SUPPORTING INFORMATION

trans-Hydroboration-Oxidation products in Δ⁵-steroids via a hydroboration-retro-hydroboration mechanism

J. Ciciolil Hilario-Martínez,[1,2] Fernando Murillo,[1] Jair García-Méndez,[1] Eugenia Dzib,[1] Jesús Sandoval-Ramírez,[2] Miguel Ángel Muñoz-Hernández,[3] Sylvain Bernès,[4] László Kürti,[5] Fernanda Duarte,[6] Gabriel Merino,[1,*] and María A. Fernández-Herrera.[1,*]

[1] Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados, Unidad Mérida. km 6 Antigua Carretera a Progreso. Apdo. Postal 73, Cordemex, 97310, Merida, Yuc., Mexico.
[2] Facultad de Ciencias Químicas, Benemérita Universidad Autónoma de Puebla, Ciudad Universitaria, 72570, Puebla, Pue., Mexico.
[3] Centro de Investigaciones Químicas, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, Cuernavaca, Mor., C. P. 62209, Mexico.
[4] Instituto de Física, Benemérita Universidad Autónoma de Puebla. Ciudad Universitaria, 72570, Puebla, Pue., Mexico.
[5] Department of Chemistry, Rice University, BioScience Research Collaborative, 6500 Main Street, Houston, Texas 77030, United States.
[6] Chemistry Research Laboratory, Oxford University, Mansfield Road, OX1 3TA Oxford, United Kingdom.

*email: mfernandez@cinvestav.mx, gmerino@cinvestav.mx

a. Cartesian coordinates of the structures at SMD-PBE0-D3/def2-TZVP level for the decalin model

Cartesian coordinates for the structures of the hydroboration mechanism for 1a' and 1b'

Decalin model

SMD-PBE0-D3/def2-TZVP
***G*= -504.610102 a.u.**
G_{corr}= 0.236682 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -504.127842171741 a.u.**
***E*(DLPNO-CCSD(T))= -504.358081241395 a.u.**
SMD CDS free energy correction energy= -0.006442930346 a.u.

O	3.485472000	0.822250000	0.106352000
H	4.136887000	0.390140000	-0.455735000
C	2.196010000	0.454940000	-0.361559000
H	2.047287000	0.842697000	-1.382009000
C	1.998082000	-1.049069000	-0.382164000
H	2.714708000	-1.506670000	-1.073736000
H	2.219785000	-1.443043000	0.615345000
C	0.578965000	-1.393074000	-0.806565000
H	0.437675000	-2.479158000	-0.822157000
H	0.426916000	-1.042380000	-1.834434000
C	-0.508292000	-0.762218000	0.082782000
C	1.178612000	1.110698000	0.554612000
H	1.295047000	2.197067000	0.521860000
H	1.412847000	0.791596000	1.578444000
C	-0.230738000	0.726073000	0.203149000
C	-0.485286000	-1.416308000	1.469599000
H	-0.621336000	-2.498420000	1.376679000
H	-1.286222000	-1.025890000	2.101638000
H	0.456118000	-1.243717000	1.994139000
C	-1.170231000	1.651368000	-0.000024000
H	-0.885308000	2.700287000	0.066185000
C	-2.605462000	1.361877000	-0.304708000
H	-2.809870000	1.607144000	-1.356454000
H	-3.245099000	2.031485000	0.281116000
C	-2.958373000	-0.091295000	-0.030612000
C	-1.871830000	-1.000377000	-0.577514000
H	-3.064287000	-0.242787000	1.048767000
H	-3.925000000	-0.340188000	-0.477957000
H	-1.776553000	-0.817678000	-1.654945000
H	-2.146115000	-2.054189000	-0.459545000

BH_3

SMD-PBE0-D3/def2-TZVP
***G*= -26.557575 a.u.**
G_{corr}= 0.008388 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -26.5297152089181 a.u.**
***E*(DLPNO-CCSD(T))= -26.539744618331 a.u.**
SMD CDS free energy correction energy= 0.001641409412 a.u.

B	0.000000000	0.000000000	0.000000000
H	-0.000000000	1.193688000	0.000000000
H	-1.033764000	-0.596844000	0.000000000
H	1.033764000	-0.596844000	0.000000000

TS1-1a'

SMD-PBE0-D3/def2-TZVP
***G*= -531.175595 a.u.** **ν_{min}= 405.6*i* cm^{-1}**
G_{corr}= 0.267079 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.653317107267 a.u.**
***E*(DLPNO-CCSD(T))= -530.915294989276 a.u.**
SMD CDS free energy correction energy= -0.005101117991 a.u.

O	3.544616000	-0.734035000	-0.379520000
H	4.257529000	-0.326888000	0.123425000
C	2.317264000	-0.365299000	0.229689000
H	2.282917000	-0.752737000	1.258981000
C	2.127404000	1.141309000	0.267459000
H	2.901974000	1.590023000	0.898911000
H	2.276641000	1.532685000	-0.744133000
C	0.750437000	1.516322000	0.799574000
H	0.621629000	2.602868000	0.779310000
H	0.675831000	1.213241000	1.850529000
C	-0.402658000	0.868827000	0.025887000
C	1.215192000	-1.033765000	-0.567733000
H	1.318099000	-2.120038000	-0.528426000
H	1.319700000	-0.738956000	-1.618312000
C	-0.163177000	-0.625300000	-0.128956000
C	-0.491213000	1.459403000	-1.388821000
H	-0.736062000	2.522743000	-1.318548000
H	-1.268337000	0.971767000	-1.980707000
H	0.446494000	1.367961000	-1.938135000
C	-1.257493000	-1.481116000	-0.361751000
H	-1.044171000	-2.379964000	-0.933217000
C	-2.654320000	-0.936253000	-0.542316000

H	-3.367547000	-1.674491000	-0.168105000
H	-2.834858000	-0.870714000	-1.621274000
C	-2.927578000	0.440622000	0.096564000
C	-1.719884000	1.103565000	0.760278000
B	-0.739255000	-1.750471000	1.243232000
H	-0.161075000	-2.803077000	1.311305000
H	0.098227000	-0.899570000	1.571021000
H	-1.677460000	-1.519870000	1.955892000
H	-3.318699000	1.108336000	-0.675121000
H	-3.721661000	0.351184000	0.841674000
H	-1.889423000	2.182615000	0.832516000
H	-1.604242000	0.737634000	1.783171000

INT-1a'

SMD-PBE0-D3/def2-TZVP
***G*= -531.185196 a.u.**
G_{corr}= 0.269444 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.666210449634 a.u.**
***E*(DLPNO-CCSD(T))= -530.930578829265 a.u.**
SMD CDS free energy correction energy= -0.005075620369 a.u.

O	3.547143000	0.783512000	0.372924000
H	4.269900000	0.329907000	-0.073174000
C	2.334424000	0.388693000	-0.248434000
H	2.322996000	0.739960000	-1.293579000
C	2.160048000	-1.122414000	-0.249020000
H	2.949089000	-1.577297000	-0.858380000
H	2.302858000	-1.485107000	0.773870000
C	0.793677000	-1.537109000	-0.784309000
H	0.687629000	-2.625696000	-0.738154000
H	0.723202000	-1.261061000	-1.844070000
C	-0.371060000	-0.879000000	-0.031895000
C	1.201001000	1.079272000	0.485402000
H	1.308380000	2.163386000	0.398151000
H	1.248806000	0.832706000	1.550037000
C	-0.142540000	0.645003000	-0.071279000
C	-0.408270000	-1.405668000	1.404480000
H	-0.544980000	-2.490865000	1.380836000
H	-1.228233000	-0.981825000	1.982155000
H	0.513792000	-1.203620000	1.950467000
C	-1.339354000	1.515499000	0.330145000
H	-1.049098000	2.244459000	1.085275000
C	-2.607249000	0.771861000	0.707489000
H	-3.450170000	1.468080000	0.657468000
H	-2.548313000	0.464477000	1.755830000

C	-2.918023000	-0.449396000	-0.169564000
C	-1.689532000	-1.184776000	-0.738651000
B	-1.078312000	1.916560000	-1.150941000
H	-0.329114000	2.817634000	-1.408712000
H	-0.003202000	0.809216000	-1.225694000
H	-1.746206000	1.438170000	-2.024368000
H	-1.855284000	-2.266403000	-0.716422000
H	-1.564275000	-0.917980000	-1.793003000
H	-3.527797000	-1.142261000	0.416385000
H	-3.544291000	-0.138564000	-1.009786000

TS2-1a'

SMD-PBE0-D3/def2-TZVP
***G*= -531.179474 a.u.** **ν_{min}= 103.7*i* cm^{-1}**
G_{corr}= 0.270221 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.662641405248 a.u.**
***E*(DLPNO-CCSD(T))= -530.927667264776 a.u.**
SMD CDS free energy correction energy= -0.005195140471 a.u.

O	3.523744000	0.755216000	0.429353000
H	4.251003000	0.352339000	-0.056331000
C	2.314393000	0.407465000	-0.228175000
H	2.298310000	0.863440000	-1.231719000
C	2.172595000	-1.101286000	-0.378055000
H	2.944680000	-1.471010000	-1.062309000
H	2.378224000	-1.554168000	0.596753000
C	0.793861000	-1.521787000	-0.882288000
H	0.711702000	-2.613876000	-0.860050000
H	0.678047000	-1.220933000	-1.930992000
C	-0.354003000	-0.905769000	-0.075614000
C	1.167989000	1.006133000	0.566069000
H	1.286526000	2.090124000	0.611768000
H	1.197506000	0.635693000	1.594090000
C	-0.152581000	0.626690000	-0.092910000
C	-0.326070000	-1.435604000	1.362655000
H	-0.721184000	-2.455557000	1.385070000
H	-0.931589000	-0.826729000	2.036535000
H	0.681032000	-1.467131000	1.776313000
C	-1.376411000	1.473904000	0.366633000
H	-1.173557000	1.869997000	1.360979000
C	-2.776776000	0.839060000	0.249417000
H	-3.269175000	1.260967000	-0.631390000
H	-3.376396000	1.161855000	1.105573000
C	-2.850082000	-0.682506000	0.122670000
C	-1.703428000	-1.237520000	-0.706385000

B	-0.959589000	2.327921000	-0.857588000
H	-0.058681000	3.116493000	-0.832263000
H	0.003430000	0.843074000	-1.196089000
H	-1.565141000	2.177939000	-1.883790000
H	-2.844340000	-1.156597000	1.107474000
H	-3.806640000	-0.952739000	-0.334761000
H	-1.794921000	-2.324894000	-0.803660000
H	-1.737758000	-0.822297000	-1.722187000

1a'

SMD-PBE0-D3/def2-TZVP
***G*= -531.194232 a.u.**
G_{corr}= 0.268409 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*=- 530.679146713334 a.u.**
***E*(DLPNO-CCSD(T))= -530.942476905762 a.u.**
SMD CDS free energy correction energy= -0.005078807571 a.u.

O	3.484342000	1.066893000	0.153058000
H	4.240541000	0.628949000	-0.251079000
B	-1.528825000	2.755510000	-0.077972000
H	-1.033628000	3.137733000	-1.103718000
C	2.305120000	0.477650000	-0.378866000
H	2.243414000	0.690771000	-1.458675000
C	2.288537000	-1.029763000	-0.187519000
H	3.113541000	-1.479362000	-0.752498000
H	2.476547000	-1.244051000	0.869606000
C	0.962814000	-1.632869000	-0.635950000
H	0.963576000	-2.714333000	-0.459368000
H	0.856602000	-1.493756000	-1.719417000
C	-0.251387000	-0.998245000	0.052704000
C	1.115529000	1.130655000	0.293602000
H	1.129476000	2.205701000	0.080543000
H	1.213664000	1.021686000	1.379398000
C	-0.194168000	0.524200000	-0.194448000
H	-0.213326000	0.648482000	-1.289031000
C	-0.239392000	-1.356405000	1.539867000
H	-0.294162000	-2.443224000	1.658553000
H	-1.084468000	-0.925330000	2.078742000
H	0.667773000	-1.018146000	2.042723000
C	-1.416001000	1.266720000	0.340258000
H	-1.493906000	1.143847000	1.427042000
C	-2.710737000	0.682103000	-0.288434000
H	-2.721957000	0.899715000	-1.365215000
H	-3.597396000	1.159261000	0.140433000
C	-2.791649000	-0.829776000	-0.097838000

C	-1.535196000	-1.531623000	-0.592086000
H	-2.205242000	3.524332000	0.547199000
H	-1.612707000	-2.611084000	-0.416961000
H	-1.457997000	-1.394528000	-1.678648000
H	-2.956217000	-1.050280000	0.961704000
H	-3.665553000	-1.214960000	-0.633685000

TS1-1b'

SMD-PBE0-D3/def2-TZVP
***G*= -531.170067 a.u.** **ν_{min}= 506.0*i* cm^{-1}**
G_{corr}= 0.266959 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.647811399509 a.u.**
***E*(DLPNO-CCSD(T))= -530.909621473477 a.u.**
SMD CDS free energy correction energy= -0.005148926032 a.u.

O	3.537686000	-0.680544000	-0.435990000
H	4.237322000	-0.271620000	0.083689000
C	2.297710000	-0.371434000	0.186036000
H	2.259719000	-0.828435000	1.185895000
C	2.098249000	1.129568000	0.328192000
H	2.861512000	1.533966000	1.002956000
H	2.267876000	1.590197000	-0.650682000
C	0.710129000	1.475919000	0.856149000
H	0.582686000	2.563523000	0.882689000
H	0.617433000	1.120452000	1.888357000
C	-0.421252000	0.852641000	0.032116000
C	1.201631000	-0.993772000	-0.655864000
H	1.337765000	-2.076344000	-0.701291000
H	1.292569000	-0.609219000	-1.678295000
C	-0.161748000	-0.652877000	-0.092356000
C	-0.453559000	1.473672000	-1.372097000
H	-0.713381000	2.534246000	-1.302640000
H	-1.197188000	0.985375000	-2.006675000
H	0.505354000	1.403524000	-1.885606000
C	-1.263599000	-1.501340000	-0.310667000
H	-1.072540000	-2.457427000	-0.790557000
C	-2.672838000	-0.998683000	-0.462466000
H	-3.358850000	-1.697503000	0.020976000
H	-2.877849000	-1.083072000	-1.535734000
C	-2.937817000	0.447022000	-0.006442000
C	-1.766429000	1.114498000	0.707508000
B	-0.466994000	-1.607252000	1.323044000
H	0.414077000	-2.413742000	1.435420000
H	-0.737236000	-0.876128000	2.231101000
H	-1.498711000	-2.267903000	1.176270000

H	-1.936060000	2.195672000	0.744903000
H	-1.715088000	0.772201000	1.743090000
H	-3.207172000	1.044207000	-0.880801000
H	-3.811611000	0.467359000	0.648990000

INT-1b'

SMD-PBE0-D3/def2-TZVP
***G*= -531.183034 a.u.**
G_{corr}= 0.269591 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.66473148302 a.u.**
***E*(DLPNO-CCSD(T))= -530.929049256081 a.u.**
SMD CDS free energy correction energy= -0.005273226939 a.u.

O	3.536247000	-0.739623000	-0.374695000
H	4.242541000	-0.265839000	0.076419000
C	2.306344000	-0.370098000	0.234668000
H	2.286557000	-0.730369000	1.276120000
C	2.111442000	1.137982000	0.244547000
H	2.886152000	1.601413000	0.866708000
H	2.261251000	1.510037000	-0.774404000
C	0.730978000	1.524957000	0.761872000
H	0.607142000	2.612966000	0.720021000
H	0.648362000	1.236231000	1.816637000
C	-0.408589000	0.843721000	-0.010532000
C	1.187172000	-1.067532000	-0.512425000
H	1.327650000	-2.149651000	-0.436430000
H	1.254197000	-0.808543000	-1.575403000
C	-0.150141000	-0.670177000	0.091039000
C	-0.400425000	1.362741000	-1.456508000
H	-0.444600000	2.456451000	-1.449462000
H	-1.258657000	1.009477000	-2.028439000
H	0.495918000	1.077722000	-2.007924000
C	-1.332557000	-1.567057000	-0.315737000
H	-1.032489000	-2.332219000	-1.032339000
C	-2.609071000	-0.837918000	-0.691194000
H	-3.444323000	-1.543660000	-0.714667000
H	-2.492326000	-0.471802000	-1.713078000
C	-2.939827000	0.308600000	0.259760000
C	-1.749069000	1.217329000	0.633315000
B	-0.519667000	-1.433763000	1.399124000
H	0.092776000	-2.429696000	1.671586000
H	-1.287021000	-0.988519000	2.202201000
H	-1.619256000	-2.228487000	0.590025000
H	-1.971205000	2.255887000	0.368966000
H	-1.623187000	1.202456000	1.718810000

H	-3.745922000	0.899692000	-0.182398000
H	-3.352742000	-0.123040000	1.176151000

TS2-1b'

SMD-PBE0-D3/def2-TZVP
***G*= -531.178523 a.u.** **ν_{min}= 118.8*i* cm^{-1}**
G_{corr}= 0.270308 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.659699147209 a.u.**
***E*(DLPNO-CCSD(T))= -530.924614400167 a.u.**
SMD CDS free energy correction energy= -0.005392747042 a.u.

O	3.532452000	-0.694374000	-0.463693000
H	4.244526000	-0.255789000	0.013234000
C	2.310098000	-0.372119000	0.187295000
H	2.306297000	-0.805300000	1.200181000
C	2.119141000	1.133179000	0.304651000
H	2.891086000	1.546133000	0.964640000
H	2.287129000	1.572295000	-0.684084000
C	0.735899000	1.508444000	0.829298000
H	0.615265000	2.597578000	0.804944000
H	0.648603000	1.203036000	1.879036000
C	-0.401375000	0.842527000	0.045987000
C	1.179984000	-1.020339000	-0.588904000
H	1.327930000	-2.104124000	-0.594682000
H	1.217553000	-0.683065000	-1.630863000
C	-0.137564000	-0.667111000	0.083263000
C	-0.421824000	1.373946000	-1.394414000
H	-0.773234000	2.410430000	-1.407677000
H	-1.086923000	0.787225000	-2.032837000
H	0.562291000	1.358502000	-1.861918000
C	-1.324908000	-1.562255000	-0.297356000
H	-1.072357000	-2.223617000	-1.126976000
C	-2.735895000	-0.963668000	-0.401916000
H	-3.396299000	-1.550764000	0.239643000
H	-3.085559000	-1.138903000	-1.421940000
C	-2.904447000	0.530298000	-0.069799000
C	-1.746086000	1.155528000	0.695530000
B	-0.428660000	-1.532655000	1.351676000
H	0.272688000	-2.486441000	1.555365000
H	-1.203306000	-1.194115000	2.199956000
H	-1.416932000	-2.369251000	0.537412000
H	-3.041934000	1.086968000	-0.999926000
H	-3.830121000	0.665700000	0.495695000
H	-1.883927000	2.242146000	0.728045000
H	-1.737226000	0.809044000	1.732114000

1b'

SMD-PBE0-D3/def2-TZVP
***G*= -531.188456 a.u.**
G_{corr}= 0.268701 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.674132399532 a.u.**
***E*(DLPNO-CCSD(T))= -530.9375681406 a.u.**
SMD CDS free energy correction energy= -0.005265258932 a.u.

O	3.515470000	-0.736700000	-0.351896000
H	4.202874000	-0.218995000	0.080744000
C	2.269661000	-0.369706000	0.211796000
H	2.215871000	-0.747597000	1.254113000
C	2.080961000	1.138505000	0.245987000
H	2.849783000	1.587489000	0.885696000
H	2.250542000	1.519380000	-0.766577000
C	0.695058000	1.531119000	0.747639000
H	0.572024000	2.617866000	0.682421000
H	0.612687000	1.274537000	1.809783000
C	-0.437012000	0.837736000	-0.020302000
C	1.170925000	-1.046750000	-0.583147000
H	1.326510000	-2.130007000	-0.565235000
H	1.226540000	-0.729375000	-1.630358000
C	-0.194057000	-0.698585000	0.032806000
C	-0.464490000	1.387981000	-1.451246000
H	-0.657193000	2.465136000	-1.422057000
H	-1.245653000	0.935427000	-2.062715000
H	0.479571000	1.242026000	-1.977207000
C	-1.334130000	-1.450531000	-0.674508000
H	-1.359995000	-1.176645000	-1.735706000
C	-2.673740000	-1.133588000	-0.016820000
H	-2.668820000	-1.526628000	1.011297000
H	-3.486861000	-1.650084000	-0.536501000
C	-2.944981000	0.365698000	0.025607000
C	-1.785614000	1.138246000	0.645960000
B	-0.137223000	-1.295146000	1.489413000
H	0.061883000	-2.476063000	1.585543000
H	-0.279904000	-0.676740000	2.504283000
H	-1.140847000	-2.527735000	-0.636906000
H	-3.129781000	0.724380000	-0.992796000
H	-3.862187000	0.563792000	0.589344000
H	-1.982470000	2.215616000	0.598206000
H	-1.717709000	0.882801000	1.710104000

Cartesian coordinates for the structures of the hydroboration mechanism for 1c' and 1d'

TS1-1c'

SMD-PBE0-D3/def2-TZVP
***G*= -531.170793 a.u.** **ν_{min}= 495.6*i* cm^{-1}**
G_{corr}= 0.267611 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.648292751364 a.u.**
***E*(DLPNO-CCSD(T))= -530.910632118026 a.u.**
SMD CDS free energy correction energy= -0.005271633337 a.u.

O	-3.503209000	-0.854137000	-0.164563000
H	-4.132351000	-0.429172000	-0.756759000
C	-2.208650000	-0.381125000	-0.495784000
H	-1.947979000	-0.691179000	-1.519858000
C	-2.083313000	1.123764000	-0.396204000
H	-2.758718000	1.607799000	-1.110124000
H	-2.386180000	1.441578000	0.606967000
C	-0.651092000	1.516229000	-0.699561000
H	-0.533424000	2.603792000	-0.686123000
H	-0.415623000	1.193032000	-1.720238000
C	0.423291000	0.926864000	0.248517000
C	-1.251316000	-1.031029000	0.483456000
H	-1.315171000	-2.117134000	0.399107000
H	-1.583508000	-0.761268000	1.489930000
C	0.184535000	-0.592316000	0.266550000
C	0.275697000	1.529767000	1.643707000
H	0.260222000	2.620906000	1.577462000
H	1.120009000	1.243148000	2.275895000
H	-0.641311000	1.210855000	2.144217000
C	1.056414000	-1.486862000	-0.405108000
H	0.590883000	-2.359781000	-0.853187000
C	2.312950000	-0.989482000	-1.077663000
H	2.089912000	-0.763381000	-2.128730000
H	3.062326000	-1.786084000	-1.080439000
C	2.855075000	0.256530000	-0.401240000
C	1.790266000	1.336438000	-0.357324000
B	1.210584000	-1.755562000	1.267392000
H	0.638341000	-0.838581000	1.868205000
H	0.635522000	-2.758683000	1.593893000
H	2.358636000	-1.580201000	1.565960000
H	3.724933000	0.631464000	-0.948287000
H	3.200425000	0.011485000	0.606280000
H	1.622566000	1.669077000	-1.386911000
H	2.160104000	2.210577000	0.186211000

INT1-1c'

SMD-PBE0-D3/def2-TZVP
***G*= -531.185478 a.u.**
G_{corr}= 0.269812 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.666939741106 a.u.**
***E*(DLPNO-CCSD(T))= -530.931762175211 a.u.**
SMD CDS free energy correction energy= -0.004989565895 a.u.

O	-3.428251000	-0.740786000	-0.194030000
H	-3.910883000	-0.490470000	-0.988651000
C	-2.056266000	-0.446111000	-0.408200000
H	-1.663160000	-1.080180000	-1.217965000
C	-1.833911000	1.009317000	-0.778949000
H	-2.352136000	1.232642000	-1.718311000
H	-2.292362000	1.634361000	-0.005462000
C	-0.349892000	1.321353000	-0.926371000
H	-0.211225000	2.388310000	-1.129124000
H	0.036814000	0.790232000	-1.799429000
C	0.484844000	0.956720000	0.312876000
C	-1.321841000	-0.785856000	0.872955000
H	-1.467645000	-1.840999000	1.118232000
H	-1.754781000	-0.196775000	1.687284000
C	0.165323000	-0.498387000	0.718507000
C	0.138883000	1.906507000	1.460140000
H	0.395947000	2.933735000	1.185872000
H	0.706959000	1.650138000	2.359543000
H	-0.920732000	1.889127000	1.719478000
C	0.904551000	-1.591196000	-0.084235000
H	0.200977000	-2.363964000	-0.391035000
C	1.744461000	-1.123749000	-1.253772000
H	1.086875000	-0.921874000	-2.105857000
H	2.392456000	-1.945466000	-1.574372000
C	2.601326000	0.108879000	-0.963145000
C	1.981770000	1.107348000	0.028657000
B	1.471416000	-1.757216000	1.351700000
H	0.570890000	-0.547855000	1.804743000
H	0.951403000	-2.527370000	2.111380000
H	2.502189000	-1.230597000	1.663811000
H	2.822926000	0.607104000	-1.910791000
H	3.566184000	-0.212197000	-0.561525000
H	2.154347000	2.132466000	-0.314298000
H	2.498400000	1.023046000	0.989433000

TS2-1c'

SMD-PBE0-D3/def2-TZVP
***G*= -531.179726 a.u.** **ν_{min}= 166.2*i* cm^{-1}**

G_{corr}= 0.268364 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.665143422001 a.u.**
***E*(DLPNO-CCSD(T))= -530.92853379212 a.u.**
SMD CDS free energy correction energy= -0.00497362988 a.u.

O	3.423685000	0.848618000	0.018132000
H	3.985477000	0.671411000	-0.743360000
C	2.086796000	0.525164000	-0.345349000
H	1.770407000	1.182025000	-1.168297000
C	1.956439000	-0.915555000	-0.806535000
H	2.522466000	-1.055504000	-1.734879000
H	2.419531000	-1.561909000	-0.053919000
C	0.498361000	-1.299450000	-1.022732000
H	0.430085000	-2.350110000	-1.325086000
H	0.089743000	-0.713454000	-1.854373000
C	-0.382032000	-1.076141000	0.215705000
C	1.218453000	0.793055000	0.869129000
H	1.291980000	1.853765000	1.130243000
H	1.640678000	0.236017000	1.710638000
C	-0.249875000	0.401953000	0.658532000
C	0.070183000	-1.994361000	1.353298000
H	-0.034664000	-3.041735000	1.052729000
H	-0.555493000	-1.838503000	2.237545000
H	1.107945000	-1.841199000	1.652378000
C	-0.940101000	1.417133000	-0.302111000
H	-0.242048000	1.663487000	-1.105345000
C	-2.246416000	0.876934000	-0.927542000
H	-2.044285000	0.506816000	-1.939534000
H	-2.983288000	1.680211000	-1.044126000
C	-2.815049000	-0.255173000	-0.097604000
C	-1.857249000	-1.435108000	-0.115031000
B	-1.271364000	2.674721000	0.556086000
H	-0.742726000	0.474223000	1.637029000
H	-0.666017000	3.708492000	0.488680000
H	-2.179818000	2.603732000	1.340437000
H	-1.893939000	-1.891805000	-1.110954000
H	-2.211257000	-2.201274000	0.581192000
H	-3.790152000	-0.567127000	-0.484308000
H	-2.984349000	0.089182000	0.929261000

INT2-1c'

SMD-PBE0-D3/def2-TZVP
***G*= -531.188312 a.u.**
G_{corr}= 0.269214 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.670952789949 a.u.**
***E*(DLPNO-CCSD(T))= -530.935100731188 a.u.**
SMD CDS free energy correction energy= -0.005066058760 a.u.

O	3.406809000	1.121541000	0.114264000
H	4.026169000	0.949848000	-0.602508000
C	2.130411000	0.644238000	-0.292243000
H	1.788870000	1.219125000	-1.166864000
C	2.159621000	-0.826423000	-0.665167000
H	2.833680000	-0.981247000	-1.515745000
H	2.571181000	-1.392248000	0.177815000
C	0.759526000	-1.305509000	-1.016086000
H	0.775942000	-2.363612000	-1.299891000
H	0.416416000	-0.756708000	-1.901657000
C	-0.265269000	-1.103047000	0.108249000
C	1.178511000	0.873068000	0.862257000
H	1.144197000	1.940501000	1.102859000
H	1.598941000	0.364597000	1.736220000
C	-0.240980000	0.368896000	0.593817000
C	0.044485000	-2.022226000	1.289273000
H	0.100195000	-3.065463000	0.963151000
H	-0.744863000	-1.949987000	2.044385000
H	0.989050000	-1.775950000	1.778628000
C	-0.996707000	1.305798000	-0.335404000
H	-0.514768000	1.423902000	-1.303844000
C	-2.483966000	0.871330000	-0.535210000
H	-2.745861000	0.927769000	-1.591781000
H	-3.193952000	1.601548000	-0.047639000
C	-2.754987000	-0.506879000	0.049271000
C	-1.671930000	-1.458207000	-0.432634000
B	-1.718433000	2.530638000	0.247444000
H	-0.761257000	0.394347000	1.557952000
H	-2.057762000	3.444129000	-0.451835000
H	-1.938236000	2.577347000	1.427464000
H	-3.742659000	-0.850682000	-0.270034000
H	-2.775757000	-0.463509000	1.141870000
H	-1.664126000	-1.427547000	-1.528524000
H	-1.920000000	-2.487922000	-0.158094000

TS3-1c'

SMD-PBE0-D3/def2-TZVP
***G*= -531.174380 a.u.** **ν_{min}= 214.2*i* cm^{-1}**
G_{corr}= 0.268354 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.659401443679 a.u.**

***E*(DLPNO-CCSD(T))= -530.922687791317 a.u.**
SMD CDS free energy correction energy= -0.005067652362 a.u.

O	3.433524000	0.876615000	0.023867000
H	4.011027000	0.653694000	-0.713523000
C	2.113672000	0.479050000	-0.324208000
H	1.763733000	1.081351000	-1.177686000
C	2.032176000	-0.986593000	-0.700939000
H	2.653493000	-1.183850000	-1.582560000
H	2.444489000	-1.580757000	0.121929000
C	0.589702000	-1.370654000	-0.988318000
H	0.526536000	-2.431224000	-1.254490000
H	0.252581000	-0.816181000	-1.872268000
C	-0.392898000	-1.094771000	0.166964000
C	1.228903000	0.747767000	0.871376000
H	1.290219000	1.807577000	1.141570000
H	1.640142000	0.187810000	1.718019000
C	-0.236677000	0.367456000	0.641354000
C	-0.096433000	-2.039829000	1.332328000
H	-0.169128000	-3.083376000	1.010170000
H	-0.819992000	-1.888016000	2.139197000
H	0.901088000	-1.893060000	1.751704000
C	-0.963970000	1.340076000	-0.287798000
H	-0.735106000	1.130888000	-1.338810000
C	-2.480673000	1.132869000	-0.073615000
H	-3.071512000	1.815071000	-0.693213000
H	-2.709330000	1.382891000	0.968753000
C	-2.918989000	-0.312760000	-0.358513000
C	-1.825397000	-1.403037000	-0.364218000
B	-0.849006000	2.846572000	0.052142000
H	-0.735388000	0.454012000	1.616584000
H	-0.984518000	3.689044000	-0.791076000
H	-0.745799000	3.199458000	1.195481000
H	-3.409934000	-0.333081000	-1.334574000
H	-3.693744000	-0.577303000	0.365764000
H	-1.717694000	-1.752345000	-1.394272000
H	-2.210820000	-2.265832000	0.185183000

1c’

SMD-PBE0-D3/def2-TZVP
***G*= -531.193386 a.u.**
G_{corr}= 0.269539 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.677948321062 a.u.**
***E*(DLPNO-CCSD(T))= -530.942390983875 a.u.**
SMD CDS free energy correction energy= -0.005096337186 a.u.

