	1.98622700	-3.34044400	0.52791400
H	-0.16847100	-4.32343100	0.83126000
H	-2.26540300	-3.22332400	0.50165700
C	-0.00864100	2.40655700	1.71097800
C	-0.01959600	1.24815900	2.50748400
C	0.06227000	2.10793300	-0.53079100
H	1.04419600	1.68880000	-0.83274300
H	-0.76167600	1.53347600	-1.02005400
H	-0.91646500	2.98830000	1.58327700
H	0.90494900	2.97569000	1.57118700
N	1.37975200	-1.36846500	0.34362200
N	-1.54360000	-1.28802700	0.33411400
C	-2.81681100	-0.79492800	-0.08238700
C	-3.48955400	-1.34500100	-1.18567400
C	-3.36953700	0.31155000	0.58503400
C	-4.70375400	-0.80041100	-1.60011900
H	-3.04860900	-2.18032400	-1.72219600
C	-4.57946800	0.85981700	0.15255100
H	-2.89182500	0.69594900	1.48468900
C	-5.24917800	0.30432200	-0.93835800
H	-5.22115100	-1.23413300	-2.45067600
H	-5.00735800	1.70454500	0.68419200
H	-6.19289300	0.72578300	-1.27006100
C	2.69175200	-0.96245300	-0.05065900
C	3.33672200	-1.55013000	-1.15073000
C	3.31654300	0.09151300	0.63689000
C	4.59403200	-1.09383500	-1.54368900
H	2.84206100	-2.34478400	-1.70202200
C	4.57035100	0.55113700	0.22726600
H	2.85442300	0.50378000	1.53213000

C	5.21172200	-0.04103900	-0.86173400
H	5.08877000	-1.55606600	-2.39271000
H	5.05312700	1.35518700	0.77481100
H	6.18908800	0.31170100	-1.17578900
H	-0.93745800	0.96756000	3.02625600
H	0.89956100	0.94185200	3.00931200
Sc	-0.04436500	0.16615000	0.52649400
C	-0.03987200	3.52627400	-0.90869700
H	-1.04580500	3.94357200	-0.92632900
C	1.00458300	4.31911000	-1.18508500
H	0.86815600	5.36862300	-1.42551600
H	2.02625100	3.94497100	-1.19293600

TS_{Sc-8a}

E(B3LYP/BS1) = -931.165085 au

H(B3LYP/BS1) = -930.772696 au

G(B3LYP/BS1) = -930.848153 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1645.74642 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1645.000915 au

C	1.24146800	-2.35581200	-0.94414900
C	-1.23755600	-2.36648700	-0.93182600
C	0.00262800	-2.95256100	-1.19115600
H	-2.12599700	-2.99007500	-1.04861600
H	0.00525300	-3.97743600	-1.54276500
H	2.13241500	-2.97486500	-1.06625300
C	0.02903400	2.82519600	-1.47879600
C	0.01027600	1.60364700	-2.22701200
C	-0.01933200	0.88561800	2.05782400
H	-1.08112100	0.62960900	2.08815500
H	0.63423700	0.30206300	2.69874100
H	0.98043700	3.34478400	-1.39641100
H	-0.81327200	3.50060300	-1.60157800
N	-1.43572700	-1.10556700	-0.53339400
N	1.43563600	-1.09357700	-0.55082400
C	2.72266700	-0.69137100	-0.08714200
C	3.41637500	-1.43469000	0.88292100
C	3.27138000	0.51598300	-0.55326100
C	4.64345500	-0.98033400	1.36197900
H	2.98105300	-2.35281700	1.26714300
C	4.49521400	0.97168100	-0.05477000
H	2.78214100	1.05793200	-1.35979600
C	5.18380300	0.22509400	0.90141500
H	5.17619600	-1.56497300	2.10618300
H	4.91926000	1.89637900	-0.43509700
H	6.13813800	0.57476100	1.28255300
C	-2.72420500	-0.70588400	-0.06916900
C	-3.39217800	-1.42190400	0.93889700
C	-3.29736500	0.47423100	-0.57423800
C	-4.61896300	-0.96657300	1.41887000
H	-2.93859000	-2.32021000	1.34822100
C	-4.52090400	0.93069700	-0.07544800
H	-2.82415200	0.99064900	-1.40670500
C	-5.18360600	0.21205800	0.91990400
H	-5.13240500	-1.52954700	2.19271400
H	-4.96476400	1.83348900	-0.48463300

H	-6.13717600	0.56275700	1.30197200
H	0.93392400	1.30084500	-2.72347500
H	-0.88403400	1.37803500	-2.80917300
C	0.41362500	2.04981700	1.47720700
C	-0.35553700	2.83051500	0.52951500
H	-1.43865900	2.68459300	0.59036700
H	-0.09979100	3.88550000	0.52229500
H	1.46050600	2.32646600	1.60841700
Sc	-0.00879200	0.42580600	-0.35010100

TS_{V-8}

E(B3LYP/BS1) = -922.625590 au

H(B3LYP/BS1) = -922.235472 au

G(B3LYP/BS1) = -922.31557 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -923.360389 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -922.598117 au

C	-1.40288000	-2.86834900	0.32450600
C	1.08168700	-2.96301500	0.33534500
C	-0.18585500	-3.54986000	0.40966800
H	1.94131500	-3.63493000	0.27734800
H	-0.22689300	-4.63162200	0.45962200
H	-2.31215000	-3.46991400	0.25339700
C	0.03664800	2.61168200	1.61063500
C	0.00973700	1.49197200	2.46169400
C	0.09405000	2.29921400	-0.66741000
H	1.06515500	1.86312900	-0.98264000
H	-0.74526200	1.75494400	-1.16465300
H	-0.86090800	3.20446300	1.46475400
H	0.95801700	3.16007300	1.44296500
N	1.33393800	-1.65234300	0.31446800
N	-1.54847300	-1.54109000	0.30952300
C	-2.77504000	-0.93976000	-0.06888900
C	-3.50664400	-1.35221800	-1.19824600
C	-3.19914100	0.20006700	0.64503200
C	-4.64323300	-0.64668400	-1.58541300
H	-3.16795500	-2.20943200	-1.77299900
C	-4.33234300	0.91253000	0.23493000
H	-2.71325300	0.45898100	1.58644100
C	-5.05478700	0.49101000	-0.87987600
H	-5.20645200	-0.97793700	-2.45292300
H	-4.66197500	1.77428700	0.80770000
H	-5.93835800	1.03655100	-1.19560300
C	2.62007500	-1.16515300	-0.03664100
C	3.32325500	-1.63289200	-1.16190900
C	3.14680500	-0.08766100	0.70349800
C	4.53204700	-1.04131000	-1.52155800
H	2.90779500	-2.44217100	-1.75555200
C	4.35330000	0.51061900	0.32267000
H	2.67018700	0.20922000	1.63796300
C	5.04664700	0.03562100	-0.78964300
H	5.07160900	-1.41433000	-2.38713900
H	4.76014000	1.32474100	0.91519000
H	5.98647000	0.49272500	-1.08266900
H	-0.90748900	1.26787100	3.00820300
H	0.92584900	1.20790300	2.98181900

Y	-0.04378300	0.16214800	0.42132000
C	0.02794400	3.72344500	-1.02947900
H	-0.96909900	4.16298400	-1.04629600
C	1.08746600	4.50631500	-1.27780400
H	0.97100100	5.56356300	-1.49338700
H	2.10311500	4.11570400	-1.28763400

TS_{Y-8a}

E(B3LYP/BS1) = -922.655987 au

H(B3LYP/BS1) = -922.264474 au

G(B3LYP/BS1) = -922.341651 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -923.373114 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -922.616149 au

C	1.26412500	-2.63198800	-0.81065000
C	-1.21809600	-2.65554200	-0.80128500
C	0.02758800	-3.25416300	-1.00634600
H	-2.10067500	-3.29682900	-0.85982400
H	0.03662100	-4.30674500	-1.26368900
H	2.15664600	-3.25912000	-0.87243200
C	0.02423200	2.99662900	-1.48195500
C	0.02546100	1.78783600	-2.25629300
C	-0.08632600	1.16401600	2.17884400
H	-1.14607000	0.89701100	2.20852400
H	0.55372100	0.65896100	2.89610000
H	0.97242300	3.51847400	-1.37562500
H	-0.81384300	3.67419600	-1.62143500
N	-1.42144200	-1.36519500	-0.52855800
N	1.44865600	-1.33854000	-0.54054900
C	2.70558000	-0.86494100	-0.08453200
C	3.43117800	-1.51271500	0.93242200
C	3.17785900	0.36441400	-0.58634300
C	4.60752300	-0.94652600	1.41742600
H	3.05675800	-2.44418700	1.34720000
C	4.35162100	0.93355000	-0.07834400
H	2.69175900	0.81698100	-1.44998800
C	5.06729100	0.28059400	0.92368300
H	5.16489300	-1.45947500	2.19580800
H	4.71773200	1.86884500	-0.49166700
H	5.98242400	0.71545300	1.31298800
C	-2.68313100	-0.90215900	-0.07754900
C	-3.39963500	-1.54103200	0.95156700
C	-3.16726900	0.31548400	-0.59726800
C	-4.57900700	-0.97678700	1.43196300
H	-3.01628000	-2.46367200	1.37786400
C	-4.34463800	0.88222300	-0.09433300
H	-2.68500800	0.75856100	-1.46880300
C	-5.05070300	0.23878000	0.92072300
H	-5.12942900	-1.48182700	2.22037200
H	-4.72060400	1.80778800	-0.52049400
H	-5.96776700	0.67214300	1.30706300
H	0.96033300	1.52327500	-2.75509500
H	-0.85239800	1.59165800	-2.87387300
C	0.33648500	2.29856900	1.52899400
C	-0.41632700	3.01959600	0.52288100
H	-1.49674000	2.84463600	0.55408500

H	-0.19368400	4.08225000	0.50195500
H	1.37143100	2.61000700	1.68194700
Y	-0.00450300	0.40058300	-0.31202300

Al_1_IV'

E(B3LYP/BS1) = -928.052998 au

H(B3LYP/BS1) = -927.593738 au

G(B3LYP/BS1) = -927.675302 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1168.807049 au

C	-1.05883700	-2.43600200	-0.95073400
C	1.42396000	-2.36755600	-0.89545300
C	0.20443700	-2.98221500	-1.19092300
H	2.32508400	-2.96800100	-1.03697500
H	0.24059300	-3.99066900	-1.58608700
H	-1.91879100	-3.08273800	-1.13759100
N	1.60057800	-1.12509900	-0.45319400
N	-1.32553600	-1.20547300	-0.51882700
C	2.90756100	-0.75912300	-0.01825100
C	3.41811100	0.50898600	-0.33634900
C	3.69126300	-1.63211200	0.75476000
C	4.69034300	0.88394300	0.09274900
H	2.82648300	1.18917100	-0.94011000
C	4.96671300	-1.25324700	1.17290600
H	3.28491800	-2.59381300	1.05436200
C	5.47374700	0.00503300	0.84404000
H	5.07215200	1.86700600	-0.16917800
H	5.55747800	-1.93999300	1.77337200
H	6.46424700	0.30122400	1.17733700
C	-2.68184500	-0.90449500	-0.19715200
C	-3.46243500	-1.78916600	0.56478400
C	-3.24909600	0.30415700	-0.62989200
C	-4.78791500	-1.47817600	0.86767000
H	-3.01679700	-2.70469400	0.94314100
C	-4.57267600	0.61145800	-0.31632400
H	-2.65999000	0.98632400	-1.23465400
C	-5.34973200	-0.27754300	0.42946100
H	-5.37690800	-2.17150200	1.46221800
H	-4.99901400	1.54812500	-0.66500600
H	-6.38001600	-0.03392000	0.67245000
C	0.15939300	0.79336100	1.64037300
C	0.07327200	1.35433900	-1.92584800
H	0.53421800	-0.08919900	2.18508900
H	0.96430200	1.53899800	1.74883400
H	1.02942300	1.21349200	-2.45756600
C	-1.08803800	1.31771400	2.38488800
H	-0.66848500	0.89734100	-2.60184200
C	-0.20829300	2.86930600	-1.83781500
H	-0.37173800	3.28610200	-2.84384000
H	-1.91257300	0.59740900	2.29644300
H	-0.87256800	1.38957100	3.46256300
C	0.91591800	3.66593800	-1.16565900
H	0.68675600	4.73805800	-1.13259100
H	1.86014800	3.54785300	-1.71416300
H	-1.14334400	3.05228000	-1.28849000
H	1.08540700	3.33008900	-0.13572000
C	-1.57599900	2.69019000	1.90924700

H	-2.42848500	3.03983600	2.50467100
H	-0.78069600	3.44194100	1.99229200
H	-1.89557600	2.66487600	0.86058400
Al	0.09456600	0.19308500	-0.27417400

Al_1_V'

E(B3LYP/BS1) = -887.534951 au

H(B3LYP/BS1) = -887.127575 au

G(B3LYP/BS1) = -887.200632 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1128.273808 au

C	-1.14186800	-2.35856400	-0.84415600
C	1.33758700	-2.28712800	-0.86817700
C	0.11241600	-2.90668000	-1.12401600
H	2.23574800	-2.89004000	-1.01620500
H	0.13830900	-3.92235900	-1.50084300
H	-2.00845200	-3.01044100	-0.97287800
N	1.52515100	-1.03582800	-0.45059100
N	-1.38839400	-1.11833400	-0.42911300
C	2.84480800	-0.67571800	-0.04381300
C	3.38337300	0.56262400	-0.42458300
C	3.61424000	-1.53340600	0.75936600
C	4.66953000	0.92324700	-0.02535300
H	2.80126900	1.22933600	-1.05151700
C	4.90340600	-1.16950600	1.14809800
H	3.18659100	-2.47068600	1.10360900
C	5.43827400	0.05919800	0.75761400
H	5.07359300	1.88308300	-0.33549300
H	5.48322300	-1.84391000	1.77267600
H	6.43959500	0.34448200	1.06725600
C	-2.72261800	-0.81254700	-0.02740100
C	-3.44141100	-1.67222500	0.81803000
C	-3.32424000	0.37675200	-0.46429200
C	-4.74482700	-1.35501700	1.20047900
H	-2.96417600	-2.57156200	1.19681700
C	-4.62476600	0.69090400	-0.07152400
H	-2.77994600	1.03628700	-1.13239700
C	-5.34241700	-0.17322600	0.75861800
H	-5.28752600	-2.02803500	1.85895300
H	-5.08019500	1.61238200	-0.42380900
H	-6.35483400	0.07554500	1.06367300
Al	0.02795800	0.28202800	-0.28687100
C	0.06321100	1.24094300	1.45492800
C	-0.02330400	1.63331000	-1.76301600
H	-0.45973700	0.71452600	2.26627400
H	1.11197300	1.30759400	1.78706300
H	0.99779300	1.77829300	-2.15216200
C	-0.50056400	2.67965600	1.32281900
H	-0.60496300	1.31466000	-2.64121100
C	-0.54755100	3.00612800	-1.26509200
H	-0.33675700	3.78715200	-2.01220100
H	-1.59938700	2.63959700	1.26833300
H	-0.27320300	3.26248800	2.22915000
C	0.00695600	3.47297900	0.09866500
H	-0.26405200	4.52985400	0.23439100
H	1.10836200	3.44683400	0.07664100
H	-1.64540600	2.97734200	-1.18203300

