

Supplementary Materials

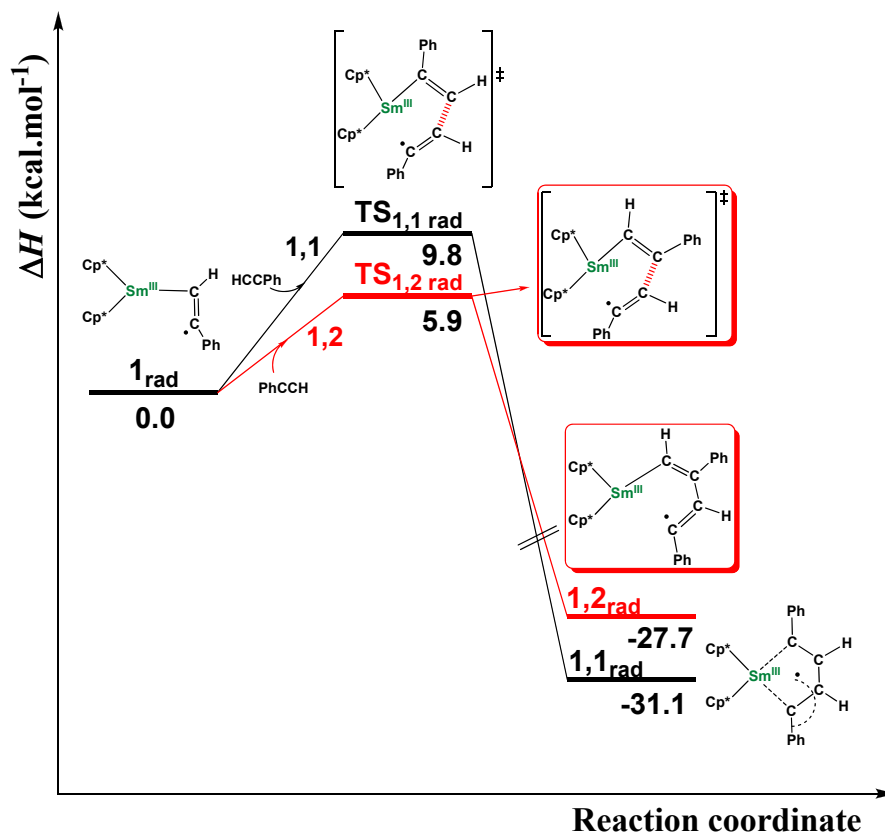


Figure S1. C-C coupling reaction of the monomers in 1,1 and 1,2 fashion.

Enthalpy Energies in a.u. Along with Cartesian Coordinates of the Optimized Structures

1-Ph

$H = -1936.840311 \text{ au}$

Sm	2.59873600	0.90371200	-0.90506800
C	0.38027400	0.30108300	-1.75577100
C	-0.10195200	-0.09501200	-0.54633700
C	3.89086000	-0.22092000	-3.08123900
C	4.92471000	0.46169600	-2.37123900
C	3.49133600	-1.34559400	-2.30533000
C	5.14056500	-0.22769700	-1.14278000
C	4.24808600	-1.34003300	-1.09939300
C	1.54758600	2.94530200	0.64031300
C	2.82399600	2.67270000	1.21736700
C	1.75811200	3.52781800	-0.63920500
C	3.82416000	3.12418600	0.30720000
C	3.16653000	3.63565300	-0.84922500
C	0.69663700	4.11459000	-1.52332700
H	0.42590300	5.12941700	-1.19823800
H	1.03142800	4.19700500	-2.56242600
H	-0.21596100	3.51469400	-1.51800600
C	3.81103600	4.39324500	-1.97558300
H	4.87300600	4.15753000	-2.07445600
H	3.34048100	4.18889000	-2.94401300
H	3.73573900	5.47692000	-1.81224100
C	5.28251200	3.26750200	0.62912100
H	5.64461000	2.47545800	1.29109500
H	5.91013300	3.25851700	-0.26632100
H	5.47283000	4.22141500	1.14031400
C	3.07596400	2.15384200	2.60669700
H	3.11713900	2.96994000	3.34091900

H	2.29046900	1.46849100	2.94350100
H	4.02897200	1.61852300	2.68018500
C	0.21478700	2.77440800	1.30361600
H	-0.23393000	3.74839200	1.54086600
H	-0.48840000	2.22686300	0.66640500
H	0.29768400	2.22316800	2.24520400
C	2.57909000	-2.43722800	-2.77445800
H	3.11014800	-3.13266000	-3.43897000
H	2.19870600	-3.02836800	-1.93728800
H	1.71808500	-2.05195200	-3.32733300
C	4.28649800	-2.41601000	-0.05038000
H	5.13728900	-3.09263400	-0.21101300
H	4.40033900	-2.01171500	0.96250400
H	3.38498200	-3.03378100	-0.05532700
C	6.26761000	-0.01081500	-0.17415400
H	7.05279400	-0.76601400	-0.31729300
H	6.73684100	0.96676700	-0.30167200
H	5.94993300	-0.08681700	0.87252100
C	5.79103600	1.54646900	-2.94325200
H	5.23608400	2.21860800	-3.60459100
H	6.25430400	2.16071300	-2.16629400
H	6.60732500	1.11715000	-3.54024500
C	3.42547200	0.08673400	-4.47656800
H	2.38241300	-0.20382200	-4.63234900
H	3.50619700	1.15335200	-4.71176600
H	4.02720200	-0.44698700	-5.22545300
Sm	-2.42414000	-1.16629800	-0.47983800
C	-3.87011000	1.02492700	0.47934300
C	-3.63019500	1.31979800	-0.89215000
C	-4.79479600	-0.06036500	0.54412500

C	-4.38255200	0.39497100	-1.67558000	C	6.41119900	0.04211600	-0.63013900
C	-5.10938200	-0.45162700	-0.78863900	C	4.97604600	-1.28965800	-1.84588900
C	-0.92276700	-3.19249600	0.68045300	C	5.93224200	-0.99309100	0.22769300
C	-2.00111500	-2.94402400	1.58030500	C	5.05884400	-1.82409200	-0.52956700
C	-1.46024300	-3.79814400	-0.49058600	C	2.31083400	3.04130700	0.07137700
C	-3.20073200	-3.42588600	0.97457100	C	3.07108700	2.93428400	1.26959200
C	-2.87032500	-3.92416000	-0.31751100	C	3.20777600	3.32446800	-1.00218100
C	-4.50139200	-3.67293600	1.67952400	C	4.44084700	3.13610300	0.93563300
H	-4.64312700	-3.01197000	2.53667200	C	4.52036600	3.39307400	-0.46419300
H	-5.36872100	-3.55798900	1.02301500	C	-2.00212500	-0.64654100	2.35077000
H	-4.52870500	-4.70284000	2.06140600	C	-1.28607000	0.48283700	2.84800600
C	-3.80681000	-4.65526800	-1.23782500	C	-3.03410400	-0.17297800	1.48512900
H	-3.84294600	-5.72742800	-1.00024300	C	-1.84672900	1.64903100	2.25455600
H	-4.83165700	-4.27876100	-1.16651800	C	-2.92041000	1.24464500	1.40128600
H	-3.50180500	-4.57679600	-2.28680200	C	0.22620100	-0.15832700	-2.43095800
C	-0.66927700	-4.43291800	-1.59826300	C	-0.21366600	-1.43809400	-1.98765800
H	-1.22439300	-4.46920100	-2.54149000	C	-0.92273800	0.67027600	-2.59780400
H	0.27325000	-3.91501700	-1.79143400	C	-1.63480600	-1.40276500	-1.87987900
H	-0.41575800	-5.47117700	-1.34433200	C	-2.07274800	-0.09908900	-2.25873200
C	0.53251600	-3.00874200	0.98626000	C	-0.28471800	0.43075900	3.96523900
H	0.69224200	-2.24489400	1.75330900	H	0.17456600	1.40552300	4.14450800
H	0.98167800	-3.93951500	1.35939000	H	-0.77549400	0.13330500	4.90133200
H	1.09427500	-2.69744500	0.10164200	H	0.52436700	-0.28290300	3.78429300
C	-1.86553500	-2.42888000	2.98642700	C	-1.56162600	3.07313000	2.64185500
H	-1.61685100	-3.23657400	3.68797100	H	-0.54636700	3.20849100	3.02410000
H	-1.07270200	-1.67830200	3.07539200	H	-1.69447600	3.76809400	1.80591300
H	-2.79118300	-1.96933800	3.34740300	H	-2.24866000	3.40018800	3.43384800
C	-6.16315800	-1.43569000	-1.20874000	C	-3.89520900	2.17993800	0.74310100
H	-5.89242600	-1.97044200	-2.12577700	H	-3.40275300	3.04922400	0.29229900
H	-6.35907500	-2.18591400	-0.43772000	H	-4.47091600	1.68534700	-0.04351900
H	-7.11734800	-0.93031800	-1.41125300	C	-4.19946400	-0.99395500	1.01633000
C	-5.52211900	-0.46060700	1.79509400	H	-3.92646500	-2.03442600	0.82210600
H	-6.22171200	0.33172700	2.09506900	H	-4.98170800	-1.01037100	1.78756300
H	-6.11015000	-1.37009300	1.65896900	H	-4.66108500	-0.59407000	0.10976200
H	-4.85167800	-0.62285100	2.64653000	C	-1.83889400	-2.05855500	2.84051000
C	-3.43813300	1.83229900	1.67034100	H	-2.10651600	-2.79693600	2.07705900
H	-3.11056100	1.20554600	2.50783300	H	-0.81051700	-2.26271700	3.15241100
H	-2.61684600	2.50999800	1.43040600	H	-2.48462100	-2.25231700	3.70821300
H	-4.26722400	2.44799400	2.04571500	C	-2.50869900	-2.60307200	-1.65043000
C	-2.89873300	2.51061100	-1.43441100	H	-2.17139200	-3.22203900	-0.81144000
H	-2.25623400	2.96627400	-0.67808500	H	-3.54418400	-2.31962700	-1.45213500
H	-2.26983900	2.25792400	-2.29278000	H	-2.51561300	-3.25056000	-2.53701600
H	-3.60725400	3.28226600	-1.76508600	C	-0.95967800	2.02578200	-3.24718200
C	-4.55091500	0.45262200	-3.16646800	H	-1.65144200	2.71893300	-2.75498800
H	-3.66572600	0.85750400	-3.66325600	H	0.02566600	2.49930500	-3.26375100
H	-4.74703300	-0.53166100	-3.60404100	H	-1.28708600	1.94610700	-4.29244100
H	-5.39995900	1.09537300	-3.43821400	C	1.63627300	0.20317600	-2.78815700
H	0.57813200	0.06732000	0.34021700	H	1.91142500	1.21521200	-2.46056700
C	-0.38946900	0.04941600	-2.97791500	H	2.33767700	-0.52317400	-2.36194300
C	-0.97456300	-1.21651700	-3.23060100	H	1.80397100	0.18354100	-3.87330400
C	-0.52260600	1.01766900	-3.99692100	C	0.64579900	-2.65316900	-1.79489800
C	-1.65043900	-1.49517500	-4.42385000	H	0.13398700	-3.41790100	-1.20326300
H	-0.76250900	-2.03045500	-2.53626400	H	0.90443400	-3.11323900	-2.75773800
C	-1.20721500	0.74428100	-5.17567100	H	1.57857400	-2.41053500	-1.27687100
H	-0.06740300	1.99293700	-3.84636200	C	4.49646700	-3.13888100	-0.07660200
C	-1.77656800	-0.51442100	-5.40202900	H	5.21667400	-3.95127900	-0.24735500
H	-2.05238200	-2.49139300	-4.59538200	H	4.25672000	-3.13675500	0.98967500
H	-1.28960000	1.51657800	-5.93674200	H	3.58322300	-3.40692500	-0.61681100
H	-2.29088500	-0.72634900	-6.33464900	C	6.43562800	-1.27069100	1.61484400
				H	7.36268100	-1.86084900	1.58938600
				H	6.66239000	-0.34962700	2.16225600
				H	5.70877100	-1.82778400	2.21014200
				C	7.56650200	0.94347200	-0.30476400
				H	7.61913900	1.81089100	-0.96648600
				H	7.53510500	1.31030400	0.72549800
				H	8.51573300	0.40076800	-0.41447000
				C	6.15079300	0.60845700	-3.17136200
				H	6.66735000	1.54966100	-2.96618000
				H	6.81829200	0.01149600	-3.80831900

1-Ph (Z-isomer)
H = -1936.835563 au

Sm	3.71524200	0.64840700	-0.19173800
Sm	-0.64714300	0.24791500	0.12799400
C	1.62257600	-0.52420000	0.86567000
H	0.81826800	-1.29200300	1.14761800
C	2.70236000	-0.54603400	1.67335000
C	5.80445400	-0.12790800	-1.90782500

H	5.26951400	0.84573000	-3.77944300	C	-1.71101100	-3.30573200	0.94847100
C	4.39428300	-1.98799500	-3.04329900	C	0.71448900	1.23219700	4.91269900
H	3.52805000	-2.60695000	-2.79096400	H	0.57002300	1.46607800	5.97604400
H	4.08543200	-1.28916300	-3.82748700	H	1.74486400	0.88339700	4.79535600
H	5.13845600	-2.65810400	-3.49620300	H	0.61463700	2.17461000	4.36748900
C	5.70591200	3.92002300	-1.21711500	C	-2.00805100	1.79130000	3.26549900
H	6.64198500	3.75618100	-0.67935100	H	-1.22695900	2.55506300	3.24313900
H	5.80835200	3.47090600	-2.21016000	H	-2.45016100	1.74560000	2.26280400
H	5.61277200	5.00463400	-1.36982300	H	-2.79652800	2.15930000	3.93594400
C	5.55942500	3.27086500	1.93037300	C	-3.70118200	-0.80828800	3.30857200
H	5.52159600	2.50330400	2.71108800	H	-3.87508200	-0.37243000	2.31758000
H	6.53936000	3.19905100	1.45206800	H	-4.07483000	-1.83386500	3.28490400
H	5.52130900	4.24334200	2.43941100	C	-2.06826800	-3.04267900	4.95081500
C	2.51741000	2.81047500	2.65684900	H	-1.28923400	-3.80629200	5.02962100
H	2.08460800	3.76110600	3.00006500	H	-2.50228600	-2.92756400	5.95350200
H	1.74453300	2.04042400	2.72215800	H	-2.85765200	-3.43992500	4.30797800
H	3.29527600	2.53643200	3.37414500	C	0.70600600	-1.78457600	5.79167800
C	0.81300100	3.03766900	0.00057400	H	0.76019800	-2.86964900	5.65502800
H	0.43046400	2.53966500	-0.90682200	H	1.70977300	-1.38325200	5.62911100
H	0.39361200	2.57494400	0.90570600	H	0.45106000	-1.61080100	6.84658200
H	0.38570000	4.04980300	-0.02721200	C	-0.59624100	-5.11784100	2.46861200
C	2.84124400	3.75083600	-2.39597100	H	0.23428100	-5.06352100	3.18186800
H	3.43619700	3.25378200	-3.17146300	H	-1.52202200	-5.13153500	3.04746300
H	1.78712400	3.56212800	-2.61899700	H	-0.51595500	-6.09083500	1.96588400
H	2.99853100	4.83035000	-2.52660200	C	-2.15148900	-1.66753000	-1.03039900
C	-3.48565500	0.32968500	-2.52671400	H	-3.04868000	-1.30489100	-0.51798900
H	-3.74845900	0.15777200	-3.57959600	H	-1.63373800	-0.79438800	-1.44291600
H	-4.21058200	-0.22331200	-1.92466600	H	-2.49657200	-2.26018000	-1.88872400
H	-3.63960100	1.39560800	-2.33296300	C	0.94549100	-2.21824700	-1.46305900
H	-4.61892500	2.57366800	1.47000800	H	0.59781800	-1.25559100	-1.84852100
C	2.87927800	-1.39221600	2.86035300	H	1.99962400	-2.10815400	-1.19774900
C	3.57865800	-0.90358400	3.97951700	H	0.88983800	-2.93478600	-2.29466600
C	2.36562900	-2.70303000	2.94021300	C	1.93137000	-4.21350700	0.80528900
C	3.72444900	-1.66721000	5.13440400	H	2.07464500	-4.71819200	1.76498000
H	4.00099500	0.09625400	3.92875700	H	2.11468800	-4.95710400	0.01748500
C	2.53420100	-3.47840500	4.08487500	H	2.70472900	-3.44465000	0.72564900
H	1.84516400	-3.11635700	2.07958500	C	5.68236900	-3.03403300	1.38973900
C	3.20702000	-2.96161700	5.19258200	H	4.80777000	-3.66130100	1.20203400
H	4.25637600	-1.25608100	5.98886800	H	6.56872400	-3.67247500	1.27113800
H	2.14005900	-4.49157500	4.11251900	H	5.64579000	-2.72496500	2.43770500
H	3.33601600	-3.56494200	6.08702000	C	7.37511500	-0.40169900	1.88700000
				H	8.39680600	-0.77493000	1.72972500
				H	7.46163000	0.66876800	2.10181200
				H	6.98940700	-0.88098000	2.78972000
				C	7.41979800	1.25813200	-0.77413000
				H	7.09288300	1.85980500	-1.62573800
				H	7.49966500	1.92356000	0.09077200
				H	8.43782500	0.91270500	-1.00107400
				C	5.61999900	-0.29816800	-2.94566400
				H	5.97891200	0.70615100	-3.17964700
				H	6.22946000	-1.00122300	-3.52974100
				H	4.59653400	-0.37895300	-3.33084600
				C	4.64472600	-2.94732000	-1.64324500
				H	4.09528800	-3.64241200	-1.00504700
				H	3.96043700	-2.60663700	-2.42677100
				H	5.43072700	-3.52900200	-2.14551000
				C	4.33709800	2.95582500	-2.36829500
				H	5.41985400	3.04914400	-2.25338100
				H	4.14922500	2.20277300	-3.13834100
				H	3.97671800	3.91471100	-2.76619300
				C	5.26966200	3.87374900	0.55154100
				H	5.72322500	3.58963000	1.50784900
				H	6.04085200	3.77061900	-0.21497900
				H	5.02689300	4.94256000	0.62242900
				C	2.87876000	3.30774500	2.53636500
				H	2.22463900	4.18792200	2.60545000
				H	2.48590400	2.55723800	3.22614900
				H	3.85832100	3.61930900	2.91122200
				C	0.53656300	1.92393500	0.90167500

TS₁₂-Ph
H = -1936.81237 au

Sm	3.89812900	0.27685100	0.46001700
Sm	-0.04428500	-1.34510700	2.12336100
C	2.34619300	-1.03209500	2.64060800
H	1.92603800	-0.67945000	0.90323500
C	3.49353200	-0.53902600	2.91995900
C	5.72129900	-0.60152900	-1.47737500
C	6.51513500	0.08836900	-0.51737700
C	5.25207600	-1.80889400	-0.87352600
C	6.51636800	-0.67849700	0.68561600
C	5.75021700	-1.85894000	0.45930200
C	1.91059600	2.21177800	0.38009500
C	2.96423100	2.81345800	1.12122700
C	2.33496300	2.09144400	-0.97571100
C	4.04585200	3.06454400	0.22385800
C	3.64619800	2.63657300	-1.07563800
C	-0.30297900	-1.14774800	4.87919500
C	-0.28863600	0.21430300	4.45868400
C	-1.53589300	-1.72857300	4.45914900
C	-1.48958900	0.46149500	3.73701500
C	-2.26222500	-0.73947200	3.73398300
C	0.13089600	-2.69483400	-0.29877500
C	0.55938700	-3.62128000	0.69123800
C	-1.26773200	-2.47632800	-0.12160300
C	-0.57675400	-3.99763600	1.46681000

H	0.02360900	1.17493700	0.28333600
H	0.56564500	1.57264400	1.94038200
H	-0.09933800	2.81974300	0.89473900
C	1.48378600	1.66544600	-2.13749800
H	2.05044000	1.10876300	-2.89171400
H	0.65207200	1.02975200	-1.82125800
H	1.04616200	2.53378200	-2.64886700
C	-3.14719500	-3.60166300	1.26331700
H	-3.52716900	-4.39181800	0.60097800
H	-3.28695600	-3.95506900	2.28788000
H	-3.79469200	-2.73218500	1.12218600
H	-4.33809600	-0.25079500	4.00952900
C	4.43117200	-0.44692100	4.02651500
C	5.03859200	0.77263400	4.37643800
C	4.76146200	-1.58774700	4.78696900
C	5.92539600	0.85314800	5.44688700
H	4.79411800	1.66563800	3.80935400
C	5.66375700	-1.50602100	5.84317700
H	4.29765800	-2.53635100	4.53452200
C	6.24968300	-0.28568200	6.18246800
H	6.37150900	1.81104800	5.70153100
H	5.90278600	-2.40103700	6.41192900
H	6.94981400	-0.22420700	7.01065300

2-Ph $H = -1936.824072$ au

Sm	3.53060400	0.28049300	0.33810100
Sm	0.16347100	-1.36557300	1.99316200
C	2.66324000	-0.87438900	2.65327600
H	1.32051500	-0.31276300	0.30947600
C	3.54453900	-0.71373600	3.51442500
C	5.44756800	-0.64962100	-1.53389600
C	6.21435600	0.04733200	-0.55960500
C	4.98252400	-1.86591300	-0.93974800
C	6.15950600	-0.69234100	0.65476400
C	5.42612000	-1.89307200	0.41200200
C	1.88904700	2.49657800	0.42646600
C	3.06804700	2.90433500	1.10560600
C	2.20594800	2.33932000	-0.95240900
C	4.11230800	3.03439600	0.14164200
C	3.57355200	2.69427100	-1.13450300
C	-0.18027200	-1.05212700	4.76969400
C	-0.20954800	0.29474300	4.29694700
C	-1.38117300	-1.69329600	4.35582400
C	-1.40436000	0.46680200	3.54531700
C	-2.12644100	-0.76567000	3.57363600
C	0.25368000	-2.82884100	-0.36815700
C	0.69182300	-3.71355900	0.65348700
C	-1.13610400	-2.58240000	-0.16665100
C	-0.43268700	-4.04512400	1.46811900
C	-1.56902500	-3.36805000	0.93963600
C	0.72521600	1.36890500	4.76675700
H	0.57019300	1.57295300	5.83479100
H	1.77478000	1.08640500	4.64102500
H	0.56330400	2.31292600	4.23937000
C	-2.00684400	1.75671000	3.06187100
H	-1.32582000	2.60134600	3.18376600
H	-2.30651000	1.73041700	2.00739100
H	-2.91307600	1.99084700	3.63690600
C	-3.56218400	-0.88709700	3.14885900
H	-3.73394100	-0.56846100	2.11399800
H	-3.93376500	-1.90883200	3.24275400
C	-1.87067800	-3.00107700	4.90484700
H	-1.07514100	-3.74740600	4.98716800
H	-2.27744300	-2.86062000	5.91593400
H	-2.67050700	-3.43568000	4.30069000
C	0.81248100	-1.61111600	5.74792300
H	0.93444000	-2.69443800	5.64039800

H	1.79939300	-1.15762400	5.62988700
H	0.49104700	-1.43131900	6.78371700
C	-0.44653700	-5.13880600	2.49905900
H	0.38097700	-5.06353400	3.21432400
H	-1.37359000	-5.14158300	3.07561300
H	-0.35980500	-6.12429500	2.02190000
C	-2.02099600	-1.77960600	-1.07851800
H	-2.92402600	-1.42900700	-0.56842000
H	-1.50648700	-0.89860600	-1.47742500
H	-2.35422200	-2.36998800	-1.94304000
C	1.03520800	-2.40379600	-1.57292300
H	0.64518600	-1.47788500	-2.00387300
H	2.08804800	-2.23635500	-1.33701000
H	0.99450900	-3.17635400	-2.35418900
C	2.04637100	-4.34426400	0.76917800
H	2.21627000	-4.75763800	1.76792800
H	2.16515400	-5.17228900	0.05600600
H	2.84654800	-3.62771500	0.57843900
C	5.37129900	-3.06031500	1.35754900
H	5.06400300	-3.97313200	0.84067500
H	6.36376400	-3.25303100	1.78179400
H	4.68245100	-2.90549900	2.19513100
C	6.96481600	-0.39153300	1.88775200
H	8.01967300	-0.66612200	1.74579200
H	6.95218300	0.67189800	2.15194600
H	6.60080800	-0.94355500	2.75676400
C	7.19231600	1.15168300	-0.82670500
H	6.87973400	1.81150800	-1.63911700
H	7.37587200	1.76955000	0.05535600
H	8.16136200	0.72462400	-1.12117700
C	5.41689900	-0.36955100	-3.01051300
H	5.75432200	0.64346300	-3.23871900
H	6.07889000	-1.05898200	-3.55275300
H	4.41828300	-0.48776600	-3.44730700
C	4.51540600	-3.03616400	-1.76057900
H	3.95371600	-3.77452800	-1.18670100
H	3.88761600	-2.73000200	-2.60235000
H	5.38388900	-3.55539400	-2.19060400
C	4.21633100	2.93564000	-2.46898700
H	5.30719100	2.94125000	-2.41268000
H	3.92928400	2.18845400	-3.21447100
H	3.91255600	3.91369800	-2.86633300
C	5.41297400	3.73637400	0.41094500
H	5.95880300	3.32167600	1.26605400
H	6.08271400	3.70274500	-0.44961200
H	5.23205300	4.79585400	0.63702300
C	3.16130500	3.36360700	2.53152000
H	2.85577900	4.41514000	2.62758100
H	2.52145300	2.78158400	3.19848700
H	4.18665200	3.30076300	2.91056100
C	0.52056700	2.42392600	1.02020600
H	-0.15779100	1.84438300	0.38791700
H	0.52944100	1.96217100	2.01069300
H	0.08448900	3.42630900	1.13401000
C	1.22860900	2.00798200	-2.04360100
H	1.72840500	1.60832100	-2.93186300
H	0.49769300	1.26200500	-1.71590900
H	0.67046600	2.89714600	-2.36688800
C	-3.00057900	-3.66618600	1.27089900
H	-3.35505000	-4.51502000	0.66979300
H	-3.14318700	-3.93952600	2.31898100
H	-3.66483400	-2.82606000	1.05458700
H	-4.20176000	-0.25358200	3.77957100
C	4.50909600	-0.58993100	4.56477600
C	4.91570700	0.67272700	5.03521200
C	5.05378100	-1.74177600	5.16508300
C	5.84543900	0.77685200	6.06432800
H	4.49083600	1.56547700	4.58766100
C	5.97805600	-1.62867800	6.19808100

H	4.74071200	-2.71901700	4.81148700
C	6.37993400	-0.37110300	6.64922000
H	6.15041200	1.75891800	6.41500300
H	6.38756300	-2.52654500	6.65252300
H	7.10381300	-0.28647300	7.45474000

TS₂₃-Ph*H* = -2244.981096 au

Sm	2.07214300	0.52052500	0.83578800
C	-0.52605200	-0.03042200	-1.11837300
C	-0.52857900	-0.28430000	0.10128000
C	3.60516600	-0.33880400	-1.32215300
C	4.55540900	0.24079600	-0.43363200
C	3.14411800	-1.55918900	-0.74164500
C	4.63230200	-0.58523200	0.72456200
C	3.77322400	-1.70714600	0.52578400
C	0.95944200	2.60818900	2.25401500
C	2.16730800	2.31284000	2.94659600
C	1.29838300	3.17606500	0.99570700
C	3.25587800	2.72465800	2.12320900
C	2.71843300	3.25470900	0.91206600
C	0.33513900	3.80099100	0.03011100
H	0.06220600	4.81699300	0.34920300
H	0.76691100	3.89374800	-0.97181900
H	-0.59559600	3.23273800	-0.05096000
C	3.46462000	4.03233800	-0.13472500
H	4.54354800	3.88676400	-0.05896900
H	3.17039100	3.76935100	-1.15755900
H	3.27680800	5.10852900	-0.02037500
C	4.67475500	2.84741000	2.59659800
H	4.97036400	2.02053100	3.24826000
H	5.38977500	2.88837700	1.77160700
H	4.80494100	3.77113700	3.17713400
C	2.28640100	1.81584200	4.35919800
H	2.33244900	2.65106200	5.07180600
H	1.44131900	1.18332900	4.64219900
H	3.19404100	1.22208900	4.50681100
C	-0.42730100	2.50781100	2.80544000
H	-1.09079600	1.92375200	2.16167700
H	-0.43277200	2.02611000	3.78381600
H	-0.87049800	3.50683000	2.92071400
C	2.35067000	-2.59616400	-1.47820400
H	2.98924700	-3.13286000	-2.19336900
H	1.92262300	-3.34315200	-0.80652100
H	1.52969700	-2.15776700	-2.05390200
C	3.77787300	-2.91852300	1.41429600
H	4.79111900	-3.33764700	1.47779200
H	3.45487800	-2.69977100	2.43738800
H	3.12977400	-3.70686300	1.02776800
C	5.63042400	-0.48557400	1.84278700
H	6.39041600	-1.27442900	1.75522500
H	6.15843600	0.47017200	1.83548000
H	5.17177900	-0.60300300	2.83157200
C	5.51961700	1.32561800	-0.81212600
H	5.07128200	2.07799500	-1.46577200
H	5.93377100	1.84344200	0.05594600
H	6.36953100	0.89595400	-1.36033700
C	3.32375300	0.12337100	-2.72436200
H	2.32140400	-0.15733200	-3.06073500
H	3.40934400	1.21037900	-2.82596600
H	4.03478600	-0.31699000	-3.43758800
C	-0.75831900	-0.79627900	3.63117100
C	-1.11190200	-0.64417700	4.80826800
Sm	-2.43208800	-1.38389400	1.64382100
C	-4.09151600	0.76954500	2.41787800
C	-3.85193000	0.98605100	1.03337400
C	-4.87951000	-0.41444400	2.54951100
C	-4.48919900	-0.06492100	0.30687000

C	-5.16450400	-0.90063400	1.24072300
C	-1.02698100	-3.74889600	1.69950900
C	-1.96211800	-3.90522700	2.76000600
C	-1.74789800	-3.78498300	0.47256100
C	-3.26097800	-4.04170300	2.19122100
C	-3.12765700	-3.97426700	0.77258100
C	-4.47503200	-4.46992400	2.96414500
H	-4.60239400	-3.90786800	3.89520900
H	-5.39480700	-4.35980700	2.38553300
H	-4.40016100	-5.52982100	3.24347600
C	-4.16957600	-4.34240700	-0.24524000
H	-3.95506700	-5.33297300	-0.66811600
H	-5.16813800	-4.39137900	0.19230500
H	-4.21575200	-3.64404200	-1.08873900
C	-1.14920400	-3.83701000	-0.90131600
H	-1.89918000	-3.63506800	-1.67280900
H	-0.34123200	-3.11255900	-1.02167500
H	-0.73223500	-4.83157300	-1.11341400
C	0.46215200	-3.69839200	1.83631200
H	0.76818000	-3.48339100	2.86298500
H	0.91665800	-4.65799800	1.55291600
H	0.90711100	-2.92288500	1.20690200
C	-1.63673900	-4.12176400	4.20758000
H	-1.48866200	-5.18998800	4.41837400
H	-0.72631500	-3.59619900	4.50580100
H	-2.44680500	-3.77752100	4.85871500
C	-6.24545500	-1.87951700	0.89275900
H	-6.09728600	-2.33211600	-0.08971400
H	-6.34133000	-2.68622300	1.62313000
H	-7.21524800	-1.36373000	0.86246100
C	-5.50052700	-0.89187500	3.83208900
H	-6.34339200	-0.25167500	4.12780700
H	-5.88934700	-1.90936800	3.74071000
H	-4.79207100	-0.88327200	4.66809900
C	-3.82508900	1.72268200	3.54537500
H	-3.55566300	1.20368300	4.46970600
H	-3.02361500	2.42689800	3.31643600
H	-4.72448200	2.31510100	3.76431400
C	-3.27812000	2.21309200	0.38863500
H	-2.78702000	2.86541500	1.11361200
H	-2.54813300	1.96866900	-0.38978500
H	-4.07389800	2.80242800	-0.08695200
C	-4.60680000	-0.12111100	-1.19001300
H	-3.67822100	0.17887300	-1.68600400
H	-4.86138000	-1.12406300	-1.54649200
H	-5.39424900	0.55423900	-1.55325000
H	1.37544700	-0.64962300	2.57240500
H	0.34167300	-0.73325500	2.96098600
C	-1.50585600	-0.44367800	6.16448000
C	-1.66609800	-1.53410100	7.04145900
C	-1.71429500	0.85940100	6.65897600
C	-2.03383700	-1.32441000	8.36557100
H	-1.49337600	-2.53861500	6.67105600
C	-2.07822100	1.06001700	7.98563900
H	-1.58170100	1.70488800	5.99194300
C	-2.24173500	-0.02940500	8.84173300
H	-2.15502000	-2.17474600	9.03074600
H	-2.23378200	2.07025400	8.35349500
H	-2.52729700	0.13045600	9.87765200
C	-0.57890600	0.23421200	-2.52729900
C	-0.72089200	-0.82217400	-3.44810300
C	-0.50868800	1.55100300	-3.02005600
C	-0.78494900	-0.56531500	-4.81377400
H	-0.78587200	-1.83952200	-3.07718300
C	-0.56572100	1.79883000	-4.38761700
H	-0.41338900	2.37232800	-2.31825900
C	-0.70369200	0.74361000	-5.28914200
H	-0.89668600	-1.39169700	-5.51016500
H	-0.50761900	2.82124200	-4.75047300