O	-2.953237000	-0.928244000	0.684470000
H	-2.929589000	-1.886646000	0.769626000
B	2.300847000	-1.126289000	1.494121000
H	3.467195000	-0.836893000	1.453747000
C	-2.327539000	-0.584502000	-0.549352000
H	-2.956784000	-0.932531000	-1.381348000
C	-2.229639000	0.927696000	-0.601672000
H	-1.928759000	1.214763000	-1.613785000
H	-3.221321000	1.358337000	-0.433392000
C	-1.246759000	1.465458000	0.427756000
H	-1.646774000	1.263755000	1.427000000
H	-1.168095000	2.554719000	0.334884000
C	0.156930000	0.849786000	0.339723000
C	-0.948770000	-1.213780000	-0.678856000
H	-0.590935000	-1.028648000	-1.696001000
H	-1.034014000	-2.303231000	-0.577830000
C	0.043937000	-0.690112000	0.356233000
H	-0.347391000	-0.966658000	1.342645000
C	0.935749000	1.307456000	1.567163000
H	1.060372000	2.395181000	1.571674000
H	1.961207000	0.902323000	1.610430000
H	0.424954000	1.018157000	2.488407000
C	1.446788000	-1.311535000	0.204660000
H	1.310406000	-2.409699000	0.181100000
C	2.129634000	-0.862111000	-1.089201000
H	1.572686000	-1.221019000	-1.962733000
H	3.127358000	-1.307576000	-1.154883000
C	2.231264000	0.656138000	-1.149319000
C	0.872818000	1.315464000	-0.937655000
H	1.824853000	-1.393356000	2.563192000
H	2.646231000	0.970677000	-2.112225000
H	2.937744000	1.000618000	-0.385669000
H	0.242746000	1.100005000	-1.806569000
H	0.983089000	2.405381000	-0.901507000

TS1-1d'

SMD-PBE0-D3/def2-TZVP
***G*= -531.169504 a.u.** □**ν_{min}= 418.6*i* cm^{-1}**
***G*$_{corr}$= 0.267075 a.u.**

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.648014998205 a.u.**
***E*(DLPNO-CCSD(T))= -530.910038281856 a.u.**
SMD CDS free energy correction energy= -0.005051716348 a.u.

O	-3.488059000	-0.740226000	-0.133535000

H	-4.039964000	-0.384478000	-0.837808000
C	-2.136606000	-0.440110000	-0.444515000
H	-1.828383000	-1.001822000	-1.341833000
C	-1.923642000	1.039558000	-0.703646000
H	-2.489477000	1.341955000	-1.592403000
H	-2.337950000	1.598959000	0.141211000
C	-0.449868000	1.369382000	-0.896963000
H	-0.327362000	2.448697000	-1.033590000
H	-0.091461000	0.896346000	-1.818576000
C	0.452241000	0.913853000	0.272663000
C	-1.284042000	-0.918454000	0.718319000
H	-1.402088000	-1.997604000	0.836527000
H	-1.640029000	-0.449794000	1.639494000
C	0.167210000	-0.580416000	0.452712000
C	0.097683000	1.707305000	1.529274000
H	0.313862000	2.767922000	1.368228000
H	0.695684000	1.365296000	2.377067000
H	-0.953792000	1.624600000	1.807008000
C	0.915557000	-1.500657000	-0.287959000
H	0.470939000	-2.473563000	-0.477577000
C	2.002172000	-1.068311000	-1.217135000
H	1.499104000	-0.795451000	-2.153866000
H	2.666838000	-1.904300000	-1.447924000
C	2.790462000	0.104545000	-0.665103000
C	1.927066000	1.230197000	-0.077723000
B	1.250470000	-1.442924000	1.523086000
H	0.563776000	-2.124979000	2.233327000
H	1.955063000	-0.597150000	1.998634000
H	2.020355000	-2.207593000	0.942192000
H	1.914071000	2.082240000	-0.763945000
H	2.422108000	1.589221000	0.827884000
H	3.443148000	0.501618000	-1.446131000
H	3.448278000	-0.285046000	0.115383000

INT1-1d'

SMD-PBE0-D3/def2-TZVP
***G*= -531.175142 a.u.**
G_{corr}= 0.269324 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.666592309439 a.u.**
***E*(DLPNO-CCSD(T))= -530.9307594154 a.u.**
SMD CDS free energy correction energy= -0.005156894039 a.u.

O	-3.442987000	-0.703656000	-0.174774000
H	-3.935164000	-0.423869000	-0.953523000
C	-2.068189000	-0.427118000	-0.406205000

H	-1.695053000	-1.074565000	-1.217166000
C	-1.834174000	1.019365000	-0.795728000
H	-2.367272000	1.246053000	-1.726741000
H	-2.267251000	1.657058000	-0.017491000
C	-0.348874000	1.303818000	-0.970042000
H	-0.198354000	2.368346000	-1.180957000
H	0.009121000	0.768647000	-1.853898000
C	0.512860000	0.921390000	0.250434000
C	-1.312082000	-0.755360000	0.863019000
H	-1.490762000	-1.799034000	1.137937000
H	-1.723643000	-0.143402000	1.672882000
C	0.184523000	-0.509760000	0.723563000
C	0.216927000	1.901261000	1.388384000
H	0.501563000	2.917572000	1.096831000
H	0.789347000	1.633267000	2.280813000
H	-0.838929000	1.921657000	1.664267000
C	0.880767000	-1.639493000	-0.078521000
H	0.172492000	-2.428466000	-0.330368000
C	1.741080000	-1.204919000	-1.247641000
H	1.074932000	-0.912712000	-2.063027000
H	2.323902000	-2.054655000	-1.614917000
C	2.674349000	-0.065031000	-0.873129000
C	2.000618000	1.089911000	-0.108643000
B	1.109020000	-1.186390000	1.769626000
H	0.672793000	-2.062763000	2.464111000
H	2.208628000	-0.761660000	1.983676000
H	1.599299000	-2.201182000	0.626477000
H	3.159129000	0.308076000	-1.778899000
H	3.474397000	-0.479671000	-0.252122000
H	2.553497000	1.258448000	0.818869000
H	2.089285000	2.019681000	-0.679637000

TS2-1d'

SMD-PBE0-D3/def2-TZVP
***G*= -531.176216 a.u.** **ν_{min}= 92.5*i* cm^{-1}**
***G*$_{corr}$= 0.269590 a.u.**

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.662220223378 a.u.**
***E*(DLPNO-CCSD(T))= -530.926646954933 a.u.**
SMD CDS free energy correction energy= -0.005163268444 a.u.

O	-3.471823000	-0.638919000	0.056113000
H	-4.034586000	-0.439246000	-0.699214000
C	-2.119518000	-0.475614000	-0.356702000
H	-1.905772000	-1.193874000	-1.159915000
C	-1.854133000	0.922299000	-0.885423000

H	-2.416397000	1.070785000	-1.814816000
H	-2.245654000	1.645433000	-0.163234000
C	-0.368958000	1.156741000	-1.129792000
H	-0.208760000	2.183937000	-1.475398000
H	-0.028025000	0.504994000	-1.941680000
C	0.491103000	0.907928000	0.121030000
C	-1.252891000	-0.805339000	0.848652000
H	-1.406913000	-1.855632000	1.116635000
H	-1.623077000	-0.212048000	1.691569000
C	0.253446000	-0.546652000	0.614141000
C	0.102913000	1.932656000	1.190552000
H	0.278708000	2.945218000	0.812749000
H	0.708757000	1.809286000	2.090762000
H	-0.945050000	1.872390000	1.487370000
C	0.772756000	-1.600362000	-0.416392000
H	-0.000271000	-1.806696000	-1.159268000
C	2.068562000	-1.196537000	-1.125168000
H	1.842732000	-0.775503000	-2.111127000
H	2.691888000	-2.077877000	-1.299878000
C	2.814608000	-0.154406000	-0.319057000
C	1.993753000	1.123907000	-0.211488000
B	0.980217000	-0.887876000	1.959230000
H	0.812338000	-1.982463000	2.424454000
H	1.686234000	-0.129270000	2.560007000
H	0.927209000	-2.547276000	0.113057000
H	2.445087000	1.775228000	0.542806000
H	2.066484000	1.665885000	-1.161459000
H	3.790071000	0.067340000	-0.762816000
H	3.028653000	-0.557606000	0.682213000

INT2-1d'

SMD-PBE0-D3/def2-TZVP
***G*= -531.171491 a.u.**
G_{corr}= 0.268339 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.66757290764 a.u.**
***E*(DLPNO-CCSD(T))= -530.930603621471 a.u.**
SMD CDS free energy correction energy= -0.005308286169 a.u.

O	-3.466317000	-0.839702000	0.060878000
H	-4.093371000	-0.499456000	-0.585892000
C	-2.161528000	-0.472678000	-0.366835000
H	-1.926824000	-0.988983000	-1.309483000
C	-2.025777000	1.021384000	-0.582047000
H	-2.715839000	1.345134000	-1.370035000
H	-2.323848000	1.535921000	0.338184000

C	-0.595681000	1.365840000	-0.965658000
H	-0.495112000	2.442628000	-1.138961000
H	-0.365948000	0.882476000	-1.921670000
C	0.441937000	0.933712000	0.081819000
C	-1.200706000	-0.944530000	0.708891000
H	-1.305395000	-2.028387000	0.826218000
H	-1.529433000	-0.489678000	1.651353000
C	0.276618000	-0.584670000	0.409269000
C	0.294815000	1.811989000	1.325288000
H	0.234594000	2.864047000	1.029936000
H	1.153081000	1.705426000	1.991319000
H	-0.599780000	1.575854000	1.905968000
C	0.839150000	-1.408943000	-0.759635000
H	0.403902000	-1.077631000	-1.706741000
C	2.369890000	-1.269686000	-0.809462000
H	2.711180000	-1.253337000	-1.849212000
H	2.851729000	-2.128350000	-0.333784000
C	2.806161000	0.020259000	-0.119928000
C	1.863855000	1.148290000	-0.501100000
B	0.942824000	-1.062001000	1.741018000
H	1.338086000	-2.193205000	1.821559000
H	0.962859000	-0.393769000	2.732870000
H	0.554316000	-2.458501000	-0.641774000
H	3.843750000	0.262188000	-0.367561000
H	2.800645000	-0.108321000	0.979014000
H	1.813379000	1.191168000	-1.595411000
H	2.252046000	2.116606000	-0.171625000

TS3-1d'

SMD-PBE0-D3/def2-TZVP
***G*= -531.168327 a.u.** □**ν_{min}= 220.7*i* cm^{-1}**
***G*$_{corr}$= 0.269212 a.u.**

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.653995699976 a.u.**
***E*(DLPNO-CCSD(T))= -530.917918537023 a.u.**
SMD CDS free energy correction energy= -0.005289162952 a.u.

O	-3.469082000	-0.770883000	-0.144372000
H	-4.042421000	-0.403177000	-0.825280000
C	-2.131035000	-0.424204000	-0.473085000
H	-1.838225000	-0.933469000	-1.402775000
C	-1.948594000	1.067360000	-0.650891000
H	-2.563376000	1.416870000	-1.488679000
H	-2.314872000	1.573791000	0.248580000
C	-0.486954000	1.392702000	-0.907488000
H	-0.360141000	2.473220000	-1.030840000

H	-0.188509000	0.943389000	-1.860945000
C	0.473377000	0.914572000	0.201998000
C	-1.258259000	-0.936120000	0.659088000
H	-1.394967000	-2.019615000	0.737919000
H	-1.646830000	-0.494084000	1.585277000
C	0.255262000	-0.603107000	0.455211000
C	0.215792000	1.753799000	1.455384000
H	0.261958000	2.817937000	1.202873000
H	0.969469000	1.563748000	2.221127000
H	-0.762560000	1.563501000	1.902427000
C	0.842257000	-1.412594000	-0.702409000
H	0.503166000	-1.029211000	-1.670555000
C	2.356276000	-1.370645000	-0.621306000
H	2.801615000	-1.906847000	-1.464505000
H	2.653646000	-1.924145000	0.277222000
C	2.921163000	0.057759000	-0.552357000
C	1.926080000	1.211764000	-0.283823000
B	0.661675000	-1.204046000	1.832645000
H	0.845687000	-2.387996000	1.906725000
H	0.662140000	-0.572816000	2.848318000
H	0.497411000	-2.450103000	-0.638529000
H	3.433945000	0.280502000	-1.491506000
H	3.701663000	0.081325000	0.212270000
H	1.842450000	1.801970000	-1.200529000
H	2.390844000	1.884784000	0.441223000

1d'

SMD-PBE0-D3/def2-TZVP
***G*= -531.187408 a.u.**
***G*$_{corr}$= 0.269136 a.u.**

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.673226319003 a.u.**
***E*(DLPNO-CCSD(T))= -530.937195863356 a.u.**
SMD CDS free energy correction energy= -0.005166455647 a.u.

O	-3.444439000	-0.648528000	-0.239939000
H	-3.954202000	-0.320671000	-0.988342000
C	-2.069948000	-0.411617000	-0.516315000
H	-1.768929000	-1.007273000	-1.389115000
C	-1.793117000	1.051447000	-0.803680000
H	-2.320347000	1.346421000	-1.718455000
H	-2.213444000	1.648846000	0.012015000
C	-0.300286000	1.312552000	-0.954120000
H	-0.124891000	2.378636000	-1.134175000
H	0.061270000	0.789856000	-1.844108000
C	0.505021000	0.878135000	0.281232000

C	-1.294766000	-0.898452000	0.698593000
H	-1.480893000	-1.970670000	0.821459000
H	-1.719888000	-0.397642000	1.576361000
C	0.235830000	-0.627840000	0.575937000
C	0.125684000	1.791063000	1.449561000
H	0.204050000	2.837031000	1.136172000
H	0.796319000	1.652039000	2.298803000
H	-0.893088000	1.631967000	1.806947000
C	0.833055000	-1.526291000	-0.520335000
H	0.359590000	-1.340234000	-1.489969000
C	2.329976000	-1.307969000	-0.664361000
H	2.742160000	-1.973023000	-1.429916000
H	2.826363000	-1.567835000	0.281524000
C	2.621296000	0.144881000	-1.002793000
C	2.009955000	1.072140000	0.035677000
B	0.625088000	-1.149237000	1.992277000
H	0.819061000	-2.325043000	2.139910000
H	0.619619000	-0.457745000	2.968326000
H	0.621810000	-2.571058000	-0.269759000
H	2.221459000	0.371304000	-1.997935000
H	3.700702000	0.319411000	-1.057759000
H	2.193314000	2.119490000	-0.232085000
H	2.523834000	0.902310000	0.991847000

Cartesian coordinates for the structures of the retrohydroboration mechanism for 1e'

TS1-1e'

SMD-PBE0-D3/def2-TZVP
***G*= -531.172106 a.u.** □**ν_{min}= 458.4*i* cm^{-1}**
***G*$_{corr}$= 0.267089 a.u.**

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.650356756252 a.u.**
***E*(DLPNO-CCSD(T))= -530.912433879938 a.u.**
SMD CDS free energy correction energy= -0.005011876314 a.u.

O	3.540671000	1.126061000	0.263739000
H	4.298871000	0.736747000	-0.184118000
C	2.364489000	0.590862000	-0.326474000
H	2.303851000	0.909283000	-1.379852000
C	2.355781000	-0.929939000	-0.283408000
H	3.176498000	-1.314641000	-0.899690000
H	2.563815000	-1.241529000	0.745143000
C	1.030778000	-1.512232000	-0.765499000
H	1.042234000	-2.602594000	-0.660559000
H	0.911698000	-1.301861000	-1.835662000
C	-0.176412000	-0.932826000	-0.022530000

C	1.172066000	1.179005000	0.402196000
H	1.178500000	2.267302000	0.285245000
H	1.259767000	0.968845000	1.473587000
C	-0.114492000	0.600136000	-0.167171000
C	-0.163226000	-1.388680000	1.436962000
H	-0.360125000	-2.463806000	1.493790000
H	-0.921586000	-0.879876000	2.036143000
H	0.797642000	-1.205501000	1.918939000
C	-1.354933000	1.269593000	0.401428000
H	-1.186495000	2.053366000	1.131663000
C	-2.571376000	0.583333000	0.471952000
H	-3.308239000	0.922021000	1.192557000
C	-2.709512000	-0.843437000	0.021327000
C	-1.476511000	-1.380116000	-0.695611000
H	-0.085865000	0.787017000	-1.245638000
B	-2.477159000	1.939370000	-0.772157000
H	-1.967663000	1.759149000	-1.842553000
H	-2.750454000	3.050294000	-0.404102000
H	-3.545855000	1.335077000	-0.807660000
H	-2.880950000	-1.415827000	0.940149000
H	-3.607961000	-0.977465000	-0.584505000
H	-1.528437000	-2.473459000	-0.726613000
H	-1.468739000	-1.032070000	-1.734417000

INT-1e'

SMD-PBE0-D3/def2-TZVP
***G*= -531.175142 a.u.**
G_{corr}= 0.267256 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.655777127806 a.u.**
***E*(DLPNO-CCSD(T))= -530.91806587233 a.u.**
SMD CDS free energy correction energy= -0.004967255475 a.u.

O	3.546753000	1.111737000	0.246535000
H	4.295850000	0.724116000	-0.217855000
C	2.359119000	0.588149000	-0.329063000
H	2.278041000	0.921665000	-1.376475000
C	2.343064000	-0.932598000	-0.307100000
H	3.156182000	-1.312529000	-0.936069000
H	2.556176000	-1.261333000	0.715106000
C	1.010815000	-1.496774000	-0.789281000
H	1.018015000	-2.589354000	-0.714022000
H	0.881107000	-1.256478000	-1.851859000
C	-0.187601000	-0.935691000	-0.018551000
C	1.184496000	1.169035000	0.432886000
H	1.190222000	2.258958000	0.333014000

H	1.294327000	0.940453000	1.498157000
C	-0.116142000	0.602511000	-0.116645000
C	-0.164856000	-1.430619000	1.427485000
H	-0.315265000	-2.514206000	1.450573000
H	-0.952338000	-0.973374000	2.030839000
H	0.782718000	-1.219707000	1.924719000
C	-1.335729000	1.240482000	0.498631000
H	-1.186678000	2.097453000	1.146793000
C	-2.549413000	0.600184000	0.512687000
H	-3.317205000	0.968112000	1.182992000
C	-2.725598000	-0.804046000	0.013204000
C	-1.494312000	-1.360396000	-0.692807000
H	-0.131744000	0.827827000	-1.189487000
B	-2.515479000	1.890139000	-0.851375000
H	-2.537330000	1.177756000	-1.821492000
H	-1.626750000	2.706544000	-0.954725000
H	-3.526481000	2.464591000	-0.537508000
H	-2.956471000	-1.407563000	0.899587000
H	-3.606321000	-0.873837000	-0.629952000
H	-1.559506000	-2.452907000	-0.725538000
H	-1.476248000	-1.012204000	-1.730873000

3

SMD-PBE0-D3/def2-TZVP
***G*= -504.604953 a.u.**
G_{corr}= 0.236849 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -504.123752253524 a.u.**
***E*(DLPNO-CCSD(T))= -504.354325651322 a.u.**
SMD CDS free energy correction energy= -0.006275602202 a.u.

O	3.472815000	0.786081000	0.193226000
H	4.172460000	0.200713000	-0.114754000
C	2.248236000	0.333424000	-0.367329000
H	2.281699000	0.447761000	-1.463372000
C	1.990683000	-1.131714000	-0.046991000
H	2.764189000	-1.746966000	-0.521193000
H	2.100646000	-1.267604000	1.033707000
C	0.609789000	-1.588933000	-0.507865000
H	0.441390000	-2.628307000	-0.205111000
H	0.570192000	-1.571564000	-1.604394000
C	-0.514789000	-0.701488000	0.031952000
C	1.139229000	1.225550000	0.155334000
H	1.327390000	2.257204000	-0.158967000
H	1.149344000	1.216486000	1.250220000
C	-0.202734000	0.749124000	-0.385327000

C	-0.624878000	-0.862067000	1.548958000
H	-0.950861000	-1.878843000	1.789623000
H	-1.347510000	-0.166194000	1.979521000
H	0.325764000	-0.694722000	2.056447000
C	-1.347937000	1.669732000	-0.086830000
H	-1.123050000	2.728544000	0.025953000
C	-2.604820000	1.245510000	0.015524000
H	-3.397511000	1.958655000	0.229691000
C	-2.998544000	-0.191476000	-0.124341000
C	-1.852017000	-1.073439000	-0.612841000
H	-0.093458000	0.726861000	-1.481938000
H	-3.374749000	-0.548853000	0.843535000
H	-3.850717000	-0.273769000	-0.808363000
H	-2.080371000	-2.127026000	-0.418703000
H	-1.750684000	-0.966356000	-1.699173000

TS2-1e'

SMD-PBE0-D3/def2-TZVP
***G*= -531.167100 a.u.** **ν_{min}= 521.4*i* cm^{-1}**
***G*$_{corr}$= 0.267673 a.u.**

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.644894449696 a.u.**
***E*(DLPNO-CCSD(T))= -530.907463144502 a.u.**
SMD CDS free energy correction energy= -0.005104305193 a.u.

O	3.506795000	1.119378000	0.143785000
H	4.294698000	0.601437000	-0.051008000
C	2.388772000	0.432972000	-0.400917000
H	2.474767000	0.406296000	-1.499695000
C	2.306350000	-1.000246000	0.104590000
H	3.177265000	-1.560792000	-0.254492000
H	2.372025000	-0.981849000	1.197145000
C	1.022664000	-1.694093000	-0.340603000
H	0.983169000	-2.706803000	0.074535000
H	1.026343000	-1.801032000	-1.432630000
C	-0.232767000	-0.916167000	0.074966000
C	1.142200000	1.224836000	-0.054169000
H	1.202895000	2.214513000	-0.518034000
H	1.094845000	1.381152000	1.027407000
C	-0.089622000	0.486107000	-0.554482000
C	-0.346151000	-0.945786000	1.601101000
H	-0.287099000	-1.984941000	1.941188000
H	-1.286916000	-0.534690000	1.961706000
H	0.453029000	-0.392885000	2.095475000
C	-1.351457000	1.315763000	-0.587234000

H	-1.295221000	2.180194000	-1.240754000
C	-2.609985000	0.710758000	-0.440121000
H	-3.463296000	1.207432000	-0.888239000
C	-2.756812000	-0.777949000	-0.205412000
C	-1.481930000	-1.551789000	-0.534046000
H	0.101779000	0.279483000	-1.620110000
B	-2.078859000	1.887516000	0.867400000
H	-2.432318000	3.023478000	0.697915000
H	-1.329113000	1.603652000	1.755211000
H	-3.102245000	1.246964000	1.125678000
H	-3.078591000	-0.978790000	0.817652000
H	-3.572016000	-1.123878000	-0.846864000
H	-1.354560000	-1.592234000	-1.622463000
H	-1.587071000	-2.585739000	-0.188943000

TS1-1f'

SMD-PBE0-D3/def2-TZVP
***G*= -531.169777 a.u.** **ν_{min}= 469.4*i* cm^{-1}**
G_{corr}= 0.267510 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.644424531816 a.u.**
***E*(DLPNO-CCSD(T))= -530.906986399557 a.u.**
SMD CDS free energy correction energy= -0.004948132259 a.u.

O	-3.515795000	-1.144244000	0.137557000
H	-4.305979000	-0.633827000	-0.067981000
C	-2.397781000	-0.450694000	-0.395461000
H	-2.468052000	-0.429427000	-1.495349000
C	-2.328991000	0.984340000	0.106385000
H	-3.200219000	1.537396000	-0.262523000
H	-2.405159000	0.968886000	1.198111000
C	-1.046696000	1.686451000	-0.330700000
H	-1.013488000	2.697238000	0.089053000
H	-1.048121000	1.799508000	-1.422115000
C	0.215280000	0.917080000	0.081279000
C	-1.151831000	-1.234866000	-0.027875000
H	-1.201186000	-2.229658000	-0.481514000
H	-1.114236000	-1.375230000	1.056615000
C	0.077483000	-0.490676000	-0.523475000
C	0.336077000	0.930624000	1.605346000
H	0.386596000	1.967288000	1.952871000
H	1.229040000	0.417800000	1.957776000
H	-0.517095000	0.462390000	2.097035000
C	1.343598000	-1.291287000	-0.573102000
H	1.252238000	-2.237897000	-1.097955000
C	2.610220000	-0.702875000	-0.488444000

H	3.408626000	-1.169908000	-1.052472000
C	2.742740000	0.789692000	-0.237799000
C	1.457187000	1.556516000	-0.542435000
H	-0.088949000	-0.318938000	-1.601533000
B	2.366780000	-1.769950000	0.874921000
H	2.583994000	-1.086809000	1.834543000
H	2.997852000	-2.777631000	0.698895000
H	1.180494000	-2.093585000	0.996767000
H	3.064202000	0.982885000	0.787817000
H	3.543224000	1.169018000	-0.878807000
H	1.310930000	1.596901000	-1.628861000
H	1.554035000	2.591474000	-0.197744000

1e'

SMD-PBE0-D3/def2-TZVP
***G*= -531.195332 a.u.**
G_{corr}= 0.269089 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.676784664189 a.u.**
***E*(DLPNO-CCSD(T))= -530.940568820199 a.u.**
SMD CDS free energy correction energy= -0.005304843990 a.u.

O	-3.562793000	-0.949006000	-0.123043000
H	-4.302653000	-0.362925000	-0.312960000
C	-2.368258000	-0.277874000	-0.501241000
H	-2.365781000	-0.119076000	-1.592111000
C	-2.234801000	1.072614000	0.181074000
H	-3.061069000	1.724462000	-0.125775000
H	-2.333159000	0.923065000	1.261590000
C	-0.904287000	1.729730000	-0.160139000
H	-0.812541000	2.690031000	0.358798000
H	-0.886168000	1.953866000	-1.233929000
C	0.312450000	0.852758000	0.161864000
C	-1.202850000	-1.175972000	-0.144045000
H	-1.303452000	-2.130179000	-0.671728000
H	-1.255035000	-1.398443000	0.925479000
C	0.123628000	-0.523396000	-0.510085000
C	0.466793000	0.713601000	1.673442000
H	0.652312000	1.689980000	2.131852000
H	1.335939000	0.096314000	1.956116000
H	-0.410793000	0.279011000	2.151814000
C	1.359422000	-1.401355000	-0.249827000
H	1.174340000	-2.375144000	-0.742329000
C	2.588794000	-0.748018000	-0.885659000
H	2.442400000	-0.672192000	-1.971479000
C	2.819522000	0.645833000	-0.316986000

C	1.567989000	1.507582000	-0.430518000
H	0.092573000	-0.328057000	-1.593101000
B	1.547344000	-1.829307000	1.238051000
H	2.635155000	-1.830577000	1.750427000
H	0.639796000	-2.290210000	1.869671000
H	3.475328000	-1.370260000	-0.727543000
H	3.650036000	1.135101000	-0.835816000
H	3.123841000	0.561760000	0.732494000
H	1.373386000	1.708289000	-1.491904000
H	1.730752000	2.480746000	0.047244000

1f'

SMD-PBE0-D3/def2-TZVP
***G*= -531.194565 a.u.**
G_{corr}= 0.267959 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.675736318344 a.u.**
***E*(DLPNO-CCSD(T))= -530.938662725212 a.u.**
SMD CDS free energy correction energy= -0.005032593132 a.u.

O	-3.573218000	-1.306249000	0.124552000
H	-4.357575000	-0.870280000	-0.224461000
C	-2.434720000	-0.628169000	-0.389301000
H	-2.393840000	-0.757248000	-1.483276000
C	-2.473941000	0.860224000	-0.085288000
H	-3.335915000	1.314058000	-0.588197000
H	-2.633668000	0.987384000	0.990383000
C	-1.190866000	1.552326000	-0.528911000
H	-1.229825000	2.616657000	-0.272103000
H	-1.116194000	1.498097000	-1.622485000
C	0.072282000	0.923753000	0.071851000
C	-1.200827000	-1.276015000	0.204841000
H	-1.175835000	-2.332923000	-0.079656000
H	-1.271159000	-1.241426000	1.297593000
C	0.062676000	-0.577674000	-0.280199000
C	0.101375000	1.177673000	1.580049000
H	0.110577000	2.255267000	1.771526000
H	0.986785000	0.755174000	2.057629000
H	-0.768376000	0.762961000	2.091979000
C	1.333169000	-1.294084000	0.168471000
H	1.269116000	-2.347054000	-0.125231000
C	2.589137000	-0.636050000	-0.464615000
H	2.500099000	-0.796634000	-1.547634000
C	2.611073000	0.863570000	-0.175891000
C	1.311923000	1.550746000	-0.575448000
H	0.054031000	-0.625083000	-1.379650000

B	3.743211000	-1.475875000	0.138617000
H	4.304817000	-1.119090000	1.139013000
H	4.030085000	-2.546052000	-0.322628000
H	1.398134000	-1.278646000	1.263748000
H	2.810024000	1.021801000	0.889810000
H	3.447281000	1.327711000	-0.709085000
H	1.198840000	1.489676000	-1.665671000
H	1.354598000	2.617216000	-0.324465000

π-complex intermediate formed from decalin model + BH_3 by α-face

SMD-PBE0-D3/def2-TZVP
***G*= -531.176421 a.u.**
G_{corr}= 0.267422 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.656545517705 a.u.**
***E*(DLPNO-CCSD(T))= -530.918882335728 a.u.**
SMD CDS free energy correction energy= -0.005085181977 a.u.

