

Supporting Information

Mechanism and Origins of Selectivity in Rhodium-Catalyzed Intermolecular [3+2] Cycloadditions of Vinylaziridines with Allenenes

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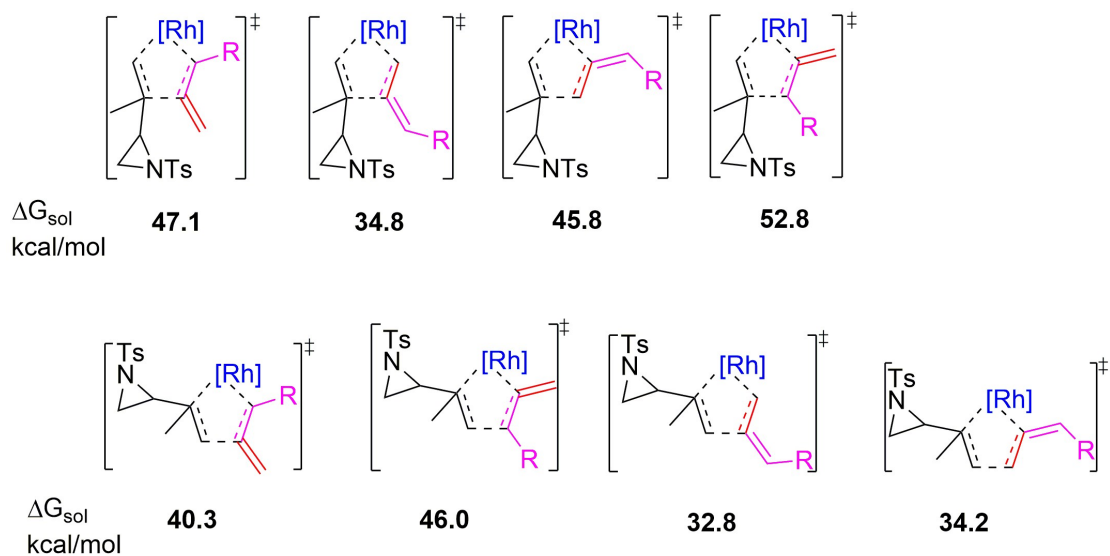
Web: <http://genpinghuang.weebly.com>

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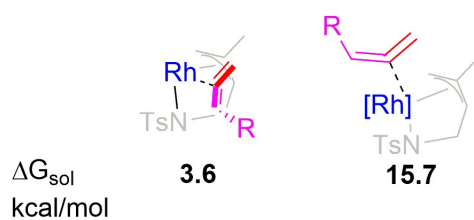
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1. Additional Results for Reaction with N-alleneamine 2a.

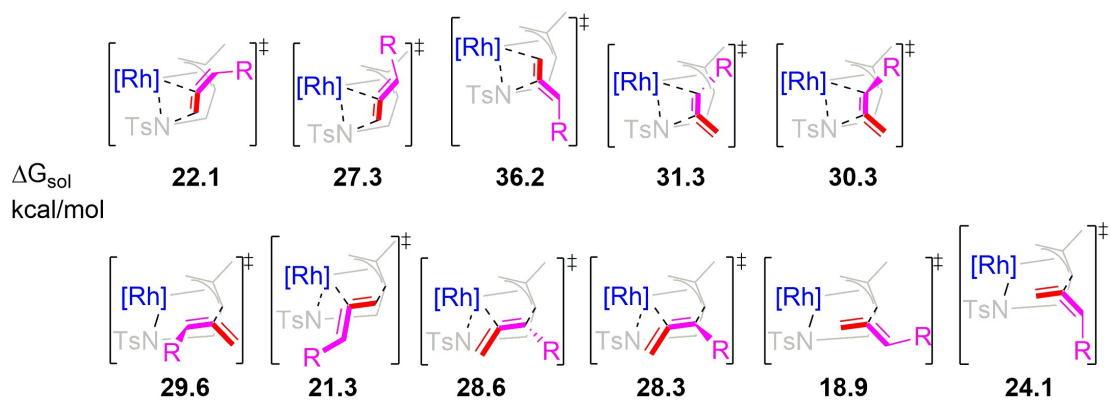
1.1. Oxidative cyclization of vinylaziridine and N-alleneamine 2a.



