

Supporting Information

Computational insights in carbon-carbon homocoupling reactions mediated by organolanthanide(III) complexes.

Christos E. Kefalidis*^[a] Lionel Perrin^[a,b] and Laurent Maron*^[a]

^a Université de Toulouse et CNRS, INSA, UPS, UMR 5215, LPCNO, 135 Avenue de Rangueil, F-31077 Toulouse (France).

^b Present address: Université Lyon 1, CNRS, UMR 5246, ICBMS, 43 Boulevard du 11 Novembre 1918, F-69622 Villeurbanne (France).

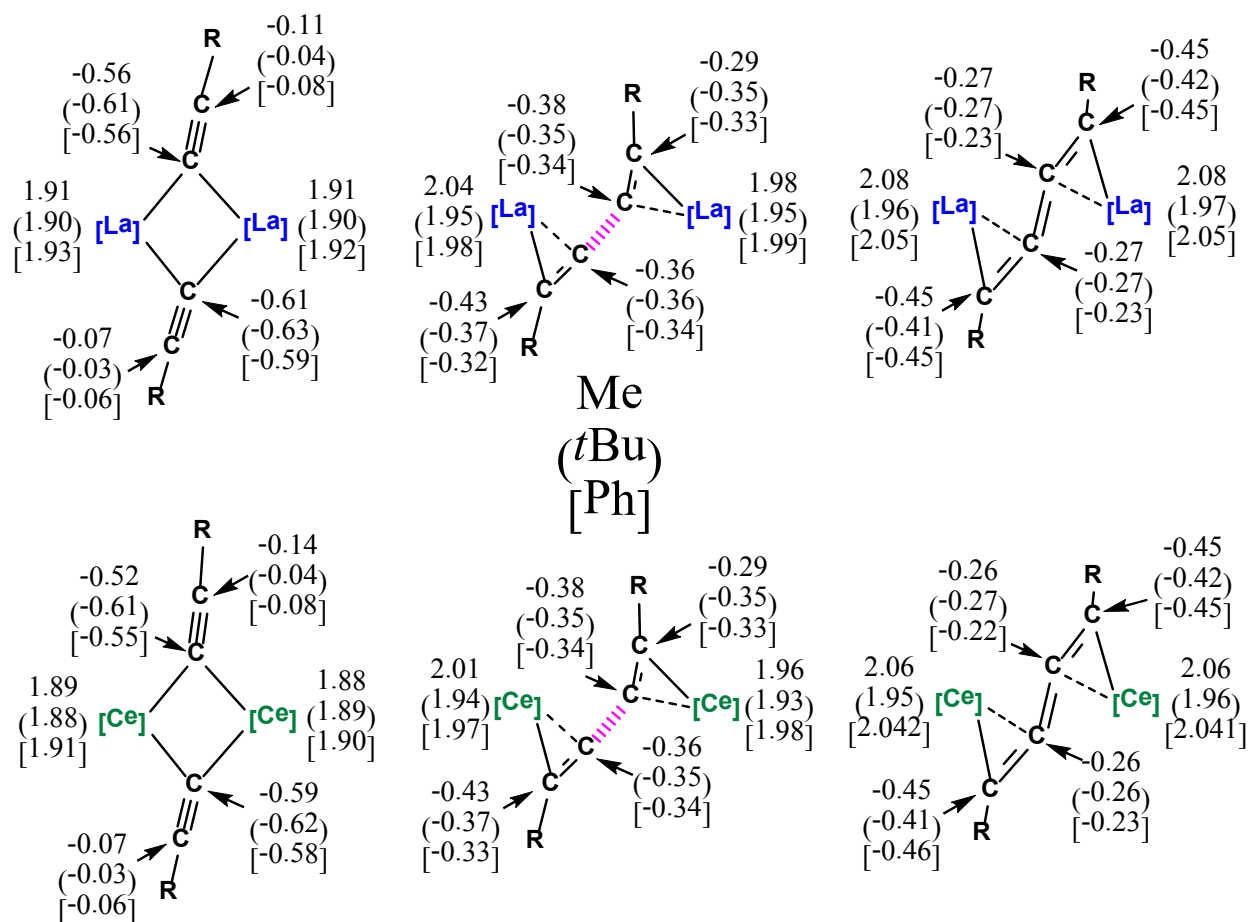


Figure S1. Selected natural charges for the C-C coupling step of $\{Cp^*Ln_2(CCR)\}_2$ intermediates (where $Ln = La, Ce$, and $R = Me, tBu, Ph$).

Cartesian Coordinates of Optimized Structures and their associated H value.

$(C_5Me_5)_2Sm-CH(SiMe_3)_2$				H	-4.13067800	-4.82792700	0.94663000
H = -1100.04458 au				H	-5.06085700	-3.50165600	1.63552000
Sm	-2.15505000	-0.99152800	3.02181300	H	-3.96039800	-3.20450600	0.28953400
C	-3.37358600	1.49618300	3.50598100	C	-1.03866500	-3.51716000	0.44479600
C	-3.50524500	1.29383600	2.10568900	H	-1.72194000	-3.09230600	-0.29767200
C	-4.19477100	0.53412400	4.17120400	H	-0.08158400	-3.00033200	0.34293600
C	-4.40493300	0.20434400	1.89808400	H	-0.87276700	-4.56469700	0.15753600
C	-4.85655900	-0.24010200	3.17606200	C	0.67218800	-3.59974300	3.11821600
C	-0.81822200	-3.44967600	3.03921700	H	1.05232700	-3.36222100	4.11567100
C	-1.72598500	-3.53630500	4.13590700	H	0.96938800	-4.63549100	2.90427600
C	-1.58578700	-3.42522400	1.84030600	H	1.19567500	-2.95780800	2.40617700
C	-3.05047200	-3.58778500	3.61460700	C	-1.37362200	-3.78339800	5.57658700
C	-2.96700400	-3.51646300	2.19367400	H	-1.46326800	-4.85074900	5.82052700
C	-4.26249900	-3.92591100	4.43352700	H	-0.34525900	-3.49253700	5.80954900
H	-4.35438400	-3.30795600	5.33432800	H	-2.03223100	-3.24758200	6.26960900
H	-5.18705900	-3.81643300	3.86385900	C	-6.03477100	-1.13455300	3.42427700
H	-4.21509200	-4.96923400	4.77392200	H	-6.14418900	-1.91052600	2.66194500
C	-4.08427400	-3.76539900	1.22123600	H	-5.98798500	-1.62810500	4.39806400

H	-6.96282500	-0.54642400	3.41003800	C	-1.00813300	1.83032600	-2.43347500
C	-4.47721300	0.48724900	5.64741300	C	0.95024300	0.88199100	-1.66377900
H	-5.34734000	1.10555900	5.90671700	C	-0.42970200	2.72613500	-1.48530200
H	-4.69612000	-0.52766300	5.99658900	C	0.79557600	2.14724600	-1.03122600
H	-3.63783600	0.86279100	6.24173600	C	-3.37303900	0.42624600	1.93074800
C	-2.68161600	2.66037600	4.15229100	C	-3.51417600	1.68266300	1.26997300
H	-3.37197100	3.50722800	4.26585100	C	-3.65023100	-0.60130200	0.98631100
H	-2.30294300	2.42833600	5.15274600	C	-3.91717000	1.42841800	-0.07408000
H	-1.83736200	3.01647400	3.55520500	C	-3.98026300	0.01695100	-0.25778400
C	-2.98196600	2.20170000	1.03212100	C	-3.51914700	3.03959900	1.91601500
H	-2.00866800	2.63432800	1.28341700	H	-4.54518500	3.36501600	2.13639400
H	-2.87244400	1.68416100	0.07526700	H	-2.97554900	3.05122300	2.86506400
H	-3.67123200	3.04069000	0.86531900	H	-3.07425000	3.80867100	1.27560700
C	-4.97028400	-0.21008900	0.56842700	C	-3.20870800	0.22155800	3.40858400
H	-4.22604800	-0.16126800	-0.23379600	H	-4.18872700	0.13300300	3.89657000
H	-5.36289300	-1.22987500	0.58879900	H	-2.65395500	-0.69130400	3.64719100
H	-5.79843500	0.44696600	0.26969700	H	-2.69129400	1.05482300	3.89328000
C	-0.06230700	0.29656100	2.34344500	C	-3.79306100	-2.06152200	1.29897500
Si	0.97961800	0.35285100	0.78748200	H	-4.82709500	-2.29988700	1.58437300
Si	0.78956700	0.50392400	3.99378500	H	-3.53480200	-2.68938800	0.44240900
C	1.92713000	2.00493900	0.61212500	H	-3.15146400	-2.37072900	2.12898400
C	2.30180600	-1.01056300	0.62350800	C	-4.50453300	-0.70027200	-1.46871400
C	-0.11357500	0.22447500	-0.77229800	H	-4.45647100	-0.07602400	-2.36579900
C	-0.39591700	-0.18168000	5.36575200	H	-3.94278100	-1.61570100	-1.67899200
C	1.15340900	2.30300300	4.50944200	H	-5.55624500	-0.98773200	-1.33444700
C	2.43042800	-0.42729700	4.22825200	C	-4.49171800	2.47022100	-0.98796200
H	1.24847100	2.86201200	0.68711200	H	-3.91530800	3.40021700	-0.98446500
H	2.68608600	2.11682900	1.39459600	H	-4.56345800	2.12498900	-2.02085100
H	2.43828600	2.06859000	-0.35568700	H	-5.50964300	2.73011400	-0.66557100
H	1.86736400	-2.00675000	0.49750300	C	-2.11683100	2.13090400	-3.39946000
H	2.91059700	-0.81021200	-0.26588100	H	-2.80078100	1.28675200	-3.53680400
H	2.97676200	-1.04487200	1.48302300	H	-2.71058400	2.99471800	-3.09586700
H	0.50223500	0.23989500	-1.67883000	H	-1.69954900	2.36044000	-4.38952600
H	-0.69585200	-0.70316200	-0.78436800	C	-0.87703100	4.13118300	-1.19215600
H	-0.81254000	1.06459300	-0.83708800	H	-0.79598300	4.38778900	-0.12948100
H	0.03189000	-0.00158100	6.35814200	H	-0.27018900	4.86422700	-1.74069100
H	-1.37699800	0.31796100	5.38434600	H	-1.91678700	4.29622300	-1.48651200
H	-0.53437800	-1.27100900	5.30613400	C	1.86458900	2.88470700	-0.27439900
H	1.85918100	2.76346800	3.81039000	H	2.44862600	2.23570900	0.38296400
H	0.25342600	2.92390600	4.52826700	H	2.57057400	3.34937900	-0.97615700
H	1.60382300	2.33579700	5.50853000	H	1.45543400	3.69261300	0.33965000
H	2.73030300	-0.39628300	5.28191200	C	2.17436900	0.01416600	-1.62165300
H	2.37576100	-1.47379900	3.92127100	H	2.83672600	0.22893400	-2.47159700
H	3.22594600	0.05168600	3.64771400	H	2.75907400	0.17612900	-0.71283600
H	-0.65312100	1.23017800	2.25126400	H	1.92825100	-1.05054900	-1.66383200
TS_{SBM}((Cp*)₂Sm-CH(SiMe₃)₂,HCCPh)				C	-0.29019600	-0.37428300	-3.58312600
H= -1408.190541 au				H	0.30876700	-1.25357600	-3.33868300
C	-0.02194700	-1.11814000	1.89523400	H	-1.32252100	-0.71095600	-3.71844700
H	-0.51677400	-1.65795600	0.29742700	H	0.05859300	0.00232700	-4.55501300
C	-1.01912100	-1.98087400	-0.73980500	Si	0.80901000	-2.81436200	2.10455700
C	-1.25397100	-2.90071200	-1.52031000	C	1.65952100	-3.11734900	3.78931000
C	-0.16405700	0.68906600	-2.53316300	H	0.94998500	-3.03032300	4.61858700
				H	2.05903200	-4.13858800	3.80411200

H	2.49492300	-2.43861300	3.98553100
C	-0.50081700	-4.19296200	1.99493700
H	-0.02220900	-5.17567100	2.07534400
H	-1.21952900	-4.11037200	2.81813500
H	-1.05781300	-4.16371000	1.05540300
C	2.13345100	-3.12932700	0.77664100
H	2.59501900	-4.11231200	0.92273900
H	1.69587500	-3.10911100	-0.22591700
H	2.92929100	-2.37851300	0.81448700
Si	0.82187900	0.25088000	2.86598500
C	2.69052100	0.36819600	2.53262200
H	3.09900300	1.31064100	2.91313000
H	3.22343600	-0.44594500	3.03360200
H	2.92206900	0.30154600	1.46636800
C	0.59268300	0.14186200	4.75650900
H	0.98340400	1.04691000	5.23708600
H	-0.46521600	0.05324500	5.02383800
H	1.11802100	-0.71646100	5.18284500
C	0.04063700	1.96566000	2.46781000
H	0.59755700	2.73231600	3.01863300
H	0.08612900	2.30247200	1.42194900
H	-0.99408500	2.01685100	2.81863900
H	-0.99987800	-1.25580900	2.39172000
Sm	-1.26997300	0.52598800	0.03717100
C	-1.53685500	-3.93893800	-2.45250400
C	-0.55600700	-4.35817600	-3.37146500
C	-2.79490100	-4.57089500	-2.46266100
C	-0.83164000	-5.37680500	-4.27594700
H	0.41804200	-3.87970500	-3.36094400
C	-3.06311000	-5.58536200	-3.37421200
H	-3.55123300	-4.25791100	-1.74986100
C	-2.08458800	-5.99093000	-4.28236600
H	-0.06653700	-5.69293800	-4.97923100
H	-4.03815200	-6.06417300	-3.37433900
H	-2.29721600	-6.78544000	-4.99203400

(C₅Me₅)₂Sm-CCPh

H= -1121.918899 au

Sm	3.24235000	0.53523900	-0.25581900
C	2.08999800	-0.81147400	1.41578800
C	1.49063200	-1.48456400	2.26259000
C	4.36179900	-0.20243700	-2.66154000
C	5.45983100	-0.11965800	-1.75195000
C	3.54682700	-1.30496100	-2.26398200
C	5.31710300	-1.17176300	-0.79736400
C	4.14312700	-1.91280600	-1.12045000
C	1.69284000	2.59301600	0.67517600
C	2.91229300	2.68405800	1.40272300
C	1.96604300	2.92980800	-0.68648500
C	3.94294000	3.07804500	0.49444900
C	3.35203400	3.24713500	-0.79406500
C	3.70103400	-3.18942900	-0.46731300
H	2.62242300	-3.34098300	-0.55635100

H	4.19670600	-4.05428700	-0.92906700
H	3.93225100	-3.20372200	0.60051200
C	6.29561300	-1.52007700	0.28916600
H	7.02007400	-2.27091700	-0.05341600
H	6.87546100	-0.65121200	0.61796400
H	5.79720300	-1.93934100	1.16936600
C	6.65650400	0.77853000	-1.88827300
H	6.41876300	1.70673800	-2.41601000
H	7.08689300	1.05210900	-0.91922600
H	7.45486600	0.28525600	-2.45894900
C	4.19357500	0.59975900	-3.92067100
H	4.66044600	1.58551200	-3.84630300
H	4.65561200	0.09034700	-4.77703500
H	3.14051300	0.75481300	-4.17962400
C	2.33591200	-1.81623000	-2.99405300
H	1.60220900	-2.26053700	-2.31317800
H	1.82908800	-1.02682700	-3.55941400
H	2.60753000	-2.59552400	-3.71850800
C	4.02495100	3.85011400	-1.99239300
H	5.08776800	3.59508400	-2.04403100
H	3.56282100	3.53297600	-2.93175700
H	3.96381500	4.94655800	-1.96293100
C	5.35644800	3.43371600	0.86381300
H	5.71570300	2.86166100	1.72585100
H	6.05506200	3.25984600	0.03922500
H	5.44141900	4.49477200	1.13430800
C	3.06190100	2.48697500	2.88432200
H	2.83168600	3.41082700	3.43152100
H	2.39375900	1.70552900	3.25706200
H	4.08283600	2.20262300	3.15981400
C	0.34081900	2.30577700	1.26178000
H	-0.35122900	1.90173800	0.51604900
H	0.39936600	1.57786600	2.07507200
H	-0.11754500	3.22101300	1.65986900
C	0.94049300	3.07293100	-1.77742300
H	1.37557800	2.93922100	-2.77332300
H	0.12281800	2.35090700	-1.67522100
H	0.48004300	4.06978400	-1.76422100
C	0.79731300	-2.26339100	3.23615600
C	1.45826400	-2.73741600	4.38574700
C	-0.56581500	-2.57619600	3.07084800
C	0.77768400	-3.49494500	5.33283300
H	2.50937900	-2.50155300	4.52202300
C	-1.23901700	-3.33540800	4.02176600
H	-1.08397000	-2.21501500	2.18762800
C	-0.57266500	-3.79817200	5.15677900
H	1.30466600	-3.85158300	6.21399500
H	-2.29097200	-3.56711500	3.87658300
H	-1.10159700	-4.39053000	5.89822800

(C₅H₅)₂Sm-CH(SiMe₃)₂

H= -707.315326 au

Sm	-2.06784700	-0.88371300	3.09875500
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C	-3.48718300	1.47758200	3.48212700	C	-1.11808000	-2.03649100	-0.60195700
C	-3.60784000	1.18367400	2.10492100	C	-1.34957900	-2.93511100	-1.40851000
C	-4.21003300	0.49203800	4.20679500	C	-0.13702900	0.54817000	-2.41405700
C	-4.39662300	0.01036100	1.97397700	C	-0.89472200	1.73611400	-2.29318000
C	-4.77860000	-0.40779100	3.27432900	C	0.97372200	0.64260500	-1.53511100
C	-0.62091000	-3.23409200	2.82951000	C	-0.26203000	2.56572600	-1.33134300
C	-1.48098000	-3.47011900	3.93174600	C	0.90185600	1.89200400	-0.87730000
C	-1.42173600	-3.13463100	1.66646200	C	-3.49913000	0.52431300	1.73361500
C	-2.81318900	-3.51613900	3.44994300	C	-3.47719200	1.77076600	1.05226200
C	-2.77715400	-3.30846700	2.04823700	C	-3.77742500	-0.48637200	0.78636800
C	-0.08978900	0.45300400	2.37252900	C	-3.75569900	1.52518900	-0.31459900
Si	0.93175200	0.29196800	0.81468500	C	-3.92766500	0.12966800	-0.48344100
Si	0.73342000	0.59872500	4.03797900	Si	0.89298700	-2.81531400	2.10833800
C	2.16701800	1.73050800	0.58941300	C	1.85375500	-3.06179300	3.73948100
C	1.94463400	-1.31606900	0.69532800	H	1.18266400	-3.05969100	4.60455800
C	-0.23243900	0.34206600	-0.69667600	H	2.34849700	-4.03998600	3.71068300
C	-0.47426600	-0.08773400	5.41348300	H	2.62982500	-2.30939900	3.90952700
C	1.06500900	2.39148400	4.57885100	C	-0.32157800	-4.27715600	2.03427800
C	2.32255300	-0.41404000	4.27381200	H	0.21993300	-5.22823000	2.08852300
H	1.65171800	2.69726100	0.60829300	H	-1.01571700	-4.24332300	2.88169500
H	2.91694400	1.74112600	1.38831800	H	-0.91071000	-4.27437600	1.11375700
H	2.70085900	1.65488800	-0.36497500	C	2.15433400	-2.96300300	0.69509600
H	1.30886500	-2.20658100	0.69959700	H	2.71044000	-3.90408100	0.76705800
H	2.51300100	-1.32205300	-0.24172300	H	1.65307200	-2.93983000	-0.27715000
H	2.66354400	-1.41198100	1.51461600	H	2.88093100	-2.14441100	0.72312600
H	0.33044100	0.31710100	-1.63648600	Si	0.72383200	0.24924200	2.87604000
H	-0.92064600	-0.51122400	-0.70019400	C	2.54639500	0.50566300	2.40562600
H	-0.83598600	1.25688800	-0.69802600	H	2.93649100	1.42066800	2.86462200
H	0.00231600	0.09379500	6.38286000	H	3.17026900	-0.32595000	2.74624300
H	-1.44045700	0.43733800	5.47591100	H	2.67284300	0.59098100	1.32217500
H	-0.63644800	-1.17843400	5.39472300	C	0.57767200	0.10442000	4.76833000
H	1.78576500	2.86189200	3.90222600	H	0.94381600	1.01767500	5.25162600
H	0.14806400	2.99006800	4.54991400	H	-0.46652500	-0.03601800	5.06837800
H	1.47025100	2.44280200	5.59557000	H	1.15334300	-0.73810000	5.15862600
H	2.66890200	-0.35026100	5.31116300	C	-0.15456800	1.93905500	2.54460200
H	2.17142700	-1.47111000	4.03452800	H	0.38345000	2.67630800	3.15239400
H	3.12540000	-0.03835100	3.63142500	H	-0.11057700	2.35664900	1.52810500
H	-0.62008800	1.41582500	2.24212800	H	-1.19164000	1.94671400	2.89442100
H	-1.17054300	-3.64371900	4.95627800	H	-1.02587500	-1.38349200	2.51547800
H	0.45924900	-3.17101100	2.86249500	Sm	-1.26500600	0.43108700	0.09272400
H	-1.05996700	-2.97969200	0.65713900	C	-1.62970900	-3.94129200	-2.37531800
H	-3.69887600	-3.71574100	4.04172700	C	-0.67713900	-4.26677500	-3.35964000
H	-3.63100400	-3.32273700	1.38125900	C	-2.86038100	-4.62475100	-2.36290100
H	-5.41019100	-1.25582200	3.50999900	C	-0.95266400	-5.24842100	-4.30431800
H	-4.34793200	0.46447000	5.28233800	H	0.27367700	-3.74305400	-3.36870100
H	-2.96551800	2.32696400	3.90753000	C	-3.12747000	-5.60362300	-3.31302800
H	-4.70480700	-0.44861400	1.04164700	H	-3.59489400	-4.37708200	-1.60298200
H	-3.18618900	1.76057700	1.29089500	C	-2.17673900	-5.91808700	-4.28483900
				H	-0.21039500	-5.49247600	-5.05896800
				H	-4.08051200	-6.12463500	-3.29538300
				H	-2.38915600	-6.68429600	-5.02508100
				H	-3.35805900	0.37568900	2.79780600
				H	-3.32964400	2.74470300	1.50488100
TS_{SBM}((Cp)₂Sm-CH(SiMe₃)₂,HCCPh)							
H= -1015.463146 au							
C	-0.08730300	-1.18748800	1.96343700				
H	-0.59521000	-1.71648000	0.48586000				

H	-3.84328500	2.27718700	-1.08900100
H	-4.16248900	-0.37714600	-1.41177500
H	-3.86581700	-1.54601900	0.99132500
H	1.62639000	2.28065000	-0.17183100
H	1.75183900	-0.10082900	-1.41189000
H	-0.57643500	3.56290000	-1.04486000
H	-1.78843000	1.97915600	-2.85474600
H	-0.35635500	-0.28237100	-3.07238500

(C₅H₅)₂Sm-CCPh

H= -729.173164 au

Sm	3.24553200	0.48664400	-0.15185400
C	2.07858100	-0.87063000	1.47311300
C	1.47246500	-1.54254300	2.31588500
C	4.64923800	-0.16954800	-2.41616700
C	5.63788800	0.17724000	-1.46120200
C	4.04162800	-1.38168500	-1.99502500
C	5.63848800	-0.82082900	-0.45159100
C	4.65615300	-1.78687900	-0.78422700
C	1.35362400	2.45842500	0.12443100
C	2.37756100	2.80598000	1.03438200
C	1.86506800	2.61457800	-1.19270000
C	3.52579300	3.17961500	0.28378700
C	3.20192000	3.07473000	-1.09197000
C	0.77138700	-2.31338400	3.28909700
C	0.99527100	-3.69829900	3.41073200
C	-0.16132600	-1.70501800	4.15104400
C	0.30837600	-4.44493900	4.36171500
H	1.71313300	-4.17399400	2.74954900
C	-0.84393500	-2.45786900	5.10002700
H	-0.33868300	-0.63754900	4.06228200
C	-0.61288200	-3.82952300	5.20982100
H	0.49267400	-5.51292200	4.44238500
H	-1.56035200	-1.97265000	5.75756300
H	-1.14768900	-4.41558700	5.95211800
H	4.41806100	-2.67619900	-0.21503400
H	6.30427500	-0.86202800	0.40375500
H	6.30415500	1.03035900	-1.51616400
H	4.42820600	0.37217600	-3.32861100
H	3.26939500	-1.92652800	-2.52728300
H	0.35326800	2.13782100	0.38917100
H	1.30993900	2.47087300	-2.11341000
H	3.85435600	3.32254800	-1.92065300
H	4.46250100	3.54540200	0.69014600
H	2.29304400	2.79959300	2.11467700

(C₅Me₅)₂La-CH(SiMe₃)₂

H= -1096.921196 au

La	-2.16277400	-0.99443100	3.01433000
C	-3.44949400	1.55184000	3.49764800
C	-3.58669800	1.34886500	2.09821000
C	-4.26454600	0.58738300	4.16702300
C	-4.48254500	0.25497800	1.89564200

C	-4.92377400	-0.19357300	3.17536100
C	-0.81353500	-3.53955100	3.06296600
C	-1.73288500	-3.61536300	4.15228000
C	-1.56671500	-3.53506000	1.85658500
C	-3.05111700	-3.67488300	3.61719700
C	-2.95242000	-3.61581200	2.19625400
C	-4.27757300	-3.99365300	4.42246800
H	-4.34320800	-3.40617500	5.34585100
H	-5.19690500	-3.82217000	3.85884700
H	-4.27809000	-5.04997200	4.72424400
C	-4.06975700	-3.84779000	1.21776800
H	-4.12702400	-4.90682500	0.93128000
H	-5.04433700	-3.58194000	1.63659000
H	-3.94583300	-3.27603400	0.29236900
C	-0.99957900	-3.59561300	0.46352200
H	-1.71230900	-4.05072500	-0.23096100
H	-0.72391200	-2.61881600	0.04697100
H	-0.09235700	-4.20889600	0.44187000
C	0.67954500	-3.66386900	3.15632800
H	1.04623600	-3.41932900	4.15733800
H	0.99887500	-4.69432700	2.94690100
H	1.19803400	-3.01279600	2.44869800
C	-1.39084300	-3.83656900	5.59959200
H	-1.45687700	-4.90187200	5.85946500
H	-0.37246900	-3.51697700	5.83982300
H	-2.06977900	-3.30707900	6.27791300
C	-6.07119200	-1.12625400	3.42749500
H	-6.15755900	-1.90128500	2.66056200
H	-5.99869200	-1.62524700	4.39745400
H	-7.02072000	-0.57335800	3.42456300
C	-4.53136200	0.53317100	5.64582200
H	-5.38729400	1.16404600	5.92169400
H	-4.76523600	-0.48098300	5.98779800
H	-3.67896600	0.88839900	6.23469700
C	-2.74150300	2.70646500	4.14476600
H	-3.41644100	3.56595200	4.25634300
H	-2.37150900	2.46695400	5.14688800
H	-1.88771800	3.04812000	3.55222500
C	-3.05570600	2.24900700	1.02141500
H	-2.09458600	2.69872300	1.28916800
H	-2.91544500	1.72035700	0.07429200
H	-3.75224900	3.07572300	0.82597200
C	-5.03916300	-0.18056600	0.56889900
H	-4.30769900	-0.08086000	-0.24033900
H	-5.37178500	-1.22244400	0.58265100
H	-5.90789900	0.42822900	0.28338700
C	-0.01383600	0.36552700	2.33247600
Si	1.03107800	0.39538000	0.78124900
Si	0.83591500	0.55035400	3.98261500
C	2.15186600	1.93990800	0.65425900
C	2.18500800	-1.10420000	0.55956800
C	-0.08266800	0.45413600	-0.77015800
C	-0.32056600	-0.15600500	5.37434800

C	1.18300200	2.34646500	4.51649400	H	-5.66506800	-0.92351000	-1.31312500
C	2.47600100	-0.39032300	4.17903000	C	-4.57179100	2.51777100	-0.91443200
H	1.56747100	2.86206700	0.74782700	H	-3.97701400	3.43695700	-0.90289300
H	2.91313400	1.95075500	1.44234100	H	-4.64289300	2.18191400	-1.95065600
H	2.67409500	1.97238000	-0.30926300	H	-5.58633500	2.79608800	-0.59702800
H	1.62793600	-2.03847000	0.44235900	C	-2.19920200	2.30971000	-3.37949800
H	2.78902100	-0.96769400	-0.34487300	H	-2.91170500	1.49202300	-3.53182400
H	2.87482400	-1.22435000	1.40000300	H	-2.75346400	3.16676500	-2.99247700
H	0.52357000	0.44828800	-1.68313600	H	-1.82800900	2.59113200	-4.37466000
H	-0.76280900	-0.40397600	-0.82251600	C	-0.76128700	4.19520500	-1.22908400
H	-0.69045200	1.36477900	-0.78540400	H	-0.42455100	4.49131300	-0.22967000
H	0.14901000	0.01177800	6.35005500	H	-0.31457300	4.90777000	-1.93608000
H	-1.29709800	0.34886600	5.43932700	H	-1.84395000	4.35042800	-1.26515000
H	-0.46708000	-1.24501700	5.31342200	C	1.97440600	2.79094700	-0.45241100
H	1.87303000	2.82419500	3.81349700	H	2.53687700	2.09551200	0.17684400
H	0.27105000	2.95029900	4.54669500	H	2.68710400	3.21840000	-1.17064400
H	1.64078700	2.38044100	5.51207200	H	1.64185700	3.61567400	0.18565600
H	2.82021600	-0.33695500	5.21801800	C	2.05825000	-0.07285600	-1.83034800
H	2.39105600	-1.44440700	3.90407100	H	2.72510800	0.11766400	-2.68257500
H	3.25376000	0.05767200	3.55154400	H	2.66231900	0.02517500	-0.92400700
H	-0.61928600	1.29016400	2.23923000	H	1.73849000	-1.11711200	-1.89562300

TS_{SBM}((Cp*)₂La-CH(SiMe₃)₂,HCCPh)

H= -1405.070489 au

C	-0.00801100	-1.16769200	1.95833900	H	-0.51781100	-0.31137100	-3.68232200
H	-0.47889300	-1.69887300	0.37460100	H	0.00438000	-1.24009900	-3.44403600
C	-0.95738000	-2.03845900	-0.68135700	H	-1.57948500	-0.55482300	-3.79090500
C	-1.15985700	-2.94892200	-1.48195800	H	-0.16261500	0.02203700	-4.66753100
C	-0.27403300	0.74607500	-2.64623700	Si	0.81697300	-2.86033900	2.19825300
C	-1.05259100	1.92727300	-2.48948300	C	1.63320400	-3.14716100	3.90283100
C	0.89100700	0.87182800	-1.83291000	H	0.90690200	-3.05093100	4.71655500
C	-0.38210400	2.77946300	-1.56276500	H	2.03350800	-4.16759700	3.93812400
C	0.83395400	2.13446600	-1.17902800	H	2.46391800	-2.46502800	4.10808000
C	-3.45796800	0.42643000	1.97839100	C	-0.48879600	-4.23966600	2.06428700
C	-3.60671400	1.69220000	1.33786700	H	-0.01459300	-5.22207800	2.17010900
C	-3.74436100	-0.58746400	1.02172700	H	-1.23400100	-4.14739400	2.86255400
C	-4.01823100	1.45872900	-0.00720600	H	-1.01440100	-4.21881200	1.10653600
C	-4.08535100	0.04934300	-0.20968000	C	2.17010200	-3.16957500	0.89815800
C	-3.58990300	3.03916900	2.00461700	H	2.62530500	-4.15555400	1.04383000
H	-4.60694900	3.36199100	2.26677200	H	1.75655000	-3.13542000	-0.11412200
H	-3.01294900	3.03588100	2.93446700	H	2.96755700	-2.42224900	0.96289200
H	-3.16831500	3.81884300	1.36074000	Si	0.84616800	0.22135000	2.88820700
C	-3.25533500	0.20564400	3.44945100	C	2.71226600	0.32401600	2.53969500
H	-4.22045900	0.14256500	3.97008000	H	3.13129300	1.26175500	2.92032900
H	-2.72022900	-0.72486900	3.66317800	H	3.24696200	-0.49702000	3.02728600
H	-2.69675800	1.01981700	3.92179300	H	2.92889300	0.26421500	1.46895900
C	-3.86449900	-2.05611300	1.30652900	C	0.60245900	0.16996600	4.77827800
H	-4.89464200	-2.31911400	1.58410900	H	1.03015200	1.06629900	5.24306100
H	-3.59271300	-2.66457400	0.43966200	H	-0.46121200	0.13526600	5.03577800
H	-3.21967800	-2.36946600	2.13258200	H	1.08270000	-0.70285500	5.22778900
C	-4.60761100	-0.65073400	-1.43221600	C	0.10219400	1.94001000	2.42028100
H	-4.54006200	-0.02128400	-2.32473400	H	0.55161200	2.69385900	3.07628100
H	-4.05981900	-1.57481500	-1.64337700	H	0.32706500	2.29159000	1.40383800
				H	-0.97893200	1.99413700	2.60231800
				H	-0.99183500	-1.28207200	2.45038600
				La	-1.29011600	0.55203200	0.04026800

C	-1.39625400	-3.97496400	-2.44040800
C	-0.36995300	-4.37701200	-3.31639800
C	-2.65035600	-4.60888200	-2.52269900
C	-0.59743700	-5.38128500	-4.24994000
H	0.60113300	-3.89664600	-3.24944900
C	-2.86973600	-5.60948000	-3.46241900
H	-3.44199800	-4.30834000	-1.84354700
C	-1.84649900	-5.99826100	-4.32769100
H	0.20238700	-5.68403300	-4.91971500
H	-3.84211800	-6.09044900	-3.51857100
H	-2.02152800	-6.78180400	-5.05948200

(C₅Me₅)₂La-CCPh

H= -1118.790113 au

La	3.17473900	0.51840300	-0.29712800
C	2.03654800	-0.86563100	1.48261500
C	1.43677800	-1.53683400	2.33173900
C	4.44271100	-0.26298700	-2.72486100
C	5.50578000	-0.16556100	-1.77793500
C	3.62970300	-1.37670000	-2.35704400
C	5.34583500	-1.22198100	-0.83023400
C	4.19327600	-1.97671000	-1.19300800
C	1.67184200	2.69122700	0.72067400
C	2.91212900	2.75733400	1.41215400
C	1.91114800	3.03322500	-0.64629500
C	3.92286100	3.14033000	0.47655900
C	3.29789000	3.32700700	-0.79289700
C	3.73926100	-3.25348800	-0.54652700
H	2.66744300	-3.42195500	-0.68124700
H	4.26370600	-4.11817400	-0.97565100
H	3.92357300	-3.25437000	0.53076300
C	6.29223300	-1.56092700	0.28715600
H	7.02576700	-2.31525600	-0.02743700
H	6.86344400	-0.68948700	0.62427400
H	5.76939200	-1.97251200	1.15703900
C	6.68615800	0.75975500	-1.86892100
H	6.44054400	1.69222900	-2.38647900
H	7.08530800	1.02589900	-0.88452300
H	7.51033600	0.29602600	-2.42761800
C	4.30027000	0.55051400	-3.98023000
H	4.72203600	1.55429400	-3.87314300
H	4.82130900	0.07508700	-4.82222200
H	3.25444400	0.66528200	-4.28627900
C	2.45141300	-1.90230400	-3.12888000
H	1.70437800	-2.36693000	-2.47608200
H	1.94795100	-1.11741000	-3.70412500
H	2.75757900	-2.67032000	-3.85166600
C	3.95007600	3.89818000	-2.01848800
H	5.01650700	3.65774500	-2.06881300
H	3.48722400	3.53840600	-2.94293800
H	3.87251300	4.99385800	-2.03190100
C	5.35001600	3.47492100	0.81144700
H	5.73069800	2.87870400	1.64778500

