**Electronic Supplementary Material**

**A Combined Gradient Projection / Single Component Artificial Force Induced Reaction (GP/SC-AFIR) Method for an Efficient Search of Minimum Energy Conical Intersection (MECI) Geometries**

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**Table SI1.** Cartesian coordinates (in Å) of the optimized MECI structures at the SF-BHHLYP/6-31G\* level for benzene. Energies in a.u. and the <S2> values for each state are also shown.

I-1 -231.886648 [0.40] -231.886648 [0.52]

C 1.30127111123500 -0.01548826045600 0.21947589424800

H 2.33679579832900 0.15091518291900 0.46428233552400

C 0.37793284027000 1.10079519141100 0.11931505403400

C 0.73073958773400 -1.26215334994300 0.05288477940900

C -0.64682186346600 -1.19181414094500 -0.01931846300800

C -0.63074537939600 1.18637845787400 -0.90091611371600

C -1.19062748334600 0.15363691602500 -0.07298491854800

H 1.28818621117400 -2.18276420391600 0.03713245731200

H -1.30192010965900 -2.04584710091900 0.01745644515900

H 0.55499561505100 1.96141107310000 0.75434658688800

H -1.17034551087600 2.10846140752400 -1.03915975449900

H -2.13687261033000 0.33670001436500 0.42341400770200

I-2 -231.882743 [0.87] -231.882743 [0.11]

C 1.06331359698100 -0.00062656407600 -0.03362999811000

H 2.08403149573000 -0.00029898040400 -0.38498224106100

C 0.46686753952600 1.23725665228900 0.26253688345800

C 0.46664827158100 -1.23782601823700 0.25931100787600

C -0.80946724156200 -1.23742717993700 0.78979185024900

C -0.81043454279600 1.23823699933600 0.78701553285100

C -1.55916454541500 -0.00078679948900 0.64440124550000

H 1.07062332182800 -2.13305820207900 0.22469894259000

H -1.21196944282000 -2.13086737584600 1.24869644505900

H 1.07168835842200 2.13202956742300 0.23172376303700

H -1.21764265414000 2.13415904914700 1.23670526336600

H -1.44895294569200 -0.00075619882000 -0.47032904168400

I-3 -231.881787 [0.42] -231.881787 [0.80]

C 1.43586825925900 -0.10006568718500 0.59697344516200

H 2.48919194717000 -0.04196472435000 0.83080322931800

C 0.68175967843400 1.05120817188700 0.39775284603900

C 0.68863567072100 -1.26212540468000 0.80310544169500

C -0.66192915729600 -1.12017613965300 0.34273142606300

C -0.70264908124000 1.01561389712500 0.76762450035600

C -1.39415015768200 -0.14547922316900 1.09163740112400

H 0.90315000849100 -1.86462807666500 1.67881095544000

H -0.91736759430800 -1.32628952729500 -0.69678153124000

H 1.14341559142000 2.00727013282800 0.21648143906000

H -1.25311057659400 1.94833046460900 0.75733536826800

H -2.44019660265200 -0.14857350443000 1.34360278850900

SI-I-6 -231.878061 [0.21] -231.878060 [0.65]

C 0.53351395523600 0.32250640657200 0.85819663882400

H 0.76485253688100 0.60090439087500 1.87446659050400

C 1.11088485045100 1.21098217082200 -0.27498335539600

C 0.40850973787700 -1.06370243699300 0.45523610072400

C -0.51343332718500 -1.18172258366800 -0.57005482088900

C -0.41280055260900 1.07193118904900 -0.01410351476700

C -1.02274629630700 0.07085088186400 -0.86511377967700

H 1.00865752082100 -1.86552296179500 0.84914137797300

H -0.73422272021200 -2.08640876521100 -1.10846131119200

H 1.51609211587500 2.15136479543400 0.09177859049200

H -0.94623846362300 1.95672618220700 0.29613654987900

H -1.71293764522600 0.29186631424300 -1.66092357472600

I-4 -231.863466 [0.78] -231.863463 [0.58]

