

Supporting Information

Insight into the Pd-Catalyzed Branching Cyclizations of Enediyne-Imides towards Furo[2,3-b]pyridines: A DFT Study

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Cartesian coordinates and electronic energies for all of the calculated structures.

PI				C	2.99704600	2.11550100	2.59757400
SCF done: -1095.25495403				C	3.53948300	2.59239300	1.47769000
C	-0.36931200	0.87107300	0.00247800	H	3.35451000	2.43415400	3.57205700
C	-1.80621300	0.93530000	0.09485700	H	2.18536200	1.39457500	2.58504500
C	-2.23508900	-0.37115900	0.04106200	H	4.35481700	3.31278100	1.55320800
C	-0.03521700	-0.49112100	-0.08863600	C	3.16103400	2.23667000	0.05412300
O	-1.16789300	-1.25044900	-0.06081700	H	2.90519100	3.16626200	-0.47463500
N	1.16079400	-1.02150300	-0.19215500	H	4.05869300	1.85958500	-0.44350300
C	0.70576200	1.76200800	0.02085900	PII			
C	2.00882600	1.25927500	-0.08017500	SCF done: -1423.13779008			
C	2.19094100	-0.14740300	-0.21148700	C	0.31331300	0.74289600	-0.45499700
C	-2.60917400	2.19803700	0.27617300	C	-0.31973100	2.03984700	-0.24658900
C	-2.95907500	2.89461900	-1.02112200	C	-1.65032800	1.86794900	-0.48723700
H	-3.52279600	1.99437800	0.84410300	C	-0.78097500	-0.16154900	-0.86262400
H	-2.01001500	2.88535000	0.89167000	O	-1.94184300	0.55100500	-0.85756400
H	-2.14203400	3.00561700	-1.73376700	N	-0.67323900	-1.40911300	-1.14610600
C	-4.16548000	3.37290200	-1.32737500	S	-2.02400400	-2.32463100	-1.67137100
H	-5.00631200	3.28295500	-0.64281500	O	-1.44103700	-3.58597000	-2.15873900
H	-4.35604200	3.87938600	-2.26880500	O	-2.91590700	-1.51716000	-2.53136900
C	-3.55008300	-1.00440600	0.11562200	C	1.59373000	0.26516600	-0.36795500
C	-3.66608300	-2.32307600	0.59556700	H	1.70576600	-0.78010100	-0.64186700
C	-4.71413300	-0.32609100	-0.28977600	C	2.77597800	0.97666000	0.02457900
C	-4.91363500	-2.93337100	0.68839300	C	4.01234400	0.41498400	0.11911400
H	-2.77135700	-2.85736700	0.89531300	C	0.37156200	3.34508200	0.06107800
C	-5.96005300	-0.94268000	-0.18861900	C	0.68106700	3.55159800	1.52849900
H	-4.63875500	0.66520300	-0.72200400	H	1.30284400	3.38427200	-0.51983800
C	-6.06691700	-2.24459700	0.30386100	H	-0.23871900	4.17731100	-0.30235200
H	-4.98643000	-3.94988500	1.06424400	H	1.12658100	2.70510700	2.04998100
H	-6.84908200	-0.40802300	-0.51085200	C	0.45038600	4.68188100	2.19733700
H	-7.03929900	-2.72273600	0.37802800	H	0.00789600	5.55142900	1.71601200
C	3.53197100	-0.78678000	-0.36552900	H	0.70480500	4.78374500	3.24796100
C	3.90476600	-1.82683100	0.49904500	C	-2.87451800	-2.66965700	-0.12312600
C	4.41019500	-0.42500600	-1.39869300	C	-2.47552700	-3.77087200	0.63681400
C	5.13592000	-2.46456000	0.35571500	C	-3.93455600	-1.85926600	0.28398800
H	3.21636100	-2.13110000	1.28088500	C	-3.13892900	-4.04582400	1.83009700
C	5.64004100	-1.06754800	-1.54665300	H	-1.67093000	-4.40444100	0.27988900
H	4.11539500	0.34098900	-2.11039200	C	-4.58691300	-2.15038200	1.48095900
C	6.01021800	-2.08400900	-0.66488600	H	-4.24331500	-1.02577400	-0.33608800
H	5.41208200	-3.26211300	1.03975200	C	-4.19859700	-3.23992100	2.27363700
H	6.30320600	-0.78066500	-2.35793700	H	-2.83685400	-4.90565200	2.42269800
H	6.96857000	-2.58280000	-0.77785300	H	-5.41761900	-1.52628200	1.80027700
H	0.55109400	2.83271300	0.12947600				

C	-2.81129600	2.75065200	-0.50414800	H	0.57211800	6.30830300	-2.69644300
C	-3.88845000	2.45280100	-1.36329100	C	1.24241800	-1.18501800	-1.14193600
C	-2.89109700	3.88474100	0.32545700	O	1.88823100	-0.36887700	-1.77641600
C	-4.99945700	3.28999900	-1.40992800	N	1.76725000	-2.36113000	-0.64443800
H	-3.83673300	1.57007200	-1.99208800	H	1.30451700	-2.83917800	0.11983900
C	-4.00784000	4.71624100	0.27029300	S	3.40728300	-2.90177600	-0.88684000
H	-2.10121200	4.08967000	1.03945800	O	3.65610500	-2.89737000	-2.33192400
C	-5.06154200	4.42666800	-0.59927200	O	3.42892800	-4.12703100	-0.06796100
H	-5.81937400	3.05487900	-2.08211800	C	4.41166400	-1.65186800	-0.10092200
H	-4.06125500	5.58520000	0.91971600	C	4.88544400	-0.57664700	-0.85429500
H	-5.93070400	5.07681000	-0.63754500	C	4.73081400	-1.79635600	1.25091400
C	4.37549200	-1.00520800	-0.01796900	C	5.68365200	0.37615600	-0.22663000
C	5.46390600	-1.40827100	-0.81323300	H	4.62515900	-0.49552200	-1.90233400
C	3.62898300	-1.99027700	0.65597500	C	5.52880500	-0.83059100	1.85711900
C	5.77286300	-2.75742400	-0.95604100	H	4.37159600	-2.65583900	1.80563800
H	6.05748900	-0.65712600	-1.32371700	C	6.01112700	0.27025600	1.13321100
C	3.94725300	-3.34000100	0.51455400	H	6.06038900	1.21676700	-0.80293700
H	2.81288700	-1.69179300	1.30539500	H	5.78440100	-0.93419900	2.90795700
C	5.01541700	-3.72821100	-0.29458900	C	6.84474400	1.33002300	1.81069700
H	6.60742800	-3.05300400	-1.58479200	H	7.43755700	0.91127200	2.62897200
H	3.36215200	-4.08653000	1.04292200	H	7.52620500	1.81556400	1.10638800
H	5.26188900	-4.78002400	-0.40453300	H	6.20397400	2.11097000	2.23845100
C	-4.89303500	-3.53089200	3.58251600	C	-1.11707200	-2.03902800	-0.93665400
H	-4.91688900	-4.60420500	3.79324900	H	-0.70975100	-3.01504900	-1.19840700
H	-4.37312700	-3.04704300	4.41897900	C	-2.49235200	-1.97269200	-0.72550900
H	-5.92220500	-3.16076600	3.58081200	C	-3.70155900	-1.97263600	-0.54476000
Br	5.48198900	1.61961700	0.49762800	C	-5.10263100	-1.96774300	-0.34173500
H	2.69960400	2.03609000	0.23330100	C	-5.85811500	-3.13543100	-0.59085500
1				C	-5.75168500	-0.79713600	0.10971900
SCF done: -1449.30389439				C	-7.23379800	-3.12721800	-0.39432600
C	-0.23153500	-0.99099100	-0.85372300	H	-5.35284600	-4.03140400	-0.93654700
C	-0.59120100	0.34126700	-0.56320400	C	-7.12919600	-0.80595600	0.30344700
C	-0.55973800	1.60332600	-0.50837900	H	-5.16281900	0.09329900	0.30697100
C	-0.28672100	2.90266400	-1.05861500	C	-7.87071600	-1.96439200	0.05257300
C	-1.09560400	4.02490300	-0.80483400	H	-7.81236100	-4.02535800	-0.58760200
C	0.84287400	3.01345500	-1.89873800	H	-7.62658100	0.09356000	0.65283800
C	-0.78030800	5.24317900	-1.39891700	H	-8.94593900	-1.96285900	0.20616000
H	-1.95672100	3.92091800	-0.15380300	Pd	-1.19777600	1.11148500	1.42231800
C	1.13771700	4.23841900	-2.48842600	Cl	0.81047900	0.31015700	2.25914300
H	1.45628800	2.13598400	-2.07655900	Cl	-3.34227400	1.96007400	1.05455300
C	0.33164600	5.35308100	-2.23880500	1'			
H	-1.40382300	6.11048800	-1.20487300	SCF done: -1449.30341327			
H	2.00142300	4.32445900	-3.14077400	C	-0.07041200	0.19844100	-1.14621800

C	0.84017200	-0.70853000	-0.58375800	H	5.13592600	6.49436400	-1.28770900
C	1.53482400	-1.69721200	-0.21818100	H	6.72733300	3.05283100	0.75328000
C	2.23252500	-2.92290400	-0.52517600	H	6.99411900	5.37775700	-0.07718000
C	3.50056500	-3.21799800	0.00571600	Pd	1.22759600	-0.90876000	1.66940700
C	1.60154800	-3.83247300	-1.39822500	Cl	-0.95037000	-1.65216000	1.97445000
C	4.13447900	-4.40443300	-0.35266600	Cl	3.41943100	-0.11421000	1.84611600
H	3.96565900	-2.51411600	0.68764700	O	-1.49184000	-1.63044900	-1.58840700
C	2.24927800	-5.01350300	-1.74721300	H	-2.45363000	-1.87741200	-1.72864500
H	0.61535100	-3.59866700	-1.78500500				
C	3.51406600	-5.30151100	-1.22660000	2			
H	5.11443700	-4.63199300	0.05557300	SCF done: -1449.321002			
H	1.76391900	-5.71257500	-2.42145000	C	-0.29260700	-0.95164700	-0.31312100
H	4.01278300	-6.22756300	-1.49728700	C	-0.50293800	0.47916200	-0.18413100
C	-1.43533100	-0.31591400	-1.46429700	C	0.67053800	1.08970700	-0.47515600
N	-2.39846200	0.54810600	-1.59198600	C	1.16468600	2.45124600	-0.55858800
S	-3.97313500	0.02995800	-1.92397100	C	0.25932600	3.51537300	-0.74222300
O	-4.01569800	-1.47587900	-1.89441900	C	2.54051200	2.73381400	-0.46052100
O	-4.46096500	0.73756400	-3.11782900	C	0.72599300	4.82459100	-0.80598100
C	-4.85130900	0.62208700	-0.48209700	H	-0.79816800	3.30279200	-0.85705900
C	-4.63763000	0.00920400	0.75667200	C	2.99616000	4.04729700	-0.53029800
C	-5.75406100	1.67189200	-0.63030100	H	3.24473000	1.92329400	-0.31115900
C	-5.34181300	0.47494200	1.86108300	C	2.09225100	5.09832700	-0.70000000
H	-3.93163700	-0.80846800	0.85905000	H	0.01758900	5.63470700	-0.95091700
C	-6.45528200	2.11858000	0.49026700	H	4.05981100	4.25232700	-0.44779600
H	-5.90340100	2.11922300	-1.60669100	H	2.45025000	6.12229700	-0.75415800
C	-6.26022600	1.53300500	1.74714000	C	1.10057200	-1.09208700	-0.65276600
H	-5.17799900	0.00824000	2.82862600	O	1.68240600	0.07351900	-0.76474600
H	-7.16533500	2.93400800	0.38353500	N	1.82828100	-2.20285200	-0.84038500
C	-7.00898500	2.02528200	2.96177300	H	1.37081300	-3.10533100	-0.78281600
H	-7.75812300	2.77511800	2.69497700	S	3.45791100	-2.34569200	-1.54335600
H	-7.51964800	1.20202300	3.47282500	O	3.51156200	-1.45843100	-2.70637200
H	-6.32451100	2.47880600	3.68813800	O	3.56383100	-3.80950500	-1.62070800
C	0.21643700	1.52879100	-1.38293400	C	4.50355700	-1.71726400	-0.24993200
H	-0.59333800	2.12059500	-1.80743400	C	5.04030600	-0.43447100	-0.37338000
C	1.41886600	2.16638600	-1.11948400	C	4.80336300	-2.53920600	0.83996000
C	2.45767400	2.78059000	-0.91394100	C	5.87735000	0.03625500	0.63518900
C	3.66677900	3.47530300	-0.68454200	H	4.81128400	0.16870700	-1.24440300
C	3.82199700	4.80171800	-1.14790500	C	5.63756300	-2.04442100	1.83671800
C	4.72687200	2.84463600	0.00528700	H	4.40276400	-3.54541500	0.89528100
C	5.01658200	5.47649000	-0.92954100	C	6.18078400	-0.75160600	1.75591400
H	3.00229500	5.27962300	-1.67432700	H	6.30480000	1.03101300	0.54880400
C	5.91478000	3.53531300	0.21904500	H	5.87766300	-2.67314500	2.68921000
H	4.58823200	1.83293400	0.37269900	C	7.05539100	-0.21485400	2.86070500
C	6.06286400	4.84524900	-0.24728600	H	7.60372100	-1.01616800	3.36343200

H	7.77811500	0.51290100	2.48199800	C	4.30067200	-1.71694100	-0.60764400
H	6.44696400	0.29215600	3.61960400	C	4.81141500	-2.86370900	-1.21794600
C	-1.15632400	-2.02515400	-0.19627000	C	4.52559300	-0.44641600	-1.14468100
H	-0.74287900	-3.03234600	-0.27164700	C	5.54890200	-2.73001900	-2.39289600
C	-2.52548600	-1.95131700	-0.02460600	H	4.64107100	-3.83590000	-0.76950000
C	-3.74831800	-1.94654400	0.05703500	C	5.26592500	-0.33755900	-2.31733400
C	-5.15423000	-1.84779100	0.12353500	H	4.12880500	0.43450100	-0.65817700
C	-5.93877100	-2.96293000	0.49604500	C	5.78456200	-1.47193200	-2.96250000
C	-5.78123600	-0.62003800	-0.19606400	H	5.95052000	-3.61869900	-2.87150200
C	-7.32128100	-2.84547500	0.56103200	H	5.44492400	0.64746800	-2.73993300
H	-5.44918500	-3.90079500	0.73745900	C	6.57100800	-1.32940500	-4.24243900
C	-7.16701200	-0.52363900	-0.13437000	H	7.39682100	-0.61972800	-4.12358200
H	-5.16897700	0.22205900	-0.50768500	H	6.98980200	-2.28582000	-4.56518900
C	-7.93601400	-1.62795800	0.24648800	H	5.93587100	-0.95132800	-5.05187000
H	-7.92363300	-3.69965900	0.85461900	C	-1.19441900	-1.97364600	0.13624400
H	-7.64994200	0.41584300	-0.38454700	H	-0.69752200	-2.90318800	0.41314100
H	-9.01767500	-1.54212700	0.29619800	C	-2.57280700	-2.01255400	-0.05440100
Pd	-2.11740800	1.27568300	0.54042500	C	-3.77266200	-2.12391400	-0.26125400
Cl	-1.40402100	0.89351200	2.72448300	C	-5.15860800	-2.17046800	-0.55363900
Cl	-3.13415600	1.77623000	-1.51355700	C	-5.96539500	-3.22100800	-0.06647000
				C	-5.73914900	-1.15778400	-1.35023200
3				C	-7.32439300	-3.24966400	-0.36024300
SCF done: -1697.866786				H	-5.51413100	-3.99826600	0.54192300
C	-0.38561500	-0.87651400	-0.02765600	C	-7.09897100	-1.20441400	-1.64131000
C	-0.65908200	0.51413500	-0.33781000	H	-5.10656600	-0.36519400	-1.73983300
C	0.53550100	1.14705400	-0.44701200	C	-7.89355200	-2.24315300	-1.14685300
C	0.97954600	2.50188600	-0.73203800	H	-7.94206000	-4.05726500	0.02142900
C	0.13705600	3.39887900	-1.41857800	H	-7.54099000	-0.42729200	-2.25767900
C	2.25777500	2.94176600	-0.33343000	H	-8.95496800	-2.27076400	-1.37624800
C	0.56021200	4.69959500	-1.67527900	Pd	-2.42028100	1.32287100	-0.25482700
H	-0.83263500	3.05870800	-1.76628600	Cl	-2.25918300	1.70492400	2.07829600
C	2.67259300	4.24516800	-0.59832200	Cl	-2.85660300	1.14949200	-2.53794900
H	2.91723000	2.26313400	0.19731800	C	1.75162900	-0.45673500	4.59638000
C	1.82562800	5.13107900	-1.26712100	O	2.80151500	-0.96893600	4.07566400
H	-0.09990400	5.37727900	-2.20863900	H	1.42515400	-0.93187800	5.52155900
H	3.65934000	4.56967600	-0.27958200	N	1.03334700	0.56024900	4.18968100
H	2.15060200	6.14659600	-1.47406000	C	-0.16463500	0.96494900	4.94569200
C	1.06372700	-0.96667400	0.12277700	H	-0.02954500	1.98741700	5.30937300
O	1.60700700	0.22821600	-0.15655300	H	-1.02870600	0.93742500	4.27575400
N	1.73333500	-2.02401000	0.49586800	H	-0.31546900	0.29354800	5.79207200
H	3.11832500	-0.78063300	3.07610800	C	1.33645800	1.38467700	3.00864500
S	3.34171000	-1.95185100	0.88713900	H	1.68500900	2.36515900	3.34758700
O	3.69136200	-3.25066000	1.47856600	H	2.09868400	0.91449800	2.39282700
O	3.59772700	-0.71176600	1.75027100	H	0.41312000	1.51447200	2.43658700

3'