H	6.02272200	3.31702600	-0.03762100
H	5.45284700	4.52791000	1.10626900
C	3.10178700	2.55097100	2.88801800
H	2.90618500	3.47634800	3.44615500
H	2.42956800	1.78176000	3.27896500
H	4.12464800	2.24581700	3.13286000
C	0.33280000	2.41580600	1.34280400
H	-0.38573200	2.02810300	0.61325700
H	0.40286800	1.68044900	2.14898600
H	-0.10406200	3.33206900	1.76223800
C	0.85888500	3.19335900	-1.70877600
H	1.26672700	3.06270200	-2.71687700
H	0.03526700	2.47996700	-1.59019000
H	0.40849900	4.19449800	-1.67905100
C	0.74315900	-2.31246800	3.30791300
C	1.40759900	-2.79589900	4.45158400
C	-0.62377500	-2.61295500	3.15111900
C	0.72689500	-3.55050300	5.40092600
H	2.46162300	-2.56951900	4.58128600
C	-1.29727700	-3.36910100	4.10424000
H	-1.14469100	-2.24466900	2.27244000
C	-0.62725400	-3.84129700	5.23319300
H	1.25669600	-3.91461100	6.27733200
H	-2.35221500	-3.59107900	3.96556300
H	-1.15631000	-4.43136300	5.97639700

TS_{SBM}((Cp*)₂La-CH(SiMe₃)₂,HCC^tBu)

H= -1331.276763 au

C	-0.01929000	-1.22015300	1.91856700
H	-0.46302700	-1.67711600	0.36851400
C	-0.96774200	-2.02069800	-0.71045200
C	-1.21602700	-2.95591500	-1.46796700
C	-0.04468300	0.80910700	-2.59536500
C	-0.90867300	1.93758700	-2.50428700
C	1.04879600	1.01157300	-1.70474300
C	-0.35950100	2.83503400	-1.54126900
C	0.86298900	2.26890200	-1.06469800
C	-3.46042000	0.51349100	1.90855200
C	-3.58883800	1.75503000	1.21697200
C	-3.73773700	-0.53520600	0.98774800
C	-3.97678600	1.47040700	-0.12563200
C	-4.05166800	0.05476000	-0.27278800
C	-3.56979600	3.12695300	1.83074000
H	-4.58456200	3.45720700	2.09238800
H	-2.98068300	3.16359900	2.75237400
H	-3.15853000	3.88044000	1.15046800
C	-3.28819500	0.34122600	3.39014200
H	-4.26292500	0.23189300	3.88434900
H	-2.70458900	-0.54967300	3.64394200
H	-2.79575500	1.19984700	3.85673800
C	-3.86721000	-1.99041700	1.33049400
H	-4.90512100	-2.24309600	1.58771400
H	-3.56673700	-2.63451800	0.49990600

H	-3.24890700	-2.26553500	2.18991500
C	-4.55937500	-0.68458200	-1.47734400
H	-4.33112600	-0.16074700	-2.41140300
H	-4.12166300	-1.68468400	-1.54685700
H	-5.65029600	-0.80929100	-1.43965500
C	-4.51004500	2.48706000	-1.09155200
H	-3.92767300	3.41360200	-1.09297900
H	-4.53851600	2.10945400	-2.11593200
H	-5.53951000	2.76241300	-0.82314700
C	-2.02217400	2.22534600	-3.46945800
H	-2.68543400	1.36672200	-3.62206800
H	-2.64066600	3.06568300	-3.14904600
H	-1.61381500	2.48519300	-4.45559800
C	-0.83837500	4.22798700	-1.24090400
H	-0.74138300	4.48693700	-0.18025200
H	-0.26311300	4.97742800	-1.80148500
H	-1.88833600	4.36672100	-1.51321000
C	1.90250600	3.00649100	-0.26717200
H	2.49046100	2.34761700	0.37825700
H	2.61144100	3.50919200	-0.93915600
H	1.46633900	3.78539200	0.36627800
C	2.27428800	0.14746600	-1.62807400
H	2.97925000	0.38880700	-2.43569100
H	2.81259800	0.28190200	-0.68616600
H	2.03429100	-0.91615800	-1.71642000
C	-0.13867100	-0.26426900	-3.63801700
H	0.34058100	-1.19005100	-3.31081700
H	-1.17717600	-0.50189000	-3.88744200
H	0.35277000	0.05297600	-4.56870000
Si	0.81433200	-2.91309900	2.13685400
C	1.66024100	-3.22103500	3.82299900
H	0.94460200	-3.15544800	4.64901600
H	2.07491100	-4.23636100	3.82796500
H	2.48448500	-2.53274400	4.03298200
C	-0.49789800	-4.28708500	2.01542000
H	-0.02723300	-5.27546200	2.06875800
H	-1.21021500	-4.21588100	2.84510600
H	-1.06116400	-4.22199100	1.08154400
C	2.14450500	-3.20052300	0.80953300
H	2.60298100	-4.18887700	0.92648100
H	1.71235700	-3.14233400	-0.19386000
H	2.94272600	-2.45405300	0.87693700
Si	0.81140200	0.14778500	2.90563100
C	2.68020800	0.28966100	2.59193700
H	3.08756700	1.18350900	3.07688300
H	3.21641900	-0.57572300	2.99281500
H	2.90899600	0.35060000	1.52414600
C	0.54154300	0.02644900	4.78852500
H	0.95254600	0.91250500	5.28696500
H	-0.52470800	-0.02738000	5.03146900
H	1.02684100	-0.85403400	5.21669500
C	0.05395000	1.86971800	2.48636400
H	0.48614600	2.60833400	3.17068400

H	0.28619200	2.25630800	1.48466400
H	-1.02932900	1.89995500	2.65528100
H	-1.00908600	-1.34792500	2.39596600
La	-1.25433900	0.56186100	0.00760200
C	-1.50474100	-4.08928600	-2.36233100
C	-2.53555500	-5.02225700	-1.69470000
H	-2.74095000	-5.87583600	-2.35013800
H	-2.16409300	-5.40525000	-0.74010600
H	-3.47840100	-4.49912000	-1.50966000
C	-0.19680500	-4.86567100	-2.61941700
H	-0.39610700	-5.72054400	-3.27521000
H	0.54957400	-4.22844400	-3.10265200
H	0.22803500	-5.24091700	-1.68424300
C	-2.07181200	-3.57986700	-3.70190100
H	-2.99191800	-3.00808900	-3.55001600
H	-1.35149200	-2.94126300	-4.21902600
H	-2.30180600	-4.43297000	-4.34943300

(C₅Me₅)₂La-CC'Bu

H= -1044.9959 au

La	3.19052500	0.51660700	-0.28844100
C	2.04596900	-0.86848300	1.46996600
C	1.44148400	-1.54306000	2.31062000
C	0.72105800	-2.34988200	3.30952700
C	4.42831600	-0.25012800	-2.74147000
C	5.50365900	-0.16223700	-1.80803400
C	3.61767800	-1.36503700	-2.37177600
C	5.35348000	-1.22524500	-0.86624400
C	4.19542600	-1.97522300	-1.22057600
C	1.69347000	2.69821600	0.72893700
C	2.93329100	2.75930400	1.42125300
C	1.93480100	3.04052400	-0.63739800
C	3.94586100	3.14032300	0.48699000
C	3.32249500	3.33060600	-0.78233000
C	3.74773400	-3.25558900	-0.57758200
H	2.67533600	-3.42388000	-0.70753200
H	4.27122300	-4.11801200	-1.01273600
H	3.93769600	-3.25901400	0.49881500
C	6.31286400	-1.57464000	0.23677000
H	7.04036500	-2.32914000	-0.09143100
H	6.89097700	-0.70721600	0.57255700
H	5.79939200	-1.98986200	1.11058100
C	6.68402000	0.76245000	-1.90504400
H	6.43432200	1.69817700	-2.41463600
H	7.09279600	1.02279500	-0.92294900
H	7.50276200	0.30160100	-2.47411600
C	4.27001900	0.57253100	-3.98893400
H	4.71183900	1.56798400	-3.88628900
H	4.76219300	0.09309500	-4.84595600
H	3.21931500	0.70794500	-4.26928800
C	2.42949800	-1.88216400	-3.13420600
H	1.68914200	-2.35076200	-2.47668500
H	1.92069000	-1.09112300	-3.69622700

H	2.72558700	-2.64412100	-3.86764500	H	-3.21749600	3.81175600	1.24386400
C	3.97672200	3.90347700	-2.00598300	C	-3.24620500	0.25781600	3.45256400
H	5.04238200	3.65974800	-2.05713200	H	-4.21263900	0.16549300	3.96628900
H	3.51275800	3.54824600	-2.93159600	H	-2.67378000	-0.64369500	3.69336900
H	3.90288100	4.99952100	-2.01598500	H	-2.72849100	1.10660000	3.91007500
C	5.37478700	3.46703100	0.82230500	C	-3.80523300	-2.07437800	1.37871700
H	5.75234800	2.86775100	1.65795700	H	-4.83124400	-2.34656000	1.66230900
H	6.04661600	3.30601700	-0.02697100	H	-3.51953400	-2.70431100	0.53202500
H	5.48415600	4.51914700	1.11812500	H	-3.15789300	-2.34977400	2.21627300
C	3.12013200	2.54954100	2.89690600	C	-4.55879800	-0.76441600	-1.40614900
H	2.91464700	3.47084600	3.45845300	H	-4.38995200	-0.21150300	-2.33575200
H	2.45355900	1.77224100	3.28168600	H	-4.07339700	-1.73936100	-1.51142900
H	4.14471700	2.25188700	3.14364900	H	-5.63981100	-0.94763900	-1.33637800
C	0.35415600	2.42560400	1.35114600	C	-4.57370900	2.40972700	-0.99496500
H	-0.37085500	2.05926600	0.61715100	H	-4.00125400	3.34267300	-1.00826100
H	0.42111200	1.67254200	2.14123700	H	-4.62263000	2.03494700	-2.01947900
H	-0.07145200	3.33777200	1.79087800	H	-5.59901900	2.67437700	-0.70125700
C	0.88449500	3.20589600	-1.70102600	C	-2.14589800	2.14749400	-3.43608400
H	1.29216600	3.06887700	-2.70840000	H	-2.81141000	1.28761800	-3.56931400
H	0.05573900	2.49877700	-1.58107100	H	-2.75515600	2.98858200	-3.10036800
H	0.44158700	4.21053900	-1.67500000	H	-1.76433300	2.40602500	-4.43342700
C	-0.74961000	-1.89188200	3.37992500	C	-0.88195700	4.17930100	-1.29939800
H	-1.24106300	-2.00921700	2.40931400	H	-0.62348400	4.51202300	-0.28809400
H	-1.29835900	-2.48816200	4.11854600	H	-0.42143900	4.89601800	-1.99330000
H	-0.81740700	-0.83874700	3.66881400	H	-1.96532200	4.28535000	-1.40896500
C	0.77299400	-3.83852900	2.91199300	C	1.88715900	2.95272700	-0.37995800
H	1.80720900	-4.19104900	2.85657300	H	2.48850600	2.29906100	0.25830400
H	0.23924400	-4.44883400	3.65023000	H	2.57973500	3.43690500	-1.08185300
H	0.30862100	-3.99685000	1.93398400	H	1.47948200	3.74679900	0.25358700
C	1.38082700	-2.16600600	4.69092700	C	2.19169600	0.06727000	-1.69334300
H	2.42709400	-2.48520100	4.66853500	H	2.87029300	0.27961100	-2.53099700
H	1.35295600	-1.11668200	4.99959500	H	2.76309900	0.22258200	-0.77428100
H	0.85386900	-2.76191100	5.44549500	H	1.93940700	-0.99602100	-1.74291800
TS_{SBM}((Cp*)₂La-CH(SiMe₃)₂,HCCMe)				H	-0.29591300	-0.36812100	-3.61603000
H= -1213.461301 au				H	0.25176500	-1.26556200	-3.31914000
C	0.02738800	-1.18938500	1.97199700	H	-1.34124000	-0.65491900	-3.77074900
H	-0.41687800	-1.67301500	0.43708100	H	0.09739500	-0.04819600	-4.59126000
C	-0.91645600	-2.02576500	-0.63801100	Si	0.87657600	-2.87390600	2.19600200
C	-1.16876900	-2.90444800	-1.45444200	C	1.72448000	-3.15947000	3.88475600
C	-0.15339800	0.72781000	-2.60131300	H	1.00953200	-3.08412000	4.71061500
C	-1.00598400	1.86342500	-2.50162000	H	2.14366800	-4.17271800	3.90423300
C	0.97127300	0.94020600	-1.75179500	H	2.54590000	-2.46415500	4.08337800
C	-0.41902900	2.77634000	-1.57601400	C	-0.41799200	-4.26478600	2.07261600
C	0.81603500	2.21180600	-1.13105500	H	0.06610900	-5.24492200	2.15182700
C	-3.44418100	0.43417800	1.97474600	H	-1.14625600	-4.19097800	2.88814000
C	-3.60937000	1.67763500	1.29466300	H	-0.96520600	-4.22854600	1.12727800
C	-3.70998700	-0.61342500	1.04881900	C	2.20820600	-3.15652600	0.86852900
C	-4.00803900	1.39530100	-0.04514200	H	2.67971400	-4.13736000	0.99629300
C	-4.05278700	-0.02068400	-0.20301500	H	1.77230400	-3.11813300	-0.13435500
C	-3.61201300	3.04486100	1.91922400	H	2.99669300	-2.39891400	0.92296700
H	-4.63144100	3.35450400	2.18794800	Si	0.86099100	0.20411100	2.91582300
H	-3.02006900	3.08390100	2.83891200	C	2.72264600	0.35285300	2.56509300
				H	3.13309700	1.26084200	3.02009800

H	3.27082000	-0.49949900	2.97785800
H	2.93178500	0.38756200	1.49190600
C	0.62391400	0.12125700	4.80524500
H	1.03329800	1.02074300	5.28032100
H	-0.43774900	0.06017600	5.06620100
H	1.12494500	-0.74622200	5.24226400
C	0.08238400	1.91213200	2.47048300
H	0.51731600	2.66871400	3.13308300
H	0.29821000	2.27961000	1.45763000
H	-0.99914500	1.93963400	2.65406900
H	-0.95396000	-1.31840900	2.46583600
La	-1.26623400	0.54261800	0.05082100
C	-1.47187000	-3.92630600	-2.44427800
H	-0.85281300	-4.81543400	-2.27846100
H	-2.52111200	-4.23654900	-2.39434100
H	-1.27072000	-3.56590000	-3.45904300

(C₅Me₅)₂La-CCMe

H= -927.178518 au

La	3.16738000	0.51396400	-0.29836400
C	2.07589500	-0.86303900	1.49658700
C	1.50320800	-1.53659600	2.35832400
C	0.82844500	-2.33642300	3.37498500
C	4.42956600	-0.25601900	-2.73780900
C	5.49224200	-0.18069300	-1.78875400
C	3.60361500	-1.36410200	-2.38296000
C	5.32010700	-1.24636000	-0.85344500
C	4.15997500	-1.98369600	-1.22574600
C	1.67225300	2.69304100	0.72376600
C	2.90876500	2.74926800	1.42232900
C	1.92019500	3.04123800	-0.63999900
C	3.92632400	3.13119800	0.49396800
C	3.30920700	3.32802300	-0.77758000
C	3.69043500	-3.26110100	-0.59213400
H	2.61845700	-3.41937200	-0.73886200
H	4.21166200	-4.12765900	-1.02177400
H	3.86422500	-3.26809200	0.48694000
C	6.25903300	-1.60652700	0.26355100
H	6.98176700	-2.37037300	-0.05340000
H	6.84281600	-0.74574000	0.60647900
H	5.72731800	-2.01352600	1.13020400
C	6.68095600	0.73530800	-1.86624700
H	6.44485500	1.67453700	-2.37604900
H	7.07801900	0.98964000	-0.87778800
H	7.50416900	0.27047100	-2.42554300
C	4.29621500	0.57354500	-3.98359200
H	4.73503100	1.56890400	-3.86689600
H	4.80600400	0.09919900	-4.83313100
H	3.25129000	0.70973500	-4.28427100
C	2.41976200	-1.86714400	-3.16151100
H	1.66396000	-2.32508600	-2.51386600
H	1.92926300	-1.07056600	-3.73191700
H	2.71580900	-2.63445500	-3.88935000

C	3.97155200	3.90132200	-1.99667800
H	5.03569200	3.65019900	-2.04511800
H	3.50834900	3.55267600	-2.92521800
H	3.90550400	4.99789800	-2.00300500
C	5.35460600	3.45312200	0.83653000
H	5.72611600	2.85130200	1.67299900
H	6.02993000	3.29111700	-0.00980300
H	5.46584200	4.50449600	1.13430100
C	3.08774900	2.53481900	2.89827000
H	2.87101200	3.45228700	3.46186900
H	2.42590100	1.74981100	3.27541500
H	4.11323900	2.24468100	3.14963000
C	0.33043400	2.41558000	1.33873400
H	-0.38971200	2.04596600	0.60135500
H	0.39680200	1.66393500	2.13032500
H	-0.10158300	3.32616700	1.77548200
C	0.87529100	3.21178700	-1.70813400
H	1.28696800	3.07498400	-2.71396500
H	0.04349600	2.50738400	-1.59301800
H	0.43549900	4.21782400	-1.68268000
H	-0.22639600	-2.05318700	3.47394800
H	0.86108600	-3.40596300	3.13515100
H	1.29459100	-2.20649000	4.35916100

(C₅Me₅)₂Ce-CH(SiMe₃)₂

H= -1097.570926 au

Ce	-2.15278800	-0.99203900	3.02190200
C	-3.41954200	1.54152800	3.51821000
C	-3.54950000	1.35060000	2.11617300
C	-4.24234600	0.57515100	4.17494700
C	-4.44782000	0.26160700	1.89948400
C	-4.89899800	-0.19488100	3.17315100
C	-0.81782100	-3.52642200	3.06050400
C	-1.74205400	-3.60268700	4.14491700
C	-1.56670100	-3.50662900	1.85094500
C	-3.05862500	-3.65203600	3.60447000
C	-2.95424000	-3.58604800	2.18475100
C	-4.28884100	-3.96580800	4.40572200
H	-4.36766400	-3.36192800	5.31738500
H	-5.20438600	-3.81348200	3.83098800
H	-4.28141900	-5.01626600	4.72704500
C	-4.06535900	-3.81140200	1.19886500
H	-4.13353500	-4.87184000	0.92068800
H	-5.04077100	-3.52667000	1.60290200
H	-3.92003000	-3.25180800	0.26895400
C	-0.99896200	-3.59277900	0.46303800
H	-1.67980500	-3.18089900	-0.28904400
H	-0.04915300	-3.05952500	0.37191100
H	-0.81091400	-4.63726500	0.17870200
C	0.67183900	-3.67024100	3.16663100
H	1.04816500	-3.33470200	4.13721700
H	0.97124300	-4.72170700	3.05715900
H	1.19958100	-3.10206000	2.39689700

C	-1.40625000	-3.83140500	5.59247900
H	-1.48867800	-4.89638700	5.84916200
H	-0.38332100	-3.52829000	5.83436000
H	-2.07817400	-3.29377800	6.27139400
C	-6.05987800	-1.11492200	3.40995200
H	-6.14819800	-1.88662800	2.64002900
H	-6.00498500	-1.61694900	4.37931400
H	-7.00191600	-0.54941900	3.39781800
C	-4.51940400	0.51161100	5.65146600
H	-5.37775900	1.14019300	5.92503100
H	-4.75470000	-0.50469500	5.98586700
H	-3.67129400	0.86398000	6.24809400
C	-2.71458400	2.69132000	4.17702700
H	-3.39112800	3.54893400	4.29336400
H	-2.34674200	2.44489100	5.17823500
H	-1.86007200	3.03854100	3.58895400
C	-3.01406900	2.26212500	1.05123500
H	-2.04140000	2.68945200	1.31417000
H	-2.89677300	1.74960300	0.09231400
H	-3.69781900	3.10492400	0.88096600
C	-5.00126400	-0.15980500	0.56692600
H	-4.26722400	-0.05411000	-0.23903600
H	-5.33557000	-1.20113100	0.57015200
H	-5.86814400	0.45338100	0.28517800
C	-0.01515500	0.34501100	2.33917700
Si	1.00328800	0.38465600	0.77028100
Si	0.83750100	0.52959600	3.98773000
C	1.94248400	2.03489400	0.54408900
C	2.32036000	-0.98401700	0.61608200
C	-0.12250900	0.21945700	-0.76326900
C	-0.32963400	-0.17235100	5.37300600
C	1.19233100	2.32360200	4.52507400
C	2.47503400	-0.41316700	4.19620800
H	1.25950600	2.89010700	0.59826300
H	2.70294000	2.17181400	1.32102300
H	2.44986500	2.07476600	-0.42698700
H	1.88216000	-1.98585000	0.57419700
H	2.88379400	-0.83788200	-0.31276600
H	3.03645800	-0.96664000	1.44208600
H	0.46781800	0.24364500	-1.68635200
H	-0.68007200	-0.72375300	-0.75359000
H	-0.84509700	1.04056000	-0.81475500
H	0.13082000	-0.00258300	6.35265100
H	-1.30701400	0.33215100	5.42857200
H	-0.47504600	-1.26141600	5.31215700
H	1.88631300	2.79918400	3.82428000
H	0.28446700	2.93326400	4.55595100
H	1.64952500	2.35246100	5.52112900
H	2.77505600	-0.42070400	5.25017000
H	2.41363700	-1.44835900	3.85251100
H	3.27352900	0.08001400	3.63193900
H	-0.62192300	1.26951300	2.25345200

TS_{SBM}((Cp*)₂Ce-CH(SiMe₃)₂,HCCPh)

H= -1405.71968 au

C	-0.00940000	-1.15213700	1.94720600
H	-0.48928400	-1.68913700	0.35953800
C	-0.97184000	-2.02646400	-0.69075400
C	-1.17629000	-2.93866900	-1.48866300
C	-0.27438600	0.73096100	-2.62672000
C	-1.05455200	1.91114500	-2.47293700
C	0.88789700	0.85809300	-1.80947000
C	-0.38816600	2.76459200	-1.54425500
C	0.82778100	2.12143900	-1.15725600
C	-3.43986100	0.42159500	1.97153200
C	-3.58854200	1.68724100	1.33082600
C	-3.72365900	-0.59246200	1.01429400
C	-3.99882200	1.45342000	-0.01451900
C	-4.06336600	0.04410700	-0.21772200
C	-3.57658900	3.03447900	1.99708300
H	-4.59616600	3.35971000	2.24600400
H	-3.01165900	3.02998800	2.93417100
H	-3.14455600	3.81277400	1.35847500
C	-3.24400700	0.20052900	3.44337000
H	-4.21192800	0.13597900	3.95859300
H	-2.70896400	-0.72939500	3.65961400
H	-2.68910700	1.01519100	3.91904600
C	-3.84763200	-2.06040800	1.30033100
H	-4.87754900	-2.31888400	1.58302400
H	-3.58258500	-2.66987000	0.43223900
H	-3.20005300	-2.37607400	2.12332100
C	-4.58383600	-0.65692500	-1.44038700
H	-4.53124800	-0.02142800	-2.32950600
H	-4.02388900	-1.57165700	-1.66037600
H	-5.63644200	-0.94537900	-1.31552500
C	-4.56014100	2.51178600	-0.91770900
H	-3.96980800	3.43374900	-0.90696900
H	-4.63517700	2.17773300	-1.95412800
H	-5.57433600	2.78468600	-0.59445400
C	-2.19545400	2.29208200	-3.37064100
H	-2.90902700	1.47537500	-3.52262200
H	-2.74919200	3.15280200	-2.99138000
H	-1.81746800	2.56703000	-4.36508200
C	-0.76894100	4.18052800	-1.21342600
H	-0.43828600	4.47693800	-0.21207200
H	-0.31765400	4.89252100	-1.91807500
H	-1.85126200	4.33580300	-1.25605500
C	1.96700900	2.78080100	-0.43143800
H	2.52488500	2.08947100	0.20609400
H	2.68331600	3.19986000	-1.15098800
H	1.63392900	3.61187700	0.19790300
C	2.05815900	-0.08262300	-1.80596200
H	2.72884000	0.11545500	-2.65347500
H	2.65673000	0.01192800	-0.89575200
H	1.74233100	-1.12741200	-1.87913900
C	-0.51253400	-0.32326400	-3.66723600

H	0.02611900	-1.24523800	-3.44017400	C	1.66002300	2.66814100	0.69428500
H	-1.57129200	-0.58238700	-3.76757300	C	2.89443700	2.75564300	1.39445900
H	-0.17138600	0.02256400	-4.65312500	C	1.90561600	2.99923900	-0.67415300
Si	0.81767300	-2.84438300	2.18363900	C	3.90754200	3.14147600	0.46271600
C	1.63675700	-3.13167000	3.88675400	C	3.28996800	3.30803100	-0.81326200
H	0.91166700	-3.03656800	4.70167900	C	3.76028600	-3.23383200	-0.49421200
H	2.03787300	-4.15183100	3.92066000	H	2.68777600	-3.40433000	-0.61942700
H	2.46721600	-2.44902000	4.09104800	H	4.28359900	-4.09892300	-0.92393400
C	-0.48628400	-4.22592300	2.05241200	H	3.95330300	-3.22960400	0.58146500
H	-0.00956800	-5.20746200	2.15511800	C	6.30632100	-1.52247700	0.32512300
H	-1.22837200	-4.13639600	2.85389600	H	7.04370600	-2.27509600	0.01552000
H	-1.01596300	-4.20518500	1.09693400	H	6.87290900	-0.64546300	0.65548700
C	2.16893900	-3.15414700	0.88174900	H	5.78634600	-1.93043900	1.19841200
H	2.62550300	-4.13930600	1.02876500	C	6.68978000	0.77986600	-1.85016800
H	1.75367700	-3.12275300	-0.12990400	H	6.44283100	1.70501500	-2.37987500
H	2.96564000	-2.40577500	0.94358300	H	7.08594600	1.05920400	-0.86822200
Si	0.84138700	0.23499800	2.88317800	H	7.51634100	0.31122300	-2.40117200
C	2.70955800	0.33912000	2.54410500	C	4.30245400	0.54409900	-3.95803500
H	3.12278200	1.28463500	2.91166000	H	4.72061700	1.55018700	-3.86044000
H	3.24290000	-0.47129600	3.05067500	H	4.82579600	0.06157100	-4.79452200
H	2.93553000	0.26077600	1.47663800	H	3.25646700	0.65205900	-4.26561900
C	0.59533600	0.17892200	4.77304400	C	2.46099000	-1.90602800	-3.08159100
H	1.01850700	1.07663300	5.23938200	H	1.71694700	-2.36694000	-2.42294900
H	-0.46815900	0.13874100	5.03024300	H	1.95402800	-1.12744700	-3.66214200
H	1.07983400	-0.69209100	5.22156600	H	2.76835600	-2.67915300	-3.79839100
C	0.08889100	1.94901800	2.41711500	C	3.94405900	3.87899000	-2.03779600
H	0.54470100	2.71017100	3.06012900	H	5.01226000	3.64556700	-2.08235500
H	0.29435900	2.29498500	1.39455300	H	3.48773800	3.51266500	-2.96271800
H	-0.98931300	1.99640900	2.61476300	H	3.85902400	4.97406100	-2.05498800
H	-0.99174300	-1.27062500	2.44103100	C	5.32839500	3.49599500	0.80363600
Ce	-1.28848400	0.54754900	0.04223400	H	5.70683500	2.91956400	1.65463200
C	-1.41493100	-3.96645700	-2.44462300	H	6.01006200	3.32822900	-0.03631700
C	-0.38902900	-4.37362600	-3.31873900	H	5.41849000	4.55543000	1.07883700
C	-2.67064400	-4.59728900	-2.52609700	C	3.07551600	2.56286500	2.87324400
C	-0.61845800	-5.37983200	-4.24968400	H	2.86120900	3.48898900	3.42314200
H	0.58331300	-3.89576800	-3.25228500	H	2.41232700	1.78589600	3.26430400
C	-2.89206000	-5.59968200	-3.46342000	H	4.10100700	2.27525000	3.12789700
H	-3.46197300	-4.29289300	-1.84832300	C	0.31915400	2.38622900	1.30918900
C	-1.86918800	-5.99352200	-4.32682500	H	-0.38861100	1.98035500	0.57907200
H	0.18107700	-5.68660500	-4.91796400	H	0.39133900	1.66269000	2.12562400
H	-3.86570300	-6.07813700	-3.51909200	H	-0.13088600	3.30346600	1.71229000
H	-2.04578500	-6.77849900	-5.05669900	C	0.85886900	3.13813100	-1.74510300
				H	1.27596800	3.00834000	-2.74942200
				H	0.04529700	2.41301900	-1.62878900
				H	0.39364100	4.13265900	-1.72346100
				C	0.74584400	-2.30460300	3.28509800
				C	1.45320100	-3.04209400	4.25410100
				C	-0.66136300	-2.35919500	3.29844800
				C	0.77522800	-3.80398700	5.19951500
				H	2.53839900	-3.00611000	4.25201900
				C	-1.33223800	-3.12538100	4.24539500
				H	-1.21566000	-1.79391200	2.55531400
				C	-0.61913500	-3.85082700	5.20024000

(C₅Me₅)₂Ce-CCPh

H= -1119.441936 au

Ce	3.19284100	0.52477200	-0.28371100
C	2.03716000	-0.84830500	1.46588700
C	1.43761800	-1.52282200	2.31243900
C	4.44729400	-0.25614200	-2.69455400
C	5.51192900	-0.14763700	-1.75024400
C	3.63909800	-1.37016300	-2.31669200
C	5.35724400	-1.19681900	-0.79398800
C	4.20695500	-1.95903600	-1.14914600

H	1.33853000	-4.36585100	5.94001900
H	-2.41869300	-3.15614300	4.23892900
H	-1.14605600	-4.44794800	5.93932500

TS_{SBM}((Cp*)₂Ce-CH(SiMe₃)₂,HCC^tBu)

H= -1331.925984 au

C	-0.02117800	-1.20593700	1.90635000
H	-0.47178500	-1.66435600	0.35459800
C	-0.98168800	-2.00529600	-0.71987300
C	-1.23014000	-2.94367200	-1.47335300
C	-0.04442000	0.79399200	-2.57458500
C	-0.91196000	1.91977600	-2.48791200
C	1.04526200	1.00043000	-1.68007100
C	-0.36902900	2.81991100	-1.52358700
C	0.85403700	2.25832800	-1.04302800
C	-3.44212000	0.50926500	1.90463700
C	-3.57087600	1.75023500	1.21215500
C	-3.71741200	-0.54029600	0.98423800
C	-3.95844900	1.46425600	-0.13029000
C	-4.03103700	0.04855700	-0.27697000
C	-3.55595900	3.12276800	1.82455200
H	-4.57270000	3.45345500	2.07779000
H	-2.97404900	3.16020000	2.75060800
H	-3.13890700	3.87520900	1.14671500
C	-3.27504000	0.33703300	3.38675100
H	-4.25138100	0.21909900	3.87574300
H	-2.68538900	-0.54926400	3.64274900
H	-2.79226000	1.19925800	3.85660600
C	-3.85050100	-1.99438000	1.32969600
H	-4.88823700	-2.24206000	1.59250700
H	-3.55714400	-2.64058400	0.49837900
H	-3.22913800	-2.27098200	2.18641700
C	-4.53797700	-0.69212400	-1.48084800
H	-4.31239900	-0.16716500	-2.41484100
H	-4.09608000	-1.69028900	-1.55103200
H	-5.62839800	-0.82059200	-1.44163000
C	-4.49971700	2.47922300	-1.09343200
H	-3.92209200	3.40858800	-1.09645700
H	-4.53137000	2.10231000	-2.11786700
H	-5.52923800	2.74919300	-0.81974600
C	-2.02110900	2.20258800	-3.45944000
H	-2.68736900	1.34520800	-3.60532500
H	-2.63696200	3.04879100	-3.14971800
H	-1.60796400	2.45061000	-4.44659500
C	-0.85066300	4.21266300	-1.22693100
H	-0.76686200	4.46966500	-0.16470100
H	-0.26763600	4.96232100	-1.77908300
H	-1.89689600	4.35264300	-1.51215600
C	1.89038200	3.00262100	-0.24763100
H	2.47803900	2.34929000	0.40342300
H	2.59937800	3.50221200	-0.92183200
H	1.45121100	3.78461100	0.37977800
C	2.27503900	0.14258200	-1.60437100

H	2.97137400	0.37862300	-2.42099400
H	2.82089300	0.29017900	-0.66897400
H	2.03968400	-0.92305800	-1.67894200
C	-0.12647900	-0.27597600	-3.62151800
H	0.35417700	-1.20093900	-3.29434400
H	-1.16190900	-0.51667500	-3.88004800
H	0.37113700	0.04759000	-4.54677700
Si	0.81254100	-2.89964200	2.12012700
C	1.66243700	-3.20952800	3.80386200
H	0.94886600	-3.14425000	4.63167900
H	2.07631800	-4.22518300	3.80673000
H	2.48766100	-2.52207500	4.01252000
C	-0.50003800	-4.27380400	2.00210000
H	-0.02869500	-5.26203900	2.05209700
H	-1.20866600	-4.20410200	2.83506300
H	-1.06752400	-4.20781600	1.07085700
C	2.13880200	-3.18823300	0.78920900
H	2.59750800	-4.17651700	0.90584000
H	1.70347300	-3.13129900	-0.21289300
H	2.93720800	-2.44169300	0.85331800
Si	0.80889300	0.15943800	2.89796700
C	2.67840300	0.30213800	2.58818600
H	3.08337500	1.19855000	3.07042600
H	3.21385900	-0.56080000	2.99535200
H	2.91101500	0.35796700	1.52110700
C	0.54113700	0.03227100	4.78092600
H	0.94638700	0.92054700	5.28019000
H	-0.52413400	-0.02996400	5.02591900
H	1.03400700	-0.84512700	5.20683100
C	0.04397300	1.87747300	2.48229300
H	0.48847500	2.62386400	3.15007700
H	0.25256700	2.25616900	1.47223900
H	-1.03528400	1.90353500	2.67235600
H	-1.00957400	-1.33623200	2.38564900
Ce	-1.25437500	0.55796600	0.00961600
C	-1.52020600	-4.08013400	-2.36337900
C	-2.56322100	-5.00186900	-1.69909100
H	-2.76838600	-5.85838700	-2.35074900
H	-2.20306900	-5.38104600	-0.73864500
H	-3.50427400	-4.47133400	-1.52625700
C	-0.21583800	-4.86728000	-2.60558100
H	-0.41613300	-5.72431300	-3.25824500
H	0.53888400	-4.23811000	-3.08642300
H	0.19894000	-5.24038500	-1.66506600
C	-2.07266800	-3.57446700	-3.71050800
H	-2.98934500	-2.99451200	-3.56935900
H	-1.34320900	-2.94491000	-4.22586400
H	-2.30432100	-4.42984700	-4.35442300