Ga_1_IV'

E(B3LYP/BS1) = -928.094583 au

H(B3LYP/BS1) = -927.635493 au

G(B3LYP/BS1) = -927.718484 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2851.220313 au

C	-1.07616800	-2.44593900	-0.92293100
C	1.41523900	-2.38254200	-0.86813300
C	0.18988100	-2.98953100	-1.15873700
H	2.30878300	-2.99481300	-1.01027900
H	0.22364400	-3.99965600	-1.55030200
H	-1.93051600	-3.10021000	-1.11159900
N	1.61053700	-1.14177800	-0.43454000
N	-1.35645600	-1.21783000	-0.49817400
C	2.91872800	-0.78537100	-0.00425800
C	3.43324300	0.48343500	-0.31541400
C	3.70531400	-1.66624700	0.75780600
C	4.70927000	0.85092400	0.10828300
H	2.84016200	1.17047700	-0.91004700
C	4.98473700	-1.29488800	1.17055800
H	3.29785800	-2.62859200	1.05365600
C	5.49465100	-0.03617000	0.84806600
H	5.09287000	1.83463500	-0.14882200
H	5.57657000	-1.98822200	1.76244000
H	6.48820300	0.25410000	1.17748000
C	-2.71261000	-0.92246300	-0.18254000
C	-3.50036500	-1.81585400	0.56270300
C	-3.27835200	0.29128500	-0.60463500
C	-4.82845600	-1.50877700	0.85829300
H	-3.05807400	-2.73561100	0.93455500
C	-4.60437700	0.59457600	-0.29856900
H	-2.68444600	0.98130300	-1.19571300
C	-5.38766600	-0.30345300	0.43000500
H	-5.42176600	-2.20939800	1.43995900
H	-5.02813300	1.53526800	-0.63969200
H	-6.42001900	-0.06308400	0.66741800
C	0.16010900	0.75668300	1.69497100
C	0.06212600	1.35510100	-1.90493000
H	0.52692200	-0.13917000	2.21823200
H	0.96377200	1.49989800	1.81130100
H	1.01868000	1.20671100	-2.42988500
C	-1.09820700	1.26944000	2.42448000
H	-0.68714400	0.90108000	-2.57093700
C	-0.21021400	2.86790300	-1.79372600
H	-0.36676500	3.29634100	-2.79574000
H	-1.91846200	0.54731300	2.31740000
H	-0.89331100	1.32780200	3.50480200
C	0.91573600	3.64834000	-1.10620200
H	0.69078300	4.72055500	-1.05648600
H	1.86097100	3.53480500	-1.65358400
H	-1.14743400	3.04707700	-1.24722900
Ga	0.08599400	0.21052700	-0.23856100
H	1.08058400	3.29538100	-0.08117900
C	-1.58210400	2.64658900	1.95886000
H	-2.44346900	2.98643100	2.54678600
H	-0.78987900	3.39898900	2.06228600

H -1.88787200 2.63326300 0.90587600

Ga_1_V'

E(B3LYP/BS1) = -887.575589 au

H(B3LYP/BS1) = -887.168372 au

G(B3LYP/BS1) = -887.242529 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2810.684650 au

C	-1.15763600	-2.38798000	-0.80373500
C	1.33003400	-2.32435900	-0.82576100
C	0.09899800	-2.93698100	-1.07430000
H	2.22077600	-2.93984300	-0.96938400
H	0.12200900	-3.95645600	-1.44134700
H	-2.01991500	-3.04626200	-0.93137300
N	1.53590400	-1.07262800	-0.42484800
N	-1.41613700	-1.14730900	-0.40299200
C	2.85631900	-0.71765700	-0.02539400
C	3.39636800	0.51978500	-0.40876000
C	3.62967900	-1.57670000	0.77337400
C	4.68551900	0.87778500	-0.01737700
H	2.81201300	1.18785300	-1.03232000
C	4.92204600	-1.21556000	1.15397200
H	3.20236900	-2.51287600	1.12088100
C	5.45748800	0.01197900	0.76066900
H	5.08976500	1.83682600	-0.32992100
H	5.50408300	-1.89130600	1.77510100
H	6.46123800	0.29510500	1.06439000
C	-2.74975900	-0.84055800	-0.00947800
C	-3.48281700	-1.70574700	0.81875700
C	-3.34175600	0.35776400	-0.43654800
C	-4.78832900	-1.38587000	1.19187000
H	-3.01485000	-2.61191000	1.19266700
C	-4.64411700	0.67458000	-0.05298200
H	-2.78721600	1.02305300	-1.09050200
C	-5.37541500	-0.19564300	0.75893200
H	-5.34090900	-2.06381600	1.83701500
H	-5.09070900	1.60307000	-0.39829500
H	-6.38939800	0.05513000	1.05707000
C	0.06325800	1.21063800	1.50789100
C	-0.02499300	1.62592300	-1.73218500
H	-0.48207100	0.67853600	2.29842800
H	1.11020700	1.24915400	1.84428400
H	0.99343000	1.75369200	-2.12917100
C	-0.47530300	2.65681200	1.37460500
H	-0.62596300	1.30686000	-2.59507700
C	-0.52902400	2.99613400	-1.21289800
H	-0.31591000	3.78081400	-1.95515700
H	-1.57442900	2.63484500	1.32172200
H	-0.23591700	3.23260600	2.28201000
C	0.04464800	3.44299400	0.15034700
H	-0.20231100	4.50460400	0.29247600
H	1.14486200	3.39237300	0.12194500
H	-1.62604000	2.97756100	-1.11992200
Ga	0.02307300	0.27502900	-0.25053700

In_1_IV'

E(B3LYP/BS1) = -927.894018 au

H(B3LYP/BS1) = -927.435801 au

G(B3LYP/BS1) = -927.521263 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1116.492734 au

C	-1.08679000	-2.53295100	-0.86720300
C	1.43351100	-2.47221900	-0.78246500
C	0.19435200	-3.06956100	-1.04340100
H	2.30540000	-3.11926700	-0.91335700
H	0.23045200	-4.09669200	-1.38979500
H	-1.91561100	-3.21924600	-1.06236500
N	1.68029500	-1.22275600	-0.40612000
N	-1.41952100	-1.29893000	-0.50556200
C	3.00885200	-0.88760000	-0.03360500
C	3.53834000	0.35877800	-0.40853800
C	3.80475500	-1.75393900	0.73670600
C	4.83291100	0.71892400	-0.03787200
H	2.94064000	1.03216100	-1.01647200
C	5.10206300	-1.39021900	1.09689800
H	3.39057700	-2.69742900	1.08013400
C	5.62438300	-0.15403400	0.71219300
H	5.22617200	1.68445000	-0.34465500
H	5.69964900	-2.07159000	1.69694800
H	6.63219100	0.12988100	1.00127100
C	-2.79040500	-1.02718100	-0.25268600
C	-3.60318100	-1.92271500	0.46458500
C	-3.35067700	0.18119800	-0.70083600
C	-4.94454800	-1.62445400	0.70339100
H	-3.17071500	-2.83695200	0.86065800
C	-4.69050600	0.47562300	-0.45208900
H	-2.73924600	0.87305900	-1.27324200
C	-5.49630900	-0.42586200	0.24713600
H	-5.55552000	-2.32710000	1.26409700
H	-5.10704700	1.41143000	-0.81502100
H	-6.53945000	-0.19317600	0.44090800
C	0.10793800	0.77766100	1.97657400
C	0.06189200	1.56888000	-1.93095300
H	0.47165800	-0.13261600	2.47349100
H	0.88700100	1.53563300	2.14399800
H	1.01157600	1.41105900	-2.46364100
C	-1.20032800	1.23893700	2.64464300
H	-0.70758900	1.14796100	-2.59396600
C	-0.17512200	3.07880600	-1.75137600
H	-0.27613200	3.56361400	-2.73529900
H	-1.97452600	0.46745800	2.53377500
H	-1.04132700	1.34683900	3.72943700
C	0.93984500	3.78904000	-0.97595300
H	0.75141900	4.86619600	-0.89358800
H	1.90907500	3.66018100	-1.47551000
H	-1.13100800	3.25502400	-1.23665200
H	1.03655600	3.39108400	0.04248300
C	-1.74136100	2.56740100	2.10598600
H	-2.63853600	2.88620300	2.65015700
H	-0.99332500	3.36518200	2.19784200
H	-2.01252700	2.48951500	1.04485800
In	0.08300200	0.30330300	-0.14839900

In_1_V'

E(B3LYP/BS1) = -887.369573 au

H(B3LYP/BS1) = -886.963243 au

G(B3LYP/BS1) = -887.039670 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1075.950153 au

C	-1.10871600	-2.57745200	-0.50053400
C	1.40865700	-2.48072600	-0.50644500
C	0.17308900	-3.12499500	-0.63161300
H	2.28827700	-3.12295500	-0.60032200
H	0.21396100	-4.18876400	-0.83815700
H	-1.93851800	-3.28382100	-0.58924900
N	1.64745800	-1.18888500	-0.30283900
N	-1.43892000	-1.30747100	-0.29880000
C	2.99499100	-0.79188300	-0.07809200
C	3.48561200	0.37168800	-0.69218600
C	3.84595700	-1.52082300	0.77019700
C	4.79944600	0.78457200	-0.47529000
H	2.84066200	0.93362100	-1.36129800
C	5.16146300	-1.10578400	0.97642400
H	3.46298900	-2.39421000	1.29015300
C	5.64593900	0.04701500	0.35561000
H	5.16379300	1.68308500	-0.96600500
H	5.80416300	-1.67926300	1.63925800
H	6.66869200	0.37179800	0.52395000
C	-2.81096800	-1.00110300	-0.08247100
C	-3.61350000	-1.77375500	0.77356900
C	-3.37510200	0.11873200	-0.71475400
C	-4.95403300	-1.44317100	0.97231300
H	-3.17456800	-2.61296100	1.30556100
C	-4.71388500	0.44695400	-0.50553700
H	-2.76634400	0.71114100	-1.39160000
C	-5.51143300	-0.33298900	0.33518700
H	-5.55942900	-2.04844500	1.64195600
H	-5.13590400	1.31227900	-1.00948700
H	-6.55353600	-0.07349800	0.49816000
C	0.00604300	1.36844100	1.78979800
C	-0.06560800	1.85326100	-1.62784100
H	-0.48574400	0.81664100	2.60029500
H	1.04423900	1.52631500	2.11648500
H	0.95369600	2.11630100	-1.94670100
C	-0.68043500	2.74032300	1.58431300
H	-0.59012300	1.54778600	-2.54263300
C	-0.73696300	3.10863200	-1.01946300
H	-0.63798500	3.95567400	-1.71682800
H	-1.76798400	2.59605100	1.49522900
H	-0.54022500	3.36133100	2.48345000
C	-0.20749800	3.56363500	0.36209100
H	-0.53021100	4.60290800	0.51530800
H	0.89354300	3.59387900	0.34250200
H	-1.82043700	2.93820500	-0.92245600
In	0.04589600	0.31240800	-0.09934200

La_1_IV'

E(B3LYP/BS1) = -957.258553 au

H(B3LYP/BS1) = -956.804963 au

G(B3LYP/BS1) = -956.897421 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -957.927385 au

C	-1.22416900	-2.82748500	-0.85701100
C	1.29185600	-2.88168400	-0.68955500
C	0.02880000	-3.45544800	-0.89099500
H	2.13755000	-3.57733400	-0.72421000
H	0.01888800	-4.52287900	-1.08464300
H	-2.08782800	-3.48641200	-1.00013900
N	1.57513100	-1.60234700	-0.48211800
N	-1.47459700	-1.53540200	-0.69241600
C	2.89186400	-1.22338300	-0.14862300
C	3.40034800	-0.02407100	-0.68881100
C	3.68611100	-1.93521700	0.77222200
C	4.66267700	0.44561300	-0.31883200
H	2.83306700	0.50680900	-1.45327600
C	4.95026500	-1.46663000	1.12267800
H	3.29089700	-2.83706500	1.23091000
C	5.44438600	-0.27361200	0.58552000
H	5.03754900	1.36784100	-0.75420300
H	5.54809300	-2.02860000	1.83560200
H	6.42646400	0.09062300	0.87222000
C	-2.80375700	-1.09531400	-0.53094300
C	-3.73675400	-1.75606900	0.29279000
C	-3.18778400	0.11520200	-1.14466100
C	-5.01249900	-1.22777700	0.47747300
H	-3.44129100	-2.66642300	0.80644100
C	-4.46465500	0.64412200	-0.94186600
H	-2.50706900	0.60423500	-1.84109700
C	-5.38310700	-0.02482000	-0.13211100
H	-5.71823800	-1.75072000	1.11767200
H	-4.74244400	1.57245200	-1.43352400
H	-6.37591900	0.38580000	0.02593400
C	0.15031500	1.26474500	2.24470100
C	0.23048600	2.22789400	-1.94436300
H	1.14295500	0.90217400	2.58541400
H	0.25152600	2.36805300	2.22230800
H	1.08893500	2.02247700	-2.61320900
C	-0.90472600	0.88439500	3.29770700
H	-0.65429700	2.07625100	-2.59500100
C	0.28327400	3.70572300	-1.51238400
H	0.20711000	4.39073200	-2.37430800
H	-0.98792700	-0.21241000	3.36919800
H	-0.61550400	1.21739700	4.30945200
C	1.56125600	4.06164200	-0.73976500
H	1.59121800	5.12319800	-0.46465000
H	2.45328800	3.85017900	-1.34423900
H	-0.58555500	3.94731600	-0.87766000
H	1.64836300	3.48233800	0.19062700
C	-2.29368600	1.46218700	2.99125900
H	-3.02289300	1.20929400	3.77121100
H	-2.25174100	2.55686900	2.91794000
H	-2.69275800	1.08487500	2.03881600
La	0.06808500	0.43100200	-0.13997200

La_1_V'

E(B3LYP/BS1) = -916.732817 au

H(B3LYP/BS1) = -916.330850 au

G(B3LYP/BS1) = -916.413311 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -917.385071 au