H -0.75036400 0.94018900 -6.35647800

3-Ph

$H = -2244.996703$ au

Sm 2.43992500 0.95234800 -0.29286600
 C -0.10085100 0.27004100 -2.35020000
 C 0.12840300 0.10899600 -1.13547400
 C 4.07722300 0.02230500 -2.29064100
 C 4.97883800 0.64600900 -1.37751300
 C 3.58456800 -1.17082500 -1.68332200
 C 4.99781500 -0.13082300 -0.18233800
 C 4.14296500 -1.25914800 -0.37683700
 C 1.16622700 2.98279400 1.02216300
 C 2.34583000 2.74914100 1.79165200
 C 1.56341400 3.53987000 -0.22522800
 C 3.46643000 3.18852200 1.02794800
 C 2.98542900 3.66578200 -0.22755200
 C 0.64964000 4.08391400 -1.28352200
 H 0.37805600 5.12627100 -1.06756100
 H 1.12140100 4.08082500 -2.27211600
 H -0.28145500 3.51611700 -1.34944400
 C 3.77040100 4.43384600 -1.25288400
 H 4.84626200 4.29785900 -1.12876400
 H 3.51954300 4.15273900 -2.28229000
 H 3.56912200 5.50964900 -1.16368300
 C 4.84775200 3.37716900 1.58114300
 H 5.12083700 2.59436400 2.29386600
 H 5.61351400 3.40172000 0.80200300
 H 4.91207000 4.33205400 2.12044600
 C 2.39308800 2.31783300 3.23055800
 H 2.45229800 3.18966100 3.89537400
 H 1.50387200 1.75448400 3.52275700
 H 3.26652400 1.69478300 3.45261700
 C -0.24351100 2.82223800 1.49739900
 H -0.91655800 2.59272700 0.66947500
 H -0.35851800 2.01193500 2.22065400
 H -0.60033500 3.74721900 1.97077300
 C 2.82058700 -2.23700200 -2.40755500
 H 3.49147600 -2.80924000 -3.06265700
 H 2.35775300 -2.94967800 -1.72212900
 H 2.02986700 -1.82293900 -3.03986300
 C 4.07806600 -2.43960700 0.55117300
 H 4.94030900 -3.10057100 0.38928700
 H 4.10460100 -2.14457300 1.60543700
 H 3.17958900 -3.04069300 0.40102700
 C 5.94281800 0.02675200 0.97522300
 H 6.76480500 -0.69839300 0.90639100
 H 6.39280400 1.02111900 1.00368100
 H 5.45731300 -0.14141100 1.94336900
 C 5.94882700 1.73071700 -1.74278900
 H 5.52295600 2.46265600 -2.43390500
 H 6.31984800 2.27368500 -0.87061500
 H 6.82534000 1.29562800 -2.24167100
 C 3.83610100 0.43362500 -3.71645400
 H 2.80926500 0.23205900 -4.03816200
 H 4.02787500 1.49956600 -3.87496000
 H 4.49714300 -0.11268400 -4.40295800
 C -1.42589900 -0.50267700 2.30993100
 C -0.97317800 -0.32519300 3.44888200
 Sm -2.34455000 -1.04257500 0.07519800
 C -3.97267500 1.18640600 0.70563700
 C -3.65463700 1.35768200 -0.66950200
 C -4.79883900 0.02969000 0.82328800
 C -4.28612300 0.30904000 -1.40461500
 C -5.02841000 -0.48582900 -0.48582600
 C -0.99588900 -3.42555100 0.41019200
 C -2.08072200 -3.54788400 1.32105000
 C -1.52060300 -3.49132000 -0.91238100

C -3.27843700 -3.68270200 0.56326200
 C -2.93302200 -3.65167500 -0.82058700
 C -4.60152000 -4.07210800 1.15685300
 H -4.90132800 -3.42003300 1.98377000
 H -5.40480100 -4.06011600 0.41697600
 H -4.55562900 -5.09253700 1.56062500
 C -3.82998300 -3.98920000 -1.97784100
 H -3.61167800 -4.99576500 -2.35976900
 H -4.88302800 -3.97990600 -1.68991800
 H -3.71873100 -3.30062700 -2.82368700
 C -0.72236600 -3.59997100 -2.17751900
 H -1.34989100 -3.43371700 -3.05908800
 H 0.10222700 -2.88324700 -2.21156900
 H -0.28389400 -4.60201800 -2.28643700
 C 0.45383200 -3.36172700 0.77899800
 H 0.59011300 -2.93388800 1.77625900
 H 0.91859200 -4.35828800 0.77965800
 H 1.01324000 -2.73776700 0.07518300
 C -1.98280000 -3.72745400 2.80641400
 H -1.87951700 -4.79164200 3.06212300
 H -1.12798400 -3.19403000 3.22681200
 H -2.87261500 -3.35460400 3.32177800
 C -6.10312500 -1.45933700 -0.86848400
 H -5.87588400 -1.98992800 -1.79623800
 H -6.29075800 -2.20493800 -0.09322400
 H -7.04985300 -0.92584700 -1.03243400
 C -5.47295300 -0.39922600 2.09524100
 H -6.24658500 0.32197300 2.39422600
 H -5.96634400 -1.36891200 1.98812200
 H -4.76742100 -0.47386600 2.92991500
 C -3.69500100 2.13026300 1.83881400
 H -3.13578700 1.65005200 2.64811600
 H -3.12028900 2.99941800 1.51103100
 H -4.63588100 2.50720000 2.26155700
 C -3.00124700 2.54754900 -1.30857200
 H -2.56670500 3.22054900 -0.56554800
 H -2.20780500 2.26584500 -2.00863000
 H -3.73555600 3.13287100 -1.87864700
 C -4.34703100 0.22469400 -2.90389600
 H -3.40229600 0.51702600 -3.37405800
 H -4.58769200 -0.78524200 -3.25122800
 H -5.12143300 0.89107400 -3.31055900
 H 2.06273900 -0.51676600 1.79828800
 H 1.32887200 -0.33845100 1.79883800
 C -0.45828100 -0.13200600 4.76703100
 C 0.50529300 -1.00997300 5.30359300
 C -0.89694300 0.94133800 5.56829400
 C 1.00743000 -0.81993100 6.58672000
 H 0.84755100 -1.84548000 4.69995200
 C -0.39175500 1.12477700 6.85115600
 H -1.64114000 1.62336000 5.16826400
 C 0.56247800 0.24736300 7.36727800
 H 1.74760100 -1.51117100 6.98158400
 H -0.74602700 1.95770200 7.45295200
 H 0.95433900 0.39288800 8.37012800
 C -0.34052600 0.45647300 -3.75302500
 C -0.45362100 -0.64881500 -4.61825700
 C -0.45232600 1.75087000 -4.29707800
 C -0.67852300 -0.46206800 -5.97819400
 H -0.36780100 -1.64937200 -4.20918700
 C -0.67005200 1.92922600 -5.65934500
 H -0.36678100 2.60954100 -3.63978000
 C -0.78644900 0.82536000 -6.50392100
 H -0.76782500 -1.32613900 -6.63058200
 H -0.75407200 2.93464800 -6.06222800
 H -0.96096900 0.96784100 -7.56657300

TS₃₄-Ph

H= -2244.991559 au

Sm	2.24264000	0.83893500	0.12367600
C	-0.26227600	0.21612700	-2.59210500
C	0.30639100	0.21604000	-1.48579600
C	4.02553600	-0.04676700	-1.80885700
C	4.87927100	0.52442600	-0.82478300
C	3.50363700	-1.27046600	-1.28474000
C	4.81287700	-0.29102200	0.34047200
C	3.98306900	-1.41868500	0.04373600
C	1.01984900	3.15317900	0.98467500
C	2.15118100	3.04555300	1.84083600
C	1.48773800	3.43863700	-0.32769900
C	3.31965500	3.29767100	1.06464800
C	2.91048500	3.53956500	-0.27917100
C	0.63885600	3.81771600	-1.50430500
H	0.34205900	4.87482600	-1.44989900
H	1.17645500	3.68341100	-2.44802200
H	-0.27379800	3.22156500	-1.55468200
C	3.74015200	4.12977400	-1.38376800
H	4.80569400	4.11327500	-1.14979400
H	3.60530400	3.62179600	-2.34529400
H	3.46240000	5.18016400	-1.54287000
C	4.67064600	3.56184800	1.66350900
H	5.00191600	2.76913900	2.34262000
H	5.44323500	3.69187600	0.90337900
H	4.64788900	4.48752800	2.25415200
C	2.12715100	2.93556500	3.33859100
H	2.03756700	3.92824100	3.80097100
H	1.28857000	2.33621200	3.70167300
H	3.04390300	2.48578600	3.73247600
C	-0.41079100	3.15370800	1.41490400
H	-1.02671400	2.49285400	0.80228500
H	-0.51882500	2.81422000	2.44627600
H	-0.83401400	4.16615300	1.35160100
C	2.82385700	-2.29645200	-2.13852900
H	3.54982200	-2.76202500	-2.81923200
H	2.36988900	-3.09744500	-1.55358600
H	2.04011200	-1.85014000	-2.75654100
C	3.88650800	-2.63609600	0.92036200
H	4.88784800	-3.03105000	1.13398200
H	3.41026200	-2.44460200	1.88958300
H	3.32141100	-3.43516700	0.43819000
C	5.72671900	-0.19278600	1.52990600
H	6.66793900	-0.72954800	1.34397400
H	5.99342400	0.84106900	1.76490700
H	5.29068000	-0.63485800	2.43234300
C	5.93835500	1.55018100	-1.09309800
H	5.67043800	2.22490200	-1.90797400
H	6.17842500	2.15353400	-0.21569700
H	6.86629800	1.04337500	-1.39275000
C	3.88470700	0.39540400	-3.23784900
H	2.87569100	0.21350200	-3.62016600
H	4.09673600	1.46165400	-3.36093400
H	4.58042800	-0.14713300	-3.89301900
C	-0.54834900	-0.24687900	1.69559300
C	-0.17657000	-0.23313300	2.88052200
Sm	-2.12964700	-0.89352400	-0.18734300
C	-3.80783500	1.22418700	0.66409400
C	-3.56722500	1.51803600	-0.70670100
C	-4.59554800	0.03374800	0.72715400
C	-4.19986100	0.50604500	-1.49068500
C	-4.87104500	-0.38326500	-0.60685100
C	-0.86806000	-3.29461900	0.29856700
C	-1.98790300	-3.32256300	1.17606200
C	-1.34828400	-3.42406600	-1.03460700
C	-3.16046400	-3.49277500	0.38594600
C	-2.76829100	-3.53843700	-0.98378900

C	-4.48704500	-3.91018700	0.94919800
H	-4.77263500	-3.33354400	1.83311600
H	-5.29590600	-3.82929900	0.22103300
H	-4.44502400	-4.96298100	1.26131900
C	-3.63837700	-3.91355400	-2.15121400
H	-3.38854600	-4.91837500	-2.51760200
H	-4.69503800	-3.93048500	-1.87645900
H	-3.53669300	-3.23226700	-3.00420300
C	-0.50558800	-3.65401700	-2.25617000
H	-1.12923100	-3.89814900	-3.12179300
H	0.12026800	-2.79817100	-2.52349500
H	0.17138100	-4.50518600	-2.10558700
C	0.57057900	-3.29425500	0.70372300
H	0.68493700	-3.06767800	1.76562500
H	1.03161200	-4.27568800	0.52157800
H	1.15129400	-2.55199000	0.14907200
C	-1.94872000	-3.38477400	2.67493400
H	-1.92486700	-4.42597000	3.02559700
H	-1.07239400	-2.87557200	3.08160300
H	-2.82956900	-2.91743500	3.12689400
C	-5.93634300	-1.34521900	-1.04144100
H	-5.65522400	-1.91982200	-1.92807300
H	-6.20576400	-2.05157100	-0.25480800
H	-6.85050400	-0.79335300	-1.30116500
C	-5.22551300	-0.48106600	1.99046600
H	-5.90123200	0.27044600	2.42175800
H	-5.82070100	-1.37883200	1.81040200
H	-4.49078600	-0.72083400	2.76847300
C	-3.55072100	2.09708200	1.85919400
H	-2.84506200	1.65432900	2.57028000
H	-3.15741800	3.07350800	1.56963300
H	-4.48824200	2.27594100	2.40146900
C	-3.02741200	2.79468500	-1.28069600
H	-2.44558300	3.36551900	-0.55526700
H	-2.39221700	2.62094800	-2.15488700
H	-3.85125000	3.44097800	-1.61387400
C	-4.38697500	0.54514300	-2.98074600
H	-3.55639800	1.03944100	-3.49074000
H	-4.48598400	-0.45529900	-3.41440300
H	-5.30143600	1.09531800	-3.24570700
H	3.10736200	-0.03568800	2.38070700
H	2.43266700	0.15417800	2.65398600
C	0.15737600	-0.25753500	4.27213000
C	1.05397500	-1.21324100	4.78957100
C	-0.42792800	0.66038300	5.16719000
C	1.35891600	-1.24149800	6.14680200
H	1.50023800	-1.93740800	4.11434900
C	-0.12243000	0.62360500	6.52332800
H	-1.12872900	1.39494800	4.78218000
C	0.77382800	-0.32397400	7.01912900
H	2.05209000	-1.98750400	6.52607900
H	-0.58659700	1.33836900	7.19743900
H	1.01160600	-0.34923600	8.07880100
C	-0.80607800	0.32108400	-3.91570700
C	-1.27679000	-0.80367100	-4.61732600
C	-0.84998500	1.57684100	-4.55286500
C	-1.78363600	-0.67280700	-5.90648100
H	-1.23242300	-1.77920600	-4.14587000
C	-1.35223900	1.69844400	-5.84425400
H	-0.48111900	2.44844300	-4.02209300
C	-1.82441900	0.57611400	-6.52530100
H	-2.14390700	-1.55274300	-6.43229400
H	-1.37619400	2.67476000	-6.32047400
H	-2.21905400	0.67428400	-7.53257400

4-Ph

 $H = -2243.833887$ au

Sm	1.91544400	0.79337800	-0.99573500
C	-0.73076500	-0.10588200	-2.52060600
C	-0.91777700	-0.15384500	-1.29163700
C	3.32097500	-0.68172900	-2.93540100
C	4.30752600	0.15939200	-2.35009700
C	2.95570400	-1.67341900	-1.97601100
C	4.50328200	-0.26537500	-1.00456500
C	3.67969000	-1.41154400	-0.77905900
C	1.14457600	3.24660900	-0.00967500
C	2.52820100	3.16101800	0.31384600
C	1.02762300	3.39308700	-1.41874100
C	3.27050300	3.29861600	-0.89413300
C	2.34329400	3.41343700	-1.97087400
C	-0.23176800	3.72060800	-2.16883400
H	-0.75311300	4.56358400	-1.69785900
H	-0.00741800	4.02392500	-3.19621700
H	-0.94581100	2.89316200	-2.21128000
C	2.66443400	3.76532600	-3.39755600
H	3.74074800	3.75334100	-3.58267900
H	2.20418100	3.08818700	-4.12709400
H	2.31251400	4.77697100	-3.63942600
C	4.73299200	3.63140800	-0.93870300
H	5.34413700	2.96190500	-0.32798700
H	5.13251500	3.61470300	-1.95387400
H	4.89198600	4.64634300	-0.54968400
C	3.11491000	3.14613000	1.69676700
H	3.20321100	4.16325700	2.10289900
H	2.50334600	2.56626600	2.39366800
H	4.12052700	2.71352500	1.70599800
C	0.02365200	3.35767900	0.97036000
H	0.36443100	3.15686500	1.98776400
H	-0.40336200	4.37061200	0.95919100
H	-0.78624500	2.65743300	0.75510500
C	2.17750900	-2.90939400	-2.31727500
H	2.79098200	-3.59070900	-2.92277500
H	1.86049100	-3.46229400	-1.43184700
H	1.28286000	-2.68401200	-2.90599800
C	3.82111100	-2.29361800	0.42938000
H	4.88229500	-2.49304300	0.62621200
H	3.40130900	-1.85426500	1.34093900
H	3.33794200	-3.26091300	0.27950500
C	5.57279400	0.19103800	-0.05246200
H	6.25899000	-0.63350100	0.18326500
H	6.17755300	0.99307000	-0.48070300
H	5.17791100	0.54999300	0.90565900
C	5.19253300	1.07349800	-3.14379700
H	4.63428300	1.75436400	-3.79250900
H	5.84134400	1.67566000	-2.50670300
H	5.84532200	0.47973500	-3.79837600
C	2.96942700	-0.70194000	-4.39570200
H	2.01571600	-1.20066100	-4.58503800
H	2.90051600	0.30359200	-4.82329300
H	3.73538900	-1.23914300	-4.97344000
C	0.92641900	0.16422100	1.30600700
C	0.80618900	0.07423500	2.54017700
Sm	-1.96952500	-0.71374300	1.00605000
C	-3.32549900	1.67254900	1.82746500
C	-3.55075600	1.58826200	0.42653100
C	-4.01011200	0.58016600	2.44780900
C	-4.36765200	0.44422600	0.17843400
C	-4.70161000	-0.13967800	1.43203100
C	-0.75691500	-3.17416800	1.25876200
C	-1.51925100	-3.06146800	2.45517500
C	-1.66375900	-3.31975500	0.17171200
C	-2.89777700	-3.17894300	2.11218200
C	-2.98914200	-3.32949500	0.69927900

C	-3.97103200	-3.43805100	3.12888700
H	-4.05559300	-2.64615900	3.88074500
H	-4.95233500	-3.56782600	2.66952800
H	-3.74822800	-4.36392700	3.67623300
C	-4.20101800	-3.72595900	-0.09583400
H	-4.08981500	-4.74890600	-0.47822100
H	-5.10907500	-3.71102100	0.51017400
H	-4.37403400	-3.08237200	-0.96555100
C	-1.30301300	-3.66610300	-1.24225000
H	-2.15710500	-3.53428900	-1.91344100
H	-0.48798900	-3.04886300	-1.62256700
H	-0.98883400	-4.71659200	-1.32065500
C	0.72948300	-3.28304700	1.16115600
H	1.21517100	-3.04982000	2.11084900
H	1.02897800	-4.30190700	0.87803300
H	1.13946300	-2.59502400	0.41973500
C	-1.00274400	-3.08026400	3.86518500
H	-1.10559600	-4.08442400	4.30014100
H	0.05312600	-2.80946100	3.92393800
H	-1.54699100	-2.39531900	4.52438700
C	-5.85784500	-1.06773800	1.65379700
H	-5.94481200	-1.83226100	0.87918900
H	-5.81313000	-1.57066600	2.62037100
H	-6.79329900	-0.49155500	1.63624100
C	-4.20254400	0.43498900	3.93153100
H	-4.87024400	1.21659800	4.32113400
H	-4.65377700	-0.52552200	4.19254400
H	-3.26567000	0.51529900	4.49388600
C	-2.76640100	2.84051500	2.59280800
H	-3.47116600	3.14921700	3.37493400
H	-1.80835800	2.64595700	3.08710900
H	-2.61363400	3.70326700	1.94112300
C	-3.27407500	2.62822200	-0.61578900
H	-2.54142300	3.36704000	-0.28870100
H	-2.90514600	2.18287600	-1.54402300
H	-4.19682900	3.17142000	-0.86263100
C	-4.97738800	0.10431700	-1.15208900
H	-4.25848500	0.20616000	-1.97154100
H	-5.36244100	-0.91909100	-1.17585700
H	-5.82239400	0.76821800	-1.38305700
C	0.85925400	-0.02123500	3.96896400
C	-0.11976600	0.56471700	4.79126000
C	1.93096600	-0.69876600	4.58368200
C	-0.03701500	0.46598700	6.17689700
H	-0.94127700	1.10638700	4.33309600
C	2.01152200	-0.78778100	5.96895900
H	2.69563900	-1.14927700	3.95848400
C	1.02719500	-0.21035800	6.77199400
H	-0.80433700	0.92517900	6.79411300
H	2.84694100	-1.31234800	6.42454700
H	1.09163500	-0.28403600	7.85378600
C	-0.65483900	-0.16462200	-3.95233200
C	-0.34888500	0.96801200	-4.72818900
C	-0.91804100	-1.38064300	-4.61350700
C	-0.29629900	0.88270000	-6.11620300
H	-0.16495800	1.91512300	-4.23269000
C	-0.86827000	-1.45676500	-6.00131600
H	-1.16585400	-2.25657300	-4.02280100
C	-0.55396200	-0.32768100	-6.75858500
H	-0.05811300	1.76824800	-6.69904000
H	-1.07640300	-2.40247000	-6.49418100
H	-0.51388700	-0.39056600	-7.84227900

TS₄₅-Ph $H = -2243.816903$ au

Sm	2.23506800	0.84611000	0.27270700
C	-0.19516600	-0.09778800	-0.51686700
C	-0.50267200	-0.31908300	0.68976600
C	3.48988600	-0.79286800	-1.62296900
C	4.51738600	0.08669900	-1.17466900
C	3.17055200	-1.68189100	-0.55591200
C	4.80975000	-0.23536400	0.18165300
C	3.97331500	-1.32741400	0.56491300
C	1.43522000	3.22790800	1.47282900
C	2.80629600	3.07428500	1.82598700
C	1.36470200	3.50492600	0.08007200
C	3.58809600	3.29410100	0.65410600
C	2.69623600	3.53211800	-0.43287200
C	0.13372400	3.96941100	-0.64581600
H	-0.19178800	4.94588200	-0.26151200
H	0.32071600	4.10442300	-1.71555600
H	-0.71538800	3.28889200	-0.53705600
C	3.09180200	3.99767700	-1.80627600
H	4.11306100	3.70048500	-2.05651900
H	2.43801600	3.60390300	-2.59259100
H	3.04999500	5.09310200	-1.87995300
C	5.06185800	3.57471700	0.65227900
H	5.59506500	3.01376700	1.42318900
H	5.53549400	3.35744300	-0.30819000
H	5.23804800	4.63986700	0.85734000
C	3.33858100	2.89123700	3.21963600
H	3.44754400	3.85387900	3.73756900
H	2.67757400	2.26984700	3.83154300
H	4.32633900	2.41867000	3.22197900
C	0.28276800	3.29638800	2.42302400
H	0.56076500	2.93875800	3.41692200
H	-0.06877000	4.33210500	2.53251500
H	-0.56340400	2.69282200	2.08884200
C	2.31867300	-2.90679300	-0.69445700
H	2.87934900	-3.71376100	-1.18608900
H	1.98712900	-3.29000900	0.27230400
H	1.42892100	-2.72146300	-1.30329700
C	4.14964000	-2.10010700	1.84034200
H	5.05222800	-2.72566900	1.79294300
H	4.26916200	-1.44625600	2.71150500
H	3.30855700	-2.76528700	2.04128500
C	5.97417300	0.24695800	0.99835300
H	6.72719400	-0.54666800	1.09781100
H	6.47070600	1.10302600	0.53775400
H	5.69232000	0.53819200	2.01713400
C	5.30155200	0.98857800	-2.08199100
H	4.66129100	1.54640000	-2.77267000
H	5.90441400	1.71295500	-1.52989800
H	5.99470600	0.40225000	-2.70084700
C	3.02768900	-0.91756600	-3.04696900
H	2.05237700	-1.40365500	-3.12489900
H	2.94666200	0.05315000	-3.54658200
H	3.73728900	-1.51728500	-3.63435900
C	0.77588600	0.03972200	2.20771300
C	0.41954800	-0.12725700	3.41148700
Sm	-2.01684700	-0.97347700	2.64930500
C	-3.32822500	1.50939700	3.16523100
C	-3.46827600	1.29618000	1.76525800
C	-4.08958100	0.50396100	3.83820200
C	-4.31849300	0.16647300	1.57194200
C	-4.74024600	-0.29192000	2.85198200
C	-0.73637000	-3.42155400	2.95107600
C	-1.52959600	-3.30042600	4.12624500
C	-1.61521900	-3.58147600	1.84220300
C	-2.89990900	-3.41964300	3.74779600
C	-2.95360900	-3.59390200	2.33454800

C	-4.01789100	-3.61795100	4.73008300
H	-4.06151900	-2.83301700	5.49390500
H	-4.99269100	-3.65745900	4.24093200
H	-3.88874100	-4.56739500	5.26712300
C	-4.14799500	-3.99830400	1.51759600
H	-4.07037200	-5.05199300	1.21844600
H	-5.07996500	-3.89556600	2.07765500
H	-4.25278500	-3.41684100	0.59487600
C	-1.20896100	-3.92652400	0.43953100
H	-2.01323900	-3.72220300	-0.27471300
H	-0.32832400	-3.36633900	0.11881500
H	-0.96780800	-4.99533800	0.34954900
C	0.75651100	-3.51682200	2.88769400
H	1.20432700	-3.41451400	3.87924000
H	1.07002300	-4.48928800	2.48615600
H	1.18737300	-2.73563600	2.25435800
C	-1.04632400	-3.28456100	5.54866900
H	-1.05856300	-4.29755300	5.97473300
H	-0.02617500	-2.90492800	5.63997800
H	-1.67827700	-2.66471800	6.19348700
C	-5.91014900	-1.19435000	3.10752500
H	-5.99375000	-2.00049900	2.37486400
H	-5.88034800	-1.64404900	4.10197600
H	-6.84299200	-0.61629700	3.04850800
C	-4.37249500	0.47699700	5.31473000
H	-5.22866600	1.11776900	5.56933700
H	-4.61435800	-0.52904500	5.67092500
H	-3.52433400	0.83535500	5.90687300
C	-2.75146500	2.72559000	3.84051900
H	-3.42312300	3.07198300	4.63443500
H	-1.76576400	2.58095700	4.29501400
H	-2.64596400	3.55084700	3.13170500
C	-3.04562400	2.21249400	0.65560300
H	-2.42155500	3.02977300	1.02239700
H	-2.48047800	1.69326400	-0.12487700
H	-3.92366500	2.66517000	0.17577600
C	-4.85811800	-0.27675400	0.24125000
H	-4.09506100	-0.24833800	-0.54408700
H	-5.25831300	-1.29408400	0.27819100
H	-5.67789400	0.37513500	-0.09224300
C	0.65419900	-0.18091900	4.82934000
C	-0.25113900	0.38048700	5.75114000
C	1.81214900	-0.80810200	5.33930600
C	-0.00637500	0.32696900	7.12099900
H	-1.14285300	0.87928700	5.38219100
C	2.04597000	-0.86378200	6.70824000
H	2.51933100	-1.24531500	4.64203300
C	1.14002900	-0.29755900	7.60801600
H	-0.71742200	0.77541400	7.80959000
H	2.94656900	-1.34796700	7.07669800
H	1.32882700	-0.34196400	8.67661200
C	-0.35159900	-0.12931000	-1.94521800
C	-0.11556200	1.00786700	-2.74299700
C	-0.75571200	-1.31803200	-2.59207600
C	-0.28231100	0.96070500	-4.12449400
H	0.17284300	1.93904400	-2.26621900
C	-0.91402300	-1.35774000	-3.97235900
H	-0.95038200	-2.20053700	-1.99200700
C	-0.67810700	-0.22091200	-4.74827400
H	-0.10258000	1.85499600	-4.71516700
H	-1.23086600	-2.28304900	-4.44626700
H	-0.80578500	-0.25663700	-5.82620000

5-Ph

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Sm	2.78036900	1.11476300	0.23816900
C	0.51702800	0.33232900	-0.50412100
C	0.24557200	0.03047500	0.75685100
C	3.91044700	-0.54765300	-1.67348500
C	4.98849600	0.27758300	-1.23424500
C	3.55987500	-1.42256300	-0.60795900
C	5.28246200	-0.06765700	0.11792800
C	4.39535700	-1.11864900	0.50463700
C	1.96712500	3.48791400	1.38815300
C	3.38198400	3.46326000	1.57325900
C	1.70571000	3.65417600	-0.00146700
C	3.99597100	3.63486200	0.30015600
C	2.96063900	3.72598700	-0.67856200
C	0.36256400	3.91088800	-0.62060600
H	0.04638300	4.94944900	-0.45215600
H	0.37682500	3.75255200	-1.70223400
H	-0.41542600	3.26152400	-0.21263800
C	3.14582600	4.06612100	-2.13087900
H	4.13977600	3.78890800	-2.49301500
H	2.41241000	3.56662600	-2.77344200
H	3.03298000	5.14489400	-2.30389400
C	5.44495400	3.96001200	0.08731200
H	6.10348000	3.40149000	0.75887800
H	5.77064000	3.76856100	-0.93753700
H	5.62599800	5.02589600	0.28353700
C	4.09517400	3.45308500	2.89642800
H	4.24672400	4.47400900	3.27339800
H	3.53277200	2.91332900	3.66471400
H	5.08748900	2.99381900	2.82744200
C	0.94565300	3.53589400	2.48553800
H	0.83871700	4.55731000	2.87570800
H	-0.03694900	3.22497300	2.12447500
H	1.20157600	2.89204500	3.33239100
C	2.60234300	-2.56961800	-0.71715300
H	3.06293900	-3.41410100	-1.24755500
H	2.30117000	-2.93873600	0.26604900
H	1.69417300	-2.29824900	-1.26394100
C	4.48994900	-1.89587100	1.78805000
H	5.16652200	-2.75446100	1.67852700
H	4.88766200	-1.28929400	2.60844400
H	3.52409800	-2.29225500	2.11375800
C	6.44944800	0.41045000	0.93520500
H	7.23574700	-0.35478100	0.98351300
H	6.90394600	1.30810700	0.50934600
H	6.17723500	0.64471600	1.97130500
C	5.81569800	1.14173400	-2.14106000
H	5.20516200	1.76409600	-2.80334700
H	6.48190700	1.80505600	-1.58556900
H	6.44943000	0.52095500	-2.78858900
C	3.38085900	-0.62552800	-3.07673600
H	2.32349700	-0.90330400	-3.10181900
H	3.48287100	0.32581800	-3.60888700
H	3.92829000	-1.37623000	-3.66363100
C	0.38579000	-0.03467300	2.06280200
C	0.07275500	-0.23578500	3.33417600
Sm	-2.08995000	-1.24896800	2.58425600
C	-3.25917300	1.14429700	3.34030600
C	-3.42056200	1.07792000	1.92699600
C	-4.08418100	0.13570500	3.92369300
C	-4.35113400	0.03563100	1.63523800
C	-4.77805300	-0.53107300	2.86960300
C	-0.62457600	-3.56852200	2.96217400
C	-1.50895900	-3.51162300	4.07466900
C	-1.40348700	-3.79897400	1.79164100
C	-2.83606100	-3.73289900	3.59746600
C	-2.77222200	-3.90434700	2.18284300

C	-4.01800200	-4.02003300	4.47737800
H	-4.10115000	-3.32278800	5.31788300
H	-4.95958100	-3.98654900	3.92583000
H	-3.93585200	-5.02570500	4.91153900
C	-3.89687800	-4.33242300	1.28294600
H	-3.88116700	-5.41862100	1.12039100
H	-4.87576400	-4.08861500	1.70357100
H	-3.84285500	-3.86690000	0.29248200
C	-0.85872200	-4.08183000	0.42024300
H	-1.61975000	-3.96320600	-0.35733000
H	-0.01948500	-3.43049400	0.16078800
H	-0.49382400	-5.11554300	0.34765300
C	0.87221400	-3.53884500	3.01726100
H	1.23643900	-3.08376500	3.94160500
H	1.28931000	-4.55330700	2.95928400
H	1.29386900	-2.96482100	2.18709400
C	-1.11374700	-3.41836500	5.52108800
H	-0.94586000	-4.41576100	5.95014600
H	-0.19297600	-2.84549100	5.66181500
H	-1.89072600	-2.94224500	6.12854700
C	-5.95139800	-1.45160300	3.03234700
H	-6.00106400	-2.21445600	2.24931200
H	-5.94660400	-1.96276400	3.99741400
H	-6.89017400	-0.88330800	2.97706600
C	-4.34169400	-0.03449300	5.39471100
H	-5.13570900	0.64158000	5.74011300
H	-4.66015000	-1.05105000	5.64450900
H	-3.45562300	0.18922700	5.99812300
C	-2.51814200	2.21092300	4.09309500
H	-3.15183700	3.09621700	4.24184800
H	-2.20232400	1.87358000	5.08417900
H	-1.61935800	2.53878500	3.56629200
C	-2.85830300	2.05113400	0.93318900
H	-1.89635300	2.44886200	1.26453800
H	-2.70280100	1.60225400	-0.05239600
H	-3.53286800	2.90721100	0.79605000
C	-4.92298100	-0.28505100	0.28262300
H	-4.21453100	-0.07986100	-0.52599100
H	-5.22340600	-1.33532000	0.20180600
H	-5.81956700	0.31620500	0.07810000
C	0.92848500	0.00017300	4.49270300
C	2.33293700	0.08800400	4.40251700
C	0.35885100	0.11779400	5.77461000
C	3.12231000	0.29940900	5.52763500
H	2.80245600	-0.04891100	3.43099000
C	1.14383800	0.34551400	6.90120800
H	-0.72010600	0.03388600	5.87071600
C	2.53040600	0.43778900	6.78479000
H	4.20355100	0.35092700	5.42778600
H	0.67248700	0.44343600	7.87563500
H	3.14564600	0.60478900	7.66435600
C	-0.33272900	0.08982600	-1.66579600
C	-1.37664400	-0.85814600	-1.66903800
C	-0.10798700	0.80128300	-2.85950700
C	-2.16013200	-1.07383700	-2.79744600
H	-1.54474700	-1.45177500	-0.77356900
C	-0.90033200	0.60042100	-3.98594100
H	0.70031400	1.52694000	-2.88420900
C	-1.93035700	-0.33940600	-3.96252000
H	-2.95052400	-1.81973100	-2.77242600
H	-0.70839900	1.17399400	-4.88896600
H	-2.54266000	-0.50541600	-4.84432600

TS₁₆-Ph $H = -2244.95793 \text{ au}$

Sm	2.79472400	0.65772400	0.54112200
C	0.41070600	0.01550000	0.16779700
C	0.23331700	-0.39384500	1.43212600
C	3.85824200	-0.51826300	-1.71036900
C	4.99211100	0.03853700	-1.04608600
C	3.38630200	-1.62061500	-0.93859500
C	5.18954000	-0.68829700	0.16250500
C	4.19939600	-1.71632500	0.22718900
C	1.85769300	2.97656000	1.85333900
C	3.06484600	2.59014400	2.50994500
C	2.19160600	3.40595000	0.54171500
C	4.15023500	2.82978300	1.61227100
C	3.60946300	3.32791000	0.39188800
C	1.25860700	4.09440800	-0.41291200
H	1.28115700	5.18317800	-0.26235000
H	1.52824800	3.92201700	-1.46067000
H	0.22181700	3.77452600	-0.27725000
C	4.37344000	3.95869200	-0.73697400
H	5.41633100	3.63716800	-0.76218300
H	3.93755200	3.73772200	-1.71765600
H	4.37608800	5.05241100	-0.63399200
C	5.60073700	2.79666400	1.99743000
H	5.84629700	1.94814700	2.64394600
H	6.25863800	2.74579500	1.12548200
H	5.87548900	3.70503600	2.55122100
C	3.22044000	2.20047400	3.95536400
H	3.52954300	3.05861400	4.56747300
H	2.28909700	1.82124400	4.38643500
H	3.98251200	1.42603500	4.10268300
C	0.49133100	3.09721600	2.46160700
H	0.10934500	4.11835700	2.34279500
H	-0.23795300	2.41737400	2.00708800
H	0.50865100	2.89141400	3.53501700
C	2.34944300	-2.59774100	-1.40918200
H	2.71945100	-3.16185100	-2.27567600
H	2.10390700	-3.32903600	-0.63601700
H	1.41701000	-2.11147000	-1.71256000
C	4.20461100	-2.81582300	1.25253100
H	5.08649300	-3.45805600	1.12620800
H	4.24043800	-2.44145600	2.28319900
H	3.32555800	-3.45696200	1.17246800
C	6.37080800	-0.59046300	1.08525800
H	7.10932900	-1.37185800	0.85823300
H	6.88382000	0.36989300	0.99729500
H	6.09579800	-0.72060200	2.13854400
C	5.95903100	1.01098200	-1.65408900
H	5.46885200	1.73851200	-2.30670500
H	6.51931900	1.56859400	-0.89867000
H	6.69764600	0.47885100	-2.26897700
C	3.35152500	-0.14387700	-3.07497400
H	2.26324400	-0.23668100	-3.15029300
H	3.61454900	0.88422500	-3.34418800
H	3.78186700	-0.79306600	-3.85006300
C	-0.49093400	0.03652500	3.59235900
C	-1.45119200	-0.38122700	4.29234900
Sm	-2.31548400	-1.44041900	2.05059200
C	-3.94002100	0.85021800	2.36113600
C	-3.85111800	0.64136500	0.95897400
C	-4.71654900	-0.20775100	2.91934700
C	-4.57779300	-0.55102200	0.64215600
C	-5.11982500	-1.06355500	1.85362400
C	-0.73178400	-3.74214500	2.24905600
C	-1.45482400	-3.72356400	3.47295000
C	-1.64675300	-4.02393500	1.19489000
C	-2.82998600	-3.97148300	3.17610900
C	-2.94368300	-4.16158700	1.76471300