(C₅Me₅)₂Ce-CC^tBu

H= -1045.64678 au

Ce	3.20660000	0.51985600	-0.27819700
C	2.05501600	-0.85734600	1.45505700

C	1.45147000	-1.53227600	2.29595600	H	-1.23060300	-2.00105500	2.39485700
C	0.73191600	-2.33980400	3.29497800	H	-1.28729000	-2.48038300	4.10399900
C	4.41086700	-0.23598600	-2.72730600	H	-0.80822600	-0.83036600	3.65456300
C	5.49389300	-0.15200300	-1.80200200	C	0.78530500	-3.82847900	2.89778300
C	3.59932500	-1.34829300	-2.35150400	H	1.81986900	-4.17989800	2.84188600
C	5.34710600	-1.21437000	-0.85918800	H	0.25263600	-4.43919400	3.63646100
C	4.18395700	-1.96076700	-1.20500500	H	0.32053100	-3.98757300	1.92009800
C	1.69784300	2.67530400	0.71912300	C	1.39156100	-2.15510000	4.67632600
C	2.93311400	2.74256200	1.41948900	H	2.43817100	-2.47319100	4.65396000
C	1.94658200	3.01625900	-0.64616700	H	1.36252500	-1.10581000	4.98499400
C	3.95010600	3.12598400	0.49114300	H	0.86527800	-2.75154500	5.43093500
C	3.33410600	3.31195700	-0.78249100				
C	3.73789500	-3.24072900	-0.56054100				
H	2.66372700	-3.40436900	-0.68048000	TS_{SBM}((Cp*)₂Ce-CH(SiMe₃)₂,HCCMe)			
H	4.25448800	-4.10372000	-1.00276100	H=- -1214.110555 au			
H	3.93808500	-3.24688900	0.51390300	C	0.02250700	-1.17620700	1.96025300
C	6.31302800	-1.56606400	0.23736500	H	-0.43082500	-1.66256000	0.42348800
H	7.03898800	-2.31936400	-0.09692000	C	-0.93569600	-2.01286400	-0.64620900
H	6.89257700	-0.69916200	0.57202300	C	-1.18886100	-2.89492500	-1.45857100
H	5.80458800	-1.98365000	1.11292900	C	-0.15484300	0.71517500	-2.58170700
C	6.67790700	0.76684700	-1.90849300	C	-1.00922900	1.84933200	-2.48450800
H	6.43002200	1.70170800	-2.42030600	C	0.96709900	0.92901900	-1.72880100
H	7.09319500	1.02872800	-0.92954900	C	-0.42664600	2.76301200	-1.55665300
H	7.49127800	0.29967600	-2.48009800	C	0.80854000	2.20071500	-1.10920900
C	4.24828000	0.58441500	-3.97559900	C	-3.42612500	0.43391400	1.96998900
H	4.69412300	1.57834400	-3.87739100	C	-3.59053100	1.67658900	1.28832200
H	4.73415400	0.10088300	-4.83390200	C	-3.69151300	-0.61474200	1.04517100
H	3.19657200	0.72283400	-4.25025300	C	-3.98961200	1.39257500	-0.05100100
C	2.40332200	-1.86134900	-3.10440000	C	-4.03358800	-0.02347400	-0.20762100
H	1.66555000	-2.32458400	-2.44033200	C	-3.59579100	3.04471900	1.91078800
H	1.89445300	-1.06892400	-3.66423900	H	-4.61693700	3.35620300	2.17065600
H	2.69083000	-2.62629800	-3.83811800	H	-3.01130400	3.08406700	2.83510800
C	3.99313600	3.89116000	-2.00040900	H	-3.19426000	3.80978800	1.23755500
H	5.05828100	3.64517000	-2.05067300	C	-3.23365600	0.25842100	3.44855500
H	3.53026300	3.54358800	-2.92924500	H	-4.20228600	0.16257700	3.95746200
H	3.92191600	4.98743000	-2.00241300	H	-2.65920300	-0.64102600	3.69217200
C	5.37615100	3.45760200	0.83375700	H	-2.72137600	1.10907400	3.90853000
H	5.74802200	2.86660600	1.67774200	C	-3.79172700	-2.07444200	1.37847100
H	6.05417400	3.28920300	-0.00914300	H	-4.81756800	-2.34046800	1.66850400
H	5.48217000	4.51263100	1.12025600	H	-3.51435300	-2.70714600	0.53122600
C	3.11105100	2.53501400	2.89650500	H	-3.14104500	-2.35165500	2.21281000
H	2.89639600	3.45563300	3.45569400	C	-4.54050800	-0.76869900	-1.40929500
H	2.44631200	1.75407200	3.27693200	H	-4.37507700	-0.21537400	-2.33918100
H	4.13561000	2.24337900	3.15029400	H	-4.05210600	-1.74200800	-1.51538800
C	0.35548700	2.40007500	1.33326300	H	-5.62084200	-0.95480000	-1.33681300
H	-0.36301200	2.02817000	0.59575800	C	-4.56361300	2.40502000	-0.99787600
H	0.42030700	1.65000000	2.12621200	H	-3.99633300	3.34096000	-1.01298800
H	-0.07603300	3.31253200	1.76659000	H	-4.61613200	2.03079900	-2.02231700
C	0.90193000	3.17678700	-1.71612700	H	-5.58875900	2.66401700	-0.69850800
H	1.31680800	3.04376300	-2.72098800	C	-2.14418100	2.13160900	-3.42538900
H	0.07716700	2.46410700	-1.60238500	H	-2.81276800	1.27366400	-3.55499100
H	0.45269600	4.17862300	-1.69091700	H	-2.75095100	2.97792100	-3.09865300
C	-0.73923800	-1.88336700	3.36546000	H	-1.75681000	2.38091500	-4.42282600
				C	-0.89039300	4.16613100	-1.28234800

H	-0.64447800	4.49596600	-0.26696400	C	0.81060800	-2.33074600	3.33735900
H	-0.41944000	4.88346300	-1.96855600	C	4.41134300	-0.24093500	-2.72415400
H	-1.97193600	4.27434400	-1.40563900	C	5.48543800	-0.16598700	-1.78763000
C	1.87817100	2.94581700	-0.36017900	C	3.58833400	-1.34793100	-2.35848900
H	2.47849500	2.29622700	0.28290900	C	5.32250700	-1.22988700	-0.84895200
H	2.57135700	3.42598500	-1.06420100	C	4.15741000	-1.96689200	-1.20731100
H	1.46910200	3.74331800	0.26800800	C	1.68286400	2.67163500	0.71610300
C	2.19080400	0.06077800	-1.67242600	C	2.91598000	2.73549400	1.42056200
H	2.86527100	0.27424100	-2.51314200	C	1.93587000	3.01712100	-0.64736700
H	2.76480200	0.22051900	-0.75591200	C	3.93618700	3.11987100	0.49619200
H	1.94276100	-1.00355900	-1.71888000	C	3.32425900	3.31060300	-0.77880400
C	-0.29034700	-0.37741000	-3.60077400	C	3.69486300	-3.24401300	-0.56843400
H	0.26109300	-1.27330100	-3.30648100	H	2.62085600	-3.40011000	-0.70081900
H	-1.33396200	-0.66845600	-3.75859000	H	4.20976500	-4.11054100	-1.00571000
H	0.10349300	-0.05110600	-4.57370000	H	3.88293100	-3.25180300	0.50817500
Si	0.87100600	-2.86180100	2.18031300	C	6.27353900	-1.58938300	0.25798800
C	1.72309300	-3.14902300	3.86668600	H	6.99414900	-2.35183200	-0.06701300
H	1.01036500	-3.07331200	4.69442100	H	6.85942900	-0.72795000	0.59563700
H	2.14093400	-4.16286200	3.88436700	H	5.75145000	-1.99813300	1.12965100
H	2.54591400	-2.45496400	4.06369900	C	6.67560400	0.74649500	-1.88058100
C	-0.42443000	-4.25250600	2.06157400	H	6.43704100	1.68454000	-2.39115500
H	0.06031400	-5.23260600	2.13736700	H	7.08374700	1.00281900	-0.89717900
H	-1.14834800	-4.17977100	2.88105000	H	7.49141200	0.27704500	-2.44682000
H	-0.97673800	-4.21564800	1.11925300	C	4.26657900	0.58442300	-3.97136200
C	2.19851100	-3.14722200	0.84937300	H	4.71115100	1.57799000	-3.86329500
H	2.66987900	-4.12805300	0.97769000	H	4.76426700	0.10417400	-4.82474000
H	1.75951400	-3.11079000	-0.15222900	H	3.21881800	0.72416700	-4.25997700
H	2.98747500	-2.38985200	0.89990200	C	2.39512700	-1.85084100	-3.12268900
Si	0.85677200	0.21448100	2.90793700	H	1.64536400	-2.30446500	-2.46524200
C	2.71915300	0.36259400	2.56015900	H	1.90058600	-1.05488500	-3.69028500
H	3.12828700	1.27260900	3.01231600	H	2.68216000	-2.62118200	-3.85091600
H	3.26609300	-0.48778400	2.97863900	C	3.98885900	3.89004000	-1.99359300
H	2.93160900	0.39219000	1.48760900	H	5.05255500	3.63740200	-2.04299700
C	0.62216100	0.12680400	4.79763000	H	3.52535300	3.54837100	-2.92433400
H	1.02751500	1.02785500	5.27326400	H	3.92466000	4.98675400	-1.99221200
H	-0.43853500	0.05951900	5.06079900	C	5.36189000	3.44804000	0.84350200
H	1.12902400	-0.73839200	5.23249400	H	5.72937700	2.85583000	1.68850200
C	0.07157600	1.91888400	2.46610200	H	6.04227400	3.27811500	0.00278800
H	0.51710600	2.68252900	3.11336300	H	5.46955600	4.50276600	1.13053200
H	0.26561900	2.27897500	1.44607100	C	3.08896800	2.52362700	2.89757000
H	-1.00601900	1.94233000	2.66900100	H	2.86795200	3.44148300	3.45882100
H	-0.95714800	-1.30694600	2.45666000	H	2.42679300	1.73793200	3.27262300
Ce	-1.26665400	0.53883300	0.05216900	H	4.11390600	2.23580400	3.15387300
C	-1.49364500	-3.91995200	-2.44448300	C	0.33899400	2.39220400	1.32537900
H	-0.88495900	-4.81404900	-2.26730300	H	-0.37540700	2.01572100	0.58602400
H	-2.54630500	-4.21954100	-2.40176700	H	0.40423000	1.64461000	2.12071200
H	-1.27989500	-3.56823200	-3.45971000	H	-0.09837800	3.30369400	1.75485800
				C	0.89467200	3.18165900	-1.72008600
				H	1.31183400	3.04832200	-2.72400700
				H	0.06745200	2.47135100	-1.60920500
				H	0.44819300	4.18474700	-1.69529000
				H	-0.24736000	-2.05424300	3.42065000
				H	0.85376000	-3.40059000	3.10060700
(C₅Me₅)₂Ce-CCMe							
H= -927.829406 au							
Ce	3.19012300	0.51828500	-0.28475200				
C	2.07416000	-0.85355300	1.47289900				
C	1.49425400	-1.52870400	2.32839300				

H	1.26187900	-2.19530500	4.32769700	C	2.96942700	-0.70194000	-4.39570200
				H	2.01571600	-1.20066100	-4.58503800
				H	2.90051600	0.30359200	-4.82329300
				H	3.73538900	-1.23914300	-4.97344000
				C	0.92641900	0.16422100	1.30600700
				C	0.80618900	0.07423500	2.54017700
				Sm	-1.96952500	-0.71374300	1.00605000
				C	-3.32549900	1.67254900	1.82746500
				C	-3.55075600	1.58826200	0.42653100
				C	-4.01011200	0.58016600	2.44780900
				C	-4.36765200	0.44422600	0.17843400
				C	-4.70161000	-0.13967800	1.43203100
				C	-0.75691500	-3.17416800	1.25876200
				C	-1.51925100	-3.06146800	2.45517500
				C	-1.66375900	-3.31975500	0.17171200
				C	-2.89777700	-3.17894300	2.11218200
				C	-2.98914200	-3.32949500	0.69927900
				C	-3.97103200	-3.43805100	3.12888700
				H	-4.05559300	-2.64615900	3.88074500
				H	-4.95233500	-3.56782600	2.66952800
				H	-3.74822800	-4.36392700	3.67623300
				C	-4.20101800	-3.72595900	-0.09583400
				H	-4.08981500	-4.74890600	-0.47822100
				H	-5.10907500	-3.71102100	0.51017400
				H	-4.37403400	-3.08237200	-0.96555100
				C	-1.30301300	-3.66610300	-1.24225000
				H	-2.15710500	-3.53428900	-1.91344100
				H	-0.48798900	-3.04886300	-1.62256700
				H	-0.98883400	-4.71659200	-1.32065500
				C	0.72948300	-3.28304700	1.16115600
				H	1.21517100	-3.04982000	2.11084900
				H	1.02897800	-4.30190700	0.87803300
				H	1.13946300	-2.59502400	0.41973500
				C	-1.00274400	-3.08026400	3.86518500
				H	-1.10559600	-4.08442400	4.30014100
				H	0.05312600	-2.80946100	3.92393800
				H	-1.54699100	-2.39531900	4.52438700
				C	-5.85784500	-1.06773800	1.65379700
				H	-5.94481200	-1.83226100	0.87918900
				H	-5.81313000	-1.57066600	2.62037100
				H	-6.79329900	-0.49155500	1.63624100
				C	-4.20254400	0.43498900	3.93153100
				H	-4.87024400	1.21659800	4.32113400
				H	-4.65377700	-0.52552200	4.19254400
				H	-3.26567000	0.51529900	4.49388600
				C	-2.76640100	2.84051500	2.59280800
				H	-3.47116600	3.14921700	3.37493400
				H	-1.80835800	2.64595700	3.08710900
				H	-2.61363400	3.70326700	1.94112300
				C	-3.27407500	2.62822200	-0.61578900
				H	-2.54142300	3.36704000	-0.28870100
				H	-2.90514600	2.18287600	-1.54402300
				H	-4.19682900	3.17142000	-0.86263100

[(C₅Me₅)₂Sm-CCPh]₂

H= -2243.833887 au

Sm	1.91544400	0.79337800	-0.99573500
C	-0.73076500	-0.10588200	-2.52060600
C	-0.91777700	-0.15384500	-1.29163700
C	3.32097500	-0.68172900	-2.93540100
C	4.30752600	0.15939200	-2.35009700
C	2.95570400	-1.67341900	-1.97601100
C	4.50328200	-0.26537500	-1.00456500
C	3.67969000	-1.41154400	-0.77905900
C	1.14457600	3.24660900	-0.00967500
C	2.52820100	3.16101800	0.31384600
C	1.02762300	3.39308700	-1.41874100
C	3.27050300	3.29861600	-0.89413300
C	2.34329400	3.41343700	-1.97087400
C	-0.23176800	3.72060800	-2.16883400
H	-0.75311300	4.56358400	-1.69785900
H	-0.00741800	4.02392500	-3.19621700
H	-0.94581100	2.89316200	-2.21128000
C	2.66443400	3.76532600	-3.39755600
H	3.74074800	3.75334100	-3.58267900
H	2.20418100	3.08818700	-4.12709400
H	2.31251400	4.77697100	-3.63942600
C	4.73299200	3.63140800	-0.93870300
H	5.34413700	2.96190500	-0.32798700
H	5.13251500	3.61470300	-1.95387400
H	4.89198600	4.64634300	-0.54968400
C	3.11491000	3.14613000	1.69676700
H	3.20321100	4.16325700	2.10289900
H	2.50334600	2.56626600	2.39366800
H	4.12052700	2.71352500	1.70599800
C	0.02365200	3.35767900	0.97036000
H	0.36443100	3.15686500	1.98776400
H	-0.40336200	4.37061200	0.95919100
H	-0.78624500	2.65743300	0.75510500
C	2.17750900	-2.90939400	-2.31727500
H	2.79098200	-3.59070900	-2.92277500
H	1.86049100	-3.46229400	-1.43184700
H	1.28286000	-2.68401200	-2.90599800
C	3.82111100	-2.29361800	0.42938000
H	4.88229500	-2.49304300	0.62621200
H	3.40130900	-1.85426500	1.34093900
H	3.33794200	-3.26091300	0.27950500
C	5.57279400	0.19103800	-0.05246200
H	6.25899000	-0.63350100	0.18326500
H	6.17755300	0.99307000	-0.48070300
H	5.17791100	0.54999300	0.90565900
C	5.19253300	1.07349800	-3.14379700
H	4.63428300	1.75436400	-3.79250900
H	5.84134400	1.67566000	-2.50670300
H	5.84532200	0.47973500	-3.79837600

C	-4.97738800	0.10431700	-1.15208900
H	-4.25848500	0.20616000	-1.97154100
H	-5.36244100	-0.91909100	-1.17585700
H	-5.82239400	0.76821800	-1.38305700
C	0.85925400	-0.02123500	3.96896400
C	-0.11976600	0.56471700	4.79126000
C	1.93096600	-0.69876600	4.58368200
C	-0.03701500	0.46598700	6.17689700
H	-0.94127700	1.10638700	4.33309600
C	2.01152200	-0.78778100	5.96895900
H	2.69563900	-1.14927700	3.95848400
C	1.02719500	-0.21035800	6.77199400
H	-0.80433700	0.92517900	6.79411300
H	2.84694100	-1.31234800	6.42454700
H	1.09163500	-0.28403600	7.85378600
C	-0.65483900	-0.16462200	-3.95233200
C	-0.34888500	0.96801200	-4.72818900
C	-0.91804100	-1.38064300	-4.61350700
C	-0.29629900	0.88270000	-6.11620300
H	-0.16495800	1.91512300	-4.23269000
C	-0.86827000	-1.45676500	-6.00131600
H	-1.16585400	-2.25657300	-4.02280100
C	-0.55396200	-0.32768100	-6.75858500
H	-0.05811300	1.76824800	-6.69904000
H	-1.07640300	-2.40247000	-6.49418100
H	-0.51388700	-0.39056600	-7.84227900

TS_{CC}[(C₅Me₅)₂Sm-CCPh]₂

H= -2243.816903 au

Sm	2.23506800	0.84611000	0.27270700
C	-0.19516600	-0.09778800	-0.51686700
C	-0.50267200	-0.31908300	0.68976600
C	3.48988600	-0.79286800	-1.62296900
C	4.51738600	0.08669900	-1.17466900
C	3.17055200	-1.68189100	-0.55591200
C	4.80975000	-0.23536400	0.18165300
C	3.97331500	-1.32741400	0.56491300
C	1.43522000	3.22790800	1.47282900
C	2.80629600	3.07428500	1.82598700
C	1.36470200	3.50492600	0.08007200
C	3.58809600	3.29410100	0.65410600
C	2.69623600	3.53211800	-0.43287200
C	0.13372400	3.96941100	-0.64581600
H	-0.19178800	4.94588200	-0.26151200
H	0.32071600	4.10442300	-1.71555600
H	-0.71538800	3.28889200	-0.53705600
C	3.09180200	3.99767700	-1.80627600
H	4.11306100	3.70048500	-2.05651900
H	2.43801600	3.60390300	-2.59259100
H	3.04999500	5.09310200	-1.87995300
C	5.06185800	3.57471700	0.65227900
H	5.59506500	3.01376700	1.42318900
H	5.53549400	3.35744300	-0.30819000

H	5.23804800	4.63986700	0.85734000
C	3.33858100	2.89123700	3.21963600
H	3.44754400	3.85387900	3.73756900
H	2.67757400	2.26984700	3.83154300
H	4.32633900	2.41867000	3.22197900
C	0.28276800	3.29638800	2.42302400
H	0.56076500	2.93875800	3.41692200
H	-0.06877000	4.33210500	2.53251500
H	-0.56340400	2.69282200	2.08884200
C	2.31867300	-2.90679300	-0.69445700
H	2.87934900	-3.71376100	-1.18608900
H	1.98712900	-3.29000900	0.27230400
H	1.42892100	-2.72146300	-1.30329700
C	4.14964000	-2.10010700	1.84034200
H	5.05222800	-2.72566900	1.79294300
H	4.26916200	-1.44625600	2.71150500
H	3.30855700	-2.76528700	2.04128500
C	5.97417300	0.24695800	0.99835300
H	6.72719400	-0.54666800	1.09781100
H	6.47070600	1.10302600	0.53775400
H	5.69232000	0.53819200	2.01713400
C	5.30155200	0.98857800	-2.08199100
H	4.66129100	1.54640000	-2.77267000
H	5.90441400	1.71295500	-1.52989800
H	5.99470600	0.40225000	-2.70084700
C	3.02768900	-0.91756600	-3.04696900
H	2.05237700	-1.40365500	-3.12489900
H	2.94666200	0.05315000	-3.54658200
H	3.73728900	-1.51728500	-3.63435900
C	0.77588600	0.03972200	2.20771300
C	0.41954800	-0.12725700	3.41148700
Sm	-2.01684700	-0.97347700	2.64930500
C	-3.32822500	1.50939700	3.16523100
C	-3.46827600	1.29618000	1.76525800
C	-4.08958100	0.50396100	3.83820200
C	-4.31849300	0.16647300	1.57194200
C	-4.74024600	-0.29192000	2.85198200
C	-0.73637000	-3.42155400	2.95107600
C	-1.52959600	-3.30042600	4.12624500
C	-1.61521900	-3.58147600	1.84220300
C	-2.89990900	-3.41964300	3.74779600
C	-2.95360900	-3.59390200	2.33454800
C	-4.01789100	-3.61795100	4.73008300
H	-4.06151900	-2.83301700	5.49390500
H	-4.99269100	-3.65745900	4.24093200
H	-3.88874100	-4.56739500	5.26712300
C	-4.14799500	-3.99830400	1.51759600
H	-4.07037200	-5.05199300	1.21844600
H	-5.07996500	-3.89556600	2.07765500
H	-4.25278500	-3.41684100	0.59487600
C	-1.20896100	-3.92652400	0.43953100
H	-2.01323900	-3.72220300	-0.27471300
H	-0.32832400	-3.36633900	0.11881500

H	-0.96780800	-4.99533800	0.34954900	H=	-2243.872862	au		
C	0.75651100	-3.51682200	2.88769400	Sm	2.78036900	1.11476300	0.23816900	
H	1.20432700	-3.41451400	3.87924000	C	0.51702800	0.33232900	-0.50412100	
H	1.07002300	-4.48928800	2.48615600	C	0.24557200	0.03047500	0.75685100	
H	1.18737300	-2.73563600	2.25435800	C	3.91044700	-0.54765300	-1.67348500	
C	-1.04632400	-3.28456100	5.54866900	C	4.98849600	0.27758300	-1.23424500	
H	-1.05856300	-4.29755300	5.97473300	C	3.55987500	-1.42256300	-0.60795900	
H	-0.02617500	-2.90492800	5.63997800	C	5.28246200	-0.06765700	0.11792800	
H	-1.67827700	-2.66471800	6.19348700	C	4.39535700	-1.11864900	0.50463700	
C	-5.91014900	-1.19435000	3.10752500	C	1.96712500	3.48791400	1.38815300	
H	-5.99375000	-2.00049900	2.37486400	C	3.38198400	3.46326000	1.57325900	
H	-5.88034800	-1.64404900	4.10197600	C	1.70571000	3.65417600	-0.00146700	
H	-6.84299200	-0.61629700	3.04850800	C	3.99597100	3.63486200	0.30015600	
C	-4.37249500	0.47699700	5.31473000	C	2.96063900	3.72598700	-0.67856200	
H	-5.22866600	1.11776900	5.56933700	C	0.36256400	3.91088800	-0.62060600	
H	-4.61435800	-0.52904500	5.67092500	H	0.04638300	4.94944900	-0.45215600	
H	-3.52433400	0.83535500	5.90687300	H	0.37682500	3.75255200	-1.70223400	
C	-2.75146500	2.72555900	3.84051900	H	-0.41542600	3.26152400	-0.21263800	
H	-3.42312300	3.07198300	4.63443500	C	3.14582600	4.06612100	-2.13087900	
H	-1.76576400	2.58095700	4.29501400	H	4.13977600	3.78890800	-2.49301500	
H	-2.64596400	3.55084700	3.13170500	H	2.41241000	3.56662600	-2.77344200	
C	-3.04562400	2.21249400	0.65560300	H	3.03298000	5.14489400	-2.30389400	
H	-2.42155500	3.02977300	1.02239700	C	5.44495400	3.96001200	0.08731200	
H	-2.48047800	1.69326400	-0.12487700	H	6.10348000	3.40149000	0.75887800	
H	-3.92366500	2.66517000	0.17577600	H	5.77064000	3.76856100	-0.93753700	
C	-4.85811800	-0.27675400	0.24125000	H	5.62599800	5.02589600	0.28353700	
H	-4.09506100	-0.24833800	-0.54408700	C	4.09517400	3.45308500	2.89642800	
H	-5.25831300	-1.29408400	0.27819100	H	4.24672400	4.47400900	3.27339800	
H	-5.67789400	0.37513500	-0.09224300	H	3.53277200	2.91332900	3.66471400	
C	0.65419900	-0.18091900	4.82934000	H	5.08748900	2.99381900	2.82744200	
C	-0.25113900	0.38048700	5.75114000	C	0.94565300	3.53589400	2.48553800	
C	1.81214900	-0.80810200	5.33930600	H	0.83871700	4.55731000	2.87570800	
C	-0.00637500	0.32696900	7.12099900	H	-0.03694900	3.22497300	2.12447500	
H	-1.14285300	0.87928700	5.38219100	H	1.20157600	2.89204500	3.33239100	
C	2.04597000	-0.86378200	6.70824000	C	2.60234300	-2.56961800	-0.71715300	
H	2.51933100	-1.24531500	4.64203300	H	3.06293900	-3.41410100	-1.24755500	
C	1.14002900	-0.29755900	7.60801600	H	2.30117000	-2.93873600	0.26604900	
H	-0.71742200	0.77541400	7.80959000	H	1.69417300	-2.29824900	-1.26394100	
H	2.94656900	-1.34796700	7.07669800	C	4.48994900	-1.89587100	1.78805000	
H	1.32882700	-0.34196400	8.67661200	H	5.16652200	-2.75446100	1.67852700	
C	-0.35159900	-0.12931000	-1.94521800	H	4.88766200	-1.28929400	2.60844400	
C	-0.11556200	1.00786700	-2.74299700	H	3.52409800	-2.29225500	2.11375800	
C	-0.75571200	-1.31803200	-2.59207600	C	6.44944800	0.41045000	0.93520500	
C	-0.28231100	0.96070500	-4.12449400	H	7.23574700	-0.35478100	0.98351300	
H	0.17284300	1.93904400	-2.26621900	H	6.90394600	1.30810700	0.50934600	
C	-0.91402300	-1.35774000	-3.97235900	H	6.17723500	0.64471600	1.97130500	
H	-0.95038200	-2.20053700	-1.99200700	C	5.81569800	1.14173400	-2.14106000	
C	-0.67810700	-0.22091200	-4.74827400	H	5.20516200	1.76409600	-2.80334700	
H	-0.10258000	1.85499600	-4.71516700	H	6.48190700	1.80505600	-1.58556900	
H	-1.23086600	-2.28304900	-4.44626700	H	6.44943000	0.52095500	-2.78858900	
H	-0.80578500	-0.25663700	-5.82620000	C	3.38085900	-0.62552800	-3.07673600	
				H	2.32349700	-0.90330400	-3.10181900	
				H	3.48287100	0.32581800	-3.60888700	

{{(C₅Me₅)₂Sm}(μ-η²:η²-PhC₄Ph)}

H	3.92829000	-1.37623000	-3.66363100
C	0.38579000	-0.03467300	2.06280200
C	0.07275500	-0.23578500	3.33417600
Sm	-2.08995000	-1.24896800	2.58425600
C	-3.25917300	1.14429700	3.34030600
C	-3.42056200	1.07792000	1.92699600
C	-4.08418100	0.13570500	3.92369300
C	-4.35113400	0.03563100	1.63523800
C	-4.77805300	-0.53107300	2.86960300
C	-0.62457600	-3.56852200	2.96217400
C	-1.50895900	-3.51162300	4.07466900
C	-1.40348700	-3.79897400	1.79164100
C	-2.83606100	-3.73289900	3.59746600
C	-2.77222200	-3.90434700	2.18284300
C	-4.01800200	-4.02003300	4.47737800
H	-4.10115000	-3.32278800	5.31788300
H	-4.95958100	-3.98654900	3.92583000
H	-3.93585200	-5.02570500	4.91153900
C	-3.89687800	-4.33242300	1.28294600
H	-3.88116700	-5.41862100	1.12039100
H	-4.87576400	-4.08861500	1.70357100
H	-3.84285500	-3.86690000	0.29248200
C	-0.85872200	-4.08183000	0.42024300
H	-1.61975000	-3.96320600	-0.35733000
H	-0.01948500	-3.43049400	0.16078800
H	-0.49382400	-5.11554300	0.34765300
C	0.87221400	-3.53884500	3.01726100
H	1.23643900	-3.08376500	3.94160500
H	1.28931000	-4.55330700	2.95928400
H	1.29386900	-2.96482100	2.18709400
C	-1.11374700	-3.41836500	5.52108800
H	-0.94586000	-4.41576100	5.95014600
H	-0.19297600	-2.84549100	5.66181500
H	-1.89072600	-2.94224500	6.12854700
C	-5.95139800	-1.45160300	3.03234700
H	-6.00106400	-2.21445600	2.24931200
H	-5.94660400	-1.96276400	3.99741400
H	-6.89017400	-0.88330800	2.97706600
C	-4.34169400	-0.03449300	5.39471100
H	-5.13570900	0.64158000	5.74011300
H	-4.66015000	-1.05105000	5.64450900
H	-3.45562300	0.18922700	5.99812300
C	-2.51814200	2.21092300	4.09309500
H	-3.15183700	3.09621700	4.24184800
H	-2.20232400	1.87358000	5.08417900
H	-1.61935800	2.53878500	3.56629200
C	-2.85830300	2.05113400	0.93318900
H	-1.89635300	2.44886200	1.26453800
H	-2.70280100	1.60225400	-0.05239600
H	-3.53286800	2.90721100	0.79605000
C	-4.92298100	-0.28505100	0.28262300
H	-4.21453100	-0.07986100	-0.52599100
H	-5.22340600	-1.33532000	0.20180600

H	-5.81956700	0.31620500	0.07810000
C	0.92848500	0.00017300	4.49270300
C	2.33293700	0.08800400	4.40251700
C	0.35885100	0.11779400	5.77461000
C	3.12231000	0.29940900	5.52763500
H	2.80245600	-0.04891100	3.43099000
C	1.14383800	0.34551400	6.90120800
H	-0.72010600	0.03388600	5.87071600
C	2.53040600	0.43778900	6.78479000
H	4.20355100	0.35092700	5.42778600
H	0.67248700	0.44343600	7.87563500
H	3.14564600	0.60478900	7.66435600
C	-0.33272900	0.08982600	-1.66579600
C	-1.37664400	-0.85814600	-1.66903800
C	-0.10798700	0.80128300	-2.85950700
C	-2.16013200	-1.07383700	-2.79744600
H	-1.54474700	-1.45177500	-0.77356900
C	-0.90033200	0.60042100	-3.98594100
H	0.70031400	1.52694000	-2.88420900
C	-1.93035700	-0.33940600	-3.96252000
H	-2.95052400	-1.81973100	-2.77242600
H	-0.70839900	1.17399400	-4.88896600
H	-2.54266000	-0.50541600	-4.84432600

[(C₅Me₅)₂Sm-CC'Bu]₂

H= -2096.23696 au

Sm	2.01519500	0.65697000	0.79748200
C	-0.67355800	-0.28986200	-1.30511500
C	-0.36574400	-0.22713200	-0.10271100
C	3.66018000	-0.84680700	-0.95557500
C	4.54872600	0.07437200	-0.33867100
C	3.29727200	-1.83184000	0.01118600
C	4.65284900	-0.27455600	1.03753500
C	3.89861900	-1.47142200	1.24794600
C	1.18155500	3.21573800	1.41861000
C	2.57081500	3.25075400	1.72623100
C	1.04545300	3.14350700	0.00473300
C	3.29399300	3.24617700	0.50060500
C	2.35542500	3.14190800	-0.56373100
C	-0.22831300	3.30916000	-0.77216800
H	-0.82025900	4.13826100	-0.36714400
H	-0.01198800	3.55207100	-1.81709000
H	-0.86079900	2.41701400	-0.76260300
C	2.64844900	3.28129200	-2.03166700
H	3.72184800	3.25676600	-2.23400300
H	2.18522900	2.49534200	-2.63805100
H	2.27577800	4.23964900	-2.41766800
C	4.71650000	3.71162100	0.39730500
H	5.39306800	3.19639400	1.08551200
H	5.12155100	3.61038500	-0.60980900
H	4.76540600	4.77886500	0.65528700
C	3.18187800	3.54902100	3.06391400
H	3.38280300	4.62412300	3.17485400

H	2.52249800	3.26175100	3.88658900	H	1.22601000	-4.46986300	2.47654700
H	4.13767000	3.03418900	3.20857100	H	1.42806400	-2.75985500	2.06659000
C	0.06864200	3.42214500	2.39241900	C	-1.30157000	-3.33554100	5.02880000
H	0.42325300	3.37738600	3.42389900	H	-1.38552300	-4.36570300	5.40305900
H	-0.39727800	4.40794900	2.25044700	H	-0.29711200	-2.98518000	5.27277000
H	-0.71126900	2.66757100	2.29240100	H	-2.01054600	-2.73181600	5.60570400
C	2.73286300	-3.16714200	-0.37304600	C	-5.68113600	-1.26842300	2.73155600
H	3.51554200	-3.77392000	-0.85010200	H	-5.69292100	-2.02836000	1.94545700
H	2.35779800	-3.73575400	0.47739900	H	-5.75283100	-1.77600100	3.69335900
H	1.91659300	-3.08131500	-1.09418900	H	-6.60169100	-0.68035000	2.61138400
C	3.99976000	-2.30537800	2.49553200	C	-3.89239400	-0.18186300	5.19400000
H	5.03419200	-2.31674300	2.85936700	H	-4.51368800	0.53773900	5.74596700
H	3.36967700	-1.94963500	3.31819900	H	-4.35639800	-1.16344200	5.31704100
H	3.71729000	-3.34308000	2.30165400	H	-2.92326400	-0.21269800	5.70504700
C	5.61286200	0.30077400	2.04061800	C	-2.48724200	2.38803500	4.21025500
H	6.50363600	-0.33516600	2.14445300	H	-3.12439300	2.52216200	5.09304300
H	5.96396400	1.29322700	1.74868500	H	-1.49136400	2.10847400	4.56949800
H	5.17396900	0.39008500	3.03983900	H	-2.39548200	3.36562800	3.73126600
C	5.48762800	0.95178100	-1.11135300	C	-3.20799900	2.74628600	1.04623000
H	4.98614100	1.58040900	-1.85217900	H	-2.45161600	3.42923800	1.43189500
H	6.07757500	1.59923600	-0.46296600	H	-2.93527700	2.50641100	0.01535800
H	6.19750100	0.32052300	-1.66363200	H	-4.15498200	3.30234800	1.00288800
C	3.42770300	-0.95821300	-2.43462500	C	-4.91692900	0.29553400	0.18325200
H	2.47622900	-1.44781800	-2.66258100	H	-4.37370600	0.78919200	-0.62607600
H	3.42525700	0.01949900	-2.92722200	H	-5.06833900	-0.74947700	-0.10814000
H	4.21533500	-1.55432700	-2.91825800	H	-5.91383600	0.75812000	0.22758000
C	0.63804000	0.00477700	3.05091200	C	1.64721200	0.31111900	5.56148800
C	1.10454000	0.14467500	4.19449500	C	-1.05346500	-0.36900900	-2.73179100
Sm	-1.75395700	-0.86873400	2.11653900	C	1.02891200	1.55148600	6.23602500
C	-3.10291800	1.37789300	3.28186100	H	1.44265800	1.67364300	7.24346100
C	-3.37948500	1.52025000	1.89382100	H	1.24080900	2.46157200	5.66820700
C	-3.77302800	0.20214200	3.74582200	H	-0.05664500	1.45099500	6.32402900
C	-4.20283900	0.42347200	1.49838800	C	3.17842000	0.47735800	5.49569200
C	-4.50096000	-0.34725600	2.65369700	H	3.57794800	0.61135500	6.50719200
C	-0.60024000	-3.34158400	2.51182500	H	3.65133300	-0.40582400	5.05737300
C	-1.56875400	-3.27513400	3.55328800	H	3.45763000	1.35071400	4.90134800
C	-1.29285100	-3.47350300	1.27632200	C	1.32240500	-0.93036000	6.41418600
C	-2.85744100	-3.41335100	2.96702300	H	0.24258600	-1.07433500	6.50644400
C	-2.69215700	-3.49440300	1.55601800	H	1.75563800	-1.83354700	5.97490300
C	-4.06244400	-3.83647500	3.75397300	H	1.73706300	-0.80732700	7.42104300
H	-4.24572800	-3.21435000	4.63509000	C	-0.14278100	0.55743700	-3.56139000
H	-4.97457800	-3.85160900	3.15669200	H	0.90512500	0.25678700	-3.47904200
H	-3.90599000	-4.85945500	4.12423300	H	-0.42980900	0.50671900	-4.61764900
C	-3.75997100	-3.81336100	0.54695800	H	-0.23318800	1.59479900	-3.23014700
H	-3.69728600	-4.86091100	0.22205700	C	-2.51636500	0.08767700	-2.89780100
H	-4.76246700	-3.66880000	0.95671000	H	-3.19547400	-0.55401100	-2.32980000
H	-3.68788100	-3.19835700	-0.35729500	H	-2.64814500	1.11785800	-2.55435900
C	-0.68290900	-3.79162100	-0.05670500	H	-2.80295700	0.03888800	-3.95433000
H	-1.45235600	-4.10771100	-0.76719700	C	-0.91484000	-1.81303100	-3.25017700
H	-0.15347200	-2.94569000	-0.50068800	H	-1.18812100	-1.85417300	-4.31064100
H	0.02942300	-4.62064300	0.03288500	H	0.11262300	-2.17380000	-3.14809700
C	0.87724100	-3.45201400	2.70353800	H	-1.56938500	-2.49458500	-2.70097100
H	1.16504100	-3.23320100	3.73401600				