C 1.27434946481600 0.17458338390400 -0.27070694874900

H 2.35053068392200 0.17486073749900 -0.32627492059600

C 0.44644994530600 1.19026034118000 -0.84307621239600

C 0.54724912530500 -0.94782898827800 0.15160342454500

C -0.79148149909200 -1.00921170044800 -0.26429857955200

C -0.79129563104800 1.37339564688600 -0.12648885366000

C -1.25346206832600 0.21255378950200 -0.84779285736300

H 1.03586151053500 -1.79794030187300 0.59853842458100

H -1.34256632138600 -1.93450882147400 -0.29227891914800

H 0.68286494844300 1.70494448297100 -1.76155942133400

H -0.76623282242700 1.32134625142300 0.95456264693700

H -1.80735941277700 0.26276028504900 -1.77183306984000

SI-I-7 -231.846532 [0.01] -231.846531 [0.01]

C 1.15857668067500 0.06743429640000 0.17786056437600

H 2.12222635077500 -0.31486337398600 0.46129594317300

C 0.78137744655000 1.34048680576600 0.06616731190000

C -0.00997534247000 -0.84033810826900 -0.16499470789800

C -0.31696039809900 -1.89196880890400 0.76855050057500

C -0.63068566835000 1.40033039649100 -0.33314750125300

C -1.11006634331100 0.16393858488300 -0.46227026091500

H 0.23484995230000 -1.35151792125200 -1.11685875568400

H -0.44809419903600 -2.89927139196100 1.08320384391600

H 1.39965807559500 2.20556777190700 0.23498473179300

H -1.17653638065600 2.31448250086400 -0.49321887297400

H -2.10753123702700 -0.13457686637700 -0.72879781796000

SI-I-8 -231.843503 [0.01] -231.843502 [0.01]

C 1.80959957287400 -0.70927405296900 -0.72916633926100

H 2.68114492815900 -1.00968868133100 -1.25129848612600

C 0.42763631366500 1.03704572032500 0.46661836992800

C 0.73526768655100 -0.42517896614700 0.18482044038600

C -0.64005622035200 -0.97365227617700 -0.16099129503300

C -0.88142785448300 1.24807903103700 0.33788119669400

C -1.54542809590200 -0.00245040062500 -0.05256037751600

H 1.01979368010300 -0.87701136828500 1.15193959820100

H -0.79829277210600 -1.99949761882800 -0.43962393328600

H 1.19059089534300 1.74604005561600 0.73155632851100

H -1.39389462612400 2.18221340362400 0.49322311477000

H -2.60480400033300 -0.09826409444400 -0.21958126172300

I-5 -231.803849 [0.02] -231.803849 [0.61]

C 1.42874700566300 -0.16512361880900 0.13820421336700

H 2.45972129132600 0.08954130893300 -0.06535694226500

C 0.56919829818900 1.32142965465400 -0.13971291883500

C 0.61383457439400 -0.68434334007400 -0.85517852176500

C -0.76773473683400 -0.94572991339100 -0.49297708690500

C -0.27160153123800 0.88204054107500 0.87048099198000

C -1.19471704161100 -0.18705722228800 0.53193047012000

H 0.99619430451600 -1.04375398818100 -1.80361384958700

H -1.35127799190100 -1.69880750075200 -0.99307519353800

H 1.30928679643800 2.08689952213800 0.04983638537900

H -0.37811474208900 1.40069446066800 1.81637736396700

H -2.13213020354600 -0.30991328519700 1.04560465274400

**Table SI2.** Cartesian coordinates (in Å) of the optimized MECI structures at the SF-BHHLYP/6-31G\* level for naphthalene. Energies in a.u. and the <S2> values for each state are also shown.