C	-3.92188500	-4.22487500	4.18098900
H	-4.58981900	-3.37114300	4.34703200
H	-4.55442200	-5.06244600	3.86745800
H	-3.50123600	-4.49732100	5.15398700
C	-4.13445200	-4.70839000	1.03076800
H	-3.96321900	-5.75582200	0.74650500
H	-5.03714700	-4.68218400	1.64368700
H	-4.35583100	-4.16467700	0.10529800
C	-1.28199600	-4.42962000	-0.20521800
H	-2.05991300	-4.17524000	-0.93329600
H	-0.34700300	-3.97413400	-0.54327200
H	-1.14348300	-5.51846700	-0.26346000
C	0.76013300	-3.69090000	2.13822400
H	1.20590200	-3.15491700	2.98151000
H	1.19711400	-4.69991600	2.12774900
H	1.07744900	-3.18005700	1.22635600
C	-0.79557900	-3.69709800	4.82331300
H	-0.10693300	-4.54560000	4.92576800
H	-0.21466300	-2.78491300	4.99577100
H	-1.51888100	-3.77371000	5.63776800
C	-6.19818400	-2.10203400	1.95570800
H	-6.22913500	-2.74887300	1.07614400
H	-6.09567900	-2.74229600	2.83722000
H	-7.18235500	-1.61809000	2.03187900
C	-5.31079300	-0.23136700	4.29730700
H	-6.32521900	0.19190800	4.28033000
H	-5.40184200	-1.24402200	4.70368500
H	-4.72692800	0.35324400	5.01066300
C	-3.48414400	2.08259400	3.08415800
H	-3.28689200	1.88939500	4.14165400
H	-2.57020900	2.49956400	2.65126200
H	-4.25039200	2.86889000	3.03414400
C	-3.32071700	1.64612400	-0.02146700
H	-2.38222900	2.09996500	0.31234000
H	-3.13580900	1.20892600	-1.00438400
H	-4.04101400	2.46494500	-0.15797600
C	-4.96084000	-1.01735400	-0.73361200
H	-4.29415500	-0.61517100	-1.49875900
H	-4.94834300	-2.10917500	-0.82838900
H	-5.97940300	-0.69122700	-0.98578100
H	1.16089800	-0.48171900	2.06073000
H	0.45411300	0.54198600	3.50336100
C	-1.97413800	-0.25051100	5.64829800
C	-2.77480100	-1.23382200	6.24645200
C	-1.66352300	0.89970600	6.40035700
C	-3.22593900	-1.09075500	7.55590600
H	-3.04367300	-2.11341800	5.67403200
C	-2.13056600	1.04978000	7.70152400
H	-1.05325600	1.67490800	5.94663800
C	-2.90881900	0.05126800	8.28882700
H	-3.83806300	-1.87081500	8.00046900
H	-1.88047400	1.94681300	8.26183100
H	-3.26920700	0.16629000	9.30723000
C	-0.46200500	0.04362600	-0.99759100
C	-1.24798500	-1.07372700	-1.34736200
C	-0.41594100	1.10492300	-1.92598200
C	-1.94200100	-1.13045200	-2.55528100
H	-1.24483500	-1.94113200	-0.69042400
C	-1.13467000	1.06383700	-3.11489000
H	0.19357400	1.97317600	-1.69709700
C	-1.89878800	-0.05868200	-3.44495700
H	-2.51691100	-2.01932200	-2.80153400
H	-1.08615800	1.90711000	-3.79929200
H	-2.43873300	-0.10110800	-4.38628700

6-Ph

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Sm	3.34533900	1.40796800	-1.02434300
C	1.03451700	0.55466500	-0.85077900
C	1.18267700	0.31634600	0.47255800
C	4.60458800	0.02437800	-3.04007600
C	5.67776400	0.46377100	-2.20930500
C	3.86024400	-0.95915500	-2.32057200
C	5.57736300	-0.22240000	-0.96331500
C	4.45865500	-1.10701700	-1.03726900
C	2.24387700	3.82197700	-0.20184600
C	3.34087200	3.56293600	0.67503400
C	2.77601800	4.08892400	-1.49368900
C	4.55009600	3.70163500	-0.06989500
C	4.20115400	4.01574000	-1.41590500
C	2.01668500	4.55855100	-2.70323500
H	2.21622800	5.61996700	-2.90192200
H	2.28599200	4.01703600	-3.61873600
H	0.93639700	4.46114600	-2.56749800
C	5.13484500	4.46157900	-2.50500100
H	6.16146200	4.13386800	-2.32643600
H	4.83893800	4.09277800	-3.49386300
H	5.15586300	5.55804500	-2.57373500
C	5.93484400	3.68876900	0.51139900
H	6.04618700	2.94609700	1.30848600
H	6.69605500	3.47502500	-0.24434900
H	6.18711700	4.66301300	0.95138800
C	3.23997100	3.35326200	2.16070100
H	3.23068500	4.31151600	2.69768600
H	2.32328900	2.82397100	2.43884300
H	4.08504700	2.78049500	2.55815400
C	0.80790000	3.93026200	0.22085300
H	0.61683100	4.89058900	0.71812100
H	0.12461500	3.86347300	-0.62985700
H	0.52199500	3.13596000	0.91674800
C	2.74876100	-1.80156400	-2.87447600
H	3.14259300	-2.71472800	-3.34156900
H	2.04708600	-2.10780400	-2.09453800
H	2.16949300	-1.27373700	-3.63791200
C	4.06276500	-2.11608100	0.00219800
H	4.50050500	-3.09972800	-0.21429700
H	4.40397700	-1.83161100	1.00278400
H	2.97847500	-2.24896000	0.05164900
C	6.58307000	-0.17087100	0.15275500
H	7.36359500	-0.93209000	0.01890100
H	7.08977700	0.79724900	0.20755300
H	6.12901300	-0.35841000	1.13182400
C	6.83937400	1.30360900	-2.65285900
H	6.56224300	2.02212600	-3.42892400
H	7.28753600	1.86444700	-1.82732200
H	7.63381100	0.67172200	-3.07319100
C	4.38850600	0.40621700	-4.47840800
H	3.33148500	0.36185100	-4.76233000
H	4.74647900	1.41798200	-4.69563800
H	4.92427600	-0.27104800	-5.15712400
C	0.35878100	0.15319400	1.67740800
C	-0.94974600	-0.17694700	1.89487700
Sm	-2.83404100	-1.34109200	0.58069600
C	-4.38911900	0.85117500	1.35172900
C	-4.31407400	0.91844400	-0.06790500
C	-5.17518600	-0.28846800	1.69765500
C	-5.06610500	-0.17022200	-0.60494500
C	-5.60181200	-0.91071000	0.48766700
C	-1.16234700	-3.65366600	0.52134300
C	-1.79068700	-3.68386800	1.79404100
C	-2.15535800	-3.89724300	-0.47177100
C	-3.18539800	-3.92037100	1.59444200
C	-3.40651300	-4.06189600	0.18936500

C	-4.17737800	-4.23982200	2.67764100
H	-3.99598100	-3.66678400	3.59258500
H	-5.20683500	-4.03746500	2.36905300
H	-4.13018700	-5.30174800	2.95455200
C	-4.65019300	-4.58884100	-0.46773700
H	-4.53107000	-5.65150700	-0.71985600
H	-5.52160500	-4.51150700	0.18468500
H	-4.89607200	-4.06931600	-1.40104900
C	-1.89010600	-4.24795200	-1.90912900
H	-2.76993400	-4.09594100	-2.54313900
H	-1.06399400	-3.67737400	-2.34467600
H	-1.62220800	-5.30954900	-1.99940600
C	0.32251500	-3.59104300	0.32012100
H	0.76913400	-2.74007800	0.84641400
H	0.80679800	-4.49977200	0.70261200
H	0.58937100	-3.51251400	-0.73793100
C	-1.03250100	-3.74127300	3.08949100
H	-0.46745300	-4.68172000	3.14927300
H	-0.31316400	-2.92247900	3.19012700
H	-1.69089700	-3.71068900	3.96095800
C	-6.68509500	-1.94309900	0.38469500
H	-6.63843400	-2.50569600	-0.55105200
H	-6.65994000	-2.66239700	1.20865600
H	-7.67263800	-1.46138600	0.41875700
C	-5.70349900	-0.61630500	3.06519700
H	-6.69630800	-0.16961700	3.21418300
H	-5.81496700	-1.69412500	3.22360800
H	-5.05324300	-0.23312000	3.85475000
C	-3.93665000	1.93605100	2.28343400
H	-3.84016800	1.58428600	3.31262100
H	-2.96854100	2.35375600	1.99332900
H	-4.66151800	2.76212100	2.28415800
C	-3.70692900	2.05732700	-0.83264800
H	-2.77124400	2.39933800	-0.37983900
H	-3.48769400	1.78745600	-1.86767800
H	-4.38800200	2.91935000	-0.85521100
C	-5.44533000	-0.37064900	-2.04513400
H	-4.76315300	0.15264100	-2.71882000
H	-5.45439400	-1.42706700	-2.33868400
H	-6.45448500	0.01737100	-2.24000700
H	2.24344400	0.40255600	0.84530700
H	0.95907800	0.40137800	2.56495600
C	-1.37703500	0.05276200	3.29841800
C	-2.26382900	-0.82318400	3.95295900
C	-0.96808400	1.18872100	4.03249200
C	-2.67706800	-0.61663200	5.26758500
H	-2.61463500	-1.71398600	3.43444100
C	-1.38493600	1.40750400	5.34165900
H	-0.33248300	1.92304800	3.54597600
C	-2.23730800	0.50173900	5.97411600
H	-3.34556800	-1.33168700	5.74073300
H	-1.04996400	2.29705500	5.86998900
H	-2.56348100	0.67103500	6.99648600
C	-0.13804600	0.43054900	-1.68962700
C	-0.94126000	-0.73541000	-1.71796200
C	-0.41834400	1.41188600	-2.66621200
C	-1.94460400	-0.90683300	-2.67758500
H	-0.66176100	-1.56520500	-1.06759000
C	-1.42525200	1.24686000	-3.60874300
H	0.19629100	2.30719500	-2.68851700
C	-2.19501500	0.08196300	-3.62847800
H	-2.50684000	-1.83637900	-2.71055300
H	-1.59989100	2.02456700	-4.34810000
H	-2.95798300	-0.06440900	-4.38677000

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H= -2245.005913 au

Sm	2.71716900	1.21802300	-1.03656500
C	0.01898600	0.04910600	-0.71310000
C	0.35274500	0.04292800	0.49394800
C	3.93554500	-0.16135100	-3.10919000
C	5.00844500	0.47918800	-2.42375400
C	3.42084900	-1.18494400	-2.25852400
C	5.13765100	-0.13350800	-1.14081800
C	4.15734500	-1.16086900	-1.04118000
C	1.75757400	3.58055300	0.16517400
C	2.94839600	3.23267700	0.86485500
C	2.12455400	3.99039000	-1.14987500
C	4.05121000	3.43082700	-0.01651800
C	3.54041000	3.88925100	-1.26798200
C	1.24462400	4.68249200	-2.15350700
H	1.35114500	5.77294100	-2.07253000
H	1.50175000	4.42195800	-3.18677300
H	0.18145900	4.46480000	-2.00802600
C	4.33637600	4.45647800	-2.40807300
H	5.37698500	4.12720000	-2.38650200
H	3.92739000	4.18205000	-3.38725800
H	4.34587400	5.55469800	-2.36728900
C	5.49082600	3.44035000	0.40839500
H	5.71774600	2.65029600	1.12954900
H	6.17524000	3.32315800	-0.43629800
H	5.74189800	4.39497500	0.89106700
C	3.05001200	2.93069200	2.33170600
H	3.21965500	3.84874700	2.91226700
H	2.13528600	2.46873200	2.71122700
H	3.87253500	2.24603400	2.55667900
C	0.39094900	3.68749400	0.77701600
H	0.27923600	4.62884400	1.33202500
H	-0.40037900	3.67328700	0.02098100
H	0.18458800	2.87318900	1.47802300
C	2.45538700	-2.26163600	-2.65818500
H	2.99073200	-3.18751700	-2.90933900
H	1.75330600	-2.50856800	-1.85551400
H	1.86835800	-1.98080900	-3.53589200
C	4.07471400	-2.17565600	0.06039900
H	4.75923200	-3.01542000	-0.12806300
H	4.34007000	-1.74564800	1.02963200
H	3.06907600	-2.59055400	0.15647300
C	6.25268100	0.06633800	-0.15538300
H	6.98862800	-0.74546600	-0.23402200
H	6.78978200	1.00227700	-0.32251600
H	5.89534300	0.06942900	0.88014100
C	5.98738100	1.42286200	-3.05844700
H	5.50987400	2.10779200	-3.76535400
H	6.51883200	2.02879800	-2.31976400
H	6.75020100	0.86600600	-3.62009500
C	3.55652300	0.06953500	-4.54498300
H	2.50580200	-0.16627100	-4.73891300
H	3.71825900	1.10864900	-4.85096200
H	4.15691300	-0.55526500	-5.22098700
C	0.13455000	0.03005800	1.91754300
C	-1.08543900	-0.28275600	2.44553300
Sm	-2.56045000	-1.29929600	0.67156300
C	-3.93350300	1.08488600	1.05285700
C	-3.76271700	0.96984000	-0.35750800
C	-4.83948700	0.06609900	1.46703500
C	-4.56692300	-0.11569100	-0.81773000
C	-5.24614600	-0.66334400	0.30935000
C	-1.07090000	-3.67173900	0.81366900
C	-1.80677300	-3.63953000	2.03191400
C	-1.99252400	-3.86755600	-0.25512100
C	-3.18929600	-3.80022300	1.71759000
C	-3.30170800	-3.95090200	0.30177500

C	-4.29271800	-4.01664700	2.71499900
H	-4.13573700	-3.45036900	3.63877400
H	-5.26968900	-3.72609600	2.31831900
H	-4.36554000	-5.07454800	3.00110700
C	-4.51186500	-4.40795200	-0.45990400
H	-4.42555700	-5.47397500	-0.71231100
H	-5.42976400	-4.29079900	0.11912900
H	-4.64791900	-3.87194100	-1.40628200
C	-1.66367700	-4.18625000	-1.68657900
H	-2.32015000	-3.67331700	-2.40030900
H	-0.62942300	-3.93385600	-1.93841800
H	-1.77917500	-5.26122000	-1.88150600
C	0.42680700	-3.68408000	0.74153200
H	0.87550500	-2.82660300	1.25518900
H	0.83095200	-4.58929000	1.21381200
H	0.78372000	-3.67697700	-0.29093200
C	-1.17425400	-3.71467700	3.39129300
H	-0.69745500	-4.69491500	3.52934000
H	-0.40267200	-2.95392800	3.54041000
H	-1.90552200	-3.60007300	4.19429100
C	-6.40929900	-1.60993900	0.25762600
H	-6.38298900	-2.25574200	-0.62303500
H	-6.47076000	-2.25307100	1.14082500
H	-7.35196600	-1.04712500	0.21328000
C	-5.44131700	-0.07824900	2.83605500
H	-6.38010400	0.48727500	2.91268300
H	-5.67926200	-1.12008800	3.07587200
H	-4.77439300	0.29452200	3.61775700
C	-3.40978100	2.20420300	1.90353100
H	-3.33685400	1.92100100	2.95621700
H	-2.41466200	2.52809700	1.58689700
H	-4.07184400	3.07921200	1.84367400
C	-3.04431700	1.96052800	-1.22626900
H	-2.12855600	2.33065900	-0.75601800
H	-2.76817700	1.53837300	-2.19631500
H	-3.68005700	2.83426700	-1.42490800
C	-4.79890600	-0.48978100	-2.25539300
H	-3.90770400	-0.33550000	-2.87308500
H	-5.09747500	-1.53752100	-2.36510400
H	-5.60016000	0.11562200	-2.70085200
H	2.37626300	0.32478300	0.79110200
H	1.00635700	0.31743200	2.50557200
C	-1.29010800	-0.05691100	3.88825600
C	-2.29698700	-0.75902800	4.57678200
C	-0.56144600	0.89700600	4.62916800
C	-2.53365600	-0.56534100	5.93468300
H	-2.89592500	-1.47811200	4.02448700
C	-0.80115000	1.10442100	5.98340700
H	0.18862400	1.50120600	4.12705500
C	-1.78300500	0.36849900	6.64787400
H	-3.31189600	-1.13631300	6.43469800
H	-0.22432100	1.85148800	6.52290300
H	-1.97169500	0.53326300	7.70514100
C	-0.13640600	0.21522200	-2.11975900
C	-0.60846900	-0.82785500	-2.94962900
C	0.15593400	1.45802700	-2.73160100
C	-0.78484600	-0.62922900	-4.31180400
H	-0.82349900	-1.79575700	-2.51157900
C	-0.00886900	1.63978900	-4.10557000
H	0.41952000	2.31120200	-2.10925400
C	-0.48170300	0.60238700	-4.90249400
H	-1.15648000	-1.44660700	-4.92372200
H	0.21181500	2.60940100	-4.54207600
H	-0.62242800	0.74841600	-5.96897500

7-Ph

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Sm	3.05895200	1.48689700	-0.87956300
C	0.22839900	0.26210400	-2.03137300
C	0.28198400	0.09678300	-0.81481000
C	4.58347500	-0.16269100	-2.53744700
C	5.52648000	0.54717900	-1.73450900
C	3.87033900	-1.05729600	-1.68625600
C	5.38595100	0.10168900	-0.38851100
C	4.36207500	-0.88865600	-0.35845200
C	1.85389700	3.92513800	-0.36646800
C	3.20867200	4.09563500	0.03203300
C	1.81814300	3.80383100	-1.78646300
C	4.01678300	4.06630500	-1.14047700
C	3.15803100	3.87637000	-2.26832900
C	0.57192200	3.81119300	-2.62430900
H	0.19984600	4.83662700	-2.75683000
H	0.73935100	3.40163100	-3.62402700
H	-0.23979900	3.23498600	-2.16911200
C	3.57168900	3.94873600	-3.71099300
H	4.57686400	3.54559700	-3.87164600
H	2.88963200	3.39286800	-4.36297500
H	3.58311900	4.98557000	-4.07505800
C	5.46922600	4.44504600	-1.18415900
H	6.04413700	3.99604400	-0.36710500
H	5.94522900	4.15146700	-2.12242600
H	5.58634400	5.53364400	-1.09230900
C	3.69227200	4.42085300	1.41478500
H	3.71302200	5.50763000	1.58067000
H	3.05184500	3.97630600	2.18009000
H	4.70446000	4.04566700	1.59085600
C	0.66003500	3.99186200	0.54047900
H	-0.17200700	3.38399200	0.17006000
H	0.90308800	3.64000500	1.54773400
H	0.28459700	5.02004800	0.63783500
C	2.90736200	-2.12151600	-2.12992900
H	3.43312900	-3.06123000	-2.34794700
H	2.16154400	-2.34427300	-1.36110700
H	2.36198800	-1.84133400	-3.03641200
C	3.97054700	-1.70505400	0.83916400
H	4.60019200	-2.60103200	0.93246100
H	4.06961600	-1.12973800	1.76336700
H	2.93265100	-2.04785700	0.78158900
C	6.24540100	0.50620100	0.77388400
H	7.09839500	-0.17539100	0.89785000
H	6.65670600	1.51251300	0.64541500
H	5.67751600	0.50590100	1.70817800
C	6.65419900	1.37081200	-2.28350200
H	6.34694300	1.98872900	-3.13364000
H	7.08991500	2.03383100	-1.53240800
H	7.46387800	0.72008600	-2.64325600
C	4.57291600	-0.15572800	-4.04096100
H	3.71031700	-0.69246400	-4.44625700
H	4.56445800	0.85608900	-4.46383900
H	5.46767800	-0.65339600	-4.44019000
C	0.40907700	-0.07384300	0.58575700
C	-0.55958100	-0.59174700	1.39249500
Sm	-2.91654000	-1.52227200	1.45820200
C	-3.63738900	1.03868100	2.21257500
C	-3.91792200	0.97125800	0.81947400
C	-4.54430000	0.16651400	2.88724400
C	-5.00819000	0.07126200	0.62763400
C	-5.40110500	-0.42106700	1.91077400
C	-1.71256500	-3.91288700	0.69847600
C	-2.57460400	-4.28516400	1.77320700
C	-2.53188400	-3.51261700	-0.39686700
C	-3.92270600	-4.11732400	1.34274300
C	-3.89825000	-3.64899400	-0.00511900

C	-5.13019700	-4.58704900	2.10303300
H	-5.04800100	-4.39407800	3.17850400
H	-6.05092100	-4.11176000	1.75568300
H	-5.26652500	-5.67117400	1.98898400
C	-5.08200000	-3.57453300	-0.92532700
H	-5.22775600	-4.53148000	-1.44430100
H	-6.00956000	-3.36111300	-0.38651800
H	-4.96776600	-2.80881600	-1.69776800
C	-2.04077500	-3.16917400	-1.77487900
H	-2.77243000	-2.57957800	-2.33635100
H	-1.10540800	-2.60195400	-1.75412600
H	-1.85163500	-4.07697600	-2.36339300
C	-0.22197900	-4.08701100	0.65836300
H	0.24406400	-3.93474900	1.63684200
H	0.04531600	-5.09937500	0.32681000
H	0.24693100	-3.38148700	-0.03149000
C	-2.16256900	-4.96263500	3.05114200
H	-2.28648800	-6.05051700	2.96858500
H	-1.11057400	-4.78569500	3.29424800
H	-2.76194800	-4.64500900	3.91231400
C	-6.62319300	-1.24199800	2.20425800
H	-6.90261900	-1.87972200	1.36062700
H	-6.49175900	-1.89073200	3.07595500
H	-7.48619500	-0.59650700	2.41626600
C	-4.66836700	0.01300600	4.37797600
H	-5.34453100	0.76819300	4.80053100
H	-5.07427300	-0.96429400	4.66094600
H	-3.70496700	0.12844600	4.88483700
C	-2.69628400	2.01056500	2.85871000
H	-2.33373500	1.65827700	3.82754000
H	-1.82066000	2.20466000	2.23356300
H	-3.19623100	2.97387200	3.02862900
C	-3.27904000	1.82247200	-0.23946800
H	-2.19616300	1.90271800	-0.10504800
H	-3.45694000	1.42701300	-1.24391900
H	-3.68609400	2.84226000	-0.22366800
C	-5.76224100	-0.10795500	-0.65969000
H	-5.10115900	-0.18398300	-1.53008200
H	-6.38902300	-1.00243400	-0.64920900
H	-6.42597700	0.74749500	-0.84271400
H	3.11533300	1.40385400	1.19257400
H	1.37982900	0.24687000	1.01122300
C	-0.31020900	-0.60840700	2.84386800
C	-0.79844700	-1.68408700	3.62062100
C	0.29610100	0.45998700	3.54181300
C	-0.69499200	-1.69540500	5.01440100
H	-1.15195600	-2.58819500	3.11938700
C	0.40359600	0.44501900	4.92650200
H	0.68387500	1.30248600	2.97718700
C	-0.10112400	-0.62463500	5.67413600
H	-1.05931300	-2.55188400	5.57558900
H	0.88586900	1.27696000	5.43325200
H	-0.01615600	-0.62511000	6.75692300
C	-0.04483600	0.36165400	-3.42737300
C	-1.36592200	0.19614600	-3.88842800
C	0.96903800	0.61500300	-4.36884700
C	-1.65509100	0.27905200	-5.24526100
H	-2.15514900	0.00544000	-3.16884600
C	0.67073900	0.69722300	-5.72479600
H	1.99182400	0.74280300	-4.02960200
C	-0.64032900	0.52922700	-6.16966100
H	-2.67940900	0.14951000	-5.58349100
H	1.46804600	0.89167300	-6.43645000
H	-0.87019800	0.59371200	-7.22918300

TS₇₅-Ph $H = -2245.004634$ au

Sm	2.47977000	1.02105600	0.18491400
C	0.18608000	0.24838600	-1.23104700
C	-0.04615000	-0.01146200	-0.02547700
C	4.05451700	-0.59726200	-1.45367300
C	4.97835600	0.04537400	-0.57489300
C	3.27422800	-1.50528100	-0.68085100
C	4.74913700	-0.44515200	0.74238100
C	3.69717800	-1.40694800	0.67512600
C	1.38288600	3.50321100	0.84925400
C	2.69506300	3.51161600	1.40470800
C	1.49979000	3.53203600	-0.56971900
C	3.62525600	3.54313500	0.32737900
C	2.88626800	3.54593200	-0.89663000
C	0.35377200	3.72328800	-1.52037200
H	0.05529500	4.78010700	-1.56291800
H	0.60378500	3.41988600	-2.54029900
H	-0.53050400	3.15143100	-1.22236100
C	3.46440600	3.74175300	-2.26951600
H	4.42501300	3.23165900	-2.39138100
H	2.79518000	3.37026400	-3.05201200
H	3.64014800	4.80529200	-2.48240400
C	5.09520000	3.81569400	0.46993100
H	5.55229900	3.25175800	1.29009900
H	5.64781600	3.57893800	-0.44197400
H	5.27079700	4.87935400	0.68312900
C	3.04572200	3.65459700	2.85806300
H	3.10597900	4.71259300	3.15002200
H	2.30630800	3.17820600	3.50776000
H	4.01420800	3.20151000	3.09064100
C	0.09782600	3.65421900	1.60899300
H	-0.70885300	3.04739600	1.18624000
H	0.21034000	3.37038800	2.65910200
H	-0.24767400	4.69729500	1.59772300
C	2.28750800	-2.49819600	-1.22183600
H	2.77242400	-3.45894800	-1.44247100
H	1.48206400	-2.70009500	-0.50972000
H	1.81779200	-2.15063400	-2.14662700
C	3.23471400	-2.27215500	1.81109300
H	3.82760100	-3.19529200	1.87278100
H	3.32510200	-1.75994600	2.77327600
H	2.18760700	-2.56585000	1.70047600
C	5.56694600	-0.12989300	1.96225700
H	6.39629700	-0.84026800	2.08495600
H	6.00957100	0.86991400	1.91189200
H	4.96499000	-0.17278000	2.87492700
C	6.16280200	0.85018500	-1.02447300
H	5.92102200	1.54774700	-1.83341800
H	6.60269900	1.42836900	-0.20884500
H	6.95129700	0.18744800	-1.40802900
C	4.10371800	-0.51899500	-2.95328600
H	3.17129600	-0.85639500	-3.41393700
H	4.30126700	0.49721600	-3.31329900
H	4.90614700	-1.15463200	-3.35370800
C	0.09800900	-0.13796200	1.34153400
C	-0.73267600	-0.68796900	2.27057700
Sm	-3.02588700	-1.76109000	2.56687400
C	-3.88721400	0.78051100	3.26102600
C	-4.16411500	0.66029900	1.87098400
C	-4.74286900	-0.12201500	3.96108700
C	-5.20587600	-0.30048600	1.70690400
C	-5.57115500	-0.77754000	3.00361700
C	-1.79955200	-4.16841800	1.87200700
C	-2.60492400	-4.50024300	3.00140400
C	-2.67275900	-3.83874800	0.79544800
C	-3.97337500	-4.38624100	2.62123700
C	-4.01726000	-3.98866400	1.25134500

C	-5.13203300	-4.85158200	3.45649000
H	-5.03066200	-4.56713200	4.51006300
H	-6.08565300	-4.45435400	3.10118000
H	-5.21264800	-5.94702600	3.43477800
C	-5.23597900	-4.00037300	0.37489700
H	-5.37392100	-4.99126800	-0.07843300
H	-6.14898700	-3.77719200	0.93364800
H	-5.16967200	-3.28137700	-0.44629700
C	-2.24461400	-3.54549600	-0.61485200
H	-3.02974600	-3.03543600	-1.18209100
H	-1.34724400	-2.91983900	-0.65663900
H	-2.01338400	-4.47069400	-1.15955900
C	-0.31250900	-4.33049400	1.76230900
H	0.20103400	-4.17706600	2.71626800
H	-0.05310900	-5.34039500	1.41704700
H	0.11571300	-3.62205600	1.04981900
C	-2.12467200	-5.08702400	4.29985300
H	-2.22872600	-6.18020300	4.29412100
H	-1.06736600	-4.87522400	4.48593600
H	-2.69339700	-4.72371000	5.16360900
C	-6.76375200	-1.62940000	3.32790000
H	-7.03184300	-2.29790000	2.50487600
H	-6.60638500	-2.24880200	4.21605400
H	-7.64377000	-1.00348600	3.52897900
C	-4.85670400	-0.24049500	5.45583500
H	-5.55886200	0.49969700	5.86263700
H	-5.22483200	-1.22470200	5.76501200
H	-3.89664000	-0.07557200	5.95573000
C	-3.01882000	1.83096800	3.88452900
H	-2.59766100	1.51283900	4.84157300
H	-2.18527000	2.10684600	3.23396000
H	-3.60060900	2.74392000	4.07242800
C	-3.57405700	1.51102000	0.78386400
H	-2.49286700	1.63106700	0.89850600
H	-3.75163500	1.08545200	-0.20823200
H	-4.01754200	2.51564300	0.78334100
C	-5.95207500	-0.54759300	0.42612700
H	-5.28795800	-0.64102700	-0.44023400
H	-6.55696700	-1.45554800	0.47125500
H	-6.63550900	0.28420100	0.20973600
H	2.23310200	0.63614400	2.28539000
H	1.28845800	0.29415700	1.92601600
C	-0.42137000	-0.64396100	3.70601400
C	-0.74314600	-1.76220200	4.51356700
C	0.04011800	0.50996000	4.38113400
C	-0.60784300	-1.73497700	5.90539500
H	-0.98337400	-2.71090000	4.03048700
C	0.18152000	0.53290000	5.76184000
H	0.28286100	1.38924100	3.79484100
C	-0.15093200	-0.58423400	6.53754000
H	-0.84046000	-2.62421700	6.48555200
H	0.55382900	1.43256800	6.24550900
H	-0.04120100	-0.55501200	7.61764000
C	-0.17726200	0.26377000	-2.61880500
C	-1.44639400	-0.20588400	-3.01692400
C	0.69809600	0.73362300	-3.61421300
C	-1.81701900	-0.20423100	-4.35591200
H	-2.13035400	-0.57113400	-2.25762100
C	0.32275700	0.73106100	-4.95388100
H	1.67723300	1.10006100	-3.32379700
C	-0.93498700	0.26280700	-5.33185100
H	-2.79957000	-0.57074100	-4.64096300
H	1.01649300	1.09739100	-5.70554200
H	-1.22664200	0.26193400	-6.37820900

TS₁₈-Ph $H = -2244.954205$ au

Sm	2.73361200	0.98102700	-0.92972700
C	0.41487000	0.15739300	-2.17242400
C	-0.12989900	-0.09719400	-1.04437800
C	4.12885000	-0.25320800	-3.03315100
C	5.11219900	0.50547200	-2.33148100
C	3.74368600	-1.34643000	-2.20246700
C	5.30064400	-0.09240200	-1.05242200
C	4.46535200	-1.24740100	-0.98163400
C	1.64378900	3.24423900	0.28167000
C	3.04045000	3.36015500	0.53793500
C	1.43120200	3.46970500	-1.10865900
C	3.69249800	3.62708800	-0.69553400
C	2.69842300	3.68645700	-1.72131000
C	0.08740700	3.65996000	-1.74804400
H	-0.44943800	4.49624300	-1.28065600
H	0.17423100	3.89848400	-2.81174400
H	-0.54448100	2.77015700	-1.66122500
C	2.93069500	4.16727500	-3.12627600
H	3.91742700	3.88181600	-3.50224700
H	2.19373700	3.77583800	-3.83419200
H	2.87472900	5.26332300	-3.18483000
C	5.11646900	4.08517900	-0.81975100
H	5.80683300	3.48424100	-0.21910400
H	5.46864200	4.06142100	-1.85295800
H	5.21630000	5.12262200	-0.47085500
C	3.69545200	3.42519200	1.88518800
H	3.76073300	4.46520000	2.23541900
H	3.14098900	2.85387600	2.63227100
H	4.71360300	3.02488400	1.86759200
C	0.56614800	3.10508100	1.31767400
H	0.25575200	4.08327800	1.71183200
H	-0.32809600	2.62985900	0.90132500
H	0.89896600	2.50159400	2.16821800
C	2.91117100	-2.51370900	-2.64490800
H	2.11605800	-2.21349700	-3.33226300
H	3.52758600	-3.25616500	-3.17097300
H	2.44525400	-3.03226600	-1.80194500
C	4.54478100	-2.28606000	0.09799200
H	5.43120000	-2.92092600	-0.04132300
H	4.61481700	-1.83402600	1.09106000
H	3.67473900	-2.94792600	0.09813500
C	6.32615000	0.28285300	-0.02141100
H	7.20530100	-0.37450700	-0.07444600
H	6.68600800	1.30683700	-0.15692800
H	5.92725200	0.20654300	0.99562300
C	5.99803500	1.53204800	-2.97447400
H	5.44656600	2.23902900	-3.60282600
H	6.56519200	2.10853000	-2.24116400
H	6.73045500	1.03931100	-3.62927400
C	3.78810500	-0.07888700	-4.48557900
H	2.82492500	-0.52634000	-4.74265600
H	3.74242400	0.97585800	-4.77700100
H	4.54692000	-0.55134900	-5.12617500
Sm	-2.22910300	-0.97548800	0.13408900
C	-3.77424600	1.27500100	-0.22054500
C	-3.69684200	0.67512900	-1.50842300
C	-4.54978600	0.41993300	0.62340300
C	-4.41916100	-0.55823100	-1.46031700
C	-4.97682800	-0.69490600	-0.15494300
C	-0.54002000	-2.87252800	1.16007500
C	-1.25274700	-2.34987500	2.27786400
C	-1.46458900	-3.59171800	0.34893800
C	-2.61349300	-2.77413600	2.17413300
C	-2.74149500	-3.55126500	0.98186000
C	-3.64884300	-2.62127700	3.25170600
H	-3.56578800	-1.66490200	3.77798600