TS_{CC}[(C₅Me₅)₂Sm-CC^tBu]₂

H= -2096.205118 au

Sm	2.26597500	0.94450200	0.30521500	H	3.64524800	-0.36772200	-3.41281400
C	-0.10960700	-0.03713100	-0.51533200	H	4.42209100	-1.90950400	-3.07610900
C	-0.42334200	-0.30993100	0.68328700	C	0.75806000	0.08355700	2.23697500
C	3.82164600	-0.85522400	-1.30290200	C	0.39915600	-0.16800500	3.43124200
C	4.75495600	0.12895900	-0.86133400	Sm	-1.95672800	-1.14250700	2.58856100
C	3.40625500	-1.61195900	-0.17232000	C	-3.18031600	1.26167600	3.40415300
C	4.90544600	-0.01184200	0.54720200	C	-3.38635600	1.20984800	1.99562300
C	4.06458500	-1.08332600	0.97265900	C	-3.97837700	0.24000600	4.00244800
C	1.48013800	3.49565300	1.20609000	C	-4.30609900	0.15681800	1.72139600
C	2.88074100	3.43159800	1.46330000	C	-4.69163000	-0.42191700	2.96254100
C	1.29350700	3.56878200	-0.20278800	C	-0.75990700	-3.70937800	2.79340300
C	3.55945800	3.49172800	0.21305700	C	-1.66679000	-3.67091500	3.88934600
C	2.58129200	3.54859300	-0.81959500	C	-1.52218100	-3.70952500	1.59182200
C	0.01061000	3.95249200	-0.88304300	C	-2.99255300	-3.67559500	3.36642100
H	-0.17340900	5.02986600	-0.76835000	C	-2.90499300	-3.68856500	1.94438300
H	0.03312000	3.75620200	-1.95900300	C	-4.20791700	-3.96895200	4.19672200
H	-0.85931200	3.43755400	-0.46993800	H	-4.29845400	-3.31847900	5.07416100
C	2.86611100	3.83046700	-2.26831900	H	-5.13123800	-3.87902100	3.62278700
H	3.80099400	3.37134000	-2.60389400	H	-4.16475600	-4.99952400	4.57559100
H	2.07265500	3.47101300	-2.93061700	C	-4.03887400	-3.90185800	0.98175100
H	2.96080700	4.91029200	-2.44818500	H	-4.11611600	-4.95833200	0.69091600
C	5.01360800	3.82094600	0.05117300	H	-5.00152800	-3.62052600	1.41515400
H	5.64802400	3.30820800	0.77782500	H	-3.91889400	-3.32820000	0.05629500
H	5.38667400	3.58840000	-0.94801700	C	-0.97739700	-3.94413100	0.21292300
H	5.16745000	4.89878600	0.20323900	H	-1.77197200	-3.90878000	-0.53785300
C	3.53811100	3.57202100	2.80687600	H	-0.21984400	-3.21231600	-0.07435000
H	3.77458000	4.62420500	3.01891300	H	-0.51724300	-4.93936500	0.14033700
H	2.89299000	3.22419200	3.61734900	C	0.72209800	-3.92148900	2.87681800
H	4.48193900	3.02055000	2.87366100	H	1.01231600	-4.31852300	3.85445800
C	0.41686000	3.72925500	2.23328000	H	1.05056400	-4.64946200	2.12640800
H	0.68035800	3.28725500	3.19631700	H	1.29333900	-3.00204900	2.71382800
H	0.26531100	4.80542300	2.39946200	C	-1.33713700	-3.91687400	5.33547000
H	-0.54293000	3.30803700	1.93259800	H	-1.42043200	-4.98660300	5.57448700
C	2.63173300	-2.89244700	-0.21401400	H	-0.32069600	-3.61047500	5.59566600
H	3.30977600	-3.75752600	-0.21266500	H	-2.01905100	-3.39315200	6.01398200
H	1.96931700	-3.00026900	0.64527500	C	-5.91133300	-1.27181100	3.15887000
H	2.01760400	-2.97183300	-1.11460500	H	-6.03958600	-2.02283000	2.37417300
C	4.12706100	-1.71368500	2.33210700	H	-5.91124300	-1.78705500	4.12103900
H	4.94059700	-2.45171100	2.38280200	H	-6.81047800	-0.63952800	3.13559100
H	4.32259700	-0.97597700	3.11686500	C	-4.24550800	0.05439400	5.47072600
H	3.20330500	-2.23428300	2.59046100	H	-5.17366500	0.55966200	5.77094100
C	5.95310200	0.62015100	1.41950100	H	-4.35858800	-1.00039900	5.74375800
H	6.65961000	-0.13933000	1.77916600	H	-3.44600100	0.46273300	6.09454000
H	6.53829500	1.36656800	0.87837200	C	-2.44791000	2.35610200	4.12753700
H	5.54271300	1.10994200	2.31047400	H	-2.81849000	3.33996900	3.81183200
C	5.61990800	0.92663900	-1.79366500	H	-2.60574300	2.29630900	5.20834200
H	5.04545000	1.52967300	-2.50594200	H	-1.36937300	2.35263100	3.94532500
H	6.28781100	1.60252400	-1.25662600	C	-2.88957700	2.22079700	1.00545300
H	6.25349400	0.25718800	-2.39089200	H	-1.87245700	2.01047500	0.66202100
C	3.62105600	-1.23413000	-2.74361300	H	-3.53334500	2.25399000	0.12145300
H	2.67693800	-1.75807400	-2.91718700	H	-2.89541900	3.22563400	1.44359500
				C	-4.97060000	-0.12707100	0.40406700
				H	-4.37343700	0.22349700	-0.44143000

H	-5.15670100	-1.19531600	0.25339200
H	-5.94560700	0.37574300	0.33737100
C	0.72707200	-0.13186600	4.90154500
C	-0.43982800	-0.02194700	-1.98178800
C	1.72542000	-1.25082300	5.24460000
H	1.94466600	-1.23478300	6.31878800
H	1.32399700	-2.23419900	4.99321500
H	2.66233600	-1.11926900	4.69988200
C	-0.53877800	-0.32287600	5.75333000
H	-0.29082200	-0.34144400	6.82099200
H	-1.24725800	0.49144900	5.58833600
H	-1.03431500	-1.27449100	5.52544200
C	1.36800400	1.21647400	5.27449100
H	2.29088200	1.37189500	4.70974900
H	0.69091600	2.04984000	5.06905000
H	1.61197300	1.23527100	6.34365800
C	0.62513200	0.75274300	-2.77424700
H	1.61502800	0.29946200	-2.65714200
H	0.39614600	0.75247800	-3.84619800
H	0.67132400	1.79359600	-2.44394200
C	-1.80477100	0.65165100	-2.20740600
H	-2.59329400	0.10715800	-1.68225800
H	-1.80322900	1.68383200	-1.84990200
H	-2.04501400	0.65994200	-3.27736400
C	-0.51214800	-1.46346700	-2.51480000
H	-0.71857500	-1.45333700	-3.59158100
H	0.42743500	-1.99803500	-2.35317600
H	-1.30705600	-2.02254200	-2.01617800

{{(C₅Me₅)₂Sm}₂(μ-η²:η²-t⁴BuC₄t⁴Bu)}

H= -2096.259488 au

Sm	2.68756800	1.12789900	0.25656800
C	0.42912700	0.16972300	-0.32843200
C	0.19855600	-0.03611700	0.95804400
C	4.11387300	-0.69992700	-1.30365100
C	5.09524000	0.22736200	-0.83502200
C	3.66361000	-1.46617700	-0.19340200
C	5.23754900	0.04403900	0.56972100
C	4.34047400	-0.99055000	0.96673300
C	1.85319100	3.62967300	1.17355000
C	3.26078600	3.60557800	1.40734500
C	1.63999900	3.67382500	-0.23167900
C	3.91557500	3.65856500	0.14278700
C	2.91441200	3.66878400	-0.87293200
C	0.32522200	3.97163100	-0.88744700
H	0.09852500	5.04510800	-0.81743300
H	0.32392800	3.71387500	-1.94913900
H	-0.50270900	3.43627000	-0.41687100
C	3.14820200	3.87350300	-2.34373100
H	4.12604900	3.49967700	-2.66215500
H	2.39081400	3.37260300	-2.95639600
H	3.11376100	4.93908200	-2.60840800
C	5.36611800	3.98451800	-0.05562100

H	6.01465600	3.49223000	0.67420800
H	5.72130400	3.72000300	-1.05371200
H	5.52567300	5.06552900	0.06136500
C	3.94558600	3.72838700	2.74034500
H	4.13139600	4.78079800	2.99510400
H	3.34927300	3.30619100	3.55468800
H	4.91820400	3.22560100	2.75277800
C	0.77689100	3.80002300	2.20600300
H	1.18585600	3.77799900	3.21851800
H	0.27406700	4.76795400	2.08238900
H	0.00364600	3.02746500	2.14797200
C	2.77080800	-2.67081900	-0.22313500
H	3.29737000	-3.55337600	0.16098600
H	1.86806200	-2.53997700	0.38223000
H	2.45022200	-2.90416200	-1.24074800
C	4.32163000	-1.64854700	2.31577600
H	5.14572100	-2.36973900	2.41087200
H	4.43766900	-0.93391000	3.13771200
H	3.39369000	-2.20147200	2.48260900
C	6.29620600	0.63052800	1.45877000
H	7.09419400	-0.10075200	1.64621700
H	6.76842900	1.50909400	1.01350800
H	5.90914700	0.92625800	2.44058700
C	6.00327600	1.00203200	-1.74601800
H	5.46056800	1.59797400	-2.48825300
H	6.66032500	1.67812000	-1.19552800
H	6.64981400	0.31566900	-2.30994100
C	3.81730600	-0.93557000	-2.75774400
H	3.06728900	-1.71686400	-2.89654300
H	3.45410700	-0.04000300	-3.27714600
H	4.72228200	-1.25734300	-3.29024300
C	0.24409000	-0.11588400	2.27848000
C	-0.14513000	-0.37720200	3.50794500
Sm	-2.26410900	-1.23627600	2.40447900
C	-3.32286500	1.19375800	3.32401200
C	-3.53819500	1.22313700	1.91718000
C	-4.16409900	0.18626500	3.87895900
C	-4.52472600	0.24322100	1.59989900
C	-4.92207300	-0.38544500	2.81260700
C	-1.03187900	-3.77920500	2.66057000
C	-1.96118600	-3.68517300	3.73335900
C	-1.77028400	-3.84790100	1.44555600
C	-3.27766100	-3.72589900	3.18253500
C	-3.16116900	-3.81060100	1.76549700
C	-4.51384300	-3.98388800	3.99394900
H	-4.59513500	-3.33387400	4.87182400
H	-5.42593400	-3.86366600	3.40705100
H	-4.50766100	-5.01659700	4.36965500
C	-4.28094400	-4.05118100	0.79303700
H	-4.41182600	-5.12343600	0.59231600
H	-5.23701700	-3.67940600	1.17157500
H	-4.10543000	-3.56918100	-0.17517900
C	-1.19351000	-4.21666900	0.10759900

H	-1.86060800	-3.95538500	-0.71929900
H	-0.22775400	-3.73852700	-0.08145200
H	-1.02882100	-5.30165100	0.04757900
C	0.45626100	-3.94504500	2.77077500
H	0.74234400	-4.29122100	3.76813100
H	0.81598400	-4.69360500	2.05617600
H	1.00608700	-3.01687100	2.58028600
C	-1.66402500	-3.79539100	5.20167800
H	-1.83219700	-4.82115400	5.55902700
H	-0.62872400	-3.53719800	5.43502100
H	-2.30522000	-3.14473900	5.80601000
C	-6.16149700	-1.21782200	2.96016100
H	-6.27444800	-1.96125600	2.16481500
H	-6.19759800	-1.74343400	3.91599300
H	-7.05167600	-0.57454000	2.91601600
C	-4.38429500	-0.06898600	5.34390000
H	-5.14641000	0.60583900	5.75720900
H	-4.72993700	-1.08990600	5.53428900
H	-3.47239500	0.07848200	5.92974200
C	-2.53994900	2.22700100	4.07861700
H	-2.95705700	3.22751100	3.90045600
H	-2.58295400	2.05433600	5.15675500
H	-1.48570100	2.26090200	3.78728000
C	-2.98300900	2.27325200	0.99910200
H	-1.88900300	2.31350300	1.01608200
H	-3.29080300	2.11105600	-0.03774800
H	-3.34508000	3.26969600	1.28567500
C	-5.21105100	0.04463100	0.27773400
H	-4.64358900	0.47372100	-0.55255000
H	-5.37582800	-1.01387800	0.04701300
H	-6.19819600	0.52674400	0.27190100
C	0.60860900	-0.15368100	4.81357500
C	-0.56867700	-0.22644800	-1.41792800
C	1.59689300	-1.31176700	5.03668700
H	2.11831500	-1.18257100	5.99301800
H	1.08181900	-2.27457300	5.06015300
H	2.34439400	-1.34925700	4.24179400
C	-0.36302300	-0.12447200	6.00389400
H	0.18694000	-0.01761500	6.94662700
H	-1.05909400	0.71415100	5.92669200
H	-0.94548100	-1.04918800	6.05548400
C	1.40120800	1.16195300	4.79245600
H	2.10732100	1.17521400	3.95476600
H	0.73424900	2.02173000	4.68638300
H	1.97371900	1.28852100	5.71941400
C	-0.94063600	0.99755400	-2.26967400
H	-0.04698400	1.44038900	-2.71988900
H	-1.61985400	0.70708800	-3.08035900
H	-1.43391300	1.76704100	-1.67161500
C	-1.85525500	-0.81637100	-0.81644700
H	-1.61777000	-1.72420600	-0.24465200
H	-2.34701500	-0.07287300	-0.17692200
H	-2.57571300	-1.10654500	-1.58994400

C	0.05973900	-1.27083400	-2.35446800
H	-0.64594700	-1.54295400	-3.14894300
H	0.96140100	-0.87276300	-2.82665300
H	0.32950400	-2.18161800	-1.81447000

[(C₅Me₅)₂Sm-CCMe]₂

H= -1860.616096 au

Sm	1.97817000	0.73531600	-0.91876900
C	-0.62320000	0.10450600	-2.46276700
C	-0.82899900	-0.14017700	-1.26376900
C	3.26913400	-0.78076400	-2.95223500
C	4.28877500	0.06356100	-2.43343700
C	2.95880800	-1.76435000	-1.96471200
C	4.55357700	-0.34370200	-1.09502000
C	3.74423600	-1.48770000	-0.81188000
C	1.14690700	3.22050400	-0.07702300
C	2.48643500	3.13052200	0.39376300
C	1.18203800	3.32888100	-1.49418600
C	3.35512300	3.22597800	-0.73163200
C	2.54815500	3.33437200	-1.90193300
C	0.01310300	3.64342300	-2.38148600
H	-0.25138900	4.70824100	-2.31424600
H	0.23422400	3.44108000	-3.43402000
H	-0.87775400	3.07253900	-2.11108200
C	3.01782600	3.69165300	-3.28363800
H	4.09913100	3.58438400	-3.38602900
H	2.55466800	3.07994500	-4.06707600
H	2.77363900	4.73671600	-3.51682200
C	4.82287300	3.52148500	-0.62961900
H	5.31143900	2.95685100	0.16875000
H	5.36159300	3.31987400	-1.55758100
H	4.97459100	4.58556700	-0.40124300
C	2.92057700	3.12937800	1.83165000
H	3.00241700	4.15180000	2.22545600
H	2.21552400	2.58402500	2.46448600
H	3.90147000	2.66071200	1.96119800
C	-0.07306400	3.35107600	0.77274400
H	0.16430100	3.21220700	1.82860200
H	-0.51850500	4.34962000	0.66162800
H	-0.83744100	2.61528700	0.51417700
C	2.19002300	-3.01535700	-2.27154000
H	2.78680700	-3.67534800	-2.91617600
H	1.93506200	-3.58474100	-1.37749700
H	1.25801000	-2.80973100	-2.80635000
C	3.94789600	-2.35118500	0.40152000
H	5.01023900	-2.60749300	0.50597500
H	3.64310200	-1.86815200	1.33663100
H	3.39842700	-3.29093500	0.32585600
C	5.68679300	0.11308900	-0.22013000
H	6.44950200	-0.67320500	-0.13251200
H	6.18305000	0.99583400	-0.62793100
H	5.37191900	0.35412500	0.80236000
C	5.14630800	0.95329000	-3.28266300

H	4.58086700	1.44773800	-4.07649800
H	5.65866000	1.72534200	-2.70624700
H	5.92564900	0.35499900	-3.77526800
C	2.83876400	-0.83488400	-4.39101100
H	1.87097900	-1.32981800	-4.51019900
H	2.76085900	0.15885400	-4.84583300
H	3.56022200	-1.40019500	-4.99797900
C	0.87842900	0.19893900	1.36342700
C	0.43285200	0.22674900	2.52150000
Sm	-1.95775300	-0.76208100	0.97850800
C	-3.35282700	1.61261200	1.76214000
C	-3.57251300	1.50809200	0.36148100
C	-4.02033000	0.51735200	2.39361600
C	-4.37029700	0.34695500	0.12692500
C	-4.69605700	-0.22850400	1.38605600
C	-0.67755800	-3.17727200	1.23281600
C	-1.40801700	-3.07946700	2.44981300
C	-1.60887100	-3.36726900	0.17422600
C	-2.79102500	-3.24896400	2.15028600
C	-2.91667500	-3.41908200	0.74189300
C	-3.83416800	-3.52163900	3.19466000
H	-3.89370900	-2.74001400	3.95984000
H	-4.82963000	-3.63804500	2.76272500
H	-3.60285800	-4.45686300	3.72231300
C	-4.13820200	-3.86722200	-0.01014400
H	-4.00279800	-4.89016400	-0.38452000
H	-5.02622300	-3.87694500	0.62495200
H	-4.36330600	-3.24203500	-0.88159100
C	-1.27980600	-3.67942700	-1.25639100
H	-2.16986300	-3.62578700	-1.89010200
H	-0.54579200	-2.98651500	-1.67028900
H	-0.87203800	-4.69509300	-1.35501700
C	0.80908500	-3.21913300	1.10323900
H	1.30486800	-2.92461100	2.03020300
H	1.15152800	-4.23308600	0.85231500
H	1.16822900	-2.54187400	0.32584100
C	-0.83244400	-3.06590300	3.83731400
H	-0.75022700	-4.08615200	4.23749500
H	0.17059800	-2.63162100	3.86159100
H	-1.45514800	-2.50430400	4.54247800
C	-5.82336600	-1.18738000	1.62472900
H	-5.90523800	-1.95015000	0.84763100
H	-5.74448400	-1.69358500	2.58809800
H	-6.77506600	-0.63795500	1.63103200
C	-4.21828500	0.39258300	3.87840700
H	-5.00721800	1.07207900	4.23165500
H	-4.51630800	-0.61730400	4.17286100
H	-3.31495000	0.64778600	4.44371400
C	-2.79551600	2.78112500	2.52573300
H	-3.55261600	3.17511100	3.21598700
H	-1.91555900	2.53383400	3.13000000
H	-2.51063100	3.59897700	1.86242200
C	-3.28296400	2.52283100	-0.70460900

H	-2.70226800	3.36617200	-0.32704200
H	-2.73041700	2.08819200	-1.54402400
H	-4.22046700	2.92946300	-1.10683200
C	-4.95757200	-0.02659700	-1.20451700
H	-4.23058700	0.07818000	-2.01682500
H	-5.32009400	-1.05852400	-1.21705600
H	-5.81363100	0.61514700	-1.45706100
C	0.07927700	0.34682400	3.94049500
H	-0.92499300	-0.03081300	4.16629800
H	0.11398100	1.39287100	4.26544700
C	-0.55527000	0.36114000	-3.90384000
H	0.37786800	0.84959700	-4.20318700
H	-1.37824100	1.01316400	-4.21658900
H	-0.63091600	-0.57211100	-4.47259300
H	0.77801400	-0.21946000	4.56617300

TS_{CC}[(C₅Me₅)₂Sm-CCMe]₂

H= -1860.59418 au

Sm	2.41215000	0.74284000	0.37957200
C	0.06297900	0.02957900	-0.48613700
C	-0.39950000	-0.26682600	0.66723200
C	3.65695400	-0.83598900	-1.60591600
C	4.70358800	-0.01302900	-1.10055500
C	3.30345700	-1.77671300	-0.59425800
C	4.95700400	-0.40357900	0.24432000
C	4.09625800	-1.50115100	0.55480100
C	1.51796800	3.19830300	1.30229800
C	2.86136500	3.11123900	1.76359800
C	1.54342700	3.33135400	-0.11292100
C	3.72332100	3.23239700	0.63528000
C	2.90727700	3.35305800	-0.52888300
C	0.35610200	3.62125200	-0.98421100
H	0.09451100	4.68849700	-0.95373000
H	0.54880100	3.37634400	-2.03389400
H	-0.52961400	3.06321700	-0.66791300
C	3.37454000	3.70323900	-1.91315800
H	4.44121300	3.50985800	-2.04378000
H	2.84361700	3.14569500	-2.69358800
H	3.21200700	4.76906000	-2.12329200
C	5.19783000	3.49817000	0.71919700
H	5.68362000	2.92507100	1.51396600
H	5.71828300	3.27559600	-0.21503200
H	5.38070500	4.55936600	0.93813200
C	3.29958800	3.05938200	3.20026800
H	3.36641200	4.06393200	3.64005500
H	2.60299500	2.48351200	3.81809700
H	4.28814300	2.60127800	3.31034800
C	0.29633300	3.30624200	2.15669400
H	0.51909400	3.08637200	3.20317000
H	-0.11885700	4.32320700	2.11579900
H	-0.48312700	2.61070300	1.83893600
C	2.43085000	-2.97376100	-0.82731300
H	2.95755500	-3.72223200	-1.43507300

H	2.14107100	-3.46300800	0.10371800
H	1.50948700	-2.72100600	-1.36120200
C	4.22522600	-2.32766200	1.80399100
H	5.24233800	-2.73255700	1.89198100
H	4.03341700	-1.76201700	2.72414900
H	3.54124800	-3.17788900	1.79959000
C	6.09786000	0.04347400	1.11420900
H	6.86026900	-0.74407500	1.19287000
H	6.59320500	0.92918200	0.71052600
H	5.78977500	0.27911300	2.14038800
C	5.56259000	0.86895600	-1.95723000
H	4.98807200	1.38242100	-2.73331600
H	6.09737200	1.62728000	-1.38113300
H	6.32397700	0.26777400	-2.47389700
C	3.21146400	-0.87886700	-3.04081000
H	2.28048500	-1.44006800	-3.15978500
H	3.05177300	0.11809500	-3.46712400
H	3.96069800	-1.37420100	-3.67424800
C	0.79277600	0.06214500	2.26867700
C	0.43406900	0.01118700	3.46694500
Sm	-1.92806500	-0.97572800	2.56555000
C	-3.23187700	1.42859000	3.27545800
C	-3.42943300	1.32000900	1.87040900
C	-3.96887200	0.37846900	3.90559100
C	-4.27689600	0.19641500	1.63211000
C	-4.64889100	-0.35444800	2.89154800
C	-0.55959700	-3.36813400	2.79346000
C	-1.32230700	-3.30063600	3.99339000
C	-1.46228500	-3.54744200	1.70792900
C	-2.69694900	-3.47264700	3.65418300
C	-2.78430300	-3.62154600	2.23956400
C	-3.77746200	-3.73668500	4.66211400
H	-3.82279600	-2.97637000	5.44996200
H	-4.76520400	-3.79252600	4.20082600
H	-3.60381900	-4.69769200	5.16527400
C	-3.99326000	-4.03802900	1.44986000
H	-3.89670900	-5.07924200	1.11558300
H	-4.90771300	-3.97799300	2.04387100
H	-4.14663700	-3.43269600	0.54911200
C	-1.08425400	-3.81184400	0.27929800
H	-1.94726900	-3.72097800	-0.38759700
H	-0.31924400	-3.11876800	-0.07704800
H	-0.69068400	-4.83040800	0.15607600
C	0.93213500	-3.38267000	2.68562700
H	1.41174100	-3.12853700	3.63446900
H	1.29375400	-4.37853200	2.39469900
H	1.29071400	-2.66338800	1.94504800
C	-0.79073600	-3.29615200	5.39910900
H	-0.77093200	-4.31288100	5.81515100
H	0.23178800	-2.91255500	5.45223400
H	-1.40529300	-2.69493000	6.07940600
C	-5.78811000	-1.30401900	3.11479000
H	-5.86088500	-2.06775900	2.33647600

H	-5.72579700	-1.81203800	4.07946300
H	-6.73893900	-0.75321200	3.10654700
C	-4.18077500	0.25438200	5.38854300
H	-4.96027500	0.94542700	5.73908400
H	-4.49674700	-0.75202500	5.67811200
H	-3.27668200	0.49285400	5.96059900
C	-2.60808200	2.57124800	4.02523800
H	-3.38308000	3.17761700	4.51326400
H	-1.92621700	2.24355800	4.81816400
H	-2.04441800	3.23491900	3.36892100
C	-3.05271600	2.31208400	0.80835000
H	-2.46529200	3.13830500	1.21288300
H	-2.47011600	1.86269200	-0.00232600
H	-3.95386700	2.74914900	0.35856100
C	-4.85615600	-0.17252300	0.29533400
H	-4.13502800	-0.03418300	-0.51726400
H	-5.19213800	-1.21347500	0.26504800
H	-5.72902300	0.44989400	0.05249300
C	0.30482200	0.08895900	4.92631600
H	-0.66442400	-0.27005200	5.30776200
H	0.41196700	1.12418700	5.26969700
C	-0.36936500	0.04078200	-1.91267300
H	-0.31565100	1.05179700	-2.33111300
H	-1.39787500	-0.31811800	-2.04148300
H	0.28191000	-0.58547700	-2.53070700
H	1.07312700	-0.51310200	5.42436100

$\{[(C_5Me_5)_2Sm]_2(\mu-\eta^2:\eta^2-MeC_4Me)\}$

H= -1860.645282 au

Sm	2.42933900	1.03719600	-1.18248900
C	0.19425500	0.21719400	-1.93484800
C	-0.11166500	0.02234400	-0.67013500
C	3.72650900	-0.71861300	-2.90237100
C	4.76135500	0.14091300	-2.42739700
C	3.29702600	-1.53630100	-1.82038900
C	4.94474500	-0.12034300	-1.03855800
C	4.03317100	-1.15390300	-0.66214500
C	1.57523800	3.47662100	-0.21813100
C	2.98806100	3.49367600	-0.02137200
C	1.32318500	3.52939700	-1.61839800
C	3.60920400	3.58106500	-1.30001400
C	2.58073900	3.57720000	-2.28954400
C	-0.02336400	3.69138500	-2.25871700
H	-0.35029100	4.74029300	-2.22988100
H	-0.01368400	3.38961600	-3.31034300
H	-0.78839900	3.09692600	-1.75402100
C	2.77132400	3.79189000	-3.76501900
H	3.75708400	3.46094600	-4.10533600
H	2.02308600	3.25779700	-4.36074100
H	2.68485600	4.85481100	-4.02840600
C	5.05230300	3.91978000	-1.53024800
H	5.72373400	3.39832500	-0.84163700
H	5.37576900	3.69217400	-2.54819700

H	5.21784200	4.99523900	-1.37745000	H	-0.96040900	-4.78970100	-1.30381100
C	3.69971800	3.58120600	1.30012600	C	0.39050500	-3.46962000	1.50502200
H	3.81502600	4.62409700	1.62558200	H	0.74696000	-3.21681600	2.50699200
H	3.15969200	3.06170200	2.09918600	H	0.78581500	-4.46419100	1.25877700
H	4.70604300	3.15226700	1.25241700	H	0.84173000	-2.75268100	0.81319500
C	0.53403700	3.56068200	0.85890900	C	-1.64601500	-3.40968500	3.98402500
H	0.95265400	3.34440500	1.84591800	H	-1.59478600	-4.42977400	4.38887500
H	0.09847000	4.56779300	0.90737900	H	-0.67250700	-2.94445400	4.16375100
H	-0.28417000	2.85436700	0.69508900	H	-2.38224200	-2.86799200	4.58759100
C	2.37262600	-2.70889300	-1.94308100	C	-6.32714500	-1.12458800	1.64932600
H	2.90184700	-3.58143500	-2.34985600	H	-6.41165300	-1.84771300	0.83201800
H	1.96128400	-3.00865400	-0.97728400	H	-6.34091300	-1.68112300	2.58860100
H	1.52966900	-2.50282900	-2.60940200	H	-7.24128900	-0.51560100	1.62553800
C	4.00742200	-1.82573500	0.68221200	C	-4.59011300	0.03301100	4.07028500
H	4.74052700	-2.64249400	0.73276400	H	-5.30854400	0.73854800	4.50945300
H	4.25700700	-1.13295100	1.49355500	H	-4.98677200	-0.97206700	4.24253100
H	3.03028800	-2.25757400	0.91261800	H	-3.66588400	0.12339900	4.65115700
C	6.02702700	0.42761200	-0.15197900	C	-2.71439100	2.29545400	2.89997500
H	6.82396200	-0.31226200	0.00242800	H	-3.29619300	3.19829500	3.13172400
H	6.49641900	1.31615400	-0.58153500	H	-2.41019900	1.85962500	3.85636800
H	5.66004700	0.70188100	0.84419000	H	-1.80485200	2.61655900	2.38635000
C	5.65314200	0.95407500	-3.31997200	C	-3.18269300	2.41284400	-0.27077100
H	5.09307000	1.55932400	-4.04120500	H	-2.30475500	2.91656700	0.13740100
H	6.30096000	1.62795600	-2.75561300	H	-2.90057200	1.99571700	-1.24317100
H	6.30840500	0.29550200	-3.90596200	H	-3.93607500	3.18872600	-0.46452000
C	3.31482800	-0.86583400	-4.33974700	C	-5.29546900	0.19722300	-1.03419600
H	2.31722900	-1.30404600	-4.43496600	H	-4.57631500	0.38960700	-1.83805800
H	3.30527100	0.09270900	-4.86979600	H	-5.68409100	-0.81687400	-1.17416800
H	4.00646400	-1.52157000	-4.88712300	H	-6.13730500	0.88424800	-1.19812600
C	0.04566900	0.03599200	0.64903200	C	0.55801500	0.17816900	3.11881100
C	-0.27689000	-0.12713600	1.91314600	H	0.71843900	-0.72894600	3.71469200
Sm	-2.46053700	-1.05244500	1.14161500	H	0.03465600	0.88031400	3.77896700
C	-3.52121000	1.33003900	2.08160900	C	-0.66538900	-0.05327600	-3.13263700
C	-3.71787100	1.37568400	0.67232100	H	-0.83056500	0.87192000	-3.69857600
C	-4.37228500	0.31206500	2.60912600	H	-1.64959000	-0.48040300	-2.89546300
C	-4.69031000	0.39008900	0.32834700	H	-0.16249300	-0.73940500	-3.82517400
C	-5.11729300	-0.24595400	1.52705200	H	1.54346400	0.60602800	2.88893200
C	-1.10502100	-3.44825500	1.42743100				
C	-2.00776900	-3.41739900	2.52586000				
C	-1.86958300	-3.57579800	0.23162600				
C	-3.33215900	-3.56160900	2.01382800				
C	-3.24787700	-3.65243300	0.59354100				
C	-4.53897200	-3.86514600	2.85312600				
H	-4.61250200	-3.22535900	3.73898200				
H	-5.46883800	-3.76101700	2.29021600				
H	-4.49907600	-4.90092800	3.21734600				
C	-4.37834100	-3.96917600	-0.34428800				
H	-4.47952500	-5.05279200	-0.49304400				
H	-5.33972200	-3.60849000	0.03207300				
H	-4.23160200	-3.52948700	-1.33681400				
C	-1.30820600	-3.75889900	-1.15023500				
H	-2.05608400	-3.56102900	-1.92491900				
H	-0.45543500	-3.10143200	-1.34124700				

[(C₅Me₅)₂La-CCPh]₂
H= -2237.597309 au

La	-1.90804700	-0.75468100	0.78672700
La	2.00961000	0.72017700	-0.70183600
C	-0.85385900	-0.12356500	-2.69745100
C	-0.53487900	-0.08514300	-1.49661200
C	3.37656100	-0.63986900	-2.87268600
C	4.41872300	0.10323800	-2.25338000
C	3.02364100	-1.71778800	-2.00467800
C	4.64693200	-0.45570400	-0.96378500
C	3.80489500	-1.60194300	-0.82311300
C	1.20679700	3.29698600	0.19406500
C	2.52149400	3.16413100	0.72188900
C	1.31178700	3.43171600	-1.21832900
C	3.44322900	3.25433300	-0.36123500