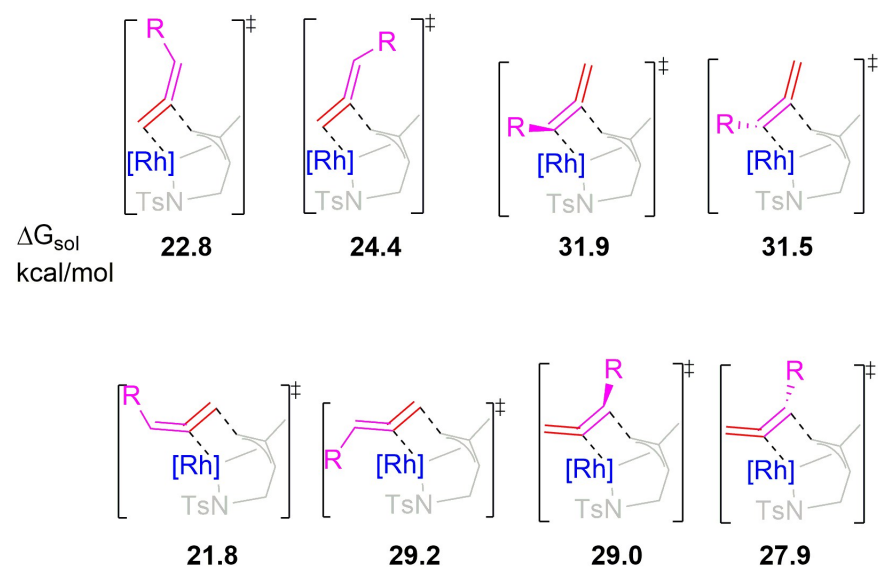
1.2. The complexations of INT2 with N-alleneamine 2a.



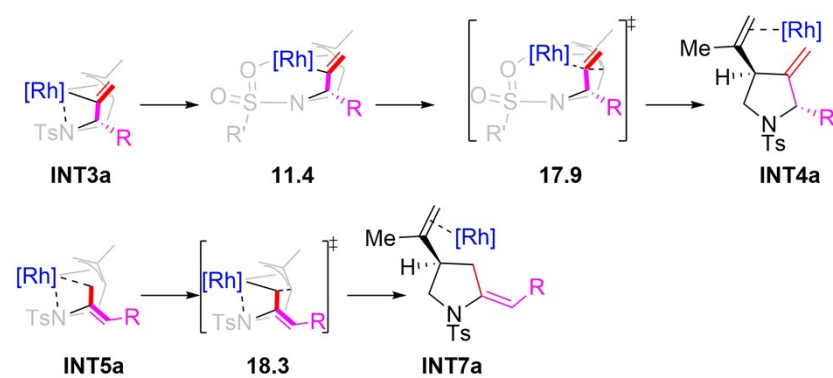
1.3. Other possibilities for migratory insertion of allene into the Rh-N and Rh-C3'