O	3.532860000	-0.705095000	-0.418925000
H	4.241216000	-0.347871000	0.126477000
C	2.299063000	-0.378886000	0.204358000
H	2.254928000	-0.837348000	1.201484000
C	2.112390000	1.122349000	0.340137000
H	2.875156000	1.523550000	1.016415000
H	2.287022000	1.578582000	-0.639792000
C	0.726425000	1.473644000	0.865276000
H	0.602009000	2.560752000	0.894378000
H	0.630391000	1.119541000	1.896799000
C	-0.415404000	0.874957000	0.035851000
C	1.207485000	-0.988487000	-0.654211000
H	1.309699000	-2.074420000	-0.692311000
H	1.338549000	-0.617143000	-1.678255000
C	-0.177436000	-0.601835000	-0.223267000
C	-0.474437000	1.562780000	-1.337970000
H	-0.742694000	2.614354000	-1.203078000
H	-1.220698000	1.102392000	-1.988540000
H	0.482080000	1.525578000	-1.860320000
C	-1.246803000	-1.451306000	-0.410585000
H	-1.050165000	-2.401974000	-0.897123000
C	-2.677837000	-0.989486000	-0.460221000
H	-3.292076000	-1.700898000	0.095711000
H	-2.994421000	-1.081247000	-1.505595000
C	-2.926096000	0.449014000	0.022780000
C	-1.745634000	1.064625000	0.763965000
B	-0.593342000	-1.778369000	1.274416000

H	-0.003747000	-2.823926000	1.172493000
H	0.102266000	-0.956235000	1.827985000
H	-1.655846000	-1.791516000	1.838698000
H	-3.169567000	1.078278000	-0.836883000
H	-3.806286000	0.473841000	0.669655000
H	-1.918244000	2.136882000	0.902654000
H	-1.656032000	0.627214000	1.761803000

π-complex intermediate formed from decalin model + BH_3 by ®-face

SMD-PBE0-D3/def2-TZVP
***G*= -531.174013 a.u.**
G_{corr}= 0.267567 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.655290896339 a.u.**
***E*(DLPNO-CCSD(T))= -530.917680285482 a.u.**
SMD CDS free energy correction energy= -0.005177610856 a.u.

O	-3.511935000	-0.878587000	-0.143772000
H	-4.182909000	-0.408247000	-0.649484000
C	-2.246906000	-0.355049000	-0.509853000
H	-2.054744000	-0.554319000	-1.575912000
C	-2.129794000	1.134139000	-0.266902000
H	-2.852312000	1.673741000	-0.888892000
H	-2.376310000	1.346331000	0.778490000
C	-0.721806000	1.578779000	-0.609327000
H	-0.614080000	2.661570000	-0.495552000
H	-0.536756000	1.357265000	-1.666985000
C	0.397209000	0.912570000	0.228593000
C	-1.218149000	-1.098986000	0.324474000
H	-1.273504000	-2.166693000	0.108428000
H	-1.491973000	-0.960712000	1.374500000
C	0.185703000	-0.597414000	0.088090000
C	0.298385000	1.386626000	1.678682000
H	0.203084000	2.476011000	1.698599000
H	1.196261000	1.113772000	2.235870000
H	-0.559993000	0.961985000	2.202244000
C	1.111970000	-1.406831000	-0.529259000
H	0.771495000	-2.362037000	-0.917575000
C	2.427264000	-0.897215000	-1.040055000
H	2.313226000	-0.682671000	-2.110991000
H	3.179896000	-1.684669000	-0.956165000
C	2.851708000	0.361724000	-0.307836000
C	1.734470000	1.383342000	-0.379621000
B	1.192560000	-1.832525000	1.296727000
H	0.860615000	-1.034269000	2.134153000
H	0.567399000	-2.857962000	1.379703000

H	2.393066000	-1.931861000	1.299777000
H	3.761856000	0.770342000	-0.754864000
H	3.087213000	0.119813000	0.733231000
H	1.574973000	1.627592000	-1.435717000
H	2.025850000	2.316219000	0.111772000

π-complex intermediate formed from BH_3 + 3 by ®-face

SMD-PBE0-D3/def2-TZVP
***G*= -531.171491 a.u.**
G_{corr}= 0.267521 a.u.

SMD-DLPNO-CCSD(T)/def2-TZVP//SMD-PBE0-D3/def2-TZVP
***G*= -530.652142854725 a.u.**
***E*(DLPNO-CCSD(T))= -530.914690224844 a.u.**
SMD CDS free energy correction energy= -0.00497362988 a.u.

O	3.509052000	1.137020000	0.109244000
H	4.298553000	0.611819000	-0.057817000
C	2.394784000	0.424955000	-0.407026000
H	2.478242000	0.356188000	-1.504243000
C	2.316448000	-0.986796000	0.155738000
H	3.192321000	-1.556612000	-0.175152000
H	2.375371000	-0.923035000	1.246939000
C	1.039970000	-1.705659000	-0.269971000
H	0.999230000	-2.698008000	0.191215000
H	1.057070000	-1.863625000	-1.355709000
C	-0.225203000	-0.918267000	0.091366000
C	1.146951000	1.225638000	-0.085403000
H	1.204960000	2.202113000	-0.576295000
H	1.099572000	1.408581000	0.991491000
C	-0.079133000	0.465943000	-0.567878000
C	-0.375563000	-0.871090000	1.612404000
H	-0.409974000	-1.894393000	1.999726000
H	-1.287724000	-0.365772000	1.925222000
H	0.455548000	-0.362854000	2.102147000
C	-1.346408000	1.262085000	-0.638456000
H	-1.261778000	2.242751000	-1.096972000
C	-2.580822000	0.682744000	-0.520443000
H	-3.449118000	1.219685000	-0.885045000
C	-2.744022000	-0.793635000	-0.263803000
C	-1.460433000	-1.581228000	-0.519483000
H	0.105839000	0.253345000	-1.635315000
B	-2.232576000	1.873006000	0.932012000
H	-2.768297000	2.909578000	0.633158000
H	-1.125371000	2.004049000	1.398350000
H	-2.872476000	1.154077000	1.656542000
H	-3.115193000	-0.964043000	0.749110000

H	-3.532122000	-1.153473000	-0.931948000
H	-1.303900000	-1.670933000	-1.601076000
H	-1.569689000	-2.598770000	-0.130605000

b. Cartesian coordinates of the structures at SMD-PBE0-D3/def2-TZVP level for the System

Cholesterol G**= -816.278930 a.u.** G_{corr}**= 0.414025 a.u.**

O	5.5975710	0.3535080	-0.1531850
H	6.1065210	-0.2388770	-0.7162620
C	4.2275660	0.2097670	-0.4984240
H	4.0684300	0.5479280	-1.5349290
C	3.7484900	-1.2224200	-0.3765880
H	4.3067530	-1.8613230	-1.0706420
H	3.9699090	-1.5787430	0.6353360
C	2.2607110	-1.3186530	-0.6763270
H	1.9388480	-2.3596450	-0.5904880
H	2.0925440	-1.0220270	-1.7189170
C	1.3739880	-0.4333590	0.2251510
C	3.4290060	1.1040490	0.4295950
H	3.7378280	2.1446600	0.3017470
H	3.6886660	0.8160160	1.4563560
C	1.9468350	0.9755240	0.2097560
C	1.4118620	-0.9647020	1.6652030
H	1.2136970	-2.0384840	1.6987580
H	0.6703270	-0.4595220	2.2886970
H	2.3870970	-0.8020160	2.1262930
C	-3.2075340	-1.0010980	1.4324520
H	-3.6959830	-1.9716820	1.5642420
H	-3.8387460	-0.2507590	1.9145000
H	-2.2632330	-1.0304510	1.9786800
C	1.1969560	2.0590780	0.0129770
H	1.6884630	3.0303710	-0.0157560
C	-0.2821540	2.0496690	-0.1636490
H	-0.5254800	2.2875990	-1.2101870
H	-0.7268040	2.8584700	0.4270930
C	-0.9165390	0.7182970	0.2103830
H	-0.9458890	0.6475890	1.3050780
C	-0.0685330	-0.4368960	-0.3448000
H	0.0313110	-0.2364020	-1.4229490
C	-0.7636960	-1.7965390	-0.2035630
H	-0.1867860	-2.5597630	-0.7328410
H	-0.7697820	-2.0978190	0.8469520
C	-2.1999580	-1.8087220	-0.7220250
H	-2.6451580	-2.7960370	-0.5524990
H	-2.2018860	-1.6401470	-1.8064800
C	-2.3295660	0.6227640	-0.3333270
H	-2.2380870	0.6803300	-1.4302580

C	-3.0253880	-0.7156320	-0.0596830
C	-3.3619830	1.6672640	0.0775680
H	-3.2080980	2.6255710	-0.4230390
H	-3.3024300	1.8583030	1.1536840
C	-4.7158900	1.0183650	-0.2962270
H	-5.4124440	1.0606450	0.5443190
H	-5.1968250	1.5441490	-1.1240790
C	-4.3968800	-0.4432350	-0.6810870
H	-4.3241760	-0.5407840	-1.7695620
H	-5.1629270	-1.1463290	-0.3416720

BH_3 G= -26.557575 a.u. G_{corr}= 0.008388 a.u.

B	0.0000000	0.0000000	0.0000000
H	-0.0000000	1.1936880	0.0000000
H	-1.0337640	-0.5968440	0.0000000
H	1.0337640	-0.5968440	0.0000000

Cartesian coordinates for the structures of the hydroboration mechanism for 1a' and 1b'

TS1-1a' *G*= -842.842486 a.u. G_{corr}=0.445893 a.u. □ν_{min}= 441.4*i* cm^{-1}

O	5.5297860	0.0372000	0.1135910
H	6.0650500	-0.6017970	-0.3682330
C	4.1972120	-0.0640150	-0.3644550
H	4.1690000	0.1857820	-1.4353020
C	3.6282690	-1.4576230	-0.1671970
H	4.1820770	-2.1674050	-0.7914290
H	3.8047090	-1.7509910	0.8725090
C	2.1432060	-1.5397890	-0.5050920
H	1.7815660	-2.5418100	-0.2639190
H	2.0033300	-1.4087900	-1.5847290
C	1.2822030	-0.5001470	0.2263320
C	3.3796920	0.9699890	0.3831590
H	3.7501500	1.9747150	0.1711990
H	3.4986140	0.8032000	1.4591470
C	1.9099410	0.8811270	0.0704860
C	1.2787630	-0.8026370	1.7346020
H	0.6851740	-1.6967750	1.9343860
H	0.8576090	0.0208740	2.3136370
H	2.2831410	-0.9874430	2.1144980
C	-3.3551560	-1.2813800	1.2737940
H	-3.8664760	-2.2479870	1.2279940
H	-3.9906800	-0.6042670	1.8490930
H	-2.4338910	-1.4239940	1.8409920
C	1.1105280	2.0427990	0.1598430
H	1.6086330	2.9245940	0.5520130
C	-0.3791240	1.9798350	0.4262560

H	-0.8873270	2.6133720	-0.3059060
H	-0.5690290	2.4434150	1.3999270
C	-1.0100760	0.5770750	0.4174300
H	-1.0993030	0.2423330	1.4558950
C	-0.1573990	-0.4623990	-0.3321470
H	-0.0735210	-0.1260340	-1.3728650
C	-0.8394330	-1.8322650	-0.3813080
H	-0.2562690	-2.5071180	-1.0125960
H	-0.8566210	-2.2842960	0.6152440
C	-2.2641300	-1.7607700	-0.9304760
H	-2.7167120	-2.7589070	-0.9168850
H	-2.2295110	-1.4409310	-1.9796620
C	-2.4034030	0.5952410	-0.1837330
H	-2.2775530	0.8346720	-1.2519450
C	-3.1095960	-0.7679700	-0.1471970
C	-3.4505940	1.5591010	0.3640360
H	-3.2787950	2.5890810	0.0450570
H	-3.4348060	1.5587240	1.4583770
C	-4.7874320	0.9924480	-0.1703990
H	-5.5227720	0.9070880	0.6329920
H	-5.2262400	1.6496540	-0.9243990
C	-4.4551470	-0.3918310	-0.7710550
H	-4.3393580	-0.3157630	-1.8573750
H	-5.2345620	-1.1343790	-0.5775930
B	1.5833990	1.8663730	-1.4668960
H	2.4510450	2.6509800	-1.7466440
H	2.1026250	0.7493810	-1.6161580
H	0.5854720	1.8006090	-2.1288520

INT-1a' ***G*= -842.850281 a.u.** **G_{corr}= 0.447654 a.u.**

O	5.5445820	0.0427570	-0.0095810
H	6.0589280	-0.6622470	-0.4164740
C	4.1988470	-0.0963380	-0.4371620
H	4.1390700	0.0631710	-1.5264550
C	3.6412400	-1.4733650	-0.1171070
H	4.1884200	-2.2295790	-0.6913240
H	3.8386100	-1.6798440	0.9395720
C	2.1490730	-1.5915260	-0.4169080
H	1.8015140	-2.5774390	-0.0984840
H	1.9894960	-1.5395530	-1.5017740
C	1.3014480	-0.4991590	0.2511150
C	3.3875270	0.9919540	0.2357860
H	3.7621410	1.9741850	-0.0621290
H	3.4965390	0.9166250	1.3215300
C	1.9210840	0.8597320	-0.1331720
C	1.3343530	-0.6719730	1.7721590
H	0.7392810	-1.5412240	2.0631310

H	0.9345530	0.2002590	2.2915990
H	2.3460280	-0.8332990	2.1444070
C	-3.4223890	-1.2934680	1.2292510
H	-3.9677160	-2.2390660	1.1499010
H	-4.0551790	-0.5986820	1.7859890
H	-2.5326170	-1.4794740	1.8329370
C	1.0646950	2.0973470	0.1347690
H	1.6258930	2.8274650	0.7153350
C	-0.3471090	1.9057190	0.6844510
H	-0.9826620	2.6703180	0.2297300
H	-0.3403420	2.1351410	1.7545360
C	-1.0089500	0.5206040	0.4989060
H	-1.1602410	0.1050550	1.5002520
C	-0.1469060	-0.4947520	-0.2738130
H	-0.0919190	-0.1546660	-1.3169920
C	-0.8245360	-1.8648480	-0.3180260
H	-0.2282150	-2.5532260	-0.9219120
H	-0.8685350	-2.2966790	0.6874630
C	-2.2307860	-1.7878850	-0.9143460
H	-2.6952360	-2.7806670	-0.9061730
H	-2.1534330	-1.4817280	-1.9654820
C	-2.3726770	0.5800060	-0.1697790
H	-2.1968140	0.8275190	-1.2288030
C	-3.0968190	-0.7780760	-0.1753870
C	-3.4380150	1.5484450	0.3353960
H	-3.2468110	2.5782440	0.0279370
H	-3.4723070	1.5457920	1.4291830
C	-4.7538930	0.9963470	-0.2631050
H	-5.5241880	0.9074990	0.5064720
H	-5.1553960	1.6647140	-1.0280630
C	-4.4051700	-0.3835670	-0.8629610
H	-4.2331690	-0.2962540	-1.9410350
H	-5.2003500	-1.1205510	-0.7181820
B	1.2963000	2.1385750	-1.4059760
H	2.2551450	2.6971920	-1.8630290
H	1.9620620	0.7516650	-1.3050690
H	0.4232030	1.7732200	-2.1424710

TS2-1a' ***G*= -842.848024 a.u.** G_{corr}**= 0.448481 a.u.** ν_{min}**= 97.1*i* cm^{-1}**

O	5.5148330	-0.1431600	0.2810310
H	6.0367200	-0.8379880	-0.1336180
C	4.2132890	-0.1783810	-0.2857010
H	4.2706640	0.0852470	-1.3544720
C	3.5807650	-1.5544220	-0.1547180
H	4.1392430	-2.2728030	-0.7657620
H	3.6969150	-1.8754810	0.8852270
C	2.1081990	-1.5821380	-0.5585850

H	1.7030610	-2.5708620	-0.3283950
H	2.0218450	-1.4536740	-1.6450230
C	1.2623020	-0.4965300	0.1239950
C	3.3754880	0.8778440	0.4057800
H	3.8363140	1.8572600	0.2659880
H	3.3530920	0.6846230	1.4816430
C	1.9616360	0.8552640	-0.1640850
C	1.2184090	-0.7473600	1.6369540
H	0.4902670	-1.5261170	1.8751250
H	0.9403810	0.1502970	2.1920420
H	2.1798780	-1.0805510	2.0256010
C	-3.2290840	-1.3344770	1.3035130
H	-3.7244390	-2.3103220	1.2851530
H	-3.8276070	-0.6769790	1.9385670
H	-2.2614930	-1.4651440	1.7911920
C	1.1296190	2.1260680	0.1777980
H	1.5236490	2.5585430	1.0971590
C	-0.4017440	1.9901770	0.1945720
H	-0.7937830	2.4101200	-0.7382280
H	-0.7988830	2.6260840	0.9912170
C	-1.0037650	0.5906390	0.3239130
H	-1.0240100	0.2984000	1.3781870
C	-0.1683910	-0.4389710	-0.4543990
H	-0.0785340	-0.0592110	-1.4852560
C	-0.8442880	-1.8116130	-0.5459730
H	-0.2918850	-2.4393700	-1.2497050
H	-0.7844350	-2.3202630	0.4212930
C	-2.3044060	-1.7491680	-0.9912310
H	-2.7373840	-2.7561530	-0.9758780
H	-2.3524210	-1.3988030	-2.0302160
C	-2.4312590	0.5812820	-0.1897770
H	-2.3780660	0.8278250	-1.2627550
C	-3.1079920	-0.7939460	-0.1226490
C	-3.4550100	1.5258250	0.4314000
H	-3.3273560	2.5573670	0.0967260
H	-3.3544290	1.5313830	1.5213890
C	-4.8181640	0.9316790	0.0042160
H	-5.4803120	0.8191170	0.8658800
H	-5.3361880	1.5845040	-0.7018710
C	-4.5039030	-0.4375890	-0.6375800
H	-4.4713320	-0.3454410	-1.7284660
H	-5.2518610	-1.1987060	-0.3973760
B	1.7080050	2.6330310	-1.1666970
H	2.8200710	3.0615110	-1.2839640
H	2.0987460	0.8317090	-1.2863720
H	1.0146740	2.5588880	-2.1444390

1a’ ***G*= -842.863478 a.u.** **G_{corr}= 0.445790 a.u.**

O	5.5403280	-0.0832810	-0.1757840
H	6.0294990	-0.7960270	-0.5996450
B	1.5517550	3.3664240	-0.1043290
H	2.0255730	3.4863220	-1.2019560
C	4.1754680	-0.2082880	-0.5533770
H	4.0785730	-0.0467880	-1.6394980
C	3.6153220	-1.5780810	-0.2199960
H	4.1467310	-2.3439340	-0.7972740
H	3.8158240	-1.7837170	0.8368190
C	2.1215720	-1.6605810	-0.5099120
H	1.7623290	-2.6561920	-0.2371410
H	1.9591310	-1.5544370	-1.5906140
C	1.2964090	-0.5824860	0.2114750
C	3.3949340	0.8766470	0.1540280
H	3.7773220	1.8557530	-0.1564930
H	3.5707020	0.7973600	1.2324680
C	1.9063950	0.7889580	-0.1622700
H	1.8115150	0.8666530	-1.2570550
C	1.3410830	-0.8367390	1.7202880
H	1.0183700	-1.8553660	1.9496190
H	0.6957070	-0.1544700	2.2756550
H	2.3487220	-0.7236590	2.1227840
C	-3.3616680	-1.0363000	1.4304510
H	-3.9044580	-1.9761430	1.5715280
H	-3.9636270	-0.2417960	1.8777590
H	-2.4344680	-1.1035610	2.0020290
C	1.1380800	1.9682460	0.4196670
H	1.1361590	1.9230880	1.5149870
C	-0.3351330	1.9214680	-0.0548600
H	-0.3793450	2.0922520	-1.1405920
H	-0.9167420	2.7206600	0.4144390
C	-0.9945440	0.5760760	0.2407100
H	-1.0750930	0.4789780	1.3297100
C	-0.1623780	-0.5960660	-0.3112440
H	-0.0903790	-0.4267110	-1.3980160
C	-0.8804230	-1.9368000	-0.1213100
H	-0.3166520	-2.7281730	-0.6214220
H	-0.8949970	-2.1996350	0.9405100
C	-2.3102010	-1.9391260	-0.6597510
H	-2.7816220	-2.9080600	-0.4580310
H	-2.2866800	-1.8179140	-1.7503220
C	-2.3894330	0.5137120	-0.3556030
H	-2.2606760	0.5392290	-1.4496540
C	-3.1257460	-0.8020220	-0.0632220
C	-3.4112630	1.5911950	-0.0058840
H	-3.2244100	2.5293530	-0.5323490
H	-3.3776260	1.8164420	1.0647130
C	-4.7683820	0.9595010	-0.3973960

H	-5.4843070	1.0374070	0.4240910
H	-5.2178620	1.4730960	-1.2501600
C	-4.4700410	-0.5173020	-0.7355910
H	-4.3640330	-0.6440170	-1.8183230
H	-5.2620060	-1.1950760	-0.4042620
H	1.2971200	4.3611350	0.5163910

TS1-1b' ***G*= -842.837334 a.u.** **G_{corr}= 0.445215 a.u.** **ν_{min}= 537.8*i* cm^{-1}**

O	5.5235710	0.0078330	0.2480980
H	6.0591400	-0.6284680	-0.2366820
C	4.2056120	-0.0396580	-0.2837490
H	4.2197420	0.2797880	-1.3354790
C	3.6204450	-1.4401610	-0.2062470
H	4.1925670	-2.1076000	-0.8610360
H	3.7625980	-1.8096700	0.8145110
C	2.1446740	-1.4931230	-0.5937510
H	1.7762520	-2.5085630	-0.4268220
H	2.0385270	-1.2884720	-1.6649040
C	1.2761210	-0.4881120	0.1774230
C	3.3642250	0.9522070	0.4939870
H	3.7680600	1.9590540	0.3669190
H	3.4316220	0.7065530	1.5594780
C	1.9227100	0.8989460	0.0287810
C	1.2712230	-0.8575450	1.6705150
H	0.7143610	-1.7819170	1.8380840
H	0.8160610	-0.0724410	2.2776830
H	2.2764740	-1.0184950	2.0572480
C	-3.3287300	-1.2599060	1.3142470
H	-3.8353280	-2.2298130	1.2942500
H	-3.9536740	-0.5785260	1.8961970
H	-2.3925040	-1.3895540	1.8596100
C	1.1056850	2.0463470	0.1171400
H	1.5775630	2.9683250	0.4452120
C	-0.3870190	1.9885500	0.3273050
H	-0.8784220	2.5871940	-0.4442950
H	-0.5817150	2.5098820	1.2699610
C	-1.0132140	0.5888010	0.3812970
H	-1.0776730	0.2898890	1.4320320
C	-0.1717750	-0.4605000	-0.3635410
H	-0.1105960	-0.1317570	-1.4074760
C	-0.8578210	-1.8298980	-0.3937470
H	-0.2858210	-2.5066720	-1.0333210
H	-0.8575040	-2.2802260	0.6031130
C	-2.2937220	-1.7626700	-0.9133100
H	-2.7461990	-2.7604870	-0.8815170
H	-2.2837230	-1.4508860	-1.9654520

C	-2.4193180	0.5992460	-0.1889130
H	-2.3168550	0.8233650	-1.2629990
C	-3.1217810	-0.7637860	-0.1188520
C	-3.4539840	1.5708060	0.3693240
H	-3.2920350	2.5960580	0.0298620
H	-3.4108550	1.5876990	1.4628180
C	-4.8030470	0.9944820	-0.1224020
H	-5.5165210	0.9184170	0.7013140
H	-5.2632670	1.6406420	-0.8731530
C	-4.4832670	-0.3969460	-0.7129450
H	-4.3951980	-0.3350380	-1.8027630
H	-5.2561740	-1.1379630	-0.4900890
B	1.8025100	1.6599340	-1.5168260
H	2.8689200	2.1345530	-1.7919630
H	1.2404740	0.9368810	-2.2874400
H	1.0484800	2.6334420	-1.4389320

INT-1b' ***G*= -842.846398 a.u.** **G_{corr}= 0.447634 a.u.**

O	5.5318300	0.0501190	0.1190880
H	6.0509090	-0.6481460	-0.2930390
C	4.1987940	-0.0558350	-0.3640300
H	4.1798930	0.1586440	-1.4446410
C	3.6307030	-1.4471130	-0.1339520
H	4.1912680	-2.1725320	-0.7354460
H	3.8081120	-1.7105380	0.9138920
C	2.1430710	-1.5530280	-0.4633110
H	1.7930050	-2.5484450	-0.1753340
H	1.9989160	-1.4671080	-1.5472980
C	1.2951150	-0.4697370	0.2201620
C	3.3599310	1.0020370	0.3238000
H	3.7627400	1.9902890	0.0846530
H	3.4365130	0.8740620	1.4093470
C	1.9303750	0.8784700	-0.1756360
C	1.3284070	-0.6805860	1.7410250
H	0.7311370	-1.5527140	2.0202540
H	0.9331100	0.1822120	2.2812880
H	2.3375310	-0.8530140	2.1144110
C	-3.4325270	-1.2402870	1.2729920
H	-3.9860110	-2.1829580	1.2203810
H	-4.0556500	-0.5271110	1.8173090
H	-2.5398670	-1.4197790	1.8743220
C	1.0415610	2.1048060	0.0300250
H	1.5850350	2.9259310	0.4971590
C	-0.3482100	1.9205110	0.6351740
H	-1.0020510	2.7010720	0.2393790
H	-0.2407260	2.1426710	1.7000670
C	-1.0196310	0.5398240	0.4848830

H	-1.1688370	0.1541960	1.4981930
C	-0.1645420	-0.4917630	-0.2734980
H	-0.1398920	-0.1779610	-1.3222940
C	-0.8446870	-1.8616810	-0.2747400
H	-0.2543560	-2.5653190	-0.8669600
H	-0.8836810	-2.2712890	0.7400300
C	-2.2551310	-1.7951030	-0.8635550
H	-2.7247550	-2.7848330	-0.8258880
H	-2.1836630	-1.5174390	-1.9229950
C	-2.3857580	0.5936290	-0.1794400
H	-2.2146000	0.8122180	-1.2455430
C	-3.1134010	-0.7626350	-0.1464700
C	-3.4456020	1.5781960	0.3063270
H	-3.2552230	2.5992170	-0.0304770
H	-3.4728560	1.6056410	1.3999880
C	-4.7667730	1.0135350	-0.2686210
H	-5.5309450	0.9450520	0.5090390
H	-5.1734120	1.6634360	-1.0466470
C	-4.4245300	-0.3813330	-0.8362990
H	-4.2582230	-0.3210750	-1.9171220
H	-5.2206880	-1.1124060	-0.6691370
B	1.7192120	1.4831680	-1.6060940
H	2.5638100	2.2319560	-2.0168590
H	0.8788340	1.1035330	-2.3689570
H	0.8409280	2.5743040	-1.0223180

TS2-1b' ***G*= -842.845113 a.u.** **G_{corr}= 0.448898 a.u.** **ν_{min}= 46.6*i* cm^{-1}**

O	5.5328330	0.0237940	0.1585600
H	6.0513340	-0.6761530	-0.2514360
C	4.2044290	-0.0701410	-0.3400400
H	4.1990700	0.1512170	-1.4192860
C	3.6239100	-1.4583430	-0.1247590
H	4.1854970	-2.1845610	-0.7243150
H	3.7872600	-1.7294270	0.9234070
C	2.1394970	-1.5505020	-0.4720630
H	1.7784680	-2.5445520	-0.1933770
H	2.0091320	-1.4581470	-1.5573050
C	1.2902400	-0.4644220	0.2056880
C	3.3652450	0.9883690	0.3458330
H	3.7783050	1.9753960	0.1194330
H	3.4281790	0.8516910	1.4311760
C	1.9399070	0.8805880	-0.1707330
C	1.3047590	-0.6785000	1.7267060
H	0.6891430	-1.5391080	2.0012550
H	0.9211260	0.1923400	2.2631320
H	2.3071210	-0.8698310	2.1087540
C	-3.3977860	-1.2527480	1.2855210

H	-3.9339800	-2.2058800	1.2427740
H	-4.0247520	-0.5516070	1.8409720
H	-2.4910780	-1.4141820	1.8707020
C	1.0651540	2.1155280	0.0373600
H	1.6020060	2.9095680	0.5563180
C	-0.3669040	1.9515230	0.5486410
H	-0.9944560	2.6873260	0.0402140
H	-0.3537970	2.2564570	1.5980450
C	-1.0171140	0.5561340	0.4493230
H	-1.1395880	0.1889730	1.4727930
C	-0.1643380	-0.4780390	-0.3060830
H	-0.1289380	-0.1628200	-1.3544210
C	-0.8426690	-1.8495900	-0.3116450
H	-0.2563040	-2.5451700	-0.9170850
H	-0.8667200	-2.2686550	0.6995670
C	-2.2614150	-1.7883720	-0.8791710
H	-2.7226580	-2.7820800	-0.8424770
H	-2.2095120	-1.5008350	-1.9371320
C	-2.3978810	0.5926170	-0.1840980
H	-2.2505880	0.8148670	-1.2532050
C	-3.1138900	-0.7682200	-0.1390360
C	-3.4542560	1.5681190	0.3270940
H	-3.2779940	2.5919890	-0.0086140
H	-3.4589840	1.5899580	1.4212410
C	-4.7828830	0.9960140	-0.2224570
H	-5.5311580	0.9214980	0.5699680
H	-5.2088210	1.6444250	-0.9913480
C	-4.4427370	-0.3957640	-0.7992240
H	-4.3009750	-0.3331980	-1.8833880
H	-5.2294210	-1.1330460	-0.6153180
B	1.7535950	1.5087980	-1.5949130
H	2.6259700	2.2295460	-1.9978240
H	0.9013890	1.1635260	-2.3613110
H	0.9374710	2.6306300	-1.0069610

1b’ ***G*= -842.857225 a.u.** **G_{corr}= 0.446391 a.u.**

O	5.5279970	0.1071240	-0.0221680
H	6.0219040	-0.6145320	-0.4258470
C	4.1733450	-0.0140990	-0.4185200
H	4.0882920	0.2156140	-1.4997310
C	3.6330780	-1.4132760	-0.1837100
H	4.1923910	-2.1296790	-0.7969250
H	3.8270150	-1.6734840	0.8624580
C	2.1442720	-1.5228060	-0.4970340
H	1.8069750	-2.5309260	-0.2426480
H	1.9931140	-1.4096280	-1.5760810
C	1.2896960	-0.4807100	0.2429520