H	-4.66742600	-2.69379300	2.86119000
H	-3.54048800	-3.40810100	4.01001800
C	-3.91552700	-4.40044300	0.58777200
H	-3.73204900	-5.44965900	0.85427000
H	-4.83241100	-4.09662300	1.09607100
H	-4.11206400	-4.38051900	-0.48986800
C	-1.11028100	-4.39411600	-0.87114100
H	-1.95755200	-4.50664800	-1.55595300
H	-0.28396700	-3.94287700	-1.42938800
H	-0.78984300	-5.40830500	-0.59686300
C	0.94261700	-2.84308400	0.95414500
H	1.43462000	-2.09516100	1.57858900
H	1.38051900	-3.81821800	1.20609800
H	1.20894300	-2.62283400	-0.08312300
C	-0.65237100	-1.59364900	3.43054500
H	-0.27936900	-2.27936600	4.20201300
H	0.19743100	-0.97533700	3.12526900
H	-1.38221200	-0.93990800	3.92061200
C	-6.04407600	-1.67206200	0.23881800
H	-5.98157400	-2.60715000	-0.32231000
H	-6.01841200	-1.91835300	1.30393600
H	-7.03568300	-1.24477000	0.03725300
C	-5.01476000	0.75606500	2.01273800
H	-5.93001700	1.36273300	1.98790200
H	-5.23997400	-0.13927400	2.59908200
H	-4.27181600	1.33650800	2.57039600
C	-3.29175800	2.64585900	0.15744900
H	-2.94647400	2.69967600	1.19570100
H	-2.47216500	2.98474100	-0.47918400
H	-4.10184400	3.38091700	0.06015400
C	-3.12759400	1.28820900	-2.75387300
H	-2.36623000	2.03818700	-2.53229200
H	-2.66355600	0.54793800	-3.41144000
H	-3.91809900	1.78412000	-3.33291500
C	-4.70168800	-1.44291200	-2.64310500
H	-3.86741400	-1.45888600	-3.35216300
H	-4.90734800	-2.47682900	-2.34784700
H	-5.58009700	-1.09123900	-3.20056800
H	0.81780000	0.10557400	0.15266900
C	0.21371000	0.06959000	-3.60254500
C	-0.21254200	-1.14564500	-4.18114900
C	0.41268600	1.16683800	-4.45909600
C	-0.43388400	-1.24856600	-5.55147600
H	-0.35553100	-2.01072700	-3.54016300
C	0.17084300	1.06377400	-5.82525200
H	0.75479600	2.10443000	-4.03669300
C	-0.24934400	-0.14360700	-6.38293600
H	-0.75597700	-2.19845600	-5.97059700
H	0.32457500	1.93180100	-6.46089800
H	-0.42432300	-0.22463000	-7.45176200
H	1.58344800	0.16988000	0.82384300
C	2.81268400	0.28913000	1.51862400
C	2.98226100	-0.02004800	2.70678500
C	3.21986500	-0.36765100	4.06557400
C	3.66920700	-1.65860300	4.41232500
C	3.01129500	0.56895100	5.09871600
C	3.90217400	-1.99358000	5.74109700
H	3.83264700	-2.38744200	3.62449300
C	3.24623800	0.22486200	6.42477900
H	2.66596800	1.56614000	4.84376100
C	3.69253400	-1.05587900	6.75327400
H	4.25068300	-2.99259800	5.98919800
H	3.08194800	0.96093100	7.20725700
H	3.87691800	-1.32100300	7.79057000

3'-Ph*H* = -1121.918899 au

Sm	3.24235000	0.53523900	-0.25581900
C	2.08999800	-0.81147400	1.41578800
C	1.49063200	-1.48456400	2.26259000
C	4.36179900	-0.20243700	-2.66154000
C	5.45983100	-0.11965800	-1.75195000
C	3.54682700	-1.30496100	-2.26398200
C	5.31710300	-1.17176300	-0.79736400
C	4.14312700	-1.91280600	-1.12045000
C	1.69284000	2.59301600	0.67517600
C	2.91229300	2.68405800	1.40272300
C	1.96604300	2.92980800	-0.68648500
C	3.94294000	3.07804500	0.49444900
C	3.35203400	3.24713500	-0.79406500
C	3.70103400	-3.18942900	-0.46731300
H	2.62242300	-3.34098300	-0.55635100
H	4.19670600	-4.05428700	-0.92906700
H	3.93225100	-3.20372200	0.60051200
C	6.29561300	-1.52007700	0.28916600
H	7.02007400	-2.27091700	-0.05341600
H	6.87546100	-0.65121200	0.61796400
H	5.79720300	-1.93934100	1.16936600
C	6.65650400	0.77853000	-1.88827300
H	6.41876300	1.70673800	-2.41601000
H	7.08689300	1.05210900	-0.91922600
H	7.45486600	0.28525600	-2.45894900
C	4.19357500	0.59975900	-3.92067100
H	4.66044600	1.58551200	-3.84630300
H	4.65561200	0.09034700	-4.77703500
H	3.14051300	0.75481300	-4.17962400
C	2.33591200	-1.81623000	-2.99405300
H	1.60220900	-2.26053700	-2.31317800
H	1.82908800	-1.02682700	-3.55941400
H	2.60753000	-2.59552400	-3.71850800
C	4.02495100	3.85011400	-1.99239300
H	5.08776800	3.59508400	-2.04403100
H	3.56282100	3.53297600	-2.93175700
H	3.96381500	4.94655800	-1.96293100
C	5.35644800	3.43371600	0.86381300
H	5.71570300	2.86166100	1.72585100
H	6.05506200	3.25984600	0.03922500
H	5.44141900	4.49477200	1.13430800
C	3.06190100	2.48697500	2.88432200
H	2.83168600	3.41082700	3.43152100
H	2.39375900	1.70552900	3.25706200
H	4.08283600	2.20262300	3.15981400
C	0.34081900	2.30577700	1.26178000
H	-0.35122900	1.90173800	0.51604900
H	0.39936600	1.57786600	2.07507200
H	-0.11754500	3.22101300	1.65986900
C	0.94049300	3.07293100	-1.77742300
H	1.37557800	2.93922100	-2.77332300
H	0.12281800	2.35090700	-1.67522100
H	0.48004300	4.06978400	-1.76422100
C	0.79731300	-2.26339100	3.23615600
C	1.45826400	-2.73741600	4.38574700
C	-0.56581500	-2.57619600	3.07084800
C	0.77768400	-3.49494500	5.33283300
H	2.50937900	-2.50155300	4.52202300
C	-1.23901700	-3.33540800	4.02176600
H	-1.08397000	-2.21501500	2.18762800
C	-0.57266500	-3.79817200	5.15677900
H	1.30466600	-3.85158300	6.21399500
H	-2.29097200	-3.56711500	3.87658300
H	-1.10159700	-4.39053000	5.89822800

1'-Bu*H* = -1863.028619 au

a Sm	-0.03911900	0.09848100	-0.05805500
Sm	5.38787600	0.15847900	0.03404600
C	2.82523100	0.40160400	-0.03299200
H	2.28047300	-0.54622900	0.28741400
C	2.01613500	1.42025200	-0.42496700
C	2.58795500	2.77127800	-0.85369900
C	-2.04398900	-1.25767100	-1.49952700
C	-2.33568900	0.12477000	-1.66854400
C	-0.83856300	-1.54254000	-2.20687900
C	-1.32326800	0.68904100	-2.50163000
C	-0.40881700	-0.34268700	-2.84839400
C	0.31258500	-0.69704000	2.56824500
C	0.31211800	0.72569200	2.63224500
C	-1.01502200	-1.12805200	2.27522500
C	-1.00424900	1.17703200	2.33743800
C	-1.83216900	0.03015900	2.14215200
C	6.99002000	2.00026000	1.43118400
C	5.86841000	1.79956300	2.29297900
C	7.75799800	0.80242500	1.41551100
C	5.91794300	0.45950300	2.76556600
C	7.08499200	-0.16220300	2.22031600
C	4.75626100	-1.81612300	-1.77263000
C	5.23311300	-0.73705500	-2.56796400
C	5.85942600	-2.34511100	-1.03898900
C	6.63363500	-0.59751100	-2.33038300
C	7.02442100	-1.61008800	-1.40574800
C	4.98629900	2.89314500	2.82027500
H	5.46999300	3.39504000	3.66961700
H	4.78366300	3.66757800	2.07400500
H	4.02422100	2.51860900	3.17358600
C	5.05180400	-0.14118300	3.83525000
H	4.06916200	0.33293400	3.88572900
H	4.89274100	-1.21529400	3.69019200
H	5.51729700	-0.02591000	4.82400600
C	7.61075400	-1.50293500	2.65042200
H	6.82539600	-2.26484900	2.70703400
H	8.38109100	-1.87961800	1.97277500
C	9.13910800	0.69395600	0.83700200
H	9.19653800	1.02958900	-0.20506100
H	9.84042700	1.31864100	1.40606600
H	9.51959200	-0.32844700	0.87318600
C	7.42381700	3.31181900	0.83807400
H	7.98040100	3.17993500	-0.09607000
H	6.57686600	3.97159900	0.62625700
H	8.08600600	3.85698400	1.52484200
C	7.56505500	0.32169100	-3.07077900
H	7.07351900	1.25155200	-3.37556400
H	8.43855000	0.59697100	-2.47099900
H	7.94484900	-0.14906600	-3.98745600
C	5.83870000	-3.59227400	-0.19977400
H	6.63155000	-3.59403200	0.55410300
H	4.88600900	-3.72482200	0.32451100
H	5.98379800	-4.48895200	-0.81749700
C	3.37949000	-2.40143100	-1.82713300
H	3.13298900	-2.95847400	-0.91718900
H	2.62089600	-1.62406500	-1.95075400
H	3.28402400	-3.10463600	-2.66603700
C	4.42481400	0.01594400	-3.58280700
H	4.92598100	0.93313100	-3.90774300
H	4.26017600	-0.59038000	-4.48349600
H	3.44106000	0.29105600	-3.19232700
C	0.65803100	-0.24321700	-3.89739100
H	1.44116400	-0.99436400	-3.76625600
H	0.23318100	-0.40039800	-4.89871900
H	1.14125700	0.73700200	-3.90279400
C	-1.40162000	2.06108700	-3.10779900

H	-2.23844100	2.12349000	-3.81775800	C	-0.32697900	-1.27184100	2.12816200
H	-1.56576400	2.85128100	-2.36542900	C	-0.64204700	0.99974500	2.35429900
H	-0.49383900	2.31224100	-3.66039900	C	-1.30675900	-0.24002800	2.11930900
C	-3.60836100	0.83323400	-1.30004200	C	6.65868600	1.98917800	1.21948100
H	-4.20443100	0.26047500	-0.58676800	C	5.68406200	1.88485000	2.25458300
H	-3.43459900	1.82374300	-0.86226300	C	7.46334700	0.81286700	1.24719000
H	-4.23421100	0.99203400	-2.18927100	C	5.83661600	0.61300800	2.87216700
C	-2.96063000	-2.30140300	-0.93246900	C	6.93566400	-0.05405300	2.24609300
H	-3.63930000	-1.89448500	-0.17899100	C	4.34406500	-1.88924800	-1.68862300
H	-3.58716800	-2.73500300	-1.72466200	C	4.99967000	-0.84116900	-2.39152300
H	-2.41666400	-3.13224700	-0.47310300	C	5.31141600	-2.55521500	-0.88094600
C	-0.28753500	-2.92358700	-2.43128000	C	6.38262800	-0.87453600	-2.03715200
H	0.74890000	-2.90280000	-2.77683900	C	6.57754400	-1.95161000	-1.12294700
H	-0.31811400	-3.54043500	-1.52550700	C	4.88507600	3.04598600	2.77037300
H	-0.86675400	-3.46211500	-3.19431100	H	5.55969400	3.85702800	3.07461400
C	-3.33211100	0.05756900	2.11884000	H	4.19850300	3.45878300	2.02822300
H	-3.72567000	0.94025200	1.60741200	H	4.29837100	2.77404300	3.65018000
H	-3.76145700	-0.82365500	1.63491900	C	5.19831400	0.14911600	4.15193300
H	-3.73014400	0.08129100	3.14302300	H	4.21975800	0.60403400	4.32471900
C	-1.49051800	2.59805700	2.40159900	H	5.06341800	-0.93739600	4.17967400
H	-0.69408100	3.31377100	2.17624900	H	5.83020500	0.40698400	5.01340200
H	-2.30805900	2.78759900	1.69716100	C	7.55741100	-1.32185200	2.76187100
H	-1.87250800	2.84824400	3.40089300	H	6.85323400	-2.16220400	2.81125100
C	1.46023200	1.56248700	3.10149800	H	8.39954700	-1.63871700	2.14277000
H	1.62947000	1.42760900	4.17926600	C	8.79364800	0.68541200	0.56547000
H	2.38188400	1.30217600	2.57287700	H	8.80445500	1.15862700	-0.42013300
H	1.27983500	2.62740000	2.93385600	H	9.57050600	1.18365200	1.16184200
C	1.45780200	-1.59171600	2.94701500	H	9.10546200	-0.35304000	0.44101700
H	1.40021200	-2.56854200	2.45367700	C	6.94709600	3.23302500	0.42713500
H	2.42228400	-1.14467800	2.68864500	H	7.39655300	3.01118900	-0.54638300
H	1.47369900	-1.78611000	4.02879400	H	6.04009900	3.81661700	0.24583000
C	-1.48645500	-2.55329400	2.33091900	H	7.65058700	3.89061800	0.95745800
H	-2.47550200	-2.67398600	1.88366800	C	7.45580400	-0.07127800	-2.71720800
H	-0.80906900	-3.24439500	1.81484300	H	7.21137300	0.99540700	-2.78126000
H	-1.55700800	-2.90357200	3.36984700	H	8.41537600	-0.15483500	-2.20268000
C	8.43531500	-2.03447700	-1.12622700	H	7.61034900	-0.41954500	-3.74707200
H	8.73443500	-2.82538700	-1.82784000	C	5.08421200	-3.80427800	-0.07625900
H	9.14785900	-1.21612900	-1.24862900	H	5.74559600	-3.86158900	0.79532700
H	8.56383500	-2.44268500	-0.12006000	H	4.05396500	-3.87968300	0.28713300
H	8.06366600	-1.44563700	3.64949500	H	5.27371000	-4.70645000	-0.67444500
C	2.13893600	3.85126900	0.14704700	C	2.94186500	-2.35315600	-1.91449600
H	2.50288000	4.84338000	-0.15004900	H	2.50861700	-2.81855500	-1.02327500
H	1.04573900	3.89487700	0.19354900	H	2.29049100	-1.52640300	-2.20562300
H	2.50762600	3.63611200	1.15345900	H	2.90250200	-3.10275000	-2.71721600
C	2.05527900	3.16703900	-2.23945200	C	4.39724400	0.03680800	-3.44955500
H	0.96447700	3.21933600	-2.22788200	H	5.00240900	0.93237900	-3.61934100
H	2.43925200	4.14987900	-2.54214300	H	4.32759100	-0.48878600	-4.41210400
H	2.35105900	2.44001800	-3.00243500	H	3.39419800	0.37364600	-3.18016200
C	4.12774000	2.78571900	-0.92397900	C	0.68638200	0.10826800	-4.08911400
H	4.55664100	2.61452000	0.07433300	H	1.39932000	-0.71729100	-4.15450700
H	4.47846800	2.03665400	-1.65319000	H	0.14399900	0.13850300	-5.04448500
H	4.52160900	3.75209900	-1.26173300	H	1.26519000	1.03464300	-4.02269200
				C	-1.34493600	2.30476300	-3.15082800
				H	-1.96350300	2.17981400	-4.05152800
				H	-1.86804900	3.02144800	-2.51100900
				H	-0.41118900	2.77051200	-3.47371300
				C	-3.30495300	1.08808600	-1.05806700
				H	-3.90488200	0.43217500	-0.42399500
				H	-3.07035100	1.98398400	-0.46991800
				H	-3.95192500	1.41525800	-1.88261100
				C	-2.66757000	-2.08275000	-0.92911700
				H	-3.46826000	-1.68148400	-0.30508400
				H	-3.14928700	-2.63923400	-1.74544200
				H	-2.11762000	-2.81789800	-0.33345100
				C	-0.23675200	-2.66256200	-2.70567000
				H	0.60241400	-2.65797000	-3.40354300
				H	0.05296700	-3.28119000	-1.84802200
				H	-1.06299200	-3.18854400	-3.20317300
				C	-2.79304400	-0.42211400	2.20660200

TS₁₂-Bu
H = -1862.999682 au

Sm	0.36568600	0.24372200	-0.13422300
Sm	4.98202100	-0.03176400	0.23387100
C	3.10338200	1.47866300	-0.37390200
H	2.60546100	-0.18644100	0.05752400
C	2.06730600	2.21796900	-0.53755600
C	1.82800200	3.67619900	-0.88327600
C	-1.78945300	-1.00288500	-1.49161200
C	-2.08451300	0.38610100	-1.58387800
C	-0.66399300	-1.27182100	-2.32695000
C	-1.14581800	0.97432800	-2.48160200
C	-0.26921900	-0.05001300	-2.94285400
C	0.93808800	-0.67281600	2.40743300
C	0.74026800	0.72755800	2.56098800

H	-3.34648300	0.37498300	1.70346300	H	1.54895700	2.40720300	3.84389400
H	-3.12440200	-1.37505300	1.78982300	C	2.48376100	-0.27581200	4.09912100
H	-3.10766200	-0.40763000	3.25956200	H	1.54793900	0.19240100	4.40927900
C	-1.33673200	2.31157300	2.58820400	H	2.30613800	-1.35496100	4.04156700
H	-0.64404400	3.15590000	2.53549700	H	3.20656800	-0.12276900	4.91287300
H	-2.13948800	2.49806500	1.86603300	C	4.76843800	-1.59437400	2.48471300
H	-1.79741400	2.34071500	3.58523900	H	4.04855500	-2.40404400	2.65089300
C	1.77548800	1.70619100	3.01136400	H	5.47345900	-1.93914300	1.72424800
H	1.88618500	1.69207600	4.10501700	C	5.91976900	0.64604900	0.47121500
H	2.74979500	1.48564900	2.57106300	H	5.87634500	0.97517400	-0.57146900
H	1.52672800	2.73150100	2.72497100	H	6.60022100	1.33518500	0.98951000
C	2.18677300	-1.44365300	2.72112800	H	6.38893500	-0.33799500	0.49093800
H	2.32882400	-2.29795900	2.05039600	C	3.97826800	3.09770700	0.51512500
H	3.07544300	-0.80807200	2.65539400	H	4.53632200	2.95326300	-0.41524000
H	2.16061900	-1.84140100	3.74583200	H	3.03978900	3.59960800	0.25943400
C	-0.57608600	-2.75386300	2.10264900	H	4.55849000	3.80164100	1.12926900
H	-1.60379100	-2.98856000	1.81620100	C	4.10764500	0.46384500	-2.99986400
H	0.08623200	-3.28913000	1.41087000	H	3.56451300	1.41528900	-3.02225400
H	-0.41133800	-3.19536600	3.09478700	H	5.08071300	0.65701400	-2.54112700
C	7.88681400	-2.56371200	-0.72059600	H	4.29582700	0.18591400	-4.04578700
H	8.07558400	-3.46759600	-1.31594800	C	3.02262900	-3.85274400	-0.40538200
H	8.72977200	-1.89187400	-0.89401800	H	3.86636000	-3.82409200	0.29078700
H	7.91262100	-2.87025700	0.32937800	H	2.13032900	-4.11631200	0.17210500
H	7.94482000	-1.18166900	3.77992500	H	3.20894600	-4.68420400	-1.09944600
C	2.77120700	4.59022700	-0.08311500	C	0.41012200	-2.92543300	-1.84956500
H	2.60352700	5.64073200	-0.35143500	H	0.26605800	-3.52001100	-0.94362900
H	2.59677900	4.48794200	0.99190500	H	-0.47974900	-2.30582700	-1.97774100
H	3.81709000	4.34565700	-0.28742800	H	0.45068000	-3.62415600	-2.69792500
C	0.38441000	4.09354800	-0.56484200	C	1.05632000	-0.10934200	-3.36696400
H	0.18979200	4.01443700	0.50978100	H	1.37357300	0.93568300	-3.43417400
H	0.19917600	5.13297300	-0.86096600	H	1.05418600	-0.51105400	-4.38919100
H	-0.33568500	3.46186200	-1.09058300	H	0.02684000	-0.10793500	-3.00553500
C	2.12043500	3.87546900	-2.38147100	C	-1.87149300	-1.49149700	-4.11406100
H	3.17400500	3.67295800	-2.59503600	H	-1.10050200	-2.24731900	-3.94796300
H	1.52226400	3.20099700	-2.99819900	H	-2.59302500	-1.92759400	-4.81900900
H	1.89592100	4.90597000	-2.68304200	H	-1.40027200	-0.64850800	-4.62245500
2-'Bu				C	-2.67522100	1.47459500	-3.42656500
<i>H = -1863.01779 au</i>				H	-2.87571800	1.31867100	-4.49456100
Sm	-2.00406900	-0.41740400	0.01426100	H	-3.25879500	2.34819000	-3.12482900
Sm	2.06727900	-0.18981600	0.14334700	H	-1.61491700	1.73227400	-3.33077900
C	-0.06334600	1.40481500	-0.33607800	C	-5.05333100	1.34109900	-1.34818100
H	0.08853700	-1.28869800	0.50228200	H	-5.70050200	1.10231400	-0.50066300
C	-0.24643900	2.61677100	-0.53768400	H	-4.49982900	2.24936300	-1.08487300
C	-0.43629500	4.05828600	-0.80728300	H	-5.71199500	1.60473700	-2.18711000
C	-4.35252600	-1.18171100	-1.37404700	C	-5.60286100	-1.79408400	-0.81360600
C	-4.14958400	0.19221800	-1.70239700	H	-6.25607900	-1.05284700	-0.35327600
C	-3.35958600	-1.94512200	-2.05044800	H	-6.17462200	-2.26072200	-1.62779600
C	-3.06614200	0.26293000	-2.62878800	H	-5.41432500	-2.57967200	-0.07598600
C	-2.60436900	-1.05986700	-2.87304900	C	-3.34397500	-3.44488200	-2.14042500
C	-1.86123800	-1.20803200	2.65157600	H	-2.36173900	-3.82845900	-2.43184400
C	-1.86952300	0.21352300	2.66763700	H	-3.61489600	-3.91924300	-1.19131400
C	-3.16450400	-1.64880400	2.27398600	H	-4.06299900	-3.80537900	-2.89055000
C	-3.17066800	0.65487800	2.29141700	C	-5.48240300	-0.46449300	2.12553800
C	-3.98332900	-0.49747800	2.09368300	H	-5.91219000	0.30153800	1.47353300
C	3.74717800	1.79948100	1.23512300	H	-5.93122600	-1.42280100	1.86194000
C	2.81247100	1.59747800	2.29236300	H	-5.81412000	-0.22647600	3.14588100
C	4.58489100	0.65339300	1.15533000	C	-3.67624100	2.06864700	2.34381100
C	3.02043600	0.28950300	2.81348100	H	-2.88157100	2.79471200	2.14702700
C	4.10447600	-0.30430000	2.09231300	H	-4.47471600	2.24903600	1.61709500
C	1.66261600	-2.10841200	-1.77887000	H	-4.08665500	2.30764200	3.33493900
C	1.96131000	-0.90094200	-2.47186600	C	-0.76804400	1.09445600	3.15112300
C	2.85585400	-2.55215300	-1.13886100	H	-0.72720400	1.11159400	4.24956300
C	3.34851500	-0.61574900	-2.28015700	H	0.20579100	0.76147500	2.78775700
C	3.90666400	-1.66144200	-1.49030600	H	-0.89907700	2.12480300	2.81501700
C	2.00531500	2.70890100	2.89875200	C	-0.77002500	-2.10362600	3.15870500
H	2.65640900	3.56541600	3.11643500	H	-0.70702800	-3.03955900	2.59504200
H	1.20575700	3.06893800	2.24533900	H	0.20666200	-1.62199100	3.09212800
				H	-0.94245700	-2.36783700	4.21183200
				C	-3.62283400	-3.07898800	2.31657100

H	-4.55186400	-3.23220600	1.76156800
H	-2.87667300	-3.76665900	1.90293100
H	-3.80894000	-3.40367500	3.34948400
C	5.36223200	-2.00164500	-1.36954600
H	5.61068700	-2.78621300	-2.09751600
H	6.01171500	-1.15246100	-1.58493800
H	5.63460100	-2.39431500	-0.38558300
H	5.33494700	-1.48190300	3.41963000
C	0.08016100	4.90827900	0.36932200
H	-0.08082900	5.97085300	0.15496600
H	-0.44948300	4.66329300	1.29465700
H	1.14907800	4.75500300	0.53727200
C	-1.93564500	4.35803600	-1.00071300
H	-2.50723100	4.09716500	-0.10505400
H	-2.07551800	5.42739700	-1.19417700
H	-2.34262900	3.80108200	-1.84643100
C	0.33204300	4.44007300	-2.08901900
H	1.40335900	4.24931500	-1.97426700
H	-0.02715700	3.86588800	-2.94759800
H	0.19595600	5.50589900	-2.30448800

TS₂₃-Bu*H* = -2097.383711 au

Sm	1.98379900	0.54843000	0.66203000
C	-0.56596900	0.07802600	-1.23268000
C	-0.78654600	-0.23759900	-0.04906200
C	3.81975000	-0.71669800	-1.12059100
C	4.60963800	0.08194000	-0.24466700
C	3.27968300	-1.80215700	-0.36881500
C	4.53435500	-0.49390200	1.05698500
C	3.71593000	-1.66043500	0.97848000
C	0.82320200	2.65421200	1.99479500
C	2.08292700	2.48119400	2.63553800
C	1.05484100	3.17342800	0.69307900
C	3.09484000	2.91596300	1.73258500
C	2.46283300	3.31602900	0.51684800
C	-0.01761500	3.69431300	-0.21904300
H	-0.54500700	4.53421400	0.25292700
H	0.39637800	4.07310300	-1.15806000
H	-0.77355900	2.93904000	-0.45702500
C	3.13275000	4.02242800	-0.62814100
H	4.19975100	3.79191600	-0.67920700
H	2.69733300	3.76163400	-1.59892100
H	3.04611400	5.11277000	-0.52465900
C	4.50586300	3.23713300	2.12815000
H	4.88425500	2.56783000	2.90407400
H	5.20159300	3.20464400	1.28683500
H	4.55407700	4.25567500	2.53802400
C	2.29488100	2.08358500	4.06804300
H	2.26582200	2.95695100	4.73413400
H	1.52662400	1.38241700	4.40591800
H	3.26507900	1.59958000	4.21904900
C	-0.52259600	2.49525700	2.62343200
H	-1.22304400	1.97579900	1.96353500
H	-0.47503900	1.92575000	3.55273300
H	-0.95815600	3.47682300	2.85851700
C	2.64364500	-3.01611300	-0.98086600
H	3.41062200	-3.66783700	-1.42201600
H	2.09479600	-3.61293000	-0.25101500
H	1.94466800	-2.76423000	-1.78399000
C	3.59961100	-2.66615300	2.08894500
H	4.59681200	-3.01590500	2.38826100
H	3.11507400	-2.26171300	2.98319300
H	3.03261300	-3.54563700	1.77927100
C	5.38066000	-0.15657300	2.25086600
H	6.12396400	-0.94649900	2.42648400
H	5.93174300	0.77523700	2.11181100
H	4.79973600	-0.06623500	3.17578400

C	5.57571200	1.13080300	-0.71325700
H	5.13411800	1.81938600	-1.44079700
H	5.96843500	1.72809700	0.11158200
H	6.43875500	0.66197400	-1.20601600
C	3.87823100	-0.64525300	-2.62082900
H	3.00247200	-1.09455600	-3.09809600
H	3.96864100	0.38099100	-2.99125300
H	4.75536700	-1.19248400	-2.99490000
C	-0.88485500	-0.80297800	3.62745800
C	-1.03362300	-0.77505300	4.85469900
Sm	-2.57170700	-1.33046700	1.60012900
C	-4.14189300	0.86564900	2.48113900
C	-4.07363100	1.00957500	1.06865200
C	-4.90231200	-0.30861500	2.76679100
C	-4.79200200	-0.07589600	0.48035300
C	-5.34374700	-0.86085400	1.53145300
C	-1.18180700	-3.69966200	1.62819600
C	-2.21752700	-3.92528400	2.57712200
C	-1.77472800	-3.64900200	0.33524600
C	-3.45048400	-4.02269200	1.87331800
C	-3.17955600	-3.84022300	0.48445500
C	-4.71931500	-4.54461800	2.48289800
H	-5.00228100	-4.01929700	3.40195600
H	-5.56400400	-4.48325500	1.79478100
H	-4.60096600	-5.60309600	2.75184700
C	-4.13405800	-4.06769700	-0.65350400
H	-3.96514000	-5.04967300	-1.11569500
H	-5.17571900	-4.04741900	-0.32473300
H	-4.02930300	-3.32258600	-1.44984200
C	-1.03915600	-3.61904700	-0.97033300
H	-1.70555200	-3.36273800	-1.79893000
H	-0.22716800	-2.88992000	-0.96732700
H	-0.60593000	-4.60303000	-1.19837900
C	0.28420100	-3.65611500	1.92094200
H	0.47831300	-3.50880100	2.98590400
H	0.77421500	-4.59424000	1.62402500
H	0.78365400	-2.83907000	1.39258200
C	-2.03712400	-4.23431700	4.03355600
H	-1.90730000	-5.31398200	4.19298500
H	-1.15980700	-3.73195600	4.44875800
H	-2.90466900	-3.92681300	4.62614600
C	-6.45996500	-1.84928400	1.37276700
H	-6.35460000	-2.47076000	0.47979700
H	-6.55462000	-2.51176600	2.23510900
H	-7.41527800	-1.31505900	1.27373600
C	-5.36340600	-0.71695800	4.13697600
H	-6.28736800	-0.19340400	4.42119800
H	-5.57341300	-1.78903700	4.20488600
H	-4.61697400	-0.47896700	4.90104500
C	-3.71425200	1.86180800	3.52013000
H	-2.94151300	1.47462100	4.19129200
H	-3.31912300	2.77178900	3.06425300
H	-4.56975900	2.15862800	4.14018200
C	-3.56018100	2.18832600	0.29564000
H	-3.00642200	2.88429700	0.92927900
H	-2.89250900	1.88788500	-0.51701600
H	-4.39185300	2.74842800	-0.15261200
C	-5.12021900	-0.20524000	-0.97924700
H	-4.29876600	0.14244900	-1.61316500
H	-5.34109000	-1.23919200	-1.26060300
H	-6.00224200	0.39425100	-1.24606800
C	-1.10346300	-0.71985300	6.32564200
C	-0.39711400	0.41639700	-2.66686000
H	1.12407700	-0.46101600	2.39619200
H	0.12451600	-0.62327400	2.86051600
C	0.28072800	-1.13340700	6.87321500
H	0.26787800	-1.10027400	7.96836300
H	0.53846200	-2.14928500	6.56076800
H	1.06349700	-0.45720300	6.51795900

C	-1.42960300	0.71319000	6.79015700
H	-2.41828000	1.02598900	6.44269900
H	-1.42322600	0.75978800	7.88483900
H	-0.69294700	1.42809400	6.41256400
C	-2.17094900	-1.68962000	6.86651000
H	-3.16482000	-1.44080600	6.48419100
H	-1.94534400	-2.72191800	6.58895500
H	-2.20079100	-1.62560100	7.95970300
C	-1.62309600	1.20131100	-3.17150700
H	-1.75038600	2.13695300	-2.62062500
H	-1.49693600	1.44372700	-4.23290600
H	-2.53738300	0.61108700	-3.06460700
C	-0.25604400	-0.87202800	-3.49922300
H	-0.12161800	-0.62082400	-4.55749100
H	0.60410300	-1.46339000	-3.17432100
H	-1.14788100	-1.49712400	-3.40508200
C	0.85944500	1.28629900	-2.84975300
H	0.75692000	2.23717900	-2.32223300
H	1.75395800	0.77132700	-2.48422400
H	1.02208900	1.50297700	-3.91156800

3-Bu $H = -2097.411034 \text{ au}$

Sm	4.08262500	1.76587100	-1.22126900
C	1.55018700	1.50637900	-3.86870800
C	2.40170300	1.58073100	-2.97692800
C	5.88072700	0.34142500	-2.70932400
C	6.64018200	0.84087400	-1.60744300
C	4.97664100	-0.64223700	-2.21683500
C	6.20099600	0.16246100	-0.43013600
C	5.16835000	-0.74576900	-0.80629000
C	2.54205500	3.76219300	-0.12757800
C	3.41765600	3.35884200	0.92741600
C	3.32297100	4.40529500	-1.12774000
C	4.73962600	3.76501400	0.58056400
C	4.68503200	4.39722200	-0.69856400
C	2.78225200	5.07692200	-2.35684700
H	2.40649800	6.08232500	-2.12291500
H	3.54915800	5.19468300	-3.12865900
H	1.96264400	4.50527400	-2.80051600
C	5.82669200	5.09380900	-1.38488100
H	6.78965600	4.62424900	-1.16230900
H	5.70979600	5.10090300	-2.47374600
H	5.90124200	6.14304000	-1.06895400
C	5.93333400	3.73056000	1.48986200
H	5.90617500	2.88352900	2.18158500
H	6.87532700	3.67320000	0.93551300
H	5.98260700	4.64077400	2.10315000
C	2.99926900	2.76591400	2.24490700
H	2.77222500	3.54923700	2.98048400
H	2.09779100	2.15052600	2.15546500
H	3.78196100	2.13916400	2.68549600
C	1.04512800	3.64196100	-0.14190700
H	0.66996300	3.40066100	-1.14106400
H	0.68991800	2.86369300	0.54079000
H	0.57065500	4.58129100	0.17214000
C	4.08937300	-1.50990500	-3.06085800
H	4.64791600	-2.36431400	-3.46674400
H	3.25034400	-1.91620000	-2.48839600
H	3.66487500	-0.95471000	-3.90087600
C	4.52319700	-1.75607100	0.10181100
H	5.13016000	-2.66849600	0.17418600
H	4.40023000	-1.38046700	1.12372400
H	3.53576800	-2.06136800	-0.25750900
C	6.85091300	0.22597400	0.92219100
H	7.62867500	-0.54390400	1.01911600
H	7.33281000	1.18977100	1.10498400
H	6.13844300	0.05533900	1.73650800