1.4. Possibilities for migratory insertion of allene into the Rh-C1'

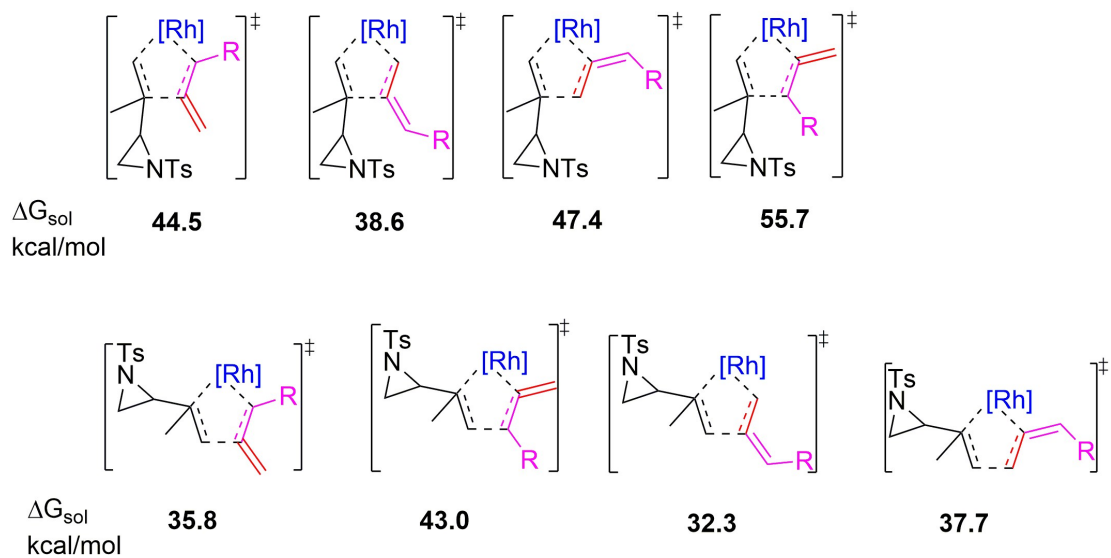


1.5. Other possibilities for C-C reductive elimination from INT3a and INT5a

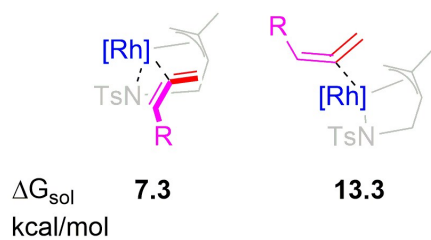


2. Additional Results for Reaction with Aryl-allene 2b.

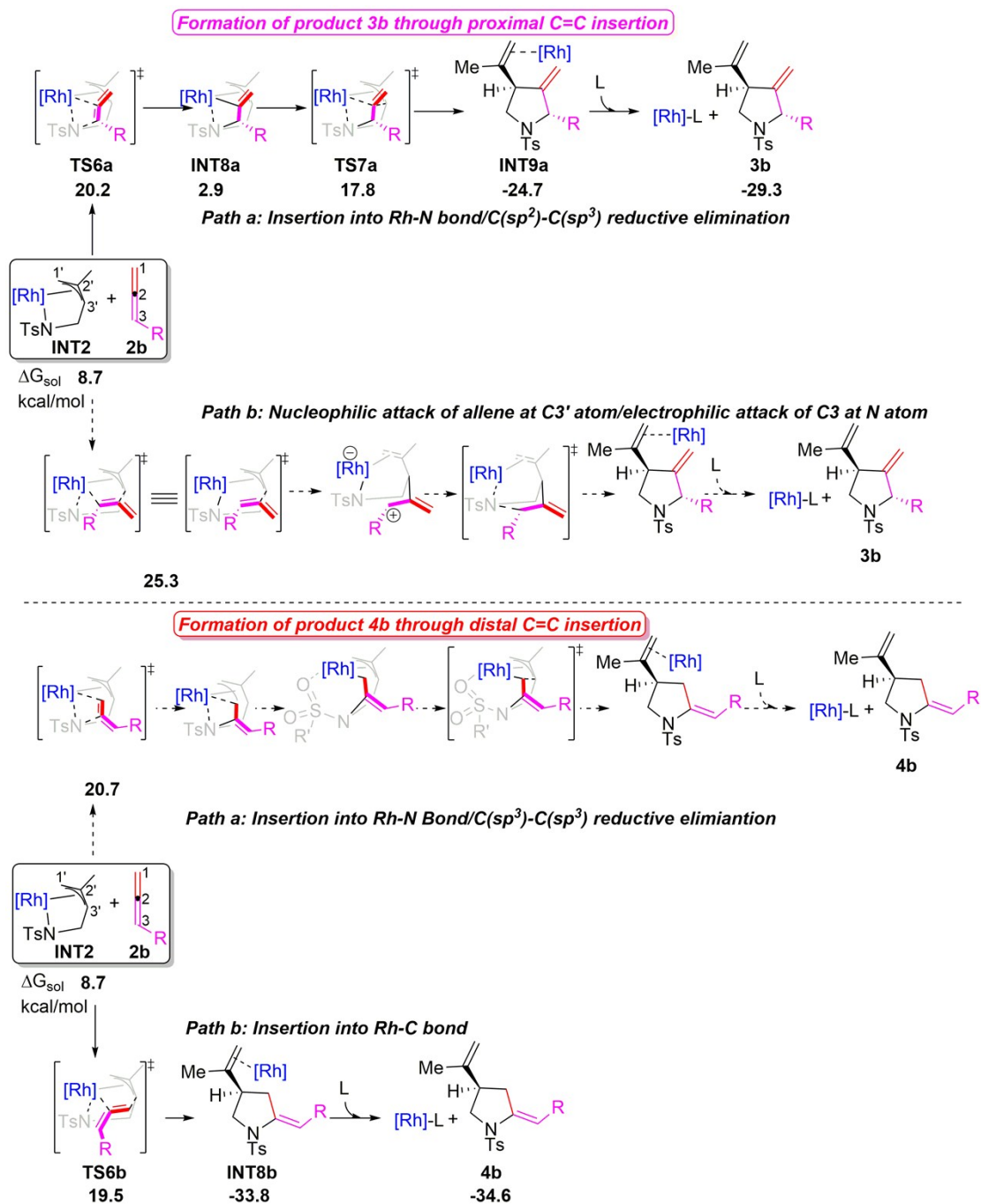
2.1. Oxidative cyclization of vinylaziridine and aryl-allene 2b.