SCF done:-1697.86365573

C	-0.26965400	-0.76650300	-0.09854800
C	-0.54339200	0.65442200	-0.17003900
C	0.64577700	1.30657600	-0.10661500
C	1.07942000	2.69422200	-0.13238400
C	0.27634400	3.68882200	-0.72316500
C	2.31774300	3.05919200	0.43181400
C	0.69967300	5.01501500	-0.72907500
H	-0.65888800	3.40928200	-1.19651700
C	2.73184700	4.38842700	0.41818100
H	2.93713900	2.29907700	0.89561100
C	1.92479100	5.37172400	-0.15897900
H	0.07352900	5.77192800	-1.19219900
H	3.68538500	4.65825000	0.86322700
H	2.25034700	6.40795200	-0.16892200
C	1.18132800	-0.86896000	0.12243000
O	1.71198200	0.37124600	0.07672400
N	1.83917100	-1.95684800	0.36762700
H	-0.51990500	1.12574300	2.92473300
S	3.46734300	-1.91199200	0.84084200
O	3.76034000	-3.29147200	1.27486800
O	3.69035000	-0.79463200	1.80492400
C	4.39041500	-1.57850700	-0.65993000
C	4.76585600	-2.65888800	-1.46159700
C	4.72978700	-0.26891000	-1.00289000
C	5.47819400	-2.41326300	-2.63237500
H	4.51353000	-3.66860300	-1.15743100
C	5.44380800	-0.04548200	-2.17809200
H	4.44416300	0.55390400	-0.35912500
C	5.82280800	-1.10725300	-3.01230100
H	5.77756500	-3.24921200	-3.25891900
H	5.71445400	0.97117000	-2.45002000
C	6.56596800	-0.84957400	-4.30049100
H	5.86552800	-0.72047400	-5.13494400
H	7.17050300	0.05981000	-4.23957000
H	7.22621200	-1.68345200	-4.55592400
C	-1.06355800	-1.88119700	-0.18102500
H	-0.55729400	-2.84007400	-0.07038400
C	-2.43617300	-1.90089900	-0.43382700
C	-3.62628900	-1.98504300	-0.69855200
C	-5.00308500	-2.00471600	-1.04043600
C	-5.79734600	-3.14044000	-0.77520600
C	-5.58739200	-0.87901000	-1.66260800

C

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SCF done: -1697.84166265

C	0.26105800	-0.60862900	0.48462200
C	-0.19234100	0.50649300	-0.31875100
C	0.85024900	1.37318300	-0.45535500
C	1.07214400	2.65904700	-1.10241100
C	0.16776800	3.16378600	-2.05804700
C	2.21366400	3.41635600	-0.77062000
C	0.39554100	4.40267700	-2.64860900
H	-0.68859500	2.57130900	-2.35375200
C	2.43054100	4.65472400	-1.36965900
H	2.91766300	3.03241700	-0.03910900
C	1.52264200	5.15555500	-2.30549400
H	-0.30601700	4.77732300	-3.38713100
H	3.31102500	5.23233200	-1.10111400
H	1.69554200	6.12002000	-2.77224100
C	1.65466100	-0.27828200	0.85358100
O	1.97973800	0.89644200	0.25217700
N	2.40955800	-0.99516400	1.60529600
S	4.01022500	-0.53926600	2.00349100

O	4.30811700	-1.24880200	3.26403900	H	-3.83092600	-0.52329100	3.93749100
O	4.19700500	0.91919600	1.92300300	Cl	-3.28651000	4.47300000	0.81013900
C	4.90463900	-1.33149100	0.64302000	H	-3.18286000	3.18439200	0.77008200
C	5.25893000	-2.67721600	0.75255300				
C	5.21876600	-0.58810100	-0.50113600	5			
C	5.92768100	-3.28576500	-0.30798100	SCF done: -1564.238336			
H	5.02578200	-3.22174200	1.65949600	C	0.55384600	-0.08602900	-0.60019100
C	5.88406400	-1.22009600	-1.55594700	C	-0.24958500	1.11185900	-0.50388800
H	4.94058700	0.45966800	-0.54812400	C	0.58140000	2.18115700	-0.38224100
C	6.24221800	-2.57393500	-1.47471700	C	0.41452700	3.61846400	-0.22385600
H	6.21324500	-4.33014000	-0.22780800	C	-0.77155300	4.26701400	-0.61872100
H	6.13562500	-0.67413100	-2.45895500	C	1.46376900	4.37835600	0.33142100
C	6.93052300	-3.25558800	-2.63286500	C	-0.91198300	5.63953600	-0.43226900
H	6.19504800	-3.70835700	-3.31327000	H	-1.55755400	3.70164100	-1.10840600
H	7.52210000	-2.54657500	-3.22069000	C	1.31092700	5.75009100	0.51311500
H	7.59679200	-4.05843700	-2.29149700	H	2.38601300	3.88427600	0.61725800
C	-0.33063600	-1.77131000	0.90095800	C	0.12371800	6.38437200	0.13857900
H	0.27345400	-2.40907000	1.54467800	H	-1.82612000	6.13194000	-0.75067000
C	-1.60072300	-2.22845300	0.53257800	H	2.12329200	6.32590600	0.94620800
C	-2.66267200	-2.70834700	0.16818200	H	0.01069100	7.45546200	0.27859100
C	-3.85688400	-3.28674300	-0.34253000	C	1.94730700	0.39558700	-0.47371700
C	-4.49357700	-4.34106400	0.34379500	O	1.92096600	1.75387500	-0.36492300
C	-4.39646300	-2.83213100	-1.56545900	N	3.00780200	-0.32094000	-0.46367100
C	-5.64429000	-4.92102100	-0.17842400	S	4.53642500	0.44552400	-0.29529500
H	-4.07334300	-4.69585700	1.28093400	O	4.55380400	1.25385100	0.94335800
C	-5.54657000	-3.42515000	-2.07777900	O	4.90359500	1.03001900	-1.60018000
H	-3.88939800	-2.03900000	-2.10505100	C	5.54691900	-1.01379100	-0.02444100
C	-6.17388200	-4.46559900	-1.38813500	C	5.84286600	-1.40936100	1.27837800
H	-6.12762300	-5.73439100	0.35561600	C	6.05324500	-1.70598000	-1.12507000
H	-5.95177000	-3.07531400	-3.02429500	C	6.64507700	-2.53250300	1.47674600
H	-7.06960500	-4.92412400	-1.79665900	H	5.46104300	-0.83445500	2.11485900
Pd	-2.06176600	0.71050400	-0.83770000	C	6.85118700	-2.82602100	-0.90759400
Cl	-1.73681800	0.08305200	-3.00858000	H	5.83329300	-1.35791200	-2.12834400
C	-2.01555700	1.27740800	2.17193400	C	7.15501100	-3.25967400	0.39245000
O	-2.73519800	1.24745300	1.13925900	H	6.88476800	-2.84472400	2.48978100
H	-0.96219400	1.56624900	2.11812800	H	7.25288600	-3.36835500	-1.75967700
N	-2.46741500	0.97925400	3.38645500	C	8.00043800	-4.49113200	0.61306000
C	-1.58972500	1.03848400	4.55493800	H	8.43533900	-4.50469200	1.61621200
H	-2.03168700	1.68387700	5.31943500	H	7.40099600	-5.40326200	0.50196000
H	-1.45134100	0.03471600	4.97174100	H	8.81690200	-4.55132700	-0.11327500
H	-0.61749800	1.44012000	4.26994900	C	0.24975500	-1.40872300	-0.75689900
C	-3.84072400	0.51787000	3.59532600	H	1.08900800	-2.10251300	-0.75262000
H	-4.32676500	1.13976000	4.35256700	C	-1.03303500	-1.93755400	-0.95260500
H	-4.38157600	0.58750000	2.65596900	C	-2.11678400	-2.45515000	-1.17890600

C	-3.39673000	-3.00290700	-1.46997300	O	4.33982000	-1.19822500	1.46470700
C	-3.71039000	-4.33110900	-1.11185000	C	5.59125400	0.67810400	0.05013700
C	-4.36713200	-2.21767800	-2.13116700	C	6.14929100	1.02391800	-1.17986100
C	-4.96697500	-4.85470100	-1.40058900	C	6.01975000	1.27482400	1.23579200
H	-2.96275300	-4.93570900	-0.60848100	C	7.14087400	2.00226500	-1.21801300
C	-5.61859500	-2.75577000	-2.41664600	H	5.81966300	0.52086600	-2.08220600
H	-4.11421900	-1.20419900	-2.42820400	C	7.01174600	2.25094600	1.17720900
C	-5.92354600	-4.07037200	-2.05139500	H	5.59079000	0.96419200	2.18211200
H	-5.20104600	-5.87711500	-1.11928600	C	7.58235900	2.63374300	-0.04614200
H	-6.35761600	-2.14889200	-2.93139300	H	7.58516100	2.27419900	-2.17183600
H	-6.90208500	-4.48390900	-2.27698000	H	7.35512300	2.71763100	2.09668200
Pd	-2.21238200	1.09716900	-0.39723500	C	8.63619000	3.71350300	-0.10063400
Cl	-2.56238500	1.37353000	-2.66221300	H	9.29383800	3.58841400	-0.96548200
C	-2.19637100	1.65862100	1.74576700	H	8.17538000	4.70597300	-0.18116600
C	-2.16624200	0.27647400	1.70324700	H	9.25482100	3.71541400	0.80157600
H	-1.28929300	2.23397600	1.89081900	C	0.35737700	1.85778200	-0.32020500
H	-3.13533800	2.18973800	1.89209900	H	1.28437400	2.41464700	-0.18419300
H	-1.21499800	-0.23943400	1.79533200	C	-0.81876200	2.60927700	-0.41045200
C	-3.38671000	-0.57629000	1.84333900	C	-1.79508400	3.34347600	-0.45667800
H	-3.33105800	-1.48910100	1.25415100	C	-2.92431400	4.20154000	-0.50947900
H	-4.31237700	-0.03923700	1.63391000	C	-2.74767200	5.60223400	-0.48166000
Br	-3.55343200	-1.19721100	3.74218500	C	-4.23038000	3.67144800	-0.58501600
6				C	-3.85181200	6.44615800	-0.52963000
SCF done: -1564.264104				H	-1.74319900	6.00817800	-0.42149500
C	0.48986500	0.49882500	-0.35742900	C	-5.32654800	4.52683400	-0.63092400
C	-0.46837300	-0.58796200	-0.57370600	H	-4.37321000	2.59575800	-0.60265800
C	0.26691000	-1.77980200	-0.55671800	C	-5.14191300	5.91209500	-0.60410000
C	0.05055700	-3.14776800	-1.04419800	H	-3.70846700	7.52222200	-0.50746500
C	-1.21157400	-3.76995700	-1.04829000	H	-6.32818400	4.11157300	-0.68563900
C	1.16210800	-3.85420300	-1.54889500	H	-6.00158800	6.57472100	-0.63956300
C	-1.36439300	-5.05085700	-1.56933900	Pd	-1.11844700	-1.36246000	1.44079000
H	-2.06315500	-3.27005000	-0.60523600	Cl	-2.20409900	-1.64791900	3.45945100
C	0.99840200	-5.13658000	-2.06577100	C	-1.93086200	-0.42730500	-0.95966700
H	2.14177800	-3.38996200	-1.53789800	C	-2.64975400	-0.47989400	0.38233600
C	-0.26162300	-5.73765400	-2.08315700	H	-2.08941700	0.51893100	-1.48409500
H	-2.34349300	-5.51960400	-1.55832500	H	-2.24208100	-1.23918900	-1.62225900
H	1.86197700	-5.66773600	-2.45387800	H	-2.71644900	0.49623200	0.86641000
H	-0.38293800	-6.74004700	-2.48260700	C	-3.90871700	-1.27273500	0.52192900
C	1.79596900	-0.15364200	-0.19837400	H	-4.28732100	-1.28191800	1.53977200
O	1.60233300	-1.51101800	-0.28833300	H	-3.85556800	-2.28363200	0.12326400
N	2.93237500	0.40041300	-0.00981400	Br	-5.37056000	-0.39771700	-0.59023100
S	4.33059300	-0.59579900	0.11747800	7			
O	4.44768300	-1.42709800	-1.10113300	SCF done: -1564.27177			

C	-0.62935300	1.21038600	-1.07217600	H	2.77245200	-5.18897700	-3.43224000
C	-0.74324400	-0.20876600	-1.40153700	C	-5.54308800	1.88397400	-0.19257600
C	0.55290400	-0.64314900	-1.67919800	C	-6.25514500	0.67702400	-0.35922100
C	0.80320400	1.53157500	-1.17550300	C	-6.24544300	3.04822600	0.18693100
O	1.46520500	0.36467000	-1.52649700	C	-7.62982500	0.63982300	-0.15090500
N	1.33763800	2.67594600	-1.02189900	H	-5.71972900	-0.22106200	-0.65026300
S	3.00950600	2.97899200	-1.34426500	C	-7.62022600	2.99966100	0.39275500
O	3.11575600	4.44281100	-1.24854700	H	-5.69909100	3.97645500	0.31715200
O	3.41312500	2.25696500	-2.56829900	C	-8.31541200	1.79860400	0.22493400
C	-1.55158700	2.16010300	-0.74262500	H	-8.16901300	-0.29372600	-0.28000500
H	-1.15253000	3.16022200	-0.57415800	H	-8.15194500	3.89975900	0.68582400
C	-2.93187200	1.99419300	-0.57772500	H	-9.38850200	1.76523600	0.38756100
C	-4.13973100	1.93648300	-0.40021700	C	5.92353700	0.59377000	3.44290000
Pd	-0.50632500	-1.39549800	0.70619400	H	5.44093500	0.86078200	4.38717900
Cl	1.32089100	-0.28148900	1.60187600	H	5.98037600	-0.49684500	3.38603800
C	-2.05027600	-0.94651700	-1.66177100	H	6.95210200	0.97488900	3.48125900
C	-2.40136800	-1.75966800	-0.42508500				
H	-2.82963800	-0.21408300	-1.87532100	8			
H	-1.96377900	-1.59954200	-2.53158600	SCF done: -1564.280896			
H	-3.17295100	-1.37909800	0.23925800	C	-0.32508500	0.43063800	-1.21150800
C	-1.84745400	-2.99718200	-0.19458000	C	-0.39462800	1.69658100	-0.50889500
H	-1.20575900	-3.47356000	-0.93138900	C	-1.71569500	2.02906800	-0.44197200
H	-2.17226200	-3.60472500	0.64158000	C	-1.72381800	0.06668400	-1.52501600
Br	-1.08165600	-2.31655700	2.92228300	O	-2.53026700	1.05782900	-1.02754100
C	3.84096000	2.25673700	0.06691800	N	-2.10252900	-0.98574800	-2.13689100
C	3.80577800	2.92806300	1.29080500	S	-3.76877800	-1.28472200	-2.49968100
C	4.54153500	1.06046600	-0.08481600	O	-3.73337300	-2.50411200	-3.31927800
C	4.46933100	2.37309300	2.38094400	O	-4.40882800	-0.04514800	-2.98244600
H	3.27188600	3.86790300	1.37787200	C	0.72481300	-0.37077600	-1.54124000
C	5.20768100	0.52708900	1.01615500	H	0.51329800	-1.31647600	-2.03663500
H	4.56285900	0.57040400	-1.05182600	C	2.07499800	-0.08919700	-1.22920100
C	5.17987700	1.16912500	2.26227700	C	3.30007500	0.05617500	-1.10627600
H	4.43717900	2.88221800	3.34036700	Pd	2.41087900	-0.34263300	1.01306600
H	5.75628700	-0.40498500	0.90876900	Cl	2.01894200	-0.71384500	3.28329400
C	1.13128500	-1.90162600	-2.17078400	C	0.77933500	2.43525000	0.07767500
C	2.33960500	-2.35077400	-1.60680700	C	1.41621000	1.80475600	1.30028300
C	0.53529400	-2.63620400	-3.20922900	H	1.54051600	2.61052900	-0.69028400
C	2.91915400	-3.53298900	-2.05808100	H	0.44311800	3.42369300	0.41019300
H	2.78911700	-1.78079100	-0.80072300	H	0.74283300	1.51254600	2.10276300
C	1.12811900	-3.81480300	-3.65986100	C	2.76234300	1.85605300	1.56193300
H	-0.36131400	-2.26882900	-3.69652700	H	3.45844600	2.26518500	0.83401300
C	2.31516500	-4.26872700	-3.08141000	H	3.13739100	1.67137700	2.56207100
H	3.84353400	-3.88229000	-1.60874100	Br	2.80651300	-2.77023200	0.66953200
H	0.66886500	-4.37061100	-4.47159200	C	-4.43977800	-1.70170200	-0.88789300