C	-1.05914200	-2.99022100	-0.24141000
C	1.46647000	-2.86381000	-0.23987500
C	0.23408900	-3.53366800	-0.24302300
H	2.35182100	-3.50952400	-0.22317500
H	0.28829500	-4.61733700	-0.24981600
H	-1.87540100	-3.72130300	-0.22551700
N	1.67751300	-1.55501500	-0.27906600
N	-1.40025000	-1.70922300	-0.28092700
C	2.98539100	-1.04994200	-0.13879400
C	3.35434900	0.06987300	-0.91329600
C	3.90867600	-1.54709300	0.80267100
C	4.60593400	0.66792900	-0.75321800
H	2.68241400	0.43070400	-1.69248500
C	5.16064600	-0.95247500	0.94489700
H	3.62452600	-2.38099900	1.43819200
C	5.51608000	0.15867300	0.17396100
H	4.87157100	1.52353200	-1.36809500
H	5.85902100	-1.35007000	1.67682900
H	6.49011000	0.62256300	0.29803100
C	-2.75184900	-1.33774600	-0.13764400
C	-3.61793700	-1.92428700	0.80676600
C	-3.23342800	-0.26155200	-0.91219500
C	-4.92297800	-1.45815200	0.95193000
H	-3.24927400	-2.72491600	1.44161300
C	-4.53827600	0.20791200	-0.74933600
H	-2.60237400	0.16359600	-1.69307200
C	-5.39003800	-0.38909100	0.18101300
H	-5.57600800	-1.92279000	1.68622300
H	-4.89009300	1.03207100	-1.36381300
H	-6.40527000	-0.02497100	0.30769200
C	0.07205300	1.83831500	1.96702900
C	-0.10919200	2.32432800	-1.71044600
H	-0.27557500	1.41180800	2.92135300
H	1.15087300	2.05354900	2.11923100
H	0.87378400	2.76675800	-1.95181000
C	-0.66349800	3.17463700	1.70879600
H	-0.59311600	2.13083400	-2.68216500
C	-0.94741500	3.37079900	-0.92801200
H	-1.16354200	4.23647700	-1.57515200
H	-1.75289300	3.00370100	1.73227700
H	-0.47127600	3.88411800	2.53184500
C	-0.33421200	3.92260500	0.39065700
H	-0.69043800	4.95468600	0.51245400
H	0.75932200	4.00200800	0.27727300
H	-1.94567500	2.95674100	-0.68873700
La	0.03831600	0.40993400	-0.08898300

Sc_1_IV'

E(B3LYP/BS1) = -972.499244 au

H(B3LYP/BS1) = -972.044030 au

G(B3LYP/BS1) = -972.132462 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1687.057772 au

C	-1.11443000	-2.52945300	-0.98444100
C	1.39498300	-2.50210800	-0.87245100
C	0.15771300	-3.07800100	-1.18521400
H	2.27143800	-3.14105800	-1.01359800
H	0.18597900	-4.08669000	-1.58268600
H	-1.95996800	-3.18877300	-1.20066100
N	1.62095600	-1.27042300	-0.42186800
N	-1.41059600	-1.30183800	-0.56106700
C	2.92906900	-0.94058700	0.02096700
C	3.46144800	0.31861000	-0.30464800
C	3.68947000	-1.81493000	0.81725500
C	4.72750200	0.68869600	0.14877600
H	2.89504700	0.99312900	-0.94282100
C	4.95945400	-1.44239700	1.25504500
H	3.26743600	-2.77058200	1.11491900
C	5.48479600	-0.19062500	0.92500600
H	5.12498600	1.66445300	-0.11672000
H	5.53433000	-2.12886900	1.87110700
H	6.47140000	0.09844000	1.27539500
C	-2.76577200	-1.01184400	-0.24709600
C	-3.55194800	-1.88941600	0.51998100
C	-3.32645300	0.20310000	-0.67649800
C	-4.87183500	-1.56441500	0.82945100
H	-3.11312600	-2.81057500	0.89281800
C	-4.64455700	0.52587600	-0.35304100
H	-2.73902600	0.87591600	-1.29669100
C	-5.42452400	-0.35657700	0.39654900
H	-5.46599700	-2.25295400	1.42447600
H	-5.06379200	1.46680800	-0.69866600
H	-6.45090300	-0.10368200	0.64614100
C	0.09694000	1.15832400	1.75508600
C	0.12141400	1.66450700	-1.95809100
H	0.62218600	0.37973300	2.34428400
H	0.80061200	2.01285800	1.72591900
H	0.97415200	1.37760700	-2.60435100
C	-1.17578600	1.58506200	2.51079200
H	-0.76567300	1.34762100	-2.54431700
C	0.10134300	3.19837500	-1.81237500
H	-0.09062200	3.68613000	-2.78242500
H	-1.90038500	0.75662600	2.52985600
H	-0.95291000	1.80252500	3.56845200
C	1.40481200	3.77252100	-1.24305100
H	1.36797400	4.86667100	-1.17217500
H	2.25892900	3.51202000	-1.88295900
H	-0.72955400	3.50571600	-1.15978400
H	1.60968000	3.38163600	-0.23821500
C	-1.85467600	2.81962900	1.90450600
H	-2.74234900	3.11505000	2.47775400
H	-1.16712200	3.67486900	1.88673200
H	-2.17596200	2.63531900	0.87117200
Sc	0.07937800	0.26903800	-0.24721300

Sc_1_V'

E(B3LYP/BS1) = -931.981402 au

H(B3LYP/BS1) = -931.577756 au

G(B3LYP/BS1) = -931.654763 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1646.523164 au

C	-1.08667900	-2.48512400	-0.81526900
C	1.43023800	-2.37196400	-0.82700200
C	0.19584700	-2.98901600	-1.06709100
H	2.31363700	-2.99438100	-0.99703700
H	0.23977700	-4.00374000	-1.44780400
H	-1.91348100	-3.18198400	-0.98116700
N	1.65193800	-1.12463700	-0.41521300
N	-1.41196900	-1.26302800	-0.39881100
C	2.97487700	-0.76865700	-0.03983600
C	3.48308800	0.48369400	-0.42455000
C	3.77758600	-1.61414800	0.74595000
C	4.76517200	0.87467100	-0.03998100
H	2.88168900	1.13618400	-1.05298500
C	5.06276000	-1.22079800	1.11689000
H	3.37721600	-2.56413800	1.08838800
C	5.56311600	0.02381800	0.72773900
H	5.14338000	1.84458100	-0.35131000
H	5.66931800	-1.88532900	1.72658100
H	6.56175400	0.33004200	1.02551000
C	-2.75899000	-1.01254300	-0.02694300
C	-3.49603900	-1.91475600	0.75979800
C	-3.36095200	0.19482900	-0.42060400
C	-4.80961700	-1.62061200	1.12285900
H	-3.02445200	-2.82951600	1.10744900
C	-4.67129600	0.48707800	-0.04277700
H	-2.81055400	0.88732900	-1.05341900
C	-5.40355400	-0.42019100	0.72556900
H	-5.36609100	-2.32765400	1.73250200
H	-5.12251200	1.42292700	-0.36085300
H	-6.42457300	-0.19193200	1.01735500
C	0.04961600	1.62148600	1.55307400
C	-0.05374000	1.92670800	-1.75135300
H	-0.33745800	1.11198000	2.45209800
H	1.10986000	1.84921200	1.77722200
H	0.99012200	2.18237900	-2.02054400
C	-0.71501900	2.94729900	1.33840000
H	-0.51162800	1.58664500	-2.69636200
C	-0.76234900	3.21324100	-1.26523400
H	-0.64857400	4.01788400	-2.01032600
H	-1.79550000	2.74143500	1.26399200
H	-0.60649400	3.59837700	2.22152800
C	-0.29618300	3.76594100	0.09832500
H	-0.70053400	4.78272200	0.20738700
H	0.79994300	3.87852800	0.08994800
H	-1.84860500	3.03556500	-1.20136700
Sc	0.04841400	0.36003900	-0.22125700

Y_1_IV'

E(B3LYP/BS1) = -963.982663 au

H(B3LYP/BS1) = -963.528199 au

G(B3LYP/BS1) = -963.618417 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -964.680969 au

C	-1.17453600	-2.68576100	-0.84148500
C	1.34334400	-2.70538000	-0.70931300

C	0.08841000	-3.28505600	-0.93539100
H	2.19915500	-3.38375300	-0.78163300
H	0.09327000	-4.33942200	-1.19019300
H	-2.02828500	-3.35211700	-1.00003000
N	1.61172700	-1.43385700	-0.42896600
N	-1.45432000	-1.40887600	-0.59670400
C	2.93429800	-1.07298100	-0.07079500
C	3.45035400	0.14777800	-0.54403600
C	3.72184700	-1.84893200	0.79982500
C	4.72106000	0.57757900	-0.15819800
H	2.87284100	0.73906200	-1.25310400
C	4.99569200	-1.41945900	1.16671900
H	3.31696000	-2.76963100	1.21000100
C	5.50115500	-0.20489600	0.69416500
H	5.10329300	1.52093700	-0.53813300
H	5.59032000	-2.02953000	1.84161300
H	6.49060500	0.12912800	0.99234600
C	-2.80892600	-1.03751800	-0.39894200
C	-3.67486400	-1.77014200	0.43332400
C	-3.28462500	0.14137400	-1.00181100
C	-4.98477900	-1.34028700	0.63763200
H	-3.30462600	-2.65820700	0.93762700
C	-4.59480800	0.57060700	-0.78244500
H	-2.64003900	0.69464000	-1.68212500
C	-5.45119100	-0.16878200	0.03467800
H	-5.64046900	-1.91611400	1.28544900
H	-4.94652200	1.47911300	-1.26346000
H	-6.47030500	0.16574400	0.20484900
C	0.15056200	1.19181800	2.02889200
C	0.17737600	1.97733900	-1.92619100
H	0.96488700	0.60584300	2.50245900
H	0.56257700	2.21874400	1.95684600
H	1.01055300	1.72337500	-2.61160300
C	-1.05676000	1.21765600	2.98617800
H	-0.72452700	1.77367300	-2.54012800
C	0.23340400	3.49017300	-1.63040100
H	0.09732300	4.08774600	-2.54758000
H	-1.45840100	0.20017400	3.11433500
H	-0.76455100	1.54451100	3.99843500
C	1.54762000	3.92990600	-0.97248900
H	1.57288800	5.01260600	-0.79703300
H	2.40613800	3.67848800	-1.60991300
H	-0.60006100	3.77742700	-0.97028900
H	1.69869700	3.43559400	-0.00314800
C	-2.18890000	2.13338100	2.50208700
H	-3.02092000	2.16626200	3.21682000
H	-1.82746900	3.16087400	2.36443200
H	-2.59888300	1.79653200	1.53977000
Y	0.07870000	0.34376700	-0.18125500

Y_1_V'

E(B3LYP/BS1) = -923.460629 au

H(B3LYP/BS1) = -923.057792 au

G(B3LYP/BS1) = -923.137570 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -924.142987 au

C	-1.05751700	-2.77497200	-0.45326700
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ESI105

C	1.46820800	-2.64545600	-0.45412500
C	0.23578200	-3.30748300	-0.54682700
H	2.35219400	-3.28866000	-0.51135700
H	0.29105100	-4.38076400	-0.69502100
H	-1.87260200	-3.50332600	-0.51252400
N	1.68808700	-1.34084900	-0.32169500
N	-1.40579700	-1.49921900	-0.31880900
C	3.01236300	-0.88771000	-0.10175300
C	3.43834000	0.28777300	-0.74796300
C	3.89302700	-1.52483900	0.79181900
C	4.71172200	0.80702300	-0.51040900
H	2.78514100	0.77024900	-1.47356500
C	5.16799700	-1.00691000	1.01281300
H	3.56026000	-2.40679300	1.33158900
C	5.58379900	0.16079400	0.36720000
H	5.02383500	1.71188700	-1.02449600
H	5.83485400	-1.51007900	1.70807100
H	6.57500700	0.56470400	0.55117900
C	-2.76738400	-1.17298200	-0.10605400
C	-3.59330600	-1.89413000	0.77588700
C	-3.29262000	-0.03596100	-0.74869400
C	-4.91209500	-1.49633900	0.98766300
H	-3.18608000	-2.74555600	1.31364600
C	-4.61014400	0.36326500	-0.51933500
H	-2.68001300	0.50846100	-1.46641600
C	-5.42705300	-0.36667400	0.34545800
H	-5.53656900	-2.06325800	1.67317000
H	-4.99896900	1.23974200	-1.03016100
H	-6.45277600	-0.05674000	0.52238500
C	0.00463900	1.68076200	1.81907200
C	-0.08361800	2.13883600	-1.67125800
H	-0.38822400	1.19914300	2.73023500
H	1.05399200	1.94067900	2.06365300
H	0.94578200	2.47310600	-1.90837800
C	-0.77906000	2.99503000	1.56852700
H	-0.53018400	1.90186800	-2.65236900
C	-0.84519600	3.33949600	-1.05067800
H	-0.81042300	4.20511200	-1.73331100
H	-1.85511200	2.77089000	1.47377600
H	-0.70377000	3.65649300	2.44798300
C	-0.35869200	3.82989600	0.33457100
H	-0.74723000	4.84845100	0.47754600
H	0.73881400	3.93115200	0.31976800
H	-1.91681700	3.09267900	-0.96072700
Y	0.04632500	0.36114200	-0.12095000

Al 1 II'

E(B3LYP/BS1) = -848.602058 au

H(B3LYP/BS1) = -848.212870 au

G(B3LYP/BS1) = -848.290135 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1089.373755 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1088.667194 au

C	-1.12906600	-2.14718500	-0.73055200
C	1.34881500	-2.08056600	-0.74233500
C	0.12576800	-2.74371800	-0.85234100

H	2.25666400	-2.66065900	-0.90537200
H	0.15302700	-3.79779600	-1.09972200
H	-2.00806700	-2.77359900	-0.88110000
C	-0.40726400	0.63148700	2.54162100
C	0.37614900	-0.45782800	2.44362900
N	1.52290600	-0.77929200	-0.47160200
N	-1.36729000	-0.85475100	-0.46322300
C	2.87400400	-0.29665100	-0.31910400
C	3.28571600	0.83997400	-1.02552700
C	3.76725500	-0.94816500	0.54265900
C	4.58734000	1.31809000	-0.87059000
H	2.60414100	1.32613500	-1.71749600
C	5.06907100	-0.46604700	0.68637200
H	3.44324000	-1.82132300	1.10300400
C	5.48087300	0.66791400	-0.01635700
H	4.90536400	2.19285900	-1.42962000
H	5.75750600	-0.97502500	1.35422300
H	6.49306300	1.04248800	0.09985300
C	-2.74388100	-0.44066900	-0.32643800
C	-3.57331100	-1.04882600	0.62500200
C	-3.24257900	0.57929400	-1.14514800
C	-4.90118100	-0.63658100	0.75055900
H	-3.17930700	-1.83454400	1.26443300
C	-4.57032200	0.98765500	-1.00951800
H	-2.60582700	1.02414400	-1.90481700
C	-5.40049600	0.38252900	-0.06289000
H	-5.54208000	-1.11096000	1.48760800
H	-4.95823800	1.77026600	-1.65442600
H	-6.43308700	0.70190300	0.03782900
H	1.45565800	-0.39154400	2.55898900
H	-0.04029900	-1.45408600	2.31232400
H	0.01118600	1.61386500	2.74364400
H	-1.49264400	0.56408100	2.49036200
C	0.09626500	2.30184800	-0.36228500
Al	0.04378200	0.35939000	-0.07498900
C	-1.01049900	3.20917100	0.21270400
H	-1.03619600	3.18689800	1.30776100
H	-0.84560600	4.25196400	-0.08026900
H	-2.00562200	2.92217900	-0.14062400
H	1.07786500	2.64804700	-0.00883400
H	0.13483000	2.43056700	-1.45588800