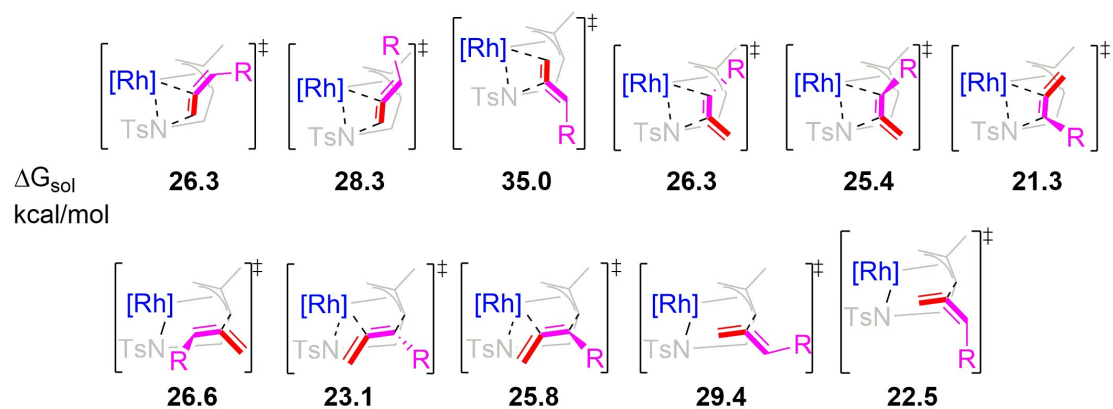
2.2. The complexations of INT2 with aryl-allene 2b.



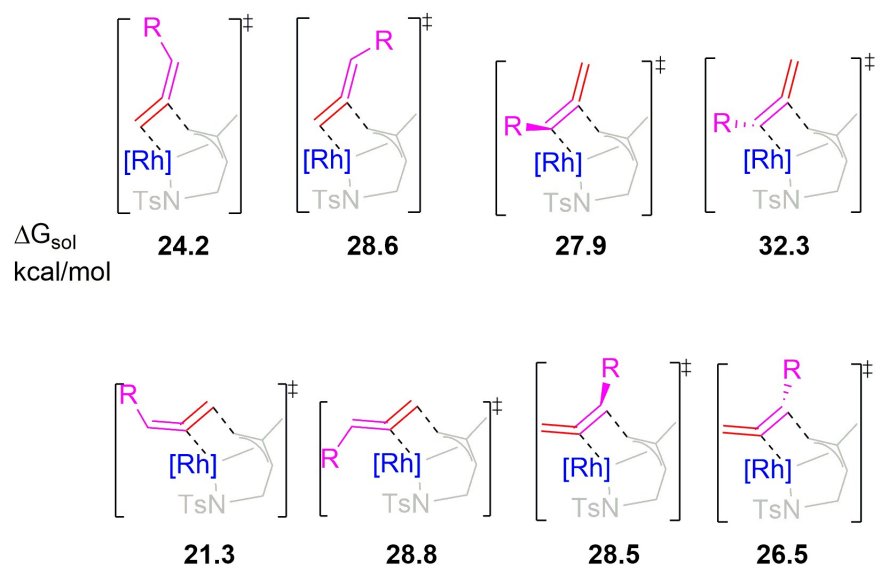
2.3. Possible pathways leading to the formation of products 3b and 4b from the Rh-allyl complex INT2 with aryl-allene 2b.