C	-4.16649600	-2.95817300	-0.34042300	C	0.38658700	5.43404000	1.76385500
C	-5.25021500	-0.78281800	-0.22289600	H	0.99419800	3.39789700	2.18241600
C	-4.69608000	-3.27893200	0.90561900	C	-0.52167400	5.82896900	-0.45367500
H	-3.55887200	-3.66851900	-0.89048300	H	-0.61525300	4.10057700	-1.75090300
C	-5.77979000	-1.12723600	1.02106900	C	-0.15792400	6.30226900	0.81100500
H	-5.46846200	0.17197400	-0.68845200	H	0.66936800	5.80878400	2.74259200
C	-5.50608300	-2.37074700	1.60704500	H	-0.94470900	6.50669100	-1.18855900
H	-4.48501900	-4.25281100	1.33924400	H	-0.29658200	7.35163600	1.05430600
H	-6.42356100	-0.42271000	1.54127300	C	-1.81540600	0.36863000	-1.66822100
C	-2.44812600	3.15805400	0.13027100	O	-2.09683800	1.61002300	-1.88203600
C	-3.68143500	2.93005400	0.76832700	N	-2.91250200	-0.30254100	-2.06643400
C	-1.95731800	4.47288100	0.04111900	H	-3.16922700	0.99095900	-2.24160800
C	-4.38581700	3.99039300	1.33171200	S	-3.58917900	-1.83326700	-1.73130500
H	-4.07099900	1.91951900	0.82679900	O	-2.54458300	-2.87945300	-1.81982400
C	-2.66920100	5.52941000	0.60469800	O	-4.79027500	-1.87568200	-2.57580700
H	-1.04292600	4.67366000	-0.50711400	C	-4.09277500	-1.69385300	-0.01418600
C	-3.88083200	5.29082900	1.25666500	C	-3.26370900	-2.18336000	0.99596500
H	-5.33207300	3.80242500	1.82982700	C	-5.32225100	-1.10069300	0.28172200
H	-2.28488600	6.54139600	0.52111600	C	-3.66852500	-2.05149900	2.32320000
H	-4.43454100	6.11595200	1.69437800	H	-2.33092200	-2.67522600	0.74436600
C	4.69850800	0.33590700	-1.25305000	C	-5.70893400	-0.98050200	1.61356000
C	5.11025500	1.57435100	-1.78559300	H	-5.96461700	-0.75909900	-0.52267400
C	5.66273000	-0.62188200	-0.88296200	C	-4.88842300	-1.44451800	2.65375500
C	6.46625500	1.84327900	-1.94998900	H	-3.02910400	-2.43438000	3.11383000
H	4.36420300	2.30626700	-2.07922300	H	-6.66740000	-0.52636500	1.85065500
C	7.01485800	-0.33811400	-1.05146500	C	-5.30434400	-1.27867500	4.09508200
H	5.33224000	-1.56651500	-0.46361000	H	-4.84656400	-2.03849900	4.73444600
C	7.41949800	0.89004600	-1.58222200	H	-4.99553500	-0.29856900	4.47931700
H	6.77919800	2.79598600	-2.36628100	H	-6.39039500	-1.34461700	4.20830200
H	7.75581400	-1.07793200	-0.76488500	C	-0.05072700	-1.32010100	-1.23685200
H	8.47644400	1.10457000	-1.70900200	H	-0.69192000	-2.04253900	-1.73869100
C	-6.05936800	-2.73106600	2.96439000	C	1.17453300	-1.79436700	-0.76620200
H	-6.82894500	-2.02397300	3.28505000	C	2.20337300	-2.31652900	-0.35858200
H	-6.49868200	-3.73390600	2.96144600	C	3.38670100	-2.93885800	0.11631100
H	-5.26768400	-2.72897700	3.72317800	C	3.83635900	-4.13860000	-0.47661800

TS1-1'

SCF done: -1449.23832668

C	-0.51554900	-0.03323100	-1.12283500	C	5.27212100	-2.99920100	1.63943800
C	0.23807400	1.04925900	-0.56179500	H	3.75288100	-1.46335500	1.65326900
C	0.34402800	2.23897800	-0.15310800	C	5.71656800	-4.18200300	1.04101000
C	0.20671000	3.61074400	0.18511800	H	5.34304600	-5.66845900	-0.47846400
C	0.56855300	4.08969300	1.46267700	H	5.82885400	-2.56371400	2.46356300
C	-0.33474800	4.49030300	-0.77900000	H	6.62214400	-4.66317400	1.39871700

Pd	2.24081400	1.05028500	-0.07831500
Cl	2.83930500	1.41178200	-2.27520000
Cl	2.03366600	0.71668100	2.22889300

TS1-2

SCF done: -1449.29851

C	-0.18446600	-0.85825500	-0.51024000
C	-0.49711200	0.51716700	-0.17646800
C	0.34386600	1.48195500	-0.35693300
C	0.88997800	2.77167700	-0.53222800
C	0.22603800	3.69850100	-1.37066300
C	2.08673100	3.14164400	0.12227700
C	0.74997000	4.97660000	-1.52781500
H	-0.70482100	3.40448100	-1.84469700
C	2.60790500	4.41464900	-0.06411400
H	2.58880800	2.41581700	0.75216900
C	1.93883700	5.33230000	-0.88355700
H	0.23453000	5.69560100	-2.15661200
H	3.52953100	4.70146100	0.43259900
H	2.34675900	6.33001700	-1.01799400
C	1.25601700	-0.94266500	-0.87232900
O	1.89144600	0.11808700	-0.99749400
N	1.85951300	-2.15495700	-1.03281200
H	1.37176800	-3.02194400	-0.84742600
S	3.49737200	-2.41440200	-1.59024500
O	3.69476000	-1.61542200	-2.80224200
O	3.56140300	-3.88569900	-1.56980600
C	4.49696900	-1.75406100	-0.26718600
C	4.95030700	-0.43602400	-0.34058300
C	4.84017800	-2.58941900	0.79841400
C	5.74933800	0.05152400	0.69096900
H	4.67829500	0.18370500	-1.18638300
C	5.63847000	-2.07954100	1.81792100
H	4.50051700	-3.61909600	0.81372400
C	6.09983600	-0.75422800	1.78469700
H	6.11339100	1.07411000	0.64251900
H	5.91424400	-2.72187400	2.64957000
C	6.93819700	-0.20435000	2.91214500
H	7.57762600	-0.97663400	3.34918100
H	7.57514600	0.61777300	2.57453800
H	6.30018900	0.18319700	3.71601100
C	-1.04923700	-1.91379600	-0.56439200
H	-0.65640700	-2.89037000	-0.84684300
C	-2.42712400	-1.87402600	-0.34092500

C	-3.64100600	-1.90632100	-0.20979500
C	-5.05203200	-1.88644800	-0.06413300
C	-5.75882600	-3.07562700	0.21362200
C	-5.75775200	-0.67120500	-0.20396200
C	-7.14153200	-3.04510900	0.35945700
H	-5.21175800	-4.00690000	0.31901200
C	-7.14183600	-0.65804100	-0.06148500
H	-5.20982400	0.23706000	-0.43708200
C	-7.83473800	-1.83850100	0.22266800
H	-7.68094300	-3.96150800	0.57918800
H	-7.68232900	0.27705400	-0.17274000
H	-8.91482500	-1.81936100	0.33573000
Pd	-2.10759000	1.16066500	0.77390800
Cl	-1.30968300	0.37588400	2.80448600
Cl	-3.15137800	2.08857700	-1.10310000

TS2-3

SCF done: -1697.851417

C	-0.01412100	-0.45568700	0.07456000
C	-0.34446100	0.95348700	0.03594700
C	0.82521500	1.63720900	0.12664200
C	1.24698000	3.02617000	0.13778600
C	0.39789800	4.03702300	-0.35452000
C	2.51411500	3.37879400	0.64570100
C	0.80800200	5.36635300	-0.32301600
H	-0.56282200	3.76916200	-0.78069200
C	2.91204900	4.71273600	0.66972900
H	3.16867800	2.60790100	1.03763200
C	2.06223200	5.71134800	0.18846000
H	0.14675800	6.13620000	-0.70974600
H	3.88734300	4.97308100	1.07087900
H	2.37622700	6.75106200	0.20849000
C	1.40893600	-0.50798500	0.40130700
O	1.92320200	0.71006300	0.31448100
N	2.06850200	-1.57610200	0.79531400
H	1.40508100	-2.21704800	1.84396800
S	3.79333100	-1.54409800	1.05637100
O	4.04242000	-2.87171900	1.64358000
O	4.18646000	-0.30431300	1.74861700
C	4.42688500	-1.51277100	-0.61881900
C	4.60467400	-2.72168200	-1.29412900
C	4.74712100	-0.29153400	-1.21539200
C	5.09998200	-2.69796500	-2.59540700
H	4.36745900	-3.65673700	-0.79878600

C	5.23776600	-0.29073900	-2.51882000	C	0.41251900	1.49266200	-0.24889900
H	4.61365100	0.63326600	-0.66657200	C	0.73343300	2.91038300	-0.21023400
C	5.42232600	-1.48757100	-3.22753200	C	-0.18593400	3.87385700	-0.66829100
H	5.24162600	-3.63400600	-3.12885800	C	1.98178500	3.33434200	0.28765000
H	5.48434900	0.65539900	-2.99288400	C	0.13593400	5.22705200	-0.61040300
C	5.98390300	-1.47202000	-4.62825800	H	-1.13281600	3.55278900	-1.08918700
H	7.07966000	-1.42294500	-4.60830200	C	2.29263300	4.69083300	0.33816000
H	5.70635500	-2.37328500	-5.18163100	H	2.68900200	2.59525000	0.64881100
H	5.63055000	-0.60261000	-5.19041800	C	1.37214000	5.64235700	-0.10758900
C	-0.71156300	-1.59156100	-0.26182400	H	-0.57920800	5.96045700	-0.97142400
H	-0.15301200	-2.52774700	-0.24306000	H	3.25569300	5.00635100	0.72972500
C	-2.03181500	-1.65456400	-0.70272100	H	1.61806400	6.69971700	-0.06854100
C	-3.16549800	-1.76789000	-1.14701600	C	1.13265100	-0.63133200	-0.11810300
C	-4.47773100	-1.80023000	-1.68135900	O	1.55831900	0.64396000	-0.19087400
C	-5.19630400	-3.01235100	-1.76466600	N	1.88099500	-1.66249000	0.11728000
C	-5.06973900	-0.60431000	-2.14688600	H	-0.60544700	0.58231100	2.70991100
C	-6.48347500	-3.02428900	-2.29061900	S	3.46741200	-1.49687400	0.67379400
H	-4.73483300	-3.92955000	-1.41237000	O	3.76117800	-2.80144900	1.31672800
C	-6.35618200	-0.63417000	-2.67615400	O	3.64138600	-0.26428500	1.48908900
H	-4.49945100	0.31940400	-2.10476100	C	4.46005700	-1.36226700	-0.81311900
C	-7.06567300	-1.83692600	-2.74599800	C	5.01176000	-2.51916600	-1.36377400
H	-7.03419100	-3.95839600	-2.34927900	C	4.66676500	-0.10973300	-1.39631800
H	-6.80661900	0.28512500	-3.03802900	C	5.77466400	-2.41468200	-2.52538400
H	-8.07038700	-1.85082500	-3.15850800	H	4.85106000	-3.47503500	-0.87785500
Pd	-2.17032900	1.60223800	0.16010700	C	5.42948900	-0.02835000	-2.55804200
Cl	-2.31352500	1.11133500	2.47331700	H	4.23782400	0.77816300	-0.94624000
Cl	-2.39734300	2.17914400	-2.08749500	C	5.99070900	-1.17462500	-3.14258300
C	-0.38478300	-2.52393700	2.81168600	H	6.21232100	-3.31063200	-2.95743900
O	0.88283500	-2.37285500	2.82738500	H	5.59659700	0.94238300	-3.01727000
H	-0.87885700	-3.04203800	1.98923900	C	6.79021800	-1.07285700	-4.41892700
N	-1.16412100	-2.09428300	3.77494800	H	6.12751300	-1.03716000	-5.29240900
C	-2.62032100	-2.24074900	3.68649300	H	7.39937700	-0.16405900	-4.43819700
H	-2.99770900	-2.68002000	4.61374700	H	7.45422700	-1.93224100	-4.54595300
H	-3.05937400	-1.25269300	3.51940600	C	-1.03586300	-1.81914800	-0.36592700
H	-2.87676500	-2.89174700	2.84925300	H	-0.45371100	-2.73903800	-0.32160900
C	-0.64834900	-1.26626400	4.87122800	C	-2.41673800	-1.93496400	-0.54148200
H	0.43926600	-1.27757300	4.84986700	C	-3.61199500	-2.09541500	-0.73761600
H	-1.01632300	-0.24547200	4.73087000	C	-5.00390300	-2.20640000	-0.99106500
H	-1.00845300	-1.66767900	5.82193500	C	-5.68648000	-3.41846000	-0.75479000
TS3'-4				C	-5.71734100	-1.09533000	-1.49298900
SCF done: -1697.848967				C	-7.05155400	-3.51184600	-1.00601000
C	-0.32953500	-0.64962500	-0.27783000	H	-5.13523400	-4.27144700	-0.37197000
C	-0.72039400	0.74544100	-0.26035600	C	-7.08186600	-1.20476300	-1.74357800
				H	-5.18286900	-0.17098000	-1.69138500

C	-7.75214900	-2.40717400	-1.49964000
H	-7.57142400	-4.44680600	-0.81842000
H	-7.62479600	-0.34864900	-2.13304100
H	-8.81765100	-2.48471100	-1.69608200
Pd	-2.52530800	1.33805000	0.16233900
Cl	-2.23585300	0.97296700	2.57602300
Cl	-3.08048300	1.81355400	-2.02499000
C	1.33844600	-0.08096400	3.43615500
O	0.44933200	0.30006000	2.60849700
H	2.02453800	0.65107400	3.86885700
N	1.55391500	-1.33587300	3.75625800
C	2.76280000	-1.72454700	4.48844200
H	2.48917400	-2.36395300	5.33154200
H	3.42293600	-2.26381300	3.80299200
H	3.27524000	-0.83486300	4.85627300
C	0.73501200	-2.42962200	3.21918400
H	0.42403200	-3.07263200	4.04675600
H	-0.13786300	-2.01659000	2.71824200
H	1.33704400	-2.99874600	2.50592100

TS5-6

SCF done: -1564.224028

C	-0.83622200	0.41399400	-0.30600400
C	0.18476700	-0.61594400	-0.45456000
C	-0.47813500	-1.81982000	-0.52342200
C	-0.06063300	-3.21063200	-0.52882700
C	1.23311000	-3.59208000	-0.93813400
C	-0.96638700	-4.20487000	-0.10201400
C	1.62042400	-4.92805500	-0.88902800
H	1.91488100	-2.84267400	-1.33187400
C	-0.56988200	-5.53794500	-0.06158700
H	-1.96753500	-3.91745700	0.20057500
C	0.72237700	-5.90406800	-0.44797000
H	2.61605400	-5.21077300	-1.21737000
H	-1.27303700	-6.29476400	0.27233400
H	1.02425500	-6.94678800	-0.41943000
C	-2.12347700	-0.30075800	-0.33505200
O	-1.85714600	-1.63657100	-0.49680400
N	-3.29760500	0.19785800	-0.23795300
S	-4.65743400	-0.85348100	-0.29802000
O	-4.54179700	-1.86435300	0.77585000
O	-4.87376900	-1.24676300	-1.70439000
C	-5.93616500	0.31532900	0.16927500
C	-6.29032800	0.44092300	1.51190200

C	-6.57679300	1.05748900	-0.82248500
C	-7.29398100	1.34159700	1.86268000
H	-5.79078800	-0.16511500	2.25967500
C	-7.57769100	1.95308600	-0.45257600
H	-6.29657400	0.92411100	-1.86157600
C	-7.95174300	2.10926400	0.89045700
H	-7.57492000	1.44703600	2.90731100
H	-8.08063600	2.53706900	-1.21891900
C	-9.06187000	3.05688500	1.27672700
H	-9.11941800	3.90754800	0.59137300
H	-10.03503800	2.55098700	1.25018700
H	-8.92398600	3.44359100	2.29059500
C	-0.75408900	1.76782300	-0.14325400
H	-1.69583100	2.29649400	-0.00108100
C	0.42015300	2.53029500	-0.14427500
C	1.39739100	3.26561800	-0.15325500
C	2.52854400	4.12505000	-0.14899400
C	2.43246500	5.40798500	0.43342900
C	3.75175200	3.71276600	-0.72180700
C	3.53747100	6.25195400	0.44922100
H	1.48995000	5.72323700	0.86944700
C	4.84780700	4.57092500	-0.70138900
H	3.82739100	2.73518400	-1.18955600
C	4.74684500	5.83612400	-0.11653100
H	3.45719400	7.23604900	0.90128200
H	5.78411500	4.24964400	-1.14753200
H	5.60711500	6.49900900	-0.10395800
Pd	2.07270300	-0.23351000	-1.11358400
Cl	4.02148600	0.24117600	-2.32203300
C	1.63030200	-0.58458600	1.12256100
C	2.98303300	-0.29791300	0.76706300
H	1.04872100	0.20000600	1.59258800
H	1.38719100	-1.60090200	1.41431800
H	3.34101900	0.71892500	0.91620300
C	4.04020600	-1.35859400	0.79309300
H	4.88639900	-1.11357600	0.15756500
H	3.65668200	-2.35206100	0.56763900
Br	4.77701600	-1.48406200	2.66071200