C	2.69506200	3.41314200	-1.56282200	C	-3.86112100	-3.39975500	3.13207300
C	0.20389800	3.77191600	-2.17170800	H	-3.83853100	-2.61098300	3.89075200
H	0.07711000	4.86085000	-2.25597600	H	-4.86376600	-3.41734400	2.70034400
H	0.40552800	3.39926000	-3.18180000	H	-3.72825400	-4.35070800	3.66594000
H	-0.75416100	3.35898100	-1.85164900	C	-4.12214100	-3.97003900	-0.04578200
C	3.22565000	3.78761800	-2.91701700	H	-4.00920700	-5.02455400	-0.33039600
H	4.31048000	3.68279200	-2.97360700	H	-5.02349900	-3.89820600	0.56524400
H	2.79485300	3.18677600	-3.72678200	H	-4.30825800	-3.41447700	-0.97266400
H	2.99036600	4.83578000	-3.14580000	C	-1.25917200	-3.93125300	-1.25665300
C	4.91911500	3.46049500	-0.18568000	H	-2.06432900	-3.68102500	-1.95522900
H	5.35732100	2.78040700	0.55109800	H	-0.34614300	-3.46037400	-1.62374400
H	5.47061900	3.33768300	-1.11985100	H	-1.11205600	-5.01914800	-1.31680600
H	5.12021500	4.48053000	0.16986200	C	0.82229500	-3.36362900	1.10331100
C	2.90312900	3.13800900	2.17391600	H	1.31281900	-2.86299900	1.94060000
H	3.08625400	4.15284700	2.55353700	H	1.15791300	-4.41057600	1.09923800
H	2.12318400	2.69257800	2.79581500	H	1.19547200	-2.89707400	0.18981800
H	3.82201800	2.56769600	2.34804600	C	-0.85276100	-2.95657000	3.78727300
C	-0.04916900	3.42556000	0.99366200	H	-0.77863000	-3.93976300	4.27284400
H	0.09827300	3.09607900	2.02383300	H	0.14777100	-2.51820900	3.78974800
H	-0.39367600	4.46888400	1.02537200	H	-1.48157300	-2.33456100	4.43356700
H	-0.86155400	2.82581000	0.57784900	C	-5.90148900	-1.20649300	1.01405100
C	2.18099700	-2.87741800	-2.44508700	H	-5.92686700	-1.88312500	0.15717500
H	2.67195400	-3.41652400	-3.26662900	H	-5.87005500	-1.81336500	1.92106400
H	2.01568600	-3.60050000	-1.64347000	H	-6.86158700	-0.67179000	1.02382400
H	1.20093200	-2.55924900	-2.81521200	C	-4.54381200	0.30179000	3.48774600
C	3.97387200	-2.60799000	0.28088800	H	-5.26450500	1.05982400	3.82662500
H	5.02448000	-2.91923400	0.34928600	H	-4.99558300	-0.67402600	3.68053500
H	3.69391800	-2.22682700	1.27012500	H	-3.66812500	0.39376700	4.14137600
H	3.38431500	-3.50904500	0.10306900	C	-3.01158700	2.74343900	2.37883900
C	5.77638800	-0.12650000	-0.02871300	H	-2.18149000	2.46398500	3.03863300
H	6.56855800	-0.88661600	-0.08624700	H	-2.67618200	3.59523100	1.78471600
H	6.23795100	0.83343000	-0.26984600	H	-3.82202200	3.10088500	3.02727400
H	5.46223400	-0.08630300	1.02135000	C	-3.21407600	2.63951700	-0.88741000
C	5.33659200	1.04177500	-2.97825500	H	-2.65510400	3.45551400	-0.42441900
H	4.82298900	1.62574700	-3.74518500	H	-2.61270200	2.24862100	-1.71515800
H	5.84727400	1.73906000	-2.31101200	H	-4.11818000	3.08065700	-1.32826000
H	6.11969800	0.46615000	-3.49133600	C	-4.79102900	0.08499000	-1.65699600
C	2.90717000	-0.48896900	-4.29267600	H	-4.00568400	0.27143900	-2.39656900
H	1.84822300	-0.74053600	-4.41002600	H	-5.09226800	-0.96278300	-1.75522300
H	3.04352100	0.53175900	-4.66380300	H	-5.65852100	0.69250300	-1.95217100
H	3.46725700	-1.14878000	-4.97077100	C	1.09536800	0.28245600	4.24270200
C	0.65046600	0.07729300	1.61424400	C	0.37420100	1.19613500	5.03483900
C	0.84104600	0.16786000	2.83923100	C	2.08315300	-0.50961800	4.85920600
C	-3.49815000	1.61422800	1.51513100	C	0.62852700	1.30558900	6.39788400
C	-3.58391000	1.57039100	0.09760000	H	-0.38196200	1.81937400	4.56717300
C	-4.20993900	0.48794300	2.03417000	C	2.33806200	-0.38813800	6.22091000
C	-4.34030700	0.41368100	-0.26167300	H	2.64455400	-1.21648400	4.25579100
C	-4.77683500	-0.21831700	0.93522100	C	1.61110600	0.51645500	6.99556800
C	-0.66599100	-3.27284000	1.20185700	H	0.06125900	2.01418200	6.99499100
C	-1.41047300	-3.08260400	2.39931400	H	3.10554200	-1.00454800	6.68073900
C	-1.58825200	-3.50836000	0.14475200	H	1.81062900	0.60670000	8.05955900
C	-2.79284200	-3.23757700	2.09036900	C	-1.23716600	-0.18114000	-4.07498800
C	-2.90423900	-3.49527100	0.69435100	C	-1.59287100	0.98849100	-4.77353100

C	-1.27096800	-1.41298100	-4.75660700
C	-1.96423700	0.92426500	-6.11241200
H	-1.57289900	1.94054100	-4.25270300
C	-1.64839000	-1.46902600	-6.09402200
H	-1.00146700	-2.31850400	-4.22221300
C	-1.99397500	-0.30230200	-6.77645400
H	-2.23475900	1.83505900	-6.63933800
H	-1.67122000	-2.42676300	-6.60640100
H	-2.28649600	-0.34883300	-7.82165100

TS_{CC}[(C₅Me₅)₂La-CCPh]₂

H= -2237.575474 au

La	-2.03685600	-0.97381700	2.80530000
La	2.22635300	0.88401200	0.10871000
C	-0.26737800	-0.15676200	-0.48940900
C	-0.52750800	-0.32888000	0.73497100
C	3.62563500	-0.90733000	-1.64872300
C	4.63249500	0.00448100	-1.21691900
C	3.26947500	-1.73140800	-0.54381700
C	4.88398800	-0.24213600	0.16349800
C	4.03554300	-1.31097900	0.58060100
C	1.55052200	3.37268600	1.39533800
C	2.95175100	3.22443800	1.60034400
C	1.32952700	3.64056900	0.01604900
C	3.60244900	3.42687700	0.34747300
C	2.59797600	3.65860900	-0.63698400
C	0.02505100	4.08864900	-0.58058800
H	-0.24248800	5.08936900	-0.21457900
H	0.07833900	4.16361600	-1.67121300
H	-0.81133700	3.42953000	-0.33260500
C	2.85126200	4.07084300	-2.05999000
H	3.77287100	3.63286400	-2.45566800
H	2.03754600	3.77521400	-2.73101500
H	2.95435100	5.16107100	-2.15014000
C	5.06717100	3.69369800	0.16423000
H	5.68778700	3.13235900	0.86640700
H	5.41228200	3.46449600	-0.84691100
H	5.27964400	4.75828000	0.33625800
C	3.62834700	3.06972400	2.93321800
H	3.75923300	4.03971600	3.43220700
H	3.05338800	2.43509200	3.61570200
H	4.62498400	2.62847900	2.83593700
C	0.50926100	3.43927000	2.46985300
H	0.86042000	2.99038000	3.40216300
H	0.23655800	4.48182300	2.68707200
H	-0.40329000	2.91240200	2.18179300
C	2.40170300	-2.95144100	-0.61870800
H	2.97849400	-3.82271500	-0.95865700
H	1.97495700	-3.20987600	0.35272400
H	1.57317600	-2.82460300	-1.32205300
C	4.15147200	-2.00521500	1.90695600
H	5.02644600	-2.67047000	1.92577900
H	4.27520400	-1.29937900	2.73580400

H	3.27698500	-2.62028400	2.12758300
C	6.01487600	0.29715300	0.99124900
H	6.77934200	-0.47601400	1.14837700
H	6.51124700	1.14133700	0.50810400
H	5.69759500	0.62651000	1.98751300
C	5.42515100	0.88046700	-2.14332500
H	4.79236900	1.49954200	-2.79016900
H	6.09543300	1.55019500	-1.60047200
H	6.05087400	0.27243400	-2.81052400
C	3.18540000	-1.08467000	-3.07363800
H	2.19755600	-1.54611900	-3.14877700
H	3.14061500	-0.13328600	-3.61422100
H	3.88621500	-1.72766200	-3.62472400
C	0.79029900	0.05073100	2.15456000
C	0.52718700	-0.12235800	3.37845700
C	-3.47427500	1.50181600	3.37815100
C	-3.53025500	1.38375700	1.96203700
C	-4.28132400	0.46343600	3.93703400
C	-4.36275500	0.27310300	1.64198800
C	-4.85678100	-0.27299000	2.86132900
C	-0.78324700	-3.54525200	3.04461800
C	-1.59875100	-3.44365100	4.20590600
C	-1.64142800	-3.65848900	1.91399000
C	-2.96323400	-3.52438400	3.79693500
C	-2.98936900	-3.65968000	2.37842000
C	-4.11111500	-3.70739000	4.74735600
H	-4.12743300	-2.95589800	5.54522400
H	-5.07595800	-3.66804900	4.23823400
H	-4.04948300	-4.68581900	5.24283300
C	-4.17583700	-4.01133800	1.52626200
H	-4.10656200	-5.05095700	1.17964400
H	-5.11406500	-3.92237400	2.07802300
H	-4.26136200	-3.38746900	0.62888500
C	-1.21289100	-3.96180800	0.50788600
H	-1.98663600	-3.68872500	-0.21715800
H	-0.30057600	-3.42793000	0.23274200
H	-1.01715600	-5.03562300	0.37579600
C	0.71027800	-3.66488100	3.01108900
H	1.13732400	-3.59615100	4.01469100
H	1.01744800	-4.63168300	2.59193100
H	1.17289600	-2.87954300	2.40504000
C	-1.14191200	-3.44863200	5.63697300
H	-1.13378800	-4.46931400	6.04431100
H	-0.13421300	-3.04328400	5.75626800
H	-1.80408400	-2.86019500	6.28137000
C	-6.01399700	-1.22069100	2.97414100
H	-6.03272300	-1.95706100	2.16700900
H	-6.02262300	-1.76155700	3.92304200
H	-6.96080300	-0.66557700	2.91752800
C	-4.64031500	0.31759700	5.38947000
H	-5.47119300	0.98093900	5.66686600
H	-4.95501200	-0.70192100	5.63177700
H	-3.80580900	0.56527200	6.05473100

C	-2.90899500	2.66384900	4.14708900	H	0.43116800	4.07667300	-2.98903000
H	-2.81414000	2.43812500	5.21412000	H	-0.50441100	3.50244700	-1.61200800
H	-1.92610200	2.98236400	3.78942900	C	3.25050000	4.21496000	-3.17059600
H	-3.57209300	3.53681200	4.07543200	H	4.19782900	3.77983400	-3.50151400
C	-3.03630500	2.38319300	0.96006500	H	2.48075800	3.90158100	-3.88380400
H	-2.36649800	3.11480600	1.41722100	H	3.34762500	5.30463300	-3.27107900
H	-2.50220100	1.91321700	0.12824200	C	5.33566900	3.82873400	-0.79000600
H	-3.87640300	2.94523500	0.52939200	H	5.88939700	3.17935500	-0.10521800
C	-4.80781700	-0.09632900	0.25514800	H	5.71767200	3.65070000	-1.79851000
H	-4.00988900	0.04321900	-0.48172000	H	5.60137100	4.86266900	-0.52995100
H	-5.13863700	-1.13776200	0.19182100	C	3.71396100	3.33471300	1.88409500
H	-5.65412100	0.52438300	-0.07159700	H	3.85137800	4.32096800	2.34841100
C	0.66204900	-0.21642600	4.79790700	H	3.08025700	2.75304400	2.56146500
C	-0.26054200	0.41497700	5.66068700	H	4.70050300	2.85869100	1.86464500
C	1.71870000	-0.95115400	5.38354800	C	0.61802300	3.63357300	1.21021600
C	-0.13022300	0.31739400	7.04467900	H	0.81538800	3.01726200	2.09236200
H	-1.05440600	1.02341600	5.23454600	H	0.46243700	4.66262700	1.56260600
C	1.83862800	-1.04190100	6.76416700	H	-0.32856400	3.29480500	0.78142000
H	2.44083100	-1.43539000	4.73449000	C	2.25979100	-2.60726500	-2.06041600
C	0.91543800	-0.41287200	7.60457100	H	2.69176000	-3.48672200	-2.55701200
H	-0.84737000	0.82258400	7.68608900	H	1.92371800	-2.93484600	-1.07259500
H	2.66462400	-1.60443200	7.19144400	H	1.37349700	-2.31423300	-2.63102300
H	1.01706800	-0.48739700	8.68316000	C	4.24020400	-2.05274100	0.39212000
C	-0.30633600	-0.15422300	-1.91702400	H	4.91671500	-2.90906000	0.26471300
C	-0.03995000	1.02169400	-2.65312800	H	4.63979400	-1.46494700	1.22609400
C	-0.60076000	-1.33388400	-2.63999200	H	3.27439600	-2.45977200	0.70788900
C	-0.07393200	1.01818500	-4.04631800	C	6.24988400	0.21833700	-0.47277700
H	0.14571700	1.95079500	-2.12025300	H	7.03640100	-0.54707300	-0.52024900
C	-0.63213900	-1.32492900	-4.02812900	H	6.68273100	1.14340700	-0.86129200
H	-0.81659800	-2.24380300	-2.08979700	H	6.03641500	0.37879500	0.59106300
C	-0.36754600	-0.15220600	-4.74177100	C	5.52097600	1.08343400	-3.47736800
H	0.12265000	1.93964100	-4.58776400	H	4.90401300	1.59362500	-4.22373400
H	-0.87158800	-2.24118500	-4.56135500	H	6.06607500	1.84876400	-2.91909600
H	-0.39658500	-0.15315500	-5.82727700	H	6.26898800	0.50141900	-4.03305500

$\{[(C_5Me_5)_2La]_2(\mu-\eta^2:\eta^2-PhC_4Ph)\}$

H= -2237.626429 au

La	-2.49144900	-1.14326100	0.97283100	H	3.56181700	-1.31355200	-5.05255100
La	2.51557900	1.09931700	-0.97803700	C	0.07854300	0.04527800	0.66069100
C	0.18791200	0.36592400	-1.89852600	C	-0.28563800	-0.12185100	1.91785300
C	-0.11942600	0.06435300	-0.65128700	C	-3.79165300	1.33101000	1.61771900
C	3.60065000	-0.59964300	-3.01702500	C	-3.79192500	1.28030500	0.19538100
C	4.70823300	0.19012200	-2.58533300	C	-4.68363100	0.32415500	2.09459000
C	3.26170600	-1.49613600	-1.96478600	C	-4.68668600	0.24633200	-0.20971200
C	5.03899600	-0.20537200	-1.25563300	C	-5.25026300	-0.33478200	0.96152600
C	4.14059200	-1.24697500	-0.87299400	C	-1.10719100	-3.56209900	1.64741900
C	1.73131300	3.57337600	0.20600300	C	-2.01717300	-3.35385200	2.72157100
C	3.12016300	3.45806300	0.50881700	C	-1.86411100	-3.88459500	0.48580900
C	1.60198400	3.80664500	-1.19253800	C	-3.33946800	-3.57414900	2.23014200
C	3.85110500	3.62808800	-0.70111900	C	-3.24612600	-3.89585200	0.84462700
C	2.91148800	3.82767700	-1.75823900	C	-4.55894500	-3.69551900	3.09730700
C	0.32501000	4.15279400	-1.90307900	H	-4.61956300	-2.90275700	3.85010000
H	0.02120400	5.18584800	-1.68534800	H	-5.48305800	-3.66977200	2.51543000

H	5.10340800	0.41422900	1.47986000	H	-1.69474100	2.26780500	3.12476800
C	5.43842700	1.03458900	-2.65826900	C	-3.35529300	2.84511000	-0.42873900
H	4.92435500	1.66794500	-3.38754600	H	-2.93547300	2.55453500	-1.39596500
H	6.00839200	1.68414700	-1.99340700	H	-4.30067400	3.36575100	-0.63400200
H	6.16651200	0.43467900	-3.22162700	H	-2.67661500	3.57544100	0.01372200
C	3.37746700	-0.86918500	-4.01528200	C	-5.10919800	0.40895400	-1.23502600
H	2.42915000	-1.36338900	-4.24745900	H	-4.49869400	0.79980600	-2.05355300
H	3.36374800	0.11645000	-4.49251500	H	-5.33433400	-0.63905600	-1.46032700
H	4.16672900	-1.44987300	-4.51462100	H	-6.06599000	0.95043000	-1.26406900
C	0.60178400	0.12049200	1.60889100	C	1.21488300	0.19837200	4.25987700
C	0.86856700	0.15569800	2.82218000	C	-1.17517600	-0.21384800	-4.22025600
La	-1.92405200	-0.75624100	0.75231300	C	2.16719500	-0.96249700	4.60861200
C	-3.34012100	1.56346400	1.86387800	H	2.41632000	-0.93527400	5.67547800
C	-3.60161700	1.66913200	0.47011800	H	1.70991900	-1.93124400	4.38939100
C	-4.02599900	0.40722300	2.35323600	H	3.09830700	-0.89060300	4.03905200
C	-4.43204500	0.57095900	0.09578500	C	-0.06595300	0.08292500	5.10983100
C	-4.74239600	-0.17051200	1.26758700	H	0.19271400	0.10946500	6.17429600
C	-0.75656400	-3.33734900	1.08664600	H	-0.74777700	0.91347500	4.90552500
C	-1.68216500	-3.27144300	2.16500300	H	-0.59219900	-0.85451400	4.91234500
C	-1.49675900	-3.43984400	-0.12289100	C	1.91002300	1.53231200	4.59368900
C	-2.99681600	-3.37009700	1.62636800	H	2.83489600	1.64858900	4.02231600
C	-2.88480800	-3.44439200	0.20830200	H	1.25756900	2.38161600	4.37106500
C	-4.19537800	-3.72730000	2.45558300	H	2.16079800	1.56378600	5.66001000
H	-4.32507000	-3.08024900	3.32921600	C	-0.25335300	0.72918900	-5.01801400
H	-5.12338600	-3.70342600	1.88317300	H	0.79483800	0.43235100	-4.92110700
H	-4.08288700	-4.75044000	2.84045400	H	-0.51854300	0.69356100	-6.08060000
C	-3.99583200	-3.71315700	-0.76871000	H	-0.35635000	1.76145200	-4.67368300
H	-3.90626200	-4.71761900	-1.20310400	C	-2.63844200	0.23094100	-4.41616800
H	-4.97623800	-3.66231200	-0.28906500	H	-3.32454000	-0.42676300	-3.87505200
H	-4.00909100	-3.00702400	-1.60776200	H	-2.78972600	1.25415300	-4.06000000
C	-0.92993400	-3.71852700	-1.48462700	H	-2.89883300	0.19565100	-5.48003900
H	-1.72844500	-3.93023900	-2.20176400	C	-1.00976500	-1.65236300	-4.74637600
H	-0.34414500	-2.88730600	-1.88501100	H	-1.25878700	-1.69012400	-5.81294100
H	-0.27729900	-4.60041400	-1.45947400	H	0.01915500	-2.00221600	-4.62292800
C	0.72942200	-3.44591800	1.20970700	H	-1.66856500	-2.34447800	-4.21539600
H	1.06549900	-3.25044900	2.23036600				
H	1.07402000	-4.45446500	0.93981600				
H	1.24833400	-2.73526700	0.56448100				
C	-1.35713100	-3.35405800	3.62796100				
H	-1.38193000	-4.39428000	3.98231500				
H	-0.35826700	-2.96717000	3.84715100				
H	-2.07136500	-2.79593200	4.24310900				
C	-5.89597000	-1.12362500	1.36281400				
H	-5.89872500	-1.87619300	0.56914000				
H	-5.92707200	-1.64488300	2.32012700				
H	-6.83881000	-0.56677100	1.27112700				
C	-4.16244500	0.05417700	3.80807300				
H	-4.81328200	0.76871700	4.33185600				
H	-4.60291600	-0.93675300	3.94676000				
H	-3.20276300	0.06195600	4.33696900				
C	-2.68044400	2.57728000	2.75782000				
H	-2.54411600	3.53206000	2.24455000				
H	-3.30585500	2.77160400	3.63774900				

TS_{CC}[(C₅Me₅)₂La-CC^tBu]₂

H= -2089.966493 au

La	2.31689600	0.96257700	0.25186700
C	-0.11356900	-0.04811800	-0.50848400
C	-0.42723500	-0.32022100	0.69145200
C	3.92092200	-0.91465500	-1.35123900
C	4.85112200	0.07599800	-0.91604500
C	3.50746600	-1.66464100	-0.21597500
C	5.00582300	-0.05929100	0.49298900
C	4.16804400	-1.13047200	0.92514200
C	1.53683600	3.59931400	1.19268300
C	2.93847200	3.53115800	1.43885300
C	1.33945200	3.67874600	-0.21455200
C	3.60911400	3.58679100	0.18339000
C	2.62176000	3.65826000	-0.84089600
C	0.04195500	4.02232200	-0.88889500
H	-0.16939200	5.09682600	-0.79757900

H	0.05827900	3.80068800	-1.96042300	H	-5.15278300	-3.89430700	3.67184000
H	-0.81100000	3.49401800	-0.45508600	H	-4.23544200	-5.07923800	4.59557300
C	2.89733400	3.92437400	-2.29447100	C	-4.07548000	-3.97003200	1.02534300
H	3.82427000	3.45122600	-2.63464600	H	-4.18163200	-5.02465200	0.73681800
H	2.09236900	3.56913700	-2.94593100	H	-5.02837400	-3.66386800	1.46422300
H	3.00400500	5.00094500	-2.48694500	H	-3.94735700	-3.40202200	0.09724000
C	5.07054200	3.87263900	0.00324200	C	-1.00910300	-4.00318300	0.23279400
H	5.69128800	3.37536700	0.75276000	H	-1.79729600	-3.90963100	-0.51983300
H	5.43508100	3.57885700	-0.98351600	H	-0.22289100	-3.28950200	-0.02455800
H	5.25898600	4.95121000	0.10200000	H	-0.58574900	-5.01138200	0.12320800
C	3.60182200	3.63751100	2.78272300	C	0.70793800	-3.99248100	2.88399400
H	3.83202700	4.68379200	3.02815100	H	1.01827700	-4.36720000	3.86429200
H	2.96248200	3.26024600	3.58587900	H	1.04413000	-4.72515200	2.14137700
H	4.55007200	3.09095200	2.82857200	H	1.26162400	-3.06536800	2.69835000
C	0.47795400	3.80142300	2.23337000	C	-1.33299900	-4.03867800	5.35872300
H	0.71415300	3.27779500	3.16291800	H	-1.41357500	-5.10819800	5.59905200
H	0.36661500	4.86704700	2.47938000	H	-0.31147300	-3.73435000	5.60395400
H	-0.49699000	3.44392000	1.89689600	H	-2.00488600	-3.51528500	6.04800400
C	2.70864800	-2.93175800	-0.24371700	C	-5.98808600	-1.26696200	3.16951300
H	3.36789100	-3.81092200	-0.26631400	H	-6.09145300	-2.00207100	2.36582000
H	2.06838200	-3.03220100	0.63436900	H	-5.96887200	-1.80842600	4.11786100
H	2.06601300	-2.99429000	-1.12610300	H	-6.90925800	-0.66685400	3.16424000
C	4.19686200	-1.73611800	2.29767000	C	-4.38767000	0.12137100	5.50515700
H	4.97458200	-2.50974200	2.37159100	H	-5.27752300	0.68925500	5.80974100
H	4.42055600	-0.99109800	3.06832800	H	-4.57841900	-0.92474900	5.76768300
H	3.24739800	-2.20723000	2.56151300	H	-3.56338500	0.46785100	6.13591100
C	6.03021000	0.61017300	1.36466300	C	-2.55970700	2.40581100	4.17271100
H	6.75998400	-0.12133000	1.73557000	H	-3.02577900	3.38285600	3.98573000
H	6.59217900	1.37226600	0.82030600	H	-2.57713500	2.25611400	5.25634900
H	5.59823400	1.09455100	2.24899700	H	-1.51336600	2.49121700	3.86368200
C	5.69102500	0.89852400	-1.85013300	C	-2.94439900	2.25655100	1.05298000
H	5.09565300	1.50147400	-2.54604800	H	-1.91714600	2.03869300	0.74339800
H	6.35267100	1.58067100	-1.31244000	H	-3.55777400	2.28615500	0.14754800
H	6.32980300	0.25098000	-2.46562000	H	-2.95730300	3.26503200	1.48240000
C	3.69332600	-1.28569900	-2.78991900	C	-5.01816200	-0.10481900	0.42112600
H	2.74440000	-1.80734500	-2.94614800	H	-4.40432500	0.24959600	-0.41114900
H	3.70483000	-0.41509500	-3.45460600	H	-5.18125400	-1.17786200	0.27404200
H	4.48513800	-1.96046200	-3.14491800	H	-6.00023800	0.37858300	0.32277900
C	0.77174200	0.07553400	2.22305100	C	0.71572000	-0.12691400	4.90704200
C	0.45803100	-0.15035100	3.42994500	C	-0.43698500	-0.02395000	-1.97452800
La	-1.99279900	-1.15539100	2.65782300	C	1.78341300	-1.17362800	5.27090500
C	-3.29823300	1.31617800	3.44790500	H	1.95293200	-1.17327500	6.35422300
C	-3.48089000	1.25759100	2.03680200	H	1.47600900	-2.17867400	4.97212900
C	-4.10601200	0.29899700	4.03899700	H	2.73030600	-0.94993400	4.77431000
C	-4.39272200	0.20149900	1.75266600	C	-0.57631500	-0.43889100	5.68241000
C	-4.79314400	-0.37795500	2.99084500	H	-0.40425000	-0.41765900	6.76461600
C	-0.78026800	-3.81090200	2.81472200	H	-1.35457600	0.29773600	5.45924500
C	-1.67971200	-3.78996200	3.91684800	H	-0.94878300	-1.44471800	5.44869600
C	-1.55060300	-3.79943000	1.61833900	C	1.22087500	1.26239600	5.33590500
C	-3.00982100	-3.77981100	3.40341500	H	2.14903300	1.51167700	4.81505600
C	-2.93067400	-3.78214800	1.98033500	H	0.48220900	2.03783800	5.11644200
C	-4.23072100	-4.04052500	4.23695500	H	1.41775700	1.27570400	6.41473500
H	-4.28564400	-3.40329800	5.12743100	C	0.65409800	0.72857700	-2.75583700

H	1.62982800	0.24072800	-2.64507900
H	0.43241100	0.74832600	-3.82912000
H	0.73037200	1.76758400	-2.41884100
C	-1.78419900	0.68238400	-2.20644200
H	-2.58871700	0.15264700	-1.69024800
H	-1.76154500	1.71131300	-1.83954700
H	-2.01768500	0.70480900	-3.27776500
C	-0.53391800	-1.46259300	-2.51160600
H	-0.74056300	-1.44851800	-3.58837500
H	0.39690700	-2.01310500	-2.35012200
H	-1.33773400	-2.00866300	-2.01251600

{{(C₅Me₅)₂La}₂(μ-η²:η²-tBuC₄tBu)}

H= -2090.019009 au

La	2.44757100	1.14473700	-0.99884500
C	0.14939900	0.21393400	-1.94388800
C	-0.11381400	0.00805700	-0.67160700
C	4.02287800	-0.61534600	-2.66320900
C	4.97605200	0.26870900	-2.07278400
C	3.53122600	-1.47616300	-1.64386600
C	5.05883700	-0.03473900	-0.68377200
C	4.16351200	-1.11378600	-0.41998300
C	1.60596300	3.76943800	-0.11505900
C	3.01893900	3.77256000	0.07556000
C	1.35052100	3.77085600	-1.51558000
C	3.63436100	3.78108800	-1.20841400
C	2.60273100	3.76128000	-2.19444400
C	0.00381600	4.00666100	-2.13099600
H	-0.30746600	5.05084100	-1.98571200
H	0.00682100	3.82035500	-3.20731100
H	-0.77305900	3.37599700	-1.69001000
C	2.80235000	3.92070100	-3.67586700
H	3.74215800	3.47370800	-4.01636800
H	1.99400700	3.46018000	-4.25315500
H	2.83352000	4.98040900	-3.96402700
C	5.07826100	4.10859000	-1.44958700
H	5.75086200	3.59701800	-0.75388000
H	5.39809200	3.86329900	-2.46442600
H	5.24833900	5.18604500	-1.31396900
C	3.75772900	3.95468500	1.37186800
H	4.09411600	4.99381700	1.49005900
H	3.13583500	3.72206600	2.24048600
H	4.65325400	3.32602000	1.43574100
C	0.55078600	3.94494300	0.93968300
H	0.97691500	3.93874200	1.94696200
H	0.03417300	4.90615000	0.81873400
H	-0.21583600	3.16298600	0.90447800
C	2.65225900	-2.67748200	-1.82480600
H	3.22083500	-3.60459600	-1.67185200
H	1.81616100	-2.69506600	-1.11837700
H	2.22916800	-2.71983300	-2.83065800
C	4.09980900	-1.91630900	0.84863000
H	4.76298100	-2.79058900	0.78774600

H	4.41997300	-1.34128800	1.72291500
H	3.09429700	-2.29820000	1.05163100
C	6.05159100	0.52931800	0.29316700
H	6.95553700	-0.09279400	0.34764100
H	6.37666700	1.53590600	0.01443100
H	5.64908900	0.58659900	1.31074100
C	5.92766800	1.11898900	-2.86323000
H	5.42858100	1.70683800	-3.64151500
H	6.48467400	1.81246800	-2.23085800
H	6.66666400	0.48655100	-3.37492600
C	3.79191200	-0.73425100	-4.14307300
H	2.96038800	-1.40383700	-4.37350200
H	3.57905800	0.22967300	-4.62048500
H	4.68054500	-1.14068400	-4.64540500
C	0.09593900	0.01005300	0.64160100
C	-0.16392800	-0.18501300	1.91704100
La	-2.45395700	-1.13934700	0.99342200
C	-3.68733200	1.30449300	1.93050700
C	-3.89830400	1.33259400	0.52280600
C	-4.48627500	0.25824700	2.47662700
C	-4.83991700	0.31202400	0.19739900
C	-5.21515300	-0.34037800	1.40568100
C	-1.16038100	-3.72436500	1.29750500
C	-2.09699400	-3.65441400	2.36464300
C	-1.88927700	-3.81569200	0.07738400
C	-3.40894000	-3.72923700	1.80558500
C	-3.28131100	-3.82310100	0.38989600
C	-4.64565900	-3.99907400	2.61224800
H	-4.73385100	-3.34847700	3.48925000
H	-5.55699900	-3.88649300	2.02220300
H	-4.63385500	-5.03120500	2.98992200
C	-4.39473800	-4.08604600	-0.58404600
H	-4.54251900	-5.16318900	-0.74154600
H	-5.34899400	-3.68254100	-0.23297400
H	-4.19901600	-3.64834000	-1.56898700
C	-1.28016300	-4.11977000	-1.26191100
H	-1.98544300	-3.95731100	-2.08250600
H	-0.38931600	-3.51705100	-1.46485100
H	-0.97035500	-5.17271600	-1.31760500
C	0.33157000	-3.83942500	1.40807700
H	0.64559500	-3.96335100	2.44737800
H	0.69729500	-4.71166200	0.85257100
H	0.85547900	-2.96004400	1.01606900
C	-1.80728500	-3.72098200	3.83752800
H	-2.10052400	-4.69593200	4.25034000
H	-0.74420900	-3.58739200	4.04928600
H	-2.35187200	-2.96326400	4.41380700
C	-6.40038600	-1.25014400	1.54266900
H	-6.46541800	-1.98861600	0.73703500
H	-6.40145300	-1.79097400	2.49104400
H	-7.33089100	-0.66632700	1.50698600
C	-4.68597300	-0.01395200	3.94170400
H	-5.46576200	0.63285500	4.36677400

H	-4.99432200	-1.04686800	4.13249000	C	1.21691400	3.39549500	-1.38733000
H	-3.77550500	0.16802900	4.52273000	C	3.38001300	3.22634600	-0.61000800
C	-2.96786900	2.36183900	2.71375700	C	2.58547900	3.36735600	-1.78477900
H	-3.61047200	3.24277100	2.85312700	C	0.06341400	3.72208200	-2.29017700
H	-2.68204200	2.01349100	3.70887100	H	-0.15609500	4.79917300	-2.27617300
H	-2.05864500	2.70554400	2.21282400	H	0.27546600	3.45783700	-3.33129700
C	-3.38538800	2.40329900	-0.39594200	H	-0.85053600	3.20261800	-1.99450700
H	-2.33443500	2.64121000	-0.20624300	C	3.07268800	3.73055200	-3.15868400
H	-3.47342300	2.12325200	-1.44975900	H	4.14759300	3.57578900	-3.26604600
H	-3.95204200	3.33580600	-0.26826200	H	2.57985000	3.15956400	-3.95440100
C	-5.50375100	0.09143800	-1.13283000	H	2.87725600	4.79100500	-3.36777300
H	-4.92143000	0.50625800	-1.96031700	C	4.85934600	3.45193800	-0.49991900
H	-5.66831600	-0.97052400	-1.34817900	H	5.31547500	2.86189000	0.29988000
H	-6.48984400	0.57499000	-1.16506300	H	5.39096700	3.22072900	-1.42552400
C	0.79456400	0.14802500	3.05217800	H	5.06524000	4.50680200	-0.27100700
C	-0.78701100	-0.12653900	-3.09392100	C	2.92697800	3.14315600	1.94905800
C	1.15677000	-1.13098500	3.82429300	H	3.07967500	4.16228500	2.33033500
H	1.82713400	-0.89516900	4.65964600	H	2.18038200	2.66127900	2.58567400
H	0.25762000	-1.59961400	4.23257400	H	3.87199700	2.60807800	2.09199900
H	1.65839500	-1.85818800	3.18057800	C	-0.05769500	3.44810000	0.86985800
C	0.12824900	1.12298800	4.03694200	H	0.12323000	3.14887700	1.90352000
H	0.80133300	1.33661400	4.87598700	H	-0.39053200	4.49587500	0.88001100
H	-0.12548300	2.06958400	3.55284400	H	-0.89019000	2.84538200	0.50080000
H	-0.79259300	0.69281500	4.44255600	C	2.22344400	-3.12576200	-2.29148900
C	2.08899200	0.79029400	2.52104300	H	2.81447400	-3.76335500	-2.96361000
H	2.61009700	0.09284800	1.85199900	H	2.00762400	-3.71667000	-1.40039000
H	1.85817800	1.71895300	1.98572100	H	1.27232400	-2.93322400	-2.79661100
H	2.78439400	1.04243300	3.33059600	C	4.05108300	-2.47545400	0.33139500
C	-1.07915200	1.13071100	-3.92890500	H	5.10899700	-2.76693700	0.37219900
H	-0.14979800	1.57290600	-4.30087200	H	3.82138200	-1.99089800	1.28794600
H	-1.70602700	0.87857900	-4.79262600	H	3.46701000	-3.39638800	0.28701400
H	-1.60074000	1.88865900	-3.33896600	C	5.74419500	0.01921800	-0.31542600
C	-2.12002700	-0.70027000	-2.58063300	H	6.52933900	-0.74955900	-0.29248500
H	-1.94429100	-1.63932100	-2.04123900	H	6.19982900	0.92943600	-0.71035100
H	-2.61274400	0.02088700	-1.91734000	H	5.47351000	0.21423500	0.72981300
H	-2.81367100	-0.92227800	-3.40042900	C	5.06366900	0.92381900	-3.32921100
C	-0.12341500	-1.16497100	-4.01352200	H	4.45946800	1.41205300	-4.09807900
H	-0.77891000	-1.39923100	-4.86102500	H	5.56511300	1.70451500	-2.75377600
H	0.82015400	-0.78009100	-4.40921600	H	5.84905900	0.36172300	-3.85381100
H	0.08395400	-2.09533600	-3.47765400	C	2.70842200	-0.87193900	-4.37462000
				H	1.71664600	-1.33128900	-4.43205300
				H	2.63648900	0.13258000	-4.80605700
				H	3.36341500	-1.45251300	-5.03992400
				C	0.70669600	0.16914200	1.55747000
				C	0.54345100	0.31740300	2.77843500
				La	-1.92002200	-0.73184100	0.89938100
				C	-3.46532400	1.65482900	1.67115100
				C	-3.63448300	1.58140500	0.26179000
				C	-4.13801900	0.53643500	2.25340500
				C	-4.40342500	0.41418100	-0.02791900
				C	-4.76137200	-0.19865900	1.20495100
				C	-0.62595800	-3.22777000	1.25007000
				C	-1.35016200	-3.08424900	2.46569500

[(C₅Me₅)₂La-CCMe]₂

H= -1854.376738 au

La	1.93414800	0.68320000	-0.83224100
C	-0.82205000	0.12283900	-2.66188900
C	-0.69906600	-0.08530900	-1.44520400
C	3.23104700	-0.85579100	-2.96613300
C	4.25810000	-0.00569500	-2.47185600
C	2.97643900	-1.86381200	-1.98782900
C	4.58175600	-0.43477700	-1.15299100
C	3.79992500	-1.59519700	-0.86101700
C	1.16673500	3.28485400	0.02950300
C	2.50006000	3.15649100	0.50921900