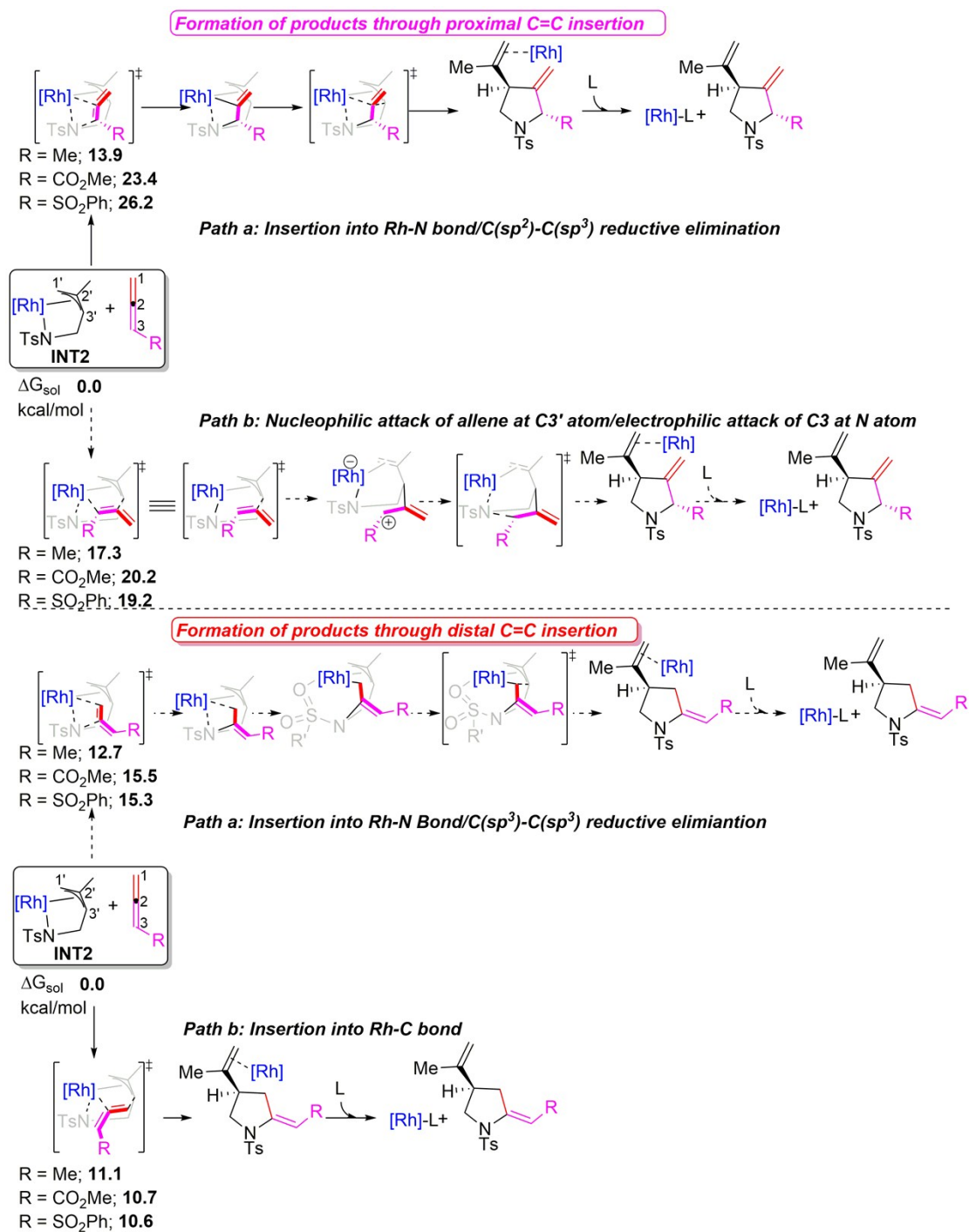
2.4. Other possibilities for migratory insertion of allene into the Rh-N and Rh-C3'



2.5. Possibilities for migratory insertion of allene into the Rh-C1'



3. Results for Reactions with General Allenes



4. Table of calculated energies and energy corrections

Stationary point	Single-point energy-B3LYP with DFT-D3 correction 6-311+G(2d,2p), lanl2tzf (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)	Optimization energy 6-31G(d,p) , lanl2dz (a.u.)	Solvation energy (dichloroethane) (a.u.)
[Rh(NBD) ₂] ⁺ -Catalyzed Reaction of Vinylaziridine 1 with N-alleneamine 2a				
Rh[NBD ₂] ⁺	-653.709296	0.221595	-652.352737	-0.080146
NBD	-271.606837	0.100709	-271.484544	-0.008391
1	-1069.986033	0.203016	-1069.588573	-0.020272
2a	-1222.470915	0.223362	-1221.994567	-0.022241
TS1	-1452.072632	0.328305	-1450.427614	-0.089557
INT1	-1452.093626	0.328180	-1450.454197	-0.083102
INT2	-1452.091277	0.331343	-1450.445298	-0.083394
TS4a	-2674.575719	0.575795	-2672.437529	-0.091015
INT5a	-2674.630019	0.581404	-2672.490401	-0.088103
TS5a	-2674.597275	0.579943	-2672.464306	-0.088102
INT6a	-2674.619339	0.579731	-2672.486816	-0.087914
TS2a	-2674.603473	0.582479	-2672.456509	-0.085270
INT3a	-2674.621190	0.584592	-2672.473248	-0.086461
TS3a	-2674.595947	0.584669	-2672.449511	-0.087074
TS2a'	-2674.596309	0.583266	-2672.449675	-0.085316
TS3a'	-2674.574658	0.583503	-2672.426328	-0.084648
TS4b	-2674.576263	0.578112	-2672.434966	-0.096601
INT7a	-2674.678240	0.584078	-2672.544926	-0.091244
TS2b	-2674.575646	0.574986	-2672.436234	-0.092926
INT3b	-2674.643022	0.581192	-2672.506815	-0.089751
TS3b	-2674.644304	0.584679	-2672.506442	-0.087632
INT4a	-2674.663812	0.585758	-2672.524159	-0.087445
4a	-2292.550871	0.456780	-2291.666942	-0.037219
3a	-2292.538477	0.456588	-2291.647949	-0.036433
[Rh(NBD) ₂] ⁺ -Catalyzed Reaction of Vinylaziridine 1 with Aryl-allene 2b				
Rh[NBD ₂] ⁺	-653.709296	0.221595	-652.352737	-0.083125
NBD	-271.606837	0.100709	-271.484544	-0.007962
1	-1069.986033	0.203016	-1069.588573	-0.021669
2a	-347.882169	0.105120	-347.722756	-0.010143
TS1	-1452.072632	0.328305	-1450.427614	-0.094679
INT1	-1452.093626	0.328180	-1450.454197	-0.087605