TS6-7

SCF done: -1564.236003

C	-0.34938500	0.61533400	0.41255600
C	0.68199700	-0.34495400	0.82508800
C	0.02524200	-1.58153500	0.93489600

C	0.37020500	-2.86687000	1.53370800	H	5.85824500	5.06074700	1.59697600
C	1.68094300	-3.37915900	1.54464800	H	5.33927900	7.43134100	1.06472500
C	-0.66459600	-3.60902100	2.14003600	Pd	1.86676700	-0.99139600	-0.98638300
C	1.95578700	-4.58631500	2.17800500	Cl	0.46962400	-2.25559000	-2.43442900
H	2.46398300	-2.86585300	0.99767600	C	2.02960800	0.02471400	1.45137200
C	-0.37810600	-4.81520600	2.77229100	C	2.99762200	0.21349500	0.28165400
H	-1.68007600	-3.22925600	2.11307600	H	1.92498100	0.94143000	2.04292800
C	0.92966100	-5.30415300	2.79903500	H	2.35570800	-0.77340800	2.12368400
H	2.96682300	-4.98141000	2.16448300	H	2.95868500	1.20598600	-0.16897400
H	-1.18085900	-5.37740200	3.23899900	C	4.29658500	-0.42639900	0.21078300
H	1.14690100	-6.25089800	3.28463300	H	4.50550000	-1.23101900	0.91210600
C	-1.58109000	-0.17158400	0.25112700	H	5.16337700	0.19196200	-0.00206000
O	-1.28492200	-1.48043400	0.57013600	Br	4.33487900	-1.56991000	-1.71935300
N	-2.74333700	0.24497200	-0.06647600				
S	-4.07771400	-0.84875200	-0.03176100	9			
O	-4.15762700	-1.44278800	1.32157400	SCF done: -1564.258313			
O	-4.04109100	-1.68356400	-1.24402100	C	-0.53181300	0.47998200	-0.71598200
C	-5.40919700	0.34232500	-0.20086000	C	0.01902400	1.80327000	-0.53774400
C	-6.02189100	0.85447000	0.94142800	C	-1.04965800	2.65979800	-0.43529400
C	-5.83016400	0.71129900	-1.47875900	C	-2.00150400	0.65166200	-0.66985000
C	-7.06546000	1.76684100	0.79445200	O	-2.26042400	1.98528400	-0.51648600
H	-5.68840700	0.53288300	1.92192000	N	-2.88285400	-0.26600300	-0.75648300
C	-6.87298000	1.62561000	-1.60525900	S	-4.56128400	0.13849500	-0.66150000
H	-5.35000100	0.28042900	-2.35053100	O	-4.98622200	0.50114400	-2.02710000
C	-7.50597900	2.16604000	-0.47538100	O	-4.80116400	1.03228300	0.48998300
H	-7.54858300	2.17206700	1.67969300	C	0.02576700	-0.76346800	-0.86377700
H	-7.20516200	1.92109100	-2.59705800	H	-0.66075400	-1.60655300	-0.92095200
C	-8.65788500	3.13039800	-0.62718500	C	1.39878000	-1.05581900	-0.93408200
H	-8.52292400	3.78071700	-1.49667400	C	2.57417000	-1.39691700	-1.16552900
H	-9.60323700	2.59194600	-0.76854200	Pd	2.54990600	-0.72557600	0.97402000
H	-8.77109600	3.76248600	0.25807400	Cl	2.58855800	-2.91762700	1.67658000
C	-0.35730300	1.97155400	0.26329500	C	1.47549700	2.14562000	-0.39723500
H	-1.31703000	2.40637000	-0.01459100	C	2.21897900	2.27994300	-1.70606000
C	0.71169800	2.86280300	0.42195900	H	1.59689800	3.05196500	0.20213300
C	1.58125200	3.71274800	0.54130800	H	1.95398100	1.34786600	0.21330400
C	2.58942200	4.70316200	0.68282200	H	1.98047000	1.54365100	-2.47152200
C	2.30501600	6.05314100	0.38457300	C	3.12315800	3.22800400	-1.96057500
C	3.88496600	4.35775000	1.12297100	H	3.38949700	3.97956300	-1.22084000
C	3.29181100	7.02388400	0.52272700	H	3.63371400	3.28268400	-2.91727400
H	1.30993300	6.32109900	0.04511800	Br	3.18487200	0.24034000	3.11553900
C	4.86425800	5.33657200	1.25769000	C	-5.21072900	-1.48272100	-0.26048700
H	4.10651500	3.32125900	1.35628300	C	-5.55856600	-2.35274900	-1.29339200
C	4.57202500	6.67032800	0.95852200	C	-5.38838500	-1.83416300	1.07768200
H	3.06332400	8.05942100	0.28936500	C	-6.07590000	-3.60544000	-0.97113600

H	-5.43751300	-2.04194500	-2.32525500	Pd	3.80472200	-1.31786000	-0.04545700
C	-5.90623000	-3.09153200	1.37932700	Cl	4.22119400	-1.54015800	-2.32306600
H	-5.13653200	-1.12712700	1.86032100	C	-1.55599900	-3.84806300	0.08735300
C	-6.25143000	-3.99668500	0.36458200	C	-1.27477800	-3.98805400	1.56976700
H	-6.35481300	-4.28835600	-1.76915200	H	-2.47293600	-4.38931600	-0.15094700
H	-6.05065900	-3.37275200	2.41901100	H	-0.75115800	-4.32853400	-0.48856200
C	-1.18725400	4.09162600	-0.22902800	H	-0.39167200	-3.47622500	1.94931500
C	-2.37874200	4.58704700	0.34167400	C	-2.03553200	-4.68802900	2.40980400
C	-0.17124600	4.99542700	-0.59843800	H	-2.92947100	-5.20952400	2.07526700
C	-2.52712000	5.95085400	0.56943100	H	-1.78979900	-4.76856600	3.46432300
H	-3.17067900	3.89401700	0.60409900	Br	3.66488400	-1.31284100	2.41294400
C	-0.33347100	6.35852200	-0.36835200	C	-4.19874500	-2.01691800	-0.78666300
H	0.71721800	4.63845800	-1.10622600	C	-5.16902100	-1.08557700	-0.37287100
C	-1.50510400	6.83891200	0.22209400	C	-4.61977400	-3.24050700	-1.33747400
H	-3.44339000	6.32278000	1.01727200	C	-6.52381100	-1.38718000	-0.48152700
H	0.45040100	7.04940100	-0.66333700	H	-4.85096900	-0.13532600	0.04196000
H	-1.62647200	7.90341100	0.39936400	C	-5.97696400	-3.53513400	-1.44400400
C	3.80997800	-1.83896700	-1.73509200	H	-3.88616100	-3.94219600	-1.71892100
C	4.76464800	-0.90051100	-2.17662100	C	-6.93265100	-2.61301400	-1.01221900
C	4.07561700	-3.21804600	-1.85065800	H	-7.26346700	-0.66359100	-0.15200900
C	5.95847900	-1.34121000	-2.73866000	H	-6.28840400	-4.47987700	-1.87924600
H	4.55613000	0.16002300	-2.07707600	H	-7.99016200	-2.84395000	-1.09877100
C	5.27465900	-3.64359600	-2.41271800	C	2.69205300	1.70857100	-0.58993300
H	3.34765500	-3.93110300	-1.48073200	C	2.86764600	2.54961900	0.53306900
C	6.21524100	-2.70997800	-2.85813500	C	2.92905100	2.20121900	-1.89250600
H	6.69164400	-0.61725200	-3.08061900	C	3.25573900	3.86878300	0.34410400
H	5.47976700	-4.70616700	-2.49821300	H	2.70829600	2.14547000	1.52711700
H	7.15012400	-3.04929900	-3.29409100	C	3.31634000	3.52344900	-2.06256400
C	-6.78230800	-5.36836600	0.70443800	H	2.81138100	1.53386200	-2.73837900
H	-5.95954900	-6.07830800	0.85501100	C	3.47574500	4.35534700	-0.95006700
H	-7.37027200	-5.35299700	1.62675300	H	3.39344400	4.52037100	1.20121600
H	-7.41276100	-5.76428600	-0.09668200	H	3.49213100	3.90957100	-3.06118600

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SCF done: -1564.257336

C	-0.54903200	-1.48044800	-0.39789400	S	-1.28817600	2.38817800	-1.34977400
C	-1.66635300	-2.40743400	-0.34677200	O	-2.18065900	2.11606100	-2.49277500
C	-2.78022800	-1.69121800	-0.65750600	O	-0.18862200	3.36230600	-1.44840300
C	-1.13385200	-0.17005200	-0.73511000	C	-2.28484700	2.81937800	0.08139400
O	-2.47800700	-0.33605300	-0.88011400	C	-3.66831500	2.65454300	0.02985800
N	-0.49454100	0.93401400	-0.85714200	C	-1.66123600	3.36250800	1.20739300
C	0.77183000	-1.75309800	-0.19359400	C	-4.43354000	3.02434600	1.13605000
C	1.83451300	-0.80759600	-0.26516700	H	-4.12654900	2.26049100	-0.87046200
C	2.26370100	0.37665900	-0.41201400	C	-2.44084300	3.71605200	2.30486100
				H	-0.58746200	3.51589500	1.20994300

C	-3.83515200	3.55003600	2.28967500
H	-5.51405600	2.91282700	1.09891600
H	-1.96296700	4.13921600	3.18452000
C	-4.66477700	3.92043000	3.49513800
H	-5.71560800	4.06463200	3.22996100
H	-4.62184900	3.13218900	4.25686900
H	-4.30124200	4.84074000	3.96240600

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SCF done: -1812.84669896

C	-0.87565400	-0.88153800	0.89460100
C	-2.15582100	-1.43061700	1.28404200
C	-2.99586700	-1.21168400	0.22326200
C	-1.05424200	-0.40055200	-0.40131900
O	-2.31309700	-0.56601800	-0.82036900
N	-0.09907600	0.21989100	-1.11797400
C	0.37258200	-0.67781500	1.49085100
C	1.40656200	-0.12316900	0.72984900
C	1.19379500	0.26373100	-0.60864200
Pd	3.13858200	0.07112700	1.60263200
Cl	3.90548200	-2.09623300	1.13175900
C	-2.43127200	-2.13472000	2.58802800
C	-2.84255400	-1.20723300	3.71168600
H	-3.19440500	-2.90689100	2.44661100
H	-1.51051800	-2.65798200	2.88262000
H	-2.22251400	-0.32203000	3.85018200
C	-3.87615700	-1.42058700	4.52634200
H	-4.51299500	-2.29673800	4.42408800
H	-4.11438000	-0.73599300	5.33459200
Br	2.56373000	2.36940000	2.37675600
C	-4.38632300	-1.53304600	-0.07759300
C	-4.79244400	-1.70888800	-1.41486000
C	-5.33767600	-1.66907100	0.94980800
C	-6.11434200	-2.03102300	-1.70948600
H	-4.06399000	-1.60134200	-2.21148200
C	-6.65701700	-1.99787000	0.64427100
H	-5.05292900	-1.48039300	1.97886600
C	-7.04999200	-2.18282700	-0.68271500
H	-6.41360800	-2.17026600	-2.74409300
H	-7.38311500	-2.09634000	1.44593800
H	-8.07963000	-2.43701400	-0.91631400
C	2.27970300	0.55747800	-1.56680800
C	3.28081000	1.50755800	-1.31022400
C	2.32588500	-0.20666100	-2.74838800

C	4.30791100	1.69455300	-2.23292900
H	3.23691100	2.10669800	-0.40739400
C	3.36477300	-0.01959300	-3.65596600
H	1.57131000	-0.96966800	-2.91437300
C	4.35449000	0.93285900	-3.40286000
H	5.07324100	2.43925300	-2.03619400
H	3.40388700	-0.62083100	-4.55958700
H	5.16245100	1.07929200	-4.11409000
H	0.55289900	-0.95381900	2.52359200
S	-0.72775700	1.41538500	-2.47077800
O	-1.57054800	0.59160300	-3.33700600
O	0.45779600	2.13487000	-2.92904800
C	-1.70158700	2.49021400	-1.43518600
C	-3.09346900	2.41709500	-1.49207000
C	-1.03732900	3.41900800	-0.62555900
C	-3.83451600	3.30164200	-0.71057700
H	-3.57677300	1.68880100	-2.13221900
C	-1.80131200	4.27967900	0.15325100
H	0.04601700	3.46473400	-0.60189000
C	-3.20619200	4.23674000	0.12384600
H	-4.91912900	3.26151400	-0.74976400
H	-1.29801300	4.99868200	0.79301300
C	-4.01337100	5.17142500	0.98952400
H	-3.95298200	4.87287000	2.04285100
H	-3.63627900	6.19684800	0.92410800
H	-5.06804600	5.17499200	0.70364400
C	0.69248500	-3.69661100	-0.94589100
O	0.32914900	-2.78926100	-1.69282000
H	0.04136700	-4.07772000	-0.13550400
N	1.87017700	-4.35794400	-1.00275000
C	2.26337100	-5.28892500	0.04298400
H	2.62454700	-6.22552100	-0.39733400
H	3.05245400	-4.85481600	0.66689500
H	1.40160800	-5.51502500	0.67654300
C	2.89804600	-3.95285100	-1.95279700
H	3.37891100	-4.84298100	-2.37229400
H	2.42536800	-3.38303500	-2.75166000
H	3.65017100	-3.32971200	-1.45620600

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SCF done: -1117.892827

C	-1.18852500	-0.28055600	0.07182500
C	-2.56370700	-0.69872800	-0.02265800
C	-3.29986400	0.46333500	-0.05983200

C	-1.20141300	1.13150100	0.07381900
O	-2.48140000	1.58313300	-0.01191300
N	-0.17416200	1.95222100	0.14178500
C	0.06307900	-0.91646400	0.10864700
C	1.16686800	-0.07421500	0.19499500
C	1.01589800	1.33159900	0.22790900
Pd	3.07224900	-0.54871900	0.12769200
C	-3.03060100	-2.12852100	-0.12285000
C	-3.21898100	-2.80603300	1.21732100
H	-3.95776300	-2.18785700	-0.70171300
H	-2.27330600	-2.68520600	-0.69380300
H	-2.40399300	-2.68090100	1.92992600
C	-4.28200700	-3.53487600	1.55855600
H	-5.11379100	-3.68859900	0.87436000
H	-4.35510100	-4.01551800	2.52944100
C	-4.72683800	0.74925600	-0.18658100
C	-5.14957800	1.95961900	-0.76873300
C	-5.69793300	-0.16195900	0.26739000
C	-6.50593700	2.23662000	-0.91290300
H	-4.40635400	2.67241700	-1.10851100
C	-7.05399600	0.12149700	0.11501500
H	-5.39141800	-1.06991300	0.77430100
C	-7.46390900	1.31689900	-0.47836700
H	-6.81679600	3.17237400	-1.36835100
H	-7.79265800	-0.58887200	0.47495800
H	-8.52164600	1.53495400	-0.59320800
C	2.26044100	2.11943100	0.32038300
C	2.47167200	3.28830400	-0.42721900
C	3.31433000	1.61620700	1.12542400
C	3.71509100	3.91086300	-0.40552900
H	1.65972200	3.67723100	-1.03238400
C	4.57352500	2.24542300	1.12174400
H	3.08543600	0.88892300	1.91228700
C	4.77524900	3.38285400	0.34950000
H	3.87343200	4.81011400	-0.99397100
H	5.36864900	1.85907700	1.75254100
H	5.74178600	3.87691000	0.34635100
H	0.17077300	-1.99273800	0.05884000
Br	2.94407700	-2.75155000	-0.88969100

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SCF done: -1119.671988

C	0.97215200	0.43154700	-0.02924100
C	2.37345200	0.74947400	-0.12700800

C	3.03057100	-0.45757700	-0.05307900
C	0.89010100	-0.97378500	0.08587500
O	2.13841200	-1.51378200	0.06599300
N	-0.19027000	-1.71767000	0.19199800
C	-0.23507900	1.14787000	-0.06656400
C	-1.39262800	0.38897500	0.06672700
C	-1.33979100	-1.01807200	0.20384500
Pd	-3.24300400	1.03104500	-0.05794000
Cl	-2.86603600	3.02470300	-1.13394400
C	2.93734500	2.13164800	-0.33713900
C	3.15805700	2.90712000	0.94357000
H	3.87214900	2.07960400	-0.90449300
H	2.22525800	2.68716300	-0.96445400
H	2.32979000	2.89843500	1.65173100
C	4.26461500	3.59058500	1.23718500
H	5.11115000	3.62864100	0.55484800
H	4.36097600	4.14754100	2.16426700
C	4.43737100	-0.84513600	-0.12118700
C	4.78991100	-2.12398200	-0.59319700
C	5.45790200	0.03477100	0.28345400
C	6.12728700	-2.50001700	-0.67860900
H	4.00768900	-2.81206400	-0.89416200
C	6.79467500	-0.34850900	0.19078500
H	5.20296600	0.99964700	0.70690600
C	7.13567800	-1.61266800	-0.29355600
H	6.38388900	-3.48827700	-1.04902100
H	7.57164900	0.33911200	0.51219400
H	8.17849700	-1.90829700	-0.36191600
C	-2.63085900	-1.71880500	0.31797500
C	-2.87725000	-2.95844000	-0.28981300
C	-3.69135500	-1.05829400	0.98715500
C	-4.15864000	-3.50044700	-0.26481200
H	-2.06212100	-3.46678200	-0.79363600
C	-4.98650700	-1.60650500	0.98745600
H	-3.45274600	-0.26133900	1.70709700
C	-5.22064800	-2.82132100	0.35360200
H	-4.34345700	-4.45723700	-0.74490900
H	-5.78666600	-1.09636900	1.51559700
H	-6.21540300	-3.25566500	0.35431200
H	-0.27637000	2.22121800	-0.20455500

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SCF done: -1250.174876

C	-1.71096800	-0.12350700	0.34837800
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C	-2.99892800	-0.76687600	0.34180100	H	4.28322100	0.25090800	-0.89007700
C	-3.83697000	0.10488700	-0.31621300	H	1.72453600	-1.47529300	-1.13803700
C	-1.86855700	1.10132100	-0.32557300	C	3.56588000	-2.38267000	-0.34987400
O	-3.15947500	1.23986200	-0.73760000	H	3.04163600	-3.07103400	0.31059200
N	-0.96098500	2.02241000	-0.54765400	H	4.51428800	-2.07889200	0.09350800
C	-0.41638400	-0.41345100	0.80034000	Br	4.06080500	-3.49453600	-1.94683100
C	0.56921100	0.53694000	0.55215300				
C	0.28558100	1.77106000	-0.08383700	17			
Pd	2.42167100	0.02017400	1.06292900	SCF done: -1250.197078			
Cl	2.06390800	0.39509100	3.31822500	C	1.46138000	-0.17845800	-0.43719100
C	-3.29119600	-2.13553100	0.90145300	C	2.74160000	-0.82429000	-0.34712600
C	-3.62625700	-2.13743600	2.37770400	C	3.64931200	0.19582000	-0.15718600
H	-4.09780000	-2.61504700	0.33758700	C	1.68883300	1.19674600	-0.28139300
H	-2.39574900	-2.75540300	0.74498500	O	3.01413000	1.42834700	-0.11012800
H	-2.96389000	-1.55256500	3.01542800	N	0.80898700	2.18038000	-0.30792000
C	-4.64459800	-2.80291200	2.92348700	C	0.12345400	-0.55694100	-0.66791300
H	-5.32632200	-3.39986400	2.32124900	C	-0.87414100	0.45860700	-0.68697400
H	-4.82892400	-2.78376300	3.99330800	C	-0.47435600	1.83437400	-0.47887200
C	-5.24838500	0.05521800	-0.69045300	Pd	-1.21599100	-0.58246600	1.31300300
C	-5.69960000	0.76804800	-1.81772100	Cl	-2.15837900	-1.37280900	3.26862400
C	-6.17762700	-0.68904000	0.05914700	C	2.97357000	-2.31353100	-0.38390800
C	-7.03811000	0.71548500	-2.19576700	C	3.13935200	-2.87942700	-1.77815300
H	-4.99162100	1.35659100	-2.39069500	H	3.84267700	-2.57669700	0.22727100
C	-7.51524700	-0.73976900	-0.32910100	H	2.10647500	-2.79520700	0.09169600
H	-5.86197400	-1.19106500	0.96663800	H	2.40921100	-2.54894400	-2.51702500
C	-7.95044100	-0.04354600	-1.45814900	C	4.08901700	-3.74290300	-2.13886200
H	-7.37050800	1.26765300	-3.07002700	H	4.83482900	-4.09967100	-1.43191600
H	-8.22249100	-1.31349700	0.26289600	H	4.14972700	-4.13348200	-3.15007700
H	-8.99424100	-0.08308500	-1.75555600	C	5.09512400	0.23785100	0.04200400
C	1.28586300	2.84474600	-0.31756300	C	5.67252800	1.30068800	0.76295400
C	1.25557000	3.55797800	-1.52819600	C	5.93257400	-0.76399300	-0.48186900
C	2.24427000	3.19169400	0.65012500	C	7.04787300	1.34437400	0.97133000
C	2.18442400	4.56548300	-1.78039500	H	5.03440600	2.08288600	1.15905400
H	0.49412800	3.31253400	-2.26119300	C	7.30832600	-0.71379300	-0.26524000
C	3.16864200	4.20666000	0.39518700	H	5.51279300	-1.55670500	-1.09075100
H	2.23979100	2.69880900	1.61709200	C	7.87078300	0.33537600	0.46402300
C	3.14863400	4.88962100	-0.82178000	H	7.47891700	2.16753800	1.53345300
H	2.15446700	5.10086400	-2.72516700	H	7.94393400	-1.49043800	-0.68048400
H	3.89431500	4.47227500	1.15857900	H	8.94358800	0.37202700	0.62864000
H	3.86991700	5.67773100	-1.01812400	C	-1.43629500	2.96870100	-0.50289800
H	-0.18889000	-1.33603200	1.32334200	C	-2.65155600	2.94345200	0.20077900
C	3.22269400	0.04003200	-1.01443400	C	-1.09422100	4.12923600	-1.21788200
C	2.72072400	-1.22674100	-0.78230300	C	-3.51217100	4.04085300	0.16983600
H	2.64797500	0.78047800	-1.55791800	H	-2.90507800	2.08450200	0.81330400