II-1 -385.449352 [0.92] -385.449351 [0.11]

C -0.50142906645500 2.43830610346900 -0.36718425531600

C -1.11566628402200 1.25553590066500 -0.02391732450400

C 0.79630887751900 2.32354083425400 -0.90292244026600

C -0.49426133540700 -0.02892482164500 -0.11979910017700

C 1.60918278132700 1.21224544905400 -0.52228385058700

C 0.88808809201800 -0.08954722201700 -0.45494047149900

C -1.22770916035400 -1.20906075468700 0.07297572080700

C 1.48844026460000 -1.33806752705700 -0.55635864216700

C -0.61302387029800 -2.43272262308600 -0.05526023789500

C 0.74550870447600 -2.49038846591000 -0.37182834485800

H -1.08012237773700 3.34879349343400 -0.41810210962300

H -2.16069412601100 1.27774824624700 0.25055564698600

H 1.12480811206000 3.07606793779700 -1.61327345268200

H 1.49877549553900 1.37891717972800 0.57829510983200

H -2.26986561681600 -1.14757841589700 0.34768207627100

H 2.53602349284100 -1.38277150819100 -0.79899128557800

H -1.17276234643900 -3.34154896732900 0.09120888147200

H 1.22197399944800 -3.45161330669000 -0.48291961214800

II-2 -385.445663 [0.59] -385.445662 [0.38]

C -0.44273762025400 2.35716305218300 0.12523466874800

C -1.37516506392700 1.22521109203900 0.21716094577200

C 0.69464475278800 2.40836819123400 0.95351805143000

C -0.78744198300400 -0.03874415870400 0.19522380105600

C 1.15445653872000 1.37270449417300 0.03322486839400

C 0.61542272349800 0.04258163911300 -0.03367612137700

C -1.41287706132800 -1.29989974636200 0.24588315974800

C 1.33033802882900 -1.11439535130900 -0.33681699511100

C -0.67516218752100 -2.43006998909100 -0.00360914657100

C 0.69216812748100 -2.33749630167700 -0.31107876693600

H -0.74679912047600 3.21187853094900 -0.47190005394600

H -2.43565236301000 1.40243490646600 0.27845010296900

H 1.26251826797400 3.31917675257900 1.04492512958400

H 2.03030780647400 1.60051162220100 -0.55921670578200

H -2.47049024232300 -1.36625094801400 0.44590043126300

H 2.38573689181100 -1.05565590767900 -0.55153845439900

H -1.14929680315100 -3.39778424087900 0.01685003148600

H 1.25122375103600 -3.23608879320200 -0.51547942929500

II-3 -385.441317 [0.20] -385.441317 [0.87]

C -0.66585083194500 2.56651657894200 0.62174171409700

C -1.32200060057800 1.41443569349400 0.36872972004200

C 0.82002879039600 2.53853061735100 0.65955437231500

C -0.58818177100700 0.19480463134800 0.10346649631900

C 1.38581937400300 1.27286440142700 0.94479201082800

C 0.82313907194600 0.12019182106700 0.31880210749400

C -1.24152664144100 -0.96673283033100 -0.33132322435800

C 1.50245218896300 -1.09488834177200 0.12022317485500

C -0.54554659456700 -2.13274237910900 -0.55357633249600

C 0.83467356768200 -2.20601647084400 -0.32689585520700

H -1.19552373266400 3.50610822535100 0.67431658354300

H -2.40023601441700 1.37534728935000 0.33967770279800

H 0.86978373418100 2.44724315968000 -0.45927882436600

H 2.18738443183000 1.12977740459700 1.66342894696800

H -2.30694494232900 -0.93829389780800 -0.49272653104000

H 2.56235145050800 -1.13482349966200 0.31588998902600

H -1.07371490613800 -3.00942230363600 -0.89265929080900

H 1.35950204921400 -3.13284102843100 -0.48943414905200

II-4 -385.439028 [0.44] -385.439028 [0.45]