C	-1.56295000	-3.45936800	0.20499600	H=	-1854.348428	au		
C	-2.73479700	-3.26096400	2.18076600	La	2.48187100	0.77877800	0.36279700	
C	-2.86798300	-3.48727600	0.78049300	C	0.04740700	0.01671800	-0.49114400	
C	-3.77913500	-3.47121100	3.23876000	C	-0.38801500	-0.27748500	0.67024600	
H	-3.78330800	-2.68231100	3.99861900	C	3.77918900	-0.88346200	-1.63956000	
H	-4.78609700	-3.53335900	2.82143000	C	4.82081100	-0.03719100	-1.16137700	
H	-3.59671400	-4.41511700	3.77049900	C	3.44108100	-1.80125500	-0.60299700	
C	-4.09924700	-3.95453200	0.05656400	C	5.09581200	-0.40110100	0.18684800	
H	-3.98653600	-4.99977000	-0.25961500	C	4.24435300	-1.49549000	0.53080800	
H	-4.98468800	-3.90807300	0.69317300	C	1.56196700	3.32700200	1.27589200	
H	-4.31644600	-3.37514600	-0.84864600	C	2.90981300	3.25652800	1.72572100	
C	-1.24246100	-3.80297000	-1.22128800	C	1.57425500	3.44803900	-0.14121900	
H	-2.14399700	-3.80257400	-1.84120300	C	3.76148800	3.36262500	0.58698300	
H	-0.53961100	-3.09856800	-1.67149300	C	2.93378700	3.47226800	-0.57002600	
H	-0.79789900	-4.80468600	-1.29843000	C	0.37206900	3.70393300	-1.00372500	
C	0.86189800	-3.26754500	1.11843200	H	0.09512900	4.76759800	-0.99399200	
H	1.35754500	-2.85062200	1.99742900	H	0.55389400	3.43867500	-2.05066300	
H	1.22033200	-4.29942700	0.99311000	H	-0.50314900	3.14164000	-0.66430600	
H	1.21018500	-2.69323500	0.25737300	C	3.39420000	3.79082200	-1.96427100	
C	-0.76466000	-2.99365800	3.84507800	H	4.44092000	3.52006100	-2.12096300	
H	-0.65858300	-3.98998200	4.29673400	H	2.80448600	3.27439600	-2.73063100	
H	0.22994600	-2.53894400	3.83672400	H	3.30545600	4.86569900	-2.17307300	
H	-1.39604500	-2.41057400	4.52551900	C	5.24156300	3.60346200	0.64663700	
C	-5.86220200	-1.20299000	1.37185200	H	5.72606300	3.03724100	1.44775200	
H	-5.91407100	-1.91184600	0.54234100	H	5.74403300	3.34656500	-0.28923400	
H	-5.77335400	-1.77477600	2.29738200	H	5.45240700	4.66475800	0.83823700	
H	-6.83187200	-0.68714900	1.40894600	C	3.36401200	3.21460700	3.15797100	
C	-4.37205600	0.36716600	3.72812600	H	3.45695300	4.22308100	3.58378900	
H	-5.10829400	1.09460400	4.09897900	H	2.66360200	2.66242900	3.79331000	
H	-4.75928200	-0.62602700	3.96892100	H	4.34513900	2.73875700	3.26355600	
H	-3.46233600	0.51919300	4.32137300	C	0.34104000	3.40162500	2.13877600	
C	-2.92689200	2.80162500	2.47943300	H	0.57776100	3.19431600	3.18518700	
H	-3.69931100	3.18244400	3.16029000	H	-0.10928400	4.40318600	2.09705600	
H	-2.06423000	2.53298300	3.10052000	H	-0.41949900	2.67901400	1.83111900	
H	-2.61823400	3.63517200	1.84636500	C	2.54225000	-2.98916900	-0.78066000	
C	-3.32234300	2.62889700	-0.76635200	H	3.02240600	-3.75132300	-1.40933600	
H	-2.73928400	3.45522200	-0.35463100	H	2.30260000	-3.46729300	0.17113600	
H	-2.76531200	2.22061200	-1.61640600	H	1.59381000	-2.72885400	-1.26222200	
H	-4.25035100	3.05967200	-1.16587100	C	4.35742900	-2.27775000	1.80893400	
C	-4.92617200	0.05018100	-1.38863400	H	5.27258900	-2.88590000	1.81850300	
H	-4.17935400	0.22306900	-2.17080800	H	4.40324000	-1.63358900	2.69556400	
H	-5.22556200	-1.00102600	-1.44570400	H	3.51649700	-2.95954000	1.94927000	
H	-5.81056900	0.64694100	-1.65382900	C	6.22973700	0.09268600	1.04014300	
C	0.44060800	0.54484400	4.22059800	H	7.03159100	-0.65603100	1.10059200	
H	-0.02311900	-0.30087900	4.73900400	H	6.67466700	1.00595200	0.63805300	
H	-0.14410200	1.44315200	4.44988200	H	5.92651200	0.30368400	2.07349600	
C	-1.04232800	0.36086500	-4.08706100	C	5.63888600	0.86956800	-2.03273300	
H	-1.24741100	1.41777200	-4.28993300	H	5.03490100	1.35971300	-2.80235500	
H	-1.90068300	-0.21992000	-4.44311000	H	6.15066000	1.65049800	-1.46484600	
H	-0.17600900	0.06412300	-4.68736400	H	6.41646700	0.29843700	-2.55908100	
H	1.43769000	0.68422200	4.65392500	C	3.30385600	-0.95249800	-3.06381000	
				H	2.35516500	-1.49057300	-3.14977000	
				H	3.16407900	0.03759800	-3.51323100	

TS_{CC}[(C₅Me₅)₂La-CCMe]₂

H	4.02532900	-1.48452100	-3.69978100
C	0.80932800	0.04554700	2.27067700
C	0.46927400	-0.03440300	3.47380400
La	-1.97549800	-1.00746600	2.61903800
C	-3.33082500	1.46017200	3.32417700
C	-3.52357200	1.35668900	1.91784400
C	-4.08595000	0.42123900	3.94959300
C	-4.38468200	0.24632100	1.67398100
C	-4.76279800	-0.30799800	2.93084700
C	-0.62708900	-3.52275800	2.83698500
C	-1.40782800	-3.45293100	4.02527300
C	-1.51554300	-3.67406900	1.73577800
C	-2.78067100	-3.58985400	3.66222600
C	-2.84762000	-3.72302300	2.24512600
C	-3.89139300	-3.81634500	4.64642800
H	-3.90811800	-3.07091800	5.45011600
H	-4.87223000	-3.80479000	4.16723700
H	-3.78332100	-4.79593000	5.13185500
C	-4.05675200	-4.08757900	1.43078100
H	-4.02460900	-5.14536300	1.13739400
H	-4.98514100	-3.93973500	1.98756900
H	-4.13486100	-3.50931700	0.50266700
C	-1.12050500	-3.93386000	0.31072300
H	-1.90593400	-3.63739500	-0.39232700
H	-0.21388600	-3.39176000	0.03390900
H	-0.93005000	-5.00294800	0.14034700
C	0.86837100	-3.55192100	2.75364700
H	1.33419800	-3.28442700	3.70607200
H	1.23066600	-4.55352800	2.48543600
H	1.24486400	-2.84852400	2.00595200
C	-0.89854800	-3.45263200	5.43934900
H	-0.89324100	-4.46813100	5.85880700
H	0.12627900	-3.07695600	5.50967200
H	-1.51974200	-2.84565700	6.10905600
C	-5.89288100	-1.27095000	3.14521700
H	-5.95551000	-2.02687400	2.35766100
H	-5.82257000	-1.79098600	4.10344300
H	-6.85217600	-0.73490700	3.14433700
C	-4.29243200	0.27925300	5.43165400
H	-5.07541100	0.95975200	5.79447800
H	-4.60074400	-0.73307800	5.71061800
H	-3.38776300	0.51760800	6.00355800
C	-2.65946600	2.57823000	4.07027100
H	-3.40360900	3.26801000	4.49142400
H	-2.05654600	2.22186200	4.91370800
H	-2.00163100	3.16601700	3.42837600
C	-3.10170900	2.33727100	0.86140600
H	-2.48028400	3.13472400	1.27366900
H	-2.53427200	1.86860000	0.05041400
H	-3.97976000	2.81691500	0.40924200
C	-4.95543800	-0.12532700	0.33434500
H	-4.23977800	0.04411700	-0.47729000
H	-5.25971100	-1.17609200	0.29270000

H	-5.84756900	0.47176900	0.09805300
C	0.35163000	-0.01056600	4.93558100
H	-0.60201500	-0.41609200	5.31541800
H	0.42677600	1.01411800	5.31639400
C	-0.35360300	0.04451700	-1.92399100
H	-0.33536000	1.06741100	-2.31683300
H	-1.36449300	-0.35143400	-2.08162600
H	0.33148000	-0.54125300	-2.54602700
H	1.14182000	-0.60564200	5.40750300

$\{[(C_5Me_5)_2La]_2(\mu-\eta^2:\eta^2-MeC_4Me)\}$

H= -1854.398602 au

La	2.44648300	1.01814200	-1.10614400
C	0.14143900	0.17813300	-1.93982300
C	-0.16366500	-0.00628500	-0.67609400
C	3.77547600	-0.76626500	-2.92413200
C	4.81358300	0.09241600	-2.45401000
C	3.37644800	-1.60808900	-1.84909900
C	5.03246100	-0.19740400	-1.07652600
C	4.13792800	-1.24616600	-0.70161400
C	1.56603900	3.57775200	-0.21185100
C	2.97762900	3.60169300	-0.01266100
C	1.31764900	3.59626300	-1.61357000
C	3.60278700	3.64919100	-1.29130300
C	2.57560500	3.62827300	-2.28294400
C	-0.03069700	3.73342600	-2.25740100
H	-0.36894000	4.77909300	-2.24893700
H	-0.01856200	3.41168100	-3.30317200
H	-0.79168600	3.14211000	-1.74144500
C	2.77195500	3.81212000	-3.76176000
H	3.74903600	3.45046700	-4.09649700
H	2.00997200	3.28820000	-4.34896900
H	2.71345300	4.87233000	-4.04342900
C	5.05369800	3.94916300	-1.52852400
H	5.71227100	3.42474800	-0.82877900
H	5.36959900	3.68685200	-2.54064800
H	5.25076800	5.02270000	-1.40184800
C	3.68691800	3.70815100	1.30855600
H	3.80758700	4.75533100	1.61788600
H	3.14263500	3.20550000	2.11591700
H	4.69192200	3.27450800	1.27042200
C	0.52028400	3.67381900	0.86064300
H	0.93474300	3.46620400	1.85147500
H	0.08437400	4.68121400	0.89980700
H	-0.29987600	2.96773600	0.70102300
C	2.44349000	-2.77561700	-1.96707100
H	2.95481100	-3.64411900	-2.40429300
H	2.05779900	-3.09150400	-0.99507800
H	1.58241600	-2.55397300	-2.60512800
C	4.12946400	-1.93772800	0.63300400
H	4.85139400	-2.76541100	0.66063200
H	4.40342900	-1.26044800	1.45005400
H	3.15021200	-2.36043100	0.87508200

C	6.12352700	0.35580900	-0.20376100
H	6.96143100	-0.34930300	-0.11852800
H	6.53242900	1.28851700	-0.60151800
H	5.78470400	0.55849900	0.81960300
C	5.66912600	0.94659700	-3.34308100
H	5.07883800	1.55490200	-4.03723700
H	6.30988200	1.62349200	-2.77373300
H	6.33020300	0.32122800	-3.95836000
C	3.33682800	-0.89203700	-4.35574600
H	2.34130300	-1.33769500	-4.43963000
H	3.30899100	0.07514400	-4.86947500
H	4.02263700	-1.53214900	-4.92852900
C	0.09811500	0.05601400	0.63737200
C	-0.22047700	-0.09756100	1.90128600
La	-2.47912000	-1.04216600	1.06545100
C	-3.60852900	1.38858900	2.09934200
C	-3.82049800	1.46862700	0.69380700
C	-4.44615600	0.35241900	2.61035700
C	-4.78904200	0.48541600	0.33586400
C	-5.19291900	-0.19006800	1.52111700
C	-1.10013800	-3.52412200	1.42853400
C	-2.00623400	-3.46905600	2.52311100
C	-1.86017400	-3.68309500	0.23427800
C	-3.32958400	-3.62415300	2.00949500
C	-3.23938100	-3.75207500	0.59288700
C	-4.54435100	-3.89477000	2.84873100
H	-4.60204500	-3.24818700	3.73091300
H	-5.47142700	-3.76917800	2.28480100
H	-4.53314900	-4.92924100	3.21901700
C	-4.37109800	-4.07360100	-0.34222200
H	-4.48131100	-5.15791200	-0.47912400
H	-5.33068200	-3.70177100	0.02938700
H	-4.22117100	-3.64746600	-1.34073500
C	-1.29229500	-3.88776200	-1.14192900
H	-2.03573100	-3.70030400	-1.92385700
H	-0.43641800	-3.23490100	-1.33827100
H	-0.94500100	-4.92089400	-1.28043400
C	0.39674200	-3.53152900	1.50856300
H	0.74880100	-3.27335100	2.51084700
H	0.80169300	-4.52328600	1.26677200
H	0.84765000	-2.81426100	0.81530400
C	-1.64939200	-3.43695000	3.98238600
H	-1.60626600	-4.44980800	4.40611700
H	-0.67319900	-2.97564300	4.15818100
H	-2.38404900	-2.88041500	4.57447500
C	-6.37300200	-1.11143900	1.62598000
H	-6.42408700	-1.83054200	0.80143000
H	-6.37060700	-1.67882400	2.55914300
H	-7.31087000	-0.53978500	1.60229300
C	-4.64986700	0.03853800	4.06655600
H	-5.36739400	0.73072000	4.52805400
H	-5.04192000	-0.97151500	4.22009700
H	-3.72148000	0.12012800	4.64240200

C	-2.79376100	2.33766000	2.93001200
H	-3.37352500	3.23385300	3.19110400
H	-2.47481200	1.88170600	3.87237000
H	-1.89214800	2.67507300	2.41171800
C	-3.28891600	2.52636000	-0.22903600
H	-2.39202500	3.00290200	0.17242200
H	-3.03709400	2.13430400	-1.22037300
H	-4.03094700	3.32190800	-0.38336300
C	-5.40083700	0.31494500	-1.02658400
H	-4.68585500	0.51722500	-1.83232700
H	-5.79547000	-0.69525000	-1.17964200
H	-6.24126400	1.00666900	-1.17751300
C	0.58536300	0.20310100	3.12541400
H	0.74109400	-0.70819100	3.71589400
H	0.04281300	0.89558200	3.78004200
C	-0.68682800	-0.08267700	-3.15893200
H	-0.83969800	0.84738900	-3.72011000
H	-1.67650600	-0.51229700	-2.95077600
H	-0.16653700	-0.76271200	-3.84418700
H	1.57219600	0.64138300	2.92194600

[(C₅Me₅)₂Ce-CCPh]₂

H= -2238.894626 au

Ce	-1.89831600	-0.74013300	0.78482700
Ce	1.99670400	0.72205000	-0.70784900
C	-0.85047000	-0.12416600	-2.69124100
C	-0.53801300	-0.08236000	-1.48881700
C	3.35009200	-0.63498900	-2.86583700
C	4.39142900	0.11264300	-2.25106900
C	3.00154100	-1.71088700	-1.99332600
C	4.62196900	-0.43975400	-0.95909200
C	3.78381100	-1.58812000	-0.81309200
C	1.19420000	3.27840600	0.18004400
C	2.50623200	3.14649500	0.71468500
C	1.30638800	3.41197600	-1.23186100
C	3.43348000	3.23813600	-0.36347300
C	2.69149000	3.39512300	-1.56900100
C	0.20469900	3.75426800	-2.19148800
H	0.07940800	4.84349400	-2.27461700
H	0.41293000	3.38325300	-3.20080000
H	-0.75543300	3.34140100	-1.87820800
C	3.22681800	3.77498800	-2.91982500
H	4.31302000	3.68249100	-2.96976100
H	2.80781500	3.16934900	-3.73213700
H	2.98094100	4.82045400	-3.14974600
C	4.90679300	3.45379700	-0.17818600
H	5.34229400	2.78346300	0.56883900
H	5.46782300	3.32631400	-1.10603500
H	5.09837000	4.47835000	0.16966800
C	2.88003300	3.12419500	2.16878500
H	3.06059400	4.14021700	2.54644700
H	2.09663100	2.67985500	2.78694300
H	3.79815200	2.55475500	2.34935600

C	-0.06438700	3.41041500	0.97401400	H	-0.79879400	-3.89864900	4.28617300
H	0.08409300	3.10051500	2.00993500	H	0.16872500	-2.50808200	3.79354200
H	-0.41646900	4.45159300	0.98658900	H	-1.45635100	-2.27277300	4.43064000
H	-0.87107100	2.79708200	0.56740100	C	-5.87975600	-1.19952300	1.02206200
C	2.17237600	-2.88000900	-2.43357900	H	-5.91429100	-1.87461700	0.16452700
H	2.68306800	-3.42902400	-3.23649000	H	-5.84628400	-1.80758600	1.92800800
H	1.99164800	-3.59210400	-1.62565000	H	-6.83645500	-0.65889700	1.03830900
H	1.20012600	-2.57041700	-2.83017400	C	-4.51636300	0.31755500	3.48564500
C	3.96477800	-2.59325200	0.28983300	H	-5.22143600	1.08995400	3.82487300
H	5.01842300	-2.89506500	0.35382200	H	-4.98682000	-0.64896200	3.67994600
H	3.68507700	-2.21539800	1.28026000	H	-3.63812400	0.39241100	4.13806600
H	3.38283100	-3.49943300	0.11329100	C	-2.99917200	2.75971200	2.36285700
C	5.75447800	-0.10682200	-0.02908600	H	-2.16022400	2.49710100	3.01801100
H	6.54346300	-0.87058700	-0.08233100	H	-2.68168600	3.61492900	1.76384400
H	6.21891200	0.84915800	-0.27953900	H	-3.81163200	3.10598700	3.01476700
H	5.44311500	-0.05647300	1.02132200	C	-3.20216400	2.63531700	-0.90368800
C	5.31006300	1.04528100	-2.98243800	H	-2.64555300	3.45684800	-0.44796300
H	4.80036100	1.61144900	-3.76498100	H	-2.60266000	2.24212300	-1.73159100
H	5.80875900	1.75840400	-2.32310700	H	-4.11084100	3.06856300	-1.34295300
H	6.10231600	0.46571900	-3.47670800	C	-4.76976200	0.07432600	-1.65707900
C	2.88016400	-0.49233800	-4.28642800	H	-3.98650800	0.25978200	-2.39901200
H	1.82169800	-0.74624500	-4.40201000	H	-5.06939300	-0.97423400	-1.75116000
H	3.01443400	0.52665200	-4.66291600	H	-5.63903700	0.67947700	-1.95190100
H	3.44134400	-1.15481400	-4.96099100	C	1.08288600	0.25516700	4.23082600
C	0.65315700	0.09199500	1.59739000	C	0.27124600	1.04261300	5.06901300
C	0.82972500	0.16894700	2.82534900	C	2.16463300	-0.44198800	4.80300900
C	-3.47434900	1.62091000	1.50529000	C	0.52943700	1.12074400	6.43356100
C	-3.56208000	1.56939400	0.08815800	H	-0.55888200	1.59323400	4.63704600
C	-4.18255200	0.49524400	2.03099300	C	2.42260400	-0.35058000	6.16635500
C	-4.31611500	0.40882700	-0.26410600	H	2.79584600	-1.05176000	4.16379500
C	-4.75101700	-0.21672000	0.93657800	C	1.60557000	0.42725700	6.98728900
C	-0.65781700	-3.23456900	1.20521000	H	-0.10883000	1.73096400	7.06659500
C	-1.40061900	-3.04263000	2.40340100	H	3.26318800	-0.89228000	6.59116500
C	-1.58174900	-3.47353600	0.15016900	H	1.80741200	0.49363800	8.05257400
C	-2.78299300	-3.20192800	2.09739600	C	-1.22945500	-0.18531700	-4.06988400
C	-2.89665800	-3.46272300	0.70235200	C	-1.57263700	0.98359500	-4.77582800
C	-3.84571600	-3.36891600	3.14395500	C	-1.27227600	-1.42047600	-4.74498200
H	-3.83410500	-2.57153100	3.89371500	C	-1.94018900	0.91544400	-6.11556900
H	-4.84917800	-3.40910600	2.71573300	H	-1.54599600	1.93818400	-4.26003400
H	-3.69468900	-4.31131900	3.68810500	C	-1.64613800	-1.48046900	-6.08321900
C	-4.11297200	-3.94679000	-0.03431800	H	-1.01277600	-2.32544900	-4.20478600
H	-3.99016400	-4.99916200	-0.32261900	C	-1.97891300	-0.31439400	-6.77306400
H	-5.01248900	-3.88618600	0.58056400	H	-2.20086300	1.82574500	-6.64827900
H	-4.30853600	-3.39029300	-0.95860000	H	-1.67611200	-2.44075500	-6.59043000
C	-1.25554200	-3.90069600	-1.25040400	H	-2.26852400	-0.36395600	-7.81893300
H	-2.06554000	-3.65887100	-1.94624400				
H	-0.34771600	-3.42484800	-1.62314200				
H	-1.10130000	-4.98786600	-1.30606900				
C	0.82977000	-3.32878700	1.10568100				
H	1.32125500	-2.83927000	1.94875300				
H	1.16131800	-4.37695000	1.09054800				
H	1.20514500	-2.85328900	0.19794500				
C	-0.84353700	-2.91807400	3.79177000				

TS_{CC}[(C₅Me₅)₂Ce-CCPh]₂
H= -2238.873919 au

Ce	-2.03725100	-0.97446900	2.76456800
Ce	2.23391500	0.87227000	0.15437000
C	-0.25202400	-0.13073200	-0.49646300
C	-0.52603400	-0.32427500	0.72205000
C	3.57662500	-0.89051600	-1.64880600

C	4.59740200	0.00719600	-1.22032800	C	-4.28340200	0.43260700	3.87773100
C	3.23336400	-1.72911700	-0.55030000	C	-4.33504500	0.25587300	1.58062900
C	4.86762100	-0.25957700	0.15256600	C	-4.84310400	-0.29904200	2.79008600
C	4.01946400	-1.32967500	0.56773400	C	-0.75633300	-3.50655700	3.04398100
C	1.55111700	3.33821900	1.43435800	C	-1.56617000	-3.39361100	4.20824800
C	2.94796800	3.18079300	1.66194800	C	-1.61956000	-3.64783600	1.92041000
C	1.35504500	3.61145400	0.05237700	C	-2.93197400	-3.49584200	3.80848100
C	3.62056700	3.38564700	0.42117700	C	-2.96472500	-3.65606800	2.39279000
C	2.63410700	3.62594700	-0.57953500	C	-4.07153300	-3.67710100	4.76904600
C	0.06300800	4.06918200	-0.56298700	H	-4.08487200	-2.91896200	5.56027100
H	-0.20978600	5.06555800	-0.18895200	H	-5.04092400	-3.64772500	4.26771600
H	0.13727200	4.15793800	-1.65131400	H	-4.00058300	-4.65104300	5.27215300
H	-0.77811800	3.40799100	-0.33840800	C	-4.15295700	-4.03436700	1.55459000
C	2.91159600	4.05245400	-1.99370500	H	-4.06787500	-5.07430300	1.21287200
H	3.84547600	3.62797300	-2.37409600	H	-5.08605000	-3.95929600	2.11665800
H	2.11474300	3.75485500	-2.68385000	H	-4.26008000	-3.41651300	0.65534400
H	3.00463300	5.14455300	-2.07128900	C	-1.19451900	-3.96909100	0.51715800
C	5.08939400	3.64814600	0.26679500	H	-1.99597800	-3.76848600	-0.20128700
H	5.69516600	3.07883400	0.97538000	H	-0.32165100	-3.38938400	0.20890800
H	5.45217800	3.42645500	-0.73981500	H	-0.93393900	-5.03234300	0.41563700
H	5.30193200	4.71052900	0.45175900	C	0.73801300	-3.60963000	3.00278700
C	3.60315900	3.01369100	3.00405700	H	1.16762900	-3.55540800	4.00621400
H	3.74635300	3.98114300	3.50457300	H	1.05264900	-4.56570800	2.56500000
H	3.00671100	2.39042600	3.67811600	H	1.19024800	-2.80766100	2.41067200
H	4.59247600	2.55308300	2.92076000	C	-1.10162900	-3.37621900	5.63682000
C	0.49047300	3.40889300	2.48938200	H	-1.09655200	-4.39024800	6.06046700
H	0.83954400	3.00139600	3.44119800	H	-0.09148500	-2.97389600	5.74363600
H	0.18538300	4.44983800	2.66740300	H	-1.75682200	-2.77385300	6.27542700
H	-0.40160900	2.84573500	2.20593200	C	-6.00062200	-1.24875800	2.88143200
C	2.35973100	-2.94412000	-0.63378400	H	-6.01915900	-1.96665800	2.05793500
H	2.92318600	-3.80555600	-1.01825400	H	-6.01129300	-1.81097100	3.81787300
H	1.96251200	-3.23097700	0.34198100	H	-6.94673100	-0.69143500	2.83628500
H	1.51027900	-2.79385200	-1.30685800	C	-4.66247400	0.28101900	5.32447500
C	4.15755500	-2.04330500	1.88160400	H	-5.48614400	0.95553400	5.59631300
H	5.05199000	-2.68235500	1.88648300	H	-4.99609500	-0.73501700	5.55460900
H	4.26285700	-1.35038800	2.72403200	H	-3.83248700	0.51050200	6.00190900
H	3.30242400	-2.68818100	2.09133100	C	-2.92502000	2.63793000	4.11864600
C	6.01320900	0.26064700	0.97212500	H	-2.86583800	2.41332500	5.18837000
H	6.76609900	-0.52502000	1.12282500	H	-1.92949200	2.95007000	3.79191500
H	6.51899200	1.09741500	0.48607500	H	-3.58066000	3.51429800	4.02422900
H	5.70845100	0.59407900	1.97112600	C	-3.01380600	2.37895200	0.92956500
C	5.38557400	0.88541200	-2.14805900	H	-2.34276800	3.10307400	1.39632900
H	4.74855600	1.49613000	-2.79795600	H	-2.48034500	1.91825100	0.09234400
H	6.05096700	1.56206900	-1.60772500	H	-3.85285100	2.94780500	0.50569600
H	6.01633400	0.27873100	-2.81190100	C	-4.75853200	-0.10787700	0.18544500
C	3.11823600	-1.05065900	-3.07021600	H	-3.95001400	0.03756200	-0.53854500
H	2.13075200	-1.51376200	-3.13830800	H	-5.08555900	-1.14988600	0.11157500
H	3.06441600	-0.09322200	-3.59909800	H	-5.60155400	0.51224500	-0.15064200
H	3.81369400	-1.68527900	-3.63755900	C	0.65655500	-0.17578500	4.81247000
C	0.78481700	0.05428000	2.17230400	C	-0.25569600	0.45350200	5.68597700
C	0.49359800	-0.10579600	3.39198700	C	1.73840400	-0.88347600	5.38366000
C	-3.47350100	1.47740500	3.33536200	C	-0.09081900	0.38108200	7.06755100
C	-3.51094600	1.36789600	1.91793700	H	-1.07375400	1.03551500	5.26951200

C	1.89266400	-0.95117800	6.76255800	H	-0.32776000	3.25791200	0.78385600
H	2.45191500	-1.36760300	4.72499400	C	2.26140200	-2.60510800	-2.04745900
C	0.97968900	-0.32320900	7.61414800	H	2.69472600	-3.47702400	-2.55597400
H	-0.80158400	0.88382000	7.71795500	H	1.93630100	-2.94380200	-1.05996000
H	2.73710600	-1.49443300	7.17855900	H	1.36856800	-2.31214700	-2.60795900
H	1.10729200	-0.37904100	8.69114500	C	4.22589300	-2.02900000	0.41653700
C	-0.33751300	-0.13420600	-1.92488500	H	4.90787200	-2.88216100	0.29736800
C	-0.09435000	1.03508600	-2.67698300	H	4.61786100	-1.43403300	1.24898400
C	-0.66384600	-1.31662800	-2.62773600	H	3.26068300	-2.43921200	0.72957500
C	-0.17951300	1.02299500	-4.06743200	C	6.23095500	0.24167700	-0.44781000
H	0.12101500	1.96440000	-2.15684900	H	7.00525800	-0.53735000	-0.45663600
C	-0.74501500	-1.31774000	-4.01442300	H	6.68473500	1.14595200	-0.86034300
H	-0.86366800	-2.22189800	-2.06392800	H	6.00329200	0.44231600	0.60635700
C	-0.50197700	-0.15111100	-4.74442000	C	5.51991600	1.08426800	-3.46575000
H	0.00168200	1.93987800	-4.62189500	H	4.90665900	1.58787300	-4.21952200
H	-1.00672700	-2.23678200	-4.53215000	H	6.06142900	1.85432600	-2.91092400
H	-0.56938400	-0.15891500	-5.82824700	H	6.27087000	0.49767400	-4.01253900

{{(C₅Me₅)₂Ce}₂(μ-η²:η²-PhC₄Ph)}

H= -2238.925891 au

Ce	-2.48845300	-1.13805700	0.98474000	C	3.02751700	-0.62538900	-4.39272600
Ce	2.51331400	1.09482600	-0.98793900	H	1.97870300	-0.93367400	-4.39662400
C	0.20499200	0.36802000	-1.89583400	H	3.08002600	0.35285500	-4.88167900
C	-0.10936200	0.06603200	-0.64950000	H	3.57700600	-1.32864200	-5.03379500
C	3.60009300	-0.59777900	-3.00450100	C	0.06904800	0.04062500	0.66330800
C	4.70288300	0.19766400	-2.57115500	C	-0.30057600	-0.12573700	1.91956600
C	3.25763400	-1.48938000	-1.94940400	C	-3.77333100	1.32140400	1.62245000
C	5.02655700	-0.18892100	-1.23702500	C	-3.77814700	1.26525800	0.20030800
C	4.12892500	-1.23093900	-0.85363200	C	-4.66288200	0.31534700	2.10588300
C	1.72759000	3.54257000	0.19767900	C	-4.67349500	0.22891200	-0.19804100
C	3.11849100	3.43207200	0.49348600	C	-5.23398900	-0.34700500	0.97714300
C	1.59024600	3.77625600	-1.20014100	C	-1.10484700	-3.53985400	1.63183800
C	3.84266400	3.60694500	-0.71983900	C	-2.01846300	-3.34514800	2.70530700
C	2.89693400	3.80244800	-1.77223100	C	-1.85776800	-3.85082700	0.46433000
C	0.30863100	4.11975100	-1.90330700	C	-3.33887800	-3.56321600	2.20778200
H	0.00316700	5.15143500	-1.68146500	C	-3.24074000	-3.86904800	0.81894100
H	0.40848600	4.04577500	-2.98991400	C	-4.55833800	-3.70494900	3.07198500
H	-0.51665700	3.46595100	-1.60891700	H	-4.62879500	-2.92088500	3.83296600
C	3.22741100	4.19265400	-3.18572700	H	-5.48195800	-3.68391800	2.48937700
H	4.17103900	3.75556900	-3.52440000	H	-4.54079100	-4.66334800	3.60831800
H	2.45148600	3.88360300	-3.89404500	C	-4.35102900	-4.33982900	-0.07774400
H	3.32693100	5.28233500	-3.28374900	H	-4.31286300	-5.42910200	-0.21366400
C	5.32434300	3.82524400	-0.81399000	H	-5.33520900	-4.10479500	0.33454700
H	5.88896500	3.18184200	-0.13273400	H	-4.30453700	-3.89946700	-1.08111600
H	5.70466700	3.65534300	-1.82440700	C	-1.29744300	-4.28541500	-0.86044800
H	5.57692600	4.86204800	-0.55220200	H	-1.99057600	-4.09090900	-1.68602200
C	3.72000000	3.31249900	1.86575000	H	-0.35158500	-3.78979800	-1.09815200
H	3.85742400	4.29993300	2.32755700	H	-1.09934700	-5.36622300	-0.86989400
H	3.09114800	2.73042200	2.54720300	C	0.38976600	-3.56265500	1.74523600
H	4.70752100	2.83872500	1.84164200	H	0.74681000	-2.92950800	2.56166000
C	0.61929400	3.60173600	1.20721600	H	0.75629300	-4.58102000	1.93360300
H	0.82308500	2.98924000	2.09044400	H	0.87158700	-3.21311600	0.82722200
H	0.46193100	4.63158800	1.55647900	C	-1.65706800	-3.13601900	4.14845800
				H	-1.48902700	-4.09515800	4.65754400
				H	-0.74526000	-2.54385200	4.26552200
				H	-2.45223400	-2.62342200	4.69993000

C	-6.40398000	-1.28672500	0.99745600
H	-6.35254000	-2.03924700	0.20443200
H	-6.49556900	-1.81373700	1.94988300
H	-7.34252700	-0.73537800	0.84794900
C	-5.08419700	0.14386300	3.53878800
H	-5.82596100	0.90054500	3.82831700
H	-5.54227300	-0.83303300	3.71590400
H	-4.24609000	0.24260000	4.23777200
C	-3.11680200	2.38147800	2.45920300
H	-3.04001900	2.07884000	3.50736000
H	-2.10753400	2.62421900	2.11642100
H	-3.69965000	3.31270700	2.44102500
C	-3.10880300	2.24089100	-0.72213000
H	-2.24662900	2.71336900	-0.24532900
H	-2.75644700	1.77232700	-1.64633600
H	-3.79801700	3.04652600	-1.01024600
C	-5.08209300	-0.08536700	-1.60984800
H	-4.27251600	0.08793600	-2.32598500
H	-5.40631200	-1.12576200	-1.72226100
H	-5.92637300	0.54177600	-1.92812000
C	0.49786400	0.08609900	3.12126900
C	-0.11427200	0.50089900	4.31919100
C	1.88749500	-0.15434700	3.15347900
C	0.62824800	0.70153400	5.47903000
H	-1.18562900	0.67879400	4.32177200
C	2.62669000	0.02332400	4.31920900
H	2.37432100	-0.52468700	2.25444300
C	2.00240600	0.46157000	5.48798500
H	0.12969600	1.03726900	6.38460400
H	3.69362900	-0.18527400	4.31809900
H	2.57899700	0.60326800	6.39758600
C	-0.57671800	0.11802100	-3.10092400
C	-0.46644900	0.97913600	-4.20914500
C	-1.42902000	-0.99845800	-3.22985300
C	-1.20065300	0.76021300	-5.37069500
H	0.19848500	1.83505000	-4.13659300
C	-2.14555300	-1.23141500	-4.39988700
H	-1.48939000	-1.70714500	-2.40713700
C	-2.04315700	-0.34694200	-5.47452100
H	-1.10732200	1.45155200	-6.20414800
H	-2.78375000	-2.10813000	-4.47644200
H	-2.60482200	-0.52580400	-6.38693500

[(C₅Me₅)₂Ce-CC^tBu]₂

H= -2091.298408 au

Ce	1.91265800	0.77439200	-0.72427500
C	-0.83310700	-0.15643000	-2.77971600
C	-0.57399700	-0.09789500	-1.56563900
C	3.59352000	-0.77605000	-2.51498500
C	4.48761400	0.13338700	-1.88759700
C	3.21099500	-1.75989100	-1.55454100
C	4.58397500	-0.22755000	-0.51382300
C	3.81468600	-1.41587300	-0.31423200