C	-1.95970400	5.21960900	-1.25549300
H	-0.14416400	4.16209100	-1.74047600
C	-3.17372900	5.17771300	-0.56525000
H	-4.44141900	4.00942000	0.73086500
H	-1.68535100	6.10477200	-1.82190600
H	-3.84645400	6.02991600	-0.59162300
H	-0.12072700	-1.56304800	-0.99680000
C	-2.29426900	0.03050200	-1.09416000
C	-2.88078300	-0.67354400	0.12842700
H	-2.23969600	-0.64897400	-1.95139400
H	-2.89333700	0.89266500	-1.39020400
H	-3.61186300	-0.08423600	0.68280300
C	-3.29547000	-2.10763200	0.00575100
H	-3.60933800	-2.53327500	0.95507200
H	-2.55780400	-2.74442100	-0.48071200
Br	-4.92089900	-2.21843800	-1.19815700

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SCF done: -1250.207469

C	-1.25649100	0.14879900	0.86081400
C	-2.58177500	-0.38468500	0.72725100
C	-3.26412800	0.53309200	-0.04130500
C	-1.22869900	1.35307300	0.13692500
O	-2.44727600	1.59374100	-0.40321100
N	-0.22185900	2.18616600	-0.01735200
C	-0.06520700	-0.20103500	1.50578200
C	1.06407300	0.64836500	1.36102400
C	0.93964000	1.83475500	0.55311200
Pd	1.73723200	-1.25823400	-0.09167800
Cl	0.38939500	-0.93999900	-1.94249300
C	-3.04608100	-1.71579700	1.25916800
C	-3.54075400	-1.67170800	2.68885700
H	-3.82336600	-2.13182600	0.61074500
H	-2.19420800	-2.40885700	1.19765300
H	-2.91232100	-1.12744800	3.39427100
C	-4.65903600	-2.25216500	3.12509900
H	-5.31367900	-2.80534300	2.45522800
H	-4.95649500	-2.20486700	4.16831100
C	-4.62333100	0.59118900	-0.57038500
C	-4.88044400	1.29273600	-1.76366400
C	-5.69110700	-0.03826100	0.09497300
C	-6.16964700	1.34230100	-2.28555200
H	-4.06222700	1.78634400	-2.27625400
C	-6.97818800	0.01430000	-0.43667000

H	-5.52035800	-0.53327000	1.04444300
C	-7.22213600	0.69963700	-1.62831100
H	-6.35315200	1.88145000	-3.21020000
H	-7.79510600	-0.47091300	0.08956400
H	-8.22688600	0.73965300	-2.03862400
C	2.06346600	2.78678300	0.34136900
C	3.33620000	2.35818900	-0.06875100
C	1.83284100	4.16263700	0.50444700
C	4.35935100	3.28159400	-0.28588200
H	3.51109600	1.30606300	-0.27210500
C	2.85854800	5.08187200	0.29668000
H	0.84206100	4.49846200	0.79223900
C	4.12639200	4.64425600	-0.09469400
H	5.33290400	2.93543000	-0.62032400
H	2.66728500	6.14199700	0.43549000
H	4.92369000	5.36238600	-0.26261500
H	-0.03194500	-1.03657900	2.19831500
C	2.28902900	0.37583600	2.24139700
C	3.09157300	-0.77066600	1.64622200
H	1.95407600	0.11661700	3.25174800
H	2.90633400	1.27099500	2.31644100
H	4.03795600	-0.53720700	1.16532800
C	2.72918200	-2.08970800	1.78867400
H	1.89873800	-2.38610000	2.42413700
H	3.37359000	-2.88351900	1.43044100
Br	3.24117800	-2.68171800	-1.41277100

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SCF done: -1248.39459615

C	-1.82635900	-0.12259100	0.22483300
C	-3.11769300	-0.75559900	0.29374600
C	-3.97265800	0.08940700	-0.37755200
C	-1.99960800	1.06871700	-0.50281200
O	-3.30288800	1.19699200	-0.87730400
N	-1.09439200	1.97019000	-0.80047800
C	-0.51953500	-0.39748600	0.65003500
C	0.46416600	0.53220500	0.32402300
C	0.16591300	1.73406200	-0.36607100
Pd	2.33517100	0.01336800	0.77582300
C	-3.39846500	-2.09191100	0.93207100
C	-3.68902000	-2.01522400	2.41573900
H	-4.22338600	-2.59593800	0.41823900
H	-2.51043500	-2.72370500	0.78150900
H	-3.00772400	-1.39854300	3.00138400

C	-4.69031700	-2.64971100	3.02615600	N	-0.98160400	2.25177300	0.18572500
H	-5.38931600	-3.27702400	2.47694200	C	-0.41782400	-0.16262800	-1.20544300
H	-4.84240500	-2.57414000	4.09854600	C	0.62228300	0.74854400	-0.86937200
C	-5.39671300	0.03487200	-0.69959800	C	0.28414600	1.94705900	-0.13323700
C	-5.88305500	0.70468200	-1.83867000	Pd	1.03356800	-0.94552800	0.60166000
C	-6.30400200	-0.66976000	0.11262700	C	-3.34573100	-1.73921500	-1.64991000
C	-7.23470400	0.64890000	-2.16607600	C	-3.20884600	-2.96283600	-0.76845400
H	-5.19194400	1.26298100	-2.46036400	H	-4.34902700	-1.70603200	-2.08635200
C	-7.65508800	-0.72426100	-0.22519600	H	-2.64672600	-1.83364300	-2.49416900
H	-5.96013800	-1.13672200	1.02849000	H	-2.30087200	-3.01874800	-0.16815900
C	-8.12560500	-0.07084000	-1.36559900	C	-4.10245400	-3.94982000	-0.69946900
H	-7.59416100	1.16789600	-3.04990200	H	-5.01936900	-3.93417700	-1.28506100
H	-8.34478700	-1.26683800	0.41491500	H	-3.94514400	-4.81477200	-0.06251900
H	-9.17976900	-0.11289500	-1.62347900	C	-5.34706100	0.49177000	-0.16243600
C	1.16080000	2.78868700	-0.69194400	C	-6.00738200	1.73097400	-0.05848400
C	1.07938000	3.44716600	-1.93118000	C	-6.10230100	-0.69206100	-0.07605400
C	2.16426400	3.17284500	0.21372200	C	-7.38871900	1.78075400	0.10424900
C	1.99998900	4.43656900	-2.27001600	H	-5.42945000	2.64715700	-0.11003500
H	0.28445500	3.17422300	-2.61729200	C	-7.48553900	-0.63249600	0.08310100
C	3.08022600	4.16995000	-0.12723800	H	-5.60299000	-1.65426400	-0.09012400
H	2.20283100	2.72227100	1.20019800	C	-8.13427600	0.60071900	0.16903200
C	3.00777300	4.79809000	-1.37136200	H	-7.88552000	2.74356100	0.17940200
H	1.92961200	4.92888800	-3.23582600	H	-8.05576200	-1.55397500	0.15560700
H	3.84104800	4.46433300	0.58998000	H	-9.21202300	0.64272000	0.29587300
H	3.72255400	5.57225800	-1.63525100	C	1.29806500	2.95585300	0.27939900
H	-0.28067100	-1.29251600	1.21390000	C	1.05964200	4.31212600	0.00533600
C	3.08191800	-0.03438300	-1.34022700	C	2.45862100	2.60174600	0.98574500
C	2.56075000	-1.28326800	-1.06833700	C	1.97713200	5.28486600	0.39671500
H	2.50647300	0.70991700	-1.87761300	H	0.14950600	4.59190000	-0.51488700
H	4.14888800	0.15774500	-1.24429000	C	3.37120300	3.57810700	1.38532500
H	1.54783200	-1.51534500	-1.38584000	H	2.62149100	1.56385200	1.26229100
C	3.39068800	-2.44726600	-0.62962600	C	3.13752900	4.92082100	1.08387300
H	2.86964900	-3.10631600	0.06240900	H	1.78421900	6.32907600	0.16864200
H	4.35803800	-2.15517100	-0.22093500	H	4.25738400	3.28970000	1.94284800
Br	2.06380800	0.43487200	3.17277500	H	3.84983700	5.68027200	1.39257100
Br	3.81393800	-3.61117700	-2.21078900	H	-0.21869700	-0.99061600	-1.87992600

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SCF done: -1248.416323

C	-1.73169800	0.13929100	-0.80488500	H	1.94692900	0.41191800	-2.56176200
C	-3.03857700	-0.44249400	-0.94530700	H	2.70062300	1.28347200	-1.22640700
C	-3.89948000	0.45317700	-0.34951100	H	2.24683600	-1.72532200	-1.45918300
C	-1.90251700	1.36514700	-0.14346200	C	3.85482800	-0.91533400	-0.27451500
O	-3.21556900	1.56263300	0.12956900	H	4.06987400	-1.86575700	0.20405300
				H	4.10192700	-0.08630500	0.38497500

Br	5.19015400	-0.76696300	-1.79220600
Br	1.93449100	-2.57668100	2.18517100

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SCF done: -1248.427202

C	-1.26928900	0.29770200	0.97700000
C	-2.58971400	-0.25352600	0.87613000
C	-3.27943200	0.61061100	0.05300900
C	-1.25159600	1.45722900	0.18321200
O	-2.47313800	1.65560500	-0.36975800
N	-0.25004700	2.28391500	-0.02526600
C	-0.07166600	-0.00836900	1.63498900
C	1.05005300	0.83929600	1.43736700
C	0.91625300	1.97296500	0.56135700
Pd	1.71602700	-1.20926000	0.11553100
C	-3.04172400	-1.55649600	1.48280700
C	-3.54649400	-1.43519500	2.90445000
H	-3.80951100	-2.01931300	0.85500700
H	-2.18119000	-2.24129800	1.46694200
H	-2.92892100	-0.84376900	3.58091400
C	-4.66117900	-2.00217900	3.36688400
H	-5.30515400	-2.60079400	2.72634300
H	-4.96612300	-1.89787700	4.40377400
C	-4.63626400	0.61963300	-0.48510700
C	-4.89416000	1.24269900	-1.72112800
C	-5.70017800	0.01729100	0.21074800
C	-6.17982100	1.24107000	-2.25386700
H	-4.07898500	1.71528900	-2.25782200
C	-6.98378000	0.01826000	-0.33181200
H	-5.52965800	-0.41559300	1.19011900
C	-7.22812400	0.62479400	-1.56535400
H	-6.36381500	1.71901400	-3.21151100
H	-7.79779500	-0.44539200	0.21780300
H	-8.23001900	0.62439400	-1.98450900
C	2.03356800	2.91707000	0.28804700
C	3.30799600	2.47133900	-0.09763700
C	1.79535800	4.29902500	0.36589200
C	4.32556100	3.38518300	-0.37359800
H	3.48887700	1.40954500	-0.23440500
C	2.81528100	5.20947200	0.09913600
H	0.80317800	4.64634500	0.63464100
C	4.08505700	4.75569600	-0.26683400
H	5.30070600	3.02446300	-0.68741600
H	2.61809800	6.27507100	0.17227000

H	4.87796900	5.46657200	-0.48024300
H	-0.03352100	-0.79970700	2.37764200
C	2.27983100	0.62552100	2.32636300
C	3.08466000	-0.55723100	1.81338900
H	1.94795800	0.43558400	3.35308500
H	2.89609200	1.52455200	2.33996400
H	4.01652000	-0.35362800	1.29210100
C	2.74412900	-1.86161600	2.07335500
H	1.92581500	-2.11318400	2.74291300
H	3.38885700	-2.67613400	1.76617500
Br	3.24420100	-2.71590100	-1.08132100
Br	0.29673700	-1.10186700	-1.88428100

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SCF done: -1564.280896

C	-0.32508500	0.43063800	-1.21150800
C	-0.39462800	1.69658100	-0.50889500
C	-1.71569500	2.02906800	-0.44197200
C	-1.72381800	0.06668400	-1.52501600
O	-2.53026700	1.05782900	-1.02754100
N	-2.10252900	-0.98574800	-2.13689100
S	-3.76877800	-1.28472200	-2.49968100
O	-3.73337300	-2.50411200	-3.31927800
O	-4.40882800	-0.04514800	-2.98244600
C	0.72481300	-0.37077600	-1.54124000
H	0.51329800	-1.31647600	-2.03663500
C	2.07499800	-0.08919700	-1.22920100
C	3.30007500	0.05617500	-1.10627600
Pd	2.41087900	-0.34263300	1.01306600
Cl	2.01894200	-0.71384500	3.28329400
C	0.77933500	2.43525000	0.07767500
C	1.41621000	1.80475600	1.30028300
H	1.54051600	2.61052900	-0.69028400
H	0.44311800	3.42369300	0.41019300
H	0.74283300	1.51254600	2.10276300
C	2.76234300	1.85605300	1.56193300
H	3.45844600	2.26518500	0.83401300
H	3.13739100	1.67137700	2.56207100
Br	2.80651300	-2.77023200	0.66953200
C	-4.43977800	-1.70170200	-0.88789300
C	-4.16649600	-2.95817300	-0.34042300
C	-5.25021500	-0.78281800	-0.22289600
C	-4.69608000	-3.27893200	0.90561900
H	-3.55887200	-3.66851900	-0.89048300

C	-5.77979000	-1.12723600	1.02106900	H	0.96163200	1.83799300	-0.13393200
H	-5.46846200	0.17197400	-0.68845200	C	2.24783000	0.08497400	0.05171900
C	-5.50608300	-2.37074700	1.60704500	C	3.47002900	0.57335000	0.34509200
H	-4.48501900	-4.25281100	1.33924400	Pd	1.88349900	-1.51309700	-1.15143000
H	-6.42356100	-0.42271000	1.54127300	Cl	1.30863600	-3.24097200	-2.72085600
C	-2.44812600	3.15805400	0.13027100	C	0.51304900	-2.00605900	1.70820000
C	-3.68143500	2.93005400	0.76832700	C	1.06030700	-2.74777000	0.50676200
C	-1.95731800	4.47288100	0.04111900	H	1.34613000	-1.57801200	2.27884500
C	-4.38581700	3.99039300	1.33171200	H	0.04773500	-2.76694700	2.34414900
H	-4.07099900	1.91951900	0.82679900	H	0.34266700	-3.32313300	-0.07462900
C	-2.66920100	5.52941000	0.60469800	C	2.41199000	-3.02434900	0.33774400
H	-1.04292600	4.67366000	-0.50711400	H	3.14885200	-2.61984300	1.02545600
C	-3.88083200	5.29082900	1.25666500	H	2.72756000	-3.82549900	-0.32258800
H	-5.33207300	3.80242500	1.82982700	Br	5.02512400	-0.42663500	-0.29072200
H	-2.28488600	6.54139600	0.52111600	C	-4.13435400	2.06561800	-0.95725300
H	-4.43454100	6.11595200	1.69437800	C	-3.95214300	2.19472200	-2.33618300
C	4.69850800	0.33590700	-1.25305000	C	-5.12376700	1.23390600	-0.43499600
C	5.11025500	1.57435100	-1.78559300	C	-4.75785600	1.45371200	-3.19607800
C	5.66273000	-0.62188200	-0.88296200	H	-3.20114200	2.87659400	-2.72022900
C	6.46625500	1.84327900	-1.94998900	C	-5.92810400	0.50663500	-1.31268900
H	4.36420300	2.30626700	-2.07922300	H	-5.26138700	1.17889900	0.63917600
C	7.01485800	-0.33811400	-1.05146500	C	-5.75312900	0.59615400	-2.70065800
H	5.33224000	-1.56651500	-0.46361000	H	-4.62091500	1.54891800	-4.27009300
C	7.41949800	0.89004600	-1.58222200	H	-6.71104400	-0.13351300	-0.91407700
H	6.77919800	2.79598600	-2.36628100	C	-2.73296100	-1.78425600	2.39676000
H	7.75581400	-1.07793200	-0.76488500	C	-4.05323200	-1.91887400	1.92914800
H	8.47644400	1.10457000	-1.70900200	C	-2.33436800	-2.51365700	3.53097100
C	-6.05936800	-2.73106600	2.96439000	C	-4.93856600	-2.78544900	2.56448200
H	-6.82894500	-2.02397300	3.28505000	H	-4.37054100	-1.34900600	1.06252700
H	-6.49868200	-3.73390600	2.96144600	C	-3.22586100	-3.37850600	4.16227600
H	-5.26768400	-2.72897700	3.72317800	H	-1.34125100	-2.37184100	3.94396700