Ga_1_II'

E(B3LYP/BS1) = -848.643481 au

H(B3LYP/BS1) = -848.254566 au

G(B3LYP/BS1) = -848.333520 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2771.786038 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2771.021190 au

C	-1.13447700	-2.18156400	-0.70141800
C	1.34890200	-2.12047200	-0.70817800
C	0.12162500	-2.77899500	-0.80378000
H	2.25236400	-2.71037300	-0.85965800
H	0.14695700	-3.83857800	-1.02694200
H	-2.01052700	-2.81374600	-0.84411200
C	-0.45570200	0.48915300	2.69389700

C	0.37109700	-0.55449400	2.51334500
N	1.53388300	-0.81653300	-0.46848800
N	-1.38203700	-0.88561600	-0.46678300
C	2.88264900	-0.32966000	-0.33004800
C	3.27944300	0.81016300	-1.03988200
C	3.78964200	-0.97776200	0.51945400
C	4.58047000	1.29437800	-0.90214700
H	2.58601900	1.29391700	-1.72213100
C	5.09094300	-0.48955200	0.64592700
H	3.47630200	-1.85033900	1.08641300
C	5.48841500	0.64680600	-0.06106700
H	4.88686300	2.17155500	-1.46390000
H	5.79010200	-0.99524700	1.30505200
H	6.50030100	1.02592500	0.04224200
C	-2.75676900	-0.46704600	-0.34880200
C	-3.60901800	-1.08562700	0.57503100
C	-3.23295600	0.56866300	-1.16115900
C	-4.93703200	-0.66784700	0.67891300
H	-3.23242200	-1.88099700	1.21280700
C	-4.56063300	0.98282200	-1.04681400
H	-2.57822700	1.02157700	-1.90084500
C	-5.41392500	0.36702200	-0.12788900
H	-5.59530800	-1.14958300	1.39558100
H	-4.93065400	1.77793000	-1.68695200
H	-6.44657300	0.69081700	-0.04331700
H	1.44821700	-0.45005200	2.62165600
H	-0.00436800	-1.55726300	2.32207100
H	-0.07588800	1.47404600	2.95223800
H	-1.53725000	0.38140300	2.64337300
C	0.10681500	2.29691200	-0.26178600
C	-1.02278600	3.13793600	0.35817900
H	-1.07283000	3.02405900	1.44600800
H	-0.85645600	4.20151500	0.15425100
H	-2.00500200	2.87417200	-0.04481200
H	1.07949900	2.60929500	0.13801800
H	0.16146300	2.48722800	-1.34333700
Ga	0.04304100	0.33815400	-0.08991900

In_1_H'

E(B3LYP/BS1) = -848.445546 au

H(B3LYP/BS1) = -848.057433 au

G(B3LYP/BS1) = -848.138934 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1037.062253 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1036.382604 au

C	-1.13913500	-2.27563100	-0.67250800
C	1.37489900	-2.21015500	-0.66070900
C	0.13342100	-2.84674800	-0.75827500
H	2.25706400	-2.83986400	-0.78283900
H	0.16194600	-3.91139100	-0.95833300
H	-1.98719200	-2.94984500	-0.79917000
C	-0.58827500	0.60260900	2.70172700
C	0.32730600	-0.37837400	2.61189600
N	1.61176100	-0.91132900	-0.45474000
N	-1.44612800	-0.98912400	-0.47369400
C	2.96994000	-0.47163300	-0.30060400

C	3.39777400	0.67748200	-0.97939900
C	3.86022400	-1.15428300	0.54067300
C	4.70703400	1.13295900	-0.82424400
H	2.72109700	1.18920200	-1.66006500
C	5.17047500	-0.69563600	0.68453300
H	3.52470100	-2.02859600	1.09171600
C	5.59697100	0.44767800	0.00615200
H	5.03416000	2.01625700	-1.36442400
H	5.85445700	-1.22947700	1.33753600
H	6.61573600	0.80328500	0.12420000
C	-2.82818400	-0.62394300	-0.33842100
C	-3.67872900	-1.32611800	0.52747800
C	-3.32171000	0.46978000	-1.06274000
C	-5.01427900	-0.94005600	0.65406200
H	-3.29323700	-2.15940800	1.10870000
C	-4.65611700	0.85294300	-0.92508900
H	-2.67462800	0.99004600	-1.76534600
C	-5.50551100	0.14954600	-0.06751900
H	-5.66744800	-1.48851200	1.32622400
H	-5.03472700	1.69211300	-1.50084300
H	-6.54377600	0.44859400	0.03658800
H	1.38601900	-0.18831700	2.77575800
H	0.03994900	-1.41275800	2.43608800
H	-0.30467300	1.62406300	2.94306200
H	-1.65302900	0.40231400	2.59676900
C	0.09495700	2.56519600	-0.39848600
C	-1.04256700	3.38338200	0.23127000
H	-2.02809700	3.07509800	-0.13217400
H	-1.05378300	3.30281800	1.32358500
H	-0.92091000	4.44591800	-0.01002500
H	1.06996700	2.89578100	-0.02326100
H	0.11963700	2.71340600	-1.48536900
In	0.04217100	0.44405000	-0.12118600

La_1_II'

E(B3LYP/BS1) = -877.849966 au

H(B3LYP/BS1) = -877.465250 au

G(B3LYP/BS1) = -877.551672 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -878.550053 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -877.816075 au

C	-1.24129500	2.73517200	0.27789800
C	1.24171900	2.73508100	0.27778500
C	0.00023000	3.37216100	0.36291200
H	2.12838500	3.37184500	0.22129400
H	0.00026800	4.45404400	0.42455800
H	-2.12793600	3.37198600	0.22158400
C	-0.00215900	-3.22008600	-1.63123400
C	-0.00048000	-2.22414900	-2.53193600
N	1.43500700	1.41766900	0.25262100
N	-1.43469300	1.41776100	0.25267800
C	2.67402600	0.85691600	-0.12285200
C	3.12057000	-0.28425400	0.58136400
C	3.40338300	1.29167000	-1.24761700
C	4.27406000	-0.96564500	0.17126900
H	2.64645500	-0.55206500	1.52730500

C	4.55845100	0.61591000	-1.63356300
H	3.05083800	2.14924900	-1.81364800
C	4.99289600	-0.51865900	-0.93602700
H	4.62248200	-1.82174200	0.74180400
H	5.12064600	0.96965600	-2.49305000
H	5.89228800	-1.03896700	-1.24987100
C	-2.67385100	0.85714900	-0.12257100
C	-3.40319100	1.29180500	-1.24738600
C	-3.12059800	-0.28374500	0.58195300
C	-4.55844400	0.61621700	-1.63308200
H	-3.05048600	2.14917700	-1.81363100
C	-4.27427500	-0.96497600	0.17210900
H	-2.64645900	-0.55145100	1.52791800
C	-4.99309400	-0.51808300	-0.93523400
H	-5.12063500	0.96988700	-2.49260400
H	-4.62284700	-1.82085800	0.74287300
H	-5.89263500	-1.03825500	-1.24887900
H	0.92620000	-1.82903100	-2.94538800
H	-0.92575300	-1.82685900	-2.94644900
H	0.92303000	-3.67134800	-1.27595100
H	-0.92881000	-3.66919300	-1.27703300
C	0.00072000	-1.54981600	2.48574000
C	0.00124800	-0.72552800	3.78145200
H	0.00177200	-1.35437400	4.68239900
H	0.88256400	-0.07501600	3.84607700
H	-0.88010700	-0.07515100	3.84696400
H	0.87827600	-2.22752200	2.46670400
H	-0.87690600	-2.22742000	2.46724700
La	-0.00004100	-0.56504300	0.23503200

Sc_1_II'

E(B3LYP/BS1) = -893.072056 au

H(B3LYP/BS1) = -892.686400 au

G(B3LYP/BS1) = -892.765848 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1607.649302 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1606.929938 au

C	1.23635600	2.30440100	-0.98487200
C	-1.23606700	2.30462800	-0.98484700
C	0.00019100	2.90235700	-1.23993200
H	-2.13200400	2.91929500	-1.09077200
H	0.00029100	3.92885100	-1.58654400
H	2.13237600	2.91894000	-1.09085400
C	-0.00010200	-1.97369700	2.00011400
C	0.00051000	-0.64250800	2.20928500
N	-1.41008600	1.03747000	-0.60040100
N	1.41023200	1.03723500	-0.60041000
C	-2.65945900	0.58926300	-0.09506900
C	-3.12381400	-0.68066400	-0.48782400
C	-3.38389500	1.32338700	0.86112400
C	-4.29437500	-1.20552400	0.07002900
H	-2.62853500	-1.21099900	-1.29991100
C	-4.55945800	0.79907100	1.39414800
H	-3.01367800	2.29038000	1.18982500
C	-5.01431200	-0.46749800	1.00866700
H	-4.65458400	-2.17726100	-0.25453800

H	-5.11897400	1.37703700	2.12381000
H	-5.92825200	-0.86981900	1.43412600
C	2.65962500	0.58895600	-0.09518900
C	3.38439900	1.32323500	0.86061900
C	3.12372700	-0.68116400	-0.48767200
C	4.55998100	0.79886900	1.39357800
H	3.01443300	2.29038000	1.18914000
C	4.29429200	-1.20606400	0.07011500
H	2.62827200	-1.21162000	-1.29956200
C	5.01453000	-0.46789200	1.00841400
H	5.11973100	1.37696400	2.12295900
H	4.65429200	-2.17794600	-0.25424500
H	5.92848600	-0.87024600	1.43380700
H	-0.92733900	-0.08985700	2.34676200
H	0.92895300	-0.09060500	2.34581800
H	-0.92681900	-2.54193900	1.95380800
H	0.92615200	-2.54262500	1.95290100
C	-0.00031100	-1.65792200	-2.27874600
C	-0.00124000	-2.96290400	-1.49472300
H	-0.00146600	-2.81686700	-0.36937500
H	-0.89005100	-3.57788400	-1.66420300
H	0.88701300	-3.57881300	-1.66355100
H	-0.88722300	-1.52079200	-2.90473100
H	0.88730800	-1.52142100	-2.90386800
Sc	-0.00013700	-0.51219400	-0.46040100

Y_1_II'

E(B3LYP/BS1) = -884.561857 au

H(B3LYP/BS1) = -884.176649 au

G(B3LYP/BS1) = -884.260321au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -885.286066 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -884.552035 au

C	-1.27009200	2.60361800	0.28195800
C	1.20377900	2.61705700	0.22654200
C	-0.03452400	3.25410700	0.34981000
H	2.09125500	3.24572600	0.12275700
H	-0.03917800	4.33629900	0.40308500
H	-2.16734100	3.22330500	0.21413700
C	-0.01869100	-3.00832500	-1.18409000
C	-0.04542300	-2.03481300	-2.11090500
N	1.38230900	1.29617400	0.20602600
N	-1.43691100	1.28068600	0.27155200
C	2.58397800	0.70116100	-0.23862100
C	3.02963200	-0.45470900	0.43994700
C	3.26004900	1.11692600	-1.40221900
C	4.12954700	-1.17762600	-0.04079200
H	2.60410300	-0.70632200	1.41262800
C	4.36437700	0.40077300	-1.85657400
H	2.90422200	1.98711200	-1.94637100
C	4.79618400	-0.75300300	-1.18839200
H	4.48002800	-2.04784200	0.50650800
H	4.88733900	0.73634600	-2.74746300
H	5.65501700	-1.30497500	-1.55693100
C	-2.64781600	0.67813300	-0.13700100
C	-3.36933300	1.10203900	-1.27019300

C	-3.05938900	-0.49053400	0.54096500
C	-4.48362900	0.38243500	-1.69366700
H	-3.04038400	1.98141600	-1.81643600
C	-4.17010100	-1.21669400	0.09115100
H	-2.59864600	-0.75185100	1.49470600
C	-4.88181000	-0.78334600	-1.02566000
H	-5.04094100	0.72501900	-2.56074900
H	-4.49314900	-2.09687100	0.63942400
H	-5.74891200	-1.33795500	-1.37005600
H	0.87022000	-1.63991900	-2.54901600
H	-0.98395900	-1.65546100	-2.51278000
H	0.91918500	-3.43847100	-0.83588600
H	-0.93458000	-3.45473600	-0.79937300
C	0.08494400	-1.28784800	2.57849900
C	0.48831800	-0.41928800	3.78219900
H	0.52220400	-0.98780200	4.72120000
H	1.47932600	0.03259800	3.64606600
H	-0.21956700	0.40515500	3.93092900
H	0.79167800	-2.14030200	2.47804300
H	-0.89035600	-1.76867500	2.78418900
Y	-0.01090600	-0.48103000	0.41386200

TS'_{Al-1}

E(B3LYP/BS1) = -848.555557 au

H(B3LYP/BS1) = -848.167918 au

G(B3LYP/BS1) = -848.242110 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1089.329616 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1088.627312 au

C	-1.15888200	2.32022000	0.05833500
C	1.32335300	2.27023800	0.08892000
C	0.09368000	2.92442000	0.18256500
H	2.22682200	2.86771600	0.21006300
H	0.11355400	3.99272900	0.35849900
H	-2.04183900	2.95055100	0.16436000
C	-0.16118500	-2.44699100	-0.50729700
C	-0.00391800	-1.66718200	-1.70480100
Al	0.04049300	-0.21178800	-0.30081400
C	0.09211700	-1.40152000	1.47216600
H	1.16507100	-1.54665800	1.64279700
H	-0.16171000	-0.40519700	1.88986600
H	-1.15340800	-2.77253600	-0.20871900
H	0.64806200	-3.07192600	-0.14242100
N	1.51684700	0.96455300	-0.14548300
N	-1.39205300	1.02444000	-0.18884500
C	-2.75929600	0.56159300	-0.18336800
C	-3.52599500	0.65097700	0.98561700
C	-3.30948200	0.00554000	-1.34474400
C	-4.84225100	0.18602100	0.98724000
H	-3.09014300	1.07498600	1.88617900
C	-4.62508000	-0.46117200	-1.33204700
H	-2.72600800	-0.01941100	-2.26052500
C	-5.39209400	-0.37370000	-0.16801100
H	-5.43519700	0.25970400	1.89392400
H	-5.05402600	-0.87900300	-2.23788200
H	-6.41568100	-0.73530500	-0.16298400