C -0.46480749720500 2.32616058334800 0.47722006301800

C -1.25293864776100 1.25709644773900 -0.08972951086600

C 0.88082095304500 2.24137125110400 0.76785964229500

C -0.69977508430200 -0.05248306421300 -0.14655526125000

C 1.15577603219300 1.31673018426800 -0.28687460276700

C 0.71197785652600 -0.05236392511900 -0.05575906423100

C -1.37252388187600 -1.28205838667900 -0.09572492614700

C 1.41279167112600 -1.19943577648900 0.27254349798900

C -0.65749601893500 -2.43543077966800 0.14342889748700

C 0.72311810135800 -2.39808846000500 0.35427393824800

H -0.96588608963100 3.28043579491800 0.60503380765200

H -2.30902211924900 1.41861630237000 -0.22560108662100

H 1.46184431549300 3.08569170589800 1.08465306948100

H 1.24739520610300 1.64310058373300 -1.32424521397400

H -2.44303512707600 -1.31513484848600 -0.22422513357100

H 2.48298052179100 -1.17172772600700 0.39683008326900

H -1.17236296783400 -3.38182400130600 0.18538551712700

H 1.26113434146700 -3.31194798958700 0.54497957439700

SI-II-10 -385.438186 [0.31] -385.438185 [0.59]

C -0.37925601654500 2.74490130233200 0.27055137876500

C -1.10751630639800 1.44588920470300 0.04107073861000

C -0.38580011621500 1.99702737423100 -1.14542610650700

C -0.31973347624200 0.26870422701200 0.46387923348900

C 0.82045337889800 1.24845487067300 -1.27325604275900

C 0.85892899142900 0.21099751899000 -0.31672254950100

C -0.52936989562500 -0.65252044139100 1.47279622389700

C 1.83487551910600 -0.76191630406600 -0.06472016302200

C 0.43019261551000 -1.62930419099200 1.69243029685700

C 1.60426041775400 -1.68156426651200 0.93321444433700

H -0.98318387159400 3.64679291949800 0.20927779206800

H -2.18731617042800 1.42594983683400 0.08458725113300

H -0.84658570064700 2.51961672607200 -1.96529728346200

H 1.60185363316700 1.45971113693400 -1.98334000538800

H -1.42027351357500 -0.61714664323500 2.07846278267800

H 2.73789400970500 -0.79750968745600 -0.65259337199200

H 0.27300884628300 -2.36260750492500 2.46683344869100

H 2.33141777029100 -2.45083685632000 1.13501763000500

II-5 -385.437787 [0.91] -385.437786 [0.43]

C -0.62535208676900 2.23699509715700 0.09847309763500

C -1.25696403984800 1.02658404795500 -0.00793829485100

C 0.75943823418600 2.32414685115500 -0.14984002141400

C -0.51533530659800 -0.12593256988600 -0.32820104456900

C 1.50845443131800 1.21488133667100 -0.44375604552000

C 0.90910018330800 -0.06092144952500 -0.43890913099700

C -1.13371220554800 -1.31473128765400 -0.81667060071200

C 1.53126030525600 -1.30902797023400 -0.69034041181700

C -0.46975121636700 -2.44958925626800 -1.29776360503800

C 0.67477604509500 -2.44677044347400 -0.47311920140600

H -1.18307850302500 3.12576547031600 0.34242304395000

H -2.32736066526700 0.95685527145600 0.11271946687400

H 1.24351658122400 3.28583136535500 -0.08213347282900

H 2.57194032720500 1.29664792041400 -0.59994344726800

H -2.21670675530900 -1.35693013753700 -0.78424110403500

H 2.06953217246500 -1.34431667276600 -1.63508174181500

H -1.01268000594900 -3.30097533917900 -1.67337269627200

H 0.74075785146200 -3.07600243377100 0.41421117052900

II-6 -385.436935 [0.29] -385.436935 [0.82]