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SCF done: -1579.839086

C	-0.17095600	0.31181400	0.71514700	H	-5.22158200	-4.19472500	4.17310600
C	-0.48834400	-0.92946500	1.39776300	C	3.77667200	1.80397800	1.10436700
C	-1.81306600	-0.88000700	1.70704200	C	2.94354900	2.19786000	2.16992000
C	-1.43540000	1.06368200	0.65011000	C	4.87223100	2.62480600	0.77524900
O	-2.40614600	0.29979000	1.24002800	C	3.18424200	3.38278000	2.86308100
N	-1.59997700	2.21432400	0.11250400	H	2.11566400	1.56337000	2.46484900
S	-3.10871200	3.03423900	0.15788500	C	5.10719500	3.80806600	1.46949500
O	-2.82801400	4.32556000	-0.48950200	H	5.53698700	2.33248300	-0.03036400
O	-3.68698700	2.96383300	1.51544700	C	4.26424900	4.19433800	2.51478700
C	1.00511900	0.80970200	0.23038200	H	2.53004000	3.66502000	3.68251000

H	5.95256200	4.43126200	1.19306000
H	4.45270400	5.11603400	3.05700100
C	-6.60361600	-0.21872400	-3.64493800
H	-6.06146600	-1.10690100	-3.99222200
H	-7.52279000	-0.56195500	-3.16232600
H	-6.87974700	0.35809600	-4.53307200
Cl	2.25527300	0.02198500	-3.27253800
H	2.79368600	1.05017800	-2.71290900

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SCF done: -1579.847381

C	0.02727000	0.31563400	-0.70813800
C	0.10178800	1.21620700	0.42988500
C	-1.12023400	1.81267500	0.53714100
C	-1.35688700	0.44388100	-1.21762700
O	-2.00878400	1.36262700	-0.43848000
N	-1.84705800	-0.17467000	-2.22208800
S	-3.45132500	0.11496500	-2.78196900
O	-3.54463000	-0.68385900	-4.01278000
O	-3.73560600	1.56458500	-2.78206400
C	0.88944900	-0.56876700	-1.29097700
H	0.42247000	-1.24108900	-2.00990700
C	2.31267100	-0.84247600	-1.09171000
C	3.38218200	0.02131000	-1.00730300
Pd	1.68892800	-1.92507500	1.06693900
Cl	0.89755600	-3.06235900	2.91883900
C	1.23038500	1.29104500	1.42039300
C	1.43976200	0.03734900	2.24674500
H	2.16493500	1.57089200	0.93017400
H	1.01120600	2.08208000	2.14622800
H	0.60044700	-0.27760400	2.86230200
C	2.68078700	-0.50430000	2.50128400
H	3.57125200	-0.10837800	2.01988500
H	2.82989300	-1.18838700	3.32870000
Br	5.10519100	-0.82796900	-0.77147400
C	-4.45045900	-0.67569900	-1.51629900
C	-4.50745100	-2.07106900	-1.46608700
C	-5.17792800	0.11067800	-0.62440700
C	-5.28648100	-2.67816500	-0.48589700
H	-3.95684500	-2.66289100	-2.18925000
C	-5.96193100	-0.51691300	0.34434800
H	-5.13651000	1.19111800	-0.70882500
C	-6.02176000	-1.91420100	0.43519400
H	-5.33199000	-3.76290900	-0.43815600

H	-6.54331100	0.08818000	1.03526000
C	-1.69220200	2.77765400	1.47422800
C	-3.03738100	2.65100600	1.86792400
C	-0.93093900	3.84823500	1.97707000
C	-3.59242500	3.55577100	2.76860700
H	-3.63259900	1.83609900	1.47043300
C	-1.49360300	4.75015600	2.87756600
H	0.08610100	3.99754500	1.62966000
C	-2.82270400	4.60366700	3.28012900
H	-4.62891200	3.44402800	3.07219400
H	-0.89840200	5.57717900	3.25278400
H	-3.26005600	5.30921600	3.98015600
C	3.42993400	1.47713700	-1.20456700
C	2.52383000	2.08926900	-2.09682600
C	4.39865300	2.28476000	-0.57282900
C	2.57886900	3.45931000	-2.33262600
H	1.79331200	1.48519200	-2.62068400
C	4.43525400	3.65725000	-0.79807500
H	5.12015800	1.83014000	0.09687000
C	3.52700400	4.25023500	-1.67874000
H	1.88369300	3.90807800	-3.03535300
H	5.18152700	4.26313500	-0.29347100
H	3.56475400	5.31968100	-1.86283800
C	-6.84736300	-2.59093000	1.50240400
H	-6.20624300	-2.99871200	2.29331600
H	-7.54858800	-1.89454800	1.97003700
H	-7.42130400	-3.42731700	1.09087200
Cl	1.33176000	-3.83394500	-0.23015000
H	2.57846800	-1.87902900	-1.29785000

TS8-22

SCF done: -1564.247202

C	-0.33499200	-0.07077800	-0.94908400
C	-0.72041200	1.31340800	-1.12950700
C	-2.07346700	1.32783500	-1.29044400
C	-1.59007000	-0.84368700	-1.02464800
O	-2.61824400	0.04380500	-1.18997600
N	-1.70168800	-2.11494700	-0.92095200
S	-3.21513400	-2.91240900	-1.08190100
O	-2.87311700	-4.34085200	-0.99479400
O	-3.95895300	-2.36858800	-2.23638100
C	0.85688400	-0.70386300	-0.74685900
H	0.79257600	-1.79158700	-0.74856200
C	2.14793200	-0.18007400	-0.39762100

C	3.30410800	-0.77395500	-0.42333500
Pd	2.39576300	1.32263100	1.03006500
Cl	2.51925900	2.72240800	2.95462700
C	0.23385800	2.46351700	-1.23879300
C	1.01871500	2.86129000	-0.00686200
H	0.94097300	2.25877300	-2.05370700
H	-0.32271800	3.36060900	-1.53042600
H	0.45432800	3.16803000	0.87121500
C	2.34045300	3.24304500	-0.11458200
H	2.87252800	3.10672000	-1.05361600
H	2.81183200	3.86088500	0.64077800
Br	4.18653500	-0.32226100	1.83271200
C	-4.07681700	-2.45383300	0.42833500
C	-3.72989400	-3.08119900	1.62719600
C	-5.10449200	-1.51293500	0.37737500
C	-4.40858300	-2.73414500	2.79199600
H	-2.95155500	-3.83653900	1.63567900
C	-5.77903000	-1.18442800	1.55350200
H	-5.37288300	-1.06670800	-0.57378800
C	-5.43806000	-1.77959600	2.77611300
H	-4.14363200	-3.21871200	3.72811100
H	-6.59101900	-0.46243600	1.51989800
C	-3.06359300	2.37939300	-1.52720000
C	-4.30819100	2.31308800	-0.87376100
C	-2.81349500	3.44643400	-2.40804300
C	-5.26131700	3.30803700	-1.07373600
H	-4.51319600	1.48404200	-0.20493400
C	-3.77241000	4.43811800	-2.60457400
H	-1.88739000	3.47798300	-2.97188700
C	-4.99563900	4.37583700	-1.93439300
H	-6.21471900	3.25009000	-0.55720000
H	-3.56927500	5.25202400	-3.29403800
H	-5.74188000	5.14908700	-2.09035000
C	4.30092800	-1.44877500	-1.18800300
C	4.32538100	-1.20536000	-2.58275300
C	5.18389200	-2.40345700	-0.63843700
C	5.19156200	-1.92095100	-3.40154500
H	3.65632300	-0.46016700	-2.99931400
C	6.04950600	-3.10589300	-1.46565500
H	5.17292800	-2.57667400	0.43107800
C	6.05567000	-2.86804300	-2.84530100
H	5.20136100	-1.73359200	-4.47069700
H	6.72284300	-3.84214900	-1.03838300
H	6.73942000	-3.41770900	-3.48533400

C	-6.14992400	-1.39782500	4.05147800
H	-7.11887800	-0.93417800	3.84690200
H	-6.31704200	-2.26949800	4.69166000
H	-5.55668500	-0.68006600	4.63148200

TS9-10

SCF done: -1564.2333485

C	0.09233400	1.07036400	-1.25597800
C	-0.59591200	2.27436100	-1.16993300
C	0.20619500	3.13463800	-0.36280500
C	1.32251900	1.21685200	-0.47481600
O	1.33300400	2.49862300	0.05446000
N	2.23599800	0.34806900	-0.29624900
S	3.58104900	0.63439000	0.76192100
O	3.12258000	0.11053900	2.06299000
O	4.10137500	2.00751300	0.61620200
C	-0.27975400	-0.18900500	-1.92798600
H	0.00559100	-0.40487600	-2.95622600
C	-0.89880900	-1.02395600	-1.11956600
C	-1.49219800	-1.85678100	-0.29301400
Pd	-3.43572300	-1.84867900	-0.39647900
Cl	-3.64663600	-3.49269000	-2.03894300
C	-1.87080100	2.57970600	-1.91590100
C	-3.12710500	2.64642200	-1.07249600
H	-1.75091700	3.50702000	-2.48994300
H	-1.99432800	1.76971900	-2.64657200
H	-3.24648600	1.87262700	-0.31610200
C	-4.09456000	3.54609900	-1.26294300
H	-4.02621500	4.32042500	-2.02637800
H	-5.00478100	3.52081900	-0.67195800
Br	-3.78490400	-0.18938300	1.42119500
C	4.74531800	-0.50471800	0.02675200
C	4.35680900	-1.82774100	-0.20883800
C	6.03549100	-0.06234300	-0.25791600
C	5.28345100	-2.70708300	-0.75534000
H	3.35033900	-2.15493300	0.02934200
C	6.95096000	-0.96360700	-0.79942600
H	6.31153700	0.96554200	-0.04975300
C	6.59149900	-2.29297500	-1.05966900
H	4.99163300	-3.73661400	-0.94483300
H	7.96076800	-0.62928800	-1.02131800
C	0.12318700	4.51401500	0.02324800
C	1.26983300	5.13803700	0.57960200
C	-1.06845600	5.26229100	-0.12865800

C	1.22308900	6.47086300	0.95097100	H	-1.82338300	-4.87672000	3.30063400
H	2.18186600	4.56207200	0.70108200	Br	3.36838900	-1.62895500	2.40050500
C	-1.10030100	6.59752300	0.25292300	C	-4.18932700	-1.88313300	-0.85855000
H	-1.97281200	4.78624800	-0.48928500	C	-5.12242200	-0.93896500	-0.39258700
C	0.04179500	7.20477200	0.78681000	C	-4.65724200	-3.05856700	-1.47248600
H	2.10449300	6.94410300	1.37051400	C	-6.48801000	-1.18089800	-0.51598100
H	-2.01850100	7.16487100	0.14813200	H	-4.76833300	-0.02662600	0.07503300
H	0.00817800	8.24985800	1.08239100	C	-6.02497700	-3.29485400	-1.59096500
C	-0.83589900	-2.76933300	0.65031500	H	-3.95023300	-3.76720900	-1.88988300
C	0.28778500	-2.33446700	1.38380800	C	-6.94410300	-2.36009400	-1.11010200
C	-1.31397500	-4.08024500	0.84160200	H	-7.19927300	-0.44814700	-0.14652800
C	0.91054200	-3.18804300	2.28657600	H	-6.37276200	-4.20312500	-2.07368500
H	0.66059600	-1.32551200	1.25414700	H	-8.00977000	-2.54485200	-1.20666100
C	-0.67526300	-4.93240000	1.73693800	C	2.46862200	1.76109500	-0.59029600
H	-2.17210200	-4.41404000	0.26697900	C	2.60730500	2.56963700	0.56130200
C	0.43341100	-4.49292100	2.46458600	C	2.93876200	2.22044100	-1.84069200
H	1.76319000	-2.83044700	2.85937300	C	3.20537800	3.81741500	0.45573900
H	-1.04731700	-5.94524800	1.87043400	H	2.26467700	2.19051400	1.51834900
H	0.91897500	-5.15675900	3.17263100	C	3.53665000	3.47018000	-1.92918700
C	7.57667900	-3.26107300	-1.66586800	H	2.85156000	1.57425800	-2.70612800
H	7.32649400	-3.46948800	-2.71303000	C	3.66441100	4.26811200	-0.78777400
H	8.59679300	-2.86740600	-1.63980800	H	3.32391600	4.43883400	1.33772000
H	7.56902500	-4.22092500	-1.13564600	H	3.90601600	3.82494500	-2.88578700

TS10-11

SCF done: -1564.254975

C	-0.52415600	-1.51885700	-0.44733200
C	-1.67745200	-2.40204500	-0.43012000
C	-2.75803500	-1.62871300	-0.71374700
C	-1.04633400	-0.18851600	-0.73585500
O	-2.38723900	-0.27463400	-0.88658500
N	-0.34616500	0.89609900	-0.82087200
C	0.79663400	-1.79410400	-0.25577400
C	1.82723000	-0.80092300	-0.30020300
C	1.88662400	0.47899200	-0.48193100
Pd	3.73076800	-1.33843400	-0.02415800
Cl	4.31460300	-1.21669300	-2.27823700
C	-1.62517500	-3.86090300	-0.05022500
C	-1.31165800	-4.06651000	1.41807300
H	-2.57406400	-4.34745500	-0.28307200
H	-0.85829500	-4.35617900	-0.66384900
H	-0.38675900	-3.62543400	1.78671200
C	-2.09285000	-4.74467300	2.25719900
H	-3.02739400	-5.19663100	1.93252800

H	-1.82338300	-4.87672000	3.30063400
Br	3.36838900	-1.62895500	2.40050500
C	-4.18932700	-1.88313300	-0.85855000
C	-5.12242200	-0.93896500	-0.39258700
C	-4.65724200	-3.05856700	-1.47248600
C	-6.48801000	-1.18089800	-0.51598100
H	-4.76833300	-0.02662600	0.07503300
C	-6.02497700	-3.29485400	-1.59096500
H	-3.95023300	-3.76720900	-1.88988300
C	-6.94410300	-2.36009400	-1.11010200
H	-7.19927300	-0.44814700	-0.14652800
H	-6.37276200	-4.20312500	-2.07368500
H	-8.00977000	-2.54485200	-1.20666100
C	2.46862200	1.76109500	-0.59029600
C	2.60730500	2.56963700	0.56130200
C	2.93876200	2.22044100	-1.84069200
C	3.20537800	3.81741500	0.45573900
H	2.26467700	2.19051400	1.51834900
C	3.53665000	3.47018000	-1.92918700
H	2.85156000	1.57425800	-2.70612800
C	3.66441100	4.26811200	-0.78777400
H	3.32391600	4.43883400	1.33772000
H	3.90601600	3.82494500	-2.88578700
H	4.13276500	5.24510100	-0.86478600
H	1.10519000	-2.81157100	-0.04976100
S	-1.10421600	2.39909800	-1.28805300
O	-1.97707400	2.15314700	-2.44882500
O	0.01413600	3.35139800	-1.35025400
C	-2.11636800	2.81167500	0.13497000
C	-3.50205100	2.68165900	0.05074600
C	-1.50240200	3.31686000	1.28394500
C	-4.28020600	3.04728600	1.14909500
H	-3.95183200	2.31599100	-0.86544400
C	-2.29575700	3.66633500	2.37226900
H	-0.42589600	3.44619900	1.31264200
C	-3.69326600	3.53434300	2.32535000
H	-5.36190000	2.96259700	1.08781200
H	-1.82599000	4.05932800	3.26992900
C	-4.53756600	3.90079600	3.52137500
H	-5.58428600	4.04956700	3.24342000
H	-4.50574500	3.10833200	4.27907400
H	-4.17693700	4.81743300	3.99804900

TS12-13

SCF done: -1812.813056

C	0.81208000	-1.67346200	-0.03077500
C	2.10374600	-2.31919700	-0.02669600
C	3.02493500	-1.31371200	0.14230100
C	1.05455200	-0.30542900	0.14984700
O	2.39380900	-0.07524500	0.27453300
N	0.16225400	0.66411700	0.21711600
C	-0.53231600	-2.06066000	-0.08980200
C	-1.50630500	-1.06609700	-0.01183500
C	-1.14181300	0.30610200	0.08488800
Pd	-3.36374900	-1.64545000	0.12382100
Cl	-3.42895400	-1.39750300	2.48262000
C	2.32431100	-3.80649300	-0.13752400
C	2.37709700	-4.30860500	-1.56445900
H	3.23559600	-4.09939900	0.39373000
H	1.48980400	-4.30382900	0.37761200
H	1.57659500	-3.96297900	-2.21778900
C	3.30698400	-5.13545400	-2.04338900
H	4.11665200	-5.50972100	-1.42028000
H	3.28441900	-5.48181300	-3.07217100
Br	-3.56349800	-2.20243200	-2.28313200
C	4.48096400	-1.26951700	0.24385100
C	5.10784300	-0.21625300	0.93950300
C	5.28312200	-2.25968300	-0.35400100
C	6.49520300	-0.17241200	1.05035600
H	4.50136800	0.56117200	1.39172200
C	6.67044000	-2.21059900	-0.23128900
H	4.82299200	-3.04203600	-0.94683600
C	7.28252100	-1.17190300	0.47310100
H	6.96304600	0.64355300	1.59362700
H	7.27591300	-2.97999300	-0.70163600
H	8.36413100	-1.13623300	0.56381700
C	-2.13304700	1.41269500	-0.00787700
C	-3.10153800	1.40481900	-1.02777600
C	-2.09270200	2.49927700	0.88090200
C	-4.00663800	2.45950600	-1.14923900
H	-3.13765800	0.58010300	-1.73159800
C	-3.00527400	3.54770400	0.75813700
H	-1.36239100	2.51160900	1.68018500
C	-3.96437100	3.53294400	-0.25777900
H	-4.74629400	2.43722200	-1.94436000
H	-2.97042200	4.37215200	1.46482500
H	-4.67549200	4.34922800	-0.34978700
H	-0.82149500	-3.10157500	-0.18268700