C	2.87027900	0.46235600	-0.12339600
C	3.64181800	0.57150300	1.04040900
C	3.40251900	-0.14634500	-1.26634600
C	4.94614400	0.07465100	1.05466000
H	3.21798600	1.03254400	1.92836100
C	4.70593000	-0.64537700	-1.24053700
H	2.81547100	-0.18891800	-2.17918800
C	5.47867400	-0.53707300	-0.08210200
H	5.54262000	0.16242700	1.95774900
H	5.12127400	-1.10497100	-2.13237000
H	6.49280700	-0.92410900	-0.06685900
H	-0.88559800	-1.57745400	-2.33716800
H	0.93643300	-1.78057800	-2.24096900
C	-0.74759700	-2.42263300	2.23969900
H	-0.55750300	-2.34539800	3.31609000
H	-1.81965500	-2.26022200	2.08239200
H	-0.51170800	-3.45184700	1.94792500

TS' _{Ga-1}

E(B3LYP/BS1) = -848.584996 au

H(B3LYP/BS1) = -848.197631 au

G(B3LYP/BS1) = -848.272439 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2771.723150 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2770.963443 au

C	-1.17191700	2.31097300	0.08662600
C	1.32029100	2.26653900	0.12315000
C	0.08334800	2.90664300	0.23274600
H	2.21604200	2.87568400	0.24321600
H	0.09993800	3.97230500	0.42467800
H	-2.04981800	2.94926300	0.18628700
C	-0.13679600	-2.45694000	-0.23487700
C	0.00780300	-1.79407100	-1.51048700
C	0.09820700	-1.25303400	1.68950100
H	1.16174000	-1.44282000	1.86349100
H	-0.10505500	-0.22531100	2.03951500
H	-1.12534500	-2.76220600	0.09357300
H	0.68287300	-3.03060500	0.18557400
N	1.53440500	0.97056000	-0.13279800
N	-1.41921800	1.02409900	-0.18230700
C	-2.78519500	0.56832400	-0.21262100
C	-3.60384900	0.71961800	0.91404000
C	-3.28635600	-0.04083100	-1.36972800
C	-4.92312700	0.26481500	0.87664900
H	-3.20542600	1.18011600	1.81394600
C	-4.60492800	-0.49744000	-1.39539000
H	-2.66153100	-0.11440800	-2.25525000
C	-5.42439000	-0.34704200	-0.27408500
H	-5.55592100	0.38563100	1.75075400
H	-4.99537300	-0.95660700	-2.29862700
H	-6.45025600	-0.70124500	-0.29891600
C	2.88830900	0.47800100	-0.13944500
C	3.70016100	0.63148500	0.99147400
C	3.38446700	-0.16427600	-1.28047300
C	5.00911700	0.14696900	0.97373300
H	3.30389800	1.11484000	1.88022400

C	4.69239800	-0.65084000	-1.28615500
H	2.76455200	-0.24271200	-2.16899600
C	5.50606200	-0.49708800	-0.16107300
H	5.63662000	0.26858100	1.85151600
H	5.07946100	-1.13639200	-2.17695800
H	6.52375400	-0.87483300	-0.17033600
H	-0.87661100	-1.78359000	-2.14447500
H	0.94867100	-1.94715500	-2.03475800
Ga	0.03796700	-0.21286400	-0.25193900
C	-0.80042100	-2.19148700	2.49161300
H	-0.63071300	-2.05186400	3.56572400
H	-1.86155400	-1.99565400	2.30030100
H	-0.60232500	-3.24676500	2.27417600

TS'_{In-1}

E(B3LYP/BS1) = -848.379111 au

H(B3LYP/BS1) = -847.992794 au

G(B3LYP/BS1) = -848.069495 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1036.986709 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1036.310868 au

C	1.21528600	-2.39629700	0.00281500
C	-1.30697100	-2.36756100	0.02533200
C	-0.05193300	-2.98233200	0.08617900
H	-2.17481800	-3.01987900	0.12942000
H	-0.06316200	-4.05837700	0.21288700
H	2.07006000	-3.06768000	0.09307400
C	0.05616300	2.70000700	-0.27448700
C	-0.01240800	2.07894900	-1.57866400
C	-0.13155500	1.50330000	1.72034100
H	-1.21559800	1.53075300	1.87541500
H	0.23470600	0.53623800	2.10972500
H	1.01098000	3.06393900	0.09059300
H	-0.81268200	3.20585700	0.13395100
N	-1.58316300	-1.07244300	-0.15905600
N	1.51626600	-1.10751400	-0.18801400
C	2.89033600	-0.69550300	-0.13802700
C	3.71855000	-1.08557100	0.92317700
C	3.39700600	0.12798700	-1.15243300
C	5.04820100	-0.66302700	0.95607600
H	3.31787200	-1.69698100	1.72680700
C	4.72548100	0.55165400	-1.10743900
H	2.76729500	0.39317300	-1.99844900
C	5.55426200	0.15682400	-0.05456900
H	5.68494300	-0.96791200	1.78115800
H	5.11622100	1.17693900	-1.90464600
H	6.58807700	0.48625200	-0.02242200
C	-2.94861300	-0.63334500	-0.09169400
C	-3.76539400	-0.99558300	0.98793100
C	-3.45712500	0.18585600	-1.10839500
C	-5.08689100	-0.54941800	1.03711100
H	-3.36175100	-1.60419800	1.79218800
C	-4.77720500	0.63306000	-1.04713300
H	-2.83594500	0.43120600	-1.96652000
C	-5.59518300	0.26613700	0.02418200
H	-5.71509100	-0.83257000	1.87635600

H	-5.17013800	1.25529700	-1.84563900
H	-6.62243700	0.61412000	0.06888900
H	0.89174400	2.13263900	-2.18270000
H	-0.93983500	2.20828000	-2.13315300
In	-0.01963300	0.28924800	-0.32203000
C	0.58599700	2.60419900	2.49567900
H	0.40168800	2.49230500	3.57099300
H	1.67113500	2.56532600	2.34714500
H	0.23902700	3.60577600	2.21801600

TS' La-1

E(B3LYP/BS1) = -877.825080 au

H(B3LYP/BS1) = -877.441524 au

G(B3LYP/BS1) = -877.521499 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -878.525531 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -877.795641 au

C	1.24535100	-2.94949500	-0.20572800
C	-1.24813600	-2.94887700	-0.20549600
C	-0.00153400	-3.58412700	-0.21005400
H	-2.13054200	-3.58894400	-0.12031000
H	-0.00178700	-4.66716600	-0.16999000
H	2.12743700	-3.59001800	-0.12069000
C	0.00324200	3.22702300	-0.88234300
C	0.00175600	2.38471700	-1.99477500
C	0.00135700	2.33757600	1.30288500
H	-0.90037500	1.77697600	1.64776300
H	0.89808900	1.77053000	1.65057900
H	0.91775000	3.72129100	-0.57228000
H	-0.90972200	3.72395800	-0.57199500
N	-1.45376500	-1.63633300	-0.30134900
N	1.45176700	-1.63702800	-0.30161500
C	2.71819200	-1.06621700	-0.05188500
C	3.50638100	-1.40155300	1.06649500
C	3.13493200	-0.00289500	-0.88412100
C	4.68444100	-0.70423200	1.32467700
H	3.17989600	-2.19630600	1.73124200
C	4.31329900	0.70129700	-0.60506700
H	2.61218600	0.17921100	-1.82536600
C	5.08761300	0.35393400	0.50046900
H	5.28901600	-0.98000800	2.18387700
H	4.63501100	1.49626100	-1.27150100
H	6.00439500	0.89329200	0.71616300
C	-2.71971900	-1.06457300	-0.05161100
C	-3.50828700	-1.39936000	1.06666300
C	-3.13545400	-0.00073000	-0.88371700
C	-4.68573200	-0.70100800	1.32486600
H	-3.18255600	-2.19449100	1.73132600
C	-4.31321600	0.70447500	-0.60464700
H	-2.61258100	0.18095400	-1.82498800
C	-5.08790300	0.35765000	0.50079600
H	-5.29061200	-0.97636600	2.18398500
H	-4.63418300	1.49981200	-1.27099600
H	-6.00421000	0.89780200	0.71651900
H	0.92253300	2.25499700	-2.56521800
H	-0.91975400	2.25758000	-2.56462500

La	-0.00033400	0.36162800	-0.29519100
C	0.00557300	3.70002900	1.97643000
H	0.00435100	3.61723000	3.07026700
H	0.89317300	4.27801800	1.69564000
H	-0.87742800	4.28429900	1.69420000

TS'_{Sc-1}

E(B3LYP/BS1) = -893.056346 au

H(B3LYP/BS1) = -892.671440 au

G(B3LYP/BS1) = -892.749099 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1607.637527 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1606.916090 au

C	-1.24995500	-2.32766700	0.81883200
C	1.25020700	-2.32766200	0.81881200
C	0.00012800	-2.90329700	1.06792200
H	2.12442800	-2.97147500	0.93406300
H	0.00013100	-3.92946600	1.41667700
H	-2.12416300	-2.97149700	0.93408300
C	-0.00062700	2.79278700	1.40393200
C	-0.00046100	1.75736000	2.32668100
C	-0.00007300	2.11895200	-0.89207100
H	0.90232200	1.57008300	-1.25542600
H	-0.90218600	1.56969300	-1.25555200
H	-0.91643200	3.31937600	1.15562500
H	0.91494400	3.31996700	1.15603100
N	1.48359200	-1.06688000	0.43106500
N	-1.48338700	-1.06687800	0.43111400
C	-2.78783500	-0.71412200	-0.03318400
C	-3.44785900	-1.48083800	-1.00609700
C	-3.39145400	0.45739900	0.45222600
C	-4.69971500	-1.08206700	-1.47269600
H	-2.96873700	-2.36962200	-1.40678400
C	-4.63948000	0.85635900	-0.03021500
H	-2.91575400	1.02116900	1.25337700
C	-5.29663200	0.08688700	-0.99167700
H	-5.20585600	-1.68187700	-2.22322300
H	-5.10513200	1.75583200	0.36143000
H	-6.26947700	0.39381300	-1.36264700
C	2.78802500	-0.71401600	-0.03317100
C	3.44819500	-1.48067000	-1.00603200
C	3.39146900	0.45759500	0.45224500
C	4.70002400	-1.08174600	-1.47257200
H	2.96920700	-2.36952300	-1.40672600
C	4.63946500	0.85671100	-0.03014200
H	2.91565800	1.02131100	1.25337600
C	5.29676400	0.08729900	-0.99155100
H	5.20628400	-1.68150700	-2.22305800
H	5.10498100	1.75625300	0.36150500
H	6.26958900	0.39434100	-1.36248000
H	-0.92319500	1.47989500	2.83797800
H	0.92227300	1.48049000	2.83830200
Sc	0.00010100	0.42116100	0.43927800
C	-0.00036700	3.52491800	-1.45586500
H	-0.00115900	3.51897400	-2.55257800
H	-0.88718700	4.08036600	-1.13254300

H 0.88698800 4.08022600 -1.13380900

TS'_{Y-1}

E(B3LYP/BS1) = -884.543937 au

H(B3LYP/BS1) = -884.159893 au

G(B3LYP/BS1) = -884.238814 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -885.264635 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -884.533415 au

C	1.24572400	-2.73210800	-0.41669500
C	-1.24530100	-2.73212800	-0.41669900
C	0.00021700	-3.36196900	-0.50275300
H	-2.12843300	-3.37481000	-0.38622100
H	0.00022100	-4.44276500	-0.58221400
H	2.12887700	-3.37476300	-0.38619100
C	-0.00063700	2.98326600	-1.10831600
C	-0.00026800	2.07025900	-2.15752500
C	-0.00026300	2.13617200	1.14358400
H	-0.90090200	1.56993300	1.48905400
H	0.90108700	1.57090400	1.48875200
H	0.91407900	3.48293600	-0.80732500
H	-0.91574300	3.48226100	-0.80738100
N	-1.45318200	-1.41458200	-0.36144300
N	1.45353100	-1.41455700	-0.36147700
C	2.73096900	-0.89336000	-0.02737300
C	3.47825900	-1.36523400	1.06695500
C	3.20190800	0.21985400	-0.75155600
C	4.67501500	-0.74115100	1.41220300
H	3.10623600	-2.20357000	1.64900900
C	4.39608500	0.85052400	-0.38504900
H	2.69123200	0.52334700	-1.66605100
C	5.13338500	0.37166600	0.69698100
H	5.24920900	-1.11744500	2.25376900
H	4.75940900	1.69360100	-0.96519500
H	6.06396600	0.85392600	0.97893000
C	-2.73070900	-0.89355000	-0.02735800
C	-3.47785100	-1.36545300	1.06705800
C	-3.20192600	0.21945200	-0.75167200
C	-4.67474000	-0.74160300	1.41227000
H	-3.10561600	-2.20363500	1.64920000
C	-4.39623500	0.84989100	-0.38520900
H	-2.69131200	0.52297600	-1.66618600
C	-5.13339100	0.37100800	0.69691100
H	-5.24881600	-1.11791800	2.25390600
H	-4.75977300	1.69280900	-0.96545300
H	-6.06407500	0.85309100	0.97882300
H	0.92124800	1.88713700	-2.71123400
H	-0.92158400	1.88650500	-2.71135800
Y	0.00014200	0.34669000	-0.36234900
C	-0.00091600	3.50445900	1.79972900
H	-0.00069800	3.43839500	2.89450600
H	0.88455400	4.08057500	1.50885800
H	-0.88711700	4.07959400	1.50913900

TS'_{AI-1 (BHT)}

E(B3LYP/BS1) = -848.571835 au

H(B3LYP/BS1) = -848.187675 au
 G(B3LYP/BS1) = -848.260879 au
 E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1089.343946 au
 E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1088.634106 au

C	-1.23370200	-2.37955500	-0.08993400
C	1.23514300	-2.37918100	0.08747500
C	0.00085100	-3.02204000	-0.00170700
H	2.12916000	-3.00105300	0.13324600
H	0.00106900	-4.10503400	-0.00242100
H	-2.12747400	-3.00172700	-0.13637100
N	1.43433500	-1.05529900	0.13517400
N	-1.43339800	-1.05569500	-0.13594700
C	2.79445300	-0.58321500	0.11775700
C	3.67159600	-0.98814900	-0.89827400
C	3.23481600	0.31102600	1.10183300
C	4.98220000	-0.50968800	-0.91723200
H	3.32188600	-1.66075900	-1.67666400
C	4.54567700	0.78989800	1.07175200
H	2.57034700	0.59263600	1.91361600
C	5.42191000	0.38119900	0.06425400
H	5.65663200	-0.82907400	-1.70610600
H	4.88555500	1.46988400	1.84732400
H	6.44173000	0.75280300	0.04537000
C	-2.79359900	-0.58402200	-0.11751900
C	-3.67080100	-0.99153100	0.89743700
C	-3.23402300	0.31257700	-1.09943700
C	-4.98150400	-0.51338800	0.91736800
H	-3.32106700	-1.66584100	1.67434200
C	-4.54497900	0.79112000	-1.06837000
H	-2.56950100	0.59631700	-1.91043800
C	-5.42128400	0.37978100	-0.06200800
H	-5.65595400	-0.83479700	1.70540500
H	-4.88488100	1.47293200	-1.84232900
H	-6.44118100	0.75113000	-0.04235900
Al	0.00030900	0.21638200	-0.00013400
C	-0.39539200	1.52109900	1.56929700
C	0.39520100	1.52127900	-1.56948600
H	-1.40290800	1.18568800	1.83490000
H	0.33414500	1.20363700	2.32024100
H	1.40455300	1.18962500	-1.83279700
C	-0.32710900	2.93464600	1.26360200
H	-0.33150300	1.20024100	-2.32169000
C	0.32060300	2.93485900	-1.26521800
H	-0.00380900	3.06884500	-0.00107200
H	1.25287800	3.49995500	-1.22303000
H	-0.50785600	3.50941200	-1.68212900
H	-1.26186800	3.49560800	1.22129500
H	0.49913100	3.51326700	1.67928000