C -0.56099692935100 2.28898209527500 0.38416749745000

C -1.16183478049500 1.10837893969900 0.06599218359900

C 0.75540457228900 2.35205198243400 0.89918724959500

C -0.55341682013500 -0.15536620698000 0.33715455390100

C 1.45944653121100 1.18787709177100 1.01704458137400

C 0.84891526344400 -0.04990223210000 0.77368251774400

C -1.23625642869700 -1.38593653871000 0.15367310326600

C 1.26711922052900 -1.22977040897900 0.14425201567700

C -0.59596308340700 -2.55907724170100 0.55986505622600

C 0.76926386351900 -2.46484166890200 0.70418648996100

H -1.10316075335600 3.20784378575900 0.22357062947800

H -2.16016472118800 1.10347262265400 -0.34103589449200

H 1.20624525571300 3.30108002144300 1.13173906100000

H 2.49445929324500 1.19614467284300 1.31980010578100

H -2.28547955467000 -1.35272878659600 -0.08611101332800

H 1.74158940821500 -1.19784776872000 -0.83685090240800

H -1.15251242151100 -3.41382487476200 0.91516867838400

H 1.25482391395900 -2.85063267219900 1.59210216204200

II-7 -385.427559 [0.21] -385.427558 [0.10]

C -0.56651872032400 2.30060196949000 -0.12216648983800

C -1.14164321723500 1.10908792553700 0.17968533422500

C 0.71380675765400 2.40573058979300 -0.73555405286100

C -0.52974158291600 -0.13583994513900 -0.27849656051200

C 1.45985420104300 1.25110144778400 -0.89941690031600

C 0.84987200432000 0.02910780078600 -0.73630342096800

C -1.35472914298500 -1.27721445620800 -0.62483625701300

C 0.98498473787000 -1.04985517394000 0.18597341125900

C -0.70873986592100 -2.50491607739000 -0.64442199765000

C 0.58444411178500 -2.41355003056600 -0.19727111229700

H -1.08325261263000 3.21030984990600 0.14374591834700

H -2.10242387262900 1.07083108508200 0.66826297083200

H 1.13481617967300 3.37510941922500 -0.93902239883900

H 2.52090615819600 1.29746054424300 -1.09588217279200

H -2.40328996846800 -1.13982626962500 -0.82448913121300

H 1.51592646801800 -0.88959197800000 1.11627242313300

H -1.16399594530400 -3.41471929192600 -0.99578028140400

H 1.28211403405200 -3.23239460615900 -0.14352082929500

II-8 -385.422156 [0.36] -385.422155 [0.76]

C -0.75517009673200 1.89877296724100 -0.08452939688000

C -1.04661842695300 1.16155558023000 -1.33041187743000

C 0.56343865738600 2.16732336608500 0.39165511424900

C -0.63397143608400 0.14847356423400 -0.43600668276000

C 1.47663861896500 1.15082002108300 0.17989284673600

C 0.84418050176300 -0.01635796672900 -0.21753314503300

C -1.46016281356300 -1.01056151352800 -0.08175460736300

C 1.37341643369000 -1.33117624436400 -0.29447899700100

C -0.88901337808700 -2.22245025995900 -0.02435731086700

C 0.54071035167800 -2.39641295277900 -0.20252499442200

H -1.59380566055500 2.38436904027700 0.39405362357500

H -2.05638030392800 1.15146663794200 -1.71138567211100

H 0.78671446850400 3.06945776054100 0.93644211622400

H 2.53202599585500 1.22239409312200 0.37848871185500

H -2.52648152633200 -0.88160851771800 0.00563890604900

H 2.44265404665300 -1.46923109838200 -0.32879264268600

H -1.49426672752200 -3.09909845314500 0.14182733045800

H 0.94057953051900 -3.39704133440700 -0.20386537228500

SI-II-11 -385.403506 [0.38] -385.403505 [0.38]