C	3.3651790	1.0110500	0.3484080
H	3.7554350	2.0124790	0.1409640
H	3.4858140	0.8380080	1.4236570
C	1.8814550	0.9302120	-0.0590410
C	1.3157990	-0.8127390	1.7404190
H	0.9980810	-1.8454810	1.9043450
H	0.6555100	-0.1725940	2.3261420
H	2.3150050	-0.7178490	2.1669050
C	-3.3885640	-1.0920600	1.3771250
H	-3.9190040	-2.0469450	1.4459200
H	-4.0112090	-0.3377850	1.8640670
H	-2.4709650	-1.1832240	1.9607900
C	1.0696850	2.0175710	0.6542050
H	1.1069730	1.8677890	1.7394620
C	-0.3708340	1.9960190	0.1676310
H	-0.3923860	2.2632240	-0.9015770
H	-0.9633560	2.7579030	0.6834000
C	-1.0251550	0.6303890	0.3390860
H	-1.1255200	0.4447380	1.4157030
C	-0.1689750	-0.4919020	-0.2827860
H	-0.1037970	-0.2560320	-1.3569130
C	-0.8640290	-1.8536680	-0.1842360
H	-0.2797620	-2.6033150	-0.7241130
H	-0.8899470	-2.1823430	0.8589320
C	-2.2854560	-1.8424690	-0.7454570
H	-2.7456300	-2.8286670	-0.6132300
H	-2.2453810	-1.6526640	-1.8257550
C	-2.4085720	0.5861320	-0.2842610
H	-2.2620530	0.6870110	-1.3719020
C	-3.1287150	-0.7567620	-0.0932790
C	-3.4538450	1.6225810	0.1162380
H	-3.2723630	2.5959950	-0.3440250
H	-3.4431270	1.7778110	1.1996760
C	-4.7934140	0.9977440	-0.3415110
H	-5.5249360	1.0095590	0.4698300
H	-5.2364870	1.5600590	-1.1664830
C	-4.4649250	-0.4485650	-0.7714120
H	-4.3363780	-0.5006160	-1.8578930
H	-5.2521530	-1.1586080	-0.5020890
B	1.8991790	1.3138670	-1.5861160
H	2.2435140	2.4312410	-1.8627030
H	1.6248240	0.5841080	-2.4942620
H	1.5195750	2.9966580	0.4589560

Cartesian coordinates for the structures of the hydroboration mechanism for 1c' and 1d'

TS1-1c' ***G*= -842.838067 a.u.** **G_{corr}= 0.446437 a.u.** **ν_{min}= 516.3*i* cm^{-1}**

O	5.4708140	0.2356260	-0.5678830
H	5.9018100	-0.2617260	-1.2707280
C	4.0699540	0.1019490	-0.7394720
H	3.7651450	0.5585560	-1.6940470
C	3.6027530	-1.3368030	-0.7184300
H	4.0509560	-1.8923610	-1.5494980
H	3.9395350	-1.8101480	0.2095790
C	2.0927800	-1.3560160	-0.8476030
H	1.7211640	-2.3829320	-0.9019400
H	1.8308390	-0.8813700	-1.8000030
C	1.3054310	-0.6368000	0.2787840
C	3.4248550	0.8546380	0.4063350
H	3.7315080	1.9015890	0.3814940
H	3.8141420	0.4248920	1.3335940
C	1.9077840	0.7778560	0.3827530
C	1.5065750	-1.3824640	1.5982310
H	1.3270490	-2.4519820	1.4792270
H	0.8301770	-1.0065930	2.3692190
H	2.5268000	-1.2619540	1.9676540
C	-3.3963270	-0.5998710	1.5299930
H	-3.9559620	-1.4796700	1.8626240
H	-3.9895570	0.2805680	1.7878270
H	-2.4763290	-0.5534880	2.1149300
C	1.2011790	1.9261880	-0.0602080
H	1.8022750	2.7117270	-0.5089620
C	-0.2185480	1.8188330	-0.5511420
H	-0.2172470	1.6963900	-1.6432900
H	-0.7431950	2.7554990	-0.3429500
C	-0.9648780	0.6479800	0.0666500
H	-1.0538900	0.8151960	1.1447830
C	-0.1842880	-0.6444760	-0.1996170
H	-0.1387690	-0.7008360	-1.2964320
C	-0.9467710	-1.8944790	0.2507910
H	-0.3971510	-2.7894070	-0.0573940
H	-0.9950520	-1.9287460	1.3419600
C	-2.3651540	-1.9585350	-0.3113460
H	-2.8761030	-2.8477300	0.0754360
H	-2.3220060	-2.0647590	-1.4028260
C	-2.3552420	0.5042230	-0.5254920
H	-2.2166540	0.2925860	-1.5981850
C	-3.1420530	-0.6934050	0.0239310
C	-3.3374920	1.6670150	-0.4278470
H	-3.1102900	2.4649330	-1.1377970
H	-3.3026290	2.1122750	0.5711820
C	-4.7144840	1.0150720	-0.6982120
H	-5.4329550	1.2900770	0.0773870
H	-5.1380250	1.3523300	-1.6468560
C	-4.4700490	-0.5096830	-0.7129010

H	-4.3620070	-0.8662780	-1.7428920
H	-5.2891580	-1.0733910	-0.2572860
B	1.3453390	2.0197160	1.6257210
H	1.7498830	0.9238310	2.0342340
H	2.1935060	2.8069480	1.9491240
H	0.2428450	2.0750360	2.0940940

INT1-1c' ***G*= -842.847107 a.u.** **G_{corr}= 0.447053 a.u.**

O	-5.4132800	-0.4353410	-0.5029370
H	-5.8077900	-0.1960730	-1.3479290
C	-4.0043650	-0.3229900	-0.6356750
H	-3.6409840	-1.0606560	-1.3684260
C	-3.5648110	1.0537940	-1.0830940
H	-3.9786980	1.2784710	-2.0727140
H	-3.9655620	1.7994870	-0.3886330
C	-2.0491270	1.1003710	-1.1403080
H	-1.7102950	2.0818130	-1.4881000
H	-1.7098890	0.3746750	-1.8884520
C	-1.3175030	0.7955090	0.1848670
C	-3.4087590	-0.6386520	0.7175350
H	-3.7137570	-1.6421980	1.0211910
H	-3.8400740	0.0561210	1.4444640
C	-1.8783740	-0.5580570	0.7309280
C	-1.6550160	1.8748710	1.2156390
H	-1.4408210	2.8754200	0.8367090
H	-1.0856410	1.7328580	2.1375260
H	-2.7125110	1.8531150	1.4815380
C	3.4319270	0.3885140	1.5558760
H	4.0739840	1.1893510	1.9357880
H	3.9448670	-0.5575990	1.7437370
H	2.5192560	0.3877690	2.1540090
C	-1.2320090	-1.8620370	0.2171740
H	-1.9608240	-2.4651830	-0.3219500
C	0.0700340	-1.6928810	-0.5422170
H	-0.1198550	-1.4713420	-1.6014920
H	0.6210450	-2.6380350	-0.5166830
C	0.9143840	-0.5762180	0.0446830
H	1.0241460	-0.7583560	1.1182490
C	0.2141490	0.7717730	-0.1775520
H	0.2498560	0.9079010	-1.2673820
C	1.0398620	1.9295190	0.3924480
H	0.5658250	2.8824320	0.1434220
H	1.0638830	1.8770440	1.4849740
C	2.4681050	1.9453780	-0.1536570
H	3.0317910	2.7637320	0.3091150
H	2.4362250	2.1512440	-1.2313770
C	2.3021970	-0.4920020	-0.5628890

H	2.1696220	-0.1979790	-1.6166240
C	3.1673440	0.6115790	0.0650350
C	3.2122180	-1.7161470	-0.5588150
H	2.9323350	-2.4448280	-1.3223510
H	3.1579010	-2.2310830	0.4052580
C	4.6248580	-1.1305690	-0.7978410
H	5.3306150	-1.5025630	-0.0514730
H	5.0206550	-1.4249190	-1.7724480
C	4.4739240	0.4034080	-0.7023330
H	4.3758790	0.8376040	-1.7031670
H	5.3311540	0.8832550	-0.2213590
B	-1.1665350	-2.0600750	1.7591510
H	-1.6279570	-0.4998090	1.8570570
H	-2.0970420	-2.5240810	2.3556850
H	-0.1526540	-1.8454730	2.3607560

TS2-1c' ***G*= -842.844838 a.u.** **G_{corr}= 0.446952 a.u.** **ν_{min}= 98.0*i* cm^{-1}**

O	5.4448940	0.2537460	-0.0738980
H	5.9391180	-0.0060120	-0.8581920
C	4.0618160	0.2256550	-0.4046650
H	3.8629770	0.9717120	-1.1884440
C	3.6223900	-1.1322010	-0.9184330
H	4.1387140	-1.3556480	-1.8593600
H	3.9301510	-1.8965620	-0.1976770
C	2.1167080	-1.1563540	-1.1351750
H	1.8029440	-2.1395880	-1.5031490
H	1.8624760	-0.4378720	-1.9238680
C	1.2944170	-0.8088820	0.1161670
C	3.2986790	0.6032580	0.8491190
H	3.6127610	1.6027210	1.1633480
H	3.6099350	-0.0793130	1.6446610
C	1.7720370	0.5633660	0.6734150
C	1.5566650	-1.8492000	1.2096540
H	1.3266840	-2.8604350	0.8690040
H	0.9537960	-1.6462400	2.0984570
H	2.5998320	-1.8504210	1.5242380
C	-3.2975950	-0.5718880	1.6263630
H	-3.8843520	-1.4206050	1.9915920
H	-3.8137550	0.3393660	1.9377010
H	-2.3348200	-0.5916450	2.1397470
C	1.2948650	1.8061500	-0.1350410
H	1.9968490	1.9710860	-0.9567910
C	-0.1288840	1.6526110	-0.6953330
H	-0.0889050	1.4074700	-1.7643860
H	-0.6685150	2.6029180	-0.6260400
C	-0.9119430	0.5538730	0.0018590
H	-0.9130760	0.7456120	1.0831600

C	-0.2214070	-0.7851510	-0.3020290
H	-0.2312480	-0.8397080	-1.4007570
C	-1.0358360	-1.9961190	0.1675610
H	-0.5683840	-2.9131330	-0.2034750
H	-1.0177840	-2.0677830	1.2578090
C	-2.4886810	-1.9595490	-0.3016690
H	-3.0283660	-2.8245090	0.1014050
H	-2.5231600	-2.0441680	-1.3954730
C	-2.3466970	0.4984570	-0.4885530
H	-2.2952020	0.2920570	-1.5700670
C	-3.1624270	-0.6578660	0.1046210
C	-3.2505130	1.7157680	-0.3130140
H	-3.0335650	2.5039790	-1.0366900
H	-3.1127750	2.1522820	0.6812690
C	-4.6807710	1.1487580	-0.4780090
H	-5.3170510	1.4516240	0.3568400
H	-5.1593890	1.5252240	-1.3848250
C	-4.5275010	-0.3865360	-0.5295340
H	-4.5150490	-0.7310830	-1.5692290
H	-5.3430930	-0.9102900	-0.0225950
B	1.3581960	2.9609500	0.9084420
H	1.3400200	0.6366360	1.6811500
H	2.2956600	3.6992200	1.0292400
H	0.4345020	3.0934800	1.6665380

INT2-1c' ***G*= -842.855716 a.u.** **G_{corr}= 0.447506 a.u.**

O	5.4841650	0.2511480	0.0136250
H	5.9995440	-0.1137250	-0.7130850
C	4.1107910	0.1715580	-0.3465620
H	3.9290320	0.8040300	-1.2293210
C	3.6845230	-1.2464750	-0.6772700
H	4.2526550	-1.6133960	-1.5401800
H	3.9344790	-1.8947050	0.1695500
C	2.1950950	-1.2859410	-0.9832750
H	1.8864620	-2.3045300	-1.2414820
H	2.0113100	-0.6744010	-1.8749970
C	1.3069220	-0.7611620	0.1560810
C	3.3088890	0.7006590	0.8228920
H	3.6003000	1.7358260	1.0277060
H	3.5909060	0.1146160	1.7033520
C	1.7945520	0.6417920	0.6030300
C	1.4099900	-1.6861010	1.3705810
H	1.2268740	-2.7307280	1.1099090
H	0.6900210	-1.3979700	2.1424600
H	2.4015180	-1.6362660	1.8227370
C	-3.2429550	-0.9558490	1.5103690
H	-3.7757170	-1.8918080	1.7051580

H	-3.8093770	-0.1528050	1.9879540
H	-2.2767940	-1.0153410	2.0141940
C	1.3355830	1.7526350	-0.3204880
H	1.7906820	1.7060880	-1.3078380
C	-0.2111080	1.7965910	-0.4500680
H	-0.4919190	1.9566460	-1.4921680
H	-0.6394580	2.7002280	0.0775710
C	-0.9108600	0.5657140	0.1233950
H	-0.8880490	0.6055040	1.2182090
C	-0.1611570	-0.6806680	-0.3805780
H	-0.0867220	-0.5312580	-1.4679700
C	-0.9486710	-1.9813370	-0.1851820
H	-0.4312920	-2.7908080	-0.7104410
H	-0.9496440	-2.2621940	0.8695790
C	-2.3969900	-1.9053620	-0.6600460
H	-2.9046940	-2.8530800	-0.4466560
H	-2.4281500	-1.7639000	-1.7478480
C	-2.3506510	0.5397900	-0.3555410
H	-2.3044780	0.5453710	-1.4564040
C	-3.1168770	-0.7388060	0.0014010
C	-3.2915590	1.6677510	0.0543710
H	-3.1011880	2.5912020	-0.4970430
H	-3.1659430	1.9001440	1.1165100
C	-4.7012490	1.0951450	-0.2254590
H	-5.3475760	1.2131490	0.6472200
H	-5.1912830	1.6208240	-1.0478630
C	-4.4956960	-0.3967970	-0.5672710
H	-4.4812740	-0.5378910	-1.6532940
H	-5.2880860	-1.0351900	-0.1664290
B	1.0484280	3.1444360	0.2666280
H	1.3349590	0.8378130	1.5788950
H	0.9664880	4.1124930	-0.4371220
H	0.9195200	3.2658740	1.4547140

TS3-1c' ***G*= -842.844839 a.u.** **G_{corr}= 0.446952 a.u.** **ν_{min}= 98.6*i* cm^{-1}**

O	5.4448940	0.2537480	-0.0738980
H	5.9391170	-0.0060100	-0.8581920
C	4.0618160	0.2256560	-0.4046650
H	3.8629760	0.9717130	-1.1884440
C	3.6223910	-1.1322000	-0.9184330
H	4.1387130	-1.3556470	-1.8593600
H	3.9301510	-1.8965610	-0.1976770
C	2.1167080	-1.1563540	-1.1351740
H	1.8029440	-2.1395890	-1.5031480
H	1.8624750	-0.4378730	-1.9238680
C	1.2944170	-0.8088820	0.1161670
C	3.2986790	0.6032580	0.8491190

H	3.6127610	1.6027220	1.1633480
H	3.6099350	-0.0793130	1.6446610
C	1.7720370	0.5633660	0.6734150
C	1.5566650	-1.8492000	1.2096550
H	1.3266830	-2.8604350	0.8690050
H	0.9537980	-1.6462390	2.0984580
H	2.5998320	-1.8504220	1.5242370
C	-3.2975940	-0.5718870	1.6263630
H	-3.8843530	-1.4206030	1.9915920
H	-3.8137520	0.3393680	1.9377010
H	-2.3348190	-0.5916470	2.1397470
C	1.2948650	1.8061500	-0.1350410
H	1.9968500	1.9710860	-0.9567900
C	-0.1288840	1.6526100	-0.6953350
H	-0.0889030	1.4074680	-1.7643870
H	-0.6685150	2.6029180	-0.6260430
C	-0.9119430	0.5538730	0.0018580
H	-0.9130750	0.7456130	1.0831590
C	-0.2214070	-0.7851510	-0.3020290
H	-0.2312480	-0.8397090	-1.4007570
C	-1.0358360	-1.9961200	0.1675610
H	-0.5683850	-2.9131330	-0.2034760
H	-1.0177840	-2.0677850	1.2578090
C	-2.4886810	-1.9595490	-0.3016690
H	-3.0283660	-2.8245090	0.1014060
H	-2.5231600	-2.0441680	-1.3954730
C	-2.3466970	0.4984570	-0.4885540
H	-2.2952020	0.2920560	-1.5700680
C	-3.1624270	-0.6578650	0.1046210
C	-3.2505130	1.7157680	-0.3130150
H	-3.0335650	2.5039780	-1.0366910
H	-3.1127730	2.1522830	0.6812680
C	-4.6807710	1.1487580	-0.4780090
H	-5.3170490	1.4516240	0.3568420
H	-5.1593890	1.5252240	-1.3848240
C	-4.5275010	-0.3865350	-0.5295330
H	-4.5150490	-0.7310830	-1.5692280
H	-5.3430930	-0.9102900	-0.0225940
B	1.3581930	2.9609480	0.9084440
H	1.3400200	0.6366360	1.6811500
H	2.2956580	3.6992160	1.0292470
H	0.4344980	3.0934760	1.6665390

1c’ ***G*= -842.862365 a.u.** **G_{corr}= 0.447373 a.u.**

O	4.7483390	-0.4313950	-0.7376780
H	5.1241460	0.3581760	-1.1396660
B	1.1422300	2.8396950	1.4534060

H	0.1046530	3.2522220	1.8999150
C	3.4944790	-0.6858800	-1.3671810
H	3.6708510	-0.9896490	-2.4092140
C	2.8420680	-1.8323210	-0.6176920
H	1.9785260	-2.1769400	-1.1953650
H	3.5437930	-2.6702290	-0.5663570
C	2.4229520	-1.4136240	0.7825620
H	3.3224540	-1.1354560	1.3418390
H	1.9824710	-2.2609970	1.3145710
C	1.4681010	-0.2094030	0.8104470
C	2.5998230	0.5444900	-1.3576160
H	1.7412100	0.3411160	-2.0037460
H	3.1341660	1.3845860	-1.8194100
C	2.1507690	0.9486460	0.0455900
H	3.0579180	1.1983180	0.6093690
C	1.3041660	0.2048640	2.2690850
H	0.8385920	-0.5814960	2.8689610
H	0.6547590	1.0872280	2.4021740
H	2.2747360	0.4328630	2.7151940
C	-3.3093100	-0.4719490	1.4951210
H	-3.8523220	-1.3189600	1.9260190
H	-3.9825660	0.3884210	1.5097310
H	-2.4749950	-0.2433860	2.1604300
C	1.2319820	2.1819060	0.0441820
H	1.7460950	2.9694210	-0.5396560
C	-0.1146760	1.8728890	-0.6057520
H	0.0115710	1.6265470	-1.6679000
H	-0.7537370	2.7606910	-0.5702910
C	-0.8166990	0.7112090	0.0860750
H	-1.0636980	1.0300110	1.1067930
C	0.0994270	-0.5276410	0.1533620
H	0.3027160	-0.7928400	-0.8929540
C	-0.6161330	-1.7367540	0.7636900
H	0.0239720	-2.6195100	0.6861910
H	-0.7789010	-1.5738700	1.8334630
C	-1.9530050	-2.0434480	0.0895770
H	-2.4390320	-2.8868290	0.5939060
H	-1.7705480	-2.3557640	-0.9468130
C	-2.1053090	0.3242100	-0.6147110
H	-1.8169770	-0.0685680	-1.6033970
C	-2.8599180	-0.8219550	0.0747510
C	-3.1813110	1.3780860	-0.8555420
H	-2.9298340	2.0491750	-1.6794540
H	-3.3090450	2.0029080	0.0339690
C	-4.4575060	0.5506880	-1.1402410
H	-5.2888120	0.8925900	-0.5192690
H	-4.7813120	0.6579340	-2.1779570
C	-4.0946670	-0.9166380	-0.8233400

H	-3.8296090	-1.4484420	-1.7435040
H	-4.9184000	-1.4643990	-0.3565460
H	2.1478960	3.0635700	2.0691590

TS1-1d' ***G*= -842.835650 a.u.** **G_{corr}= 0.446415 a.u.** **ν_{min}= 489.9*i* cm^{-1}**

O	5.4650570	0.2667000	-0.6254670
H	5.8774900	-0.2541420	-1.3223050
C	4.0579530	0.1392390	-0.7640000
H	3.7317820	0.6194500	-1.7011730
C	3.5958040	-1.3012010	-0.7737010
H	4.0365620	-1.8349950	-1.6236550
H	3.9485450	-1.7952100	0.1378150
C	2.0831220	-1.3281590	-0.8794700
H	1.7216230	-2.3585310	-0.9542420
H	1.8059950	-0.8333770	-1.8178120
C	1.3174550	-0.6321410	0.2731270
C	3.4320110	0.8631860	0.4088600
H	3.7392960	1.9115900	0.4009260
H	3.8490740	0.4224350	1.3197350
C	1.9105540	0.7866160	0.4362330
C	1.5469780	-1.4208600	1.5647350
H	1.3892300	-2.4907760	1.4135020
H	0.8804920	-1.0855020	2.3597740
H	2.5692180	-1.2890250	1.9243380
C	-3.4118780	-0.5810890	1.5186110
H	-3.9815950	-1.4550810	1.8492030
H	-4.0014830	0.3049260	1.7655200
H	-2.4980240	-0.5395030	2.1135240
C	1.1868050	1.9207030	0.0080950
H	1.7544840	2.7927720	-0.3048370
C	-0.2122880	1.8231910	-0.5164260
H	-0.1364520	1.6897990	-1.6043330
H	-0.7402430	2.7650180	-0.3485380
C	-0.9695260	0.6518280	0.0822480
H	-1.0785570	0.8224650	1.1569030
C	-0.1818560	-0.6394420	-0.1813850
H	-0.1505690	-0.6957450	-1.2790030
C	-0.9458660	-1.8866890	0.2719760
H	-0.3943690	-2.7817810	-0.0316970
H	-0.9963420	-1.9171570	1.3633460
C	-2.3610220	-1.9541600	-0.2991730
H	-2.8767790	-2.8387410	0.0918140
H	-2.3087520	-2.0714910	-1.3891780
C	-2.3493130	0.5091020	-0.5329630
H	-2.1949860	0.2913950	-1.6022400
C	-3.1413250	-0.6857360	0.0160470
C	-3.3335160	1.6718480	-0.4545250

H	-3.0995980	2.4647760	-1.1680960
H	-3.3105710	2.1244700	0.5415660
C	-4.7069920	1.0167150	-0.7352060
H	-5.4336430	1.2963310	0.0310090
H	-5.1206790	1.3473620	-1.6904700
C	-4.4609870	-0.5077530	-0.7369720
H	-4.3409890	-0.8710640	-1.7632740
H	-5.2847060	-1.0690750	-0.2869130
B	1.3811670	1.7138260	1.8011500
H	2.3500220	2.1768890	2.3345620
H	0.5906900	1.0778900	2.4310770
H	0.7408660	2.6997070	1.4144780

INT1-1d' ***G*= -842.845801 a.u.** **G_{corr}= 0.445300 a.u.**

O	-5.3585450	-0.6578760	-0.5722610
H	-5.7025930	-0.5803210	-1.4681160
C	-3.9452010	-0.5242810	-0.6370750
H	-3.5178260	-1.3869260	-1.1751570
C	-3.5117980	0.7429740	-1.3416270
H	-3.8753170	0.7442640	-2.3762140
H	-3.9716900	1.6004170	-0.8384940
C	-1.9964120	0.8381370	-1.3313950
H	-1.6725680	1.7491080	-1.8467240
H	-1.5993310	0.0004410	-1.9160760
C	-1.3359350	0.8098430	0.0672080
C	-3.4212170	-0.5198280	0.7800060
H	-3.7333820	-1.4368030	1.2880020
H	-3.9082880	0.3045850	1.3117770
C	-1.9001210	-0.3870070	0.8791460
C	-1.7311230	2.0815810	0.8226730
H	-1.5130840	2.9820090	0.2434520
H	-1.2036370	2.1523630	1.7763840
H	-2.7997700	2.0939570	1.0421670
C	3.4930750	0.4158260	1.4896360
H	4.1751300	1.2171400	1.7902360
H	3.9856670	-0.5327790	1.7153130
H	2.6087740	0.4845360	2.1253810
C	-1.1979350	-1.7507190	0.6670410
H	-1.9190410	-2.5352950	0.4363230
C	0.0248910	-1.7484470	-0.2295480
H	-0.2931500	-1.6828250	-1.2759260
H	0.5633480	-2.6935030	-0.1162040
C	0.9113460	-0.5762180	0.1313650
H	1.0791430	-0.6303680	1.2114890
C	0.2164750	0.7540180	-0.2094150
H	0.3007340	0.8216610	-1.3027230
C	1.0575280	1.9214100	0.3156830

H	0.5995580	2.8740140	0.0408560
H	1.0902160	1.9010770	1.4098840
C	2.4784140	1.8922870	-0.2555970
H	3.0638010	2.7198710	0.1615130
H	2.4241270	2.0570460	-1.3395780
C	2.2730590	-0.5691860	-0.5356650
H	2.1117050	-0.3403940	-1.6008620
C	3.1706830	0.5599220	-0.0001280
C	3.1689660	-1.8013370	-0.4823660
H	2.8526270	-2.5759420	-1.1843070
H	3.1491570	-2.2503380	0.5154110
C	4.5760140	-1.2475430	-0.8146580
H	5.3096760	-1.5849000	-0.0789110
H	4.9255670	-1.6026380	-1.7866670
C	4.4451190	0.2920130	-0.8026960
H	4.3147190	0.6696560	-1.8224880
H	5.3252320	0.7865590	-0.3819400
B	-1.3562070	-0.6998260	2.2996270
H	-2.0730690	-1.2664200	3.0787720
H	-0.3004110	-0.2864450	2.6811290
H	-0.8015960	-2.1113470	1.6867190

TS2-1d’ ***G*= -842.841288 a.u.** **G_{corr}= 0.448419 a.u.** **□ν_{min}= 60.0*i* cm^{-1}**

O	-5.4113770	-0.5487550	-0.1639980
H	-5.8649220	-0.5473730	-1.0132760
C	-4.0118400	-0.5441600	-0.4207740
H	-3.7422530	-1.4683510	-0.9523260
C	-3.5895450	0.6311170	-1.2799260
H	-4.0497930	0.5444640	-2.2713070
H	-3.9748610	1.5524390	-0.8318660
C	-2.0746820	0.6781530	-1.4139820
H	-1.7808310	1.5348410	-2.0307360
H	-1.7395610	-0.2153070	-1.9528030
C	-1.3308260	0.7579180	-0.0665920
C	-3.3155820	-0.5243410	0.9273690
H	-3.5836250	-1.4308630	1.4796550
H	-3.7274570	0.3142610	1.4980660
C	-1.7764770	-0.4318880	0.8347430
C	-1.7346050	2.0666290	0.6214720
H	-1.5590900	2.9282630	-0.0271520
H	-1.1785770	2.2270730	1.5469140
H	-2.7939270	2.0745340	0.8778500
C	3.3512690	0.5400650	1.5496960
H	3.9793030	1.3808440	1.8603540
H	3.8495310	-0.3762080	1.8748380
H	2.4109390	0.6127740	2.0988320
C	-1.2505230	-1.8211860	0.3363960

H	-2.0182950	-2.3055550	-0.2717660
C	0.0676630	-1.7652330	-0.4253140
H	-0.1127780	-1.6579550	-1.5013810
H	0.6079680	-2.7066240	-0.2929840
C	0.9034100	-0.5934450	0.0434040
H	0.9652990	-0.6484470	1.1399680
C	0.2155150	0.7203640	-0.3719780
H	0.2961770	0.7290840	-1.4690330
C	1.0283630	1.9305470	0.1009070
H	0.5752200	2.8533780	-0.2685260
H	1.0045440	1.9949560	1.1928490
C	2.4798770	1.8798430	-0.3783470
H	3.0278930	2.7473020	0.0076210
H	2.4978700	1.9542210	-1.4734700
C	2.3187510	-0.5883740	-0.5002200
H	2.2381620	-0.4236640	-1.5866430
C	3.1600530	0.5819240	0.0315830
C	3.2180690	-1.8045280	-0.3039310
H	2.9700360	-2.6199800	-0.9864700
H	3.1142650	-2.1989130	0.7117620
C	4.6448570	-1.2540340	-0.5428960
H	5.3112500	-1.5340680	0.2762380
H	5.0846560	-1.6645490	-1.4545660
C	4.5006400	0.2806590	-0.6404350
H	4.4548970	0.5911120	-1.6898390
H	5.3370340	0.8134770	-0.1790490
B	-1.2051180	-0.3715500	2.2889950
H	-1.6750910	-1.1129910	3.1090380
H	-0.3090890	0.3456400	2.6324710
H	-1.1246060	-2.4802120	1.2066890

INT2-1d' ***G*= -842.848410 a.u.** **G_{corr}= 0.445376 a.u.**

O	-5.4459760	-0.4249110	0.0135970
H	-5.9941040	-0.0016420	-0.6554570
C	-4.0895240	-0.2917000	-0.3906840
H	-3.9272480	-0.8617720	-1.3174510
C	-3.7031910	1.1536160	-0.6358730
H	-4.3096980	1.5631590	-1.4522590
H	-3.9388380	1.7362690	0.2611230
C	-2.2260670	1.2519820	-0.9851830
H	-1.9495770	2.2951130	-1.1709010
H	-2.0570880	0.7207360	-1.9279920
C	-1.2968960	0.6753490	0.0972870
C	-3.2411900	-0.8936080	0.7142140
H	-3.5228230	-1.9439670	0.8440390
H	-3.5092120	-0.3787190	1.6439980
C	-1.7216130	-0.7905880	0.4367770

C	-1.3990310	1.5634720	1.3406010
H	-1.3418030	2.6209740	1.0718650
H	-0.6068140	1.3592870	2.0609760
H	-2.3467960	1.4113950	1.8597120
C	3.1344090	0.8219100	1.5483590
H	3.6348550	1.7558500	1.8225890
H	3.6884840	0.0051420	2.0170850
H	2.1392390	0.8367180	1.9963890
C	-1.3020150	-1.7129790	-0.7146070
H	-1.6574280	-1.3235340	-1.6725240
C	0.2235140	-1.8409160	-0.7320420
H	0.5857270	-1.9057580	-1.7639090
H	0.5397660	-2.7604410	-0.2324400
C	0.8982990	-0.6412640	-0.0611440
H	0.8338720	-0.7547020	1.0422080
C	0.1643400	0.6458500	-0.4749950
H	0.0711260	0.5666270	-1.5679220
C	0.9483290	1.9367470	-0.2084550
H	0.4528810	2.7636250	-0.7280240
H	0.9107720	2.1877070	0.8523210
C	2.4157410	1.8736530	-0.6228530
H	2.9142810	2.8109250	-0.3497730
H	2.4981910	1.7737720	-1.7126130
C	2.3654690	-0.5806600	-0.4390940
H	2.3829290	-0.5298870	-1.5396120
C	3.1016310	0.6795910	0.0255520
C	3.2863270	-1.7263690	-0.0337300
H	3.1333580	-2.6197300	-0.6426760
H	3.0973080	-2.0138830	1.0053420
C	4.7070870	-1.1364640	-0.1970280
H	5.2995340	-1.2961770	0.7067710
H	5.2499510	-1.6184470	-1.0130670
C	4.5139480	0.3703010	-0.4754510
H	4.5636720	0.5654480	-1.5520520
H	5.2774670	0.9899230	0.0034150
B	-1.1155120	-1.3558750	1.7668270
H	-0.9194280	-2.5370700	1.8600530
H	-0.9563740	-0.6909260	2.7483830
H	-1.7682220	-2.6948820	-0.5904070