INT2	-1452.091277	0.331343	-1450.445298	-0.087695
TS6a	-1799.989467	0.459404	-1798.164652	-0.086437
INT8a	-1800.023833	0.463655	-1798.197579	-0.083749
TS7a	-1799.998797	0.463531	-1798.173805	-0.084847
TS6b	-1799.978212	0.459853	-1798.154662	-0.099222
TS6b'	-1799.975565	0.461171	-1798.148056	-0.095226
INT8b	-1800.077804	0.464877	-1798.265814	-0.089530
INT9a	-1800.068047	0.465754	-1798.249234	-0.085713
4b	-1417.956391	0.338900	-1417.391439	-0.029592
3b	-1417.947659	0.336697	-1417.378555	-0.027629

5. Cartesian coordinates

1

C	1.29466400	-0.65080500	-1.24279400
C	2.13498700	-0.91305200	-2.25040500
H	1.77376800	-1.09631000	-3.25780500
H	3.21050800	-0.95113700	-2.10240700
C	-0.19873500	-0.57341900	-1.42200800
H	-0.58086100	0.38518400	-1.05644200
H	-0.47267100	-0.68468600	-2.47367100
H	-0.71387100	-1.35964700	-0.85566800
C	1.84985000	-0.42896300	0.12325100
C	1.18333200	-0.85130900	1.39290100
H	1.84605300	-1.13388000	2.20744100
H	0.20687600	-1.32683300	1.38329000
H	2.93716300	-0.42453700	0.17966400
N	1.15918700	0.56397000	0.99431900
S	2.20061500	1.63993700	1.84202100
O	2.50981100	2.72050000	0.90451000
O	3.28413900	0.89070100	2.50126100
C	1.08507200	2.24378500	3.10049500
C	0.11066800	3.18381000	2.75448700
C	1.20844500	1.77980300	4.40943500
C	-0.75526400	3.65015600	3.73861900
H	0.04219400	3.54343600	1.73359200
C	0.33252300	2.26119400	5.38239800
H	1.98547800	1.06471300	4.65600200
C	-0.65901300	3.19878700	5.06502000
H	-1.51712300	4.37958100	3.47634400
H	0.42375900	1.90442900	6.40483600
C	-1.58639600	3.73711700	6.12755400
H	-1.24033600	4.71262300	6.49085400
H	-2.59986100	3.87799100	5.73941100
H	-1.64104100	3.06663800	6.98951100

2a

C	-2.65117500	2.52440200	-0.27371300
C	-3.34525900	2.74579700	-1.35837400
H	-3.12921900	3.58462700	-2.01945800
H	-4.16823400	2.09697200	-1.65659300
C	-2.01469900	2.31288600	0.85447700
H	-2.36616700	2.75311800	1.78240600
N	-0.89661300	1.45318600	1.03513400
C	-0.28039400	0.79339500	-0.08376700
C	-0.19073200	-0.60197400	-0.08256900

C	0.22304800	1.53156900	-1.16187600
C	0.40343500	-1.25696300	-1.16106300
H	-0.57871000	-1.15293400	0.76614800
C	0.80511800	0.86864700	-2.24199600
H	0.15198200	2.61378200	-1.14993500
C	0.89786300	-0.52486500	-2.24267400
H	0.47522600	-2.34050200	-1.15753300
H	1.19113100	1.44167700	-3.08002200
H	1.35410500	-1.03850900	-3.08399100
S	0.05315000	1.68906700	2.44742100
O	0.77575600	0.43640300	2.65704800
O	-0.86224000	2.23933700	3.44994600
C	1.25356000	2.95326200	2.03912100
C	2.48680100	2.58240100	1.49841200
C	0.93160900	4.29747300	2.24365300
C	3.40207800	3.57673000	1.15824600
H	2.72423000	1.53315600	1.36458600
C	1.85984100	5.27582900	1.89623100
H	-0.02196300	4.56480700	2.68534300
C	3.10633900	4.93384700	1.35026200
H	4.36439900	3.29293200	0.74058100
H	1.61568300	6.32247600	2.05798000
C	4.11744700	6.00219200	1.01101500
H	3.63025200	6.92173400	0.67340900
H	4.72377600	6.25900300	1.88852800
H	4.80358500	5.67073000	0.22651400
3a			
C	1.68749100	-0.78483000	-1.56449900
C	0.64404000	0.04125100	-1.69511300
H	-0.26164900	-0.27467400	-2.20559800
H	0.65845600	1.05718500	-1.30971000
C	1.68110600	-2.18661300	-2.12175900
H	1.80887500	-2.92964500	-1.32325700
H	0.74980800	-2.40939600	-2.64946700
H	2.51742100	-2.33360400	-2.81668800
C	2.97736900	-0.36248800	-0.87257100
C	2.80859200	0.30096400	0.52963300
H	3.02461600	-0.40141200	1.33937100
H	1.79777800	0.68670600	0.65958200
H	3.60635300	-1.25216100	-0.74864800
N	3.78756700	1.42593600	0.58100900
S	3.14820800	2.97519800	0.90676600
O	1.77322900	3.08475700	0.39600500
O	4.17569500	3.93683600	0.49257300