C -0.79785739913200 2.29745714032700 0.29856794730200

C -1.58671679514300 1.19537266814000 0.29321476298700

C 0.61201366641000 2.21371121446300 0.00666427445600

C -1.16716734735800 -0.13452881557000 -0.03140395537200

C 1.20443118991000 1.05152433269000 -0.29643495701800

C 0.49178138829000 -0.22951152602600 -0.27363339274200

C -0.16646152129800 -0.86528909703000 0.89929194408700

C 0.74751466600500 -1.31170517002500 -1.17428763522100

C -0.15505673008000 -2.29121188676100 0.63986608917800

C 0.36347150401900 -2.52670050859800 -0.61247403230000

H -1.23213657785300 3.27189968555200 0.45976182560700

H -2.64937451076000 1.33016844374600 0.45118760898200

H 1.19184499077700 3.12300706468700 -0.00247505209400

H 2.24732069122700 1.03158287044600 -0.57416923739900

H -0.06885638503000 -0.46309308787200 1.89537467448900

H 1.14578530560600 -1.18392608250700 -2.16657788265900

H -0.58146225586800 -3.02896290003100 1.29677256111500

H 0.40092769773700 -3.47979485240600 -1.10924180577800

II-9 -385.399863 [0.36] -385.399863 [0.26]

C -0.63415522419200 2.16122875419100 0.22411517654600

C -1.44205996979000 1.15573379889800 0.85176124767700

C 0.68340217373800 1.93692485648600 0.01773549922400

C -0.83415422987200 -0.00122358315800 1.30070867020200

C 1.38035974192800 0.85676095760200 0.72001343149700

C 0.61727694893100 0.01087697944500 1.62693870090600

C -1.43380633091300 -1.18081296354900 0.88773966899800

C 1.38159445990700 -0.83307989372100 0.73380725125500

C -0.61113090785900 -2.17424868789400 0.25622924667100

C 0.69759702149700 -1.92978205228700 0.03036396182200

H -1.11694460271300 3.02105858016200 -0.21083742630500

H -2.51218145454900 1.18569342422500 0.71110785541900

H 1.26979811522500 2.64143361545300 -0.55111634533700

H 2.40265066415500 1.10372608248800 0.97242244370000

H -2.50484931569000 -1.23476316138300 0.76611965465300

H 2.40807696543500 -1.06363503822200 0.98632945845000

H -1.08267748763000 -3.04825719892600 -0.16294440856000

H 1.28952263345900 -2.61977484264400 -0.54978143165500

SI-II-12 -385.339474 [0.66] -385.339474 [1.37]

C -0.35626277897900 2.76880715159800 0.20473697541700

C -1.10827034032300 2.61179122355200 -0.96417489685600

C 0.49269465883700 1.90646972632900 0.89581718028300

C 0.06425705550600 -1.63954591767900 -0.22005473091300

C 0.72166077342400 0.56250733402600 0.69024898239300

C 0.15689279014100 -0.26073069776000 -0.34341008198100

C -0.50478283539700 -2.50374340138700 -1.10426004307300

C -0.35282107294000 0.22722187201600 -1.55805609856400

C -1.00780716689900 -1.96840136596400 -2.29663371872700

C -0.93761009893100 -0.60080643787300 -2.50451664118000

H -0.37137143197300 3.80688867621600 0.52666556001700

H -2.11237202369300 2.18890509157900 -0.92325225072200

H 1.01909629734900 2.35520515263800 1.72329248190200

H 1.31377908013300 0.04667422205400 1.42795581635700

H -0.57794786517600 -3.55948919189400 -0.89764720813600

H -0.23713153275300 1.29317158032600 -1.80338511299900

H -1.44467583737200 -2.61522568941400 -3.04044259977000

H -1.31718595712700 -0.17265483889800 -3.41794252839100

SI-II-13 -385.334561 [0.80] -385.334525 [1.14]