TS3-1d' ***G*= -842.841288 a.u.** **G_{corr}= 0.448419 a.u.** **□ν_{min}= 60.8*i* cm^{-1}**

O	-5.4113800	-0.5487280	-0.1639700
H	-5.8649350	-0.5474030	-1.0132430
C	-4.0118460	-0.5441620	-0.4207610
H	-3.7422820	-1.4683670	-0.9523010
C	-3.5895430	0.6310950	-1.2799370
H	-4.0497920	0.5444230	-2.2713170

H	-3.9748570	1.5524280	-0.8318980
C	-2.0746800	0.6781260	-1.4139950
H	-1.7808290	1.5348020	-2.0307650
H	-1.7395620	-0.2153440	-1.9528010
C	-1.3308260	0.7579140	-0.0666060
C	-3.3155760	-0.5243370	0.9273770
H	-3.5836140	-1.4308590	1.4796660
H	-3.7274500	0.3142650	1.4980750
C	-1.7764720	-0.4318830	0.8347410
C	-1.7346140	2.0666330	0.6214370
H	-1.5591200	2.9282550	-0.0272080
H	-1.1785760	2.2271050	1.5468680
H	-2.7939320	2.0745290	0.8778300
C	3.3512630	0.5400630	1.5497050
H	3.9792780	1.3808550	1.8603680
H	3.8495470	-0.3762000	1.8748430
H	2.4109300	0.6127480	2.0988390
C	-1.2505200	-1.8211850	0.3364000
H	-2.0182930	-2.3055590	-0.2717570
C	0.0676650	-1.7652350	-0.4253120
H	-0.1127760	-1.6579630	-1.5013800
H	0.6079710	-2.7066250	-0.2929770
C	0.9034100	-0.5934440	0.0434000
H	0.9652940	-0.6484400	1.1399650
C	0.2155150	0.7203640	-0.3719850
H	0.2961840	0.7290890	-1.4690400
C	1.0283600	1.9305450	0.1009090
H	0.5752180	2.8533780	-0.2685210
H	1.0045370	1.9949480	1.1928520
C	2.4798760	1.8798430	-0.3783380
H	3.0278900	2.7473030	0.0076340
H	2.4978740	1.9542250	-1.4734610
C	2.3187520	-0.5883730	-0.5002170
H	2.2381690	-0.4236640	-1.5866400
C	3.1600520	0.5819240	0.0315920
C	3.2180710	-1.8045250	-0.3039240
H	2.9700300	-2.6199870	-0.9864470
H	3.1142790	-2.1988940	0.7117770
C	4.6448540	-1.2540320	-0.5429160
H	5.3112720	-1.5340900	0.2761900
H	5.0846200	-1.6645290	-1.4546100
C	4.5006430	0.2806650	-0.6404210
H	4.4549170	0.5911420	-1.6898180
H	5.3370340	0.8134680	-0.1790120
B	-1.2051080	-0.3715350	2.2889900
H	-1.6750590	-1.1129900	3.1090330
H	-0.3090980	0.3456790	2.6324650
H	-1.1245990	-2.4802040	1.2066970

1d' ***G*= -842.860931 a.u.** **G_{corr}= 0.452339 a.u.**

O	4.4128160	0.2331420	-0.4133390
H	4.8840160	-0.5613020	-0.1292450
C	3.4201110	-0.0934460	-1.4583450
H	3.9345700	0.0028780	-2.4157590
C	2.8665500	-1.4836270	-1.2372250
H	2.0924790	-1.6381310	-1.9956970
H	3.6391620	-2.2380160	-1.4232310
C	2.3039620	-1.6421700	0.1706500
H	3.1405800	-1.7027920	0.8763030
H	1.7948020	-2.6049150	0.2528000
C	1.3905320	-0.4980280	0.6501690
C	2.3671840	0.9487000	-1.2046010
H	1.5053450	0.7628100	-1.8472690
H	2.7508550	1.9440470	-1.4515470
C	2.0934270	0.8601980	0.3113770
C	1.2453620	-0.6740790	2.1646330
H	0.9338770	-1.6939320	2.4069480
H	0.5130280	0.0043560	2.6038280
H	2.2001030	-0.4966860	2.6626810
C	-3.4090060	-0.8407540	1.3717970
H	-3.9763140	-1.7676230	1.5026670
H	-4.0519930	-0.0175340	1.6920230
H	-2.5599720	-0.8756030	2.0564120
C	1.2207960	2.0318230	0.7504790
H	1.7208850	2.9702320	0.4852170
C	-0.1650610	1.9891650	0.1232780
H	-0.0842140	2.1478220	-0.9599820
H	-0.7760170	2.8136940	0.5057060
C	-0.8814160	0.6684410	0.3758740
H	-1.0946450	0.6080590	1.4503640
C	-0.0113910	-0.5437870	-0.0215860
H	0.1406960	-0.4598940	-1.1060720
C	-0.7706080	-1.8594430	0.1890720
H	-0.1742950	-2.6969310	-0.1825840
H	-0.9135420	-2.0403880	1.2584180
C	-2.1282220	-1.8842230	-0.5129380
H	-2.6375070	-2.8328840	-0.3059900
H	-1.9737620	-1.8370650	-1.5988170
C	-2.1994370	0.5853750	-0.3729790
H	-1.9458130	0.5453580	-1.4450270
C	-2.9889440	-0.7019070	-0.0934360
C	-3.2372120	1.6914400	-0.2103280
H	-2.9713130	2.5962580	-0.7606800
H	-3.3295230	1.9770930	0.8422160
C	-4.5475370	1.0521100	-0.7289300

H	-5.3582030	1.1882990	-0.0092890
H	-4.8786670	1.5173250	-1.6601550
C	-4.2376860	-0.4463920	-0.9392570
H	-4.0052460	-0.6413150	-1.9917700
H	-5.0761510	-1.0935480	-0.6658700
B	3.6240500	0.9640600	0.8393690
H	4.0472920	2.1035770	0.8375520
H	3.9714590	0.3368050	1.8170680
H	1.1268270	2.0381260	1.8424200

Cartesian coordinates for the structures of the retrohydroboration mechanism for 1e'

TS1-1e' ***G*= -842.840942 a.u.** **G_{corr}= 0.445586 a.u.** **ν_{min}= 338.5*i* cm^{-1}**

O	5.5856280	0.1196300	-0.0336940
H	6.1160880	-0.5685040	-0.4485280
C	4.2435010	-0.0423760	-0.4707670
H	4.1871190	0.1312770	-1.5575800
C	3.7211730	-1.4390000	-0.1769620
H	4.2911070	-2.1708720	-0.7610740
H	3.9202100	-1.6582620	0.8769720
C	2.2336750	-1.5879660	-0.4839810
H	1.9077590	-2.5885200	-0.1865680
H	2.0769190	-1.5165040	-1.5678090
C	1.3683390	-0.5227790	0.2018830
C	3.4007070	1.0164710	0.2096480
H	3.7605610	2.0082720	-0.0819130
H	3.5187430	0.9365210	1.2955580
C	1.9450970	0.8509860	-0.2014650
C	1.3913820	-0.7334640	1.7172460
H	0.8090300	-1.6163860	1.9936470
H	0.9814030	0.1209510	2.2601560
H	2.4044220	-0.8875260	2.0897070
C	-3.2726800	-1.3500420	1.2968700
H	-3.7907170	-2.3134680	1.2685660
H	-3.8993360	-0.6603340	1.8667520
H	-2.3488580	-1.4937410	1.8601670
C	1.0798730	2.0010020	0.2845230
H	1.5866370	2.7866340	0.8340290
C	-0.2802440	1.8181290	0.5364570
H	-0.7811900	2.5273720	1.1880580
C	-0.9510050	0.4830330	0.4017040
H	-1.0550560	0.1611350	1.4476140
C	-0.0806040	-0.5434930	-0.3401820
H	-0.0210880	-0.2076230	-1.3861650
C	-0.7532160	-1.9168450	-0.3615960
H	-0.1677790	-2.5970390	-0.9848790

H	-0.7540070	-2.3481690	0.6445690
C	-2.1839770	-1.8648620	-0.9006690
H	-2.6312750	-2.8645190	-0.8628710
H	-2.1579170	-1.5672210	-1.9565340
C	-2.3424130	0.5089850	-0.1996360
H	-2.2164590	0.7286870	-1.2703180
C	-3.0345710	-0.8615330	-0.1340690
C	-3.3896400	1.4761020	0.3369850
H	-3.2259900	2.4998170	-0.0064480
H	-3.3671020	1.4988470	1.4308410
C	-4.7248300	0.8873780	-0.1785160
H	-5.4522940	0.8080780	0.6323980
H	-5.1750940	1.5286050	-0.9391550
C	-4.3844170	-0.5032230	-0.7596310
H	-4.2720990	-0.4424460	-1.8471410
H	-5.1577130	-1.2480330	-0.5522800
H	1.9361320	0.8551830	-1.2962680
B	0.1360610	2.8342160	-0.9493930
H	0.5013940	2.3497820	-1.9836770
H	0.2630250	4.0143890	-0.7583510
H	-1.0687980	2.6064820	-0.8920120

INT-1e' ***G*= -842.843155 a.u.** **G_{corr}= 0.445300 a.u.**

O	5.5817480	0.1587810	-0.1274930
H	6.1051640	-0.5207860	-0.5648330
C	4.2278200	-0.0157280	-0.5172030
H	4.1278210	0.1676920	-1.5995140
C	3.7289020	-1.4191050	-0.2173750
H	4.2926450	-2.1419890	-0.8182960
H	3.9525290	-1.6413870	0.8311470
C	2.2373470	-1.5782970	-0.4941310
H	1.9273600	-2.5871940	-0.2089470
H	2.0565260	-1.4878260	-1.5728840
C	1.3722140	-0.5385980	0.2298540
C	3.4005850	1.0254360	0.2071350
H	3.7384060	2.0254890	-0.0826750
H	3.5595510	0.9301310	1.2863980
C	1.9314280	0.8524230	-0.1484900
C	1.4195800	-0.7797230	1.7392730
H	0.9025520	-1.7078320	1.9962610
H	0.9493080	0.0305410	2.3010590
H	2.4431120	-0.8688310	2.1052550
C	-3.3250480	-1.3178210	1.2906130
H	-3.8758650	-2.2629660	1.2608650
H	-3.9390670	-0.6000980	1.8395210
H	-2.4192610	-1.4881250	1.8755840
C	1.0757140	1.9627370	0.4075080

H	1.5789020	2.7991690	0.8808460
C	-0.2729380	1.7952250	0.6097100
H	-0.7876320	2.5050010	1.2472390
C	-0.9519480	0.4664000	0.4383110
H	-1.0931130	0.1262930	1.4746890
C	-0.0814710	-0.5644530	-0.2944720
H	-0.0292510	-0.2401300	-1.3437960
C	-0.7595230	-1.9355480	-0.2992460
H	-0.1697090	-2.6329680	-0.8992100
H	-0.7817850	-2.3463870	0.7152740
C	-2.1803450	-1.8808860	-0.8661640
H	-2.6378010	-2.8756070	-0.8170780
H	-2.1296600	-1.6059720	-1.9273070
C	-2.3244900	0.5067900	-0.2054500
H	-2.1653780	0.7070770	-1.2739760
C	-3.0379610	-0.8531470	-0.1390210
C	-3.3712180	1.4996900	0.2806270
H	-3.1780550	2.5108700	-0.0834690
H	-3.3798940	1.5497110	1.3740000
C	-4.7009140	0.9186570	-0.2579020
H	-5.4486840	0.8593080	0.5362620
H	-5.1260990	1.5530190	-1.0386050
C	-4.3636240	-0.4847540	-0.8094580
H	-4.2175310	-0.4403710	-1.8938390
H	-5.1541760	-1.2153100	-0.6161570
H	1.8655150	0.9033370	-1.2416110
B	0.0249780	2.7747260	-0.9451950
H	-0.3812460	2.0041790	-1.7750820
H	1.1309770	3.1499820	-1.2686650
H	-0.6396980	3.7423240	-0.6772480

3 **G= -816.272127 a.u.** **G_{corr}= 0.414958 a.u.**

O	5.5796370	0.3010890	-0.1896530
H	6.1076770	-0.4315230	-0.5235000
C	4.2292710	0.0725420	-0.5676690
H	4.1430790	0.1155950	-1.6658720
C	3.7363740	-1.2870490	-0.0991830
H	4.3073220	-2.0746180	-0.6048550
H	3.9601500	-1.3764010	0.9687750
C	2.2450190	-1.4937410	-0.3516280
H	1.9436290	-2.4566790	0.0702900
H	2.0634270	-1.5545870	-1.4325340
C	1.3792590	-0.3660830	0.2240350
C	3.3861590	1.1933000	0.0049140
H	3.7249720	2.1490780	-0.4076720
H	3.5295430	1.2425030	1.0893420
C	1.9230640	0.9604650	-0.3496020

C	1.4393640	-0.3959260	1.7525240
H	0.9079200	-1.2705020	2.1372810
H	0.9887150	0.4946510	2.1945490
H	2.4636680	-0.4541800	2.1218540
C	-3.3350740	-1.0087590	1.3771810
H	-3.8854540	-1.9513200	1.4570960
H	-3.9551980	-0.2300560	1.8271680
H	-2.4356160	-1.1033420	1.9879100
C	1.0298000	2.1207480	-0.0311660
H	1.4723830	3.1143240	-0.0728360
C	-0.2597260	1.9832500	0.2650260
H	-0.8572280	2.8645610	0.4865910
C	-0.9434100	0.6546480	0.3497310
H	-1.0992510	0.4411850	1.4174480
C	-0.0827780	-0.4640450	-0.2631970
H	-0.0486790	-0.2628020	-1.3453530
C	-0.7553210	-1.8265410	-0.1010110
H	-0.1642040	-2.5939090	-0.6075620
H	-0.7822250	-2.1088780	0.9566400
C	-2.1724350	-1.8381420	-0.6796900
H	-2.6377420	-2.8160420	-0.5107030
H	-2.1119020	-1.6992720	-1.7667240
C	-2.3113830	0.6185460	-0.3151420
H	-2.1389260	0.6886850	-1.4000010
C	-3.0309760	-0.7236750	-0.0955970
C	-3.3675620	1.6609830	0.0330570
H	-3.1770160	2.6219370	-0.4491650
H	-3.3864410	1.8452280	1.1116500
C	-4.6919690	1.0172190	-0.4437680
H	-5.4462160	1.0509510	0.3457410
H	-5.1121550	1.5531430	-1.2976780
C	-4.3479830	-0.4406360	-0.8208600
H	-4.1887920	-0.5251540	-1.9011480
H	-5.1408300	-1.1444130	-0.5519590
H	1.9001310	0.8405080	-1.4452810

TS2-1e' ***G*= -842.835360 a.u.** **G_{corr}= 0.445670 a.u.** **ν_{min}= -509.3*i* cm^{-1}**

O	5.5584290	0.0559780	-0.1730200
H	6.0846420	-0.7107120	-0.4226170
C	4.2199250	-0.1813510	-0.5855830
H	4.1796890	-0.2351500	-1.6859820
C	3.6800370	-1.4864650	-0.0228650
H	4.2480670	-2.3246530	-0.4431950
H	3.8635880	-1.4929350	1.0562970
C	2.1930220	-1.6812660	-0.3077760
H	1.8625880	-2.6116980	0.1612020
H	2.0380630	-1.7996400	-1.3878660

C	1.3371190	-0.5041200	0.1899200
C	3.3783790	1.0015460	-0.1501820
H	3.7349560	1.9050730	-0.6549930
H	3.5002490	1.1674790	0.9238990
C	1.9221630	0.7466280	-0.5070080
C	1.3984450	-0.4806520	1.7199830
H	1.1316700	-1.4654040	2.1137200
H	0.7222810	0.2475600	2.1627760
H	2.3977660	-0.2481330	2.0882890
C	-3.3117010	-0.9401650	1.4879080
H	-3.8366370	-1.8742440	1.7098030
H	-3.9312630	-0.1217200	1.8610240
H	-2.3868960	-0.9399360	2.0673050
C	1.0525250	1.9780910	-0.4863770
H	1.3582090	2.7422640	-1.1936880
C	-0.3163580	1.8881560	-0.2048380
H	-0.9680630	2.6424120	-0.6318020
C	-0.9730450	0.5751350	0.1745630
H	-1.0783120	0.5319740	1.2605530
C	-0.1233050	-0.6233910	-0.2980540
H	-0.0817410	-0.5558770	-1.3967420
C	-0.8112630	-1.9485150	0.0329050
H	-0.2346300	-2.7731850	-0.3929990
H	-0.8148880	-2.1050440	1.1160620
C	-2.2409470	-2.0187790	-0.5032320
H	-2.7031150	-2.9678840	-0.2093300
H	-2.2141670	-2.0041290	-1.6002710
C	-2.3634460	0.4605510	-0.4313730
H	-2.2346700	0.3973790	-1.5229220
C	-3.0737740	-0.8400830	-0.0208570
C	-3.4050400	1.5431620	-0.1648660
H	-3.2400820	2.4413030	-0.7634740
H	-3.3775200	1.8516190	0.8842900
C	-4.7476640	0.8542600	-0.5075900
H	-5.4691950	0.9895430	0.3010970
H	-5.2000670	1.2852150	-1.4032680
C	-4.4208440	-0.6402190	-0.7175280
H	-4.3096120	-0.8582450	-1.7849850
H	-5.1997320	-1.3018610	-0.3286110
H	1.9276340	0.4705090	-1.5742250
B	0.7250670	2.8222020	0.9870770
H	0.8437160	3.9989620	0.7737620
H	1.3727720	2.2825280	1.8363290
H	-0.4434370	2.6626430	1.3464340

TS1-1f' ***G*= -842.838257 a.u.** **G_{corr}= 0.445275 a.u.** **ν_{min}= -465.8*i* cm^{-1}**

O	5.5646340	0.0534100	-0.2220710

H	6.0843580	-0.7191110	-0.4675090
C	4.2185760	-0.1872060	-0.6034710
H	4.1529100	-0.2481120	-1.7022050
C	3.6881350	-1.4852400	-0.0167590
H	4.2461570	-2.3282190	-0.4405580
H	3.8951260	-1.4813100	1.0579930
C	2.1958160	-1.6827410	-0.2696410
H	1.8732750	-2.6017320	0.2261500
H	2.0219070	-1.8270510	-1.3437350
C	1.3432300	-0.4967980	0.2116340
C	3.3906600	1.0007210	-0.1555610
H	3.7412690	1.9036300	-0.6651700
H	3.5292540	1.1624150	0.9175550
C	1.9287240	0.7473250	-0.4858630
C	1.4097190	-0.4235310	1.7373840
H	1.0001950	-1.3385200	2.1731040
H	0.8513990	0.4191440	2.1410460
H	2.4341370	-0.3284830	2.0984740
C	-3.3170750	-0.9380630	1.4847460
H	-3.8378110	-1.8734000	1.7118280
H	-3.9448410	-0.1199340	1.8444890
H	-2.3976080	-0.9239810	2.0720720
C	1.0538430	1.9614600	-0.4740660
H	1.4237900	2.7832460	-1.0804400
C	-0.3177780	1.9003660	-0.2146580
H	-0.9454060	2.6123740	-0.7373740
C	-0.9719410	0.5822890	0.1729130
H	-1.0884710	0.5456550	1.2586020
C	-0.1176940	-0.6212470	-0.2779130
H	-0.0704120	-0.5664100	-1.3774870
C	-0.7975660	-1.9485300	0.0617260
H	-0.2157170	-2.7753250	-0.3530480
H	-0.8081150	-2.0965950	1.1461240
C	-2.2228870	-2.0318130	-0.4839140
H	-2.6827830	-2.9798750	-0.1830380
H	-2.1869100	-2.0295340	-1.5808190
C	-2.3553980	0.4469910	-0.4412250
H	-2.2178130	0.3717770	-1.5315630
C	-3.0647950	-0.8514360	-0.0224630
C	-3.4054550	1.5265570	-0.1975140
H	-3.2367910	2.4211440	-0.8002920
H	-3.3908650	1.8436570	0.8492460
C	-4.7411440	0.8292410	-0.5503810
H	-5.4764420	0.9736740	0.2443910
H	-5.1812520	1.2456170	-1.4591520
C	-4.4058380	-0.6671860	-0.7349360
H	-4.2835510	-0.8998560	-1.7981780
H	-5.1863220	-1.3266190	-0.3450770

H	1.9044690	0.4989880	-1.5613340
B	0.4682790	2.8474960	1.0259260
H	0.1331650	2.3343020	2.0554020
H	0.2391150	4.0117660	0.8330270
H	1.6953190	2.7049680	1.0041920

1e' ***G*= -842.864015 a.u.** **G_{corr}= 0.447066 a.u.**

O	5.5578510	-0.0267530	-0.5112530
H	6.0342820	-0.8088690	-0.8152010
C	4.1667140	-0.2408670	-0.7390490
H	3.9831760	-0.3243710	-1.8244370
C	3.6641500	-1.5063150	-0.0607240
H	4.1788250	-2.3833780	-0.4765830
H	3.9313900	-1.4574580	1.0031050
C	2.1551320	-1.6730540	-0.2354290
H	1.8353950	-2.5770520	0.2943250
H	1.9361850	-1.8420270	-1.3002370
C	1.3274370	-0.4593260	0.2381950
C	3.4200530	0.9695740	-0.2127860
H	3.7710320	1.8709560	-0.7309740
H	3.6678080	1.0970670	0.8473210
C	1.9139480	0.8164330	-0.4232480
C	1.3995050	-0.3542810	1.7641860
H	0.9914350	-1.2481800	2.2479990
H	0.8036560	0.4867650	2.1612320
H	2.4236190	-0.2286630	2.1237000
C	-3.3465490	-0.7161700	1.5474160
H	-3.8738910	-1.6148780	1.8900360
H	-3.9643630	0.1466980	1.8177250
H	-2.4176540	-0.6410690	2.1199400
C	1.0989330	2.0536600	-0.0009930
H	1.5677420	2.9331800	-0.4872740
C	-0.3362390	1.9080980	-0.5113180
H	-0.3389640	1.8555370	-1.6122010
C	-1.0003910	0.6473660	0.0393790
H	-1.0980560	0.7693020	1.1285440
C	-0.1430870	-0.6066860	-0.2522740
H	-0.0757460	-0.6725420	-1.3532410
C	-0.8386050	-1.8938460	0.2209120
H	-0.2621850	-2.7671950	-0.1028310
H	-0.8516390	-1.9272310	1.3172960
C	-2.2717400	-2.0338520	-0.3055450
H	-2.7295940	-2.9463400	0.1005920
H	-2.2459220	-2.1512740	-1.3991840
C	-2.3929350	0.4340520	-0.5370240
H	-2.2570320	0.2276860	-1.6138520
C	-3.1106800	-0.8041980	0.0324680

C	-3.4369420	1.5478710	-0.4279700
H	-3.2659400	2.3513600	-1.1517550
H	-3.4039940	2.0072490	0.5681460
C	-4.7881600	0.8208970	-0.6638760
H	-5.5018350	1.0581150	0.1325010
H	-5.2550970	1.1354390	-1.6029550
C	-4.4625460	-0.6930460	-0.6846970
H	-4.3526940	-1.0439990	-1.7195510
H	-5.2446460	-1.3018800	-0.2153680
H	1.7618760	0.6891150	-1.5089680
B	1.2159080	2.4300650	1.5133580
H	0.2482590	2.7760770	2.1415080
H	2.2842560	2.5092740	2.0536240
H	-0.9300220	2.7884190	-0.2354830

1f' ***G*= -842.864149 a.u.** **G_{corr}= 0.446325 a.u.**

O	5.633843000	0.198200000	-0.253112000
H	6.154034000	-0.524175000	-0.619954000
C	4.273183000	-0.029280000	-0.595022000
H	4.154157000	0.031224000	-1.689270000
C	3.789477000	-1.391123000	-0.134588000
H	4.359700000	-2.176387000	-0.644797000
H	4.004519000	-1.488974000	0.934789000
C	2.301612000	-1.579807000	-0.403917000
H	1.997566000	-2.565142000	-0.041678000
H	2.130257000	-1.578293000	-1.488518000
C	1.421890000	-0.487846000	0.226288000
C	3.444989000	1.071726000	0.029946000
H	3.772961000	2.039661000	-0.363139000
H	3.632483000	1.088768000	1.109204000
C	1.963482000	0.874354000	-0.266811000
C	1.476608000	-0.609087000	1.750886000
H	1.210420000	-1.621144000	2.065464000
H	0.790236000	0.079170000	2.246332000
H	2.474495000	-0.405337000	2.141637000
C	-3.232591000	-1.080576000	1.469953000
H	-3.709198000	-2.043144000	1.679903000
H	-3.897802000	-0.299762000	1.845896000
H	-2.312953000	-1.034108000	2.055463000
C	1.126910000	2.047174000	0.227535000
H	1.561281000	2.979361000	-0.150384000
C	-0.338118000	1.909001000	-0.241723000
H	-0.324626000	1.961111000	-1.339329000
C	-0.923018000	0.556090000	0.169070000
H	-1.006055000	0.545086000	1.263062000
C	-0.034515000	-0.617017000	-0.286174000
H	0.027667000	-0.537571000	-1.383592000

C	-0.685272000	-1.970774000	0.019781000
H	-0.079322000	-2.774772000	-0.405292000
H	-0.697203000	-2.138763000	1.101119000
C	-2.106456000	-2.090378000	-0.527733000
H	-2.532139000	-3.061635000	-0.250523000
H	-2.073804000	-2.058735000	-1.624345000
C	-2.308607000	0.371365000	-0.420675000
H	-2.175295000	0.322106000	-1.513594000
C	-2.985420000	-0.950693000	-0.034379000
C	-3.383514000	1.418549000	-0.158368000
H	-3.227214000	2.336450000	-0.735697000
H	-3.397042000	1.699041000	0.898507000
C	-4.699208000	0.702718000	-0.550986000
H	-5.454575000	0.825816000	0.228185000
H	-5.124053000	1.121742000	-1.465604000
C	-4.330570000	-0.786232000	-0.745540000
H	-4.203727000	-1.007748000	-1.810449000
H	-5.098668000	-1.463712000	-0.361795000
H	1.859881000	0.854506000	-1.362020000
B	-1.034809000	3.149623000	0.380983000
H	-1.373811000	3.127193000	1.532806000
H	-1.141794000	4.183581000	-0.219222000
H	1.177758000	2.101895000	1.321545000

π-complex intermediate formed from cholesterol + BH_3 by α-face

***G*= -842.844508 a.u.** **G_{corr}= 0.445497 a.u.**

O	5.5279030	0.0634570	0.0645610
H	6.0585360	-0.5509920	-0.4528470
C	4.1838190	-0.0410640	-0.3832870
H	4.1256070	0.2286440	-1.4459490
C	3.6311380	-1.4409360	-0.1915030
H	4.1791240	-2.1402130	-0.8325330
H	3.8268270	-1.7435020	0.8425130
C	2.1424630	-1.5273190	-0.5069890
H	1.7909290	-2.5354480	-0.2755310
H	1.9867620	-1.3790310	-1.5806120
C	1.2807980	-0.5109740	0.2587330
C	3.3812100	0.9663310	0.4150490
H	3.7388100	1.9799250	0.2268110
H	3.5463090	0.7612860	1.4798260
C	1.9016970	0.8757510	0.1712870
C	1.2745210	-0.8790230	1.7537270
H	0.7414050	-1.8196680	1.9053490
H	0.7908900	-0.1108870	2.3594910
H	2.2846580	-1.0114910	2.1412880
C	-3.3762280	-1.2839130	1.2506000

H	-3.8916440	-2.2475040	1.1902360
H	-4.0148620	-0.6089170	1.8249890
H	-2.4619960	-1.4364500	1.8266400
C	1.1111950	2.0015140	0.2294840
H	1.5982630	2.9404950	0.4751430
C	-0.3749260	1.9662690	0.4520570
H	-0.8537110	2.6105790	-0.2897640
H	-0.5636120	2.4432010	1.4203830
C	-1.0158900	0.5719740	0.4394220
H	-1.1163810	0.2366480	1.4766810
C	-0.1563920	-0.4613380	-0.3089810
H	-0.0601640	-0.1099200	-1.3439810
C	-0.8427550	-1.8280270	-0.3802300
H	-0.2541950	-2.4994860	-1.0099560
H	-0.8744290	-2.2883540	0.6120350
C	-2.2606920	-1.7466560	-0.9456150
H	-2.7163460	-2.7434520	-0.9465210
H	-2.2129320	-1.4170780	-1.9912100
C	-2.4013070	0.6017930	-0.1783920
H	-2.2605720	0.8495590	-1.2427050
C	-3.1124860	-0.7587210	-0.1627150
C	-3.4504630	1.5659640	0.3645830
H	-3.2703480	2.5975870	0.0553140
H	-3.4478180	1.5571800	1.4589880
C	-4.7831020	1.0090280	-0.1902730
H	-5.5279360	0.9197220	0.6038530
H	-5.2105640	1.6743770	-0.9436080
C	-4.4491340	-0.3714030	-0.7989290
H	-4.3202800	-0.2863680	-1.8830900
H	-5.2337030	-1.1123450	-0.6210160
B	1.6430520	1.8119300	-1.5296210
H	2.5085630	2.6368260	-1.6777380
H	2.0059720	0.7337630	-1.9419160
H	0.5695500	2.0485110	-2.0171090

π-complex intermediate formed from cholesterol + BH_3 by ®-face

***G*= -842.842276 a.u. G_{corr}= 0.445691 a.u.**

O	5.4980930	0.1602050	-0.4534940
H	5.9661420	-0.4027550	-1.0789590
C	4.1099070	0.0284590	-0.7066460
H	3.8784720	0.3969760	-1.7184930
C	3.6182250	-1.3971720	-0.5870230
H	4.1007450	-2.0253000	-1.3439780
H	3.9019300	-1.7928030	0.3933910
C	2.1152760	-1.4193590	-0.7851820