S	1.51469000	3.09386400	0.84938900
O	2.84964300	2.71850700	1.33557900
O	0.69088300	4.20925200	1.32803200
C	1.46406000	3.06849300	-0.93322100
C	2.52248200	2.47999000	-1.62927400
C	0.35607400	3.63824200	-1.57050300
C	2.47699400	2.50865100	-3.01935100
H	3.34933100	2.02343500	-1.10045000
C	0.34115300	3.64190100	-2.95917100
H	-0.46104300	4.05893000	-0.99703600
C	1.39081600	3.07645700	-3.70495300
H	3.29920800	2.07661800	-3.58199200
H	-0.50568600	4.08525000	-3.47457000
C	1.33004600	3.05799200	-5.21017500
H	0.61169000	2.30460000	-5.55530000
H	0.99950200	4.02319000	-5.60629300
H	2.30093500	2.81849700	-5.65034200
C	0.66017500	0.86349800	3.16523500
O	0.54716700	2.05790600	2.81889400
H	1.49321700	0.24676500	2.80160300
N	-0.18030400	0.23082000	3.98235800
C	-0.05607800	-1.19912300	4.25284200
H	0.03636500	-1.37331100	5.33013900
H	-0.94667100	-1.71250300	3.87432400
H	0.83028400	-1.59471800	3.75229800
C	-1.35891700	0.90485300	4.53041300
H	-1.39459600	0.74358600	5.61254400
H	-1.28320700	1.97053100	4.32200500
H	-2.25923500	0.48812700	4.06742800

TS13-14

SCF done: -1812.833171

C	2.40638600	-1.10911200	-0.18721500
C	3.69724100	-1.24410400	-0.81234300
C	4.61093700	-0.87803800	0.14943300
C	2.64531400	-0.68890500	1.13551100
O	3.98469200	-0.54451100	1.34271800
N	1.76332800	-0.46066800	2.08246000
C	1.06624300	-1.27820400	-0.56283600
C	0.10489000	-1.03130100	0.41073000
C	0.47425500	-0.66072200	1.72994200
Pd	-1.83754200	-0.98078600	0.01998500
C	3.93334500	-1.74489700	-2.21445900
C	3.83997300	-0.66845000	-3.27384400

H	4.90242000	-2.24950500	-2.28301800
H	3.17051500	-2.50867700	-2.42423300
H	2.96845100	-0.01710900	-3.21124200
C	4.72413600	-0.48880200	-4.25569400
H	5.60295400	-1.12226000	-4.35682500
H	4.59621300	0.28899700	-5.00258600
C	6.06983400	-0.81156300	0.18249500
C	6.74990100	-0.95305800	1.40761900
C	6.82061400	-0.59906500	-0.98853200
C	8.14028900	-0.90674100	1.45255400
H	6.17740400	-1.10366500	2.31615300
C	8.21278500	-0.55911700	-0.93523600
H	6.31342600	-0.42507400	-1.93071000
C	8.87879400	-0.71648000	0.28164400
H	8.64994600	-1.02269900	2.40478800
H	8.77809600	-0.38982700	-1.84728300
H	9.96373000	-0.68230500	0.31938300
C	-0.55184600	-0.44926100	2.77484500
C	-0.43421400	0.61375400	3.68271800
C	-1.68011700	-1.29137200	2.85345700
C	-1.44236000	0.86099700	4.60936900
H	0.44616300	1.24592500	3.63732000
C	-2.69498000	-1.03177100	3.78376400
H	-1.71877900	-2.20327300	2.26347500
C	-2.58317700	0.04701700	4.65527800
H	-1.34760200	1.69707800	5.29668300
H	-3.55532000	-1.69239800	3.83341300
H	-3.36706200	0.25014300	5.37904500
H	0.78333400	-1.57161200	-1.56645300
S	-2.29949400	2.27312300	-0.58691100
O	-1.97797800	1.31229200	0.55146700
O	-3.68339500	2.84293300	-0.69262400
C	-1.11565800	3.62738200	-0.39132700
C	0.17973600	3.34744900	0.04815500
C	-1.49712100	4.90420000	-0.80289900
C	1.09734400	4.39235000	0.10913000
H	0.45383900	2.34217700	0.34814500
C	-0.55986600	5.93306100	-0.72835800
H	-2.50741400	5.08295700	-1.15350800
C	0.74606200	5.69694800	-0.27500800
H	2.10553700	4.19079300	0.46120300
H	-0.84891000	6.93631100	-1.02994700
C	1.74866700	6.82089700	-0.18074100
H	2.75682000	6.47922500	-0.43361800

H	1.48964200	7.64674100	-0.84892600
H	1.78927000	7.22349000	0.83904800
C	-4.70888600	-1.44043800	-1.02627900
O	-4.03641200	-0.75475900	-0.23643600
H	-4.36456500	-2.42802600	-1.36078900
N	-5.88769900	-1.04188800	-1.52485500
C	-6.68388100	-1.91655500	-2.37205600
H	-7.64543200	-2.14589000	-1.89785300
H	-6.87825600	-1.43899900	-3.33867800
H	-6.14804500	-2.85210100	-2.54464500
C	-6.42659400	0.27630500	-1.19886700
H	-7.23475100	0.19460900	-0.46240100
H	-5.62826000	0.89979200	-0.79671900
H	-6.82506500	0.73584600	-2.10841200
Br	-1.84701500	-3.49011200	-0.25164100
Cl	-1.58511000	0.05266300	-2.18894400

TS13-15

SCF done: -1812.832607

C	2.48008800	-1.17874400	-0.07568600
C	3.77136000	-1.32172300	-0.69776700
C	4.67805800	-0.85885300	0.22845800
C	2.71210200	-0.65714600	1.21101300
O	4.04777600	-0.45818400	1.39849900
N	1.82812100	-0.39495200	2.14690200
C	1.14328500	-1.41267300	-0.42805300
C	0.17732100	-1.11799100	0.52775400
C	0.54292400	-0.65619400	1.81968500
Pd	-1.76621300	-1.17797100	0.14174200
Cl	-1.67792800	-3.55137000	0.10835100
C	4.01593500	-1.91738600	-2.06067500
C	3.87998100	-0.92599100	-3.19572500
H	5.00103300	-2.39333100	-2.09934500
H	3.27808100	-2.71954700	-2.20699700
H	2.98628200	-0.30254900	-3.17474100
C	4.75269100	-0.78817900	-4.19444800
H	5.65296100	-1.39618400	-4.25553300
H	4.59390000	-0.07203200	-4.99514500
Br	-1.60682600	-0.23720900	-2.31054400
C	6.13431500	-0.74599400	0.24569900
C	6.82481100	-0.77632200	1.47282300
C	6.87223100	-0.59770300	-0.94328200
C	8.21336200	-0.68499600	1.50386100
H	6.26175600	-0.87683800	2.39409800

C	8.26280300	-0.51228200	-0.90347500	H	-7.32587800	-0.58633500	-0.20779500
H	6.35505000	-0.50846100	-1.89187200	H	-5.80616900	0.21021700	-0.70095000
C	8.93967400	-0.55963700	0.31668100	H	-7.00813800	-0.26872200	-1.93069700
H	8.73127400	-0.71500300	2.45823600				
H	8.81790800	-0.39357500	-1.82966900	TS16-17			
H	10.02325700	-0.49032800	0.34375700	SCF done: -1250.153863			
C	-0.47210700	-0.43287800	2.87459100	C	2.04133400	-0.34723500	0.20504300
C	-0.38535700	0.68420900	3.71883600	C	3.39127100	-0.77996900	0.46110500
C	-1.54644700	-1.33034800	3.03873800	C	4.17679000	0.32655200	0.23214600
C	-1.37357600	0.92695100	4.66815400	C	2.11485500	1.01514600	-0.14742100
H	0.45659500	1.35945300	3.60892400	O	3.40950900	1.42785700	-0.12608900
C	-2.53941600	-1.07767100	3.99317900	N	1.12765500	1.83002900	-0.43787600
H	-1.56195800	-2.26482600	2.48468200	C	0.75503400	-0.88436600	0.28626500
C	-2.46102400	0.05259600	4.80159100	C	-0.32862500	-0.06602000	-0.07391200
H	-1.30378300	1.80416700	5.30538300	C	-0.11658300	1.30329200	-0.42074500
H	-3.35808900	-1.78136500	4.11126100	Pd	-1.86478400	-1.21418300	-0.85319500
H	-3.22965300	0.25009700	5.54318300	Cl	-3.18202600	-2.60215200	-2.18137100
H	0.86837000	-1.79346100	-1.40412400	C	3.79000300	-2.15336100	0.93725900
S	-2.45476900	2.00960500	-0.57164200	C	3.99446000	-3.15751100	-0.17704400
O	-2.01218300	1.07698800	0.55392400	H	4.69299100	-2.09526700	1.55350200
O	-3.88040300	2.46973400	-0.61946400	H	2.99039500	-2.52033600	1.59788600
C	-1.37272500	3.44996000	-0.41245700	H	3.21628900	-3.18735600	-0.93934600
C	-0.04478000	3.27259200	-0.01843700	C	5.03297200	-3.98884200	-0.26567400
C	-1.86827800	4.69363900	-0.80344600	H	5.82783500	-3.99088100	0.47720300
C	0.78843000	4.38685200	0.01658700	H	5.12202200	-4.70451200	-1.07719900
H	0.31868400	2.29189100	0.26728700	C	5.61151300	0.58182100	0.33208300
C	-1.01339100	5.79351300	-0.75597200	C	6.07470000	1.88359600	0.60299100
H	-2.90120900	4.79259600	-1.11784400	C	6.54999000	-0.45168300	0.15745800
C	0.32191000	5.66048100	-0.34901500	C	7.43852600	2.13568200	0.71982300
H	1.82076400	4.26520400	0.33364300	H	5.35751300	2.68793600	0.72366600
H	-1.39124100	6.77140000	-1.04210500	C	7.91348100	-0.19096400	0.28001400
C	1.23618100	6.85930200	-0.28461200	H	6.21503300	-1.44613900	-0.11461400
H	2.24996900	6.60620300	-0.60941300	C	8.36316100	1.09945900	0.56580800
H	0.87035100	7.67689800	-0.91155100	H	7.78116100	3.14393800	0.93319000
H	1.31061200	7.23906400	0.74192900	H	8.62723500	-0.99693400	0.13648400
C	-4.62804200	-2.00967300	-0.66781400	H	9.42670600	1.29899000	0.65789400
O	-3.98050900	-1.11823100	-0.09189900	C	-1.20826100	2.26290300	-0.73112400
H	-4.19535100	-3.00341000	-0.84242600	C	-1.12641500	3.56688000	-0.20973500
N	-5.88115900	-1.83449100	-1.11263200	C	-2.30584300	1.93554900	-1.54525900
C	-6.62821000	-2.92766600	-1.71498100	C	-2.12854800	4.49988700	-0.46449300
H	-7.52186700	-3.15888500	-1.12340100	H	-0.26663500	3.83431500	0.39528200
H	-6.94308700	-2.66257100	-2.73041600	C	-3.30638800	2.87407800	-1.80486600
H	-6.00126600	-3.82030000	-1.76397700	H	-2.36166700	0.95679200	-2.01518600
C	-6.54570000	-0.54125200	-0.97672400	C	-3.22544700	4.15576900	-1.25868800

H	-2.05303100	5.49826800	-0.04358500
H	-4.13792700	2.60515400	-2.44966900
H	-4.00446900	4.88503200	-1.46055900
H	0.58783200	-1.90405700	0.62262200
C	-1.94925800	-0.33034100	1.25690000
C	-3.07615700	-1.10641100	0.82871900
H	-1.28448700	-0.77338200	1.98925400
H	-2.07977300	0.74389500	1.34161800
H	-3.14999100	-2.13152600	1.18733700
C	-4.38366000	-0.46851200	0.47400200
H	-4.98920300	-1.10224500	-0.16832300
H	-4.27516200	0.52893000	0.05262900
Br	-5.45986400	-0.22191600	2.15886000

TS17-18

SCF done: -1250.17037

C	-1.12756900	0.28135100	0.54664200
C	-2.39185900	-0.39218500	0.52047500
C	-3.27024900	0.51488400	-0.03852200
C	-1.33436800	1.55910500	-0.00641100
O	-2.63622600	1.70057500	-0.37083000
N	-0.46939700	2.53595200	-0.13091400
C	0.18051800	0.02160100	0.99534500
C	1.16232000	1.03858700	0.85866800
C	0.79406000	2.28796400	0.27734600
Pd	1.69552900	-1.34369300	-0.41742800
Cl	-0.05033900	-2.60203400	-1.41656100
C	-2.64586400	-1.81097000	0.96050300
C	-2.91561500	-1.95031500	2.44170600
H	-3.47634900	-2.23753800	0.38986000
H	-1.75909400	-2.39676100	0.68258500
H	-2.23357300	-1.41626400	3.10445600
C	-3.89676600	-2.68007400	2.97436400
H	-4.59785400	-3.23301300	2.35295300
H	-4.02655000	-2.76447800	4.04920900
C	-4.68958000	0.46066500	-0.37452100
C	-5.18847800	1.24452700	-1.43255300
C	-5.57891200	-0.35632300	0.34749100
C	-6.53694400	1.19122000	-1.77215300
H	-4.50916900	1.88384700	-1.98545900
C	-6.92734500	-0.40402700	-0.00043300
H	-5.22181900	-0.92120600	1.20112000
C	-7.41054300	0.36342800	-1.06200100
H	-6.90721300	1.79509400	-2.59538500

H	-7.60460800	-1.03462200	0.56814000
H	-8.46230600	0.32313000	-1.32984900
C	1.71162000	3.45979100	0.16566100
C	3.00337300	3.38105000	-0.37678800
C	1.23876100	4.71677100	0.58170600
C	3.80638300	4.51799800	-0.48047100
H	3.37442200	2.43726900	-0.76005300
C	2.04244700	5.84987900	0.48507100
H	0.23114000	4.79110400	0.97665800
C	3.33226700	5.75472100	-0.04329200
H	4.79843200	4.43643600	-0.91533200
H	1.66038000	6.80999000	0.81979300
H	3.95813900	6.63881900	-0.12211000
H	0.38654100	-0.85038500	1.61519400
C	2.56088900	0.71372100	1.36546800
C	3.27637800	-0.14296600	0.31969500
H	2.48174900	0.15812100	2.30793200
H	3.13111500	1.62413800	1.57464800
H	3.55515800	0.39780400	-0.58702800
C	4.20713100	-1.16578200	0.69255700
H	4.19108000	-1.54589900	1.71030600
H	5.17440400	-1.21057200	0.20609700
Br	3.50516100	-3.13498700	-0.39345200

TS19-20

SCF done: -1248.37394325

C	2.23491800	-0.22081500	0.33609700
C	3.57560000	-0.66563800	0.61889600
C	4.39385000	0.35778300	0.19839400
C	2.34788900	1.06532100	-0.22843300
O	3.65688600	1.42193300	-0.30565500
N	1.38315400	1.86389900	-0.62186000
C	0.93242300	-0.68510300	0.53390200
C	-0.12880200	0.11001300	0.07171900
C	0.12200700	1.39631100	-0.49490600
Pd	-1.72459100	-1.09053400	-0.47981200
C	3.93920900	-1.96702800	1.28667500
C	4.05990000	-3.13537500	0.33136700
H	4.86738300	-1.85651300	1.85631700
H	3.15277300	-2.19445000	2.02162400
H	3.24952400	-3.24604500	-0.38886100
C	5.06243800	-4.01418900	0.33150600
H	5.88783400	-3.93957800	1.03633300
H	5.09016300	-4.84623300	-0.36537000