TS'_{Ga-1 (BHT)}

E(B3LYP/BS1) = -848.610470 au
 H(B3LYP/BS1) = -848.226561 au
 G(B3LYP/BS1) = -848.300362 au
 E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2771.752809 au
 E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2770.985277 au

C	1.23774800	-2.39754800	0.09174900
C	-1.23738200	-2.39766400	-0.09192700
C	0.00021400	-3.03474000	-0.00011000
H	-2.12609900	-3.02676700	-0.14303800
H	0.00026900	-4.11779500	-0.00014000
H	2.12652000	-3.02657100	0.14285000
N	-1.45021200	-1.07763700	-0.13710400
N	1.45046800	-1.07750300	0.13699400
C	-2.80968600	-0.61110600	-0.11824800
C	-3.69530700	-1.04653400	0.87777400
C	-3.24432400	0.30864200	-1.08142500
C	-5.00816000	-0.57403900	0.89624800
H	-3.35056300	-1.73698100	1.64255700
C	-4.55718300	0.78099600	-1.05187400
H	-2.57225500	0.61631700	-1.87742400
C	-5.44211600	0.34108200	-0.06506400
H	-5.68860900	-0.91678700	1.67001400
H	-4.89203100	1.48091000	-1.81176700
H	-6.46361400	0.70803400	-0.04637200
C	2.80990900	-0.61086500	0.11821500
C	3.69557900	-1.04611400	-0.87784000
C	3.24446900	0.30880100	1.08150200
C	5.00841100	-0.57355200	-0.89621600
H	3.35090100	-1.73647100	-1.64273600
C	4.55730500	0.78122300	1.05204900
H	2.57235200	0.61638100	1.87749600
C	5.44229800	0.34146900	0.06522200
H	5.68889500	-0.91617400	-1.67000700
H	4.89208500	1.48107300	1.81203200
H	6.46377700	0.70847200	0.04660900
C	0.40800300	1.51675500	-1.58299800
C	-0.40814800	1.51653600	1.58310300
H	1.41765800	1.18106400	-1.83454100
H	-0.32009600	1.18987500	-2.32963200
H	-1.41735300	1.17991400	1.83522200
C	0.32672300	2.92527400	-1.26642100
H	0.32062100	1.19050900	2.32945000
C	-0.32845800	2.92511200	1.26629400
H	-0.00106500	3.04511900	-0.00006100
H	-1.25952100	3.49146700	1.21879600
H	0.50143100	3.49922200	1.68053400
H	1.25714600	3.49266400	-1.21875500
H	-0.50372300	3.49841900	-1.68087700
Ga	0.00006800	0.20844300	0.00001200

TS_{In-1} (BHT)

E(B3LYP/BS1) = -848.409792 au

H(B3LYP/BS1) = -848.026593 au

G(B3LYP/BS1) = -848.102666 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1037.024973 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1036.340924 au

C	-1.25563300	-2.37489200	-0.64232300
C	1.25554600	-2.37491900	-0.64232700
C	-0.00005100	-2.96493900	-0.80937300
H	2.12049300	-3.03322900	-0.73670600

H	-0.00006200	-4.01957700	-1.05838300
H	-2.12059600	-3.03318300	-0.73669600
N	1.52854700	-1.09291500	-0.37897000
N	-1.52860700	-1.09288100	-0.37896700
C	2.88726300	-0.74051000	-0.08005000
C	3.47887800	0.35347600	-0.72646500
C	3.62064200	-1.45912000	0.87522500
C	4.79169000	0.71829700	-0.42606700
H	2.93020100	0.88573300	-1.49917100
C	4.93515700	-1.09208200	1.16561200
H	3.15469500	-2.28718600	1.40200700
C	5.52374500	-0.00313400	0.51950800
H	5.24723300	1.55684200	-0.94456400
H	5.49531700	-1.65441800	1.90678600
H	6.54571400	0.28100200	0.75032600
C	-2.88731600	-0.74044900	-0.08004400
C	-3.62069600	-1.45902900	0.87525200
C	-3.47892100	0.35352900	-0.72648100
C	-4.93520400	-1.09196900	1.16564100
H	-3.15475500	-2.28709100	1.40204700
C	-4.79172700	0.71837300	-0.42608000
H	-2.93024200	0.88576300	-1.49920200
C	-5.52378400	-0.00302800	0.51951700
H	-5.49536600	-1.65428100	1.90683100
H	-5.24726300	1.55691300	-0.94459100
H	-6.54574700	0.28112600	0.75033600
C	0.00003800	1.48078200	1.80945800
C	0.00003500	2.13134100	-1.57769100
H	-0.90700000	1.06984300	2.25957700
H	0.90701300	1.06966600	2.25954700
H	0.90458700	1.91038500	-2.14756200
C	0.00017900	2.91847100	1.66820500
H	-0.90462500	1.91060700	-2.14747400
C	0.00022800	3.41187000	-0.92321300
H	0.00001800	3.23175400	0.40230900
H	0.91167700	4.00916500	-0.96648200
H	-0.91097700	4.00952900	-0.96664200
H	-0.90975100	3.45179800	1.94786800
H	0.91028900	3.45159400	1.94766600
In	-0.00001700	0.34725300	-0.14718500

TS'_{La-1 (BHT)}

E(B3LYP/BS1) = -877.818108 au

H(B3LYP/BS1) = -877.437998 au

G(B3LYP/BS1) = -877.516108 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -878.508365 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -877.774209 au

C	1.24448800	2.75943700	-0.70163900
C	-1.24519000	2.75939800	-0.70152800
C	-0.00035900	3.37759000	-0.85619300
H	-2.12819600	3.40264500	-0.74383100
H	-0.00037500	4.44312100	-1.05415500
H	2.12746700	3.40270100	-0.74417900
N	-1.44833800	1.45740800	-0.50671700
N	1.44776500	1.45747400	-0.50659100

C	-2.70970200	0.95963700	-0.11442000
C	-3.14857700	-0.25403600	-0.68915900
C	-3.47478500	1.53756100	0.91734700
C	-4.32614400	-0.86889400	-0.24371400
H	-2.64721700	-0.63931000	-1.57907700
C	-4.65160800	0.92518100	1.34078100
H	-3.12957600	2.45296900	1.38930400
C	-5.07707600	-0.28280300	0.77315100
H	-4.66662100	-1.78504400	-0.71761400
H	-5.23798600	1.38684700	2.12999200
H	-5.99312200	-0.75296200	1.11635400
C	2.70928400	0.95997100	-0.11445300
C	3.47429900	1.53800200	0.91730700
C	3.14839200	-0.25359000	-0.68923900
C	4.65128300	0.92587000	1.34065200
H	3.12890500	2.45330500	1.38933200
C	4.32611400	-0.86821500	-0.24387700
H	2.64704600	-0.63897500	-1.57911500
C	5.07698100	-0.28199900	0.77295600
H	5.23760400	1.38763300	2.12984900
H	4.66675300	-1.78428200	-0.71782000
H	5.99314800	-0.75197200	1.11608900
C	0.00087000	-1.38776100	2.29343600
C	0.00025400	-2.30379000	-2.17282800
H	0.92187400	-0.97995200	2.70910200
H	-0.92004600	-0.98033400	2.70967300
H	-0.91752500	-2.10336500	-2.72435400
C	0.00099600	-2.69696300	1.76299400
H	0.91763700	-2.10248100	-2.72469100
C	0.00090600	-3.29836300	-1.17067700
H	0.00085600	-2.80625600	0.26380900
H	-0.91023000	-3.87436400	-1.00560300
H	0.91267100	-3.87345500	-1.00589700
H	0.91295900	-3.28983800	1.84281000
H	-0.91076300	-3.29010900	1.84315500
La	-0.00006700	-0.51154600	-0.20132200

TS'_{sc-1} (BHT)

E(B3LYP/BS1) = -893.046783 au

H(B3LYP/BS1) = -892.665165 au

G(B3LYP/BS1) = -892.739977 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1607.622315 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1606.902412 au

C	-1.23988100	2.27100800	0.95337600
C	1.23985600	2.27102200	0.95338100
C	-0.00001600	2.85915600	1.21484100
H	2.12976200	2.89129700	1.07774700
H	-0.00002300	3.87995700	1.57824600
H	-2.12979300	2.89127400	1.07774100
N	1.43259600	1.01339500	0.54507900
N	-1.43260900	1.01338000	0.54507300
C	2.70597700	0.60332800	0.06052300
C	3.21745100	-0.64091100	0.47182000
C	3.41831200	1.36187400	-0.88416100
C	4.42194600	-1.11750400	-0.05444300

H	2.72262000	-1.19453200	1.26824600
C	4.62675100	0.88642100	-1.38918900
H	3.01083100	2.30744000	-1.23021600
C	5.12904800	-0.35502900	-0.98357200
H	4.81702600	-2.07075300	0.28422800
H	5.17438300	1.48290200	-2.11288400
H	6.06837900	-0.72021900	-1.38664400
C	-2.70599100	0.60330800	0.06052000
C	-3.41832400	1.36184800	-0.88416900
C	-3.21747000	-0.64092500	0.47182900
C	-4.62676600	0.88639500	-1.38919300
H	-3.01084000	2.30740900	-1.23023300
C	-4.42196700	-1.11751800	-0.05442800
H	-2.72263800	-1.19454200	1.26825700
C	-5.12906700	-0.35505000	-0.98356400
H	-5.17439600	1.48287100	-2.11289400
H	-4.81704900	-2.07076300	0.28425200
H	-6.06839900	-0.72024000	-1.38663300
C	-0.00001500	-0.98281800	-1.92965500
C	0.00000700	-1.70538200	2.31777800
H	-0.92477100	-0.52854700	-2.28215800
H	0.92469100	-0.52847400	-2.28219300
H	0.91836200	-1.39713600	2.81461600
C	0.00004800	-2.32224600	-1.49656700
H	-0.91839000	-1.39720200	2.81457800
C	0.00006600	-2.82429300	1.46643400
H	0.00009900	-2.46197500	-0.01007800
H	0.91286500	-3.40937000	1.35482200
H	-0.91268500	-3.40942800	1.35475600
H	-0.91456600	-2.90741700	-1.59405600
H	0.91470700	-2.90734000	-1.59411400
Sc	0.00000600	-0.51279800	0.32781800

TS'_{Y-1} (BHT)

E(B3LYP/BS1) = -884.536814 au

H(B3LYP/BS1) = -884.156161 au

G(B3LYP/BS1) = -884.232742 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -885.248900 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -884.516831 au

C	1.24197400	2.55018400	-0.82933700
C	-1.24198300	2.55018300	-0.82933800
C	-0.00000400	3.15855100	-1.03344600
H	-2.12917500	3.18435700	-0.89689900
H	-0.00000500	4.20906800	-1.29937700
H	2.12916700	3.18435900	-0.89689800
N	-1.43519800	1.26048600	-0.54874900
N	1.43519100	1.26048700	-0.54874800
C	-2.68709400	0.78461900	-0.09014400
C	-3.13067600	-0.46754500	-0.56418000
C	-3.43117500	1.43944300	0.90877000
C	-4.29403300	-1.05129600	-0.04749100
H	-2.63878600	-0.92282500	-1.42445600
C	-4.59629600	0.85782400	1.40218800
H	-3.07906300	2.38760700	1.30471000
C	-5.02691300	-0.39120400	0.93675900

H	-4.63842600	-2.00339300	-0.44060200
H	-5.16789700	1.37583000	2.16678200
H	-5.93310500	-0.83722500	1.33411200
C	2.68708900	0.78462100	-0.09014600
C	3.43117100	1.43944600	0.90876900
C	3.13067500	-0.46754000	-0.56418400
C	4.59629400	0.85783000	1.40218400
H	3.07905600	2.38760900	1.30471100
C	4.29403300	-1.05128900	-0.04749900
H	2.63878400	-0.92282000	-1.42446000
C	5.02691400	-0.39119700	0.93675200
H	5.16789400	1.37583600	2.16677800
H	4.63842900	-2.00338300	-0.44061100
H	5.93310700	-0.83721500	1.33410300
C	0.00001600	-1.10896700	2.09664900
C	-0.00000100	-2.02209600	-2.25568800
H	-0.91701900	-1.78520500	-2.79319600
C	0.00002600	-2.44599700	1.64397900
H	0.91701600	-1.78520700	-2.79319700
C	-0.00000400	-3.06208700	-1.30347600
H	0.00000600	-2.61192800	0.15361900
H	-0.91240100	-3.63986600	-1.15419400
H	0.91238800	-3.63987800	-1.15420300
H	0.91314500	-3.03283100	1.74908000
H	-0.91307700	-3.03285300	1.74910500
Y	-0.00000300	-0.49067700	-0.28969200
H	-0.92301500	-0.67068300	2.47443300
H	0.92304800	-0.67066600	2.47441100

Ni_10_II

E(B3LYP/BS1) = -937.814437 au

H(B3LYP/BS1) = -937.474135 au

G(B3LYP/BS1) = -937.54447 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2277.180603 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2276.473393 au

C	-0.66493000	-1.76067700	-0.08099100
C	0.79617500	-1.71618200	-0.10270200
H	-1.17999300	-2.71578200	-0.19371600
H	1.36769300	-2.64350400	-0.14382000
Ni	0.07408900	0.96775800	0.04916300
C	-1.31688200	2.46144800	0.67044000
H	-0.74917500	3.20799300	1.21595400
H	-2.05437000	1.90358800	1.23764100
C	-1.30538800	2.40352100	-0.69882800
N	1.38134600	-0.56523800	-0.08801700
N	-1.29756700	-0.65145800	0.08634500
H	-0.72379500	3.09925500	-1.29545200
H	-2.02298800	1.78639400	-1.23459100
C	1.47559000	2.26738200	-0.00364700
H	2.14987400	1.97614300	0.80862900
H	1.97560100	2.15991400	-0.96980500
H	1.13496600	3.29508100	0.13012100
C	2.81427000	-0.56286300	-0.03794100
C	3.46481100	-1.14583100	1.05831800
C	3.54993700	0.00015000	-1.08810300