H	1.7398720	-2.4456000	-0.7606900
H	1.8938410	-1.0296370	-1.7855880
C	1.3002210	-0.5953140	0.2472900
C	3.4028700	0.9068890	0.3108250
H	3.7194320	1.9426420	0.1824460
H	3.7313460	0.5848400	1.3029540
C	1.8997300	0.8138340	0.2025090
C	1.4703980	-1.2238230	1.6323890
H	1.3429920	-2.3068750	1.5807790
H	0.7413290	-0.8256620	2.3391160
H	2.4622680	-1.0283830	2.0414760
C	-3.3476920	-0.6317000	1.5572840
H	-3.8810180	-1.5223660	1.9038170
H	-3.9506020	0.2368340	1.8323410
H	-2.4133360	-0.5676760	2.1172420
C	1.1824500	1.9020540	-0.2332300
H	1.7361530	2.7707240	-0.5770010
C	-0.2562420	1.8154340	-0.6316390
H	-0.3009700	1.6962650	-1.7233870
H	-0.7545630	2.7597520	-0.4006380
C	-0.9694730	0.6480230	0.0264790
H	-1.0169900	0.8332700	1.1058020
C	-0.1783980	-0.6368380	-0.2463800
H	-0.1249900	-0.6958160	-1.3432580
C	-0.9222400	-1.8948550	0.2137210
H	-0.3692980	-2.7842540	-0.1035210
H	-0.9517410	-1.9297410	1.3050480
C	-2.3513500	-1.9724590	-0.3181660
H	-2.8429090	-2.8696920	0.0749580
H	-2.3332940	-2.0710580	-1.4110280
C	-2.3755030	0.4891730	-0.5217620
H	-2.2646700	0.2809970	-1.5983870
C	-3.1335730	-0.7181510	0.0446570
C	-3.3661770	1.6416860	-0.3939880
H	-3.1660700	2.4445260	-1.1066210
H	-3.3094200	2.0832270	0.6056490
C	-4.7427540	0.9760270	-0.6306390
H	-5.4438250	1.2419360	0.1637500
H	-5.1938320	1.3108930	-1.5673260
C	-4.4829490	-0.5461850	-0.6554830
H	-4.3995470	-0.8996040	-1.6888310
H	-5.2833720	-1.1191920	-0.1788710
B	1.3790740	2.1324250	1.6186230
H	1.5333730	1.1859090	2.3455860
H	2.2748630	2.9302250	1.7195130
H	0.2612190	2.5592960	1.7574430

π-complex intermediate formed from BH_3 + 3 by ®-face

***G*= -842.839574 a.u. G_{corr}= 0.445376 a.u.**

O	5.5537660	0.0493830	-0.2786610
H	6.0721120	-0.7274610	-0.5129410
C	4.2028960	-0.2045340	-0.6328650
H	4.1203920	-0.2961120	-1.7284820
C	3.6849600	-1.4874060	-0.0029280
H	4.2440200	-2.3403200	-0.4049540
H	3.9000150	-1.4491760	1.0697800
C	2.1918400	-1.6981260	-0.2389100
H	1.8753990	-2.6050380	0.2826700
H	2.0107870	-1.8701590	-1.3077900
C	1.3401100	-0.5033870	0.2179640
C	3.3776280	0.9917470	-0.2027740
H	3.7214710	1.8837870	-0.7356810
H	3.5294260	1.1761640	0.8640560
C	1.9126980	0.7280980	-0.5149050
C	1.4126990	-0.3912280	1.7416300
H	1.0341890	-1.3090930	2.1993970
H	0.8294790	0.4424460	2.1289390
H	2.4352380	-0.2546570	2.0945150
C	-3.3461640	-0.8819690	1.4895280
H	-3.8911650	-1.7990560	1.7331460
H	-3.9600640	-0.0406370	1.8185950
H	-2.4346130	-0.8746360	2.0895110
C	1.0309750	1.9367620	-0.5011010
H	1.4142410	2.8024320	-1.0333970
C	-0.3036380	1.8691850	-0.2091720
H	-0.9476920	2.6829200	-0.5227600
C	-0.9725230	0.5709020	0.1749480
H	-1.1077640	0.5534180	1.2592340
C	-0.1235910	-0.6427990	-0.2542540
H	-0.0869110	-0.6148060	-1.3550040
C	-0.8129650	-1.9540030	0.1227030
H	-0.2329530	-2.7969900	-0.2608760
H	-0.8331380	-2.0653130	1.2112380
C	-2.2352540	-2.0419160	-0.4324660
H	-2.7058990	-2.9761890	-0.1061720
H	-2.1897540	-2.0746850	-1.5285410
C	-2.3486980	0.4410480	-0.4610960
H	-2.1947490	0.3342690	-1.5459250
C	-3.0731750	-0.8410580	-0.0160490
C	-3.3913390	1.5367330	-0.2630370
H	-3.2093890	2.4065150	-0.8976170
H	-3.3827010	1.8920380	0.7715170
C	-4.7297750	0.8379230	-0.6025130

H	-5.4643880	1.0042190	0.1885050
H	-5.1667260	1.2357750	-1.5209510
C	-4.4033080	-0.6639080	-0.7505000
H	-4.2679200	-0.9207090	-1.8065550
H	-5.1934160	-1.3090510	-0.3563570
H	1.8871460	0.4544370	-1.5843000
B	0.6324410	2.8730130	1.1095350
H	0.4837230	4.0286820	0.8039550
H	1.7619690	2.5924490	1.4367210
H	-0.1229520	2.4620210	1.9529210

c. Cartesian coordinates of the structures at SMD-B3LYP-D3/def2-TZVP level for the decalin model

Cholesterol G= -505.228424 a.u. G_{corr}= 0.236114 a.u.

O	3.489820000	0.791820000	0.206096000
H	4.200087000	0.218782000	-0.109084000
C	2.259081000	0.337544000	-0.373479000
H	2.306876000	0.460938000	-1.465544000
C	2.003501000	-1.137873000	-0.062291000
H	2.772615000	-1.746915000	-0.548495000
H	2.123614000	-1.282074000	1.014347000
C	0.611692000	-1.598939000	-0.515300000
H	0.449407000	-2.636455000	-0.208354000
H	0.566777000	-1.586179000	-1.609905000
C	-0.518103000	-0.708171000	0.033587000
C	1.144519000	1.233400000	0.151394000
H	1.330712000	2.262711000	-0.167033000
H	1.157855000	1.228980000	1.244533000
C	-0.207206000	0.753262000	-0.385351000
C	-0.620371000	-0.875907000	1.560364000
H	-0.948720000	-1.891337000	1.797862000
H	-1.336221000	-0.181246000	1.999908000
H	0.332318000	-0.715397000	2.062679000
C	-1.356969000	1.678381000	-0.083433000
H	-1.129004000	2.734781000	0.030372000
C	-2.616336000	1.256943000	0.012619000
H	-3.408828000	1.969160000	0.223400000
C	-3.016798000	-0.185904000	-0.125023000
C	-1.866641000	-1.082476000	-0.607597000
H	-0.103797000	0.734261000	-1.480504000
H	-3.396402000	-0.537752000	0.842019000
H	-3.864754000	-0.268695000	-0.812476000
H	-2.099812000	-2.131342000	-0.401523000
H	-1.769497000	-0.988340000	-1.693905000

BH_3 G= -26.615656 a.u. G_{corr}= 0.008471 a.u.

B	0.000000000	0.000000000	0.000000000

H	0.000000000	1.189962000	0.000000000
H	-1.030538000	-0.594981000	0.000000000
H	1.030538000	-0.594981000	0.000000000

Cartesian coordinates for the structures of the hydroboration mechanism for 1a' and 1b'

TS1-1a' ***G*= -531.835037 a.u.** **G_{corr}= 0.266969 a.u.** **ν_{min}= 535.9*i* cm^{-1}**

O	3.566617000	-0.748905000	-0.372804000
H	4.288435000	-0.346838000	0.126708000
C	2.331380000	-0.368414000	0.244047000
H	2.306198000	-0.746740000	1.274434000
C	2.146147000	1.145912000	0.268851000
H	2.917194000	1.595711000	0.901583000
H	2.302504000	1.528572000	-0.743035000
C	0.760065000	1.532260000	0.793329000
H	0.636788000	2.617568000	0.761146000
H	0.683764000	1.240693000	1.845287000
C	-0.400749000	0.875083000	0.019262000
C	1.222464000	-1.049847000	-0.546072000
H	1.327680000	-2.133408000	-0.489355000
H	1.323450000	-0.772649000	-1.599623000
C	-0.163097000	-0.633041000	-0.108412000
C	-0.476628000	1.453507000	-1.411908000
H	-0.691077000	2.522639000	-1.352661000
H	-1.266900000	0.984505000	-1.997344000
H	0.455939000	1.330719000	-1.960578000
C	-1.269011000	-1.492805000	-0.358824000
H	-1.052175000	-2.367997000	-0.962809000
C	-2.647117000	-0.902120000	-0.602224000
H	-3.400580000	-1.651630000	-0.352764000
H	-2.742896000	-0.729758000	-1.678723000
C	-2.952059000	0.416900000	0.149308000
C	-1.726656000	1.136835000	0.749331000
B	-0.810900000	-1.777758000	1.243635000
H	-0.231351000	-2.821672000	1.349415000
H	0.055647000	-0.920025000	1.514566000
H	-1.713685000	-1.495126000	1.975600000
H	-3.467270000	1.089192000	-0.539048000
H	-3.655782000	0.220765000	0.959829000
H	-1.903469000	2.215126000	0.762023000
H	-1.599276000	0.834767000	1.789480000

INT-1a' ***G*= -531.847459 a.u.** **G_{corr}= 0.268555 a.u.**

O	3.564069000	0.826894000	0.394350000
H	4.305408000	0.401544000	-0.054845000
C	2.353245000	0.420640000	-0.256492000

H	2.358410000	0.787874000	-1.293128000
C	2.206267000	-1.100926000	-0.281317000
H	2.997635000	-1.529587000	-0.904474000
H	2.367556000	-1.474918000	0.732647000
C	0.835631000	-1.543846000	-0.810604000
H	0.754266000	-2.633206000	-0.758339000
H	0.757113000	-1.275430000	-1.869532000
C	-0.344900000	-0.900173000	-0.049424000
C	1.196139000	1.092093000	0.472703000
H	1.293710000	2.176392000	0.389594000
H	1.237913000	0.843368000	1.535840000
C	-0.137842000	0.637565000	-0.117236000
C	-0.365313000	-1.444756000	1.390745000
H	-0.515867000	-2.527095000	1.360809000
H	-1.165292000	-1.019069000	1.990562000
H	0.567425000	-1.261796000	1.922273000
C	-1.368636000	1.495660000	0.343312000
H	-1.062780000	2.152193000	1.157393000
C	-2.614827000	0.698135000	0.738019000
H	-3.478583000	1.368252000	0.721337000
H	-2.519725000	0.374635000	1.776004000
C	-2.914024000	-0.526619000	-0.153367000
C	-1.668774000	-1.221505000	-0.758268000
B	-1.300490000	2.114100000	-1.072956000
H	-0.550756000	3.012576000	-1.313076000
H	-0.016529000	0.804679000	-1.226156000
H	-1.970556000	1.666288000	-1.955086000
H	-1.814981000	-2.304847000	-0.770278000
H	-1.561673000	-0.915795000	-1.803086000
H	-3.487791000	-1.243250000	0.438216000
H	-3.566811000	-0.226070000	-0.975124000

TS2-1a' ***G*= -531.843919 a.u.** **G_{corr}= 0.268983 a.u.** **ν_{min}= 118.7*i* cm^{-1}**

O	3.559122000	0.830066000	0.398491000
H	4.306583000	0.405737000	-0.041400000
C	2.355658000	0.409439000	-0.258759000
H	2.363666000	0.775279000	-1.295769000
C	2.226939000	-1.113113000	-0.278919000
H	3.022385000	-1.537167000	-0.900168000
H	2.393635000	-1.479301000	0.737117000
C	0.860234000	-1.574741000	-0.801346000
H	0.782721000	-2.662601000	-0.715139000
H	0.783593000	-1.340003000	-1.868550000
C	-0.328608000	-0.917420000	-0.070932000
C	1.186359000	1.066263000	0.463503000
H	1.292790000	2.150556000	0.406828000

H	1.214369000	0.796639000	1.521894000
C	-0.137986000	0.617837000	-0.162163000
C	-0.379835000	-1.403771000	1.388652000
H	-0.680011000	-2.454317000	1.417928000
H	-1.092353000	-0.836585000	1.987677000
H	0.585480000	-1.327182000	1.886178000
C	-1.375489000	1.453174000	0.347922000
H	-1.102832000	1.862571000	1.320828000
C	-2.756482000	0.738809000	0.443579000
H	-3.478209000	1.329311000	-0.124006000
H	-3.092941000	0.792512000	1.481008000
C	-2.863772000	-0.737217000	-0.023920000
C	-1.643527000	-1.257943000	-0.784539000
B	-1.235498000	2.444556000	-0.833241000
H	-0.400059000	3.297089000	-0.850954000
H	-0.026966000	0.796050000	-1.253855000
H	-1.912889000	2.287660000	-1.806935000
H	-3.024742000	-1.378877000	0.844383000
H	-3.752239000	-0.856717000	-0.647983000
H	-1.727028000	-2.342541000	-0.906766000
H	-1.611381000	-0.829324000	-1.792511000

1a’ ***G*= -531.860443 a.u.** **G_{corr}= 0.268347 a.u.**

O	3.505512000	1.065323000	0.158058000
H	4.268842000	0.643618000	-0.256312000
B	-1.515350000	2.781868000	-0.065515000
H	-1.015365000	3.173828000	-1.079477000
C	2.317296000	0.471238000	-0.385670000
H	2.268821000	0.684928000	-1.463681000
C	2.299916000	-1.042430000	-0.189932000
H	3.120036000	-1.493353000	-0.758307000
H	2.492815000	-1.254356000	0.864867000
C	0.963994000	-1.649280000	-0.632451000
H	0.965163000	-2.727540000	-0.445945000
H	0.859333000	-1.520416000	-1.715449000
C	-0.256731000	-1.003978000	0.056189000
C	1.123743000	1.136909000	0.282941000
H	1.144442000	2.207567000	0.058227000
H	1.221886000	1.040167000	1.367905000
C	-0.196821000	0.527781000	-0.200991000
H	-0.215138000	0.646316000	-1.293676000
C	-0.243676000	-1.358449000	1.554002000
H	-0.288720000	-2.444055000	1.676669000
H	-1.091624000	-0.933571000	2.089877000
H	0.658336000	-1.010959000	2.056483000
C	-1.425440000	1.281822000	0.331604000

H	-1.503030000	1.154740000	1.416526000
C	-2.728519000	0.688945000	-0.297707000
H	-2.740778000	0.903810000	-1.373100000
H	-3.613446000	1.166427000	0.131061000
C	-2.812900000	-0.829694000	-0.101260000
C	-1.549698000	-1.542895000	-0.587726000
H	-2.172491000	3.549121000	0.573794000
H	-1.631602000	-2.618613000	-0.400989000
H	-1.473471000	-1.419164000	-1.674206000
H	-2.985254000	-1.045895000	0.956349000
H	-3.683080000	-1.214331000	-0.641500000

TS1-1b' ***G*= -531.829962 a.u.** **G_{corr}= 0.266604 a.u.** **ν_{min}= 552.3*i* cm^{-1}**

O	3.567547000	-0.743177000	-0.331382000
H	4.268123000	-0.323269000	0.183184000
C	2.307695000	-0.377377000	0.249662000
H	2.249626000	-0.771390000	1.272722000
C	2.120722000	1.137100000	0.293054000
H	2.877444000	1.579049000	0.949259000
H	2.298063000	1.535957000	-0.709555000
C	0.721950000	1.512184000	0.791433000
H	0.601367000	2.599409000	0.785128000
H	0.620085000	1.189550000	1.831750000
C	-0.417026000	0.867436000	-0.026084000
C	1.220851000	-1.039883000	-0.582843000
H	1.347656000	-2.122734000	-0.558551000
H	1.348896000	-0.723388000	-1.622592000
C	-0.168554000	-0.656453000	-0.087016000
C	-0.422643000	1.446674000	-1.459985000
H	-0.496707000	2.535979000	-1.416935000
H	-1.275179000	1.081664000	-2.033608000
H	0.477237000	1.202064000	-2.022533000
C	-1.266672000	-1.487716000	-0.398142000
H	-1.069394000	-2.437815000	-0.882717000
C	-2.631893000	-0.902198000	-0.626003000
H	-3.398463000	-1.673900000	-0.534021000
H	-2.637130000	-0.586020000	-1.673961000
C	-2.960748000	0.280144000	0.295838000
C	-1.769679000	1.213403000	0.637276000
B	-0.606347000	-1.566568000	1.324654000
H	0.253035000	-2.364637000	1.555343000
H	-0.995243000	-0.826025000	2.173225000
H	-1.606329000	-2.248425000	1.046892000
H	-2.015301000	2.243823000	0.370856000
H	-1.631102000	1.207283000	1.718451000
H	-3.774698000	0.849237000	-0.155639000

H	-3.354647000	-0.128042000	1.227950000

INT-1b' ***G*= -531.844974 a.u.** **G_{corr}= 0.268763 a.u.**

O	3.546978000	-0.738966000	-0.399017000
H	4.267140000	-0.270020000	0.041018000
C	2.315652000	-0.361955000	0.233909000
H	2.326139000	-0.705586000	1.278852000
C	2.115861000	1.152738000	0.226497000
H	2.888225000	1.624191000	0.843192000
H	2.264382000	1.513333000	-0.794480000
C	0.726774000	1.545843000	0.742188000
H	0.600193000	2.630905000	0.677856000
H	0.651655000	1.282676000	1.802576000
C	-0.419570000	0.839777000	-0.017338000
C	1.184476000	-1.086218000	-0.483735000
H	1.335939000	-2.163783000	-0.385871000
H	1.231705000	-0.854284000	-1.551302000
C	-0.162021000	-0.685542000	0.130583000
C	-0.404012000	1.329507000	-1.484241000
H	-0.434999000	2.422414000	-1.501133000
H	-1.264313000	0.974997000	-2.047835000
H	0.486899000	1.023765000	-2.029481000
C	-1.353054000	-1.595384000	-0.347011000
H	-1.017632000	-2.249769000	-1.152530000
C	-2.635135000	-0.840546000	-0.700470000
H	-3.470607000	-1.544295000	-0.734617000
H	-2.538190000	-0.437132000	-1.708328000
C	-2.956918000	0.278082000	0.296741000
C	-1.774143000	1.233799000	0.611249000
B	-0.419214000	-1.355789000	1.508506000
H	0.184580000	-2.348120000	1.790476000
H	-1.225809000	-0.944506000	2.282279000
H	-1.624858000	-2.320634000	0.462879000
H	-2.014458000	2.247714000	0.281870000
H	-1.653098000	1.290922000	1.694500000
H	-3.810815000	0.846599000	-0.077432000
H	-3.289306000	-0.189313000	1.226900000

TS2-1b' ***G*= -531.840481 a.u.** **G_{corr}= 0.268848 a.u.** **□ν_{min}= 176.7*i* cm^{-1}**

O	3.555633000	-0.696841000	-0.465576000
H	4.280814000	-0.235097000	-0.026174000
C	2.333236000	-0.343972000	0.198552000
H	2.364563000	-0.714134000	1.233573000
C	2.125342000	1.169330000	0.229216000
H	2.900781000	1.631202000	0.849256000

H	2.267142000	1.550791000	-0.785153000
C	0.738518000	1.553758000	0.760778000
H	0.602576000	2.636726000	0.680266000
H	0.680045000	1.307276000	1.826552000
C	-0.414667000	0.829806000	0.034932000
C	1.193594000	-1.055010000	-0.518195000
H	1.359959000	-2.133540000	-0.466889000
H	1.207285000	-0.780895000	-1.576880000
C	-0.137829000	-0.688452000	0.149295000
C	-0.478378000	1.301740000	-1.434050000
H	-0.788858000	2.349191000	-1.474957000
H	-1.193769000	0.721281000	-2.018392000
H	0.479956000	1.228686000	-1.944671000
C	-1.327021000	-1.595971000	-0.330713000
H	-1.022424000	-2.108565000	-1.243783000
C	-2.732933000	-0.961440000	-0.472096000
H	-3.445168000	-1.612199000	0.035944000
H	-2.997901000	-1.007525000	-1.529433000
C	-2.946933000	0.498065000	0.016808000
C	-1.750716000	1.164683000	0.708508000
B	-0.358666000	-1.448280000	1.486217000
H	0.316583000	-2.405741000	1.723074000
H	-1.206268000	-1.147237000	2.267928000
H	-1.434009000	-2.454161000	0.381121000
H	-3.227794000	1.106915000	-0.844234000
H	-3.804774000	0.528123000	0.691596000
H	-1.897008000	2.249242000	0.698782000
H	-1.706741000	0.870566000	1.757785000

1b’ ***G*= -531.853477 a.u.** **G_{corr}= 0.268565 a.u.**

O	3.535634000	-0.733520000	-0.391048000
H	4.242817000	-0.237878000	0.041414000
C	2.293215000	-0.370035000	0.218868000
H	2.284208000	-0.743355000	1.258652000
C	2.097860000	1.145104000	0.251004000
H	2.864254000	1.595878000	0.890027000
H	2.266985000	1.525450000	-0.759544000
C	0.703055000	1.542356000	0.753400000
H	0.581856000	2.626945000	0.674533000
H	0.623426000	1.301269000	1.816803000
C	-0.435715000	0.837799000	-0.013316000
C	1.178601000	-1.069757000	-0.549330000
H	1.340133000	-2.149961000	-0.511840000
H	1.224625000	-0.776482000	-1.601692000
C	-0.199598000	-0.711652000	0.060929000
C	-0.451994000	1.378156000	-1.459918000

H	-0.644759000	2.454275000	-1.441991000
H	-1.227435000	0.921742000	-2.072326000
H	0.492792000	1.229131000	-1.980325000
C	-1.341394000	-1.463187000	-0.667617000
H	-1.339801000	-1.200909000	-1.729997000
C	-2.702213000	-1.127038000	-0.042938000
H	-2.733578000	-1.526644000	0.979885000
H	-3.504405000	-1.629375000	-0.590583000
C	-2.963695000	0.382815000	0.004298000
C	-1.798773000	1.154840000	0.637640000
B	-0.164249000	-1.300367000	1.523919000
H	0.001643000	-2.479775000	1.633763000
H	-0.285423000	-0.668117000	2.525915000
H	-1.163466000	-2.540861000	-0.616125000
H	-3.142167000	0.747549000	-1.011278000
H	-3.881469000	0.582129000	0.564798000
H	-1.989450000	2.231216000	0.577012000
H	-1.750708000	0.911361000	1.703582000

Cartesian coordinates for the structures of the hydroboration mechanism for 1c' and 1d'

TS1-1c' ***G*= -531.831188 a.u.** G_{corr}**= 0.265983 a.u.** ν_{min}**= 579.0*i* cm^{-1}**

O	-3.518756000	-0.818026000	-0.150877000
H	-4.128080000	-0.443301000	-0.799491000
C	-2.193869000	-0.398963000	-0.491877000
H	-1.923734000	-0.799636000	-1.478694000
C	-2.043357000	1.113452000	-0.514233000
H	-2.670307000	1.541047000	-1.302558000
H	-2.398510000	1.518096000	0.437045000
C	-0.584662000	1.481077000	-0.764075000
H	-0.467581000	2.566439000	-0.796762000
H	-0.294133000	1.106931000	-1.750651000
C	0.439397000	0.933945000	0.280089000
C	-1.269231000	-0.996277000	0.561196000
H	-1.351796000	-2.082374000	0.545984000
H	-1.613575000	-0.656017000	1.539357000
C	0.180368000	-0.588598000	0.328664000
C	0.196843000	1.588708000	1.647867000
H	0.228663000	2.675866000	1.550094000
H	0.973817000	1.292368000	2.355177000
H	-0.768028000	1.320918000	2.078150000
C	1.019576000	-1.501801000	-0.375994000
H	0.516511000	-2.353142000	-0.822244000
C	2.224703000	-0.992701000	-1.145427000
H	1.908912000	-0.712949000	-2.158076000
H	2.951619000	-1.800884000	-1.256300000
C	2.867091000	0.208942000	-0.462996000

C	1.857702000	1.336522000	-0.244926000
B	1.252903000	-1.784104000	1.282822000
H	0.665771000	-0.859630000	1.872811000
H	0.690846000	-2.779630000	1.639225000
H	2.393782000	-1.585078000	1.576248000
H	3.693580000	0.586234000	-1.070157000
H	3.298445000	-0.103118000	0.488581000
H	1.726455000	1.851010000	-1.199537000
H	2.285520000	2.075747000	0.434979000

INT1-1c' ***G*= -531.847487 a.u.** **G_{corr}= 0.268064 a.u.**

O	-3.449149000	-0.851934000	-0.077078000
H	-3.998200000	-0.642738000	-0.843141000
C	-2.091625000	-0.508788000	-0.395709000
H	-1.758689000	-1.124893000	-1.240678000
C	-1.949822000	0.957995000	-0.781286000
H	-2.495906000	1.148654000	-1.711110000
H	-2.420885000	1.567749000	-0.006127000
C	-0.478293000	1.341002000	-0.955863000
H	-0.400620000	2.406416000	-1.190691000
H	-0.072323000	0.806559000	-1.818421000
C	0.400067000	1.043348000	0.283852000
C	-1.254147000	-0.843270000	0.830889000
H	-1.341989000	-1.910771000	1.039429000
H	-1.687140000	-0.320495000	1.686653000
C	0.229821000	-0.460203000	0.672936000
C	-0.049014000	1.932052000	1.458151000
H	0.092898000	2.985968000	1.203503000
H	0.551265000	1.722093000	2.347033000
H	-1.095924000	1.798917000	1.727664000
C	0.963085000	-1.478456000	-0.300274000
H	0.214754000	-1.905791000	-0.968868000
C	2.102787000	-0.852188000	-1.123780000
H	1.715843000	-0.411207000	-2.047878000
H	2.805872000	-1.633044000	-1.427437000
C	2.814583000	0.224265000	-0.316603000
C	1.885229000	1.407026000	-0.029966000
B	1.422673000	-2.485959000	0.788026000
H	0.683076000	-0.551314000	1.673952000
H	0.653447000	-3.252741000	1.284016000
H	2.536687000	-2.446879000	1.220733000
H	3.705922000	0.579609000	-0.840002000
H	3.165003000	-0.211197000	0.624097000
H	1.891295000	2.081261000	-0.891536000
H	2.299415000	1.982410000	0.801209000

TS2-1c' ***G*= -531.846277 a.u.** **G_{corr}= 0.268194 a.u.** **ν_{min}= 155.7*i* cm^{-1}**

O	3.449162000	0.845670000	0.019390000
H	4.014740000	0.683063000	-0.745975000
C	2.097962000	0.528349000	-0.350982000
H	1.791529000	1.192486000	-1.168550000
C	1.964601000	-0.916083000	-0.822302000
H	2.519998000	-1.047959000	-1.756779000
H	2.436585000	-1.564989000	-0.080181000
C	0.498059000	-1.307415000	-1.027294000
H	0.435229000	-2.358413000	-1.324453000
H	0.084624000	-0.727435000	-1.858104000
C	-0.383439000	-1.081723000	0.221810000
C	1.229481000	0.799978000	0.871314000
H	1.304383000	1.859540000	1.129239000
H	1.652175000	0.245608000	1.711889000
C	-0.248714000	0.406219000	0.666891000
C	0.074225000	-2.006479000	1.364213000
H	-0.032110000	-3.052795000	1.064771000
H	-0.545804000	-1.849517000	2.250765000
H	1.112152000	-1.855110000	1.657818000
C	-0.952484000	1.430652000	-0.294709000
H	-0.256093000	1.676967000	-1.096692000
C	-2.258919000	0.880341000	-0.933599000
H	-2.047350000	0.515748000	-1.943978000
H	-2.998121000	1.679111000	-1.052615000
C	-2.834536000	-0.261712000	-0.108765000
C	-1.868474000	-1.445185000	-0.108054000
B	-1.284197000	2.692573000	0.560731000
H	-0.733914000	0.477590000	1.646396000
H	-0.668592000	3.715214000	0.495748000
H	-2.195346000	2.634376000	1.335580000
H	-1.903884000	-1.916695000	-1.095125000
H	-2.225969000	-2.198996000	0.597215000
H	-3.800913000	-0.578690000	-0.510736000
H	-3.022207000	0.081012000	0.913853000

INT2-1c' ***G*= -531.852818 a.u.** **G_{corr}= 0.268449 a.u.**

O	3.444035000	1.009824000	0.121430000
H	4.065600000	0.827797000	-0.594519000
C	2.144865000	0.561225000	-0.293064000
H	1.830691000	1.137910000	-1.174033000
C	2.134736000	-0.920414000	-0.648683000
H	2.809243000	-1.105830000	-1.491081000
H	2.521493000	-1.487169000	0.203260000
C	0.716406000	-1.362600000	-1.009124000
H	0.703702000	-2.424263000	-1.273494000

H	0.408483000	-0.820542000	-1.909020000
C	-0.328675000	-1.107689000	0.099142000
C	1.191063000	0.832141000	0.858079000
H	1.195209000	1.900558000	1.091725000
H	1.588732000	0.317772000	1.737357000
C	-0.253649000	0.372597000	0.589031000
C	-0.088772000	-2.046620000	1.291193000
H	-0.062246000	-3.089706000	0.964557000
H	-0.894081000	-1.947997000	2.024353000
H	0.849216000	-1.838011000	1.807325000
C	-1.002792000	1.325414000	-0.351007000
H	-0.602873000	1.263470000	-1.363131000
C	-2.544897000	0.973015000	-0.413449000
H	-2.888211000	1.101781000	-1.440065000
H	-3.153623000	1.664696000	0.193906000
C	-2.812332000	-0.461749000	0.065516000
C	-1.741592000	-1.397704000	-0.485781000
B	-1.276789000	2.756892000	0.150082000
H	-0.767311000	0.421107000	1.554202000
H	-1.592930000	3.625434000	-0.607616000
H	-1.305470000	2.981559000	1.324622000
H	-3.806275000	-0.770815000	-0.268548000
H	-2.825256000	-0.504641000	1.157444000
H	-1.720689000	-1.280865000	-1.574029000
H	-2.007910000	-2.440993000	-0.296179000

TS3-1c' ***G*= -531.841284 a.u.** **G_{corr}= 0.267507 a.u.** **□ν_{min}= 217.5*i* cm^{-1}**

O	3.459626000	0.852261000	0.032908000
H	4.038219000	0.649833000	-0.713037000
C	2.122994000	0.469932000	-0.324524000
H	1.786118000	1.088048000	-1.168377000
C	2.030492000	-0.996630000	-0.721239000
H	2.641468000	-1.183747000	-1.610652000
H	2.448542000	-1.602114000	0.087972000
C	0.576951000	-1.378566000	-1.000346000
H	0.513790000	-2.438126000	-1.264364000
H	0.237678000	-0.825110000	-1.881696000
C	-0.404558000	-1.098984000	0.167976000
C	1.239962000	0.740001000	0.880432000
H	1.314173000	1.795520000	1.156630000
H	1.646093000	0.172200000	1.721786000
C	-0.238474000	0.370441000	0.650565000
C	-0.107472000	-2.057132000	1.334187000
H	-0.186463000	-3.097627000	1.007281000
H	-0.825239000	-1.906219000	2.144920000
H	0.890992000	-1.920574000	1.750591000