C	7.82285200	1.76311900	-1.70103900
H	7.71052100	2.50860600	-2.49498700
H	7.99537300	2.30491400	-0.76615700
H	8.74320200	1.20481800	-1.91927700
C	6.05942000	0.71159100	-4.15472000
H	5.10271000	0.74329800	-4.68544200
H	6.53469300	1.69096700	-4.27128100
H	6.69831200	-0.01418700	-4.67564700
C	-2.86696200	-1.26337900	3.40243700
C	-2.24393800	-0.93471500	4.41694000
Sm	-4.11616800	-1.95333700	1.43633600
C	-5.35525600	0.48456400	1.72636900
C	-5.10429800	0.36002900	0.32708400
C	-6.33480000	-0.48607900	2.08082900
C	-5.94774400	-0.66896400	-0.18748700
C	-6.70455300	-1.20051700	0.90009600
C	-2.10253200	-3.73385000	0.92495800
C	-2.96938200	-4.41390300	1.82565100
C	-2.78488800	-3.58765700	-0.32243400
C	-4.19285000	-4.68500600	1.14023300
C	-4.07095400	-4.19118200	-0.19274100
C	-5.34415800	-5.49438500	1.67023200
H	-5.44626000	-5.40552200	2.75695200
H	-6.29855600	-5.19405100	1.22536400
H	-5.21525900	-6.56322000	1.45300600
C	-5.03727400	-4.45412400	-1.31053800
H	-4.85837500	-5.44315900	-1.75403500
H	-6.07867200	-4.44474000	-0.97257800
H	-4.94539300	-3.72301500	-2.11831600
C	-2.19631000	-3.03592900	-1.59190800
H	-2.95718800	-2.58870800	-2.24024000
H	-1.43954900	-2.26835700	-1.39791600
H	-1.70242400	-3.82166300	-2.17888500
C	-0.68620900	-3.33152600	1.22182900
H	-0.58169000	-2.95656400	2.24422800
H	-0.00018200	-4.18123500	1.10474700
H	-0.33390400	-2.54495000	0.54647100
C	-2.60746400	-4.85580700	3.21416900
H	-1.99672900	-5.76826600	3.18983900
H	-2.04246000	-4.08617200	3.74739900
H	-3.49458300	-5.08168100	3.81378700
C	-7.82324900	-2.19963400	0.79748600
H	-7.69318800	-2.88232800	-0.04787400
H	-7.91854500	-2.81173800	1.70080100
H	-8.79030500	-1.69886700	0.65470400
C	-6.94384200	-0.65065600	3.44467500
H	-7.78270900	0.04280300	3.59195900
H	-7.34007900	-1.65966800	3.60192800
H	-6.21806400	-0.45218800	4.23939800
C	-4.79148400	1.53492900	2.63818200
H	-4.60160900	1.14369200	3.64080500
H	-3.84084000	1.92696200	2.26583900
H	-5.48074300	2.38547600	2.72917100
C	-4.21218700	1.25373300	-0.48961400
H	-4.73658300	2.16857200	-0.79626900
H	-3.32366600	1.57298100	0.06588700
H	-3.86982800	0.76580500	-1.40823900
C	-6.14118100	-0.98889300	-1.64191500
H	-5.20219000	-0.96781600	-2.20604200
H	-6.58852200	-1.97506600	-1.78809400
H	-6.81022400	-0.25932000	-2.11778700
C	-1.50310400	-0.53847300	5.62634100
C	0.54273100	1.42373000	-4.93981300
H	2.08542000	0.32755100	-0.07161800
H	1.86641000	0.47512400	-0.77884900
C	-0.00637300	-0.38986300	5.28685300
H	0.55786200	-0.09238400	6.17865600
H	0.40543900	-1.33409600	4.91783100
H	0.14365400	0.37119200	4.51506000

C	-2.04313300	0.80615700	6.15251700
H	-3.10355200	0.72531200	6.40979000
H	-1.49352100	1.11213100	7.05055100
H	-1.93627300	1.59145100	5.39827800
C	-1.67608400	-1.61841000	6.71324700
H	-2.73217500	-1.74859900	6.96790800
H	-1.28865700	-2.58270200	6.37102900
H	-1.13485500	-1.33196500	7.62271100
C	-0.75712400	2.11719100	-4.48565000
H	-0.57695100	3.17188200	-4.25703100
H	-1.51510800	2.06072800	-5.27587000
H	-1.16060400	1.63987000	-3.58731300
C	0.24680500	-0.05420700	-5.26393100
H	-0.50327300	-0.12647000	-6.06042700
H	1.15256300	-0.56967000	-5.59688400
H	-0.13571100	-0.57792200	-4.38252300
C	1.08144700	2.12604700	-6.20248100
H	1.29947300	3.17881500	-5.99986400
H	2.00297700	1.64955000	-6.54992900
H	0.34088000	2.07541600	-7.00937700

3'-Bu $H = -1048.124628 \text{ au}$

Sm	3.24871300	0.52935700	-0.25275900
C	2.09464200	-0.81717500	1.40415200
C	1.49168500	-1.49221600	2.24436000
C	0.77288600	-2.30184200	3.24225300
C	4.34807600	-0.19114200	-2.67766800
C	5.45496300	-0.11485200	-1.77892300
C	3.53724000	-1.29674900	-2.28003700
C	5.32182500	-1.17353600	-0.83031500
C	4.14558300	-1.91282100	-1.14777500
C	1.71135600	2.59764200	0.68393700
C	2.93103900	2.67899600	1.41169600
C	1.98636400	2.93727500	-0.67643800
C	3.96390900	3.07023700	0.50495800
C	3.37403300	3.24738800	-0.78263100
C	3.71021700	-3.19357400	-0.49922100
H	2.63049000	-3.34256100	-0.57825900
H	4.20071400	-4.05613800	-0.97101000
H	3.95239000	-3.21292000	0.56616100
C	6.31097900	-1.52883700	0.24425600
H	7.03360700	-2.27608400	-0.11012500
H	6.89253000	-0.66152000	0.57421500
H	5.82107700	-1.95458800	1.12615700
C	6.65090800	0.78343000	-1.92028300
H	6.41015300	1.71291200	-2.44427400
H	7.08734600	1.05475100	-0.95323800
H	7.44589300	0.29155000	-2.49695300
C	4.16598200	0.61999900	-3.92911400
H	4.63962300	1.60248400	-3.85513900
H	4.61206400	0.11375100	-4.79581300
H	3.11010200	0.78320100	-4.17132100
C	2.31912100	-1.80256900	-3.00187600
H	1.59118300	-2.24954800	-2.31655500
H	1.80782900	-1.00895900	-3.55727300
H	2.58267400	-2.57765800	-3.73389300
C	4.04955600	3.85437200	-1.97746300
H	5.10991800	3.59033700	-2.03442600
H	3.58203000	3.54976700	-2.91828700
H	3.99850600	4.95110000	-1.93849300
C	5.37997700	3.41542100	0.87456800
H	5.73718700	2.83642300	1.73289000
H	6.07623100	3.24141700	0.04796000
H	5.47245000	4.47451300	1.15052400
C	3.07749300	2.47586900	2.89264200
H	2.82804300	3.39183900	3.44487900
H	2.42196400	1.67935100	3.25607900

H	4.10202900	2.20774200	3.17063900
C	0.35903100	2.31533900	1.27143500
H	-0.34282500	1.94024500	0.51994100
H	0.41398200	1.56414500	2.06372200
H	-0.08381000	3.22602300	1.69691600
C	0.96228700	3.08975100	-1.76748200
H	1.39650600	2.95205300	-2.76325800
H	0.13874200	2.37441100	-1.66563700
H	0.51026700	4.09052200	-1.75474400
C	-0.69998300	-1.85055000	3.30951600
H	-1.18865300	-1.96887200	2.33765700
H	-1.24765100	-2.45022600	4.04615800
H	-0.77355300	-0.79811200	3.59957600
C	0.83240300	-3.79060600	2.84641500
H	1.86834400	-4.13811600	2.79180300
H	0.30133900	-4.40278400	3.58501800
H	0.36919800	-3.95240500	1.86843600
C	1.42931400	-2.11371200	4.62465300
H	2.47698900	-2.42848000	4.60468900
H	1.39630400	-1.06428900	4.93242300
H	0.90350300	-2.71117900	5.37874700

4'-Bu $H = -2096.23696 \text{ au}$

Sm	2.01519500	0.65697000	0.79748200
C	-0.67355800	-0.28986200	-1.30511500
C	-0.36574400	-0.22713200	-0.10271100
C	3.66018000	-0.84680700	-0.95557500
C	4.54872600	0.07437200	-0.33867100
C	3.29727200	-1.83184000	0.01118600
C	4.65284900	-0.27455600	1.03753500
C	3.89861900	-1.47142200	1.24794600
C	1.18155500	3.21573800	1.41861000
C	2.57081500	3.25075400	1.72623100
C	1.04545300	3.14350700	0.00473300
C	3.29399300	3.24617700	0.50060500
C	2.35542500	3.14190800	-0.56373100
C	-0.22831300	3.30916000	-0.77216800
H	-0.82025900	4.13826100	-0.36714400
H	-0.01198800	3.55207100	-1.81709000
H	-0.86079900	2.41701400	-0.76260300
C	2.64844900	3.28129200	-2.03166700
H	3.72184800	3.25676600	-2.23400300
H	2.18522900	2.49534200	-2.63805100
H	2.27577800	4.23964900	-2.41766800
C	4.71650000	3.71162100	0.39730500
H	5.39306800	3.19639400	1.08551200
H	5.12155100	3.61038500	-0.60980900
H	4.76540600	4.77886500	0.65528700
C	3.18187800	3.54902100	3.06391400
H	3.38280300	4.62412300	3.17485400
H	2.52249800	3.26175100	3.88658900
H	4.13767000	3.03418900	3.20857100
C	0.06864200	3.42214500	2.39241900
H	0.42325300	3.37738600	3.42389900
H	-0.39727800	4.40794900	2.25044700
H	-0.71126900	2.66757100	2.29240100
C	2.73286300	-3.16714200	-0.37304600
H	3.51554200	-3.77392000	-0.85010200
H	2.35779800	-3.73575400	0.47739900
H	1.91659300	-3.08131500	-1.09418900
C	3.99976000	-2.30537800	2.49553200
H	5.03419200	-2.31674300	2.85936700
H	3.36967700	-1.94963500	3.31819900
H	3.71729000	-3.34308000	2.30165400
C	5.61286200	0.30077400	2.04061800
H	6.50363600	-0.33516600	2.14445300
H	5.96396400	1.29322700	1.74868500

H	5.17396900	0.39008500	3.03983900
C	5.48762800	0.95178100	-1.11135300
H	4.98614100	1.58040900	-1.85217900
H	6.07757500	1.59923600	-0.46296600
H	6.19750100	0.32052300	-1.66363200
C	3.42770300	-0.95821300	-2.43462500
H	2.47622900	-1.44781800	-2.66258100
H	3.42525700	0.01949900	-2.92722200
H	4.21533500	-1.55432700	-2.91825800
C	0.63804000	0.00477700	3.05091200
C	1.10454000	0.14467500	4.19449500
Sm	-1.75395700	-0.86873400	2.11653900
C	-3.10291800	1.37789300	3.28186100
C	-3.37948500	1.52025000	1.89382100
C	-3.77302800	0.20214200	3.74582200
C	-4.20283900	0.42347200	1.49838800
C	-4.50096000	-0.34725600	2.65369700
C	-0.60024000	-3.34158400	2.51182500
C	-1.56875400	-3.27513400	3.55328800
C	-1.29285100	-3.47350300	1.27632200
C	-2.85744100	-3.41335100	2.96702300
C	-2.69215700	-3.49440300	1.55601800
C	-4.06244400	-3.83647500	3.75397300
H	-4.24572800	-3.21435000	4.63509000
H	-4.97457800	-3.85160900	3.15669200
H	-3.90599000	-4.85945500	4.12423300
C	-3.75997100	-3.81336100	0.54695800
H	-3.69728600	-4.86091100	0.22205700
H	-4.76246700	-3.66880000	0.95671000
H	-3.68788100	-3.19835700	-0.35729500
C	-0.68290900	-3.79162100	-0.05670500
H	-1.45235600	-4.10771100	-0.76719700
H	-0.15347200	-2.94569000	-0.50068800
H	0.02942300	-4.62064300	0.03288500
C	0.87724100	-3.45201400	2.70353800
H	1.16504100	-3.23320100	3.73401600
H	1.22601000	-4.46986300	2.47654700
H	1.42806400	-2.75985500	2.06659000
C	-1.30157000	-3.33554100	5.02880000
H	-1.38552300	-4.36570300	5.40305900
H	-0.29711200	-2.98518000	5.27277000
H	-2.01054600	-2.73181600	5.60570400
C	-5.68113600	-1.26842300	2.73155600
H	-5.69292100	-2.02836000	1.94545700
H	-5.75283100	-1.77600100	3.69335900
H	-6.60169100	-0.68035000	2.61138400
C	-3.89239400	-0.18186300	5.19400000
H	-4.51368800	0.53773900	5.74596700
H	-4.35639800	-1.16344200	5.31704100
H	-2.92326400	-0.21269800	5.70504700
C	-2.48724200	2.38803500	4.21025500
H	-3.12439300	2.52216200	5.09304300
H	-1.49136400	2.10847400	4.56949800
H	-2.39548200	3.36562800	3.73126600
C	-3.20799900	2.74628600	1.04623000
H	-2.45161600	3.42923800	1.43189500
H	-2.93527700	2.50641100	0.01535800
H	-4.15498200	3.30234800	1.00288800
C	-4.91692900	0.29553400	0.18325200
H	-4.37370600	0.78919200	-0.62607600
H	-5.06833900	-0.74947700	-0.10814000
H	-5.91383600	0.75812000	0.22758000
C	1.64721200	0.31111900	5.56148800
C	-1.05346500	-0.36900900	-2.73179100
C	1.02891200	1.55148600	6.23602500
H	1.44265800	1.67364300	7.24346100
H	1.24080900	2.46157200	5.66820700
H	-0.05664500	1.45099500	6.32402900
C	3.17842000	0.47735800	5.49569200

H	3.57794800	0.61135500	6.50719200
H	3.65133300	-0.40582400	5.05737300
H	3.45763000	1.35071400	4.90134800
C	1.32240500	-0.93036000	6.41418600
H	0.24258600	-1.07433500	6.50644400
H	1.75563800	-1.83354700	5.97490300
H	1.73706300	-0.80732700	7.42104300
C	-0.14278100	0.55743700	-3.56139000
H	0.90512500	0.25678700	-3.47904200
H	-0.42980900	0.50671900	-4.61764900
H	-0.23318800	1.59479900	-3.23014700
C	-2.51636500	0.08767700	-2.89780100
H	-3.19547400	-0.55401100	-2.32980000
H	-2.64814500	1.11785800	-2.55435900
H	-2.80295700	0.03888800	-3.95433000
C	-0.91484000	-1.81303100	-3.25017700
H	-1.18812100	-1.85417300	-4.31064100
H	0.11262300	-2.17380000	-3.14809700
H	-1.56938500	-2.49458500	-2.70097100

TS₄₅-Bu*H* = -2096.205118 au

Sm	2.26597500	0.94450200	0.30521500
C	-0.10960700	-0.03713100	-0.51533200
C	-0.42334200	-0.30993100	0.68328700
C	3.82164600	-0.85522400	-1.30290200
C	4.75495600	0.12895900	-0.86133400
C	3.40625500	-1.61195900	-0.17232000
C	4.90544600	-0.01184200	0.54720200
C	4.06458500	-1.08332600	0.97265900
C	1.48013800	3.49565300	1.20609000
C	2.88074100	3.43159800	1.46330000
C	1.29350700	3.56878200	-0.20278800
C	3.55945800	3.49172800	0.21305700
C	2.58129200	3.54859300	-0.81959500
C	0.01061000	3.95249200	-0.88304300
H	-0.17340900	5.02986600	-0.76835000
H	0.03312000	3.75620200	-1.95900300
H	-0.85931200	3.43755400	-0.46993800
C	2.86611100	3.83046700	-2.26831900
H	3.80099400	3.37134000	-2.60389400
H	2.07265500	3.47101300	-2.93061700
H	2.96080700	4.91029200	-2.44818500
C	5.01360800	3.82094600	0.05117300
H	5.64802400	3.30820800	0.77782500
H	5.38667400	3.58840000	-0.94801700
H	5.16745000	4.89878600	0.20323900
C	3.53811100	3.57202100	2.80687600
H	3.77458000	4.62420500	3.01891300
H	2.89299000	3.22419200	3.61734900
H	4.48193900	3.02055000	2.87366100
C	0.41686000	3.72925500	2.23328000
H	0.68035800	3.28725500	3.19631700
H	0.26531100	4.80542300	2.39946200
H	-0.54293000	3.30803700	1.93259800
C	2.63173300	-2.89244700	-0.21401400
H	3.30977600	-3.75752600	-0.21266500
H	1.96931700	-3.00026900	0.64527500
H	2.01760400	-2.97183300	-1.11460500
C	4.12706100	-1.71368500	2.33210700
H	4.94059700	-2.45171100	2.38280200
H	4.32259700	-0.97597700	3.11686500
H	3.20330500	-2.23428300	2.59046100
C	5.95310200	0.62015100	1.41950100
H	6.65961000	-0.13933000	1.77916600
H	6.53829500	1.36656800	0.87837200
H	5.54271300	1.10994200	2.31047400
C	5.61990800	0.92663900	-1.79366500

H	5.04545000	1.52967300	-2.50594200
H	6.28781100	1.60252400	-1.25662600
H	6.25349400	0.25718800	-2.39089200
C	3.62105600	-1.23413000	-2.74361300
H	2.67693800	-1.75807400	-2.91718700
H	3.64524800	-0.36772200	-3.41281400
H	4.42209100	-1.90950400	-3.07610900
C	0.75806000	0.08355700	2.23697500
C	0.39915600	-0.16800500	3.43124200
Sm	-1.95672800	-1.14250700	2.58856100
C	-3.18031600	1.26167600	3.40415300
C	-3.38635600	1.20984800	1.99562300
C	-3.97837700	0.24000600	4.00244800
C	-4.30609900	0.15681800	1.72139600
C	-4.69163000	-0.42191700	2.96254100
C	-0.75990700	-3.70937800	2.79340300
C	-1.66679000	-3.67091500	3.88934600
C	-1.52218100	-3.70952500	1.59182200
C	-2.99255300	-3.67559500	3.36642100
C	-2.90499300	-3.68856500	1.94438300
C	-4.20791700	-3.96895200	4.19672200
H	-4.29845400	-3.31847900	5.07416100
H	-5.13123800	-3.87902100	3.62278700
H	-4.16475600	-4.99952400	4.57559100
C	-4.03887400	-3.90185800	0.98175100
H	-4.11611600	-4.95833200	0.69091600
H	-5.00152800	-3.62052600	1.41515400
H	-3.91889400	-3.32820000	0.05629500
C	-0.97739700	-3.94413100	0.21292300
H	-1.77197200	-3.90878000	-0.53785300
H	-0.21984400	-3.21231600	-0.07435000
H	-0.51724300	-4.93936500	0.14033700
C	0.72209800	-3.92148900	2.87681800
H	1.01231600	-4.31852300	3.85445800
H	1.05056400	-4.64946200	2.12640800
H	1.29333900	-3.00204900	2.71382800
C	-1.33713700	-3.91687400	5.33547000
H	-1.42043200	-4.98660300	5.57448700
H	-0.32069600	-3.61047500	5.59566600
H	-2.01905100	-3.39315200	6.01398200
C	-5.91133300	-1.27181100	3.15887000
H	-6.03958600	-2.02283000	2.37417300
H	-5.91124300	-1.78705500	4.12103900
H	-6.81047800	-0.63952800	3.13559100
C	-4.24550800	0.05439400	5.47072600
H	-5.17366500	0.55966200	5.77094100
H	-4.35858800	-1.00039900	5.74375800
H	-3.44600100	0.46273300	6.09454000
C	-2.44791000	2.35610200	4.12753700
H	-2.81849000	3.33996900	3.81183200
H	-2.60574300	2.29630900	5.20834200
H	-1.36937300	2.35263100	3.94532500
C	-2.88957700	2.22079700	1.00545300
H	-1.87245700	2.01047500	0.66202100
H	-3.53334500	2.25399000	0.12145300
H	-2.89541900	3.22563400	1.44359500
C	-4.97060000	-0.12707100	0.40406700
H	-4.37343700	0.22349700	-0.44143000
H	-5.15670100	-1.19531600	0.25339200
H	-5.94560700	0.37574300	0.33737100
C	0.72707200	-0.13186600	4.90154500
C	-0.43982800	-0.02194700	-1.98178800
C	1.72542000	-1.25082300	5.24460000
H	1.94466600	-1.23478300	6.31878800
H	1.32399700	-2.23419900	4.99321500
H	2.66233600	-1.11926900	4.69988200
C	-0.53877800	-0.32287600	5.75333000
H	-0.29082200	-0.34144400	6.82099200
H	-1.24725800	0.49144900	5.58833600

H	-1.03431500	-1.27449100	5.52544200
C	1.36800400	1.21647400	5.27449100
H	2.29088200	1.37189500	4.70974900
H	0.69091600	2.04984000	5.06905000
H	1.61197300	1.23527100	6.34365800
C	0.62513200	0.75274300	-2.77424700
H	1.61502800	0.29946200	-2.65714200
H	0.39614600	0.75247800	-3.84619800
H	0.67132400	1.79359600	-2.44394200
C	-1.80477100	0.65165100	-2.20740600
H	-2.59329400	0.10715800	-1.68225800
H	-1.80322900	1.68383200	-1.84990200
H	-2.04501400	0.65994200	-3.27736400
C	-0.51214800	-1.46346700	-2.51480000
H	-0.71857500	-1.45333700	-3.59158100
H	0.42743500	-1.99803500	-2.35317600
H	-1.30705600	-2.02254200	-2.01617800

5-Bu $H = -2096.259488 \text{ au}$

Sm	2.68756800	1.12789900	0.25656800
C	0.42912700	0.16972300	-0.32843200
C	0.19855600	-0.03611700	0.95804400
C	4.11387300	-0.69992700	-1.30365100
C	5.09524000	0.22736200	-0.83502200
C	3.66361000	-1.46617700	-0.19340200
C	5.23754900	0.04403900	0.56972100
C	4.34047400	-0.99055000	0.96673300
C	1.85319100	3.62967300	1.17355000
C	3.26078600	3.60557800	1.40734500
C	1.63999900	3.67382500	-0.23167900
C	3.91557500	3.65856500	0.14278700
C	2.91441200	3.66878400	-0.87293200
C	0.32522200	3.97163100	-0.88744700
H	0.09852500	5.04510800	-0.81743300
H	0.32392800	3.71387500	-1.94913900
H	-0.50270900	3.43627000	-0.41687100
C	3.14820200	3.87350300	-2.34373100
H	4.12604900	3.49967700	-2.66215500
H	2.39081400	3.37260300	-2.95639600
H	3.11376100	4.93908200	-2.60840800
C	5.36611800	3.98451800	-0.05562100
H	6.01465600	3.49223000	0.67420800
H	5.72130400	3.72000300	-1.05371200
H	5.52567300	5.06552900	0.06136500
C	3.94558600	3.72838700	2.74034500
H	4.13139600	4.78079800	2.99510400
H	3.34927300	3.30619100	3.55468800
H	4.91820400	3.22560100	2.75277800
C	0.77689100	3.80002300	2.20600300
H	1.18585600	3.77799900	3.21851800
H	0.27406700	4.76795400	2.08238900
H	0.00364600	3.02746500	2.14797200
C	2.77080800	-2.67081900	-0.22313500
H	3.29737000	-3.55337600	0.16098600
H	1.86806200	-2.53997700	0.38223000
H	2.45022200	-2.90416200	-1.24074800
C	4.32163000	-1.64854700	2.31577600
H	5.14572100	-2.36973900	2.41087200
H	4.43766900	-0.93391000	3.13771200
H	3.39369000	-2.20147200	2.48260900
C	6.29620600	0.63052800	1.45877000
H	7.09419400	-0.10075200	1.64621700
H	6.76842900	1.50909400	1.01350800
H	5.90914700	0.92625800	2.44058700
C	6.00327600	1.00203200	-1.74601800
H	5.46056800	1.59797400	-2.48825300
H	6.66032500	1.67812000	-1.19552800

H	6.64981400	0.31566900	-2.30994100
C	3.81730600	-0.93557000	-2.75774400
H	3.06728900	-1.71686400	-2.89654300
H	3.45410700	-0.04000300	-3.27714600
H	4.72228200	-1.25734300	-3.29024300
C	0.24409000	-0.11588400	2.27848000
C	-0.14513000	-0.37720200	3.50794500
Sm	-2.26410900	-1.23627600	2.40447900
C	-3.32286500	1.19375800	3.32401200
C	-3.53819500	1.22313700	1.91718000
C	-4.16409900	0.18626500	3.87895900
C	-4.52472600	0.24322100	1.59989900
C	-4.92207300	-0.38544500	2.81260700
C	-1.03187900	-3.77920500	2.66057000
C	-1.96118600	-3.68517300	3.73335900
C	-1.77028400	-3.84790100	1.44555600
C	-3.27766100	-3.72589900	3.18253500
C	-3.16116900	-3.81060100	1.76549700
C	-4.51384300	-3.98388800	3.99394900
H	-4.59513500	-3.33387400	4.87182400
H	-5.42593400	-3.86366600	3.40705100
H	-4.50766100	-5.01659700	4.36965500
C	-4.28094400	-4.05118100	0.79303700
H	-4.41182600	-5.12343600	0.59231600
H	-5.23701700	-3.67940600	1.17157500
H	-4.10543000	-3.56918100	-0.17517900
C	-1.19351000	-4.21666900	0.10759900
H	-1.86060800	-3.95538500	-0.71929900
H	-0.22775400	-3.73852700	-0.08145200
H	-1.02882100	-5.30165100	0.04757900
C	0.45626100	-3.94504500	2.77077500
H	0.74234400	-4.29122100	3.76813100
H	0.81598400	-4.69360500	2.05617600
H	1.00608700	-3.01687100	2.58028600
C	-1.66402500	-3.79539100	5.20167800
H	-1.83219700	-4.82115400	5.55902700
H	-0.62872400	-3.53719800	5.43502100
H	-2.30522000	-3.14473900	5.80601000
C	-6.16149700	-1.21782200	2.96016100
H	-6.27444800	-1.96125600	2.16481500
H	-6.19759800	-1.74343400	3.91599300
H	-7.05167600	-0.57454000	2.91601600
C	-4.38429500	-0.06898600	5.34390000
H	-5.14641000	0.60583900	5.75720900
H	-4.72993700	-1.08990600	5.53428900
H	-3.47239500	0.07848200	5.92974200
C	-2.53994900	2.22700100	4.07861700
H	-2.95705700	3.22751100	3.90045600
H	-2.58295400	2.05433600	5.15675500
H	-1.48570100	2.26090200	3.78728000
C	-2.98300900	2.27325200	0.99910200
H	-1.88900300	2.31350300	1.01608200
H	-3.29080300	2.11105600	-0.03774800
H	-3.34508000	3.26969600	1.28567500
C	-5.21105100	0.04463100	0.27773400
H	-4.64358900	0.47372100	-0.55255000
H	-5.37582800	-1.01387800	0.04701300
H	-6.19819600	0.52674400	0.27190100
C	0.60860900	-0.15368100	4.81357500
C	-0.56867700	-0.22644800	-1.41792800
C	1.59689300	-1.31176700	5.03668700
H	2.11831500	-1.18257100	5.99301800
H	1.08181900	-2.27457300	5.06015300
H	2.34439400	-1.34925700	4.24179400
C	-0.36302300	-0.12447200	6.00389400
H	0.18694000	-0.01761500	6.94662700
H	-1.05909400	0.71415100	5.92669200
H	-0.94548100	-1.04918800	6.05548400
C	1.40120800	1.16195300	4.79245600

H	2.10732100	1.17521400	3.95476600
H	0.73424900	2.02173000	4.68638300
H	1.97371900	1.28852100	5.71941400
C	-0.94063600	0.99755400	-2.26967400
H	-0.04698400	1.44038900	-2.71988900
H	-1.61985400	0.70708800	-3.08035900
H	-1.43391300	1.76704100	-1.67161500
C	-1.85525500	-0.81637100	-0.81644700
H	-1.61777000	-1.72420600	-0.24465200
H	-2.34701500	-0.07287300	-0.17692200
H	-2.57571300	-1.10654500	-1.58994400
C	0.05973900	-1.27083400	-2.35446800
H	-0.64594700	-1.54295400	-3.14894300
H	0.96140100	-0.87276300	-2.82665300
H	0.32950400	-2.18161800	-1.81447000

1-"Bu $H = -1863.036762 \text{ au}$

Sm	3.99280900	0.62859200	-0.06436400
Sm	0.04601600	-1.71725400	2.69089800
C	2.07030000	-0.54441400	1.69434700
H	1.85824300	-0.30322800	0.60035600
C	3.29116200	-0.14556400	2.13191700
C	3.76389200	-0.44606900	3.53202800
H	4.43618400	-1.31819900	3.47846600
H	2.93132300	-0.75975100	4.19131700
C	4.53981900	0.68857300	4.20793700
H	5.35780400	0.99801800	3.54339300
H	3.88823400	1.56600500	4.31216700
C	5.11282500	0.31398900	5.57503500
H	4.29795300	-0.01196900	6.23715700
H	5.77203200	-0.55819100	5.46225300
C	5.88206100	1.45221600	6.24167500
H	6.72529500	1.77624600	5.62098000
H	5.23845900	2.32480500	6.40162100
H	6.28342300	1.15291700	7.21566900
C	5.98465900	-0.12650200	-1.87129300
C	6.68038300	0.32638600	-0.71281800
C	5.32233600	-1.34572500	-1.53755400
C	6.45029000	-0.61694200	0.33329600
C	5.62557200	-1.65564900	-0.18097500
C	1.93652800	2.45642600	-0.46719800
C	2.72625500	3.03000600	0.56889100
C	2.69160300	2.50394500	-1.67798200
C	3.97378400	3.42377200	0.00309900
C	3.94149800	3.12346900	-1.39056600
C	-0.27238700	-1.19217900	5.38864000
C	-0.07992900	0.09502500	4.80242300
C	-1.54643800	-1.68415900	4.97329300
C	-1.21597000	0.37683900	3.99306200
C	-2.12700100	-0.71648200	4.10263500
C	0.32800500	-3.19073800	0.38680800
C	0.61275300	-4.09339300	1.45007200
C	-1.06115600	-2.87082100	0.44410300
C	-0.60221900	-4.35202900	2.15198200
C	-1.64047000	-3.60390500	1.52174200
C	0.99675900	1.07943200	5.15361900
H	0.58727400	1.89024300	5.77076200
H	1.79769300	0.61117700	5.73043500
H	1.45678800	1.53686700	4.27388100
C	-1.50404300	1.68269500	3.30870400
H	-0.58767100	2.22144100	3.05404600
H	-2.08152600	1.55481400	2.38648400
H	-2.09506700	2.34324600	3.95819200
C	-3.53402300	-0.70736800	3.57690900
H	-3.59615800	-0.32935500	2.54989800
H	-3.98476700	-1.70201900	3.58815800
C	-2.23197200	-2.89156100	5.54365900

H	-1.53624400	-3.71128900	5.74856600
H	-2.72054700	-2.64684600	6.49653100
H	-3.01010600	-3.27802900	4.87994300
C	0.62539300	-1.84417700	6.40452000
H	0.52826000	-2.93528900	6.39924300
H	1.68176800	-1.60905700	6.23735800
H	0.38347300	-1.51284100	7.42322600
C	-0.78571300	-5.39183100	3.22176800
H	0.06126600	-5.43688300	3.91566900
H	-1.68519200	-5.21429400	3.81617900
H	-0.88353800	-6.39342900	2.78219600
C	-1.81367200	-2.04726300	-0.56409600
H	-2.71358000	-1.59205300	-0.13768000
H	-1.20194400	-1.23839800	-0.97732400
H	-2.14242400	-2.66006700	-1.41418000
C	1.27646400	-2.79738300	-0.70270700
H	1.01225400	-1.83334300	-1.15005600
H	2.30154400	-2.71788300	-0.33134400
H	1.27137300	-3.53736500	-1.51447600
C	1.93844300	-4.74661800	1.71747900
H	2.00984600	-5.12224900	2.74353500
H	2.09848300	-5.60844900	1.05582600
H	2.77409700	-4.05890200	1.55817700
C	5.28498200	-2.92072000	0.54973200
H	4.56912800	-3.52983900	-0.00907100
H	6.17882800	-3.54070300	0.70048700
H	4.85356100	-2.72635700	1.53754800
C	7.13813400	-0.62857300	1.66748400
H	8.09734300	-1.16359200	1.61440000
H	7.36147500	0.38105200	2.02700800
H	6.53452700	-1.12277700	2.43365400
C	7.65994600	1.46321000	-0.63845400
H	7.50926900	2.19067100	-1.44050100
H	7.59855900	2.00681500	0.31093200
H	8.69292900	1.09998200	-0.72663500
C	6.11022200	0.41031900	-3.26806000
H	6.56826300	1.40142200	-3.28549700
H	6.74269700	-0.24676100	-3.88079100
H	5.14612900	0.48573400	-3.78483900
C	4.61359200	-2.22280600	-2.53228100
H	3.96178500	-2.95620500	-2.05036400
H	3.99557000	-1.64752600	-3.23188100
H	5.33079600	-2.78718100	-3.14442900
C	4.92106700	3.62288300	-2.41101700
H	5.94914800	3.63333600	-2.03745900
H	4.90685500	3.02612400	-3.32624200
H	4.68099000	4.65564000	-2.70042300
C	5.05135700	4.19849900	0.70876900
H	5.14239500	3.91306000	1.76224300
H	6.03165800	4.05340000	0.24438000
H	4.84689400	5.27786700	0.68990800
C	2.25279200	3.32485800	1.95984700
H	1.63792900	4.23571200	1.98771400
H	1.65118500	2.50226100	2.35594800
H	3.08634000	3.47769500	2.65156000
C	0.49842200	2.04644400	-0.33673000
H	0.20655100	1.31451400	-1.09819100
H	0.29435700	1.60515700	0.64458200
H	-0.17493700	2.90724000	-0.45090700
C	2.18759000	2.13316700	-3.04506600
H	2.99536600	1.81020200	-3.71040700
H	1.45092100	1.32270200	-3.01035500
H	1.69370100	2.98253800	-3.53712000
C	-3.11228500	-3.76087900	1.76900800
H	-3.51718000	-4.58329100	1.16374200
H	-3.33873800	-3.99542500	2.81284800
H	-3.67647100	-2.86300700	1.50259700
H	-4.17372700	-0.05699900	4.18851300