C	4.85889100	-1.15476200	1.10333700
H	2.88245400	-1.55685600	1.87818100
C	4.94224000	-0.03737100	-1.04138200
H	3.03749400	0.42277700	-1.94575800
C	5.59863400	-0.60505700	0.05454200
H	5.36366000	-1.59310800	1.95870200
H	5.51501400	0.37828400	-1.86463100
H	6.68349400	-0.61804500	0.08994400
C	-2.72447100	-0.67488200	0.04064000
C	-3.45967500	-0.22524900	1.14716900
C	-3.38312200	-1.14510800	-1.10561000
C	-4.85253700	-0.26112900	1.10505900
H	-2.94417100	0.09000600	2.04934400
C	-4.77750300	-1.15214400	-1.14349200
H	-2.80544400	-1.47039800	-1.96638400
C	-5.51347800	-0.71388600	-0.04051600
H	-5.42178800	0.06203000	1.97116000
H	-5.28643800	-1.50215300	-2.03632200
H	-6.59841600	-0.72613100	-0.07183700

TS_{Ni-10}

E(B3LYP/BS1) = -937.798141 au

H(B3LYP/BS1) = -937.458151 au

G(B3LYP/BS1) = -937.526056 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2277.161549 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2276.456615 au

C	0.47957700	-3.03208300	-0.76574300
C	1.52262700	-2.12134500	-0.59006300
C	-1.50788000	-2.22699500	-0.31309100
H	-1.83920000	-2.01564900	0.70770100
H	-2.04500000	-1.63442100	-1.05752800
H	-1.69191300	-3.27798800	-0.51497600
H	0.13519900	-3.27587900	-1.76566900
H	0.31466300	-3.79807400	-0.01555900
H	1.98425700	-1.65319700	-1.45764400
H	2.14378700	-2.18531300	0.29928500
C	0.69887000	1.76744400	-0.12286300
C	-0.75511400	1.76721700	-0.12076700
H	1.24679600	2.70813800	-0.16971000
H	-1.30216000	2.70689700	-0.19788200
Ni	0.02874900	-0.90800800	-0.13153300
N	1.30254300	0.63314100	0.03295700
N	-1.35157900	0.63646800	0.06999500
C	2.72752800	0.63594800	0.11775100
C	3.50187300	1.31261600	-0.83624000
C	3.34276900	-0.03151200	1.18658700
C	4.89087900	1.32118500	-0.71379300
H	3.02165200	1.79503200	-1.68301900
C	4.72974300	0.00579800	1.31186600
H	2.73218000	-0.53380200	1.93088400
C	5.50618400	0.67500100	0.36082000
H	5.49096800	1.83054600	-1.46147300
H	5.20492900	-0.48971100	2.15286100
H	6.58756100	0.68758000	0.45473300
C	-2.77333500	0.62412800	0.12676100

C	-3.53651700	1.21297800	-0.89393700
C	-3.40469700	0.01784300	1.22333000
C	-4.92758600	1.19718600	-0.80964200
H	-3.04188300	1.64696200	-1.75849700
C	-4.79535200	0.03028800	1.30766500
H	-2.80651000	-0.41035300	2.02157600
C	-5.55852900	0.61193000	0.29118600
H	-5.51772000	1.64058400	-1.60573300
H	-5.28337300	-0.41578300	2.16871000
H	-6.64217900	0.60562400	0.35522600

Pd_10_II

E(B3LYP/BS1) = -895.260123 au

H(B3LYP/BS1) = -894.919571 au

G(B3LYP/BS1) = -894.991161 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -896.7604279 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -896.1185431 au

C	-0.67456900	-1.90576300	-0.04578600
C	0.78584900	-1.85858600	-0.06405500
H	-1.16062800	-2.87801500	-0.14734900
H	1.33447100	-2.80140200	-0.07564000
C	-1.30677800	2.60924500	0.73497200
H	-0.69083700	3.35019700	1.23437500
H	-2.02780100	2.08849200	1.35635800
C	-1.39311800	2.54916200	-0.63883900
N	1.41790700	-0.73075400	-0.08965100
N	-1.35309800	-0.81940500	0.10475000
H	-0.84139400	3.23838000	-1.27109100
H	-2.17597700	1.97029500	-1.12234000
C	1.54431100	2.37261400	-0.16609200
H	2.36009400	2.01718100	0.46738300
H	1.83389500	2.37219000	-1.22074900
H	1.22069400	3.36899800	0.13851700
Pd	0.06769600	0.98870400	0.02564400
C	2.84245000	-0.75561900	-0.02762600
C	3.58886300	-0.07073200	-0.99648400
C	3.48804700	-1.47075600	0.99354200
C	4.98011000	-0.12828600	-0.95492500
H	3.08051100	0.46204300	-1.79250900
C	4.88086200	-1.49965900	1.03749200
H	2.90185100	-1.96333500	1.76414000
C	5.62837400	-0.83503800	0.06248000
H	5.55924000	0.38125800	-1.71883200
H	5.38024300	-2.03909900	1.83637300
H	6.71300200	-0.86266100	0.09763600
C	-2.76965300	-0.87214200	0.03948800
C	-3.52197300	-0.23930900	1.04161600
C	-3.41720700	-1.53699000	-1.01545600
C	-4.91305000	-0.29617000	0.99854000
H	-3.01444000	0.23336200	1.87646400
C	-4.80993400	-1.56366900	-1.06156800
H	-2.83159300	-1.98907800	-1.81089500
C	-5.55968000	-0.94968700	-0.05507100
H	-5.49340800	0.16919400	1.78928700
H	-5.30880500	-2.06205400	-1.88705700

H -6.64420800 -0.97690000 -0.09277000

TS_{Pd-10}

E(B3LYP/BS1) = -895.232616 au

H(B3LYP/BS1) = -894.892683 au

G(B3LYP/BS1) = -894.962369 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -896.731436 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -896.092997 au

C	0.39644700	-3.29596800	-0.02815300
C	1.48632600	-2.39050700	-0.12159300
C	-1.53648400	-2.45483900	0.14766900
H	-1.82374400	-2.13399100	1.14972800
H	-2.06304400	-1.92186800	-0.64868900
H	-1.76401200	-3.51118200	0.04292700
H	0.11323800	-3.84266800	-0.92183000
H	0.24300200	-3.82778600	0.90575600
H	1.98188000	-2.28366500	-1.08408700
H	2.12572100	-2.24302500	0.74809100
C	0.69660500	1.93876700	-0.01905400
C	-0.76237500	1.94427700	-0.00102700
H	1.22964600	2.88993800	-0.00281800
H	-1.28472400	2.90084100	-0.05461600
N	1.33824200	0.81782300	-0.07477800
N	-1.40099600	0.82704700	0.09464300
C	2.76263300	0.84202000	-0.02149500
C	3.49982500	0.16359300	-1.00198600
C	3.41913600	1.54637500	0.99946800
C	4.89161000	0.21325400	-0.97059600
H	2.98161600	-0.35170900	-1.80389200
C	4.81276400	1.56704700	1.03413000
H	2.84117300	2.03622000	1.77789200
C	5.55066400	0.90691200	0.04905500
H	5.46290800	-0.29035500	-1.74438500
H	5.32029400	2.09708400	1.83422200
H	6.63562700	0.92881100	0.07711700
C	-2.81895700	0.83347900	0.03349100
C	-3.48762100	1.50181900	-1.00575500
C	-3.54848200	0.15239200	1.02002900
C	-4.88033400	1.48939800	-1.04864800
H	-2.91643400	1.99056500	-1.78993000
C	-4.94102200	0.16951200	0.97989000
H	-3.02516600	-0.33393000	1.83654500
C	-5.60903000	0.82972000	-0.05549400
H	-5.39572600	1.99379700	-1.86024000
H	-5.50551000	-0.33360300	1.75896400
H	-6.69405000	0.82664600	-0.09010000
Pd	0.05187700	-0.90973300	-0.00455000

Ni_10_IV

E(B3LYP/BS1) = -977.921648 au

H(B3LYP/BS1) = -977.540969 au

G(B3LYP/BS1) = -977.614691 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2317.257690 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2316.518098 au

C	0.74524500	-1.95371800	0.22652900
C	-0.69507800	-1.97402300	0.23314800
H	1.31059900	-2.88042300	0.33435900
H	-1.23386500	-2.89908900	0.44499100
N	-1.30955800	-0.86056400	-0.03205500
N	1.33084900	-0.79918300	0.09461400
C	-2.73171200	-0.88276100	0.03840000
C	-3.48986800	-0.58801700	-1.10272300
C	-3.37829600	-1.19876400	1.24184400
C	-4.88182600	-0.62675800	-1.03842800
H	-2.98262700	-0.35600400	-2.03289500
C	-4.77201100	-1.21631600	1.30112500
H	-2.78403800	-1.39904100	2.12898800
C	-5.52778700	-0.93458700	0.16169300
H	-5.46339800	-0.41055600	-1.93029000
H	-5.26540300	-1.44973400	2.24065200
H	-6.61292100	-0.95069700	0.20868300
C	2.75247100	-0.82464600	-0.00054900
C	3.38032800	-1.57476400	-1.00594300
C	3.52887800	-0.09922000	0.91281200
C	4.77260400	-1.60101000	-1.09153900
H	2.77243900	-2.10772400	-1.73165800
C	4.91939900	-0.14745100	0.83129000
H	3.03717800	0.48047100	1.68551500
C	5.54653100	-0.89306100	-0.17066800
H	5.25011100	-2.17531800	-1.88071000
H	5.51500100	0.40658800	1.55148500
H	6.63056900	-0.91576300	-0.23657600
C	-1.42789800	2.02518700	-0.49669700
H	-1.95179600	1.51325800	-1.31792900
H	-2.04853700	1.88458300	0.40363100
C	-1.32575100	3.50923900	-0.83195300
H	-0.77082800	3.68104800	-1.76270900
H	-2.32517800	3.95190500	-0.96809700
H	-0.82837300	4.08767400	-0.04540700
C	1.28000300	2.20143000	-0.03999500
H	1.09091000	2.98044400	-0.78161200
H	2.24547200	1.74452300	-0.29236500
C	1.33234700	2.80950500	1.36627100
H	2.12661600	3.56847100	1.45688800
H	0.38770200	3.29774600	1.63218400
H	1.52335400	2.05477200	2.14154800
Ni	0.00223200	0.76176800	-0.17479600

Ni_10_V

E(B3LYP/BS1) = -937.404524 au

H(B3LYP/BS1) = -937.078090 au

G(B3LYP/BS1) = -937.144771 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -2276.726710 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -2276.025671 au

C	-0.72073500	-1.88397500	0.01928600
C	0.71902300	-1.88427700	-0.00813100
H	-1.27713600	-2.82235400	-0.00107000
H	1.27525700	-2.82256100	0.01893800
N	1.31013700	-0.72585700	-0.08108600

N	-1.31167300	-0.72503100	0.08368200
C	2.72580400	-0.68953900	-0.02839500
C	3.43691300	-1.41380500	0.94268100
C	3.42497100	0.09437800	-0.95776100
C	4.82979800	-1.36103400	0.97267300
H	2.89245400	-1.98277700	1.69105800
C	4.81745700	0.12544000	-0.93179600
H	2.86664200	0.65447400	-1.69817300
C	5.52509100	-0.59779700	0.03239400
H	5.37095900	-1.91275600	1.73652200
H	5.35200100	0.72378200	-1.66436500
H	6.61042600	-0.55839500	0.05678600
C	-2.72721700	-0.68867800	0.02883500
C	-3.42775100	0.10194800	0.95148300
C	-3.43696500	-1.41946500	-0.93839200
C	-4.82017200	0.13334600	0.92281600
H	-2.87054900	0.66700300	1.68893300
C	-4.82977900	-1.36643100	-0.97117800
H	-2.89144300	-1.99379700	-1.68188200
C	-5.52642700	-0.59637600	-0.03749700
H	-5.35575700	0.73698800	1.65026000
H	-5.36980200	-1.92329900	-1.73209300
H	-6.61170400	-0.55676900	-0.06404500
C	0.00331700	3.43612200	0.00022200
C	-1.10832700	2.40375100	0.18919800
C	1.11331700	2.40166400	-0.18653200
H	-1.56064600	2.39790700	1.18785900
H	-1.88413200	2.38745900	-0.58506300
H	1.88650800	2.38280700	0.59023200
H	1.56883100	2.39547900	-1.18373000
H	-0.14301300	4.08532000	-0.87325200
H	0.15043600	4.08846000	0.87125600
Ni	0.00041200	0.83705700	-0.00092000

Pd_10_IV

E(B3LYP/BS1) = -935.369063 au

H(B3LYP/BS1) = -934.988405 au

G(B3LYP/BS1) = -935.063513 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -936.840489 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -936.168221 au

C	0.72526400	-2.10163900	-0.01343200
C	-0.72718000	-2.10147100	0.01255800
H	1.24023700	-3.06466400	-0.06275000
H	-1.24228800	-3.06447000	0.06126400
N	-1.37773200	-0.98532000	-0.03793100
N	1.37603900	-0.98560000	0.03774000
C	-2.78984000	-1.02717900	0.06005300
C	-3.55216700	-0.25116800	-0.82534400
C	-3.43488300	-1.81132400	1.03104100
C	-4.94314900	-0.29417500	-0.76360300
H	-3.04316000	0.36046000	-1.56136300
C	-4.82717000	-1.82921800	1.09954300
H	-2.84266800	-2.36872300	1.75117200
C	-5.58559300	-1.07909100	0.19812600

H	-5.52734800	0.29708300	-1.46307500
H	-5.31873900	-2.42549900	1.86332200
H	-6.67036000	-1.09515000	0.25317100
C	2.78820000	-1.02794900	-0.06005900
C	3.43295500	-1.81124400	-1.03189500
C	3.55077400	-0.25351800	0.82646700
C	4.82525000	-1.82977100	-1.10023700
H	2.84052900	-2.36748300	-1.75275700
C	4.94174400	-0.29717700	0.76488200
H	3.04197900	0.35744700	1.56318600
C	5.58393100	-1.08118000	-0.19777200
H	5.31660600	-2.42537300	-1.86467900
H	5.52614400	0.29287400	1.46520300
H	6.66869800	-1.09773800	-0.25266500
C	-1.38289200	2.37109600	-0.13176800
H	-2.31426700	1.92853900	0.24802000
H	-1.10999000	3.18740600	0.54566400
Pd	0.00079600	0.85010700	-0.00007800
C	-1.58779000	2.91684400	-1.54736000
H	-1.86913000	2.13253300	-2.26253400
H	-2.38330700	3.67974400	-1.57600800
H	-0.67638800	3.38577600	-1.93606100
C	1.38598400	2.37000700	0.13214600
H	1.11367200	3.18618900	-0.54565200
H	2.31691700	1.92646800	-0.24753400
C	1.59128300	2.91631700	1.54742000
H	1.87139000	2.13212500	2.26317700
H	2.38786400	3.67812700	1.57558900
H	0.68053500	3.38686100	1.93564900

Pd_10_V

E(B3LYP/BS1) = -894.848475 au

H(B3LYP/BS1) = -894.520454 au

G(B3LYP/BS1) = -894.592329 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -896.305893 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -895.672924 au