C	-0.963769000	1.359691000	-0.280489000
H	-0.727178000	1.147284000	-1.327740000
C	-2.492305000	1.157009000	-0.082993000
H	-3.066724000	1.833364000	-0.721490000
H	-2.736974000	1.423586000	0.949779000
C	-2.942337000	-0.296840000	-0.353522000
C	-1.851110000	-1.401889000	-0.359072000
B	-0.801432000	2.868454000	0.051265000
H	-0.731439000	0.455692000	1.626423000
H	-0.877748000	3.705050000	-0.799048000
H	-0.709826000	3.227279000	1.188576000
H	-3.442331000	-0.324353000	-1.323476000
H	-3.709629000	-0.550369000	0.380749000
H	-1.753152000	-1.756073000	-1.386564000
H	-2.242473000	-2.256093000	0.196292000

1c' ***G*= -531.859717 a.u.** **G_{corr}= 0.268621 a.u.**

O	-2.958370000	-0.978139000	0.663430000
H	-2.931875000	-1.940269000	0.733324000
B	2.339874000	-1.282437000	1.449978000
H	3.519040000	-1.081620000	1.412768000
C	-2.329038000	-0.601598000	-0.575327000
H	-2.953322000	-0.948232000	-1.409091000
C	-2.256287000	0.918883000	-0.599772000
H	-1.954916000	1.228608000	-1.603604000
H	-3.254029000	1.330747000	-0.427557000
C	-1.281872000	1.455641000	0.448921000
H	-1.688719000	1.235129000	1.439144000
H	-1.218772000	2.545633000	0.371358000
C	0.142705000	0.862459000	0.369457000
C	-0.935010000	-1.208814000	-0.709916000
H	-0.577357000	-0.998199000	-1.720290000
H	-1.004939000	-2.299655000	-0.630994000
C	0.057606000	-0.692160000	0.343533000
H	-0.327364000	-1.003765000	1.319004000
C	0.893486000	1.320930000	1.627456000
H	0.948394000	2.412325000	1.667430000
H	1.929361000	0.965493000	1.669121000
H	0.389534000	0.975207000	2.532097000
C	1.469437000	-1.310236000	0.162035000
H	1.323080000	-2.404923000	0.064281000
C	2.161455000	-0.795648000	-1.113526000
H	1.612964000	-1.120897000	-2.003492000
H	3.161850000	-1.229484000	-1.192057000
C	2.249724000	0.732276000	-1.111528000
C	0.876398000	1.375656000	-0.891807000

H	1.847759000	-1.559314000	2.503587000
H	2.671292000	1.086393000	-2.056571000
H	2.943068000	1.052703000	-0.327859000
H	0.261449000	1.183957000	-1.774754000
H	0.979461000	2.463121000	-0.820332000

TS1-1d' ***G*= -531.829856 a.u.** **G_{corr}= 0.266691 a.u.** **ν_{min}= 500.9*i* cm^{-1}**

O	-3.506376000	-0.725878000	-0.141395000
H	-4.051764000	-0.389885000	-0.863926000
C	-2.135936000	-0.437588000	-0.444240000
H	-1.828084000	-1.018364000	-1.326582000
C	-1.913792000	1.042816000	-0.730396000
H	-2.465353000	1.328684000	-1.632057000
H	-2.337912000	1.618356000	0.096356000
C	-0.428576000	1.370172000	-0.909771000
H	-0.306584000	2.447206000	-1.053583000
H	-0.065168000	0.892896000	-1.824512000
C	0.466233000	0.918194000	0.277910000
C	-1.298510000	-0.901437000	0.742788000
H	-1.432453000	-1.974895000	0.882900000
H	-1.661381000	-0.411640000	1.648167000
C	0.172015000	-0.581931000	0.498251000
C	0.115630000	1.742749000	1.526783000
H	0.357750000	2.795284000	1.356877000
H	0.691902000	1.397988000	2.386729000
H	-0.939808000	1.689292000	1.790870000
C	0.903652000	-1.519504000	-0.260899000
H	0.436940000	-2.478184000	-0.458013000
C	1.969549000	-1.098644000	-1.228519000
H	1.434523000	-0.838364000	-2.148867000
H	2.622955000	-1.938354000	-1.472286000
C	2.786636000	0.086898000	-0.723796000
C	1.955195000	1.212521000	-0.066129000
B	1.239335000	-1.427503000	1.566232000
H	0.581956000	-2.114010000	2.292809000
H	2.022348000	-0.641783000	2.008453000
H	1.933409000	-2.218970000	0.911679000
H	1.965689000	2.100892000	-0.701636000
H	2.464018000	1.502405000	0.853900000
H	3.379694000	0.487557000	-1.547497000
H	3.499088000	-0.297062000	0.008329000

INT1-1d' ***G*= -531.847378 a.u.** **G_{corr}= 0.268303 a.u.**

O	-3.464834000	-0.690812000	-0.159094000
H	-3.963001000	-0.436146000	-0.945960000

C	-2.075741000	-0.426834000	-0.405937000
H	-1.719481000	-1.092912000	-1.205299000
C	-1.834366000	1.015951000	-0.826601000
H	-2.362594000	1.225066000	-1.763063000
H	-2.264414000	1.672098000	-0.064714000
C	-0.339463000	1.288479000	-1.005099000
H	-0.184781000	2.346994000	-1.234348000
H	0.010879000	0.738194000	-1.879659000
C	0.530785000	0.922140000	0.227151000
C	-1.318905000	-0.737595000	0.873881000
H	-1.509804000	-1.772208000	1.168184000
H	-1.727941000	-0.107583000	1.668726000
C	0.195127000	-0.508542000	0.745730000
C	0.243613000	1.939871000	1.347446000
H	0.525278000	2.946947000	1.026506000
H	0.822983000	1.701537000	2.242585000
H	-0.808415000	1.968373000	1.631662000
C	0.872563000	-1.679768000	-0.076143000
H	0.114096000	-2.406401000	-0.364380000
C	1.738172000	-1.241414000	-1.252676000
H	1.090179000	-0.915093000	-2.067680000
H	2.300523000	-2.099860000	-1.629202000
C	2.703653000	-0.129814000	-0.849541000
C	2.027781000	1.074582000	-0.150333000
B	1.046383000	-1.072958000	1.907193000
H	0.600624000	-1.931454000	2.609002000
H	2.156255000	-0.683477000	2.103098000
H	1.546252000	-2.274379000	0.595999000
H	3.257298000	0.205927000	-1.728918000
H	3.443854000	-0.563870000	-0.171481000
H	2.588853000	1.302280000	0.757619000
H	2.110808000	1.964919000	-0.779167000

TS2-1d' ***G*= -531.842209 a.u.** **G_{corr}= 0.269025 a.u.** **ν_{min}= 78.2*i* cm^{-1}**

O	-3.495995000	-0.640024000	0.063506000
H	-4.068905000	-0.448475000	-0.689790000
C	-2.133222000	-0.480530000	-0.363773000
H	-1.933834000	-1.198501000	-1.167188000
C	-1.868707000	0.925327000	-0.892116000
H	-2.426869000	1.072794000	-1.822688000
H	-2.265410000	1.644412000	-0.171306000
C	-0.376001000	1.171792000	-1.131667000
H	-0.225018000	2.202920000	-1.464468000
H	-0.030813000	0.533780000	-1.949884000
C	0.491961000	0.914421000	0.123746000
C	-1.259464000	-0.823547000	0.841922000

H	-1.415092000	-1.875122000	1.096371000
H	-1.627707000	-0.240385000	1.690379000
C	0.259490000	-0.559805000	0.605694000
C	0.103643000	1.943239000	1.202627000
H	0.252227000	2.955175000	0.814915000
H	0.724732000	1.839819000	2.092243000
H	-0.936148000	1.866406000	1.518283000
C	0.776453000	-1.594790000	-0.456771000
H	0.030940000	-1.733951000	-1.239120000
C	2.121613000	-1.208097000	-1.105218000
H	1.948918000	-0.810438000	-2.109871000
H	2.750609000	-2.093207000	-1.225228000
C	2.838444000	-0.142847000	-0.287567000
C	2.002827000	1.137184000	-0.219447000
B	0.956738000	-0.913878000	1.966247000
H	0.863726000	-2.036047000	2.369685000
H	1.553826000	-0.131512000	2.638550000
H	0.870370000	-2.566095000	0.035195000
H	2.449736000	1.814420000	0.511803000
H	2.072909000	1.646868000	-1.185298000
H	3.821890000	0.079677000	-0.710311000
H	3.031969000	-0.527046000	0.723865000

INT2-1d' ***G*= -531.845779 a.u.** **G_{corr}= 0.268561 a.u.**

O	-3.496849000	-0.824668000	0.013358000
H	-4.120950000	-0.481085000	-0.638565000
C	-2.174423000	-0.449073000	-0.397983000
H	-1.940603000	-0.940647000	-1.350887000
C	-2.028804000	1.055416000	-0.568135000
H	-2.709798000	1.405522000	-1.350906000
H	-2.328029000	1.545992000	0.362555000
C	-0.587110000	1.398292000	-0.936418000
H	-0.478569000	2.476650000	-1.083689000
H	-0.361889000	0.937518000	-1.902305000
C	0.457094000	0.932352000	0.105542000
C	-1.225871000	-0.964566000	0.677666000
H	-1.338939000	-2.049190000	0.752914000
H	-1.569524000	-0.541021000	1.627490000
C	0.276373000	-0.602093000	0.417130000
C	0.324901000	1.797921000	1.369423000
H	0.278643000	2.854744000	1.093826000
H	1.181434000	1.668345000	2.031290000
H	-0.570753000	1.565018000	1.947399000
C	0.858744000	-1.419922000	-0.757715000
H	0.430000000	-1.081989000	-1.703677000
C	2.397658000	-1.280697000	-0.805682000

H	2.736435000	-1.304451000	-1.844717000
H	2.872523000	-2.125448000	-0.301300000
C	2.851914000	0.034729000	-0.153157000
C	1.878725000	1.156671000	-0.501918000
B	0.850469000	-1.124089000	1.775891000
H	1.179344000	-2.270736000	1.858992000
H	0.865000000	-0.469451000	2.769713000
H	0.577500000	-2.470352000	-0.652847000
H	3.867506000	0.287070000	-0.468429000
H	2.905671000	-0.078763000	0.938888000
H	1.806705000	1.211954000	-1.592642000
H	2.265526000	2.123927000	-0.171931000

TS3-1d' ***G*= -531.834786 a.u.** **G_{corr}= 0.268194 a.u.** **□ν_{min}= 229.1*i* cm^{-1}**

O	-3.494623000	-0.768565000	-0.112623000
H	-4.069096000	-0.441860000	-0.816878000
C	-2.140354000	-0.444623000	-0.459989000
H	-1.861965000	-0.994744000	-1.367024000
C	-1.951881000	1.044483000	-0.701988000
H	-2.551887000	1.355065000	-1.563910000
H	-2.334647000	1.588565000	0.165956000
C	-0.479189000	1.371462000	-0.947722000
H	-0.361529000	2.448589000	-1.093956000
H	-0.167094000	0.904958000	-1.885772000
C	0.474351000	0.923749000	0.193697000
C	-1.270223000	-0.921808000	0.697519000
H	-1.411430000	-1.999302000	0.814455000
H	-1.655320000	-0.447075000	1.605363000
C	0.255947000	-0.600236000	0.488599000
C	0.193345000	1.805850000	1.423730000
H	0.250560000	2.860876000	1.141647000
H	0.925583000	1.637850000	2.212747000
H	-0.794765000	1.634954000	1.852146000
C	0.826393000	-1.435071000	-0.674924000
H	0.453010000	-1.077247000	-1.637368000
C	2.350753000	-1.389410000	-0.657864000
H	2.750419000	-1.890979000	-1.542764000
H	2.694395000	-1.977010000	0.198947000
C	2.930777000	0.042148000	-0.556833000
C	1.944534000	1.212876000	-0.273175000
B	0.727369000	-1.160522000	1.868827000
H	0.923452000	-2.335217000	1.971748000
H	0.778370000	-0.501237000	2.858924000
H	0.492205000	-2.472224000	-0.581040000
H	3.460264000	0.276255000	-1.482193000
H	3.697065000	0.042368000	0.220592000

H	1.882137000	1.826018000	-1.174376000
H	2.413696000	1.856001000	0.473310000

1d' ***G*= -531.853722 a.u.** **G_{corr}= 0.268398 a.u.**

O	-3.472574000	-0.653694000	-0.226543000
H	-3.988117000	-0.350140000	-0.984612000
C	-2.085150000	-0.419318000	-0.512200000
H	-1.795576000	-1.022187000	-1.380546000
C	-1.809279000	1.048003000	-0.813419000
H	-2.332841000	1.332794000	-1.732028000
H	-2.233101000	1.651254000	-0.006289000
C	-0.308793000	1.314384000	-0.962878000
H	-0.139510000	2.378844000	-1.148566000
H	0.051827000	0.791234000	-1.850210000
C	0.507453000	0.885975000	0.279570000
C	-1.306353000	-0.901692000	0.710102000
H	-1.492505000	-1.971158000	0.839408000
H	-1.729544000	-0.396833000	1.583485000
C	0.235613000	-0.631997000	0.592336000
C	0.130585000	1.814619000	1.449033000
H	0.197323000	2.857432000	1.126819000
H	0.806563000	1.689665000	2.294301000
H	-0.882783000	1.651003000	1.814682000
C	0.835946000	-1.540319000	-0.511223000
H	0.355905000	-1.362023000	-1.476759000
C	2.339046000	-1.318427000	-0.671503000
H	2.741901000	-1.984119000	-1.440060000
H	2.846870000	-1.576234000	0.267015000
C	2.630240000	0.140301000	-1.019259000
C	2.019892000	1.079975000	0.020662000
B	0.670292000	-1.136654000	2.007490000
H	0.878245000	-2.303795000	2.164743000
H	0.697646000	-0.436147000	2.970156000
H	0.632368000	-2.583921000	-0.256145000
H	2.227447000	0.361011000	-2.012819000
H	3.708679000	0.313398000	-1.077433000
H	2.201352000	2.122882000	-0.259961000
H	2.541790000	0.920831000	0.972382000

Cartesian coordinates for the structures of the retrohydroboration mechanism for 1e'

TS1-1e' ***G*= -531.832127 a.u.** **G_{corr}= 0.266857 a.u.** **ν_{min}= 545.1*i* cm^{-1}**

O	3.555967000	1.135425000	0.273964000
H	4.325024000	0.763059000	-0.175564000
C	2.376011000	0.591282000	-0.333569000

H	2.333659000	0.905449000	-1.386466000
C	2.371457000	-0.936329000	-0.281106000
H	3.190569000	-1.322203000	-0.896380000
H	2.580908000	-1.240410000	0.747357000
C	1.039635000	-1.529931000	-0.758949000
H	1.056048000	-2.617437000	-0.639836000
H	0.924016000	-1.334549000	-1.830531000
C	-0.178018000	-0.942571000	-0.019767000
C	1.173674000	1.189521000	0.384831000
H	1.179518000	2.274549000	0.251551000
H	1.259527000	0.996929000	1.457881000
C	-0.121343000	0.599549000	-0.175282000
C	-0.166416000	-1.394246000	1.450911000
H	-0.361381000	-2.468223000	1.513613000
H	-0.925136000	-0.884505000	2.045892000
H	0.791630000	-1.207668000	1.933962000
C	-1.366608000	1.282352000	0.393607000
H	-1.186811000	2.009650000	1.175862000
C	-2.595139000	0.587227000	0.455467000
H	-3.315048000	0.901908000	1.201156000
C	-2.729792000	-0.849682000	0.003904000
C	-1.482889000	-1.399817000	-0.697655000
H	-0.097804000	0.777014000	-1.253405000
B	-2.457295000	1.985256000	-0.752621000
H	-2.008812000	1.809184000	-1.846317000
H	-2.782069000	3.075605000	-0.378564000
H	-3.508532000	1.330143000	-0.736739000
H	-2.914485000	-1.416328000	0.921537000
H	-3.617894000	-0.985496000	-0.614327000
H	-1.537999000	-2.491934000	-0.713445000
H	-1.469620000	-1.068549000	-1.740196000

INT-1e' ***G*= -531.840952 a.u.** **G_{corr}= 0.265240 a.u.**

O	3.559246000	1.130800000	0.280190000
H	4.315196000	0.795321000	-0.217998000
C	2.363495000	0.619173000	-0.322431000
H	2.284535000	0.999025000	-1.351315000
C	2.364269000	-0.908773000	-0.366695000
H	3.167658000	-1.249982000	-1.027161000
H	2.600884000	-1.277691000	0.634349000
C	1.021912000	-1.475986000	-0.847401000
H	1.045797000	-2.568787000	-0.806311000
H	0.873682000	-1.205606000	-1.898388000
C	-0.176379000	-0.950869000	-0.034241000
C	1.184125000	1.165778000	0.471353000
H	1.178705000	2.256680000	0.404999000

H	1.305294000	0.906214000	1.526357000
C	-0.124201000	0.601135000	-0.085796000
C	-0.116961000	-1.495790000	1.403506000
H	-0.260944000	-2.579205000	1.394173000
H	-0.890289000	-1.064782000	2.040574000
H	0.839118000	-1.296484000	1.885242000
C	-1.351114000	1.213246000	0.550306000
H	-1.218786000	2.103306000	1.153776000
C	-2.546127000	0.564200000	0.577262000
H	-3.339048000	0.947756000	1.206376000
C	-2.730736000	-0.829564000	0.043358000
C	-1.501046000	-1.375653000	-0.694139000
H	-0.147118000	0.861497000	-1.148933000
B	-2.589053000	1.983820000	-0.928983000
H	-2.634539000	1.197844000	-1.830744000
H	-1.707735000	2.792402000	-1.038529000
H	-3.616820000	2.464837000	-0.543079000
H	-2.964461000	-1.455384000	0.911984000
H	-3.614948000	-0.873853000	-0.595855000
H	-1.561958000	-2.466249000	-0.741081000
H	-1.506347000	-1.013742000	-1.725526000

3 **G= -505.223088 a.u.** **G_{corr}= 0.236347 a.u.**

O	3.489820000	0.791820000	0.206096000
H	4.200087000	0.218782000	-0.109084000
C	2.259081000	0.337544000	-0.373479000
H	2.306876000	0.460938000	-1.465544000
C	2.003501000	-1.137873000	-0.062291000
H	2.772615000	-1.746915000	-0.548495000
H	2.123614000	-1.282074000	1.014347000
C	0.611692000	-1.598939000	-0.515300000
H	0.449407000	-2.636455000	-0.208354000
H	0.566777000	-1.586179000	-1.609905000
C	-0.518103000	-0.708171000	0.033587000
C	1.144519000	1.233400000	0.151394000
H	1.330712000	2.262711000	-0.167033000
H	1.157855000	1.228980000	1.244533000
C	-0.207206000	0.753262000	-0.385351000
C	-0.620371000	-0.875907000	1.560364000
H	-0.948720000	-1.891337000	1.797862000
H	-1.336221000	-0.181246000	1.999908000
H	0.332318000	-0.715397000	2.062679000
C	-1.356969000	1.678381000	-0.083433000
H	-1.129004000	2.734781000	0.030372000
C	-2.616336000	1.256943000	0.012619000
H	-3.408828000	1.969160000	0.223400000
C	-3.016798000	-0.185904000	-0.125023000

C	-1.866641000	-1.082476000	-0.607597000
H	-0.103797000	0.734261000	-1.480504000
H	-3.396402000	-0.537752000	0.842019000
H	-3.864754000	-0.268695000	-0.812476000
H	-2.099812000	-2.131342000	-0.401523000
H	-1.769497000	-0.988340000	-1.693905000

TS2-1e' ***G*= -531.827379 a.u.** **G_{corr}= 0.267050 a.u.** **ν_{min}= 613.1*i* cm^{-1}**

O	3.525924000	1.131627000	0.150109000
H	4.323742000	0.634202000	-0.069689000
C	2.399799000	0.438879000	-0.406201000
H	2.491779000	0.424064000	-1.502163000
C	2.325487000	-1.005399000	0.090527000
H	3.192413000	-1.560067000	-0.282729000
H	2.402528000	-0.996054000	1.180518000
C	1.031367000	-1.703836000	-0.348283000
H	0.997931000	-2.715001000	0.067171000
H	1.030832000	-1.812457000	-1.438324000
C	-0.231458000	-0.923362000	0.077183000
C	1.147907000	1.232262000	-0.050681000
H	1.206341000	2.221033000	-0.513561000
H	1.106378000	1.387004000	1.029597000
C	-0.094179000	0.491580000	-0.549058000
C	-0.336496000	-0.963627000	1.613670000
H	-0.276524000	-2.003547000	1.947096000
H	-1.271797000	-0.554783000	1.984214000
H	0.465221000	-0.414906000	2.104657000
C	-1.362316000	1.331391000	-0.568068000
H	-1.303778000	2.170537000	-1.251996000
C	-2.630030000	0.712151000	-0.450416000
H	-3.468305000	1.189306000	-0.941657000
C	-2.772624000	-0.784022000	-0.205548000
C	-1.489653000	-1.562765000	-0.531839000
H	0.090951000	0.292395000	-1.614663000
B	-2.092974000	1.905640000	0.869607000
H	-2.436937000	3.042846000	0.715866000
H	-1.431006000	1.577928000	1.804095000
H	-3.152891000	1.274173000	1.024184000
H	-3.085355000	-0.976644000	0.819971000
H	-3.588362000	-1.138708000	-0.839002000
H	-1.365195000	-1.608846000	-1.618604000
H	-1.597312000	-2.593213000	-0.181610000

TS1-1f' ***G*= -531.829707 a.u.** **G_{corr}= 0.267199 a.u.** **ν_{min}= 545.6*i* cm^{-1}**

O	-3.536055000	-1.157270000	0.151592000
H	-4.335914000	-0.663511000	-0.069285000

C	-2.412522000	-0.458030000	-0.398225000
H	-2.493185000	-0.448971000	-1.495105000
C	-2.349219000	0.988142000	0.094044000
H	-3.216510000	1.535946000	-0.287745000
H	-2.434867000	0.981793000	1.183305000
C	-1.057025000	1.693508000	-0.339798000
H	-1.029057000	2.703470000	0.078368000
H	-1.056014000	1.805331000	-1.429569000
C	0.213380000	0.923674000	0.081829000
C	-1.160290000	-1.243727000	-0.026345000
H	-1.208347000	-2.236907000	-0.480203000
H	-1.125381000	-1.384473000	1.056196000
C	0.078837000	-0.496900000	-0.519398000
C	0.328957000	0.949361000	1.615704000
H	0.381513000	1.987602000	1.954267000
H	1.216646000	0.438072000	1.976648000
H	-0.526910000	0.489208000	2.106839000
C	1.350161000	-1.304402000	-0.561544000
H	1.256604000	-2.235629000	-1.109182000
C	2.629811000	-0.712360000	-0.483266000
H	3.400306000	-1.154983000	-1.101147000
C	2.757715000	0.793560000	-0.242819000
C	1.463810000	1.564898000	-0.545502000
H	-0.078255000	-0.332714000	-1.597683000
B	2.424569000	-1.761348000	0.877803000
H	2.560067000	-1.104513000	1.864255000
H	3.051328000	-2.770121000	0.721129000
H	1.228198000	-2.104108000	0.917349000
H	3.079810000	0.993947000	0.779594000
H	3.552832000	1.173693000	-0.887982000
H	1.318475000	1.607557000	-1.630402000
H	1.562566000	2.597861000	-0.199485000

1e’ ***G*= -531.861461 a.u.** **G_{corr}= 0.268263 a.u.**

O	-3.570278000	-0.983755000	-0.102049000
H	-4.324199000	-0.419517000	-0.315149000
C	-2.374075000	-0.300839000	-0.505024000
H	-2.382240000	-0.173053000	-1.597411000
C	-2.260840000	1.075615000	0.144100000
H	-3.086201000	1.710041000	-0.195347000
H	-2.375948000	0.957322000	1.224850000
C	-0.922721000	1.739644000	-0.193665000
H	-0.850716000	2.711089000	0.304463000
H	-0.891870000	1.939066000	-1.270399000
C	0.303941000	0.876758000	0.173276000
C	-1.194636000	-1.184673000	-0.128001000

H	-1.281168000	-2.143602000	-0.646650000
H	-1.250418000	-1.397202000	0.941194000
C	0.134440000	-0.516414000	-0.494342000
C	0.425310000	0.778657000	1.701767000
H	0.556766000	1.774883000	2.132486000
H	1.293737000	0.192720000	2.019535000
H	-0.452076000	0.330465000	2.164989000
C	1.383945000	-1.399249000	-0.260001000
H	1.204724000	-2.350331000	-0.803328000
C	2.617932000	-0.717007000	-0.878117000
H	2.478275000	-0.620947000	-1.961705000
C	2.832647000	0.675796000	-0.281104000
C	1.573544000	1.539436000	-0.405121000
H	0.094714000	-0.319694000	-1.574508000
B	1.587372000	-1.978457000	1.169120000
H	2.686461000	-2.120719000	1.620844000
H	0.666965000	-2.388513000	1.807292000
H	3.508086000	-1.333063000	-0.726391000
H	3.668094000	1.175045000	-0.780138000
H	3.118618000	0.577013000	0.770692000
H	1.396524000	1.746535000	-1.466665000
H	1.730317000	2.508444000	0.079532000

1f' ***G*= -531.861336 a.u.** **G_{corr}= 0.267358 a.u.**

O	-3.598671000	-1.310336000	0.135814000
H	-4.389019000	-0.892729000	-0.229199000
C	-2.450692000	-0.631445000	-0.393662000
H	-2.419798000	-0.772344000	-1.484108000
C	-2.491310000	0.866163000	-0.099825000
H	-3.347230000	1.315649000	-0.614009000
H	-2.660697000	1.000964000	0.971612000
C	-1.197395000	1.560639000	-0.538702000
H	-1.239518000	2.623177000	-0.281234000
H	-1.120046000	1.507491000	-1.630377000
C	0.071182000	0.928746000	0.071373000
C	-1.213137000	-1.283965000	0.205489000
H	-1.189853000	-2.338906000	-0.081133000
H	-1.286882000	-1.251666000	1.296260000
C	0.061081000	-0.584211000	-0.276688000
C	0.095246000	1.192401000	1.587716000
H	0.101958000	2.269835000	1.773318000
H	0.978356000	0.774422000	2.069653000
H	-0.773929000	0.779313000	2.098414000
C	1.335451000	-1.305614000	0.179593000
H	1.272845000	-2.356767000	-0.115134000
C	2.604651000	-0.648849000	-0.450943000
H	2.514681000	-0.809297000	-1.533433000
C	2.627312000	0.862237000	-0.172318000
C	1.322459000	1.554758000	-0.576670000
H	0.056272000	-0.636948000	-1.373729000
B	3.792625000	-1.468252000	0.124307000
H	4.402076000	-1.084718000	1.080523000
H	4.067441000	-2.541263000	-0.326876000
H	1.397050000	-1.290781000	1.272816000
H	2.828466000	1.029034000	0.889895000
H	3.461612000	1.320500000	-0.711564000
H	1.214473000	1.494058000	-1.665728000
H	1.368907000	2.619760000	-0.326196000

π-complex intermediate formed from decalin model + BH_3 by α-face

***G*= -531.841684 a.u.** **G_{corr}= 0.265790 a.u.**

O	3.545697000	-0.681435000	-0.459511000
H	4.256292000	-0.388451000	0.124609000
C	2.295736000	-0.389616000	0.180055000
H	2.247252000	-0.914280000	1.140202000
C	2.116518000	1.106770000	0.414995000
H	2.868616000	1.454479000	1.129570000
H	2.310038000	1.626107000	-0.527392000

C	0.716549000	1.432795000	0.941808000
H	0.598339000	2.515380000	1.036414000
H	0.605656000	1.015829000	1.945235000
C	-0.424279000	0.891949000	0.052460000
C	1.208453000	-0.940224000	-0.736393000
H	1.310557000	-2.019816000	-0.841438000
H	1.362139000	-0.505315000	-1.730407000
C	-0.188723000	-0.572014000	-0.305341000
C	-0.457298000	1.684161000	-1.277597000
H	-0.714758000	2.725353000	-1.070637000
H	-1.196997000	1.280930000	-1.969643000
H	0.505703000	1.671863000	-1.785724000
C	-1.243275000	-1.421426000	-0.487719000
H	-1.048787000	-2.379223000	-0.957835000
C	-2.692081000	-0.997753000	-0.466610000
H	-3.254468000	-1.707218000	0.141882000
H	-3.066889000	-1.124895000	-1.487419000
C	-2.944853000	0.451380000	-0.000541000
C	-1.770952000	1.043475000	0.781604000
B	-0.541922000	-1.931158000	1.336774000
H	0.112253000	-2.899924000	1.073370000
H	0.045749000	-1.101196000	1.968675000
H	-1.652098000	-2.109528000	1.747213000
H	-3.150339000	1.080681000	-0.868186000
H	-3.844726000	0.486898000	0.616192000
H	-1.950780000	2.105193000	0.970928000
H	-1.693488000	0.557418000	1.756290000

π-complex intermediate formed from decalin model + BH_3 by ®-face

***G*= -531.840082 a.u. G_{corr}= 0.266278 a.u.**

O	-3.532090000	-0.910315000	-0.149402000
H	-4.230212000	-0.430874000	-0.613232000
C	-2.275207000	-0.338245000	-0.523638000
H	-2.122930000	-0.463044000	-1.604921000
C	-2.175370000	1.139737000	-0.180623000
H	-2.920530000	1.705469000	-0.748082000
H	-2.402539000	1.274880000	0.879999000
C	-0.776248000	1.642510000	-0.519616000
H	-0.688325000	2.712175000	-0.315437000
H	-0.615436000	1.515870000	-1.594903000
C	0.378007000	0.919933000	0.236130000
C	-1.204477000	-1.129781000	0.222983000
H	-1.253881000	-2.177389000	-0.070887000
H	-1.446262000	-1.076237000	1.287313000
C	0.186543000	-0.583685000	-0.013149000
C	0.316021000	1.277657000	1.732327000

H	0.222674000	2.360709000	1.840958000
H	1.225423000	0.962583000	2.242475000
H	-0.527828000	0.814361000	2.242489000
C	1.140495000	-1.347997000	-0.621166000
H	0.845619000	-2.311005000	-1.022747000
C	2.475613000	-0.812702000	-1.064310000
H	2.409574000	-0.582056000	-2.134869000
H	3.233756000	-1.591103000	-0.962017000
C	2.855576000	0.443790000	-0.289110000
C	1.708517000	1.444320000	-0.361239000
B	1.275926000	-2.018962000	1.327163000
H	0.927001000	-1.266815000	2.184523000
H	0.623706000	-3.018321000	1.238631000
H	2.463711000	-2.123797000	1.223421000
H	3.764859000	0.883819000	-0.704447000
H	3.071951000	0.182798000	0.749972000
H	1.549445000	1.695237000	-1.414314000
H	1.970496000	2.376852000	0.143943000