TS₁₂-ⁿBu $H = -1863.013768$ au

Sm	3.81794200	0.27214100	0.39664000
Sm	0.03573700	-1.35246000	2.20487100
C	2.42465400	-0.99193500	2.68156700
H	1.89786500	-0.65707900	0.98196200
C	3.58541300	-0.49035700	2.88180900
C	4.55050400	-0.40892700	4.02657900
H	5.41931800	-1.03990300	3.79882200
H	4.10069100	-0.83573500	4.93458500
C	5.04618600	1.00696900	4.34164100
H	5.51507500	1.43792000	3.44573600
H	4.18513700	1.64625800	4.57273000
C	6.03836100	1.04606500	5.50383500
H	5.56766900	0.60692900	6.39403100
H	6.89772400	0.40337300	5.26853000
C	6.52782800	2.45534400	5.82901900
H	7.03654900	2.90723500	4.96976500
H	5.69374600	3.11207700	6.10075600
H	7.23330300	2.45184700	6.66619300
C	5.62208200	-0.58311900	-1.57953200
C	6.42508100	0.13225500	-0.64817200
C	5.20135400	-1.79833900	-0.95369800
C	6.47858100	-0.62485800	0.55908900
C	5.73861000	-1.82731900	0.36467600
C	1.71501700	2.06155600	0.12735900
C	2.61386100	2.68357700	1.03749600
C	2.32461800	2.05523300	-1.16255100
C	3.78395800	3.06003700	0.31243500
C	3.59206500	2.69317000	-1.05168700
C	-0.44432900	-1.31327300	4.94387300
C	-0.14333800	0.05307300	4.66868600
C	-1.72055500	-1.60784400	4.38093700
C	-1.20009200	0.58393400	3.88067200
C	-2.17125200	-0.44933900	3.68636500
C	0.25953000	-2.73770600	-0.18569700
C	0.71211700	-3.63504400	0.82174800
C	-1.14551100	-2.56026100	-0.02006400
C	-0.41760900	-4.03233600	1.59737900
C	-1.56934600	-3.38494100	1.06053800
C	0.97183300	0.81815800	5.31838900
H	0.83391000	0.84211600	6.40747700
H	1.95355300	0.37845800	5.12077100
H	1.00166500	1.85661100	4.98032000
C	-1.43272700	2.03205000	3.55031200
H	-0.50304400	2.60305900	3.48235400
H	-1.96714700	2.16369900	2.60352900
H	-2.04738800	2.51038600	4.32529500
C	-3.53182800	-0.23758600	3.08393100
H	-3.49700700	0.37955200	2.17869200
H	-4.01409100	-1.18158300	2.81642700
C	-2.54600300	-2.81146600	4.72877300
H	-1.95977700	-3.73459500	4.75649400
H	-2.98467800	-2.68819700	5.72863800
H	-3.37556900	-2.96100800	4.03526300
C	0.34282300	-2.20763200	5.85940100
H	0.23022600	-3.26553400	5.60017800
H	1.41133900	-1.97460000	5.82930200
H	0.01661100	-2.10062300	6.90367300
C	-0.40222500	-5.11706900	2.63784800
H	0.42098500	-5.00559900	3.35291900
H	-1.33133200	-5.14346400	3.21211500
H	-0.28385100	-6.10522800	2.17383000
C	-2.06091000	-1.81179400	-0.94826600
H	-2.93889800	-1.41276200	-0.42908600
H	-1.55873000	-0.97143600	-1.43949200
H	-2.43838100	-2.46265700	-1.74930100
C	1.06246500	-2.24143700	-1.34918300

H	0.70675000	-1.27404000	-1.71642700	H	4.84153100	0.12699300	4.49327000
H	2.11853800	-2.13197400	-1.09050700	C	4.53094100	2.07711900	5.36553100
H	1.00681500	-2.94349100	-2.19298800	H	5.04736600	2.64289600	4.58201200
C	2.09766300	-4.19368300	0.95263200	H	3.71688400	2.70549600	5.74380400
H	2.24962000	-4.66795900	1.92632100	H	5.23968100	1.92319700	6.18534400
H	2.29329100	-4.95872200	0.18828000	C	3.29189700	-0.07027800	-3.16177900
H	2.86189000	-3.41840800	0.85369400	C	4.03019200	0.69969400	-2.22088200
C	5.68937700	-2.98692600	1.32105000	C	2.90299300	-1.28708700	-2.52276700
H	5.36957500	-3.90020600	0.81176400	C	4.03407900	-0.00615900	-0.98562100
H	6.68245900	-3.18726700	1.73976400	C	3.37402500	-1.25515200	-1.18086800
H	5.00403300	-2.82927700	2.16178900	C	-0.53179500	2.82066600	-1.61714800
C	7.40419800	-0.32164700	1.70346100	C	0.38014200	3.29202400	-0.63603400
H	8.44665800	-0.53213600	1.42560200	C	0.15343600	2.77472400	-2.86544200
H	7.37247300	0.72936900	2.01151000	C	1.62363700	3.57308200	-1.28136700
H	7.18032500	-0.92857500	2.58377800	C	1.46710600	3.28708500	-2.66885300
C	7.29815600	1.32038700	-0.93073400	C	-2.26679300	-0.52516400	3.37927600
H	7.01959200	1.82522300	-1.85802800	C	-2.09193500	0.82718800	2.96137100
H	7.27829300	2.06579000	-0.12803000	C	-3.51607600	-0.98799800	2.88115200
H	8.34599400	1.00792300	-1.03935200	C	-3.19673900	1.17431700	2.13805900
C	5.46562000	-0.28884000	-3.04507800	C	-4.07131200	0.04257200	2.07082900
H	5.82635700	0.71066400	-3.29735800	C	-1.77399600	-2.50183500	-1.62448300
H	6.04502200	-0.99972800	-3.64959700	C	-1.23025100	-3.27257700	-0.56253800
H	4.42750000	-0.35915400	-3.39143200	C	-3.15983500	-2.30682500	-1.35728900
C	4.61134200	-2.95853500	-1.70648100	C	-2.28855400	-3.59388000	0.34251800
H	4.05446100	-3.64549800	-1.06573200	C	-3.48828900	-3.02339800	-0.17114300
H	3.93525100	-2.63464000	-2.50371200	C	-1.06636000	1.75502700	3.54537700
H	5.40784600	-3.54210000	-2.18957200	H	-1.04493200	1.65161200	4.63755500
C	4.42045100	3.15178700	-2.21464600	H	-0.05486000	1.55849500	3.17622500
H	5.46167000	3.33343300	-1.93871700	H	-1.30381100	2.79993600	3.33075900
H	4.41262500	2.43613600	-3.04114200	C	-3.62305000	2.55920700	1.73633700
H	4.02680700	4.09805000	-2.61134900	H	-2.78556200	3.25290800	1.63338200
C	4.91054500	3.89769000	0.85014000	H	-4.17431200	2.56985500	0.79082800
H	5.19284800	3.61777800	1.87105100	H	-4.29740100	2.98063600	2.49556800
H	5.80805200	3.81902500	0.23043000	C	-5.46353400	0.09844100	1.50602000
H	4.63547100	4.96068700	0.87957700	H	-5.49074100	0.44324200	0.46526400
C	2.31546400	3.03407700	2.46505900	H	-5.95488900	-0.87641100	1.53833800
H	1.59072500	3.85745900	2.52776700	C	-4.22796700	-2.19851300	3.40872600
H	1.90787200	2.18568400	3.02134600	H	-3.59649400	-3.09124300	3.43822100
H	3.21489100	3.36205500	2.99295500	H	-4.55702600	-2.01290600	4.44037500
C	0.30053200	1.66442300	0.43075400	H	-5.12104600	-2.44009600	2.83056400
H	-0.02096600	0.79885400	-0.16237100	C	-1.40675200	-1.23864700	4.38331100
H	0.18028500	1.43540700	1.49744800	H	-1.48024600	-2.32736900	4.29034600
H	-0.40712100	2.47776700	0.21660500	H	-0.35225700	-0.96856000	4.27566000
C	1.66196600	1.65809600	-2.45108300	H	-1.69936100	-0.98895700	5.41354400
H	2.36783400	1.22852000	-3.16989500	C	-2.16541700	-4.58547300	1.46620900
H	0.86662300	0.92304100	-2.29496400	H	-1.35631500	-4.34334200	2.16593900
H	1.19904500	2.52476900	-2.94311600	H	-3.08707000	-4.65746000	2.04771500
C	-3.00264000	-3.71228300	1.35836000	H	-1.95248100	-5.59042600	1.07828100
H	-3.41762500	-4.35063600	0.56633200	C	-4.14713400	-1.64575300	-2.27697100
H	-3.11406200	-4.25881300	2.29665300	H	-5.00629800	-1.24048600	-1.73259200
H	-3.64182400	-2.82488700	1.41114000	H	-3.69472300	-0.82223900	-2.83892200
H	-4.20339900	0.27579100	3.78610100	H	-4.54617400	-2.35379700	-3.01673700
				C	-1.08917800	-2.14702600	-2.90778400
				H	-1.51358900	-1.24711100	-3.36100600
				H	-0.02270100	-1.96861600	-2.76109900
				H	-1.18591100	-2.96405300	-3.63715800
				C	0.15769200	-3.83226100	-0.48583700
				H	0.44879700	-4.06506900	0.54312400
				H	0.24637200	-4.76392200	-1.06275500
				H	0.89633500	-3.13158600	-0.87697100
				C	3.41205400	-2.39656600	-0.20357300
				H	3.16364800	-3.34283200	-0.69098500
				H	4.42195700	-2.50949900	0.20897700
				H	2.72315300	-2.26750700	0.63820800
				C	4.83850200	0.38653000	0.22052900
				H	5.90277300	0.14474700	0.08638200
				H	4.78766500	1.46190900	0.42580400
				H	4.50208300	-0.13642500	1.11882800
				C	4.92949700	1.86325300	-2.51620400

2-Bu
H = -1863.027434 au

Sm	1.34598200	0.80135300	-1.28574900
Sm	-1.80001400	-0.85723700	0.62015100
C	0.72086200	-0.22272900	1.10439000
H	-0.79272800	0.06907500	-1.20814100
C	1.53644400	-0.30277200	2.03503800
C	2.47665200	-0.41727200	3.15103400
H	3.32066600	-1.05570000	2.85356200
H	1.97841500	-0.95447100	3.97052100
C	3.00988100	0.92477900	3.68003600
H	3.49078300	1.46897900	2.85793000
H	2.16538500	1.54242600	4.00819600
C	4.00108800	0.74906700	4.83018000
H	3.51796200	0.19118200	5.64394500

H	4.71306100	2.31932500	-3.48323400	C	-0.45503000	2.52554200	2.58661000
H	4.87973600	2.64914700	-1.75648300	H	-1.12076500	1.93328300	1.95322900
H	5.97453600	1.52519700	-2.54875100	H	-0.44257700	2.04715200	3.56695400
C	3.19251500	0.16688500	-4.64317300	H	-0.90802700	3.51913000	2.70750800
H	3.56063200	1.15749100	-4.91900900	C	2.45584100	-2.87124900	-1.22854100
H	3.79640400	-0.56343800	-5.19872900	H	3.12400900	-3.46036700	-1.87160200
H	2.16842800	0.08024000	-5.02584500	H	2.03904100	-3.55329000	-0.48582800
C	2.46347800	-2.50382300	-3.29513600	H	1.62769200	-2.53036600	-1.85672500
H	1.98519200	-3.26262700	-2.67267300	C	3.83930300	-2.82389300	1.69927700
H	1.76692900	-2.25531700	-4.10169100	H	4.85034800	-3.24414300	1.78666700
H	3.33342400	-2.98036400	-3.76953600	H	3.54378600	-2.48704800	2.69829600
C	2.36564100	3.73881900	-3.78173700	H	3.17427700	-3.64331400	1.42231700
H	3.36140200	4.00803400	-3.42642700	C	5.63767300	-0.31554400	1.86478600
H	2.48182000	2.99199400	-4.57238800	H	6.42732000	-1.07953300	1.85427900
H	1.94258600	4.63482200	-4.25599100	H	6.12838600	0.65493100	1.76820900
C	2.76867500	4.29682700	-0.62944900	H	5.17785000	-0.35723600	2.85902300
H	3.08139800	3.83533900	0.31484500	C	5.48556800	1.20573600	-0.97364700
H	3.64707500	4.33919300	-1.27740200	H	5.00975600	1.86728100	-1.70261200
H	2.49353200	5.33358600	-0.39386100	H	5.87635100	1.82821900	-0.16559600
C	0.05838100	3.62641100	0.78805600	H	6.35287200	0.75322500	-1.47429800
H	-0.34715000	4.64430300	0.87820900	C	3.37782100	-0.28714600	-2.76064000
H	-0.67937200	2.93868700	1.20252300	H	2.44455500	-0.74399300	-3.10327700
H	0.94153200	3.57602000	1.43239500	H	3.32400100	0.78567500	-2.97831400
C	-2.00484000	2.61900200	-1.43944100	H	4.17862100	-0.69437600	-3.39373500
H	-2.40463600	1.89512300	-2.15464300	C	-0.75510700	-0.75531900	3.61675100
H	-2.24749600	2.26343100	-0.43567700	C	-1.20478800	-0.71888500	4.76710000
H	-2.54699500	3.56436100	-1.58442900	Sm	-2.41990500	-1.38615000	1.70052700
C	-0.46649700	2.43930400	-4.19224800	C	-4.02910600	0.83520000	2.45425500
H	0.28066900	2.10891500	-4.92083700	C	-3.90133300	0.94665900	1.04329000
H	-1.21428600	1.64404700	-4.10392300	C	-4.79724500	-0.33570600	2.73419000
H	-0.97628400	3.30832500	-4.63104900	C	-4.59171700	-0.15437100	0.44979000
C	-4.89034300	-3.36796200	0.23443200	C	-5.18605500	-0.91738200	1.49373100
H	-5.31052900	-4.09690000	-0.47200900	C	-1.01437000	-3.73641000	1.76495500
H	-4.93693700	-3.82291800	1.22499500	C	-1.96005800	-3.90704300	2.81366500
H	-5.56204200	-2.50494100	0.22919500	C	-1.71873500	-3.77111600	0.52761500
H	-6.09273100	0.79219200	2.08048200	C	-3.24921200	-4.05700200	2.22738900
				C	-3.10015800	-3.97406300	0.81111700
				C	-4.46337600	-4.51591600	2.98264400
				H	-4.69926500	-3.88200600	3.84472900
				H	-5.35130500	-4.55144300	2.34824900
				H	-4.30976300	-5.53064900	3.37362500
				C	-4.13646700	-4.30951500	-0.22397300
				H	-3.90045900	-5.26459100	-0.71135200
				H	-5.13010700	-4.41347400	0.21653900
				H	-4.20924800	-3.55981000	-1.02019000
				C	-1.10750700	-3.78654900	-0.84255100
				H	-1.86371700	-3.63410700	-1.61870500
				H	-0.35305900	-3.00671800	-0.96326500
				H	-0.62368400	-4.75132500	-1.04956200
				C	0.47089600	-3.65904000	1.92610200
				H	0.75451000	-3.46951000	2.96408900
				H	0.94980900	-4.60043400	1.62171500
				H	0.90808800	-2.85626500	1.32496900
				C	-1.65199700	-4.11059500	4.26779400
				H	-1.46336700	-5.17120700	4.48499700
				H	-0.77122100	-3.54569800	4.58287800
				H	-2.48605200	-3.80000300	4.90589100
				C	-6.28083600	-1.92640300	1.31440700
				H	-6.18694000	-2.48670600	0.38142300
				H	-6.32827100	-2.64493900	2.13544200
				H	-7.25391500	-1.41662400	1.28152100
				C	-5.31507200	-0.71182000	4.09346100
				H	-6.19585100	-0.11234700	4.36499000
				H	-5.62004100	-1.76118900	4.14248900
				H	-4.56907200	-0.54803400	4.87796100
				C	-3.64750900	1.85268100	3.49099300
				H	-2.90339600	1.48181100	4.20378000
				H	-3.23416800	2.75469800	3.03536200
				H	-4.52936900	2.15868100	4.06827500

TS₂₃-ⁿBu
H = -2097.391879 au

Sm	2.07063300	0.48715100	0.75539900
C	-0.41630000	0.07831700	-1.07561800
C	-0.55617700	-0.33948700	0.08696500
C	3.63655600	-0.57046800	-1.30768400
C	4.55941800	0.13327200	-0.48124600
C	3.20338000	-1.73224000	-0.60147200
C	4.65133800	-0.56146600	0.75901000
C	3.82121700	-1.71989700	0.68013700
C	0.91817200	2.64066800	2.00674100
C	2.14568400	2.44797300	2.70291300
C	1.22108900	3.10719800	0.69817300
C	3.20826400	2.82528900	1.83148600
C	2.63731900	3.22341000	0.58548000
C	0.22424000	3.58935900	-0.31475600
H	-0.07142100	4.62827100	-0.11136500
H	0.63068600	3.57220400	-1.33145400
H	-0.68786500	2.98751800	-0.30738900
C	3.34691300	3.92590500	-0.53714300
H	4.42919000	3.79565400	-0.48216600
H	3.02591100	3.58350800	-1.52778200
H	3.15049900	5.00594100	-0.50020600
C	4.62502300	3.05288400	2.27015500
H	4.94799300	2.33138400	3.02554800
H	5.33556300	3.00532800	1.44142000
H	4.72812700	4.05008000	2.71994900
C	2.29730700	2.07333300	4.14975600
H	2.33238400	2.96542900	4.79009400
H	1.46927700	1.44895400	4.49526200
H	3.22071200	1.51397200	4.33150600

C	-3.37594800	2.11305700	0.25921600
H	-2.87016800	2.84158900	0.89614000
H	-2.66467000	1.80582600	-0.51453800
H	-4.19768700	2.63948200	-0.24475700
C	-4.84553700	-0.30971600	-1.02270900
H	-3.97208400	-0.02865800	-1.62100900
H	-5.11123500	-1.33709500	-1.28930600
H	-5.67563800	0.32971000	-1.35545900
C	-1.68961800	-0.69633000	6.14551400
C	-0.55885700	-0.86892600	7.17655100
H	-2.42687700	-1.49901800	6.28507700
H	-2.21996600	0.24590200	6.34177400
C	-1.07315200	-0.85032000	8.61572400
H	-0.03651700	-1.81265900	6.97782500
H	0.18039200	-0.07107500	7.03404700
C	0.04007900	-1.02461700	9.64594900
H	-1.60134100	0.09497800	8.80062700
H	-1.82025700	-1.64546100	8.74402800
H	-0.35505000	-1.00990800	10.66665400
H	0.56395700	-1.97665200	9.50588100
C	0.78381700	-0.22402500	9.56585000
H	-0.36267700	0.55550000	-2.46335800
C	-0.87193400	-0.47148500	-3.48891600
H	0.66547000	0.83955200	-2.72621400
H	-0.95436800	1.47771500	-2.54777000
C	-0.83851100	0.06423400	-4.92009200
H	-0.26755500	-1.38410000	-3.41626400
H	-1.89608200	-0.76206600	-3.22398000
C	-1.35122600	-0.94427200	-5.94534200
H	-1.43775900	0.98321700	-4.97705600
H	0.18947000	0.35666000	-5.17460800
H	-1.31526800	-0.53500400	-6.95988500
H	-0.75083600	-1.86071700	-5.93519800
H	-2.38912500	-1.22764500	-5.73810000
H	1.37994500	-0.53851100	2.60143600
H	0.42787400	-0.62684900	2.93965200

3-"Bu $H = -2097.405543$ au

Sm	2.38689000	1.07064400	-0.38600000
C	-0.19931100	0.46816200	-2.32140800
C	0.06230200	0.20537400	-1.13373700
C	4.02623200	0.10917000	-2.37418800
C	4.92556800	0.77610400	-1.48986200
C	3.56674000	-1.07850300	-1.72959200
C	4.97080400	0.03626300	-0.27353800
C	4.14143800	-1.11737000	-0.42776900
C	1.06909000	3.17370300	0.75488800
C	2.22369400	2.99149100	1.57336800
C	1.50429300	3.65437400	-0.51108000
C	3.36841700	3.38831000	0.82245600
C	2.92514200	3.79024500	-0.47305200
C	0.62519700	4.11305000	-1.63813500
H	0.33132800	5.16293400	-1.50434700
H	1.13258900	4.04970000	-2.60678900
H	-0.29412100	3.52643100	-1.70285200
C	3.73282500	4.52048700	-1.50778900
H	4.80592300	4.40157100	-1.34981300
H	3.51128300	4.19567500	-2.53086900
H	3.51824600	5.59671100	-1.46812300
C	4.73422000	3.60708200	1.40354700
H	4.99023100	2.85927000	2.15961200
H	5.52031800	3.59418900	0.64442100
H	4.78558900	4.58691400	1.89752000
C	2.21053100	2.64522000	3.03577700
H	2.16938800	3.55427400	3.65067600
H	1.33945400	2.03871400	3.29756700
H	3.10575700	2.09504500	3.34534700

C	-0.35073100	3.04102500	1.20521700
H	-1.01720600	2.87272400	0.35855600
H	-0.50521400	2.20877200	1.89764600
H	-0.68175000	3.95980800	1.70868800
C	2.81678100	-2.18021400	-2.41633500
H	3.48593600	-2.74013700	-3.08350000
H	2.39273200	-2.89581000	-1.70965500
H	1.99286400	-1.80187500	-3.02892800
C	4.12772600	-2.27466700	0.53089700
H	5.05137000	-2.86063500	0.43110400
H	4.07226200	-1.95666200	1.57753800
H	3.29360500	-2.95355500	0.35010000
C	5.92499200	0.24744300	0.86739100
H	6.78903000	-0.42547400	0.78133700
H	6.31343000	1.26757800	0.89389400
H	5.46705000	0.04409500	1.84200200
C	5.88058700	1.85771800	-1.89938200
H	5.45115700	2.54246600	-2.63479000
H	6.23090000	2.45381200	-1.05336100
H	6.77119200	1.41134200	-2.36242500
C	3.77511400	0.47074700	-3.81153500
H	2.79480900	0.12426400	-4.15386900
H	3.82437400	1.55117300	-3.98420900
H	4.52124100	0.01081700	-4.47388200
C	-1.33462900	-0.21136100	2.43445600
C	-1.02472000	0.05843500	3.60049500
Sm	-2.27295300	-0.86231000	0.24297200
C	-3.95036900	1.35829400	0.84064400
C	-3.72424800	1.45866900	-0.55954700
C	-4.72538700	0.18454200	1.07578800
C	-4.35995600	0.34646100	-1.19084500
C	-5.01634700	-0.41527900	-0.18256600
C	-0.82969700	-3.20483300	0.46940900
C	-1.82398400	-3.34259300	1.47466600
C	-1.46695400	-3.29849000	-0.80115000
C	-3.08053600	-3.51879400	0.82784100
C	-2.85866900	-3.50150000	-0.58175300
C	-4.33456800	-3.93106000	1.54370000
H	-4.58719100	-3.26065000	2.37201000
H	-5.19697900	-3.97094700	0.87466600
H	-4.21912600	-4.93458500	1.97514200
C	-3.84242000	-3.88773900	-1.64974900
H	-3.60843200	-4.88300300	-2.05110300
H	-4.86237300	-3.93178100	-1.26289900
H	-3.84860200	-3.19909600	-2.50312800
C	-0.77506900	-3.37349900	-2.13023600
H	-1.48561200	-3.28122100	-2.95715900
H	-0.02556600	-2.58708600	-2.25119400
H	-0.26098200	-4.33679600	-2.25785300
C	0.64697500	-3.12255300	0.69650500
H	0.87793500	-2.84944100	1.72934000
H	1.13563400	-4.08739400	0.49617200
H	1.11284100	-2.37699500	0.04423200
C	-1.59153100	-3.49235200	2.94836800
H	-1.46624300	-4.55079900	3.21830000
H	-0.70167200	-2.95114000	3.27617600
H	-2.42946800	-3.10212200	3.53316500
C	-6.08634100	-1.43466800	-0.43828500
H	-5.91394600	-1.99922500	-1.35750000
H	-6.19168700	-2.15010000	0.38028600
H	-7.05903100	-0.93528000	-0.55088600
C	-5.29958500	-0.19375200	2.41086300
H	-6.09953300	0.49867500	2.70928400
H	-5.73510300	-1.19661500	2.39767600
H	-4.54201400	-0.16894900	3.20160400
C	-3.64469400	2.37362100	1.90215900
H	-2.99584900	1.96681400	2.68436500
H	-3.15247800	3.25752300	1.49031600
H	-4.57177200	2.71442900	2.38197900

C	-3.13935000	2.62592800	-1.30279000
H	-2.93844700	3.46512400	-0.63174900
H	-2.19896200	2.38704500	-1.81271100
H	-3.83768300	2.98998600	-2.06703800
C	-4.53239200	0.17569400	-2.67412300
H	-3.67604300	0.56535600	-3.23471800
H	-4.66134300	-0.87360600	-2.96035400
H	-5.41913900	0.71299600	-3.04119400
C	-0.69816300	0.35486200	4.99743000
C	0.11435100	-0.74445600	5.70131200
H	-1.63044200	0.52131100	5.55702500
H	-0.14713600	1.30504200	5.06420500
C	0.43362500	-0.40916100	7.15780600
H	-0.44533700	-1.68647900	5.65001900
H	1.04664400	-0.91250400	5.14623700
C	1.23374600	-1.50194800	7.86290100
H	0.98921900	0.53808900	7.19950200
H	-0.50409800	-0.23229200	7.70239600
H	1.44907000	-1.23528900	8.90282900
H	0.68639800	-2.45121600	7.86992000
H	2.19155000	-1.67931900	7.36048700
C	-0.50909000	0.79621100	-3.71749900
C	-0.84023400	-0.40965300	-4.61129300
H	0.34613300	1.33745300	-4.14639400
H	-1.34610300	1.50773500	-3.74340700
C	-1.14425600	0.00014000	-6.05214200
H	-0.00217000	-1.11698200	-4.59335200
H	-1.69971800	-0.94301200	-4.18828900
C	-1.48508900	-1.18792900	-6.94868900
H	-1.97776400	0.71557500	-6.05749000
H	-0.28067000	0.53818300	-6.46701100
H	-1.69507400	-0.86674600	-7.97373900
H	-0.65824500	-1.90572500	-6.98772600
H	-2.36813100	-1.72153500	-6.58037800
H	2.08420300	-0.28557400	1.79101300
H	1.34638000	-0.12567700	1.83384600

TS₃₄-ⁿBu*H* = -2097.400502 au

Sm	2.11294000	0.93019800	-0.03754000
C	-0.34640200	0.45884500	-2.58270700
C	0.00047500	0.25002500	-1.40910300
C	3.86796600	0.07188100	-2.00702200
C	4.73288500	0.66743100	-1.04614400
C	3.39318200	-1.16506800	-1.46862300
C	4.71241000	-0.14378300	0.12294100
C	3.91138100	-1.29633600	-0.15315800
C	0.90233200	3.23757700	0.83129400
C	2.01521200	3.09317800	1.70679300
C	1.39999400	3.54655600	-0.46353700
C	3.20212000	3.35603600	0.96216000
C	2.82235600	3.63501000	-0.38270500
C	0.58413800	3.95422500	-1.65448000
H	0.41760600	5.04084000	-1.66187900
H	1.07890100	3.70248500	-2.59817500
H	-0.39503700	3.47273800	-1.65655400
C	3.66769700	4.26638300	-1.45157200
H	4.72796700	4.26384100	-1.19511700
H	3.56171400	3.78322500	-2.42939600
H	3.37221300	5.31515800	-1.58849400
C	4.54428700	3.58972300	1.59185500
H	4.81315100	2.81487500	2.31692100
H	5.34782100	3.64660200	0.85496500
H	4.54659100	4.54301200	2.13766800
C	1.94906800	2.92718200	3.19799600
H	1.83928300	3.89932500	3.69773200
H	1.09943400	2.30819100	3.49792000
H	2.85616600	2.46469600	3.60008500

C	-0.53308500	3.25303900	1.23848700
H	-1.16054100	2.69521100	0.54195500
H	-0.67608900	2.80072200	2.21956900
H	-0.91217300	4.28412400	1.27987200
C	2.72533200	-2.21858300	-2.29856600
H	3.45493700	-2.68800100	-2.97286000
H	2.28358400	-3.01321100	-1.69545200
H	1.93100500	-1.80080600	-2.927334800
C	3.90049200	-2.52218000	0.71607400
H	4.92736800	-2.87072800	0.88550500
H	3.45527300	-2.36049300	1.70444600
H	3.35559000	-3.34315200	0.24798700
C	5.63595000	-0.01614400	1.30148200
H	6.55554300	-0.59761100	1.14330200
H	5.93987300	1.01850300	1.47774600
H	5.18799600	-0.39146500	2.22827000
C	5.77223200	1.70217000	-1.35351200
H	5.47751900	2.36479500	-2.16868900
H	6.02999600	2.31968800	-0.49109100
H	6.69704700	1.20020100	-1.67040900
C	3.68697800	0.51023100	-3.43299700
H	2.68432200	0.27503200	-3.80407000
H	3.83960200	1.58694400	-3.55550400
H	4.40053200	0.00750100	-4.10070300
C	-0.57108600	-0.05850800	1.95526900
C	-0.47890400	0.02510100	3.18893100
Sm	-2.12845600	-0.76517400	0.08586300
C	-3.86231200	1.37974900	0.84251200
C	-3.67130500	1.57301500	-0.55254200
C	-4.60340600	0.17131500	1.02090100
C	-4.28921100	0.48116900	-1.23525300
C	-4.91055700	-0.35320400	-0.26623800
C	-0.81641200	-3.14316100	0.43171200
C	-1.86500300	-3.22272800	1.38894800
C	-1.39345300	-3.25768500	-0.86462900
C	-3.09026700	-3.40611700	0.68746800
C	-2.80021600	-3.42091900	-0.70777200
C	-4.36819000	-3.83301600	1.34974000
H	-4.67426800	-3.16505000	2.16091500
H	-5.19846300	-3.89781000	0.64377500
H	-4.24800200	-4.83086600	1.79286400
C	-3.73684600	-3.80631000	-1.81909800
H	-3.42055200	-4.74983900	-2.28262200
H	-4.75431200	-3.95852400	-1.45292700
H	-3.79053600	-3.06305200	-2.62414800
C	-0.65267500	-3.39519700	-2.16290100
H	-1.34600000	-3.52951300	-2.99827200
H	-0.03177800	-2.52546600	-2.38981100
H	0.00764500	-4.27271000	-2.14908400
C	0.64488700	-3.10102500	0.74011500
H	0.82487000	-2.80661100	1.77682000
H	1.11168800	-4.08513000	0.58960400
H	1.17613400	-2.38936600	0.10133200
C	-1.70677300	-3.32205800	2.87763700
H	-1.54331400	-4.36332100	3.18951400
H	-0.86065900	-2.72922000	3.23351600
H	-2.59818700	-2.96769400	3.40586100
C	-5.96779400	-1.36801300	-0.58160500
H	-5.72349700	-1.97836600	-1.45417900
H	-6.16186900	-2.04255200	0.25381000
H	-6.91515500	-0.85815100	-0.80644000
C	-5.16105000	-0.28003500	2.34139300
H	-5.84872700	0.47055900	2.75504600
H	-5.72638800	-1.20988500	2.24484200
H	-4.38437000	-0.44228600	3.09861600
C	-3.59871400	2.34394900	1.96295600
H	-2.87449700	1.96426600	2.69173300
H	-3.22447400	3.30146900	1.59568100
H	-4.52936200	2.55069100	2.50750700

C	-3.17768700	2.80681200	-1.25150000	C	-0.03401300	3.37843400	0.95192300
H	-2.82019300	3.56173400	-0.54829500	H	0.23839500	3.18329500	1.99038400
H	-2.36128000	2.59982900	-1.95213400	H	-0.48045100	4.38196300	0.90920100
H	-3.98784400	3.26732800	-1.83242300	H	-0.80857700	2.65793300	0.68081800
C	-4.50899200	0.40472800	-2.71946400	C	2.33132200	-2.77459600	-2.46991700
H	-3.67436200	0.83457000	-3.28185800	H	2.94656900	-3.35986300	-3.16685300
H	-4.64674600	-0.62435600	-3.06765200	H	2.05070300	-3.43978900	-1.65246300
H	-5.40961100	0.96042700	-3.01924600	H	1.41316000	-2.50934200	-3.00416400
C	-0.42707800	0.10091600	4.65227700	C	3.89935700	-2.36727400	0.37452000
C	0.81376100	-0.55027500	5.28525400	H	4.95544600	-2.62369100	0.53070400
H	-1.32660700	-0.38644300	5.05519600	H	3.52165100	-1.97667800	1.32558000
H	-0.48819100	1.14920300	4.97936100	H	3.37236300	-3.30040100	0.17002800
C	0.79684800	-0.49127900	6.81245800	C	5.62442400	0.15923300	0.14871000
H	0.88012100	-1.59428600	4.95380900	H	6.33987100	-0.65771400	0.31462300
H	1.71523300	-0.04908600	4.91019600	H	6.20422100	1.02878600	-0.16820100
C	2.03102400	-1.12599800	7.44894000	H	5.18832500	0.39198600	1.12789800
H	0.71493000	0.55608700	7.13390800	C	5.37586000	1.23759800	-2.89201000
H	-0.10710800	-0.99331400	7.18340700	H	4.85580700	1.94099400	-3.54729600
H	1.99082400	-1.07167600	8.54157400	H	5.98146500	1.81595300	-2.19361000
H	2.12103600	-2.18240200	7.17219900	H	6.07154000	0.67080700	-3.52635200
H	2.94851900	-0.62134800	7.12553900	C	3.17977000	-0.42606400	-4.33712500
C	-0.70492700	0.73345900	-3.97596000	H	2.23446700	-0.91562900	-4.58937400
C	-1.08034400	-0.50682900	-4.80241300	H	3.13039700	0.60636800	-4.70146300
H	0.14727700	1.23980000	-4.45136400	H	3.96092700	-0.92730800	-4.92682900
H	-1.53036100	1.45807700	-4.00833200	C	0.88521900	0.19224000	1.38238800
C	-1.42805900	-0.16247100	-6.25040700	C	0.46771000	0.16096800	2.55172600
H	-0.24852500	-1.22110300	-4.77797300	Sm	-1.92659200	-0.74074900	0.88806600
H	-1.93127100	-1.01044300	-4.32738200	C	-3.31159600	1.58384500	1.83607200
C	-1.80899800	-1.38796400	-7.07768600	C	-3.56282300	1.55406600	0.43761000
H	-2.25470400	0.56086300	-6.26311200	C	-3.95778100	0.45156900	2.42232300
H	-0.57354800	0.34583400	-6.71789800	C	-4.36306700	0.40469500	0.15891300
H	-2.05020500	-1.11405100	-8.10961700	C	-4.65681700	-0.24000200	1.39272800
H	-0.99017400	-2.11527000	-7.10921800	C	-0.68282600	-3.18268600	0.94058800
H	-2.68395400	-1.89445800	-6.65539900	C	-1.40454800	-3.17091400	2.16586400
H	2.81957200	-0.04304800	2.23326400	C	-1.62117200	-3.28102200	-0.12334600
H	2.08192200	-0.01505000	2.39590000	C	-2.79095100	-3.30523100	1.86381100
4-"Bu				C	-2.92600500	-3.36364500	0.44734700
<i>H</i> = -2096.248857 au				C	-3.82740200	-3.65881500	2.89063200
Sm	2.00635800	0.84475900	-0.86243100	H	-3.88495300	-2.93972300	3.71530600
C	-0.54478600	0.26153000	-2.50041700	H	-4.82536300	-3.74231300	2.45729900
C	-0.77223700	-0.02621900	-1.31429100	H	-3.59068200	-4.63179500	3.34191900
C	3.47907700	-0.50348100	-2.86692100	C	-4.15660900	-3.72770600	-0.33541400
C	4.44957800	0.28816300	-2.19303100	H	-4.00084100	-4.66970400	-0.87632100
C	3.08796600	-1.56719900	-1.99831600	H	-5.02190700	-3.87485400	0.31475000
C	4.59735800	-0.23112400	-0.87638500	H	-4.43301900	-2.97705200	-1.08486300
C	3.77356200	-1.39464500	-0.76406700	C	-1.30559500	-3.50044400	-1.57353000
C	1.15385600	3.29060600	0.05300700	H	-2.14631100	-3.22198600	-2.21595600
C	2.51318400	3.22263500	0.46737600	H	-0.44431100	-2.91416100	-1.89615400
C	1.12955100	3.42930500	-1.36130700	H	-1.08332900	-4.55872700	-1.77206500
C	3.33358500	3.36851700	-0.68882000	C	0.80145300	-3.22975300	0.80317300
C	2.47766800	3.47614800	-1.82331500	H	1.29996500	-2.99144300	1.74416900
C	-0.07955800	3.73526800	-2.19527400	H	1.13505400	-4.23122200	0.49634100
H	-0.40114600	4.77610300	-2.04861500	H	1.16558700	-2.51445600	0.06257300
H	0.12694500	3.61575500	-3.26312100	C	-0.81719200	-3.26706000	3.54492300
H	-0.92889700	3.09594300	-1.94555800	H	-0.68377000	-4.31610400	3.84441500
C	2.87512800	3.84615300	-3.22551500	H	0.16523800	-2.79044800	3.60830100
H	3.96001900	3.90317500	-3.33749700	H	-1.46151500	-2.80667800	4.30195200
H	2.50812700	3.14233600	-3.98289800	C	-5.77745700	-1.21292100	1.60513600
H	2.47460200	4.83198500	-3.49453100	H	-5.84861100	-1.96377600	0.81566600
C	4.79427000	3.70954100	-0.62955500	H	-5.69884500	-1.73444900	2.56014000
H	5.37892200	3.00520600	-0.03086000	H	-6.73334300	-0.67109500	1.61604900
H	5.24892800	3.75991900	-1.62035300	C	-4.09960400	0.23562000	3.90328800
H	4.92508500	4.69785000	-0.16851500	H	-4.86140600	0.90303500	4.33120900
C	3.00983100	3.20981900	1.88496600	H	-4.40302300	-0.78667400	4.14546600
H	3.08115400	4.22779400	2.29272100	H	-3.16906300	0.43878500	4.44499200
H	2.34679200	2.63824000	2.54061000	C	-2.75336700	2.71943800	2.64694600
H	4.00822100	2.76704900	1.96242100	H	-3.49326500	3.05148400	3.38654200
				H	-1.84469400	2.46235300	3.20197100
				H	-2.51575300	3.58191700	2.02236600