C	-0.72647500	-2.03001500	0.00923500
C	0.72607300	-2.03015400	-0.00884600
H	-1.24290200	-2.99354800	-0.00431300
H	1.24234100	-2.99376300	0.00499500
N	1.36935500	-0.90928400	-0.05926400
N	-1.36959400	-0.90903700	0.05935900
C	2.78122500	-0.91334800	-0.01290600
C	3.50163600	-1.79366500	0.81340900
C	3.47269400	0.01605700	-0.80516600
C	4.89459800	-1.75658300	0.82341500
H	2.96922800	-2.47081400	1.47510900
C	4.86521400	0.03055300	-0.80424300
H	2.90150600	0.70457500	-1.41699400
C	5.58116100	-0.85306700	0.00844900
H	5.44424900	-2.42853300	1.47686700
H	5.39337400	0.74309000	-1.43157400
H	6.66712500	-0.82665600	0.01924800
C	-2.78148300	-0.91304300	0.01291500

C	-3.47307800	0.01581500	0.80569800
C	-3.50175600	-1.79298200	-0.81391600
C	-4.86560200	0.03021200	0.80464800
H	-2.90203900	0.70395900	1.41806900
C	-4.89472500	-1.75599000	-0.82403400
H	-2.96921100	-2.46974500	-1.47589700
C	-5.58141800	-0.85295000	-0.00866000
H	-5.39387700	0.74232600	1.43236300
H	-5.44426700	-2.42762500	-1.47790100
H	-6.66738200	-0.82659200	-0.01953900
C	-0.00025100	3.64336200	-0.00000900
C	-1.14163800	2.62740100	0.11808900
C	1.14186300	2.62814000	-0.11779100
H	-1.66262900	2.63995700	1.08108400
H	-1.85597700	2.62600000	-0.71108300
H	1.85582400	2.62708900	0.71169700
H	1.66326200	2.64117300	-1.08055200
H	-0.09124100	4.29358900	-0.88011300
H	0.09026700	4.29414300	0.87974200
Pd	0.00034300	0.92067800	-0.00007800

Ti_4_IIa

E(B3LYP/BS1) = -872.686281 au

H(B3LYP/BS1) = -872.356975 au

G(B3LYP/BS1) = -872.427445 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1664.339769 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1663.844284 au

C	0.11558700	0.23217500	-1.56814700
C	1.41041300	-0.07538000	-1.04132500
C	1.30223400	-1.26908800	-0.25841100
C	-0.81109300	-0.75070400	-1.09530300
C	-0.05936500	-1.68677600	-0.28669100
Si	-2.60248600	-0.34888900	-0.66976600
N	-2.07059400	0.45177700	0.81807900
Ti	-0.18553300	0.37394500	0.78347200
H	-2.66527300	0.67369700	1.61641700
H	-3.25957700	0.56329400	-1.63266000
H	-3.44972800	-1.53459400	-0.41134000
C	0.51974800	-0.32050800	2.58359300
H	0.06372200	0.36944100	3.31660800
H	1.61304300	-0.24019700	2.66221100
C	1.06942100	2.66887900	0.83741900
H	1.82903700	2.31829000	1.53529900
H	1.39445600	2.87729300	-0.17669700
C	-0.18306800	2.95419900	1.24930300
H	-0.47876800	2.83839400	2.29096200
H	-0.92574000	3.37572500	0.57729800
C	2.70333700	0.61068400	-1.38570000
H	3.37104800	0.70280400	-0.52298200
H	3.24088100	0.02601300	-2.14349600
H	2.54626200	1.60683100	-1.80758900
C	2.44920300	-2.00515800	0.36931500
H	2.13653400	-2.58899500	1.23875200
H	2.88702700	-2.70525200	-0.35428500
H	3.24710400	-1.32701900	0.68622700

C	-0.59869100	-2.93998600	0.34399700
H	-0.54240300	-3.76182200	-0.38183200
H	-0.02337500	-3.24029000	1.22323900
H	-1.64684500	-2.84373400	0.63916400
C	-0.20236000	1.37154300	-2.49878800
H	0.00013200	1.06467400	-3.53307000
H	-1.25544700	1.66153800	-2.45343100
H	0.40673300	2.26045400	-2.30738600
H	0.22967500	-1.34060200	2.85679700

TS_{Ti-4-IIa}

E(B3LYP/BS1) = -872.673953 au

H(B3LYP/BS1) = -872.344681 au

G(B3LYP/BS1) = -872.410492 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -1664.325795 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -1663.834238 au

C	-0.25650800	0.47094400	1.55268800
C	1.03248200	0.91205700	1.11563600
C	0.87822800	1.56823900	-0.14119000
C	-1.22817400	0.87116600	0.56969100
C	-0.51455900	1.55408200	-0.47578100
Si	-2.73505500	-0.18867700	0.17385500
N	-1.69577200	-1.35672900	-0.65216900
Ti	0.06181500	-0.68588600	-0.50221800
H	-2.00079200	-2.22677800	-1.08775400
H	-3.41011800	-0.74862100	1.36649800
H	-3.72024400	0.46190000	-0.71963200
C	1.21236600	-1.08568900	-2.23257800
H	1.18517900	-1.85359600	-3.00536200
H	0.37692500	-0.36975600	-2.49944800
H	2.15328400	-0.53213900	-2.28823900
C	1.15995000	-2.26897700	0.58429700
H	1.84916600	-1.83056500	1.29960700
H	0.34033700	-2.85169900	1.00141900
C	1.63543300	-2.59614400	-0.69477000
H	2.67726800	-2.43324300	-0.95131600
H	1.13713900	-3.37264600	-1.26726400
C	-1.12371500	2.21629900	-1.68419300
H	-1.34839000	3.26443800	-1.44821500
H	-0.44841900	2.21939400	-2.54519000
H	-2.06322200	1.74763800	-1.98866500
C	-0.54539000	-0.19920700	2.86822100
H	0.24450800	-0.89499900	3.16698100
H	-0.62329100	0.55957500	3.65741100
H	-1.49164500	-0.74558600	2.85268000
C	2.31530200	0.80565700	1.88893600
H	3.17876300	0.62000000	1.24164700
H	2.51004900	1.74794400	2.41766300
H	2.27769600	0.01865400	2.64695900
C	1.96869600	2.26256400	-0.90939800
H	2.05832600	3.30579000	-0.57992000
H	2.94477500	1.79262500	-0.75407600
H	1.76927800	2.28377300	-1.98511600

Zr_4_IIa

E(B3LYP/BS1) = -861.198663 au
 H(B3LYP/BS1) = -860.870056 au
 G(B3LYP/BS1) = -860.942899 au
 E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -861.968390 au
 E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -861.467984 au

C	0.05900900	0.23264200	1.69265300
C	0.83629700	1.26505400	1.07485800
C	0.00909700	1.92259800	0.10228300
C	-1.23962000	0.21702000	1.08621400
C	-1.26676300	1.29085800	0.11185100
Si	-2.28333700	-1.34448600	0.88306800
N	-1.28170900	-1.91887800	-0.45326900
H	-1.55221700	-2.67582700	-1.08100400
H	-2.25195200	-2.22055100	2.07777500
H	-3.68468800	-1.06930000	0.49016500
C	0.11057900	0.25645600	-2.76335400
H	0.25801700	-0.62996200	-3.41073900
H	0.93919800	0.95399600	-2.96713200
C	2.91975400	-1.25037600	-0.08889000
H	3.43999900	-0.37215800	-0.46702700
H	2.92401900	-1.39490900	0.98811300
C	2.38053600	-2.16710200	-0.91927500
H	2.46759000	-2.07140000	-2.00245100
H	1.94365700	-3.09037300	-0.54102900
Zr	0.20280500	-0.53982400	-0.70177500
C	-2.47028400	1.73478600	-0.67371000
H	-3.05742400	2.43862400	-0.06915600
H	-2.19390600	2.24792200	-1.59792900
H	-3.13257900	0.90361900	-0.93078800
C	0.39124200	3.14982700	-0.67635600
H	0.18654600	4.05158700	-0.08438400
H	1.45676000	3.16482300	-0.92576500
H	-0.17312400	3.23613900	-1.60820600
C	2.19493900	1.74810600	1.50874100
H	2.08445000	2.59700800	2.19586800
H	2.76221100	0.98038600	2.04174700
H	2.80075200	2.10037400	0.66758000
C	0.50507300	-0.64261200	2.83498100
H	0.18991200	-0.19266800	3.78515600
H	0.06046400	-1.64175800	2.79655700
H	1.59254300	-0.75214000	2.88290900
H	-0.81289700	0.74090600	-3.09928300

TS_{Zr-4-IIa}

E(B3LYP/BS1) = -861.183231 au
 H(B3LYP/BS1) = -860.854945 au
 G(B3LYP/BS1) = -860.922702 au
 E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -861.950226 au
 E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -861.452643 au

C	-0.80103000	0.67950000	1.41608100
C	0.04427400	1.68249200	0.84424300
C	-0.30870900	1.83227700	-0.53333300
C	-1.69600700	0.20361800	0.39236100
C	-1.38760500	0.92690400	-0.81086500

Si	-2.30373500	-1.58206700	0.34280200
N	-0.72819300	-2.17250100	-0.19829900
H	-0.52898400	-3.15244200	-0.39782700
H	-2.70439400	-2.10589200	1.66909900
H	-3.38786900	-1.81570500	-0.63997600
C	2.17697300	-0.92458900	-1.84690500
H	3.18383000	-0.90060600	-2.25913200
H	1.69561500	-1.86125300	-2.18552400
H	1.64483200	-0.05350800	-2.31379800
C	2.19531100	-0.93745600	1.27812000
H	2.28049200	-0.03313000	1.87518000
H	1.82663600	-1.81985600	1.80115200
C	3.08299500	-1.11244900	0.20579900
H	3.78890600	-0.32708400	-0.04490300
H	3.37687700	-2.10901700	-0.11017500
Zr	0.52189800	-0.56647100	-0.35506700
C	-2.11287300	0.82234900	-2.12940300
H	-2.88726400	1.59826600	-2.18511400
H	-1.45128900	0.97362400	-2.98907600
H	-2.61491700	-0.14094900	-2.25186000
C	-0.82715300	0.29273000	2.87163900
H	0.17009800	0.28590200	3.32240300
H	-1.42995700	1.01661000	3.43481400
H	-1.27640700	-0.69109000	3.02845400
C	1.03214700	2.53987600	1.58635100
H	1.89943900	2.80587600	0.97301900
H	0.55637200	3.48164600	1.88994700
H	1.39345800	2.05903300	2.49973200
C	0.23824600	2.87801400	-1.47061000
H	-0.31919900	3.81652800	-1.35349300
H	1.29037500	3.10512200	-1.27155000
H	0.14767200	2.58362000	-2.52068200

Hf_4_IIa

E(B3LYP/BS1) = -863.537005 au

H(B3LYP/BS1) = -863.208336 au

G(B3LYP/BS1) = -863.281345 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -862.926188 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -862.441906 au

C	0.17688200	0.62448800	1.73409400
C	1.23656500	1.21307100	0.96797900
C	0.65081200	1.90052400	-0.14694000
C	-1.06892400	0.91609100	1.08904500
C	-0.76248000	1.72423900	-0.07693500
Si	-2.55409200	-0.25139900	1.11155400
N	-1.81590900	-1.33776500	-0.08201800
H	-2.34978100	-2.05454200	-0.57219800
H	-2.77529600	-0.88249600	2.43313600
H	-3.80566600	0.37189900	0.62423700
C	0.23571500	-0.32828500	-2.65784800
H	0.03486000	-1.30518100	-3.13516600
H	1.26035900	-0.04012200	-2.94586400
C	2.29199900	-1.92021300	0.28796400
H	2.99038800	-1.40902200	-0.37364000
H	2.42024600	-1.75612400	1.35368700

C	1.38282800	-2.80081300	-0.18621100
H	1.33427700	-3.04675700	-1.24832100
H	0.74903500	-3.38152100	0.48143600
Hf	-0.00998500	-0.55423400	-0.48825100
C	-1.77079300	2.36542000	-0.99385800
H	-2.07848400	3.33215600	-0.57447100
H	-1.36168000	2.55528700	-1.98931000
H	-2.67625500	1.76305600	-1.10831000
C	0.34103400	-0.10822700	3.04091100
H	1.30930800	-0.61082900	3.12756900
H	0.28138900	0.60707800	3.87112000
H	-0.44569600	-0.85016900	3.20552900
C	2.68440500	1.31253600	1.37062700
H	3.36092300	1.27593700	0.51069000
H	2.86399100	2.27089300	1.87450700
H	2.97896900	0.52705800	2.07189900
C	1.39462100	2.76861100	-1.12369200
H	0.87828300	2.84095900	-2.08430300
H	1.49127300	3.78735400	-0.72610400
H	2.40715500	2.39978100	-1.31376500
H	-0.43600000	0.38945100	-3.14672700

TS_{Hf4-IIa}

E(B3LYP/BS1) = -863.519262 au

H(B3LYP/BS1) = -863.191013 au

G(B3LYP/BS1) = -863.25906 au

E(B3LYP/BS2//B3LYP/BS1, solvent = dichloromethane) = -862.904708 au

E(M06/BS2//B3LYP/BS1, solvent = dichloromethane) = -862.424050 au

C	-0.87199900	0.93268500	1.37029900
C	0.09595900	1.81512100	0.79649500
C	-0.15904100	1.90714600	-0.60940700
C	-1.74785900	0.47276500	0.31913100
C	-1.29795500	1.08711000	-0.90366100
Si	-2.52022900	-1.25199400	0.33689300
N	-0.97612000	-2.03272700	-0.04986800
H	-0.88991600	-3.04109700	-0.16474800
H	-3.05977400	-1.63882100	1.66069300
H	-3.55251600	-1.44528700	-0.70800900
C	1.97600700	-0.96877300	-1.68649900
H	2.94158100	-0.76955100	-2.14886100
H	1.67355200	-1.99607600	-1.94881800
H	1.27074800	-0.25314700	-2.20595300
C	2.01035700	-0.94538700	1.40456600
H	2.09331900	-0.06701900	2.04032400
H	1.70055300	-1.86177200	1.90876800
C	2.91018700	-1.05884000	0.32401200
H	3.57521500	-0.23370000	0.08854000
H	3.26476800	-2.03298600	0.00056300
Hf	0.37371500	-0.54467300	-0.19526600
C	-1.95790700	0.96701900	-2.25592900
H	-2.68332600	1.78060700	-2.38291000
H	-1.24387400	1.04542700	-3.08214700
H	-2.50713800	0.02843800	-2.36968100
C	-1.02104900	0.64107000	2.84160500
H	-0.05827200	0.59110800	3.35933600

H	-1.60274400	1.44013800	3.31850300
H	-1.55235500	-0.29636900	3.02470600
C	1.11611700	2.62416200	1.54953700
H	2.03263000	2.78246800	0.97180100
H	0.71033300	3.61745000	1.78166700
H	1.38836200	2.16287700	2.50322000
C	0.53998200	2.83738200	-1.56681500
H	0.07264300	3.83013100	-1.53760200
H	1.59648200	2.97360600	-1.31542800
H	0.48153100	2.48829400	-2.60223000