C	1.09337400	3.39808400	-0.06117200
C	2.48384100	3.41039500	0.24339800
C	0.95330000	3.35199600	-1.47620100
C	3.20393600	3.40908300	-0.98443000
C	2.26060200	3.34039900	-2.04835500
C	-0.32520500	3.52336600	-2.24598700
H	-0.11682100	3.83983500	-3.27294700
H	-0.92956900	2.61181700	-2.29555000
H	-0.94694900	4.30243700	-1.79053400
C	2.55707900	3.49738600	-3.51361800
H	3.61240500	3.32129000	-3.73596600
H	1.97429700	2.81388900	-4.14019800
H	2.32648100	4.51548900	-3.85660600
C	4.63966100	3.83095800	-1.09122900
H	5.29713900	3.30721200	-0.39048500
H	5.04291100	3.69657100	-2.09541600
H	4.72314600	4.90099900	-0.85397900
C	3.10565500	3.65595100	1.58727300
H	3.39068500	4.71129500	1.70199400
H	2.41882700	3.41836100	2.40187700
H	4.01663600	3.06682500	1.74135800
C	-0.02177600	3.57780000	0.91824800
H	0.32384900	3.46532900	1.94795000
H	-0.46618600	4.57966400	0.82939600
H	-0.81983800	2.84948100	0.76929300
C	2.58340900	-3.06948500	-1.93185800
H	3.32074600	-3.70444300	-2.44291800
H	2.21843600	-3.62945300	-1.07060000
H	1.74229200	-2.94729100	-2.61979800
C	3.88922700	-2.24872500	0.93579900
H	4.92895300	-2.32522600	1.27710200
H	3.30404900	-1.84674000	1.77019500
H	3.53660400	-3.26703000	0.75660500
C	5.52899200	0.34266600	0.50636400
H	6.41423800	-0.29740500	0.62963800
H	5.89058500	1.33355100	0.22101800
H	5.07122000	0.43428200	1.49815900
C	5.41922900	1.03325600	-2.64297700
H	4.91158500	1.66369200	-3.37899300
H	5.99136900	1.68401600	-1.98149900
H	6.14501400	0.42382800	-3.19909600
C	3.35813500	-0.86853900	-3.99524900
H	2.41228700	-1.36672300	-4.22858500
H	3.34233100	0.11556200	-4.47537400
H	4.15107900	-1.44801700	-4.49020200
C	0.58805800	0.12059500	1.60119900
C	0.86402600	0.16097100	2.81232500
Ce	-1.91641100	-0.75449500	0.73663100
C	-3.30634600	1.54428200	1.87576000
C	-3.57185200	1.66982100	0.48439400
C	-3.99363500	0.38268400	2.35104400
C	-4.40438800	0.57788100	0.09708000
C	-4.71451600	-0.17818700	1.25934900

H	-0.50654300	3.41698900	1.90062100	H	-2.00412300	-3.49816500	6.04479600
C	2.69033700	-2.92762400	-0.23878000	C	-5.97059600	-1.26958000	3.16309200
H	3.35431700	-3.80327700	-0.26071700	H	-6.07805700	-2.00680400	2.36200600
H	2.04934800	-3.03159800	0.63801100	H	-5.95602300	-1.80719600	4.11353600
H	2.04987400	-2.99282700	-1.12241500	H	-6.88765100	-0.66319500	3.15435500
C	4.18252400	-1.73391600	2.30187500	C	-4.36401000	0.10892500	5.49687000
H	4.96644200	-2.50181700	2.37029100	H	-5.26365800	0.66325400	5.79759100
H	4.40321100	-0.98998400	3.07435700	H	-4.53818300	-0.93940600	5.76216500
H	3.23777300	-2.21323900	2.56703100	H	-3.54686300	0.47024200	6.12828100
C	6.01539000	0.60755300	1.36850500	C	-2.54255500	2.39914400	4.16535500
H	6.74277300	-0.12961400	1.73293800	H	-3.00291800	3.37603500	3.96436100
H	6.57920100	1.36846500	0.82452600	H	-2.57532700	2.25802300	5.24971900
H	5.59031200	1.09049100	2.25681400	H	-1.49209300	2.47862400	3.86976800
C	5.67138900	0.89956700	-1.84518900	C	-2.93252000	2.25249800	1.04518000
H	5.07886400	1.50208900	-2.54368700	H	-1.90812000	2.03549500	0.72641800
H	6.33491900	1.58083600	-1.30885800	H	-3.55362800	2.28596100	0.14513800
H	6.30853400	0.24762100	-2.45774900	H	-2.94206400	3.25906600	1.47909400
C	3.67147700	-1.28022500	-2.78299700	C	-5.00308100	-0.11001400	0.41532700
H	2.72218300	-1.80032000	-2.94139200	H	-4.39414200	0.24876700	-0.41851500
H	3.68692200	-0.41115500	-3.44945500	H	-5.16476400	-1.18272300	0.26520500
H	4.46340900	-1.95723700	-3.13345800	H	-5.98649000	0.37207600	0.32403500
C	0.76915000	0.07880300	2.22434200	C	0.71387800	-0.12602600	4.90734600
C	0.45259300	-0.14852900	3.43031600	C	-0.43820400	-0.02064300	-1.97428800
Ce	-1.98283300	-1.14824900	2.64707400	C	1.77707000	-1.17786000	5.26934400
C	-3.27623900	1.30685700	3.43980100	H	1.94948300	-1.17644400	6.35219800
C	-3.46076100	1.24939600	2.02884100	H	1.46351300	-2.18164100	4.97337500
C	-4.08170500	0.28761200	4.03089100	H	2.72373300	-0.95999800	4.76985200
C	-4.37201700	0.19253500	1.74496200	C	-0.57745800	-0.43052800	5.68610200
C	-4.77088900	-0.38744900	2.98300800	H	-0.39980500	-0.41934600	6.76757500
C	-0.76954900	-3.78324600	2.81335200	H	-1.34879800	0.31484100	5.47094500
C	-1.67109400	-3.76234000	3.91381700	H	-0.96163700	-1.42995800	5.44511000
C	-1.53756700	-3.77291400	1.61553400	C	1.22837700	1.26011000	5.33519700
C	-3.00000900	-3.75503000	3.39785100	H	2.15752900	1.50356500	4.81344600
C	-2.91837200	-3.75645500	1.97492200	H	0.49433800	2.04026600	5.11713800
C	-4.22030300	-4.02424800	4.22946900	H	1.42664300	1.27194000	6.41379600
H	-4.28383200	-3.38505100	5.11788200	C	0.64579700	0.73469900	-2.76208300
H	-5.14240200	-3.88972900	3.66172000	H	1.62460100	0.25369900	-2.65170000
H	-4.21470600	-5.06187300	4.59119400	H	0.41969900	0.74904200	-3.83457200
C	-4.05989200	-3.94799700	1.01681300	H	0.71751700	1.77440700	-2.42774900
H	-4.15739900	-5.00191700	0.72277100	C	-1.78933900	0.67910500	-2.20282800
H	-5.01577200	-3.65114500	1.45532700	H	-2.58951300	0.14734500	-1.68208400
H	-3.93386700	-3.37402000	0.09216200	H	-1.76984500	1.70930600	-1.83950700
C	-0.99433400	-3.98127100	0.23151000	H	-2.02687000	0.69714900	-3.27335000
H	-1.78519500	-3.90846500	-0.52054300	C	-0.53220200	-1.46065400	-2.50803000
H	-0.22046300	-3.25748900	-0.03402300	H	-0.74053600	-1.44909300	-3.58450600
H	-0.55463200	-4.98346300	0.13194800	H	0.40022200	-2.00848900	-2.34713200
C	0.71745900	-3.96985100	2.88611700	H	-1.33383000	-2.00792600	-2.00681300
H	1.02413700	-4.34649300	3.86681400				
H	1.05273900	-4.70311200	2.14367700				
H	1.27365200	-3.04410600	2.70261200				
C	-1.32785800	-4.01588400	5.35566000				
H	-1.40527300	-5.08689100	5.59039500				
H	-0.30849600	-3.70879500	5.60602900				

{{(C₅Me₅)₂Ce}(μ-η²:η²-tBuC₄tBu)}
H= -2091.317239 au

Ce	2.43967400	1.14057300	-1.00622000				
C	0.15986200	0.21721600	-1.94505200				
C	-0.10624100	0.01043400	-0.67310400				

C	4.00712400	-0.60426400	-2.66082200	C	-3.66686300	1.29358200	1.93314100
C	4.95736500	0.28074100	-2.06745200	C	-3.87628900	1.32117500	0.52521700
C	3.51361800	-1.46607100	-1.64317000	C	-4.46665400	0.24765400	2.47877100
C	5.03503000	-0.02144800	-0.67782300	C	-4.81831800	0.30109000	0.19918700
C	4.14102700	-1.10244000	-0.41717600	C	-5.19600400	-0.34962100	1.40749800
C	1.59835400	3.74163100	-0.11424800	C	-1.15627700	-3.70286300	1.29087800
C	3.01117500	3.74509900	0.07845600	C	-2.09097300	-3.63654000	2.35991700
C	1.34503000	3.74688000	-1.51508300	C	-1.88742400	-3.78907900	0.07171400
C	3.62824600	3.75923300	-1.20454400	C	-3.40378300	-3.70974300	1.80300300
C	2.59830100	3.73980800	-2.19221000	C	-3.27891600	-3.79713600	0.38659700
C	0.00001300	3.98885500	-2.13132800	C	-4.63750800	-3.98759000	2.61143100
H	-0.31032600	5.03202700	-1.97702100	H	-4.72796800	-3.33939400	3.48991000
H	0.00553300	3.81243400	-3.20921300	H	-5.55046400	-3.87974300	2.02317300
H	-0.77802100	3.35481700	-1.69775800	H	-4.61840000	-5.02039100	2.98699300
C	2.79953200	3.90612300	-3.67264100	C	-4.39326600	-4.05949000	-0.58630000
H	3.74035000	3.46208100	-4.01400500	H	-4.53809700	-5.13651700	-0.74729700
H	1.99259100	3.44694400	-4.25285700	H	-5.34774300	-3.65990200	-0.23185400
H	2.82933200	4.96723300	-3.95574600	H	-4.20061400	-3.61752400	-1.56986800
C	5.06989300	4.09903800	-1.44176600	C	-1.28080500	-4.09448300	-1.26832100
H	5.74623400	3.58871100	-0.74896500	H	-1.98773800	-3.93395500	-2.08776900
H	5.39276300	3.86437400	-2.45804400	H	-0.39087100	-3.49150100	-1.47385600
H	5.23003000	5.17696700	-1.29791000	H	-0.97055300	-5.14738800	-1.32227000
C	3.74844300	3.92834300	1.37543700	C	0.33527200	-3.82243700	1.39764900
H	4.08742600	4.96693400	1.49093000	H	0.65138000	-3.95291200	2.43548000
H	3.12458800	3.69988800	2.24363000	H	0.69721800	-4.69255800	0.83638000
H	4.64189500	3.29720500	1.44228500	H	0.85968900	-2.94206000	1.00906700
C	0.54171300	3.91831400	0.93867700	C	-1.79965300	-3.70874100	3.83215900
H	0.96703600	3.91878000	1.94627400	H	-2.10676400	-4.67970300	4.24418200
H	0.02225000	4.87723900	0.81209000	H	-0.73427700	-3.59157000	4.04174100
H	-0.22202700	3.13360000	0.90668600	H	-2.33147800	-2.94344200	4.41037000
C	2.64209600	-2.67202000	-1.82774500	C	-6.38744100	-1.25106600	1.54489000
H	3.21540200	-3.59550700	-1.67043000	H	-6.45894700	-1.98900600	0.73947800
H	1.80226700	-2.69368400	-1.12610600	H	-6.39276500	-1.79122800	2.49352200
H	2.22518900	-2.71797900	-2.83594900	H	-7.31301800	-0.65942300	1.50925700
C	4.07939100	-1.90871900	0.84908900	C	-4.66828400	-0.02335300	3.94374300
H	4.74102600	-2.78375200	0.78262900	H	-5.44776100	0.62463000	4.36758200
H	4.40346700	-1.33712300	1.72405400	H	-4.97785700	-1.05583000	4.13448000
H	3.07404200	-2.28956300	1.05419300	H	-3.75809200	0.15772700	4.52538300
C	6.02416800	0.54264400	0.30260900	C	-2.95430300	2.35501100	2.71687200
H	6.92803900	-0.07929100	0.36016400	H	-3.60030400	3.23467000	2.84845200
H	6.34956400	1.54940800	0.02533700	H	-2.67444300	2.01115500	3.71513600
H	5.61754100	0.59964600	1.31847300	H	-2.04290500	2.69907100	2.22049800
C	5.91424600	1.12655800	-2.85633100	C	-3.36508800	2.39414100	-0.39162400
H	5.41982000	1.71853300	-3.63436700	H	-2.31403500	2.63157200	-0.20277800
H	6.47582900	1.81515700	-2.22285300	H	-3.45490600	2.11728900	-1.44606400
H	6.64901900	0.48934600	-3.36820500	H	-3.93195300	3.32597700	-0.25996500
C	3.78298200	-0.72417800	-4.14159900	C	-5.48308200	0.08140200	-1.13067700
H	2.95870600	-1.40134900	-4.37547600	H	-4.90473600	0.50286200	-1.95746500
H	3.56306300	0.23791500	-4.61938900	H	-5.64121100	-0.98071600	-1.34961400
H	4.67742200	-1.12222100	-4.64030000	H	-6.47211800	0.55913200	-1.15901100
C	0.08668600	0.00477500	0.64108700	C	0.78835400	0.14234800	3.04922900
C	-0.17431000	-0.19133200	1.91658600	C	-0.77809600	-0.12449900	-3.09463800
Ce	-2.44812800	-1.13664300	1.00302800	C	1.15425400	-1.13572500	3.82103900

H	1.82797600	-0.89820200	4.65321400
H	0.25730600	-1.60429900	4.23400800
H	1.65395200	-1.86335900	3.17646100
C	0.12588400	1.11677900	4.03695100
H	0.80201500	1.32865400	4.87400800
H	-0.12819200	2.06427400	3.55500900
H	-0.79402200	0.68715100	4.44521400
C	2.08019300	0.78510800	2.51338800
H	2.59934100	0.08849100	1.84221400
H	1.84715500	1.71287700	1.97793800
H	2.77808300	1.03784800	3.32059900
C	-1.06600500	1.12934400	-3.93605100
H	-0.13513400	1.56919300	-4.30700300
H	-1.69014100	0.87355600	-4.80068700
H	-1.58945700	1.89023400	-3.35173300
C	-2.11308100	-0.69082900	-2.57928700
H	-1.94185600	-1.62786500	-2.03531900
H	-2.60252000	0.03392600	-1.91803200
H	-2.80728900	-0.91319600	-3.39850500
C	-0.11839300	-1.16885500	-4.01023300
H	-0.77513400	-1.40355300	-4.85667000
H	0.82638000	-0.78897200	-4.40770000
H	0.08533800	-2.09816900	-3.47136200

[(C₅Me₅)₂Ce-CCMe]₂

H= -1855.674399 au

Ce	1.93857200	0.69303900	-0.84592800
C	-0.79940900	0.12944400	-2.63370500
C	-0.70220300	-0.09122300	-1.41684700
C	3.21279400	-0.84005100	-2.97172300
C	4.24412900	0.00694500	-2.48150900
C	2.95731800	-1.84593200	-1.99127500
C	4.56952800	-0.42118400	-1.16279600
C	3.78503000	-1.57881100	-0.86720400
C	1.17164300	3.27058400	0.02283700
C	2.50560100	3.13994000	0.50066400
C	1.22026700	3.38622100	-1.39355500
C	3.38434000	3.21661300	-0.61893400
C	2.58841600	3.36050600	-1.79239700
C	0.06811900	3.72011000	-2.29527500
H	-0.12317800	4.80269300	-2.30587100
H	0.26270300	3.42516100	-3.33163300
H	-0.85563200	3.23199700	-1.97862200
C	3.07191500	3.73264300	-3.16516200
H	4.14774800	3.58608700	-3.27470500
H	2.58183100	3.16180800	-3.96266800
H	2.86860300	4.79260900	-3.36933000
C	4.86293700	3.44759400	-0.51017500
H	5.32181100	2.86120900	0.29057500
H	5.39524300	3.21690000	-1.43547800
H	5.06436400	4.50381700	-0.28365300
C	2.93211400	3.11662300	1.94063200
H	3.05601600	4.13342500	2.33812600

H	2.20029100	2.60191700	2.56871700
H	3.89141000	2.60581100	2.07500900
C	-0.05043900	3.43423200	0.86652300
H	0.14456700	3.17046300	1.90719100
H	-0.40261800	4.47546600	0.84772800
H	-0.87372400	2.80423900	0.52371500
C	2.20166800	-3.10649800	-2.29315500
H	2.79326600	-3.74786200	-2.96122900
H	1.98047900	-3.69373100	-1.40106800
H	1.25324200	-2.91201800	-2.80249700
C	4.04272600	-2.46092000	0.32241200
H	5.10215600	-2.74734500	0.35906100
H	3.81328900	-1.97995800	1.28061900
H	3.46325800	-3.38459600	0.27651800
C	5.73755000	0.02757100	-0.33018300
H	6.51702400	-0.74696500	-0.30731400
H	6.19862600	0.93292900	-0.72977500
H	5.47135700	0.22804800	0.71503900
C	5.05205400	0.93112500	-3.34230800
H	4.44936600	1.41827300	-4.11297900
H	5.55542500	1.71256000	-2.76974200
H	5.83591800	0.36474200	-3.86456100
C	2.68897900	-0.85858100	-4.37966200
H	1.69203000	-1.30676300	-4.43490800
H	2.62933800	0.14436100	-4.81682700
H	3.33731300	-1.45013600	-5.04180700
C	0.74426500	0.18502600	1.52681900
C	0.46998600	0.30525600	2.73083300
Ce	-1.91056700	-0.73825900	0.90769100
C	-3.43904600	1.63498500	1.68243800
C	-3.60283600	1.56547600	0.27226100
C	-4.11590900	0.51567500	2.25862300
C	-4.37169800	0.39959600	-0.02404400
C	-4.73651500	-0.21518800	1.20538700
C	-0.61007500	-3.20523900	1.26415000
C	-1.32882400	-3.05845000	2.48272900
C	-1.55129400	-3.44497900	0.22447800
C	-2.71403000	-3.24279900	2.20498000
C	-2.85320900	-3.47632900	0.80656600
C	-3.75054000	-3.45591000	3.26990000
H	-3.74980200	-2.66810100	4.03068600
H	-4.76063800	-3.51976800	2.86048000
H	-3.56210000	-4.40013300	3.79905000
C	-4.08493000	-3.95531400	0.09115400
H	-3.96602900	-5.00122300	-0.22049500
H	-4.96752500	-3.91206600	0.73180900
H	-4.31066200	-3.38180500	-0.81566500
C	-1.23692700	-3.79348900	-1.20192800
H	-2.14261500	-3.80491300	-1.81562100
H	-0.54379400	-3.08484600	-1.66017100
H	-0.78363400	-4.79147900	-1.27655400
C	0.87674500	-3.24215500	1.12469800
H	1.37636400	-2.83634500	2.00653400

H	1.23433900	-4.27248300	0.98532400	H	-0.50758500	3.12308100	-0.66453000
H	1.22073100	-2.65659200	0.26961400	C	3.39096300	3.77009600	-1.95313700
C	-0.73906900	-2.96311700	3.86028800	H	4.44300900	3.51812500	-2.10410600
H	-0.64662200	-3.95751300	4.31907400	H	2.81476900	3.24352800	-2.72288000
H	0.26110700	-2.52188700	3.84685400	H	3.28402900	4.84332200	-2.16176500
H	-1.35826600	-2.36447900	4.53787200	C	5.23354700	3.57724500	0.66259800
C	-5.84336400	-1.21383000	1.36553900	H	5.71907100	3.00663300	1.45979500
H	-5.90263000	-1.91337400	0.52883600	H	5.73987700	3.33231900	-0.27422200
H	-5.75625400	-1.79587600	2.28475300	H	5.43736900	4.63798000	0.86464500
H	-6.80899800	-0.69110400	1.41090300	C	3.35200700	3.17571600	3.16686600
C	-4.36866000	0.34916800	3.73045900	H	3.44013800	4.18296200	3.59661100
H	-5.11248600	1.07510200	4.08896200	H	2.65218600	2.61828100	3.79815300
H	-4.75493600	-0.64475000	3.96907200	H	4.33450700	2.70298500	3.27251100
H	-3.46844000	0.50719600	4.33644200	C	0.33292500	3.37776100	2.14314500
C	-2.90519700	2.77962200	2.49700200	H	0.56743700	3.16910600	3.18970000
H	-3.68353000	3.16103300	3.17082500	H	-0.11145400	4.38199100	2.10061400
H	-2.04903000	2.50853200	3.12571400	H	-0.43059100	2.65917900	1.83439900
H	-2.58954400	3.61328100	1.86768000	C	2.51375600	-2.98285700	-0.79697800
C	-3.28895800	2.61529400	-0.75256400	H	3.00166900	-3.74027800	-1.42541200
H	-2.71751300	3.44652200	-0.33481800	H	2.26469200	-3.46643000	0.14944800
H	-2.71973600	2.21045100	-1.59607500	H	1.57001600	-2.72109900	-1.28660600
H	-4.21672300	3.03745100	-1.16156500	C	4.32193800	-2.28880700	1.80687800
C	-4.88943800	0.04082700	-1.38807600	H	5.28146800	-2.82219500	1.85029100
H	-4.13883500	0.21376400	-2.16644300	H	4.27347500	-1.66237000	2.70630600
H	-5.19145900	-1.00936000	-1.44944000	H	3.53331800	-3.03836400	1.89386300
H	-5.77113600	0.64090200	-1.65477300	C	6.19542100	0.07987500	1.06148600
C	0.25066800	0.50739200	4.16487200	H	6.98475300	-0.68127300	1.13222700
H	-0.78176000	0.28984900	4.46102000	H	6.65796000	0.98372900	0.65827700
H	0.45886400	1.54483500	4.45086900	H	5.88708500	0.30079400	2.09118700
C	-0.99587800	0.37792400	-4.06093200	C	5.62281600	0.87187100	-2.01279800
H	-1.37367200	1.39002700	-4.24270800	H	5.02607700	1.37101700	-2.78206600
H	-1.72061900	-0.33063500	-4.47754500	H	6.14240100	1.64474900	-1.44134600
H	-0.06502200	0.26084900	-4.62540200	H	6.39484700	0.29317000	-2.53909600
H	0.90162100	-0.14056600	4.76182300	C	3.28523100	-0.93171000	-3.06114300

TS_{CC}[(C₅Me₅)₂Ce-CCMe]₂

H= -1855.64786 au

Ce	2.46523500	0.76980600	0.36580500	H	2.33987000	-1.47384200	-3.15638900
C	0.04857300	0.01880300	-0.49200400	H	3.14301800	0.06047000	-3.50497600
C	-0.39132800	-0.27577500	0.66795100	H	4.01337900	-1.45609100	-3.69586200
C	3.75156000	-0.86997600	-1.63359400	C	0.80552500	0.04827000	2.26910000
C	4.79373900	-0.02959500	-1.14663400	C	0.46020300	-0.02463900	3.47102800
C	3.40865900	-1.79458300	-0.60436900	Ce	-1.96517200	-0.99975100	2.60666300
C	5.06167300	-0.40125200	0.20081300	C	-3.31115900	1.45184700	3.31228900
C	4.20783000	-1.49714300	0.53447300	C	-3.50436700	1.34701800	1.90612100
C	1.55400100	3.29675800	1.28184900	C	-4.06214000	0.41026000	3.93854200
C	2.90090300	3.22128400	1.73382500	C	-4.36187000	0.23338100	1.66328900
C	1.56898900	3.42109300	-0.13481000	C	-4.73873400	-0.32041700	2.92062500
C	3.75476300	3.33022900	0.59719100	C	-0.60947100	-3.48668900	2.82793100
C	2.92941500	3.44354400	-0.56117100	C	-1.38480000	-3.41667800	4.01980100
C	0.36976000	3.68488100	-0.99883200	C	-1.50267400	-3.64495800	1.73160000
H	0.09602700	4.74933800	-0.98382600	C	-2.75859500	-3.56182800	3.66392900
H	0.55371400	3.42482700	-2.04664300	C	-2.83194100	-3.69923600	2.24760400
				C	-3.86195500	-3.79407300	4.65493400
				H	-3.88502300	-3.04198300	5.45209200
				H	-4.84486700	-3.79994400	4.17998300

H	-3.73836300	-4.76791200	5.14812200	C	3.35716300	-1.59325400	-1.83768800
C	-4.04164700	-4.07588000	1.43970300	C	5.00779400	-0.17707900	-1.06346300
H	-3.99475100	-5.13062400	1.13768600	C	4.11038600	-1.22293500	-0.68734100
H	-4.96741200	-3.94739700	2.00531700	C	1.56519900	3.55446200	-0.21402100
H	-4.13656500	-3.49152200	0.51701600	C	2.97722900	3.57588500	-0.01678000
C	-1.11474500	-3.90824100	0.30541200	C	1.31467800	3.58109900	-1.61527700
H	-1.91000100	-3.62706000	-0.39274000	C	3.60036700	3.63197900	-1.29604500
H	-0.21828400	-3.35509700	0.01842800	C	2.57190200	3.61601300	-2.28623100
H	-0.91087200	-4.97569400	0.14034700	C	-0.03376700	3.72526200	-2.25698800
C	0.88530400	-3.51046400	2.73786200	H	-0.36766000	4.77231200	-2.24503600
H	1.35401100	-3.25123500	3.69105300	H	-0.02415400	3.40654000	-3.30368700
H	1.24854300	-4.50874100	2.45854000	H	-0.79602800	3.13535200	-1.74174500
H	1.25715200	-2.79815900	1.99642900	C	2.76579300	3.80735900	-3.76442500
C	-0.86899400	-3.41492700	5.43149600	H	3.74296800	3.44899900	-4.10230200
H	-0.85649600	-4.43106900	5.84926700	H	2.00384600	3.28486800	-4.35292800
H	0.15401700	-3.03383800	5.49756500	H	2.70490700	4.86879700	-4.04089600
H	-1.49044600	-2.81221600	6.10465400	C	5.04961400	3.93982400	-1.53271000
C	-5.87142400	-1.27989200	3.13651700	H	5.71168500	3.41086200	-0.83998600
H	-5.93706700	-2.03690200	2.35045800	H	5.36479100	3.69080700	-2.54836600
H	-5.80350600	-1.79799000	4.09585900	H	5.24146100	5.01285600	-1.39430500
H	-6.82844300	-0.73978100	3.13441200	C	3.68878200	3.67630700	1.30367400
C	-4.27036600	0.27227600	5.42073300	H	3.80633800	4.72194300	1.61936600
H	-5.05152200	0.95638200	5.78077800	H	3.14819100	3.16622800	2.10879100
H	-4.58223700	-0.73827400	5.70167700	H	4.69504300	3.24632000	1.26002900
H	-3.36559700	0.50899700	5.99305500	C	0.52168000	3.64769000	0.86078700
C	-2.65081500	2.57580100	4.05924400	H	0.94081100	3.44789000	1.85121500
H	-3.40294900	3.25207900	4.48801600	H	0.07896100	4.65222000	0.89612600
H	-2.03724500	2.22516600	4.89726400	H	-0.29352900	2.93474400	0.70707600
H	-2.00633900	3.17628800	3.41585100	C	2.42873500	-2.76402700	-1.95632900
C	-3.09218800	2.33067300	0.84886300	H	2.94574500	-3.63184500	-2.38819400
H	-2.47232400	3.13057600	1.25850700	H	2.03947600	-3.07814600	-0.98537000
H	-2.52721700	1.86528500	0.03439300	H	1.57031300	-2.54746100	-2.59958500
H	-3.97511600	2.80647500	0.40210400	C	4.09635900	-1.90557100	0.65173800
C	-4.93332000	-0.13880400	0.32412000	H	4.81821600	-2.73304300	0.68735000
H	-4.21640900	0.02534500	-0.48747700	H	4.36738600	-1.22239800	1.46472000
H	-5.24233900	-1.18817100	0.28492300	H	3.11622600	-2.32611600	0.89317700
H	-5.82248000	0.46201100	0.08605000	C	6.09294400	0.37910700	-0.18512900
C	0.34319500	0.01225400	4.93280700	H	6.90963600	-0.34391900	-0.05623900
H	-0.60659700	-0.39689100	5.31661500	H	6.53475700	1.28594300	-0.60642000
H	0.41137500	1.04134200	5.30292900	H	5.73778500	0.62750100	0.82260200
C	-0.35690200	0.04517600	-1.92398900	C	5.66118200	0.94790700	-3.33587100
H	-0.32601800	1.06556300	-2.32228600	H	5.07639900	1.55504100	-4.03565300
H	-1.37335600	-0.33826500	-2.07654800	H	6.30387800	1.62486900	-2.76899500
H	0.31894200	-0.55258900	-2.54450700	H	6.32046200	0.31490600	-3.94518800
H	1.13878000	-0.57188800	5.40934400	C	3.33325200	-0.89305500	-4.34880800
{{(C₅Me₅)₂Ce}₂(μ-η²:η²-MeC₄Me)}				H	2.33780700	-1.33820900	-4.43585700
H= -1855.698089 au				H	3.30950300	0.07091400	-4.86865200
Ce	2.43692700	1.02159400	-1.12427200	H	4.02201600	-1.53743300	-4.91318900
C	0.14717200	0.18590100	-1.94066200	C	0.09125300	0.05011700	0.63808300
C	-0.15560000	-0.00196800	-0.67643200	C	-0.22610200	-0.10610700	1.90238600
C	3.76325900	-0.75841600	-2.91543600	Ce	-2.47008000	-1.04317200	1.08132600
C	4.79864500	0.10313300	-2.44453600	C	-3.58275500	1.37545500	2.09760400
				C	-3.79122500	1.45020700	0.69126700

C	-4.42401800	0.34294700	2.61058200	H	-1.68133100	-0.49499500	-2.93946000
C	-4.76124400	0.46770900	0.33481700	H	-0.17754900	-0.76271100	-3.83853200
C	-5.17062000	-0.20086400	1.52201100	H	1.57393300	0.62862000	2.91316100
C	-1.09934000	-3.50766600	1.42706900				
C	-2.00566600	-3.45705600	2.52166000	[(C₅H₄Me)₂Sm-CC'Bu]₂			
C	-1.85939800	-3.65861700	0.23163600	H= -1467.928718 au			
C	-3.32894100	-3.60813500	2.00705400	Sm	1.58533600	0.79507600	-0.74894600
C	-3.23879800	-3.72781400	0.58964900	C	-0.76990500	-0.22162900	-2.79762700
C	-4.54275500	-3.88556900	2.84534000	C	-0.68826700	-0.16958900	-1.56331200
H	-4.60335600	-3.24161900	3.72919400	C	3.14973700	-0.71818700	-2.42710900
H	-5.47013200	-3.76274200	2.28153100	C	4.06529900	0.11259100	-1.73297000
H	-4.52667500	-4.92095200	3.21285500	C	2.62363800	-1.65348500	-1.50128700
C	-4.36949500	-4.04758100	-0.34719300	C	4.10473400	-0.29431500	-0.37356100
H	-4.47673800	-5.13162700	-0.48852400	C	3.20721500	-1.38966100	-0.23999700
H	-5.33001900	-3.67973600	0.02558000	C	0.66003600	3.34483300	-0.15867100
H	-4.22004500	-3.61679100	-1.34365000	C	2.04544100	3.39023100	0.15837300
C	-1.29186300	-3.85978300	-1.14518800	C	0.52115600	3.20664500	-1.56048300
H	-2.03549200	-3.67019400	-1.92631400	C	2.75616700	3.26135300	-1.06188700
H	-0.43613300	-3.20655900	-1.34002300	C	1.81931300	3.14272400	-2.12308900
H	-0.94492700	-4.89273600	-1.28593200	C	0.66549100	0.16370300	1.57611000
C	0.39714200	-3.52021300	1.50799800	C	0.83804000	0.03079900	2.79490800
H	0.74956700	-3.26532100	2.51096800	Sm	-1.63195700	-0.74519300	0.76547000
H	0.79892500	-4.51274500	1.26407000	C	-2.62262400	1.55809300	1.91493100
H	0.84975500	-2.80258900	0.81660200	C	-2.92286800	1.70055900	0.53918600
C	-1.64943900	-3.43080400	3.98113500	C	-3.41051300	0.49740600	2.42531500
H	-1.60968300	-4.44514000	4.40161200	C	-3.91440200	0.74347100	0.18874200
H	-0.67194400	-2.97303400	4.15867900	C	-4.20870400	0.00075700	1.36048300
H	-2.38265800	-2.87369000	4.57444000	C	-0.49382900	-3.25417400	1.02011300
C	-6.35799700	-1.11235000	1.62865800	C	-1.41190300	-3.14482400	2.09371800
H	-6.41358400	-1.83428200	0.80710200	C	-1.23767800	-3.31591300	-0.18170700
H	-6.36265300	-1.67525500	2.56442000	C	-2.72073000	-3.14970200	1.54888400
H	-7.29052900	-0.53222400	1.60037000	C	-2.62245000	-3.25326200	0.13601200
C	-4.63072200	0.03451500	4.06748100	C	1.08824300	-0.13016800	4.23897500
H	-5.34506400	0.73172900	4.52630500	C	-0.89662100	-0.31981900	-4.26326600
H	-5.02789500	-0.97312400	4.22325000	C	1.89127700	-1.42331700	4.48396000
H	-3.70237600	0.11288500	4.64380400	H	2.07807700	-1.55144900	5.55608500
C	-2.76933800	2.32612700	2.92755700	H	1.34599700	-2.30002800	4.12268000
H	-3.34975900	3.22280400	3.18548200	H	2.85630500	-1.38848100	3.96987300
H	-2.45243000	1.87197800	3.87142300	C	-0.25495900	-0.20426600	4.99138900
H	-1.86665600	2.66197600	2.41039300	H	-0.07319500	-0.32668700	6.06477500
C	-3.25766700	2.50362900	-0.23504700	H	-0.83909500	0.70863000	4.84396500
H	-2.36556300	2.98608300	0.16945700	H	-0.85335100	-1.05385500	4.64869200
H	-2.99743900	2.10568700	-1.22177400	C	1.89218300	1.08072500	4.75327400
H	-4.00207300	3.29490900	-0.39942100	H	2.84842400	1.16971900	4.22971900
C	-5.37236200	0.29591400	-1.02777400	H	1.33497200	2.01114900	4.61097700
H	-4.65600700	0.49422500	-1.83315700	H	2.09709900	0.96293100	5.82312000
H	-5.76971900	-0.71340100	-1.17891600	C	-0.08503400	0.80717300	-4.93177700
H	-6.21048900	0.99002300	-1.18062100	H	0.97546800	0.73856400	-4.67092100
C	0.58698100	0.19346600	3.12237500	H	-0.17366300	0.73272200	-6.02121000
H	0.74302400	-0.71766100	3.71305600	H	-0.45034700	1.79117900	-4.62432500
H	0.04963100	0.88803000	3.77912300	C	-2.38167500	-0.17519500	-4.65222300
C	-0.68924500	-0.07457000	-3.15475900	H	-2.98860600	-0.95774900	-4.18781100
H	-0.83701900	0.85339500	-3.72072400	H	-2.77656600	0.79612100	-4.34091000