C	-3.32238800	2.63794400	-0.57014800	H	-0.11533700	4.32660100	2.01442000
H	-2.63179800	3.40151900	-0.20882100	H	-0.43658100	2.59185700	1.83344200
H	-2.91879500	2.24180900	-1.50706500	C	2.62550200	-2.97897900	-0.85813900
H	-4.26626500	3.14433200	-0.81514100	H	3.22350000	-3.70740900	-1.42252000
C	-4.99023500	0.11015200	-1.17443500	H	2.23907700	-3.49446600	0.02248700
H	-4.27353500	0.20442900	-1.99777600	H	1.76392700	-2.72081700	-1.48277400
H	-5.40882900	-0.89929400	-1.21449100	C	3.99407300	-2.31842800	2.02359300
H	-5.81407700	0.80548500	-1.38885600	H	5.01096200	-2.54781000	2.36624700
C	0.17015400	0.20993300	3.99086000	H	3.47806100	-1.82702800	2.85658300
C	1.40570200	-0.07097300	4.86455200	H	3.49339100	-3.27292700	1.85140100
H	-0.61690300	-0.50985800	4.25416300	C	5.89095700	0.09244600	1.65288700
H	-0.23003500	1.20072100	4.24815900	H	6.69124900	-0.64201500	1.82160300
C	1.10057300	0.01069500	6.35986700	H	6.37624200	1.03030100	1.37133600
H	1.80101900	-1.06365300	4.61599500	H	5.40685100	0.25144400	2.62346900
H	2.19328100	0.64660800	4.60321600	C	5.91478100	0.84528800	-1.48820400
C	2.32384800	-0.26137600	7.23219600	H	5.46180500	1.51203400	-2.22912400
H	0.69672400	1.00516800	6.59420000	H	6.49827200	1.45864700	-0.79976200
H	0.30565200	-0.70577700	6.60836300	H	6.62634600	0.21013300	-2.03426200
H	2.07826300	-0.19323500	8.29675800	C	3.82631100	-0.93161000	-2.93447100
H	2.72781100	-1.26304600	7.04784900	H	2.97190200	-1.54659200	-3.22616300
H	3.12374500	0.45928700	7.02886000	H	3.70289100	0.04878300	-3.40793600
C	-0.45126400	0.56771200	-3.93372400	H	4.71786500	-1.38851500	-3.38728100
C	-1.00412500	-0.55238600	-4.83130100	C	0.84138700	0.03884400	2.23607100
H	0.58961900	0.77162800	-4.21868700	C	0.53097200	-0.03629000	3.44596400
H	-1.00098900	1.49734400	-4.13430500	Sm	-1.91027600	-0.98253900	2.58977300
C	-0.92614900	-0.20590700	-6.31788900	C	-3.13321400	1.42434400	3.43724700
H	-0.45114000	-1.47906900	-4.63379500	C	-3.40956400	1.35263900	2.04318100
H	-2.04492300	-0.75225700	-4.54788200	C	-3.85676600	0.37344900	4.08216400
C	-1.47665100	-1.31121300	-7.21601300	C	-4.29162700	0.25281600	1.82510900
H	-1.47724600	0.72639700	-6.50251200	C	-4.60659700	-0.32002600	3.09036300
H	0.11842100	0.00117700	-6.58799100	C	-0.62712400	-3.42808800	2.62591700
H	-1.40834700	-1.03772700	-8.27372300	C	-1.38283700	-3.42297800	3.83120300
H	-0.92324600	-2.24682500	-7.07840100	C	-1.53667700	-3.49833300	1.53389400
H	-2.52973400	-1.51555800	-6.99287800	C	-2.76286300	-3.52728000	3.48751700
				C	-2.85886000	-3.56629200	2.06608600
				C	-3.84461600	-3.84850000	4.47711400
				H	-3.86408200	-3.16248200	5.33173000
				H	-4.83610300	-3.83536600	4.02168700
				H	-3.69411700	-4.85578300	4.88906900
				C	-4.08420400	-3.87593200	1.25398300
				H	-4.06645400	-4.91724500	0.90577300
				H	-5.00263800	-3.74897800	1.83149600
				H	-4.16898300	-3.24781300	0.36047200
				C	-1.16740800	-3.67663200	0.08987100
				H	-1.98701800	-3.38747400	-0.57559700
				H	-0.29683800	-3.07650100	-0.18420300
				H	-0.93290600	-4.72728700	-0.13166900
				C	0.86083700	-3.48357200	2.50994700
				H	1.35223300	-3.26051800	3.46007900
				H	1.19399500	-4.48301100	2.19760300
				H	1.23362100	-2.76079200	1.78119600
				C	-0.84518100	-3.52825400	5.23056800
				H	-0.84495900	-4.57119400	5.57658900
				H	0.18646500	-3.17197700	5.30405100
				H	-1.44407600	-2.96221500	5.95373700
				C	-5.76332800	-1.23604400	3.35891700
				H	-5.90710800	-1.98211800	2.57322900
				H	-5.66673400	-1.76422600	4.30956900
				H	-6.69274900	-0.65221200	3.41260800
				C	-3.98882400	0.20525400	5.57055100
				H	-4.75172800	0.87999300	5.98344900
				H	-4.28357500	-0.81157500	5.84778600
				H	-3.05628900	0.43152000	6.09939800
				C	-2.45271000	2.54415500	4.17141100
				H	-3.19395900	3.25665600	4.55891200
				H	-1.88279600	2.19092900	5.03764200
				H	-1.76649500	3.10473400	3.53613100
				C	-3.06837700	2.36069800	0.98441900
				H	-2.46411100	3.17806500	1.38164500

TS₄₅-ⁿBu*H* = -2096.221854 au

Sm	2.38411700	0.73801900	0.28526500
C	-0.02738300	0.02182000	-0.52233100
C	-0.44883900	-0.26790500	0.65007200
C	3.97302200	-0.84901500	-1.44130700
C	4.91206000	-0.01248800	-0.77421400
C	3.45320000	-1.77993000	-0.49421200
C	4.93351000	-0.38616200	0.59806800
C	4.04559200	-1.49188800	0.76850700
C	1.49443800	3.21958400	1.11777800
C	2.87125800	3.20304300	1.47947100
C	1.41024800	3.26875500	-0.30110000
C	3.64088000	3.28254300	0.28391900
C	2.73892500	3.29612400	-0.81992600
C	0.15866800	3.49235600	-1.09741900
H	-0.05862500	4.56554500	-1.19481700
H	0.23839500	3.09263900	-2.11354100
H	-0.71009100	3.02778800	-0.62533100
C	3.09821800	3.54249500	-2.25832800
H	4.11668400	3.21968800	-2.49113400
H	2.42575900	3.02391100	-2.95049500
H	3.03781300	4.61149800	-2.50499100
C	5.09776700	3.63630400	0.23853700
H	5.69765200	3.07144900	0.95837500
H	5.53058900	3.48236600	-0.75102100
H	5.23114900	4.69879900	0.48525500
C	3.42524900	3.28090400	2.87444300
H	3.55294500	4.32314300	3.19848800
H	2.76758900	2.79812400	3.60431500
H	4.40737500	2.80315500	2.95281000
C	0.33875700	3.32672200	2.06042400
H	0.65117900	3.15706200	3.09362500

H	-2.51738500	1.92129000	0.14632200	C	2.67326300	-2.58752600	-0.70975200
H	-3.98331500	2.80733700	0.57359800	H	3.14132200	-3.37890800	-1.31055900
C	-4.95483300	-0.06422800	0.51409600	H	2.40136400	-3.03546400	0.24848300
H	-4.26944200	0.05017500	-0.33274300	H	1.74447800	-2.30225700	-1.21405700
H	-5.34590700	-1.08548500	0.48650800	C	4.43545000	-1.94117900	1.88880200
H	-5.80400100	0.60772500	0.32506400	H	5.11158700	-2.80076800	1.78423400
C	0.44692500	-0.00549200	4.91375700	H	4.80718400	-1.35105800	2.73230700
C	1.76673900	-0.37020700	5.61776900	H	3.45677800	-2.33713400	2.17319400
H	-0.33766600	-0.68659300	5.28776900	C	6.40447900	0.41445500	1.16592800
H	0.13669600	1.00004000	5.22927500	H	7.26363300	-0.26879000	1.11862600
C	1.65434500	-0.32657700	7.14125300	H	6.76597100	1.39957300	0.85905300
H	2.08227600	-1.36914900	5.29272300	H	6.12039900	0.48638100	2.22166100
H	2.54512500	0.32400700	5.27780300	C	5.93643800	1.14438100	-1.92229500
C	2.96476900	-0.67448900	7.84360100	H	5.37669600	1.74992300	-2.64228300
H	1.32475700	0.67409000	7.45258800	H	6.56148900	1.81891800	-1.33372000
H	0.86755700	-1.02064800	7.46703300	H	6.61519000	0.50958000	-2.50858800
H	2.85565200	-0.63748500	8.93204800	C	3.55383700	-0.58695500	-3.00004400
H	3.30208300	-1.68234700	7.57745100	H	2.58913100	-1.09089000	-3.10485500
H	3.76154900	0.02425000	7.56562600	H	3.45799600	0.40638000	-3.45180200
C	-0.66724200	0.06098900	-1.88163000	H	4.27403900	-1.14515000	-3.61471100
C	0.26809000	-0.08656200	-3.08161100	C	0.37789700	0.00863800	2.04693400
H	-1.19210900	1.02181800	-1.97103500	C	0.03937800	-0.19990600	3.30161800
H	-1.44540100	-0.71262700	-1.94516500	Sm	-2.09170100	-1.19923900	2.51135100
C	-0.46192600	0.03257700	-4.41958200	C	-3.15557800	1.16060500	3.49962100
H	1.05798200	0.67637500	-3.02745000	C	-3.45581000	1.18051200	2.10726000
H	0.77613900	-1.05702400	-3.02779000	C	-3.93517000	0.13081200	4.10327600
C	0.45930700	-0.11681500	-5.62796200	C	-4.42741200	0.16793600	1.85101400
H	-1.25400800	-0.72746700	-4.46635800	C	-4.73723000	-0.46793500	3.08607600
H	-0.97404100	1.00368200	-4.46636700	C	-0.63367300	-3.54096500	2.85020900
H	-0.09508700	-0.02691400	-6.56773300	C	-1.50505000	-3.49560200	3.97292200
H	1.24037600	0.65179000	-5.62920900	C	-1.42525500	-3.75497600	1.68569300
H	0.95827200	-1.09233000	-5.62906900	C	-2.83683400	-3.70967200	3.50695000
				C	-2.79018100	-3.85900900	2.09020400
				C	-4.00174700	-4.03646600	4.39485000
				H	-4.06897200	-3.37913400	5.26804800
				H	-4.95431800	-3.98272500	3.86424300
				H	-3.90765800	-5.06086500	4.78105300
				C	-3.93500500	-4.25717100	1.20193000
				H	-4.00372900	-5.34935500	1.10534700
				H	-4.89823400	-3.91168900	1.58877300
				H	-3.83107800	-3.85811500	0.18726500
				C	-0.88866700	-4.03099300	0.31013700
				H	-1.65558900	-3.91044100	-0.46133700
				H	-0.05103100	-3.37736000	0.04969200
				H	-0.52339100	-5.06435200	0.23126200
				C	0.86345300	-3.50422000	2.87890400
				H	1.24146800	-3.16209700	3.84590800
				H	1.28830500	-4.50008000	2.69396800
				H	1.26416500	-2.82699100	2.11904100
				C	-1.10268500	-3.42920300	5.41881300
				H	-1.05103000	-4.43277500	5.86315000
				H	-0.11853300	-2.97059100	5.54933900
				H	-1.81341700	-2.85421900	6.02238100
				C	-5.90853300	-1.38048100	3.30056400
				H	-6.00538100	-2.13874800	2.51669600
				H	-5.85852500	-1.89927900	4.25990300
				H	-6.84412100	-0.80411400	3.29664200
				C	-4.03965300	-0.12819100	5.58013800
				H	-4.76014400	0.55203100	6.05436700
				H	-4.37504700	-1.14666400	5.79701500
				H	-3.08349300	0.01660200	6.09400500
				C	-2.32861400	2.17659800	4.23000800
				H	-2.90386900	3.09625600	4.40658500
				H	-2.00674400	1.80898700	5.20863700
				H	-1.43077500	2.45663400	3.67367300
				C	-2.97418000	2.21414000	1.13235900
				H	-1.90720000	2.42003600	1.24922700
				H	-3.13348700	1.90853200	0.09402900
				H	-3.50439200	3.16623300	1.27004800

5-ⁿBu
H = -2096.274955 au

Sm	2.75095600	1.09819700	0.32436100
C	0.55529700	0.29096100	-0.52032000
C	0.22168000	0.02783700	0.72450200
C	3.99726600	-0.52917000	-1.56600400
C	5.04815600	0.29329300	-1.06352000
C	3.60679200	-1.42783400	-0.53412700
C	5.27840200	-0.06826600	0.29526700
C	4.38679100	-1.13640100	0.62077600
C	1.83694700	3.55778900	1.24373100
C	3.24821200	3.60740000	1.44473800
C	1.59074600	3.57449200	-0.15853300
C	3.87409000	3.67000000	0.16879000
C	2.85101500	3.62423700	-0.82549200
C	0.24870300	3.71488500	-0.81519600
H	-0.13094100	4.74137800	-0.71971300
H	0.30068300	3.49368100	-1.88512800
H	-0.50057500	3.04733200	-0.38145500
C	3.04408600	3.81584000	-2.30380300
H	4.04142400	3.50821500	-2.63005300
H	2.31819700	3.24726500	-2.89490600
H	2.92746200	4.87052400	-2.58787300
C	5.31387000	4.02926000	-0.05091900
H	5.99283200	3.48378600	0.61206300
H	5.63442700	3.84877600	-1.07876600
H	5.47170600	5.09818100	0.14902800
C	3.94707800	3.80451000	2.76024200
H	4.11424600	4.87195300	2.96167200
H	3.36392200	3.41487900	3.60031200
H	4.93058100	3.32284100	2.78720900
C	0.79924700	3.70090600	2.31677700
H	0.66543200	4.75495900	2.59676500
H	-0.17190400	3.33188600	1.98197400
H	1.05614300	3.15701600	3.23144200

C	-5.16025500	-0.06392000	0.55971700
H	-4.59832000	0.30327200	-0.30414700
H	-5.37599700	-1.12407300	0.38549400
H	-6.12644300	0.45924700	0.55351400
C	0.82105500	0.10387900	4.54469600
C	2.33043200	0.31352600	4.38759400
H	0.65267100	-0.69576000	5.27922700
H	0.37807900	0.99870000	5.00878100
C	3.03316100	0.62394200	5.71050900
H	2.76875500	-0.58719400	3.93902800
H	2.50645300	1.13683800	3.67699200
C	4.54997700	0.74828400	5.58951900
H	2.61996500	1.55131800	6.13032800
H	2.79099500	-0.16621200	6.43448400
H	5.01085800	0.98198000	6.55483800
H	4.99667600	-0.18513400	5.22868900
H	4.82982800	1.54328000	4.88961300
C	-0.21788500	0.08545300	-1.78653000
C	-1.54558100	-0.67257700	-1.69590800
H	0.43088300	-0.42527400	-2.51278200
H	-0.39694100	1.07392900	-2.23587800
C	-2.22240300	-0.85227600	-3.05628400
H	-1.36027700	-1.65699400	-1.24627700
H	-2.22103900	-0.13500200	-1.01466500
C	-3.50353200	-1.68101900	-3.00299500
H	-2.44069800	0.13561800	-3.48442100
H	-1.51185800	-1.32789100	-3.74632400
H	-3.95673200	-1.78231200	-3.99457500
H	-3.30578600	-2.69128100	-2.62668200
H	-4.24934400	-1.22330900	-2.34411100

9

 $H = -1629.81826 au$

Sm	3.26628100	0.42269900	0.28900800
Sm	0.31817000	-1.54134200	1.89455500
H	1.14478700	-0.36770800	0.13284300
C	5.66026900	-0.47935600	-0.89500000
C	6.07301700	0.19190300	0.29105000
C	4.97551900	-1.67297300	-0.50758400
C	5.60456900	-0.56133400	1.40597600
C	4.95401600	-1.73170000	0.91109100
C	1.48469200	2.50224100	-0.31077500
C	2.40354100	3.08486500	0.60201700
C	2.18859300	2.22627800	-1.52191100
C	3.67147300	3.19323900	-0.04886900
C	3.52858300	2.68704800	-1.37176100
C	0.62451900	-1.43249400	4.64939900
C	0.66777900	-0.06122200	4.25392400
C	-0.71343200	-1.89803800	4.49422500
C	-0.62919600	0.30124700	3.80365000
C	-1.48476100	-0.83561500	3.94392600
C	0.01015000	-2.95770400	-0.51098200
C	0.39688900	-3.95019500	0.42794800
C	-1.29519100	-2.50291000	-0.15171700
C	-0.67438400	-4.12846900	1.35709900
C	-1.73169400	-3.25454800	0.97786100
C	1.82419500	0.86435700	4.48592200
H	1.78567500	1.28977000	5.49856400
H	2.78122700	0.34665200	4.38174000
H	1.82930800	1.70254800	3.78516500
C	-1.12911000	1.68676100	3.51267500
H	-0.31128800	2.38326600	3.31650400
H	-1.81233200	1.72502300	2.65680700
H	-1.68472400	2.08616500	4.37269200
C	-2.98206700	-0.76635500	3.84706300
H	-3.32644200	-0.26604200	2.93486000
H	-3.44441300	-1.75485200	3.87145200
C	-1.25029600	-3.18477000	5.04863500

H	-0.54429300	-4.01462400	4.95179300
H	-1.46977300	-3.07766300	6.11977500
H	-2.18120300	-3.48763400	4.56235000
C	1.75562500	-2.19312500	5.28197600
H	1.63838800	-3.27581400	5.16633700
H	2.72289300	-1.91858200	4.84859200
H	1.82030700	-1.99628400	6.36096000
C	-0.75987200	-5.27928600	-2.31864100
H	0.15657100	-5.41176100	2.90498400
H	-1.58552600	-5.16839100	3.02402300
H	-0.92316000	-6.22200100	1.77785200
C	-2.12961700	-1.53148200	-0.93788300
H	-2.89141900	-1.04753400	-0.31752500
H	-1.51994800	-0.74082300	-1.38672700
H	-2.66237800	-2.03044600	-2.31864100
C	0.73385300	-2.59693000	-1.77386400
H	0.50220500	-1.57747900	-2.09260200
H	1.81874100	-2.66224400	-1.66016700
H	0.45164900	-3.27291000	-2.59320700
C	1.56429600	-4.88762800	0.31876600
H	2.04707300	-5.08724300	1.28191800
H	1.24015300	-5.86152800	-0.07421400
H	2.32695700	-4.51131100	-0.36598800
C	4.52829200	-2.89709400	1.75280400
H	3.74965700	-3.49093800	1.26886400
H	5.37544200	-3.57052000	1.94449900
H	4.13964600	-2.57329900	2.72197800
C	5.89429800	-0.27317600	2.85204500
H	6.78785000	-0.81058900	3.19834600
H	6.07909800	0.79138200	3.03038400
H	5.06674600	-0.57696200	3.50155200
C	7.03256100	1.34228800	0.37129300
H	7.03647400	1.94211400	-0.54253600
H	6.81496800	2.01587400	1.20531200
H	8.05813300	0.97650900	0.51702000
C	6.13780500	-0.21054200	-2.29351500
H	6.52682700	0.80270300	-2.41024100
H	6.95104100	-0.89966000	-2.56109200
H	5.35259000	-0.34893600	-3.04536600
C	4.62648800	-2.77736100	-1.46291500
H	3.99140200	-3.53463500	-0.99876100
H	4.11402500	-2.41882500	-2.36266400
H	5.53434600	-3.29283400	-1.80616000
C	4.51725300	2.84441400	-2.48888800
H	5.54558900	2.91529600	-2.12506200
H	4.47850400	2.02102900	-3.20777200
H	4.31398100	3.76603700	-3.05134500
C	4.81444400	4.01207100	0.47985300
H	5.03213400	3.80684600	1.53418500
H	5.73593000	3.84713000	-0.08161200
H	4.58412500	5.08452800	0.41147600
C	2.07821400	3.75447300	1.90565800
H	2.01928200	4.84427000	1.77671100
H	1.11256500	3.43217600	2.30064800
H	2.83285000	3.57365700	2.67920600
C	0.00064000	2.38507600	-0.13036700
H	-0.40776300	1.54172700	-0.69325800
H	-0.27646900	2.24307800	0.91701000
H	-0.50906500	3.29426700	-0.47895100
C	1.57420300	1.70198400	-2.78920700
H	2.31541700	1.22282800	-3.43770900
H	0.78945500	0.96620700	-2.58686200
H	1.11449200	2.50789000	-3.37773200
C	-3.13790400	-3.29614700	1.49780600
H	-3.74778700	-3.98298000	0.89495200
H	-3.18649100	-3.65161200	2.53022900
H	-3.63103100	-2.32079100	1.46184600
H	-3.39592000	-0.19657500	4.69078200
H	2.44184100	-0.73802600	2.05511300

9-monomer $H = -814.895960$ au

Sm	4.33799200	1.88935500	0.43703100
C	5.47203500	0.07488900	-1.28029300
C	6.58237400	0.72707600	-0.66404500
C	4.81403600	-0.70973500	-0.28384100
C	6.59580600	0.36134100	0.71383500
C	5.50647200	-0.53381900	0.94648400
C	2.72286800	4.10200500	0.56899600
C	3.95210000	4.49590900	1.17287600
C	2.96727700	3.90306500	-0.82260300
C	4.95356400	4.55002300	0.15695500
C	4.34125300	4.18726300	-1.08080800
C	1.92291000	3.57249800	-1.85226800
H	1.38483100	4.47278100	-2.17775900
H	2.35830900	3.12384600	-2.75112400
H	1.16818100	2.87791400	-1.46723600
C	4.98356300	4.26473700	-2.43619700
H	6.06428100	4.10289600	-2.38850200
H	4.57196100	3.53048800	-3.13653000
H	4.83030600	5.25334500	-2.88968600
C	6.35916000	5.05499100	0.33044700
H	6.76563000	4.82518400	1.32149900
H	7.04468700	4.63184000	-0.41051100
H	6.40624400	6.14659000	0.21870100
C	4.13299300	4.87322500	2.61666600
H	3.86289100	5.92299200	2.79214600
H	3.50474000	4.26870500	3.27962100
H	5.17087400	4.75809400	2.94763500
C	1.38168200	4.05502300	1.24256200
H	0.87290800	5.02669000	1.17202700
H	0.72409700	3.30691400	0.79198800
H	1.46819200	3.80266400	2.30215900
C	3.64992600	-1.63113100	-0.51066500
H	3.98868500	-2.64585400	-0.75979800
H	3.01429800	-1.70319100	0.37610200
H	3.01581900	-1.29886600	-1.33949400
C	5.21255800	-1.24960600	2.23351200
H	5.75829900	-2.20138000	2.29025500
H	5.50751000	-0.66193700	3.10893500
H	4.14725400	-1.46871500	2.33904700
C	7.65225400	0.73758300	1.71588500
H	8.47553800	0.01075700	1.72150000
H	8.09773900	1.71512400	1.50201200
H	7.25985100	0.77004100	2.73836200
C	7.64891800	1.51125500	-1.37275500
H	7.26670900	2.01620700	-2.26482100
H	8.10173300	2.27337000	-0.73014600
H	8.46391500	0.85408400	-1.70529700
C	5.15405300	0.07473200	-2.74999600
H	4.08527300	-0.06814200	-2.94234500
H	5.45401800	1.00720100	-3.23871800
H	5.67711000	-0.73869000	-3.27051000
H	2.79961200	1.11947600	1.63610000

TS₉₂-Ph $H = -1937.958777$ au

Sm	1.95693500	0.41487800	0.90885300
C	3.27428000	-0.23178600	-1.44723800
C	4.32224000	0.24995800	-0.61230400
C	2.86235900	-1.50619000	-0.94848200
C	4.50106900	-0.68482100	0.44688000
C	3.62326600	-1.78566100	0.22048000
C	0.88884600	2.55212500	2.28050200
C	2.07963000	2.23231600	2.99195700
C	1.26083200	3.08813800	1.01555100
C	3.19045300	2.59597500	2.17405600
C	2.68220600	3.13748000	0.95659700

C	0.34458900	3.71274200	0.00303400
H	0.25927500	4.79695000	0.16335800
H	0.70391800	3.57714900	-1.02332500
H	-0.66529600	3.30167900	0.05596600
C	3.43859000	3.93206100	-0.06815000
H	4.51827200	3.80762900	0.02425000
H	3.16263000	3.67869500	-1.09789000
H	3.22639900	5.00249600	0.05824400
C	4.61490600	2.63189900	2.64656400
H	4.89101900	1.73620000	3.21172900
H	5.32217900	2.72812000	1.81893800
H	4.78232500	3.49023200	3.31145700
C	2.17112400	1.77313800	4.41895700
H	2.24254900	2.62971500	5.10389200
H	1.30082700	1.18314800	4.71638600
H	3.05534100	1.15188900	4.59198100
C	-0.50127600	2.51773900	2.82820300
H	-1.22319700	2.18483300	2.08036200
H	-0.58388600	1.83392800	3.67385600
H	-0.81478100	3.51481400	3.16929000
C	1.99426700	-2.45984500	-1.71429300
H	2.53740600	-2.86457200	-2.57952200
H	1.68021400	-3.30968700	-1.10580500
H	1.08921300	-1.98375300	-2.10580000
C	3.73792600	-3.08864000	0.95973500
H	4.76804100	-3.46370100	0.89932700
H	3.48840100	-3.00483400	2.02243000
H	3.09320500	-3.85759700	0.53071000
C	5.60507600	-0.68605900	1.46543100
H	6.41573500	-1.36505900	1.16481300
H	6.04844700	0.30415700	1.59298200
H	5.26219400	-1.02401600	2.44970200
C	5.29001800	1.33532000	-0.97677600
H	4.84313800	2.10389200	-1.61063900
H	5.71999100	1.83102000	-0.10302100
H	6.12890600	0.90551400	-1.54155100
C	2.82514800	0.37135400	-2.74934700
H	1.75702100	0.20933400	-2.93469700
H	3.00363600	1.45085700	-2.78666000
H	3.36018400	-0.06852700	-3.60256600
C	-0.71399800	-0.82202500	3.76815500
C	-1.14221800	-0.61842600	4.91161100
Sm	-2.29118800	-1.48495400	1.172570000
C	-3.98881800	0.74386800	2.18075100
C	-3.69697600	0.77801300	0.78980800
C	-4.76829200	-0.42469900	2.43727700
C	-4.30959000	-0.36213100	0.18319300
C	-5.01714000	-1.07194500	1.19417900
C	-0.88045500	-3.82326400	1.80252600
C	-1.74897000	-3.95295900	2.92126400
C	-1.67200200	-3.91008400	0.62114600
C	-3.07814500	-4.11722100	2.43551500
C	-3.02703600	-4.11169200	1.00986000
C	-4.25141300	-4.49959800	3.29179700
H	-4.31783800	-3.90023100	4.20618100
H	-5.20129600	-4.39315300	2.76260900
H	-4.17896200	-5.54928600	3.60755200
C	-4.11124400	-4.56740800	0.07534500
H	-3.88472800	-5.57512500	-0.29745900
H	-5.08217500	-4.62210000	0.56940700
H	-4.22550200	-3.92404600	-0.80333800
C	-1.16480900	-3.94884700	-0.79226800
H	-1.98560800	-4.08044700	-1.50293400
H	-0.62842000	-3.03901700	-1.07684500
H	-0.47136100	-4.78629600	-0.94301400
C	0.61232600	-3.76349700	1.85037500
H	0.97756600	-3.40308000	2.81534400
H	1.05330900	-4.75596700	1.68130300
H	1.01271200	-3.08960600	1.09011400

C	-1.32983800	-4.12693400	4.35031500
H	-1.10241400	-5.18101000	4.56121500
H	-0.44152100	-3.54014800	4.59672200
H	-2.12543500	-3.82847700	5.04006200
C	-6.10926800	-2.07173100	0.96120000
H	-6.00536100	-2.59071600	0.00718200
H	-6.17368700	-2.82464300	1.75076400
H	-7.07838900	-1.55440400	0.93946000
C	-5.42603400	-0.74804700	3.74907800
H	-6.37527100	-0.20545300	3.86443100
H	-5.65556900	-1.81370300	3.84001000
H	-4.79792300	-0.47238600	4.60231600
C	-3.76831000	1.82470900	3.19934900
H	-3.13788900	1.50453400	4.03483400
H	-3.30370700	2.70933300	2.76043400
H	-4.72823600	2.14175000	3.62613000
C	-3.07836900	1.89890700	0.00497500
H	-2.81330600	2.74012700	0.64973500
H	-2.17393000	1.59553600	-0.53287000
H	-3.78593600	2.28150000	-0.74191500
C	-4.37349900	-0.60476300	-1.29894000
H	-3.42246300	-0.37970700	-1.79429700
H	-4.62951100	-1.64152700	-1.53653000
H	-5.13441800	0.02907000	-1.77577100
H	1.44991400	-0.75393400	2.72142700
H	0.39036200	-0.80596500	3.11913600
H	-0.35809600	-0.45149600	0.65361000
C	-1.62968500	-0.36606800	6.22837700
C	-1.83197800	-1.42187300	7.13822300
C	-1.89261500	0.95239100	6.64994900
C	-2.29585500	-1.16416000	8.42297500
H	-1.61400300	-2.43704000	6.82462000
C	-2.35449900	1.20097600	7.93738400
H	-1.72124200	1.77319500	5.96094100
C	-2.56053800	0.14532300	8.82590900
H	-2.44819600	-1.98781300	9.11472300
H	-2.55204300	2.22248700	8.24962300
H	-2.92197900	0.34283800	9.83115700

TS₉₂-^tBu*H* = -1864.169423 au

Sm	1.70927800	0.62822400	0.91506800
C	2.57161300	0.14897500	-1.68326300
C	3.78536900	0.39212900	-0.97749800
C	2.03270400	-1.08777800	-1.22084300
C	3.97183300	-0.66948800	-0.04458900
C	2.89669900	-1.58931300	-0.20683900
C	0.98702400	2.76988500	2.59459200
C	2.20078800	2.23907400	3.12186700
C	1.28484300	3.38812600	1.34666700
C	3.25337500	2.55635800	2.21470900
C	2.68642300	3.26837300	1.11731600
C	0.37405900	4.24891400	0.51634300
H	0.60970900	5.31278300	0.65768400
H	0.46608600	4.05076800	-0.55812200
H	-0.67741100	4.11763200	0.78154500
C	3.42145000	4.05654600	0.07237500
H	4.47234700	3.77178700	0.00076700
H	2.98261700	3.95689100	-0.92688300
H	3.39506000	5.12721100	0.31917500
C	4.71628600	2.36959400	2.49970200
H	4.93187100	1.40411900	2.96904100
H	5.32436000	2.43538500	1.59351200
H	5.08311700	3.14438200	3.18666800
C	2.37119800	1.64405900	4.48981800
H	2.51714300	2.42936600	5.24570200
H	1.49935300	1.05431200	4.78529400
H	3.24106500	0.98268800	4.54171300

C	-0.29853700	2.87735800	3.35870600
H	-1.11018200	3.26037100	2.73557600
H	-0.62154100	1.92005800	3.77512600
H	-0.18660700	3.57797300	4.19760100
C	0.87772300	-1.81756800	-1.83970600
H	1.21078800	-2.42890500	-2.69034700
H	0.39504300	-2.48526000	-1.12426600
H	0.11082900	-1.13462200	-2.21781100
C	2.78428100	-2.92079200	0.46858300
H	3.09480800	-3.73537400	-0.20065100
H	3.41256500	-2.97542300	1.36148200
H	1.76069900	-3.12307900	0.78602900
C	5.19643500	-0.89970800	0.79506500
H	5.90647600	-1.56446200	0.28443500
H	5.72659700	0.03190600	1.00835600
H	4.95956700	-1.36740200	1.75655600
C	4.83590400	1.38213800	-1.38248700
H	4.41350900	2.27347700	-1.85134900
H	5.45469200	1.70886500	-0.54256200
H	5.51487500	0.92596100	-2.11627200
C	2.04666400	0.95636300	-2.83739400
H	0.95676800	0.88875200	-2.92495200
H	2.30290000	2.01735500	-2.75025300
H	2.45986300	0.60765300	-3.79385700
C	-0.67913200	-0.75619600	3.85701900
C	-1.07514600	-0.50909000	5.00089800
Sm	-2.07096400	-1.71613200	1.76778600
C	-3.74905800	0.51004800	1.91208400
C	-3.12744000	0.59261000	0.63708200
C	-4.62370300	-0.61720100	1.90551300
C	-3.61911300	-0.48019900	-0.16456400
C	-4.56922500	-1.20766800	0.60867500
C	-0.82252700	-4.13045300	2.53836700
C	-1.97458300	-4.01482700	3.37082600
C	-1.27306300	-4.37178700	1.20942100
C	-3.13359200	-4.19963900	2.56485500
C	-2.70108400	-4.40794600	1.22393100
C	-4.52126300	-4.40818500	3.09912000
H	-4.77211100	-3.71356800	3.90701900
H	-5.28351500	-4.29646400	2.32414700
H	-4.62999700	-5.42221100	3.50746500
C	-3.52628300	-4.92852600	0.08180000
H	-3.32899300	-5.99819400	-0.07439400
H	-4.59683200	-4.82473600	0.26659000
H	-3.30661400	-4.42934300	-0.86912200
C	-0.46501900	-4.86081500	0.04125500
H	-0.56850300	-5.95077700	-0.05674700
H	-0.79523900	-4.43265000	-0.91096600
H	0.59945800	-4.64929700	0.14491100
C	0.59181100	-4.17125100	3.04975400
H	0.62557900	-4.66100600	4.02906200
H	1.23616800	-4.74922200	2.38149200
H	1.04855100	-3.18165100	3.17000300
C	-1.95302800	-3.97546700	4.86992300
H	-1.77067300	-4.97756100	5.28324600
H	-1.17112500	-3.31365300	5.24983900
H	-2.90919300	-3.63554000	5.27902400
C	-5.55452100	-2.19495500	0.05750600
H	-5.15047500	-2.76424800	-0.78280300
H	-5.89734000	-2.91022500	0.80933300
H	-6.44585400	-1.66934300	-0.31181600
C	-5.62056200	-0.93040000	2.98497800
H	-6.44769300	-0.20674400	2.97645000
H	-6.06220200	-1.92130400	2.85775200
H	-5.18055100	-0.89445900	3.98752200
C	-3.67923600	1.53374000	3.01016800
H	-2.99762000	1.25928200	3.82175800
H	-3.34185000	2.49827900	2.62124700
H	-4.67002800	1.69176100	3.45149200