C 1.48005406087500 3.07633592632000 -0.38873173987900

C -2.33659527163100 -0.39265213385200 0.16873578502000

C 0.40437798837800 2.59283285646800 -1.19188703668700

C -0.94085464142200 -0.51575866076200 0.44600366091000

C -0.21045237224100 1.40162934247500 -0.97975634462200

C 0.10358086909300 0.34286237306400 -0.02574513353900

C -0.59743820573800 -1.56396209029000 1.31841164816200

C 1.41072800728600 0.10269079909800 0.38454793793200

C 0.70631031371400 -1.78909436994700 1.71104251700700

C 1.70548409843000 -0.95024871364400 1.23917351926800

H 1.79792713584600 4.06822309984600 -0.72302629134000

H -2.57891192845900 0.41686004356100 -0.52352214711900

H -0.01180418176300 3.18351895863100 -2.00343714369900

H -1.06516672573500 1.19409669453200 -1.60484429864100

H -1.40284857376100 -2.18400598951700 1.67334353230600

H 2.19372776528900 0.74838176779200 0.03740766333500

H 0.94592767109500 -2.60171496735200 2.37655328366900

H 2.72980410558700 -1.11535571404200 1.53249628585200

SI-II-14 -385.327487 [1.05] -385.327252 [0.72]

C -1.80490761076600 2.24538359729700 -0.67856147660000

C -0.73725392980000 1.51355128301600 -0.92913090361700

C 0.99114437221600 2.58253173651500 0.20732073786600

C -0.41396507852300 0.16626676124900 -0.41984757209500

C 1.42875042935600 1.29835400373500 0.63349735210100

C 0.77618346543100 0.08753159089300 0.34637122588000

C -1.16697543821800 -0.95960442896600 -0.67856027124900

C 1.19710125256000 -1.18462148028600 0.78098325226800

C -0.75336989834900 -2.20222856060900 -0.21304539203400

C 0.43649525511500 -2.29929972856100 0.50367570906600

H -2.12418064280400 3.23089876669400 -0.96891580110400

H -0.02240540338800 1.95438699042400 -1.62859940944100

H 0.34193322753700 3.09800655994100 0.92853690953300

H 2.38747477440200 1.32363144384000 1.13896100680900

H -2.07275271080600 -0.87051793015600 -1.25677827813600

H 2.11183207970600 -1.27485166286600 1.34552129875200

H -1.34478002986100 -3.07990626517600 -0.41102961573400

H 0.76953681613900 -3.26346724926100 0.85412885448000

SI-II-15 -385.316360 [0.93] -385.316298 [0.69]

C -0.58096669252500 2.38255765038800 0.80910758048900

C -1.89253077611900 2.20163715497100 1.04584647088800

C 0.65270424028300 2.25250902944700 0.26727411998800

C -0.98637841454500 -0.20233658139700 -0.55485608422600

C 1.03465553658300 1.27436480923700 -0.65725324419900

C 0.22909981193300 0.17101371375100 -1.09590316487100

C -1.78203257667400 -1.24592825232200 -0.89408586561700

C 0.63862437052000 -0.67062331314400 -2.15253310197100

C -1.33247967485700 -2.04975397423200 -1.94804331585400

C -0.12564654316600 -1.74855410742400 -2.56191068893800

H -0.87641454731300 3.30689108056200 1.44526380286000

H -2.10369170673200 1.58130958388800 1.92728294398500

H 1.38267443758900 2.99731365222400 0.53682871719700

H 2.01349001027500 1.36683758554700 -1.09558113474700

H -2.71193143513100 -1.45826948906700 -0.39247952465400

H 1.57761880981600 -0.45673733388500 -2.64022863961300

H -1.92482771091200 -2.89060842084300 -2.27146914822900

H 0.22817457478100 -2.36457829824600 -3.37231863748200