C	3.04649700	2.96682100	2.69488600
C	1.79688900	2.91852000	3.30910800
C	4.22058100	3.04951700	3.44971600
C	1.72565700	2.94033700	4.70328300
H	0.90051600	2.87662200	2.70056500
C	4.12842800	3.07043300	4.83676000
H	5.18498900	3.10207200	2.95756500
C	2.88332600	3.01477100	5.48622000
H	0.75336400	2.90428200	5.18709500
H	5.03835600	3.13462400	5.42799900
C	2.80652600	3.04229500	6.99387400
H	3.24897700	3.96097300	7.39556800
H	1.77256000	2.98739800	7.34389600
H	3.35604000	2.20251800	7.43434100
C	4.69875300	1.31904300	-0.57248800
H	5.03934600	2.30799400	-0.87843800
N	5.86292900	0.47927100	-0.10352100
C	6.65451000	1.13452600	0.92005800
C	7.30166400	2.35657300	0.69751200
C	6.74693600	0.51601700	2.17046500
C	8.04254700	2.94633200	1.72285300
H	7.23445300	2.83515400	-0.27341000
C	7.49271100	1.10553600	3.19119200
H	6.23097100	-0.42545800	2.32477400
C	8.14202900	2.32258300	2.96908900
H	8.54299700	3.89377400	1.54595600
H	7.56429200	0.61661400	4.15848800
H	8.72304800	2.78346500	3.76286500
S	6.79689500	-0.20123500	-1.40396500
O	7.31955800	0.87097100	-2.26793400
O	5.99274900	-1.28429300	-1.97969800
C	8.17627500	-0.95548000	-0.54362700
C	9.42110000	-0.32762100	-0.55073300
C	8.00492600	-2.21361200	0.03855300
C	10.50172000	-0.96303600	0.05888700
H	9.53590000	0.63391800	-1.03785500
C	9.09448700	-2.83048200	0.64647500
H	7.03844600	-2.70347200	-0.00522400
C	10.35604500	-2.21522100	0.67126700
H	11.47550800	-0.48087300	0.05271900
H	8.96897500	-3.81131400	1.09768900
C	11.52410400	-2.88564100	1.35308500
H	11.50942800	-3.96880900	1.19821700
H	12.47860200	-2.50103900	0.98364700

H	11.49689500	-2.71268600	2.43613100
C	3.83039800	0.65373400	-1.61531400
C	3.73907600	1.05460000	-2.87991600
H	3.00240600	0.62882700	-3.55297100
H	4.40566900	1.81119800	-3.28123700
3b			
C	1.31149100	-0.95252300	-1.44580300
C	0.93819100	-0.55891900	-2.66755900
H	0.06197800	-0.98168100	-3.15083700
H	1.49124200	0.19079700	-3.22366900
C	0.54419600	-1.99881700	-0.67457100
H	0.19457800	-1.60688500	0.28949300
H	-0.32711800	-2.35337500	-1.23118500
H	1.18070700	-2.86371200	-0.44631300
C	2.49282900	-0.34069600	-0.70753400
C	2.14537700	0.98454400	0.00228700
H	1.57659400	0.84148300	0.92602800
H	1.56858500	1.63530100	-0.66521200
H	2.81029000	-1.04779000	0.07401300
N	3.47613300	1.54527000	0.30606100
S	3.49829800	3.14556800	0.87696900
O	2.28982300	3.84877400	0.42312000
O	4.83201100	3.67285500	0.57452400
C	3.35159500	2.92294100	2.64894500
C	2.15338100	3.24101000	3.28526600
C	4.45228600	2.45592600	3.37352900
C	2.05587800	3.07794600	4.66835600
H	1.32076400	3.61954200	2.70262800
C	4.33609800	2.30109600	4.75086100
H	5.37989100	2.22092800	2.86246300
C	3.13967700	2.60920400	5.42037700
H	1.12350500	3.32454600	5.16923500
H	5.18847300	1.93845300	5.31975300
C	3.04119800	2.46018600	6.91954600
H	3.56213200	3.27948800	7.42988500
H	2.00117500	2.47051700	7.25648400
H	3.50043600	1.52610200	7.25881800
C	4.44937000	1.18910800	-0.76659700
H	4.58369400	2.02179900	-1.46740100
C	3.74234500	0.03637100	-1.49144500
C	4.19392200	-0.52244600	-2.61176400
H	3.65179300	-1.32436100	-3.10097400
H	5.12432900	-0.19928500	-3.06979200
C	5.81615800	0.80654000	-0.21926700