π-complex intermediate formed from BH_3 + 3 by ®-face

***G*= -531.836515 a.u. G_{corr}= 0.266506 a.u.**

O	3.520271000	1.162755000	0.098205000
H	4.324186000	0.654933000	-0.069318000
C	2.407334000	0.421798000	-0.417783000
H	2.509558000	0.328348000	-1.509068000
C	2.335836000	-0.982540000	0.183979000
H	3.214172000	-1.554481000	-0.132067000
H	2.393706000	-0.890740000	1.271266000
C	1.057076000	-1.726317000	-0.224295000
H	1.022537000	-2.700416000	0.271518000
H	1.082354000	-1.922637000	-1.301898000
C	-0.222163000	-0.929402000	0.106070000
C	1.147652000	1.230096000	-0.129298000
H	1.204309000	2.187881000	-0.652856000
H	1.092752000	1.449423000	0.938136000
C	-0.079507000	0.445200000	-0.597905000
C	-0.381300000	-0.839294000	1.633809000
H	-0.422941000	-1.850445000	2.048013000
H	-1.290607000	-0.324021000	1.930701000
H	0.448683000	-0.323667000	2.113661000
C	-1.358443000	1.233026000	-0.693485000
H	-1.274317000	2.223995000	-1.125062000
C	-2.582195000	0.652260000	-0.580403000
H	-3.460702000	1.196463000	-0.902939000
C	-2.752976000	-0.817869000	-0.284397000

C	-1.459687000	-1.621261000	-0.491900000
H	0.115219000	0.205422000	-1.655403000
B	-2.268549000	1.969074000	1.014245000
H	-2.798826000	2.966452000	0.612746000
H	-1.160351000	2.102863000	1.451190000
H	-2.946877000	1.236370000	1.676228000
H	-3.139543000	-0.950907000	0.727871000
H	-3.532455000	-1.199314000	-0.949231000
H	-1.295483000	-1.757733000	-1.565607000
H	-1.574556000	-2.619373000	-0.061089000

d. Cartesian coordinates of the structures at SMD-B3LYP-D3/def2-TZVP level for the System

Cholesterol G= -817.277375 a.u. G_{corr}**= 0.413237 a.u.**

O	5.632101000	0.353501000	-0.138499000
H	6.152591000	-0.226760000	-0.708214000
C	4.251792000	0.209010000	-0.498160000
H	4.107544000	0.547167000	-1.534342000
C	3.772353000	-1.230611000	-0.378867000
H	4.328932000	-1.865457000	-1.076041000
H	3.996930000	-1.589313000	0.629514000
C	2.275828000	-1.331011000	-0.675526000
H	1.958858000	-2.370799000	-0.580739000
H	2.106526000	-1.045076000	-1.719054000
C	1.381584000	-0.434716000	0.224326000
C	3.447140000	1.111484000	0.427711000
H	3.759520000	2.148957000	0.294669000
H	3.702843000	0.830249000	1.455318000
C	1.957435000	0.982571000	0.205215000
C	1.414503000	-0.961972000	1.676632000
H	1.206230000	-2.032246000	1.716818000
H	0.678258000	-0.447298000	2.295828000
H	2.388992000	-0.808374000	2.138755000
C	-3.215303000	-1.013891000	1.445071000
H	-3.701718000	-1.984559000	1.574495000
H	-3.841809000	-0.268126000	1.936856000
H	-2.268073000	-1.046588000	1.982009000
C	1.206025000	2.066162000	0.008494000
H	1.692319000	3.038310000	-0.020597000
C	-0.279656000	2.059900000	-0.172510000
H	-0.517416000	2.297879000	-1.218913000
H	-0.722778000	2.869345000	0.416176000
C	-0.922896000	0.723878000	0.204151000
H	-0.948217000	0.658043000	1.296581000
C	-0.070360000	-0.440007000	-0.352905000
H	0.033158000	-0.237374000	-1.427641000

C	-0.769166000	-1.808987000	-0.222813000
H	-0.199198000	-2.562180000	-0.770318000
H	-0.765233000	-2.127401000	0.820150000
C	-2.219455000	-1.817460000	-0.729583000
H	-2.662675000	-2.803389000	-0.555400000
H	-2.230823000	-1.652338000	-1.812908000
C	-2.345352000	0.627283000	-0.335728000
H	-2.258253000	0.686229000	-1.430680000
C	-3.044029000	-0.718895000	-0.056285000
C	-3.379890000	1.680147000	0.076799000
H	-3.225986000	2.633051000	-0.430971000
H	-3.316371000	1.877946000	1.149817000
C	-4.744494000	1.028917000	-0.291023000
H	-5.437923000	1.078997000	0.549885000
H	-5.223649000	1.549257000	-1.121712000
C	-4.429817000	-0.445326000	-0.667624000
H	-4.374162000	-0.553789000	-1.754427000
H	-5.192680000	-1.141225000	-0.311184000

Cartesian coordinates for the structures of the retrohydroboration mechanism for 1e'

1a' ***G*= -843.909912 a.u.** **G_{corr}= 0.445413 a.u.**

O	5.574352000	-0.094953000	-0.148518000
H	6.076781000	-0.797937000	-0.579281000
B	1.593260000	3.388925000	-0.082078000
H	2.084208000	3.526822000	-1.164741000
C	4.201830000	-0.216565000	-0.551542000
H	4.128794000	-0.052905000	-1.636744000
C	3.634118000	-1.593313000	-0.228552000
H	4.163883000	-2.354589000	-0.810940000
H	3.831137000	-1.808316000	0.825322000
C	2.132846000	-1.669997000	-0.523237000
H	1.772750000	-2.663566000	-0.251840000
H	1.974404000	-1.564750000	-1.602725000
C	1.303424000	-0.584449000	0.202230000
C	3.416811000	0.879182000	0.149590000
H	3.806864000	1.852243000	-0.164275000
H	3.586394000	0.804276000	1.227277000
C	1.919756000	0.796697000	-0.173748000
H	1.831994000	0.874565000	-1.266698000
C	1.349241000	-0.842650000	1.720335000
H	1.063497000	-1.871696000	1.944731000
H	0.677091000	-0.187235000	2.272778000
H	2.347920000	-0.693718000	2.128522000
C	-3.378891000	-1.040097000	1.449950000
H	-3.919049000	-1.980071000	1.591402000

H	-3.979070000	-0.248952000	1.902102000
H	-2.450156000	-1.107308000	2.015382000
C	1.144383000	1.984477000	0.407673000
H	1.135929000	1.927693000	1.501275000
C	-0.338107000	1.934424000	-0.070623000
H	-0.380812000	2.105511000	-1.153904000
H	-0.916339000	2.733777000	0.398620000
C	-1.002619000	0.584367000	0.231744000
H	-1.076601000	0.494365000	1.319202000
C	-0.167009000	-0.599082000	-0.320500000
H	-0.097828000	-0.436098000	-1.405577000
C	-0.889521000	-1.946973000	-0.123899000
H	-0.332775000	-2.738089000	-0.628830000
H	-0.897587000	-2.210240000	0.935612000
C	-2.332465000	-1.950513000	-0.653039000
H	-2.800833000	-2.917179000	-0.440710000
H	-2.316451000	-1.839233000	-1.743237000
C	-2.409232000	0.517112000	-0.359415000
H	-2.285600000	0.537829000	-1.451948000
C	-3.148996000	-0.804124000	-0.054249000
C	-3.433485000	1.605137000	-0.015817000
H	-3.246444000	2.534423000	-0.554915000
H	-3.396708000	1.843960000	1.049949000
C	-4.801011000	0.968874000	-0.399249000
H	-5.513821000	1.057602000	0.421965000
H	-5.248792000	1.472732000	-1.257151000
C	-4.506195000	-0.521575000	-0.722021000
H	-4.414392000	-0.663181000	-1.802573000
H	-5.296050000	-1.190758000	-0.373302000
H	1.357271000	4.369417000	0.560005000

TS1-1e’ ***G*= -843.881030 a.u.** **G_{corr}= 0.445133 a.u.** **ν_{min}= 530.5*i* cm^{-1}**

O	5.618592000	0.115688000	-0.042498000
H	6.158312000	-0.562677000	-0.467600000
C	4.263908000	-0.049711000	-0.484682000
H	4.215112000	0.118451000	-1.570245000
C	3.741734000	-1.452100000	-0.182809000
H	4.305706000	-2.184027000	-0.770158000
H	3.948507000	-1.669103000	0.868364000
C	2.243318000	-1.603761000	-0.478127000
H	1.923720000	-2.601324000	-0.169774000
H	2.080091000	-1.543886000	-1.559857000
C	1.374163000	-0.528736000	0.209767000
C	3.421403000	1.019116000	0.195457000
H	3.779167000	2.007031000	-0.107052000
H	3.548470000	0.948819000	1.279197000

C	1.953143000	0.854230000	-0.199996000
C	1.400767000	-0.742624000	1.734242000
H	0.835278000	-1.634432000	2.011690000
H	0.978872000	0.101970000	2.279769000
H	2.415068000	-0.880033000	2.105605000
C	-3.291713000	-1.352710000	1.309288000
H	-3.799325000	-2.320408000	1.285020000
H	-3.923718000	-0.669533000	1.878175000
H	-2.368040000	-1.484585000	1.872860000
C	1.090596000	2.019307000	0.287478000
H	1.595410000	2.750174000	0.907379000
C	-0.287341000	1.834132000	0.533041000
H	-0.773645000	2.516662000	1.220009000
C	-0.961785000	0.490184000	0.398566000
H	-1.068740000	0.176438000	1.442992000
C	-0.084338000	-0.549909000	-0.337494000
H	-0.020525000	-0.221112000	-1.382466000
C	-0.763026000	-1.930237000	-0.359900000
H	-0.181476000	-2.608374000	-0.986116000
H	-0.761613000	-2.363414000	0.642840000
C	-2.203275000	-1.877763000	-0.899354000
H	-2.650406000	-2.875815000	-0.854551000
H	-2.176993000	-1.588524000	-1.955764000
C	-2.359398000	0.513564000	-0.208589000
H	-2.230726000	0.727255000	-1.277884000
C	-3.056976000	-0.864509000	-0.133272000
C	-3.412745000	1.491762000	0.318307000
H	-3.246159000	2.510707000	-0.032455000
H	-3.396542000	1.523140000	1.410286000
C	-4.754548000	0.900072000	-0.202285000
H	-5.490099000	0.841924000	0.601271000
H	-5.189068000	1.530365000	-0.979233000
C	-4.417938000	-0.511650000	-0.759529000
H	-4.318069000	-0.473819000	-1.847728000
H	-5.190093000	-1.248714000	-0.529405000
H	1.934308000	0.854536000	-1.292635000
B	0.198119000	2.874050000	-0.924793000
H	0.471934000	2.397312000	-1.985577000
H	0.285884000	4.053772000	-0.735306000
H	-1.005625000	2.623520000	-0.778371000

INT-1e' ***G*= -843.888489 a.u.** **G_{corr}= 0.443310 a.u.**

O	5.615972000	0.168299000	-0.075513000
H	6.155578000	-0.478386000	-0.547575000
C	4.255288000	0.007387000	-0.497044000
H	4.178015000	0.237019000	-1.569827000

C	3.757852000	-1.417073000	-0.264755000
H	4.322712000	-2.105890000	-0.901065000
H	3.983962000	-1.689450000	0.769449000
C	2.257314000	-1.574537000	-0.546464000
H	1.956899000	-2.593027000	-0.292932000
H	2.076032000	-1.452139000	-1.620088000
C	1.381660000	-0.557876000	0.216293000
C	3.415412000	1.023450000	0.262414000
H	3.752122000	2.032379000	0.010281000
H	3.565756000	0.890781000	1.336746000
C	1.941769000	0.857641000	-0.114880000
C	1.431706000	-0.855030000	1.725300000
H	0.916864000	-1.790639000	1.950586000
H	0.964052000	-0.066812000	2.316271000
H	2.453764000	-0.956674000	2.086996000
C	-3.327921000	-1.363427000	1.286533000
H	-3.863285000	-2.315165000	1.236714000
H	-3.947104000	-0.671823000	1.859604000
H	-2.416655000	-1.533958000	1.860174000
C	1.066895000	1.954109000	0.450535000
H	1.555530000	2.824767000	0.871359000
C	-0.266779000	1.777272000	0.654299000
H	-0.813010000	2.514342000	1.229111000
C	-0.954677000	0.454683000	0.454621000
H	-1.095072000	0.096807000	1.482634000
C	-0.082905000	-0.569285000	-0.308941000
H	-0.031115000	-0.218105000	-1.346158000
C	-0.768176000	-1.945739000	-0.354080000
H	-0.186994000	-2.621417000	-0.983735000
H	-0.781455000	-2.391050000	0.643319000
C	-2.203043000	-1.870211000	-0.908289000
H	-2.661391000	-2.863880000	-0.880656000
H	-2.160043000	-1.569371000	-1.960871000
C	-2.339111000	0.514092000	-0.183835000
H	-2.186309000	0.739036000	-1.245240000
C	-3.057122000	-0.855380000	-0.142292000
C	-3.386530000	1.503498000	0.330376000
H	-3.193163000	2.520080000	-0.013199000
H	-3.391656000	1.530046000	1.422826000
C	-4.727558000	0.935412000	-0.218497000
H	-5.475843000	0.874286000	0.573139000
H	-5.143424000	1.581353000	-0.992779000
C	-4.400087000	-0.472947000	-0.790159000
H	-4.277651000	-0.420152000	-1.875442000
H	-5.187839000	-1.201617000	-0.587221000
H	1.896201000	0.941366000	-1.205354000
B	0.025462000	2.886379000	-1.078174000
H	-0.426680000	2.065805000	-1.821328000

H	1.125379000	3.251538000	-1.393549000
H	-0.683185000	3.785437000	-0.724027000

3 G= -817.270389 a.u. G_{corr}= 0.414135 a.u.

O	5.612343000	0.311782000	-0.194290000
H	6.151130000	-0.406018000	-0.550267000
C	4.250193000	0.081905000	-0.581569000
H	4.172654000	0.138280000	-1.677332000
C	3.762327000	-1.292068000	-0.127688000
H	4.327785000	-2.068713000	-0.653155000
H	3.999084000	-1.398360000	0.934042000
C	2.259942000	-1.501593000	-0.366181000
H	1.969117000	-2.467992000	0.050658000
H	2.069041000	-1.555182000	-1.444065000
C	1.389482000	-0.375506000	0.230717000
C	3.404690000	1.202147000	0.006616000
H	3.738141000	2.159205000	-0.403909000
H	3.557043000	1.246972000	1.088255000
C	1.930318000	0.967608000	-0.337513000
C	1.460417000	-0.424596000	1.767296000
H	0.937096000	-1.305869000	2.143091000
H	1.008649000	0.455659000	2.224193000
H	2.486094000	-0.481063000	2.128013000
C	-3.369621000	-1.014530000	1.384048000
H	-3.921463000	-1.955393000	1.458087000
H	-3.990746000	-0.238200000	1.833174000
H	-2.476090000	-1.112415000	1.999763000
C	1.032613000	2.129244000	-0.004425000
H	1.475937000	3.121082000	-0.035004000
C	-0.259682000	1.990119000	0.283553000
H	-0.856347000	2.868223000	0.511441000
C	-0.950141000	0.657008000	0.360617000
H	-1.109478000	0.443580000	1.424993000
C	-0.084449000	-0.472374000	-0.253815000
H	-0.052120000	-0.276060000	-1.334163000
C	-0.764147000	-1.840582000	-0.090192000
H	-0.177214000	-2.609142000	-0.596334000
H	-0.794521000	-2.122638000	0.965245000
C	-2.189228000	-1.849850000	-0.674672000
H	-2.656120000	-2.824745000	-0.501452000
H	-2.124067000	-1.719300000	-1.760818000
C	-2.322686000	0.623238000	-0.313402000
H	-2.142789000	0.694049000	-1.394998000
C	-3.052830000	-0.724738000	-0.095507000
C	-3.382323000	1.677124000	0.021970000
H	-3.181094000	2.632838000	-0.463165000
H	-3.412429000	1.866724000	1.097706000

C	-4.712505000	1.035094000	-0.470513000
H	-5.475773000	1.080290000	0.307614000
H	-5.114578000	1.566205000	-1.334554000
C	-4.372509000	-0.437583000	-0.832844000
H	-4.212986000	-0.534125000	-1.910443000
H	-5.170277000	-1.131680000	-0.559333000
H	1.898423000	0.859126000	-1.431924000

TS2-1e' ***G*= -843.876031a.u.** **G_{corr}= 0.444793 a.u.** **□ν_{min}= 589.4*i* cm^{-1}**

O	5.594407000	0.058036000	-0.136466000
H	6.134843000	-0.697562000	-0.399631000
C	4.249861000	-0.178989000	-0.576752000
H	4.233961000	-0.221631000	-1.675767000
C	3.704234000	-1.497671000	-0.032469000
H	4.272065000	-2.328835000	-0.463410000
H	3.883790000	-1.520330000	1.045168000
C	2.209375000	-1.690284000	-0.325325000
H	1.880504000	-2.622979000	0.136108000
H	2.060208000	-1.803567000	-1.404919000
C	1.344746000	-0.509374000	0.179729000
C	3.401160000	1.007351000	-0.139780000
H	3.761011000	1.910797000	-0.639356000
H	3.518752000	1.170050000	0.933430000
C	1.937425000	0.756939000	-0.505533000
C	1.397307000	-0.501215000	1.719413000
H	1.127863000	-1.487744000	2.102577000
H	0.719084000	0.220898000	2.163334000
H	2.392062000	-0.271727000	2.096795000
C	-3.305518000	-0.954645000	1.509457000
H	-3.809369000	-1.897915000	1.735307000
H	-3.931632000	-0.150358000	1.897673000
H	-2.372578000	-0.940059000	2.072213000
C	1.069476000	2.002030000	-0.470979000
H	1.372461000	2.744437000	-1.200738000
C	-0.318628000	1.902442000	-0.230944000
H	-0.959270000	2.632608000	-0.708355000
C	-0.979339000	0.583074000	0.155251000
H	-1.068442000	0.546148000	1.239618000
C	-0.123453000	-0.624887000	-0.320277000
H	-0.077446000	-0.556273000	-1.416002000
C	-0.815761000	-1.960156000	0.004949000
H	-0.248143000	-2.778880000	-0.439962000
H	-0.803943000	-2.130875000	1.083618000
C	-2.261256000	-2.026826000	-0.513182000
H	-2.717959000	-2.975585000	-0.214822000
H	-2.249196000	-2.010784000	-1.608760000
C	-2.384473000	0.465109000	-0.434064000

H	-2.268666000	0.405252000	-1.525200000
C	-3.092260000	-0.844270000	-0.012288000
C	-3.429471000	1.552182000	-0.156442000
H	-3.268479000	2.450740000	-0.752840000
H	-3.397591000	1.856389000	0.891991000
C	-4.781734000	0.861181000	-0.496867000
H	-5.505356000	1.010845000	0.305482000
H	-5.225094000	1.281608000	-1.400523000
C	-4.459476000	-0.646913000	-0.688771000
H	-4.375076000	-0.882388000	-1.753297000
H	-5.231437000	-1.297554000	-0.272463000
H	1.945891000	0.493077000	-1.572954000
B	0.726993000	2.841296000	0.985954000
H	0.864540000	4.016811000	0.799434000
H	1.263894000	2.287788000	1.894832000
H	-0.484756000	2.706367000	1.222617000

TS1-1f' ***G*= -843.878311 a.u.** **G_{corr}= 0.444644 a.u.** **ν_{min}= 546.4*i* cm^{-1}**

O	5.601972000	0.062158000	-0.203130000
H	6.135922000	-0.698196000	-0.466034000
C	4.247621000	-0.182333000	-0.603124000
H	4.198887000	-0.235067000	-1.700708000
C	3.716358000	-1.493186000	-0.027685000
H	4.272671000	-2.329555000	-0.463115000
H	3.925466000	-1.501608000	1.044756000
C	2.214863000	-1.690600000	-0.280130000
H	1.896459000	-2.611267000	0.211297000
H	2.041737000	-1.831398000	-1.352910000
C	1.353394000	-0.501960000	0.211051000
C	3.413745000	1.008722000	-0.151276000
H	3.763283000	1.910892000	-0.659842000
H	3.553513000	1.168944000	0.919944000
C	1.942605000	0.756267000	-0.481064000
C	1.419956000	-0.443270000	1.747074000
H	1.016323000	-1.363947000	2.172366000
H	0.857575000	0.389177000	2.160296000
H	2.442289000	-0.345887000	2.108375000
C	-3.329997000	-0.957797000	1.496091000
H	-3.841913000	-1.898136000	1.717112000
H	-3.961242000	-0.148919000	1.865930000
H	-2.409180000	-0.941228000	2.077890000
C	1.065313000	1.978036000	-0.464260000
H	1.428985000	2.783167000	-1.092980000
C	-0.320643000	1.918280000	-0.213107000
H	-0.935261000	2.593455000	-0.793626000
C	-0.977079000	0.587199000	0.169448000

H	-1.088337000	0.546418000	1.252560000
C	-0.117060000	-0.624662000	-0.285462000
H	-0.067166000	-0.567620000	-1.382246000
C	-0.801692000	-1.962109000	0.046412000
H	-0.224941000	-2.784092000	-0.380790000
H	-0.806271000	-2.121653000	1.127044000
C	-2.238783000	-2.041530000	-0.494241000
H	-2.695839000	-2.989661000	-0.193708000
H	-2.207726000	-2.037603000	-1.589673000
C	-2.370713000	0.450535000	-0.440147000
H	-2.236549000	0.382115000	-1.529395000
C	-3.083499000	-0.857217000	-0.021368000
C	-3.425786000	1.535301000	-0.192709000
H	-3.255796000	2.429496000	-0.793056000
H	-3.413221000	1.849165000	0.853348000
C	-4.769454000	0.836959000	-0.551817000
H	-5.507998000	0.988052000	0.236829000
H	-5.199634000	1.249264000	-1.465765000
C	-4.437223000	-0.671065000	-0.727923000
H	-4.329014000	-0.911968000	-1.789219000
H	-5.215838000	-1.322668000	-0.325172000
H	1.915250000	0.518817000	-1.556423000
B	0.419972000	2.868067000	1.029037000
H	0.169222000	2.353379000	2.075904000
H	0.197871000	4.031714000	0.849534000
H	1.653274000	2.735382000	0.926747000

1e' ***G*= -843.910487 a.u.** **G_{corr}= 0.445695 a.u.**

O	5.581270000	-0.024547000	-0.452644000
H	6.067168000	-0.797957000	-0.765477000
C	4.186816000	-0.235499000	-0.720000000
H	4.032937000	-0.294515000	-1.807558000
C	3.673056000	-1.520263000	-0.082775000
H	4.189757000	-2.381587000	-0.519235000
H	3.929917000	-1.502642000	0.980181000
C	2.161768000	-1.680713000	-0.273124000
H	1.839562000	-2.594836000	0.227985000
H	1.951960000	-1.820235000	-1.339542000
C	1.329108000	-0.476331000	0.230951000
C	3.428565000	0.966815000	-0.185117000
H	3.783198000	1.872176000	-0.685735000
H	3.663432000	1.080576000	0.874592000
C	1.921687000	0.813627000	-0.413479000
C	1.396277000	-0.414595000	1.764807000
H	1.027556000	-1.339585000	2.210829000
H	0.781458000	0.390824000	2.180391000

H	2.412504000	-0.265244000	2.125675000
C	-3.341160000	-0.730601000	1.565498000
H	-3.856835000	-1.632773000	1.905328000
H	-3.958553000	0.122767000	1.850286000
H	-2.408881000	-0.654864000	2.124041000
C	1.100274000	2.059119000	-0.015764000
H	1.562860000	2.924121000	-0.534375000
C	-0.337280000	1.904377000	-0.527824000
H	-0.337923000	1.842994000	-1.623829000
C	-1.002348000	0.644821000	0.032854000
H	-1.084839000	0.770447000	1.117149000
C	-0.146654000	-0.615646000	-0.265352000
H	-0.080486000	-0.674876000	-1.361231000
C	-0.847634000	-1.908260000	0.198870000
H	-0.280604000	-2.776209000	-0.141409000
H	-0.849597000	-1.956030000	1.289781000
C	-2.290494000	-2.037166000	-0.314455000
H	-2.745585000	-2.947441000	0.089569000
H	-2.276529000	-2.148087000	-1.404638000
C	-2.404271000	0.437469000	-0.529587000
H	-2.280498000	0.237318000	-1.604005000
C	-3.122850000	-0.804986000	0.042345000
C	-3.446460000	1.555830000	-0.409449000
H	-3.276304000	2.360098000	-1.126159000
H	-3.411758000	2.006242000	0.585702000
C	-4.804341000	0.833592000	-0.648247000
H	-5.518202000	1.079830000	0.139289000
H	-5.259779000	1.143366000	-1.589926000
C	-4.487038000	-0.687270000	-0.658813000
H	-4.398118000	-1.046598000	-1.688098000
H	-5.264150000	-1.282193000	-0.173456000
H	1.787854000	0.686837000	-1.496309000
B	1.231563000	2.556067000	1.452564000
H	0.290447000	3.024076000	2.024897000
H	2.287083000	2.580606000	2.007281000
H	-0.929152000	2.783522000	-0.261696000

1f' ***G*= -843.910359 a.u.** **G_{corr}= 0.445677 a.u.**

O	5.670054000	0.191881000	-0.248036000
H	6.200064000	-0.521825000	-0.624776000
C	4.298344000	-0.036710000	-0.602958000
H	4.193739000	0.022939000	-1.696308000
C	3.811661000	-1.404639000	-0.141703000
H	4.376799000	-2.188179000	-0.657429000
H	4.032136000	-1.506073000	0.924448000
C	2.313698000	-1.592938000	-0.404526000

H	2.013067000	-2.575131000	-0.036394000
H	2.139863000	-1.598100000	-1.486912000
C	1.430267000	-0.491095000	0.227565000
C	3.469081000	1.074701000	0.018404000
H	3.797694000	2.037105000	-0.383684000
H	3.659837000	1.100108000	1.094992000
C	1.977219000	0.877810000	-0.272120000
C	1.487397000	-0.611227000	1.761850000
H	1.223640000	-1.622019000	2.077465000
H	0.800692000	0.074827000	2.256072000
H	2.483439000	-0.404965000	2.151547000
C	-3.254190000	-1.083489000	1.483343000
H	-3.731385000	-2.044739000	1.692159000
H	-3.916845000	-0.303202000	1.860605000
H	-2.335609000	-1.038898000	2.067345000
C	1.142119000	2.059150000	0.227062000
H	1.574226000	2.987580000	-0.158268000
C	-0.338867000	1.928647000	-0.232349000
H	-0.330641000	1.988730000	-1.328052000
C	-0.932639000	0.565933000	0.171637000
H	-1.016568000	0.551063000	1.262567000
C	-0.037790000	-0.617681000	-0.285248000
H	0.022651000	-0.541393000	-1.380294000
C	-0.692509000	-1.979719000	0.021894000
H	-0.090052000	-2.781341000	-0.408300000
H	-0.700268000	-2.150738000	1.100567000
C	-2.123384000	-2.100608000	-0.522708000
H	-2.547790000	-3.068906000	-0.238056000
H	-2.092956000	-2.077627000	-1.617965000
C	-2.326427000	0.377276000	-0.424055000
H	-2.188343000	0.325098000	-1.514008000
C	-3.006095000	-0.952988000	-0.030805000
C	-3.413185000	1.428662000	-0.176357000
H	-3.258634000	2.336859000	-0.764890000
H	-3.432489000	1.723298000	0.874603000
C	-4.733387000	0.702203000	-0.567702000
H	-5.490775000	0.833223000	0.206337000
H	-5.152765000	1.109104000	-1.488876000
C	-4.360884000	-0.796926000	-0.743750000
H	-4.241311000	-1.032410000	-1.804877000
H	-5.125966000	-1.468154000	-0.347111000
H	1.870363000	0.859390000	-1.364640000
B	-1.018229000	3.176370000	0.400247000
H	-1.373078000	3.148861000	1.541852000
H	-1.098128000	4.213239000	-0.189858000
H	1.203538000	2.117208000	1.318348000

π-complex intermediate formed from BH_3 + 3 by ®-face

***G*= -843.884551 a.u. G_{corr}= 0.444493 a.u.**

O	5.583795000	0.047551000	-0.278562000
H	6.116162000	-0.722595000	-0.514678000
C	4.224326000	-0.217501000	-0.647754000
H	4.160096000	-0.318261000	-1.741216000
C	3.707543000	-1.505207000	-0.009096000
H	4.264012000	-2.357107000	-0.413277000
H	3.927754000	-1.465278000	1.060445000
C	2.204615000	-1.720802000	-0.236287000
H	1.894749000	-2.621323000	0.296571000
H	2.020570000	-1.907026000	-1.300211000
C	1.347565000	-0.514698000	0.213480000
C	3.392944000	0.989602000	-0.234589000
H	3.735234000	1.870674000	-0.783387000
H	3.547380000	1.192546000	0.825894000
C	1.918190000	0.719107000	-0.541322000
C	1.428977000	-0.387309000	1.744891000
H	1.070747000	-1.306855000	2.211910000
H	0.834136000	0.435369000	2.131863000
H	2.449075000	-0.229089000	2.090632000
C	-3.363750000	-0.837503000	1.522973000
H	-3.906558000	-1.745929000	1.796574000
H	-3.973508000	0.011981000	1.833203000
H	-2.449635000	-0.812597000	2.115382000
C	1.029476000	1.931085000	-0.532784000
H	1.429387000	2.813899000	-1.018997000
C	-0.297571000	1.863478000	-0.253648000
H	-0.931673000	2.704507000	-0.502996000
C	-0.978979000	0.575066000	0.146815000
H	-1.115392000	0.588196000	1.228938000
C	-0.127980000	-0.662481000	-0.250628000
H	-0.095610000	-0.665806000	-1.349003000
C	-0.826856000	-1.967669000	0.164588000
H	-0.257113000	-2.821964000	-0.204450000
H	-0.837986000	-2.053500000	1.253428000
C	-2.262694000	-2.063576000	-0.379425000
H	-2.734433000	-2.983096000	-0.019402000
H	-2.224906000	-2.133667000	-1.472219000
C	-2.364852000	0.431547000	-0.485996000
H	-2.211411000	0.290800000	-1.564621000
C	-3.097800000	-0.840257000	0.005701000
C	-3.407579000	1.543970000	-0.328233000
H	-3.220838000	2.386472000	-0.995012000
H	-3.400201000	1.936614000	0.690938000
C	-4.757142000	0.836731000	-0.647384000
H	-5.494375000	1.042724000	0.129848000
H	-5.182242000	1.196979000	-1.585120000

C	-4.439721000	-0.681899000	-0.729746000
H	-4.319841000	-0.986104000	-1.773411000
H	-5.230575000	-1.300371000	-0.299980000
H	1.893941000	0.435491000	-1.605820000
B	0.682583000	2.973593000	1.238061000
H	0.536851000	4.095073000	0.841164000
H	1.798419000	2.663769000	1.546581000
H	-0.147765000	2.567000000	1.999291000