C	5.83977800	0.56450300	0.21550600	C	0.81400900	2.43744400	0.25911400
C	6.35956200	1.87164800	0.27447900	Pd	1.71625900	-1.18567700	-0.29063500
C	6.73276800	-0.52156400	0.16791900	C	-2.65647300	-1.57916000	1.19854900
C	7.73499600	2.08178100	0.30873600	C	-2.94468200	-1.62194500	2.68256400
H	5.67677100	2.71378600	0.29681900	H	-3.47826300	-2.04443700	0.64595800
C	8.10850300	-0.30203100	0.20628600	H	-1.76650900	-2.18319200	0.97439800
H	6.35169400	-1.53060300	0.05875400	H	-2.27189500	-1.04381200	3.31704300
C	8.61500600	0.99676200	0.28143700	C	-3.93186900	-2.31751200	3.24864700
H	8.12161400	3.09547400	0.35818800	H	-4.62389600	-2.91139700	2.65557500
H	8.78683500	-1.14912100	0.16201400	H	-4.07624900	-2.33111000	4.32484100
H	9.68781200	1.16343400	0.30831200	C	-4.68450700	0.62028700	-0.28217500
C	-0.94405600	2.33308400	-0.93565100	C	-5.17292400	1.34525700	-1.38614500
C	-0.81614000	3.69782000	-0.62075300	C	-5.58275600	-0.14934200	0.47955400
C	-2.06215200	1.91827100	-1.67844800	C	-6.51970200	1.28022500	-1.73023400
C	-1.79540700	4.61102800	-1.00423900	H	-4.48664200	1.94773500	-1.97081300
H	0.06013100	4.02801700	-0.07298400	C	-6.92944400	-0.20953300	0.12662800
C	-3.03951000	2.83620800	-2.06781000	H	-5.23468300	-0.66641400	1.36649600
H	-2.15122900	0.88044800	-1.99057300	C	-7.40226000	0.49896200	-0.97960200
C	-2.91365900	4.18319600	-1.72461000	H	-6.88147700	1.83820400	-2.58887800
H	-1.68543400	5.65913500	-0.74152400	H	-7.61350400	-0.80324900	0.72595100
H	-3.88817100	2.49777000	-2.65500600	H	-8.45264500	0.44914800	-1.25120400
H	-3.67479300	4.89656500	-2.02661400	C	1.74179200	3.59283100	0.08252100
H	0.73872000	-1.63134400	1.03184300	C	3.03227600	3.47224900	-0.45516000
C	-1.73886200	0.12644400	1.45632900	C	1.28135200	4.87492500	0.43029900
C	-2.91528400	-0.64070300	1.17007200	C	3.84665600	4.59379700	-0.61943700
H	-1.08186100	-0.23510100	2.23868600	H	3.39246600	2.50555800	-0.78838500
H	-1.80874800	1.20613200	1.37221200	C	2.09636400	5.99306900	0.27326100
H	-3.03973300	-1.58913200	1.68937800	H	0.27471700	4.98025000	0.82066000
C	-4.19175100	0.00974300	0.73458700	C	3.38512000	5.85674600	-0.24872700
H	-4.85629400	-0.68235800	0.22472300	H	4.83752200	4.47922600	-1.04950000
H	-4.03940600	0.91298600	0.14730100	H	1.72409900	6.97356100	0.55587300
Br	-5.19985600	0.60742100	2.37460600	H	4.01981500	6.72904400	-0.37447700
Br	-3.14674200	-2.73474300	-1.64050000	H	0.38780200	-0.62478500	1.76137000
TS20-21				C	2.56698200	0.92002400	1.44947200
SCF done: -1248.388869				C	3.29840100	0.00514000	0.46810000
C	-1.12433300	0.46987100	0.65266800	H	2.47463300	0.42239800	2.42244800
C	-2.39465000	-0.19284600	0.66969000	H	3.13505800	1.84140900	1.61171200
C	-3.26612900	0.68473500	0.05622700	H	3.61793300	0.49838100	-0.45220500
C	-1.32127000	1.71339500	0.02476600	C	4.19661300	-1.01824100	0.91712000
O	-2.62221800	1.84332200	-0.34601400	H	4.14209500	-1.34606400	1.95168600
N	-0.44735600	2.67323700	-0.16028800	H	5.18062100	-1.09555100	0.46937700
C	0.18316100	0.22084900	1.10636800	Br	3.49107900	-3.00946000	-0.09303800
C	1.17397800	1.21821900	0.90885900	Br	-0.09833400	-2.49881600	-1.44599600

TS23-24

SCF done: -1579.8109586

C	-0.13212000	0.65502400	0.20581100
C	-0.31108600	0.09417000	1.53763500
C	-1.60425900	0.32700300	1.88939000
C	-1.44792900	1.22047800	-0.16365100
O	-2.30987000	0.98025200	0.87292500
N	-1.72896900	1.81510400	-1.25883800
S	-3.28580700	2.49163400	-1.55551400
O	-3.12911900	3.18672500	-2.84208700
O	-3.77323400	3.19811500	-0.35338500
C	0.93973200	0.72366900	-0.62381500
H	0.76798600	1.22977000	-1.57510900
C	2.24405100	0.06120500	-0.45053300
C	3.41466900	0.71063200	-0.18492900
Pd	1.88674300	-2.04616300	-0.33864300
Cl	1.26686300	-4.32098200	-0.43930800
C	0.75305900	-0.62016600	2.32342000
C	1.16312200	-1.97599100	1.78709800
H	1.64111000	0.01515100	2.42045800
H	0.38723400	-0.80445700	3.33943600
H	0.37862100	-2.72630100	1.71588200
C	2.48199100	-2.39965000	1.75232500
H	3.28955500	-1.71871900	2.00651900
H	2.71837600	-3.45658300	1.69734700
Br	5.03876200	-0.34619600	-0.19330000
C	-4.29870500	1.03172700	-1.82260600
C	-4.19171900	0.34252400	-3.03336300
C	-5.19478100	0.62615500	-0.83458000
C	-4.98134900	-0.78535900	-3.23683500
H	-3.51150100	0.69630100	-3.80051800
C	-5.98471800	-0.50122100	-1.06408600
H	-5.27708700	1.20354400	0.07882300
C	-5.88336800	-1.22787400	-2.25576000
H	-4.90422300	-1.32765800	-4.17551800
H	-6.69862300	-0.81382900	-0.30473800
C	-2.40683600	0.02428600	3.07535000
C	-3.74757100	-0.37238500	2.91991800
C	-1.87550000	0.13914800	4.37193300
C	-4.52388700	-0.67562300	4.03522400
H	-4.16655300	-0.44600200	1.92235500
C	-2.65836800	-0.16481400	5.48372300
H	-0.86437400	0.50671200	4.51251700
C	-3.98189100	-0.57809300	5.31903900

H	-5.55521200	-0.98533200	3.90259000
H	-2.23858200	-0.06677600	6.48001100
H	-4.59085300	-0.81259200	6.18692700
C	3.60838000	2.15278000	0.05692700
C	2.65662300	2.87859400	0.80090300
C	4.72383300	2.83817100	-0.46268900
C	2.81583600	4.24619400	1.01076400
H	1.80109800	2.36990000	1.22622800
C	4.86677500	4.20767900	-0.26521200
H	5.46867400	2.29491100	-1.03304900
C	3.91889200	4.91644600	0.47375000
H	2.08044500	4.78724900	1.59431600
H	5.72400500	4.72274800	-0.68755900
H	4.03697500	5.98409400	0.63537300
C	-6.70685600	-2.47525800	-2.47775700
H	-6.09637300	-3.38512600	-2.28346700
H	-7.57754500	-2.50599700	-1.79868700
H	-7.06706200	-2.53912500	-3.52244100
Cl	2.32230800	-1.53271500	-3.25531600
H	2.52851600	-0.47795900	-2.10974000

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SCF done: -1564.30263800

C	-0.53087600	-1.81397800	-0.33682300
C	-1.72243200	-2.63164000	-0.23843600
C	-2.77596400	-1.77258500	-0.38231300
C	-0.98230400	-0.50912000	-0.52913600
O	-2.32160400	-0.45151600	-0.55208800
N	-0.17581100	0.56514800	-0.67184800
C	0.84961500	-2.02602600	-0.30663300
C	1.70774700	-0.92000300	-0.35926800
C	1.19609700	0.38157000	-0.52373500
Pd	3.61018700	-1.24756700	-0.12249600
Cl	3.97136200	-1.57500300	-2.42353000
C	-1.74330900	-4.10730400	0.07015800
C	-1.24204900	-4.41398400	1.46576400
H	-2.75621600	-4.50031900	-0.04593600
H	-1.11462900	-4.62879100	-0.66793900
H	-0.23593300	-4.07218300	1.70702000
C	-1.95199400	-5.06526300	2.38640200
H	-2.96153800	-5.41939600	2.18604600
H	-1.54726800	-5.27266400	3.37183100
Br	3.45378700	-1.06551200	2.34287200
C	-4.23107900	-1.92677100	-0.37489000

C	-5.03945400	-0.99404900	0.29634700	C	0.03864600	1.07405700	-0.24818300
C	-4.84103100	-3.00203700	-1.04196100	O	-1.16673400	1.70437500	-0.18470600
C	-6.42400700	-1.14222900	0.31158400	N	0.13752200	-0.21185600	-0.51839100
H	-4.57372200	-0.16304500	0.82057100	C	2.39042000	1.49790700	0.02040500
C	-6.22858500	-3.15136000	-1.01648000	C	2.52910800	0.14632900	-0.27832600
H	-4.23260300	-3.70242900	-1.60437600	C	1.40472400	-0.66433400	-0.55559400
C	-7.02277500	-2.22307000	-0.34101500	Pd	4.15244000	-0.95758200	-0.24323500
H	-7.03760700	-0.42003300	0.83940500	C	1.15677600	4.53798000	0.62502200
H	-6.68649700	-3.98404400	-1.54083200	C	1.66593600	5.33145000	-0.55883700
H	-8.10222300	-2.33920100	-0.32634200	H	0.50923600	5.16862800	1.24259200
C	2.06508200	1.57691700	-0.40580600	H	2.01292800	4.26031000	1.25670700
C	1.59918200	2.68325900	0.32239700	H	2.21155700	4.76304700	-1.31167300
C	3.36637500	1.58759300	-0.93079300	C	1.50358900	6.64516700	-0.71878000
C	2.42123200	3.79139800	0.51399100	H	0.97092100	7.24853700	0.01324900
H	0.61533500	2.64816300	0.77882500	H	1.90861600	7.16853200	-1.57957400
C	4.17381000	2.70799300	-0.75170800	Br	5.60487700	0.44710400	1.10962900
H	3.73557700	0.72120700	-1.46825900	C	-2.09251600	3.88077900	0.24821200
C	3.70604700	3.81142100	-0.03242400	C	-3.31020700	3.31430300	0.67291700
H	2.06691000	4.63050100	1.10652500	C	-2.04587400	5.25754900	-0.03591200
H	5.17693400	2.71642900	-1.16913100	C	-4.44260600	4.11064500	0.82507100
H	4.34766300	4.67610300	0.11599800	H	-3.35533200	2.25294000	0.89173300
H	1.26434100	-3.02301300	-0.21288300	C	-3.18324800	6.04787200	0.12316100
S	-0.94538500	2.06450900	-1.62326600	H	-1.13100000	5.69899000	-0.41542800
O	-1.84609900	1.39100800	-2.56225100	C	-4.38322500	5.48093400	0.55590000
O	0.20274700	2.85899300	-2.04528600	H	-5.37181700	3.66227900	1.16491600
C	-1.86967100	2.91041800	-0.36203500	H	-3.13356700	7.10862200	-0.10495600
C	-3.21911400	2.58871000	-0.18388700	H	-5.26711500	6.10001600	0.67791800
C	-1.25377700	3.94215400	0.35215200	C	1.69468500	-2.08055900	-0.85922100
C	-3.94981300	3.30691100	0.75814800	C	2.83772300	-2.36919700	-1.65166800
H	-3.67687500	1.80585700	-0.77528700	C	0.94827500	-3.13981100	-0.32227700
C	-2.01017800	4.64114100	1.28933400	C	3.24792800	-3.70331000	-1.84089500
H	-0.21615500	4.19355600	0.16984000	H	3.25273600	-1.58957400	-2.29736000
C	-3.36039300	4.33278100	1.51203100	C	1.35166700	-4.45283000	-0.54166100
H	-5.00221600	3.07361600	0.90084400	H	0.06543800	-2.93293700	0.27047900
H	-1.54300400	5.44598000	1.84950800	C	2.51304300	-4.73946300	-1.27758700
C	-4.15694200	5.08255000	2.54937300	H	4.11405300	-3.91486500	-2.46105000
H	-5.22724900	5.06089700	2.32819100	H	0.76004000	-5.26196200	-0.12431500
H	-4.01692800	4.63358600	3.54112200	H	2.81949900	-5.77006100	-1.42741600
H	-3.84055500	6.12685700	2.61972500	H	3.24542600	2.11798000	0.25870400
11* Toluene				S	-3.52162400	-3.83115100	0.65973500
SCF done: -1564.32837094				O	-4.49653800	-4.92593600	0.59117300
C	1.07638700	1.99356700	0.00868000	O	-2.10943200	-4.01911800	0.29615400
C	0.44167800	3.26678500	0.24444700	C	-4.17751500	-2.37695300	-0.14111100
C	-0.90676800	3.03890200	0.10666800	C	-5.55479900	-2.30202100	-0.35200400

C	-3.30655800	-1.35926900	-0.53807300	H	7.17930500	-0.68824800	2.55596300
C	-6.06861300	-1.16803600	-0.97720600	H	6.86314200	-2.97061800	-1.07430600
H	-6.20062000	-3.11411500	-0.03792300	C	8.25495800	-2.84519900	1.27395500
C	-3.84774300	-0.23677300	-1.15768700	H	9.00308300	-2.29480600	1.85223200
H	-2.23552700	-1.42944100	-0.37786300	H	7.85513100	-3.63310000	1.92413100
C	-5.22926700	-0.12094800	-1.38456000	H	8.75994200	-3.33640400	0.43785900
H	-7.13871300	-1.09633400	-1.15017500	C	-0.46907900	-1.71243500	-0.23830300
H	-3.17950300	0.56432300	-1.45761800	H	0.25632900	-2.50897700	-0.40919900
C	-5.78651900	1.10628700	-2.06281200	C	-1.85247900	-1.96402200	-0.17442700
H	-5.49411000	1.13518800	-3.11910400	C	-3.07055900	-2.17729800	-0.24077900
H	-6.87838000	1.13026200	-2.01840700	C	-4.41876800	-2.64820300	-0.25228900
H	-5.40240300	2.02053300	-1.59834300	C	-4.74285100	-3.84788900	0.41792000
Cl	-3.49947800	-3.19329200	2.70236400	C	-5.43147300	-1.92695400	-0.91997500
TS2-4^{Toluene}				C	-6.05380400	-4.31003400	0.41212200
SCF done: -1449.29985516				H	-3.96241600	-4.39841300	0.93248400
C	-0.12756000	-0.39578700	-0.13911200	C	-6.74099600	-2.39877700	-0.91041600
C	-1.09615100	0.67260300	0.03370400	H	-5.17732200	-1.01192900	-1.44590100
C	-0.43800600	1.85303200	-0.11925000	C	-7.05409700	-3.58764600	-0.24736400
C	-0.72249800	3.27675400	-0.18971600	H	-6.29903500	-5.23405000	0.92644600
C	-1.98070100	3.75242700	-0.60080900	H	-7.51632100	-1.83982100	-1.42470000
C	0.30154600	4.19983700	0.10725900	H	-8.07658300	-3.95282500	-0.24388900
C	-2.21561600	5.12054600	-0.68484200	Pd	-2.92430500	0.04797400	0.47315700
H	-2.76440300	3.04990600	-0.85244100	Cl	-3.69804800	1.91334800	1.52472500
C	0.05323800	5.56649300	0.02562700	H	2.47326700	-1.48800500	-0.60460200
H	1.28269400	3.83895200	0.39554400	Cl	2.54169100	-3.02696300	-0.87542700
C	-1.20418100	6.03115000	-0.36721000	TS11-11^{Toluene}			
H	-3.19007600	5.47727400	-1.00417300	SCF done: -1564.25096029			
H	0.84512000	6.26974100	0.26486800	C	0.80536800	1.56934900	0.01004300
H	-1.39323400	7.09869700	-0.43393800	C	2.09978500	2.21006500	0.02093100
C	1.17163900	0.26808700	-0.29651300	C	3.00076200	1.24153100	-0.34376300
O	0.95899900	1.58757000	-0.30354000	C	1.04665500	0.24158500	-0.39013600
N	2.35712700	-0.24705000	-0.41455800	O	2.35256000	0.02822300	-0.59004700
S	3.78243200	0.80730600	-0.61846700	N	0.12060100	-0.70416600	-0.55050100
O	3.65923400	1.92101400	0.33786300	C	-0.51565400	1.95751400	0.26789200
O	3.90123100	1.02097400	-2.06806000	C	-1.47434100	0.96148000	0.10883400
C	5.06324500	-0.29729700	-0.05525600	C	-1.16092200	-0.33613700	-0.31022900
C	5.65955900	-0.05116800	1.18359000	Pd	-3.42532000	1.00030700	0.24813600
C	5.48961600	-1.33798500	-0.88270700	C	2.34143100	3.66945700	0.30921100
C	6.70213900	-0.87464200	1.59771100	C	2.51207700	3.98421900	1.77973900
H	5.31574800	0.77601600	1.79398000	H	3.21397000	4.02141400	-0.24989100
C	6.52972400	-2.15194600	-0.44351400	H	1.47966100	4.23225700	-0.07676900
H	5.01656300	-1.51112400	-1.84151700	H	1.76203200	3.56067200	2.44747700
C	7.14826400	-1.93724700	0.79645200	C	3.48632400	4.74129500	2.28468900

H	4.24950900	5.18862300	1.65154900	H	-5.08164100	-2.15811300	1.39891900
H	3.54880100	4.95417900	3.34751500	H	-4.38775800	-2.61316900	-2.82496800
Br	-3.79459600	3.39169800	0.44160900	H	-5.84599800	-2.92179400	-0.83842600
C	4.43936000	1.20949200	-0.58082100	H	-0.78559500	2.96488800	0.55895700
C	4.97005900	0.28760900	-1.50451600	S	0.73551400	-2.59120400	-1.20584200
C	5.30807200	2.08324600	0.09770200	O	2.06210500	-2.55614200	-1.83061100
C	6.33970300	0.25897200	-1.75168200	O	-0.46170100	-3.35843400	-1.57360400
H	4.30251300	-0.38834000	-2.02888700	C	1.05809600	-3.04027900	0.52368000
C	6.67675200	2.04838800	-0.16154000	C	2.33197200	-2.84336800	1.05673500
H	4.91701100	2.75897800	0.85035400	C	0.03452200	-3.61324300	1.28007400
C	7.19619000	1.14066100	-1.08690400	C	2.57100000	-3.21444600	2.37898600
H	6.73839500	-0.44984800	-2.47115100	H	3.11873200	-2.41956700	0.44446000
H	7.34031200	2.72374500	0.37052700	C	0.29680200	-3.97826900	2.59861100
H	8.26370400	1.11630800	-1.28518200	H	-0.93722000	-3.79140600	0.83446400
C	-2.38737600	-1.17276700	-0.48546600	C	1.56228600	-3.78032400	3.17156600
C	-3.21242500	-1.36173200	0.66007700	H	3.56313000	-3.06988700	2.79786800
C	-2.82192500	-1.63154700	-1.75012400	H	-0.49221200	-4.43641300	3.18918800
C	-4.46413900	-1.99739100	0.52056400	C	1.82464700	-4.15415300	4.60998500
H	-2.81606100	-1.16087600	1.65177800	H	1.24874200	-5.03589300	4.90573800
C	-4.05512200	-2.25974400	-1.85377700	H	2.88374100	-4.36382000	4.78272900
H	-2.16971500	-1.47663800	-2.60965000	H	1.53836400	-3.33721300	5.28397800
C	-4.88225100	-2.43326200	-0.72979400	Cl	0.05416100	-0.93362200	-3.42843800