C	-2.26037500	1.71575300	0.15403100
H	-2.86167400	2.60331900	-0.08873600
H	-1.52205200	2.01307100	0.90229000
H	-1.71628100	1.43834600	-0.75318600
C	-3.32311600	-0.69188200	-1.62223600
H	-2.29134100	-0.42590100	-1.87243000
H	-3.47221800	-1.73323700	-1.92508700
H	-3.97633600	-0.07935600	-2.25852100
H	1.43895100	-0.67576200	2.68373800
H	0.38753800	-0.73394300	3.15822400
H	-0.33553000	-0.56165800	0.77902500
C	-1.50115700	-0.21309300	6.38210300
C	-0.63210200	-1.03069700	7.36045500
C	-1.31589300	1.28993000	6.67465500
C	-2.98469500	-0.58451300	6.57267300
H	-0.76601400	-2.10470800	7.20671700
H	0.42851100	-0.79630800	7.23260700
H	-0.91505600	-0.79322900	8.39193000
H	-1.93326900	1.90249200	6.01187700
H	-1.61026400	1.50032600	7.70874600
H	-0.27346300	1.59360700	6.54648800
H	-3.28690300	-0.36521800	7.60251400
H	-3.62463700	-0.00605600	5.90035800
H	-3.15369400	-1.64774300	6.38567200

I_{rad} (C₅Me₅)₂Sm^{III}(HCCPh)*H* = -1122.487388 au

Sm	2.71940500	0.93367600	-1.21513700
C	0.25517800	-0.30146700	-1.04058700
C	1.00628500	-0.47601700	-0.02315700
C	4.23286900	-0.51673900	-3.01720400
C	5.17580300	0.24177400	-2.26077000
C	3.67268600	-1.50774100	-2.15795600
C	5.17938200	-0.26905000	-0.92683500
C	4.24541400	-1.34510800	-0.86586900
C	1.44835200	3.09434000	-0.02211700
C	2.66383500	2.91711700	0.69776800
C	1.77576200	3.52726200	-1.33925300
C	3.74521000	3.27887400	-0.16161000
C	3.19704600	3.64400600	-1.42647200
C	0.80339900	3.93743300	-2.41044000
H	0.51167400	4.99043900	-2.29834200
H	1.23441800	3.83890800	-3.41260900
H	-0.11456600	3.34234700	-2.39460500
C	3.95191700	4.25231200	-2.57481200
H	4.99812100	3.93543600	-2.59357100
H	3.51527300	3.99426500	-3.54620600
H	3.95004700	5.34915800	-2.51268300
C	5.16026800	3.50788100	0.28318100
H	5.46221900	2.82154800	1.07907100
H	5.87880900	3.40439100	-0.53493200
H	5.27750500	4.52572700	0.67987700
C	2.76568800	2.58151400	2.15884900
H	2.74046600	3.48766200	2.78008100
H	1.93794700	1.94447500	2.48501000
H	3.69759100	2.05961900	2.40073900
C	0.07339600	2.98642500	0.57032200
H	-0.06153400	3.72277700	1.37286700
H	-0.69574500	3.18688600	-0.17943700
H	-0.12777000	1.99697300	0.99519900
C	2.77432300	-2.64172800	-2.55913400
H	3.31035800	-3.59811100	-2.50390100
H	1.89224200	-2.72974500	-1.91528000
H	2.42811600	-2.53745300	-3.59154500
C	4.03767500	-2.26456000	0.30232800
H	4.74832500	-3.10262200	0.27897700
H	4.18079100	-1.75343500	1.25978700
H	3.03180700	-2.69421900	0.30633100

C	6.15491200	0.07716500	0.16182400
H	6.94735700	-0.68040800	0.22765000
H	6.64397500	1.03738600	-0.01503300
H	5.68429100	0.12485500	1.15055500
C	6.14378900	1.23757800	-2.83167500
H	5.71087000	1.81159500	-3.65682200
H	6.48877500	1.95390900	-2.08104200
H	7.03665200	0.73517200	-3.22815100
C	3.98795400	-0.38290000	-4.49527600
H	2.97087600	-0.67391500	-4.77744400
H	4.13984000	0.64355100	-4.84581600
H	4.67264800	-1.01708100	-5.07431700
H	0.90975100	-1.13553300	0.83790100
C	-0.49521300	0.01000400	-2.17800100
C	-0.25780600	-0.62301900	-3.43793500
C	-1.57290800	0.94792000	-2.11344500
C	-1.01907300	-0.30314600	-4.54990000
H	0.52038600	-1.37555200	-3.50550100
C	-2.32169400	1.24867000	-3.23820200
H	-1.80745100	1.40591200	-1.15866300
C	-2.05224900	0.63870500	-4.47036000
H	-0.81378100	-0.80211300	-5.49377800
H	-3.13758100	1.96254400	-3.15598400
H	-2.64469600	0.88214100	-5.34682000

TS_{1,1 rad}*H* = -1430.628991 au

C	-0.96312300	-0.61717900	0.59547300
C	-0.41214600	-0.20782100	1.66299600
C	-0.52300000	-1.20580300	3.70655200
C	-1.01554100	-0.83011000	4.80500100
Sm	-2.71222000	-1.65495000	2.23211700
C	-3.90799600	0.77763200	2.88997200
C	-3.99890700	0.73127600	1.46949700
C	-4.77961900	-0.22102400	3.42234400
C	-4.91356500	-0.30213900	1.11911200
C	-5.40100200	-0.88675800	2.32812100
C	-1.28220600	-4.06744700	2.11486400
C	-2.21585400	-4.23697400	3.17721700
C	-2.00974000	-4.00575500	0.89316800
C	-3.52353700	-4.28235800	2.61433800
C	-3.39672700	-4.13366700	1.19833200
C	-4.76876400	-4.67090900	3.35973700
H	-4.87921000	-4.14198100	4.31358200
H	-5.66941100	-4.47515200	2.77449700
H	-4.76441300	-5.74438700	3.59286900
C	-4.48663600	-4.32949600	0.18355800
H	-4.57141400	-5.38578900	-0.10668100
H	-5.46684100	-4.02434500	0.56032600
H	-4.29859300	-3.76512800	-0.73555100
C	-1.39487100	-4.05034300	-0.47517700
H	-2.05403900	-3.63977100	-1.24460500
H	-0.45713400	-3.49016900	-0.52365500
H	-1.17076500	-5.08688200	-0.76415000
C	0.21313200	-4.13826600	2.22326800
H	0.54886300	-4.04495900	3.26058200
H	0.58934000	-5.10260500	1.85646700
H	0.71280600	-3.36014400	1.63380000
C	-1.87722700	-4.50782100	4.61509500
H	-1.57335500	-5.53509000	4.75989900
H	-1.05758100	-3.88070600	4.98047700
H	-2.73879800	-4.33978900	5.26961900
C	-6.59355400	-1.79283700	2.42474300
H	-6.66030000	-2.48785300	1.58242100
H	-6.59605100	-2.38380500	3.34438100
H	-7.52267000	-1.20514200	2.42166600
C	-5.14885400	-0.40261600	4.86686800
H	-6.03863100	0.18896300	5.12316600

H	-5.38626000	-1.44543700	5.10492600
H	-4.34964900	-0.08844500	5.54266400
C	-3.17855300	1.83778000	3.66323200
H	-3.08060800	1.57990100	4.72004400
H	-2.17021900	2.01637200	3.27311700
H	-3.71371000	2.79595200	3.61255500
C	-3.38182600	1.73972000	0.54565000
H	-2.37576000	2.02471500	0.86752600
H	-3.29659800	1.36977800	-0.47902600
H	-3.98505500	2.65746400	0.51287500
C	-5.47900200	-0.56842400	-0.24759600
H	-4.87308800	-0.11134500	-1.03478200
H	-5.56472800	-1.63727000	-0.47145000
H	-6.48846200	-0.14496800	-0.34162700
H	0.31272600	0.42507900	2.14886000
H	0.35415000	-1.77509500	3.42652100
C	-0.81461400	-0.51440100	-0.85237900
C	-1.88178200	-0.76371200	-1.72821100
C	0.43307000	-0.17219500	-1.40749000
C	-1.72038800	-0.65010200	-3.10656200
H	-2.84535000	-1.04567900	-1.31457800
C	0.59793500	-0.07598900	-2.78499900
H	1.27113700	0.01322600	-0.74174400
C	-0.47923100	-0.30880100	-3.64143300
H	-2.56429100	-0.83845200	-3.76486200
H	1.57048600	0.18720700	-3.19281700
H	-0.34969900	-0.22971600	-4.71719500
C	-1.45305100	-0.37956600	6.06058900
C	-2.25167300	-1.18899000	6.90804700
C	-1.04309900	0.89160500	6.54051400
C	-2.62395800	-0.73934800	8.16615000
H	-2.56042300	-2.17019100	6.56268700
C	-1.41793900	1.32174900	7.80477800
H	-0.42808700	1.52014500	5.90439000
C	-2.21237600	0.51542100	8.62478400
H	-3.23603200	-1.37485500	8.80030000
H	-1.09149400	2.29716600	8.15507500
H	-2.50607200	0.86034600	9.61166500

TS_{1,2} rad $H = -1430.63513 \text{ au}$

C	-1.16718800	-0.43343700	1.00986900
C	-0.36146000	-0.07754800	1.94265400
C	-0.66159100	-1.14274400	3.93263000
C	-1.14060700	-0.71118600	5.01907800
Sm	-2.83386000	-1.64910900	2.38834100
C	-4.20745100	0.69401000	3.00209600
C	-4.20378200	0.64091000	1.57869100
C	-5.04473700	-0.35871500	3.47921400
C	-5.03131700	-0.44400900	1.17371400
C	-5.55840500	-1.05919400	2.34956500
C	-1.22432800	-3.91373500	2.00351700
C	-2.10788600	-4.25769000	3.06588500
C	-1.99371000	-3.78411900	0.81316200
C	-3.42529300	-4.35849600	2.52951500
C	-3.35264600	-4.07195100	1.13198600
C	-4.61290700	-4.90896400	3.26762500
H	-4.71535200	-4.49433000	4.27744200
H	-5.54887400	-4.71310200	2.73970400
H	-4.53211600	-5.99840500	3.38403300
C	-4.44149200	-4.28829500	0.12100700
H	-4.37960700	-5.29826400	-0.30699300
H	-5.43895500	-4.18997000	0.55742100
H	-4.37663500	-3.58547500	-0.71507500
C	-1.43455500	-3.56486400	-0.56298600
H	-2.16301100	-3.09809500	-1.23378100
H	-0.55062200	-2.92058600	-0.54214400
H	-1.13563200	-4.51463500	-1.02846100

C	0.27393600	-3.86046400	2.06265600
H	0.64281900	-3.90617900	3.09209300
H	0.71810400	-4.71351700	1.53329000
H	0.67485200	-2.95278100	1.59590900
C	-1.71874400	-4.61219600	4.47299000
H	-1.47714300	-5.68008800	4.56306900
H	-0.84454600	-4.05273000	4.81910300
H	-2.53016100	-4.41414600	5.18135700
C	-6.68036500	-2.05458600	2.39949600
H	-6.68986100	-2.71789000	1.53041800
H	-6.64048000	-2.68210300	3.29448400
H	-7.65165900	-1.54050300	2.41591800
C	-5.48776700	-0.57694800	4.89798700
H	-6.46638700	-0.11193500	5.08057000
H	-5.59795500	-1.64012900	5.18134400
H	-4.78961000	-0.14622700	5.62008700
C	-3.58531200	1.78808000	3.82030800
H	-3.52642900	1.52895300	4.87984100
H	-2.56837600	2.02353900	3.48814300
H	-4.16951000	2.71524600	3.74462200
C	-3.60159400	1.67140300	0.66997000
H	-2.66881500	2.07871200	1.07051600
H	-3.37907500	1.26428500	-0.32109400
H	-4.29020700	2.51538100	0.52412800
C	-5.44015900	-0.73712700	-0.24152400
H	-4.60415600	-0.65008800	-0.94449600
H	-5.85529500	-1.74242200	-0.34753700
H	-6.21230200	-0.03369000	-0.58187800
H	0.13990200	-1.83608700	3.70671900
C	-1.59400500	-0.13193100	6.21127100
C	-2.53980700	-0.77949000	7.04699300
C	-1.05278800	1.10806800	6.64314500
C	-2.93087400	-0.20273600	8.24614700
H	-2.94500500	-1.73926500	6.74201600
C	-1.44650900	1.66290600	7.85122500
H	-0.32417600	1.60835300	6.01310100
C	-2.38959700	1.01882700	8.65829500
H	-3.65740100	-0.71302400	8.87260900
H	-1.01931500	2.61073400	8.16745000
H	-2.69772700	1.46286800	9.60015700
C	0.79539200	0.63576900	2.41446700
C	2.05801600	0.01280200	2.46724100
C	0.69116200	1.97788100	2.83197400
C	3.17396300	0.71115500	2.91627500
H	2.15519300	-1.01746700	2.13797600
C	1.81210500	2.66955100	3.27557200
H	-0.27551100	2.47015500	2.79029500
C	3.05797100	2.04008000	3.32410400
H	4.14111100	0.21632700	2.94305500
H	1.71560200	3.70810400	3.58107100
H	3.93150900	2.58310800	3.67334700
H	-1.10672900	-0.13784300	-0.03802500

1,1 rad $H = -1430.694206 \text{ au}$

C	-0.87193400	-0.62101300	1.08789100
C	0.14796700	-0.54837200	2.03669500
C	-0.05635500	-0.66788700	3.43329200
C	-1.30193700	-0.87515200	4.02397800
Sm	-2.96987100	-1.67557500	2.20828000
C	-4.15140500	0.79071900	2.82603300
C	-4.09517100	0.76022200	1.40212100
C	-5.09328600	-0.19006100	3.25078900
C	-4.99630100	-0.24652500	0.94624900
C	-5.62225900	-0.82651300	2.08988900
C	-1.49811800	-4.05020500	1.83528600
C	-2.08195600	-4.18209900	3.12882300
C	-2.54647200	-4.10787600	0.87237900

C	-3.49438700	-4.31266500	2.96427300
C	-3.77975800	-4.27283400	1.56813000
C	-4.47860900	-4.63295600	4.05426100
H	-4.14911800	-4.25812600	5.02886700
H	-5.46977600	-4.20984700	3.86023300
H	-4.61327100	-5.71767000	4.16562100
C	-5.09274000	-4.60383100	0.92035600
H	-5.11127500	-5.65214400	0.59118800
H	-5.93334400	-4.46989700	1.60494100
H	-5.29094800	-3.99265000	0.03291800
C	-2.37638700	-4.21453500	-0.61619600
H	-3.20207400	-3.75079300	-1.16828600
H	-1.44636800	-3.75251700	-0.95930600
H	-2.34501500	-5.26684200	-0.93159400
C	-0.02549700	-4.05727800	1.54784100
H	0.53862000	-3.48817000	2.29318500
H	0.37279600	-5.08140400	1.55317600
H	0.20385600	-3.62462000	0.56996000
C	-1.31221800	-4.40126900	4.39982800
H	-1.02131700	-5.45634000	4.49937300
H	-0.39397200	-3.80817700	4.43326200
H	-1.89257200	-4.14763100	5.29114700
C	-6.81313100	-1.74025100	2.07511500
H	-6.88865800	-2.30480400	1.14249500
H	-6.80153700	-2.46260800	2.89839900
H	-7.74379100	-1.16448000	2.17618500
C	-5.59865700	-0.38857700	4.65167200
H	-6.49632200	0.21767200	4.83737400
H	-5.87816100	-1.42971700	4.84938700
H	-4.85741700	-0.09882900	5.40175000
C	-3.47835400	1.80861400	3.70058000
H	-3.31895400	1.43574600	4.71573900
H	-2.50045900	2.10243200	3.30658700
H	-4.08257200	2.72319100	3.77926300
C	-3.38720600	1.76580500	0.54126700
H	-2.45511800	2.11213500	0.99690300
H	-3.13368600	1.36600300	-0.44416000
H	-4.01768800	2.65125100	0.37953900
C	-5.35565200	-0.52191400	-0.48726300
H	-4.52904400	-0.29200900	-1.16725000
H	-5.63511400	-1.56850000	-0.65127400
H	-6.21035800	0.08746200	-0.81200800
H	1.19009900	-0.41819200	1.71874000
H	0.84704000	-0.61178100	4.05400800
C	-0.58513200	-0.19175000	-0.27006300
C	-1.32895800	-0.71957400	-1.35002700
C	0.39470300	0.78333500	-0.57896300
C	-1.07998500	-0.33816600	-2.66240400
H	-2.10167500	-1.45245400	-1.13811700
C	0.62757000	1.18462700	-1.88767300
H	0.95691000	1.24132800	0.22985900
C	-0.10093700	0.61900600	-2.93716200
H	-1.65556600	-0.77630000	-3.47324000
H	1.37850700	1.94227400	-2.09578200
H	0.08538100	0.93122300	-3.96103300
C	-1.43225400	-0.68877400	5.45844400
C	-0.63154600	0.22072500	6.19153300
C	-2.42114300	-1.39873900	6.17682100
C	-0.80065400	0.39182100	7.55931200
H	0.11147100	0.81274100	5.66456400
C	-2.57317800	-1.24921400	7.54946800
H	-3.06237000	-2.08654900	5.63228200
C	-1.76476600	-0.34919800	8.24715000
H	-0.18089400	1.10551300	8.09573200
H	-3.33015400	-1.82297700	8.07710400
H	-1.89287700	-0.21733400	9.31797500

1,2rad

 $H = -1430.688691 \text{ au}$

C	-1.00078400	-0.75621800	1.26359400
C	0.14404200	-0.59978900	2.04483400
C	0.02705600	-0.70973000	3.46962500
C	-1.17593500	-0.98274900	4.11065900
Sm	-3.00503400	-1.77038900	2.39922300
C	-3.97403800	0.80595100	2.85792500
C	-4.02257300	0.65199800	1.44141800
C	-4.94357800	-0.06824300	3.42822200
C	-5.01939900	-0.31803300	1.13523500
C	-5.59399200	-0.76185600	2.36441800
C	-1.54821800	-4.14929800	2.09253200
C	-2.46208900	-4.42209500	3.14969100
C	-2.29853300	-4.00560800	0.88910400
C	-3.78019700	-4.44810800	2.60259200
C	-3.67737200	-4.19509500	1.20343500
C	-5.02495500	-4.86428500	3.33381400
H	-5.00807600	-4.56596200	4.38800600
H	-5.92679400	-4.43422900	2.88882100
H	-5.14991600	-5.95581300	3.31846600
C	-4.78401700	-4.31977500	0.19611700
H	-4.84228600	-5.34295400	-0.20047100
H	-5.76435800	-4.09203000	0.62561800
H	-4.63887600	-3.65630100	-0.66223400
C	-1.73576000	-3.84652200	-0.49467400
H	-2.37701700	-3.23151400	-1.13569600
H	-0.74662200	-3.38028600	-0.48130700
H	-1.62946200	-4.81884400	-0.99514800
C	-0.05343600	-4.18741700	2.21017400
H	0.29208200	-3.75502500	3.15475400
H	0.31963200	-5.22014200	2.17103600
H	0.43585000	-3.63534900	1.40310900
C	-2.07808700	-4.82035300	4.54616600
H	-1.80271400	-5.88329000	4.58966500
H	-1.22099800	-4.25174400	4.92052400
H	-2.90061900	-4.68313400	5.25584900
C	-6.81415000	-1.62592600	2.50449700
H	-6.90403000	-2.35038600	1.68924900
H	-6.82196200	-2.18696600	3.44448200
H	-7.73029400	-1.01925700	2.49090500
C	-5.32639200	-0.13314900	4.88004400
H	-6.08711000	0.62067300	5.12566200
H	-5.75146400	-1.10571800	5.15200300
H	-4.47336100	0.04774600	5.54124300
C	-3.16158600	1.83085000	3.59485100
H	-3.00031200	1.54957000	4.63894000
H	-2.17533400	1.97367200	3.14175900
H	-3.66312100	2.80858800	3.59508700
C	-3.29523100	1.50464000	0.44212600
H	-2.32803400	1.84571900	0.82354000
H	-3.10828000	0.97229800	-0.49607300
H	-3.87767400	2.40152800	0.18897700
C	-5.50965000	-0.65719600	-0.24383400
H	-4.70079500	-0.65947400	-0.98294400
H	-5.98957500	-1.63924900	-0.28151200
H	-6.25170800	0.07426100	-0.59265100
H	0.94160900	-0.55446300	4.05374100
C	-1.25644200	-0.76616800	5.54606000
C	-0.50557500	0.22966400	6.21799000
C	-2.14258800	-1.54192100	6.32820400
C	-0.62292900	0.41993600	7.58862100
H	0.15518000	0.87020000	5.64066800
C	-2.23935200	-1.37167500	7.70358700
H	-2.74136100	-2.30231800	5.83468300
C	-1.48222900	-0.38599100	8.33987500
H	-0.04394600	1.19874500	8.07792800
H	-2.91369000	-1.99770600	8.28147600

H	-1.56889400	-0.23897200	9.41288400
H	-0.85746200	-0.49575400	0.20687600
C	1.48335800	-0.34593100	1.44988200
C	2.63454000	-0.96588500	1.96396500
C	1.62855600	0.50942600	0.34575400
C	3.88270800	-0.74498800	1.38930900
H	2.54363700	-1.64837800	2.80456200
C	2.87798800	0.74096500	-0.22088400
H	0.75253100	1.01267000	-0.05412500
C	4.01049000	0.11246800	0.29660700
H	4.75811700	-1.24624100	1.79335400
H	2.96890600	1.41731300	-1.06653000
H	4.98558600	0.28912300	-0.14875200

(C₅Mes)₂Sm^{II}(THF)*H* = -1040.025538 au

C	2.22332700	3.49554500	12.65133700
C	3.55305700	2.99528500	12.54396700
C	4.32135400	3.55939400	13.60201800
C	3.46549200	4.40507900	14.36370600
C	2.17197900	4.37250000	13.77112300
C	1.11028900	3.24275400	11.67188300
H	1.11382300	3.96806300	10.84567700
H	0.11931100	3.31339400	12.13740300
H	1.18092200	2.25034700	11.21097500
C	4.08399700	2.14948800	11.42048000
H	4.40707800	2.76205900	10.56655200
H	3.33414000	1.44954900	11.03366300
H	4.95251000	1.55581100	11.72508200
C	5.80540500	3.41332300	13.79019000
H	6.36081700	4.21053600	13.27573000
H	6.17917200	2.46407100	13.39309500
H	6.10090700	3.46140100	14.84508700
C	3.88538900	5.27781600	15.51404200
H	4.21137300	6.27355600	15.18060300
H	4.72553100	4.84954700	16.07320800
H	3.07037500	5.44555700	16.22933700
C	1.00377200	5.22730500	14.17288500
H	1.05098200	6.22636300	13.71614400
H	0.95341300	5.38503600	15.25709800
H	0.04668900	4.79244700	13.86245700
C	2.05768800	-1.02468900	15.55004600
C	3.03483200	-1.05547100	14.51431500
C	4.25665900	-0.55547400	15.04790500
C	4.03191500	-0.20720900	16.41034800
C	2.67396900	-0.50279200	16.72152700
C	0.65641300	-1.55974400	15.45300200
H	0.60976000	-2.63721600	15.66679400
H	0.22690400	-1.42754100	14.45205300
H	-0.02052400	-1.07352400	16.16544600
C	2.84566100	-1.64090900	13.14223800
H	3.07370900	-2.71617700	13.11923400
H	3.49496400	-1.16824800	12.39695600
H	1.81399000	-1.53674600	12.78496000
C	5.58680400	-0.55402700	14.34899900
H	6.12856400	-1.49766200	14.50707100
H	6.24355400	0.24686000	14.70568100
H	5.48521600	-0.43100500	13.26527500
C	5.08030200	0.25546700	17.38426200
H	5.56214600	-0.58661600	17.90147500
H	4.66792700	0.90233400	18.16853600
H	5.88235000	0.81653500	16.89140500
C	2.04228400	-0.40411600	18.08178000
H	2.16117800	-1.33181800	18.65982900
H	0.96436900	-0.20991500	18.02586700
H	2.48886600	0.39308900	18.68908800
Sm	2.52793200	1.74015500	14.91532600
O	0.24396900	2.38921900	16.23432400

C	0.17705300	2.97316500	17.55111500
C	-1.07758000	2.30200400	15.66308600
H	0.56606900	3.99860700	17.50279400
H	0.80949100	2.38206900	18.21951500
C	-1.29762300	2.95425300	17.93381900
C	-1.97724500	3.12967100	16.57343400
H	-1.38099200	1.24765800	15.64289400
H	-1.03464800	2.67916200	14.63682900
H	-1.55199300	3.73976700	18.64993200
H	-1.56623400	1.98866800	18.37586600
H	-3.01417000	2.78449900	16.55888800
H	-1.96228100	4.18207800	16.27050900

(C₅Mes)₂Sm^{II}*H* = -808.436425 au

C	2.30684100	3.45511300	12.62037400
C	3.69078600	3.13363200	12.51640900
C	4.36712800	3.74111700	13.61422700
C	3.40106200	4.43775100	14.39531600
C	2.12775600	4.26027800	13.78188800
C	1.24007600	3.10231800	11.62073300
H	1.12323400	3.88077900	10.85385600
H	0.25430600	2.97942300	12.08605800
H	1.46477000	2.17239300	11.08604000
C	4.34398800	2.40048500	11.37754700
H	4.65978000	3.08675600	10.57936400
H	3.67043200	1.67149000	10.91303700
H	5.24085000	1.85652400	11.69413500
C	5.85471000	3.75552900	13.83263700
H	6.33330500	4.60436000	13.32443300
H	6.33800800	2.85006100	13.44937300
H	6.11943200	3.83998000	14.89309300
C	3.69052200	5.29841200	15.59434300
H	3.90444800	6.33831900	15.31056700
H	4.56304500	4.94704700	16.15767200
H	2.84638600	5.33841200	16.29355800
C	0.83837500	4.89635500	14.22323100
H	0.68812800	5.88295500	13.76296000
H	0.80132000	5.05551400	15.30783700
H	-0.03779400	4.29481300	13.95198200
C	2.01021000	-0.92949100	15.58366500
C	2.94699000	-1.13983100	14.53165100
C	4.23470700	-0.75496200	15.00546900
C	4.09278000	-0.30710300	16.35068100
C	2.71793000	-0.41516900	16.70782700
C	0.54997200	-1.28804800	15.54948500
H	0.37302900	-2.32148800	15.87891700
H	0.12548900	-1.20999500	14.54143900
H	-0.05239700	-0.64943200	16.20711600
C	2.65084100	-1.78008700	13.20345100
H	2.71880600	-2.87576800	13.25528600
H	3.35238400	-1.46125700	12.42462400
H	1.64059400	-1.55045500	12.84402500
C	5.53254100	-0.92440800	14.26582800
H	5.96922100	-1.91907100	14.43255200
H	6.28728200	-0.19549800	14.58145100
H	5.41024400	-0.81505500	13.18251000
C	5.21401500	0.09284100	17.27005000
H	5.63284800	-0.77153500	17.80404200
H	4.88841400	0.80259500	18.03990800
H	6.04761000	0.55823800	16.73177300
C	2.13270800	-0.13654700	18.06486800
H	2.13260900	-1.03096500	18.70343800
H	1.09006900	0.20036300	18.00994800
H	2.69447300	0.63069300	18.61079800
Sm	2.78427000	1.69138500	14.80168900

(C₅Me₅)₂Sm^{III}(HCC^tBu)*H* = -1042.806690 au

Sm	3.00548400	1.01541400	0.10796700
C	0.44066200	-0.92617800	0.24245200
H	0.31832400	-0.96473000	-0.81789400
C	0.51693800	-0.95181800	1.45320700
C	0.58478400	-1.00067700	2.92300100
C	4.71188200	-0.18234900	-1.85805700
C	5.60690400	0.37180900	-0.89804200
C	4.05574000	-1.29373200	-1.25682300
C	5.49798900	-0.39392100	0.29814600
C	4.54349600	-1.42694300	0.07392600
C	1.19982200	3.21137100	0.63601400
C	2.42501900	3.61088800	1.24190600
C	1.39019400	3.20519400	-0.77521500
C	3.36876700	3.86138900	0.20451600
C	2.72709700	3.61553400	-1.04283500
C	0.32253100	2.94539300	-1.80185600
H	-0.22468200	3.86115200	-2.06811900
H	0.73391400	2.55011500	-2.73831900
H	-0.42898800	2.23042400	-1.44553700
C	3.30128500	3.90049700	-2.40221300
H	4.39258600	3.81154200	-2.41605700
H	2.91135500	3.22491400	-3.17199500
H	3.06537400	4.92157800	-2.73417500
C	4.73641800	4.45392100	0.39812400
H	5.20018700	4.12952300	1.33712300
H	5.42346200	4.18578300	-0.41051400
H	4.70082100	5.55229900	0.43230200
C	2.65541200	3.88393000	2.70300200
H	2.57536300	4.95520900	2.93545900
H	1.92523600	3.37428500	3.34129900
H	3.65232100	3.57131800	3.03881900
C	-0.11473700	2.99863100	1.33282000
H	-0.76197200	3.88363800	1.25513000
H	-0.68347800	2.15824000	0.91663700
H	0.01523100	2.80586400	2.40365600
C	3.13052600	-2.25105400	-1.95518600
H	3.68237300	-3.04920100	-2.47193200
H	2.44597700	-2.74742600	-1.25810900
H	2.51992900	-1.75737700	-2.72166600
C	4.22468900	-2.55506800	1.01389300
H	4.85769400	-3.43415900	0.82625100
H	4.38785600	-2.27951900	2.06265300
H	3.18601400	-2.89276500	0.91980000
C	6.34508400	-0.22324800	1.52923900
H	7.28790400	-0.78444000	1.46125900
H	6.62023100	0.82372300	1.70192600
H	5.84036400	-0.57851700	2.43576100
C	6.61526000	1.45488900	-1.15739100
H	6.26605300	2.17516900	-1.90494600
H	6.86052800	2.02082500	-0.25225500
H	7.56152400	1.04310800	-1.53646200
C	4.59745300	0.22944300	-3.29959000
H	3.59792200	0.03941100	-3.70858800
H	4.80819600	1.29411400	-3.44382200
H	5.30333300	-0.32125600	-3.93754900
C	0.76733900	-2.46469800	3.36944300
H	-0.06778400	-3.08408200	3.03040800
H	1.69372500	-2.88721300	2.97137900
H	0.80782500	-2.51152600	4.46279800
C	1.78185900	-0.15574600	3.40113200
H	1.67956800	0.88869400	3.08546500
H	1.83504200	-0.16647600	4.49448600
H	2.72544200	-0.56444500	3.02189200
C	-0.72537800	-0.43610700	3.50633100
H	-0.68441000	-0.47116000	4.60004000
H	-0.88182300	0.60071000	3.19787800

H -1.58528900 -1.02570400 3.17613500

THF*H* = -232.249985 au

C	10.91869000	0.97458100	-0.04839400
O	10.39033700	-0.15162300	-0.74455300
C	9.48830200	-0.86302000	0.09698300
C	9.72686600	-0.34731300	1.51494800
C	10.10875400	1.10916200	1.24167400
H	8.45096200	-0.66992000	-0.22001000
H	9.67845100	-1.93713600	-0.01120200
H	8.85229200	-0.45815300	2.16223400
H	10.56459300	-0.87980400	1.97980500
H	10.67613900	1.57422700	2.05277400
H	9.20906700	1.71106500	1.06926700
H	11.98373200	0.80206700	0.17085100
H	10.84799200	1.85880700	-0.69321900

HC≡CPh*H* = -308.157204 au

C	0.00000000	0.00000000	2.02025700
C	0.00000000	0.00000000	3.23137300
H	0.00000000	0.00000000	4.29776100
C	0.00000000	0.00000000	0.59283900
C	0.00000000	1.21176200	-0.11986800
C	0.00000000	-1.21176200	-0.11986800
C	0.00000000	1.20706500	-1.51056000
H	0.00000000	2.14841700	0.42904500
C	0.00000000	-1.20706500	-1.51056000
H	0.00000000	-2.14841700	0.42904500
C	0.00000000	0.00000000	-2.20995800
H	0.00000000	2.14968500	-2.05073700
H	0.00000000	-2.14968500	-2.05073700
H	0.00000000	0.00000000	-3.29631600

HC≡C^tBu*H* = -234.366058 au

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

HC≡CⁿBu*H* = -234.364604 au

C	-1.30320000	2.60805700	0.00000000
C	-1.37690100	1.08294100	0.00000000
H	-0.77192700	2.97900700	0.88361800
H	-0.77192700	2.97900700	-0.88361800
C	0.00000000	0.42068100	0.00000000
H	-1.94370200	0.74242000	0.87737600
H	-1.94370200	0.74242000	-0.87737600
C	-0.08374900	-1.11485900	0.00000000
H	0.57158900	0.74682000	-0.87773800
H	0.57158900	0.74682000	0.87773800
H	-0.65359100	-1.45078200	0.87732900

H	-0.65359100	-1.45078200	-0.87732900
C	1.22239500	-1.76519900	0.00000000
C	2.31234400	-2.28808000	0.00000000
H	3.27148100	-2.75309200	0.00000000
H	-2.30156500	3.05691800	0.00000000

H₂ $H = -1.16406 \text{ au}$

H	0.74333400	-0.07163300	0.00000000
H	-0.00006800	-0.07163300	0.00000000