H	-2.48948900	-0.25753200	-5.73943100	C	0.80519900	0.10437700	2.18193400
C	-0.37194400	-1.68913000	-4.73906500	C	0.56729700	-0.18864000	3.38870100
H	-0.46575600	-1.76891200	-5.82790900	Sm	-1.80059700	-1.02535200	2.61058300
H	0.68096700	-1.82138000	-4.47423100	C	-2.75035400	1.36008500	3.61943000
H	-0.94134700	-2.50562100	-4.28539200	C	-3.04638600	1.43474900	2.23666700
H	-3.43508700	0.15207400	3.45257600	C	-3.57408200	0.35516200	4.18625700
H	-4.95244100	-0.78413300	1.43640900	C	-4.06309400	0.48823500	1.93796100
H	-3.64517600	-3.11913200	2.11415800	C	-4.37900200	-0.18213800	3.14911500
H	-0.82703900	-3.41062300	-1.17968100	C	-0.69779500	-3.56133400	2.69441600
H	0.58523800	-3.28635700	1.10423200	C	-1.67465900	-3.55584700	3.72001500
H	-1.16313400	-3.11059900	3.14804100	C	-1.37276500	-3.49816700	1.45136600
H	-1.90873600	2.15056800	2.47374000	C	-2.95104900	-3.49210800	3.10443900
H	-2.49361900	2.43158900	-0.13548300	C	-2.77328400	-3.46157800	1.69616000
H	-0.14874600	3.43411900	0.55657900	C	0.97813600	-0.27119900	4.82747100
H	3.83467900	3.29405300	-1.16633600	C	-0.43379400	-0.31417700	-1.99549300
H	2.05830000	3.06360900	-3.17742000	C	1.99310300	-1.41934100	4.98528800
H	-0.41399000	3.14893300	-2.10338300	H	2.31796200	-1.49194600	6.02975800
H	4.66335300	0.90385100	-2.17031000	H	1.55154800	-2.37803400	4.69795800
H	2.93081200	-0.67277500	-3.48780100	H	2.87409100	-1.25064200	4.36030200
H	1.90262300	-2.43094100	-1.72043100	C	-0.22454400	-0.54256600	5.74936400
H	3.01894700	-1.93657000	0.67601400	H	0.10135800	-0.62103700	6.79259800
C	5.01874300	0.24249300	0.69074000	H	-0.96228800	0.26277700	5.68958100
H	4.55857100	0.19877500	1.68326000	H	-0.71589300	-1.49092600	5.49688500
H	5.94806600	-0.33912900	0.74065400	C	1.63408200	1.05625700	5.24989400
H	5.29996800	1.28224200	0.49584000	H	2.52488100	1.25720900	4.64860500
C	2.63643100	3.64846200	1.51395700	H	0.94081800	1.89333600	5.12348700
H	3.67262100	3.30144300	1.57700400	H	1.93130000	1.01456600	6.30452400
H	2.64113600	4.72242800	1.73947300	C	0.63744000	0.30850800	-2.90879800
H	2.06564700	3.15072200	2.30327400	H	1.61223600	-0.16944400	-2.75970200
C	-3.76495700	-3.40497800	-0.82717500	H	0.36763600	0.17780200	-3.96278200
H	-3.56243700	-2.91389700	-1.78485600	H	0.74017300	1.38380000	-2.72678100
H	-3.95836000	-4.46342800	-1.04313500	C	-1.78474600	0.36852800	-2.27706100
H	-4.69090000	-2.98444400	-0.42289800	H	-2.58108700	-0.09852800	-1.69168300
C	-4.60548300	0.63011300	-1.13904900	H	-1.75165600	1.43161700	-2.02057700
H	-5.02491600	-0.36866500	-1.29483200	H	-2.03989400	0.28055300	-3.33969900
H	-5.43612100	1.34396900	-1.20873000	C	-0.54507700	-1.81666200	-2.31529200
H	-3.92243200	0.84159700	-1.96677100	H	-0.78582500	-1.96014400	-3.37526300

TS_{CC}[(C₅H₄Me)₂Sm-CC^tBu]₂

H= -1467.870119 au

Sm	2.13566500	0.96303200	0.25493200	H	0.39506500	-2.33550000	-2.10597600
C	-0.09191400	-0.15541800	-0.54277500	H	-1.33171100	-2.28355600	-1.71636700
C	-0.40625200	-0.32068900	0.67277600	H	-3.61476200	0.07033800	5.23196000
C	4.03215700	-0.41036800	-1.20161300	H	-5.14541300	-0.93950100	3.26893300
C	4.78069300	0.37505100	-0.28900600	H	-3.90617000	-3.51333800	3.61707500
C	3.35548500	-1.41082900	-0.45969900	H	-0.90081500	-3.51149500	0.47673600
C	4.57329100	-0.13098600	1.02070400	H	0.37543100	-3.61648600	2.82806700
C	3.68510700	-1.23586100	0.90638800	H	-1.48829600	-3.64384300	4.78447200
C	1.05597300	3.44284100	0.90417900	H	-2.03463600	1.97908700	4.14701200
C	2.42932500	3.56594100	1.24670100	H	-2.59850200	2.11914800	1.52605300
C	0.94875800	3.33588300	-0.50381800	H	0.22970500	3.45973900	1.60497300
C	3.16828400	3.51691500	0.03554500	H	4.24396500	3.62040000	-0.04985300
C	2.25861600	3.37711500	-1.04426200	H	2.52286500	3.34679700	-2.09570100
				H	0.02470300	3.26092600	-1.06437000
				H	5.43653700	1.19805500	-0.54863000
				H	4.02339000	-0.29156400	-2.27941900

H	2.71594100	-2.18684100	-0.86222100	C	-0.11066800	0.77196900	4.12049300
H	3.34160100	-1.85727100	1.72439400	H	0.46315800	0.93353600	5.04060500
C	5.27133300	0.33316800	2.26736600	H	-0.34741000	1.75141900	3.69201700
H	4.63768300	0.23984000	3.15553400	H	-1.05246000	0.28246400	4.38627700
H	6.17497700	-0.26031200	2.45570700	C	2.00147800	0.63905800	2.77458200
H	5.58434400	1.37900500	2.18755800	H	2.60167000	0.02636100	2.08922900
C	2.98002800	3.84869400	2.61485300	H	1.77973900	1.60523800	2.30248200
H	3.98340600	3.43202000	2.75207900	H	2.61424200	0.83817400	3.66164100
H	3.05694200	4.92989900	2.78654800	C	0.13745100	-0.86074800	-4.10169300
H	2.33576400	3.44259800	3.39950800	H	0.35322300	-1.83313000	-3.64715700
C	-3.86400300	-3.53334500	0.66551000	H	-0.41780700	-1.03534600	-5.03076200
H	-3.63902500	-2.93457900	-0.22363300	H	1.09081200	-0.38854400	-4.35680300
H	-4.01257300	-4.56596000	0.32531500	C	-0.97089100	1.36936400	-3.84705400
H	-4.82021700	-3.18712700	1.06949300	H	-1.57520300	2.02328700	-3.20992400
C	-4.78476900	0.34935700	0.62814600	H	-0.04134900	1.89528800	-4.08547600
H	-5.09583300	-0.68123500	0.42966200	H	-1.52088200	1.20235800	-4.78059800
H	-5.69348200	0.96471000	0.62018900	C	-2.00862300	-0.66905100	-2.81782700
H	-4.16477000	0.68332100	-0.20856000	H	-2.60709200	-0.85612300	-3.71721100
{{(C₅H₄Me)₂Sm}₂(μ-η²:η²-tBuC₄tBu)}							
H= -1467.914549 au							
Sm	2.19320400	1.22331200	-0.81093200	H	-1.81903600	-1.63857800	-2.33883600
C	0.12693200	0.28771300	-1.89546000	H	-2.60766600	-0.04242000	-2.14525600
C	-0.16960300	-0.01919200	-0.65629200	H	-3.91514800	-0.51360100	3.60554500
C	3.87811500	-0.05487400	-2.54213800	H	-5.47751000	-1.61500200	1.70991900
C	4.74613300	0.66652800	-1.68037800	H	-4.09761300	-3.92379000	1.79929600
C	3.29748600	-1.10533800	-1.79097300	H	-0.85938800	-3.77840700	-1.09597700
C	4.70119300	0.07650900	-0.39208400	H	0.21753200	-3.57190000	1.35413300
C	3.79041000	-1.01698800	-0.46718800	H	-1.78499300	-3.67314600	3.15337500
C	1.26699500	3.69191300	0.04949100	H	-2.65531100	1.60114700	2.50740600
C	2.68495900	3.81208800	0.11983600	H	-3.44421600	1.79720900	-0.05231500
C	0.88834300	3.59607500	-1.31113800	H	0.58842100	3.73128800	0.89480700
C	3.17137800	3.76697400	-1.21096000	H	4.21001900	3.86967600	-1.50316300
C	2.06765900	3.62916900	-2.09422500	H	2.11887500	3.59686000	-3.17674100
C	0.14235000	-0.02544200	0.65177200	H	-0.12349300	3.50794200	-1.68421700
C	-0.14052700	-0.33902300	1.89298700	H	5.37413500	1.50256400	-1.96572900
Sm	-2.21124500	-1.28308600	0.83141600	H	3.72245300	0.14020200	-3.59702700
C	-3.34085700	0.93383600	2.00211800	H	2.59524600	-1.84174800	-2.15938200
C	-3.74144500	1.02331800	0.64707400	H	3.56316800	-1.70490300	0.34016100
C	-3.99312100	-0.18497400	2.57526000	C	5.57187200	0.43565400	0.77864500
C	-4.66877800	-0.02373900	0.37680000	H	5.07357600	0.25890500	1.73738800
C	-4.81327300	-0.76944300	1.57361400	H	6.48893300	-0.16709100	0.78037000
C	-0.83787700	-3.65946100	1.13055000	H	5.87862300	1.48586000	0.74858800
C	-1.89159800	-3.69703700	2.07509600	C	3.49522200	4.10612800	1.35040300
C	-1.40927500	-3.74334400	-0.16152400	H	4.52121600	3.73530100	1.26287100
C	-3.11170800	-3.82426900	1.36018000	H	3.55824700	5.18808300	1.52267900
C	-2.82349300	-3.85610700	-0.02796900	H	3.05483900	3.66608400	2.25058200
C	0.69171700	-0.08847500	3.12854000	C	-3.80605000	-4.12010300	-1.13379900
C	-0.67764200	0.03016900	-3.14728000	H	-3.51782900	-3.63140400	-2.07041900
C	1.02554500	-1.43470100	3.79580600	H	-3.87612900	-5.19492700	-1.34402600
H	1.61101800	-1.27548200	4.70896300	H	-4.81267500	-3.77860400	-0.87271600
H	0.11127200	-1.97254800	4.06414900	C	-5.47630100	-0.19841900	-0.87828800
H	1.60844300	-2.07426200	3.12519500	H	-5.73295800	-1.24665100	-1.06158400
				H	-6.42118500	0.35531100	-0.80875100
				H	-4.95200800	0.17798500	-1.76189700

[(C₅H₅)₂Sm-CC^tBu]₂

H= -1310.829534 au

Sm	1.68656900	0.78971000	-0.41559800
C	-0.75786400	-0.10782800	-2.85065900
C	-0.41211900	-0.01911900	-1.66593800
C	3.29423700	-0.75888700	-2.03902800
C	4.18332500	0.08888300	-1.33547400
C	2.74234900	-1.68221300	-1.11369100
C	4.17040300	-0.29942800	0.02867200
C	3.28660900	-1.40148300	0.16075200
C	0.75108600	3.32287600	0.21928300
C	2.10125900	3.29968900	0.65452800
C	0.74667300	3.27418700	-1.19397800
C	2.93052400	3.24179800	-0.49154700
C	2.09344400	3.21374000	-1.63624200
C	0.36995900	0.02396000	1.66420600
C	0.74113800	0.06843800	2.84372800
Sm	-1.74035900	-0.75791600	0.41406900
C	-2.86347500	1.47446100	1.60223000
C	-2.96682400	1.72230400	0.21361900
C	-3.72489100	0.39312000	1.92134300
C	-3.89748300	0.79912500	-0.32833900
C	-4.37213600	-0.01618000	0.72741600
C	-0.62589500	-3.27813400	0.71641500
C	-1.64869900	-3.19703000	1.69678300
C	-1.24198400	-3.30425000	-0.55588400
C	-2.89654400	-3.17828100	1.02836400
C	-2.64630900	-3.23158900	-0.36663600
C	1.16498800	0.11083900	4.25295300
C	-1.15286400	-0.20853000	-4.26526700
C	2.17847900	-1.01706800	4.52935200
H	2.48734100	-0.99457100	5.58035000
H	1.74097900	-1.99754800	4.32015700
H	3.07193800	-0.90238900	3.90840600
C	-0.07704200	-0.07924300	5.14815100
H	0.21890600	-0.05069800	6.20259100
H	-0.81165100	0.71254900	4.97522500
H	-0.55798400	-1.04256700	4.95410800
C	1.81229200	1.47638100	4.55754800
H	2.70357900	1.63425000	3.94259600
H	1.11293400	2.29495900	4.36489400
H	2.11315100	1.51918200	5.61009000
C	-0.29503700	0.77204400	-5.09109200
H	0.76852900	0.52901800	-5.00844300
H	-0.57846500	0.71332600	-6.14768400
H	-0.43922900	1.80205000	-4.75252900
C	-2.64189600	0.16386900	-4.41059500
H	-3.27547600	-0.52017600	-3.83773500
H	-2.82846200	1.18225800	-4.05784000
H	-2.93992400	0.10267800	-5.46304900
C	-0.92634100	-1.64666900	-4.77138900
H	-1.21189700	-1.72235500	-5.82660700
H	0.12478500	-1.93469100	-4.67782800

H	-1.52776700	-2.36213700	-4.20276100
H	-3.89658900	-0.01687400	2.91015000
H	-5.11676000	-0.79848300	0.64285400
H	-3.39843800	-3.26421100	-1.14676300
H	-3.87136700	-3.15131100	1.49989900
H	-0.73166900	-3.37132200	-1.50850500
H	0.43816000	-3.32157600	0.91095600
H	-1.50176200	-3.18863800	2.77063900
H	-2.23950900	2.01742400	2.30102000
H	-2.43956000	2.48937500	-0.33936500
H	-4.21732300	0.75195700	-1.36273400
H	-0.12055000	3.38198000	0.85872400
H	2.43881200	3.35542900	1.68283900
H	4.01376800	3.24295400	-0.49470900
H	2.42695200	3.19935400	-2.66765900
H	-0.13061100	3.28351600	-1.82862700
H	4.77109200	0.13646100	0.81899300
H	4.78513300	0.87957700	-1.76675800
H	3.09879900	-0.73203300	-3.10481700
H	2.04056100	-2.47279000	-1.34752000
H	3.07183200	-1.93835100	1.07620700

TS_{CC}[(C₅H₅)₂Sm-CC^tBu]₂

H= -1310.77394 au

Sm	2.14502500	0.88702100	0.26262600
C	-0.14538100	-0.05968300	-0.49495900
C	-0.44387300	-0.28516700	0.71618400
C	4.08044900	-0.46028800	-1.17876900
C	4.77868500	0.12866400	-0.09576800
C	3.24777300	-1.48562100	-0.65724000
C	4.36823800	-0.52193500	1.09430800
C	3.42640100	-1.52353100	0.74542700
C	1.26943400	3.36538300	1.13990600
C	2.66213300	3.34420600	1.40708900
C	1.09435800	3.39827700	-0.26341000
C	3.34790600	3.37379300	0.16735700
C	2.37989600	3.39948800	-0.86692700
C	0.79335500	0.13417900	2.20513700
C	0.55891600	-0.06826900	3.42629100
Sm	-1.77414800	-1.03558500	2.66655100
C	-2.91234500	1.35596900	3.49501300
C	-3.07961400	1.33715100	2.09086800
C	-3.73825500	0.34162900	4.04957500
C	-4.00420700	0.30920500	1.77342700
C	-4.41817100	-0.29854500	2.98502000
C	-0.68619800	-3.57107200	2.96192400
C	-1.89017700	-3.59966900	3.71497200
C	-1.02926000	-3.47166100	1.59328900
C	-2.97534400	-3.52082700	2.80880700
C	-2.44418400	-3.43149300	1.49760300
C	0.86566600	-0.05058500	4.88742200
C	-0.56013100	-0.13283700	-1.93526900
C	2.12813100	-0.89451800	5.14458400

H	2.37183700	-0.89271800	6.21346600	C	3.38091500	-1.59595200	-0.57976800
H	1.98072800	-1.93138500	4.82841300	C	1.44465800	3.49934400	-0.21626100
H	2.98183000	-0.49041600	4.59375600	C	2.84585500	3.48451200	0.02151900
C	-0.30418600	-0.63165400	5.70368600	C	1.23774600	3.36665300	-1.60966800
H	-0.07514000	-0.62382800	6.77495900	C	3.49987000	3.33974200	-1.22485200
H	-1.21863200	-0.04062200	5.56684000	C	2.50629500	3.25405900	-2.23374400
H	-0.50317300	-1.67476400	5.42628800	C	0.11795200	0.00792200	0.67163000
C	1.11664700	1.40336400	5.32938400	C	-0.17371000	-0.16406700	1.94182100
H	1.96030800	1.83340800	4.78277400	Sm	-2.35162400	-0.95355700	1.01048400
H	0.23865600	2.02917700	5.14413000	C	-3.32814900	1.45478200	1.93645700
H	1.34294400	1.43793600	6.40144200	C	-3.48224300	1.51971000	0.53150900
C	0.54178000	0.40761200	-2.86518100	C	-4.22110200	0.46848400	2.43043500
H	1.46471800	-0.17605700	-2.76565600	C	-4.47877600	0.57955300	0.15539200
H	0.23012000	0.34888000	-3.91409800	C	-4.93991500	-0.06337000	1.32959800
H	0.76234800	1.45993600	-2.64902700	C	-1.43610000	-3.46542000	1.69738900
C	-1.83754200	0.70431600	-2.13081200	C	-2.74605900	-3.37780600	2.23652200
H	-2.64928500	0.32360800	-1.50491100	C	-1.54486600	-3.49434200	0.28697500
H	-1.66738100	1.75157300	-1.86359100	C	-3.66514500	-3.36982600	1.15641900
H	-2.15906500	0.66689800	-3.17845400	C	-2.92412700	-3.43336100	-0.04846100
C	-0.84588400	-1.60158700	-2.29947100	C	0.71064300	0.11203000	3.13613000
H	-1.15047600	-1.67947600	-3.34987100	C	-0.61821000	-0.11146500	-3.18298600
H	0.04298500	-2.22339600	-2.15577200	C	2.06956800	0.69360000	2.70439000
H	-1.64676700	-2.00698200	-1.67501300	H	2.72265900	0.89500700	3.56167400
H	-3.87264500	0.13073800	5.10498500	H	2.59700000	-0.01927700	2.05615800
H	-5.14831600	-1.09245600	3.08298800	H	1.92643700	1.64351700	2.17301800
H	-3.02120900	-3.38952300	0.58079100	C	0.94608200	-1.20301500	3.90086900
H	-4.02566300	-3.55567900	3.07069100	H	1.56186300	-1.02557300	4.79042600
H	-0.33416000	-3.43783100	0.76461700	H	-0.00333600	-1.64098100	4.22428800
H	0.31884100	-3.64841400	3.35914000	H	1.46033200	-1.93713600	3.27187200
H	-1.97072400	-3.72034900	4.78984900	C	0.00673800	1.11272900	4.06989100
H	-2.29395200	2.05108400	4.05046700	H	-0.16647700	2.06876600	3.56499900
H	-2.59122900	1.99421300	1.38306400	H	-0.96226500	0.72373300	4.39792000
H	-4.36712700	0.06166800	0.78246600	H	0.61727900	1.30403700	4.96010500
H	0.47923600	3.36421100	1.87966700	C	0.22588500	0.39283300	-4.36525100
H	3.12295200	3.35046900	2.38841300	H	1.18959900	-0.12529700	-4.40596500
H	4.42224100	3.40258300	0.03337100	H	-0.29220400	0.22112100	-5.31571800
H	2.58889500	3.46362400	-1.92920000	H	0.42287900	1.46602200	-4.27609600
H	0.14502900	3.45170300	-0.78261300	C	-1.96105900	0.64057100	-3.17279400
H	4.74258800	-0.31801400	2.09117200	H	-2.60713900	0.28111700	-2.36456000
H	5.51779800	0.91696500	-0.16936600	H	-1.81126800	1.71490500	-3.02629400
H	4.20555800	-0.20784000	-2.22604300	H	-2.49126900	0.49866500	-4.12199300
H	2.61390300	-2.14839500	-1.23393200	C	-0.87904100	-1.61845200	-3.36312500
H	2.93603200	-2.20307100	1.43060000	H	-1.38679700	-1.80947800	-4.31589100
{{(C₅H₅)₂Sm}₂(μ-η²:η²-tBuC₄tBu)}				H	0.05775900	-2.18431100	-3.36001300
H= -1310.815421 au				H	-1.50696100	-2.00747000	-2.55508400
Sm	2.25038700	0.92055200	-0.81145400	H	-4.36980700	0.20707400	3.47231800
C	0.11519600	0.11928100	-1.88283400	H	-5.72356000	-0.80911800	1.38142000
C	-0.22263600	-0.06611000	-0.63398200	H	-3.34108800	-3.48256100	-1.04842600
C	4.11223100	-0.35469100	-2.36454600	H	-4.74480200	-3.34818400	1.23960400
C	4.83787300	0.05891300	-1.21746100	H	-0.72172900	-3.58031500	-0.41194900
C	3.22107600	-1.38548300	-1.97044000	H	-0.51636400	-3.52138500	2.26513900
C	4.38479200	-0.70486500	-0.11586800	H	-3.00383600	-3.37393900	3.28984700
				H	-2.66128800	2.06474400	2.53175000

H	-2.95546400	2.19109300	-0.13578000
H	-4.86018300	0.41999800	-0.84713700
H	0.67086100	3.63243200	0.53056600
H	3.33254000	3.61040900	0.98232900
H	4.57104900	3.32454800	-1.38414800
H	2.68821500	3.17087200	-3.29915700
H	0.27892300	3.36704200	-2.11188400
H	4.77245900	-0.64945800	0.89524600
H	5.62282700	0.80480400	-1.19446600
H	4.25373800	0.01584500	-3.37342300
H	2.55151100	-1.93159400	-2.62227800
H	2.85801300	-2.33488000	0.01571700

(C₅Me₅)₂Sm(CCPH)(THF)

H= -1354.190104 au

O	2.49415500	3.01719900	17.46439300
C	2.31446400	3.45498200	12.86709900
C	3.60015000	2.85512700	12.72711100
C	4.46095000	3.42244100	13.71611600
C	3.70408800	4.37738100	14.45662100
C	2.37869700	4.39479100	13.93501200
C	1.13226100	3.24524600	11.96584700
H	1.09482100	4.00959700	11.17734900
H	0.19221600	3.29026200	12.52253800
H	1.16620800	2.27217300	11.46641700
C	4.02839900	1.98603300	11.57949800
H	4.32000900	2.59899700	10.71563900
H	3.22809200	1.32187100	11.23999500
H	4.89132700	1.36159500	11.82831300
C	5.94754800	3.22651900	13.81168500
H	6.48706000	4.00733500	13.25803300
H	6.26078500	2.26589700	13.39524300
H	6.31204200	3.26677400	14.84476100
C	4.26005700	5.32823000	15.47774600
H	4.55721500	6.27895100	15.01460700
H	5.15490400	4.92905700	15.96775200
H	3.53160600	5.57106000	16.25821100
C	1.26796200	5.31750500	14.34490700
H	1.15509200	6.14581300	13.63234400
H	1.45540400	5.76645100	15.32558700
H	0.30930600	4.79245000	14.40057900
C	1.99342200	-0.78497300	15.43619800
C	2.98447000	-0.74307000	14.41248500
C	4.22101700	-0.35618900	15.01005200
C	3.98872300	-0.14383000	16.40042300
C	2.61214000	-0.40938200	16.66214900
C	0.59424800	-1.30308100	15.27811400
H	0.56081800	-2.39073000	15.43223500
H	0.19455800	-1.09967700	14.28121600
H	-0.09336100	-0.84224900	15.99126200
C	2.79250400	-1.22837200	13.00353600
H	2.85598700	-2.32390800	12.95233000
H	3.55312300	-0.83277000	12.32521300

H	1.81318200	-0.95029900	12.59952300
C	5.57468100	-0.41167000	14.36443000
H	6.03273200	-1.40094300	14.50389000
H	6.26956700	0.32055400	14.78750900
H	5.52626500	-0.23642000	13.28624500
C	5.06006500	0.11844200	17.42185800
H	5.63084100	-0.79447500	17.64032800
H	4.64288900	0.46055700	18.37344600
H	5.78960100	0.86801800	17.09221800
C	1.94269800	-0.41614400	18.00604300
H	1.93954700	-1.42133400	18.44883800
H	0.89892100	-0.09247500	17.93865700
H	2.44760400	0.24280100	18.72001300
C	0.14943400	2.02171300	15.13385400
C	-1.08368600	2.11090300	15.18110100
C	-2.50667700	2.20707400	15.24664500
C	-3.21177700	3.11019900	14.42737800
H	-2.65532300	3.73489000	13.73511500
C	-4.59770400	3.20188200	14.49832800
H	-5.12272000	3.90418400	13.85601800
C	-5.31374600	2.39921800	15.38693400
H	-6.39643600	2.47302900	15.44045000
C	-4.62936400	1.49985300	16.20499600
H	-5.17907600	0.86888000	16.89870700
C	-3.24379600	1.40203600	16.13726100
H	-2.71157400	0.69928100	16.77134600
C	1.23328300	3.30650900	18.10747000
H	1.02051500	2.50946000	18.83274200
H	0.46453900	3.30017800	17.33320700
C	1.47354300	4.64508200	18.79468200
H	0.82055100	4.78081500	19.66059700
H	1.27857600	5.46434800	18.09719200
C	2.97081500	4.59490500	19.17560900
H	3.48763900	5.50924900	18.87411000
H	3.11570200	4.47487100	20.25267800
C	3.50946500	3.36837200	18.41791800
H	4.43346600	3.55566100	17.86793100
H	3.66745600	2.51993100	19.09579600
Sm	2.60898000	1.90950800	15.14423200

(C₅Me₅)₂Sm(CC^tBu)(THF)

H= -1280.396213 au

O	2.53586600	2.98715300	17.49765500
C	2.30074900	3.49584600	12.89944200
C	3.58139300	2.88860500	12.74493000
C	4.45223200	3.43938000	13.73432600
C	3.70653200	4.39096100	14.48987200
C	2.37810100	4.42300700	13.97701300
C	1.11018500	3.30387100	12.00541800
H	1.06719500	4.08147100	11.23019300
H	0.17611600	3.34126400	12.57276700
H	1.13821400	2.33916100	11.48947700
C	3.99701300	2.02861900	11.58585700

H	4.29633700	2.64806000	10.72921500
H	3.18738200	1.37964300	11.23905900
H	4.85140000	1.38916100	11.82608500
C	5.93813300	3.23365700	13.81819600
H	6.47897200	4.01530400	13.26687800
H	6.24297200	2.27430400	13.39281100
H	6.30937800	3.26395400	14.84924400
C	4.27478700	5.32862800	15.51630900
H	4.56744300	6.28494500	15.06176700
H	5.17477500	4.92283000	15.99120900
H	3.55539000	5.56247000	16.30797300
C	1.27585400	5.34728500	14.40530200
H	1.16587400	6.18782000	13.70657500
H	1.47067500	5.77904400	15.39238500
H	0.31479500	4.82646800	14.45676600
C	1.98398800	-0.78179400	15.42451400
C	2.96759500	-0.72867800	14.39424900
C	4.20861700	-0.34975800	14.98765500
C	3.98618400	-0.15313700	16.38157700
C	2.61120000	-0.42004800	16.64992000
C	0.58357500	-1.29802400	15.27331400
H	0.54435100	-2.38136200	15.45490000
H	0.19261900	-1.11932200	14.26812000
H	-0.10543300	-0.81403800	15.96970500
C	2.76701400	-1.19834700	12.98113000
H	2.83474800	-2.29295800	12.91588300
H	3.52058600	-0.79126200	12.30160800
H	1.78363400	-0.91922300	12.58762200
C	5.55767100	-0.39956100	14.33196500
H	6.01123400	-1.39405700	14.44743700
H	6.25906000	0.31980700	14.76613700
H	5.50411200	-0.20082500	13.25797600
C	5.06450500	0.09712100	17.39861600
H	5.63903900	-0.81734700	17.60022200
H	4.65307900	0.42481400	18.35772600
H	5.78985100	0.85325700	17.07464200
C	1.94952200	-0.44047600	17.99751500
H	1.94130400	-1.45162600	18.42668400
H	0.90789700	-0.10797700	17.94013200
H	2.46351700	0.20488400	18.71751500
C	0.14350000	2.04832400	15.17744300
C	-1.08919200	2.12584000	15.19765500
C	1.28236200	3.27404100	18.15506100
H	1.07968700	2.47687200	18.88329500
H	0.50617700	3.26429500	17.38764900
C	1.52927000	4.61291000	18.83916200
H	0.88313900	4.75158900	19.70987200
H	1.33163100	5.43160500	18.14157900
C	3.02898800	4.55971700	19.20942200
H	3.54420000	5.47635600	18.91211300
H	3.18039300	4.43105200	20.28463400
C	3.56228900	3.33846900	18.43877900
H	4.47786400	3.53210200	17.87718200

H	3.73318300	2.48775800	19.11058100
Sm	2.59484500	1.91989800	15.15791700
C	-2.56139700	2.19736400	15.20738500
C	-3.10099000	1.66390600	16.54954400
C	-3.01752100	3.65803000	15.02075900
C	-3.12140100	1.33738200	14.05652000
H	-2.79390400	0.62577100	16.70784000
H	-2.72501600	2.26028600	17.38697500
H	-4.19661000	1.70582600	16.56421400
H	-2.65486700	4.06103700	14.07036000
H	-4.11229700	3.72163400	15.02600900
H	-2.63373100	4.29241300	15.82592800
H	-4.21723200	1.37842200	14.04830100
H	-2.75546800	1.69586100	13.08976400
H	-2.81572700	0.29293100	14.16770500

CH₂(SiMe₃)₂

H= -286.329373 au

C	0.27519200	2.71177700	-2.13487900
H	0.87163600	1.90136100	-2.57838100
H	0.18744100	3.47551500	-2.92115600
Si	1.32624600	3.45140600	-0.73294200
Si	-1.47743600	2.04044600	-1.83575300
C	-2.01628400	1.05907700	-3.37111200
H	-3.03689900	0.67783400	-3.25691800
H	-1.99298000	1.68666700	-4.26847300
H	-1.35764600	0.20182100	-3.54723900
C	-2.69609100	3.47446800	-1.58547100
H	-2.45840600	4.05844500	-0.69141200
H	-2.68454000	4.15609200	-2.44287500
H	-3.71865700	3.09713500	-1.47596900
C	-1.54897000	0.89098100	-0.32726800
H	-2.55116200	0.46228400	-0.21887600
H	-0.84058800	0.06120200	-0.42082000
H	-1.31683800	1.42837000	0.59790200
C	0.33079800	4.63372000	0.36942700
H	-0.13525000	5.43179100	-0.21784700
H	-0.46173000	4.11089400	0.91458900
H	0.98577500	5.10613300	1.10976600
C	2.05705500	2.06596700	0.33936300
H	2.65547000	1.37463800	-0.26376800
H	2.71124000	2.48238700	1.11296800
H	1.27722600	1.48335500	0.83905400
C	2.75764100	4.42668200	-1.51517600
H	3.41821300	4.84574700	-0.74832300
H	3.36354500	3.78557600	-2.16436900
H	2.38426800	5.25743400	-2.12379300

HCCPh

H= -308.157204 au

C	0.00000000	0.00000000	2.02025700
C	0.00000000	0.00000000	3.23137300
H	0.00000000	0.00000000	4.29776100

C	0.00000000	0.00000000	0.59283900
C	0.00000000	1.21176200	-0.11986800
C	0.00000000	-1.21176200	-0.11986800
C	0.00000000	1.20706500	-1.51056000
H	0.00000000	2.14841700	0.42904500
C	0.00000000	-1.20706500	-1.51056000
H	0.00000000	-2.14841700	0.42904500
C	0.00000000	0.00000000	-2.20995800
H	0.00000000	2.14968500	-2.05073700
H	0.00000000	-2.14968500	-2.05073700
H	0.00000000	0.00000000	-3.29631600

HCCMe

H= -116.548258 au

C	0.21625200	-0.00000100	-0.00002300
C	1.42454400	0.00000100	0.00000400
H	2.49040900	-0.00000300	0.00003300
C	-1.23917700	0.00000000	0.00000600
H	-1.63340100	-0.64698500	-0.79102300
H	-1.63335400	-0.36156700	0.95584100
H	-1.63336700	1.00856100	-0.16476800

HCC'Bu

H= -234.366058 au

C	0.00000000	0.00000000	1.17077500
C	0.00000000	0.00000000	2.38017600
H	0.00000000	0.00000000	3.44618800
C	0.00000000	0.00000000	-0.29962600
C	0.00000000	1.45525500	-0.80657300
C	1.26028700	-0.72762700	-0.80657300
C	-1.26028700	-0.72762700	-0.80657300
H	-0.88564600	1.99268500	-0.45490900
H	0.88564600	1.99268500	-0.45490900
H	0.00000000	1.46983800	-1.90212200
H	1.28289300	-1.76333400	-0.45490900
H	1.27291700	-0.73491900	-1.90212200
H	2.16853900	-0.22935100	-0.45490900
H	-1.27291700	-0.73491900	-1.90212200
H	-1.28289300	-1.76333400	-0.45490900
H	-2.16853900	-0.22935100	-0.45490900

C₅Me₅

H= -389.73602 au

C	-3.50759000	1.60825700	3.51290300
C	-3.67503300	1.45130600	2.11475800
C	-4.37633600	0.69739000	4.16320200
C	-4.64753500	0.44340400	1.90092100
C	-5.08087100	-0.02252300	3.16690300
C	-6.11253600	-1.08402600	3.40734300
H	-6.12356300	-1.83616400	2.60414900
H	-5.92985900	-1.63137700	4.34422500
H	-7.14996100	-0.70556400	3.47815700
C	-4.53093000	0.53254600	5.64578700

H	-4.81420000	-0.49522400	5.91785400
H	-3.59641600	0.75100200	6.18420200
H	-5.29919700	1.18617800	6.10056400
C	-2.58215600	2.57796900	4.18506500
H	-3.02471200	3.57380500	4.37732600
H	-2.24033900	2.20941700	5.16375400
H	-1.67628600	2.76469100	3.58860000
C	-2.95453300	2.22537400	1.05133200
H	-3.45002300	3.17041500	0.75852100
H	-1.93755100	2.50674400	1.36413800
H	-2.84522400	1.64516100	0.12303600
C	-5.14152900	-0.03963200	0.56993700
H	-4.38317500	0.08188000	-0.21754900
H	-5.40214700	-1.10894000	0.58840800
H	-6.04476100	0.48227700	0.20112300

C₅H₄Me

H= -232.629903 au

C	-3.51148500	1.60746300	3.51007800
C	-3.62977600	1.39433000	2.11730400
C	-4.32061900	0.64313800	4.15421100
C	-4.50564000	0.30824100	1.90415900
C	-4.93418900	-0.15652000	3.16616700
C	-2.71941900	2.69401400	4.17810300
H	-3.28556700	3.62807800	4.35856200
H	-2.33853800	2.37981600	5.16228000
H	-1.84191400	2.98541500	3.58073800
H	-3.12637000	1.97749600	1.34591600
H	-4.78487200	-0.10946800	0.93753100
H	-5.60308600	-0.99704000	3.34724600
H	-4.44528900	0.54373500	5.23271000

C₅H₅

H= -193.352617 au

C	0.00000000	1.20138400	0.00000000
C	1.14258400	0.37124800	0.00000000
H	2.17902500	0.70800800	0.00000000
C	0.70615600	-0.97194000	0.00000000
H	1.34671200	-1.85359000	0.00000000
C	-1.14258400	0.37124800	0.00000000
H	-2.17902500	0.70800800	0.00000000
C	-0.70615600	-0.97194000	0.00000000
H	-1.34671200	-1.85359000	0.00000000
H	0.00000000	2.29116300	0.00000000

THF

H= -232.249985 au

C	10.91869000	0.97458100	-0.04839400
O	10.39033700	-0.15162300	-0.74455300
C	9.48830200	-0.86302000	0.09698300
C	9.72686600	-0.34731300	1.51494800
C	10.10875400	1.10916200	1.24167400
H	8.45096200	-0.66992000	-0.22001000

H	9.67845100	-1.93713600	-0.01120200
H	8.85229200	-0.45815300	2.16223400
H	10.56459300	-0.87980400	1.97980500
H	10.67613900	1.57422700	2.05277400
H	9.20906700	1.71106500	1.06926700
H	11.98373200	0.80206700	0.17085100
H	10.84799200	1.85880700	-0.69321900