C	5.94506600	-0.04426300	0.88639600
C	6.97288900	1.26249500	-0.85894400
C	7.20608000	-0.43567600	1.33571700
H	5.05258500	-0.38599500	1.40225000
C	8.23626000	0.86791100	-0.41416600
H	6.88486800	1.94346100	-1.70150200
C	8.35675100	0.01606400	0.68391500
H	7.29156700	-1.09561600	2.19485900
H	9.12477900	1.23589600	-0.91941000
H	9.33863500	-0.28853500	1.03476400
4a			
C	1.72497700	-0.65286700	-1.60783700
C	0.52911200	-0.24333800	-1.17135500
H	-0.38427700	-0.55929500	-1.66741100
H	0.40490500	0.41107600	-0.31512600
C	1.85142400	-1.57735600	-2.79628000
H	2.41546700	-2.48186800	-2.53427400
H	0.87104500	-1.88357000	-3.16979000
H	2.39298700	-1.09897400	-3.62133900
C	3.03648500	-0.26965400	-0.95411000
C	2.95634500	0.67733500	0.25200900
H	2.67229500	0.17126700	1.17786900
H	2.24254300	1.48384400	0.05135600
H	3.52647000	-1.19812400	-0.62448600
N	4.33694700	1.23147100	0.37396600
S	4.36592900	2.84599100	0.98524400
O	3.35985400	3.69669200	0.32666500
O	5.77034900	3.27334200	0.99601900
C	3.83070000	2.55815600	2.66861400
C	2.66076400	3.16301700	3.12419700
C	4.61574000	1.77174700	3.51693000
C	2.26971800	2.96843500	4.44950400
H	2.07378900	3.77247900	2.44596800
C	4.20673800	1.58516400	4.83333500
H	5.52611600	1.31216200	3.14752200
C	3.03197800	2.18124900	5.32172300
H	1.35698400	3.43565000	4.80934800
H	4.80924400	0.96932300	5.49589600
C	2.61909300	1.99283100	6.76142800
H	3.19717700	2.64980100	7.42280400
H	1.56119500	2.22578200	6.90950700
H	2.79284800	0.96518600	7.09551700
N	7.20842300	0.98265700	-2.05417400
C	6.73135300	1.15964600	-3.39984300

C	7.01149000	0.17987200	-4.35847100
C	6.01253100	2.30879500	-3.75662800
C	6.56381900	0.34711400	-5.66927700
H	7.58315400	-0.69323600	-4.06678600
C	5.55864200	2.46136400	-5.06609600
H	5.80830600	3.06633700	-3.00689800
C	5.83330900	1.48279300	-6.02485200
H	6.78384700	-0.41432300	-6.41176500
H	4.99749100	3.35040400	-5.33875400
H	5.48019200	1.60616400	-7.04453800
S	8.88399600	1.34815700	-1.79067400
O	9.61453400	0.68715900	-2.87097700
O	9.13927100	1.03719400	-0.38398900
C	9.02204100	3.11826700	-2.02840600
C	9.64649300	3.59902100	-3.17975200
C	8.49194200	3.99187500	-1.07195100
C	9.74861300	4.97674500	-3.36887300
H	10.04674800	2.89945000	-3.90459900
C	8.59685400	5.36312400	-1.28712700
H	7.99342400	3.61917100	-0.18394000
C	9.22901700	5.87767500	-2.43023700
H	10.23769800	5.35614900	-4.26213000
H	8.17837200	6.04508900	-0.55190300
C	9.36220900	7.36839500	-2.62769500
H	10.20368000	7.76639600	-2.04713200
H	9.53939700	7.62002800	-3.67699400
H	8.46295200	7.89659200	-2.29607400
C	4.04596900	0.46184000	-1.87750700
H	4.50993600	-0.19762900	-2.61123500
H	3.53433200	1.26766000	-2.42283600
C	5.03529600	0.99982800	-0.87928000
C	6.37014500	1.13696500	-0.92972500
H	6.90071000	1.37266000	-0.01911400
4b			
C	1.73131000	-0.66003500	-1.59958100
C	0.50351500	-0.15438700	-1.44159100
H	-0.35004700	-0.59077300	-1.95259300
H	0.29422200	0.70071000	-0.80778100
C	1.97838900	-1.86194200	-2.48096600
H	2.46540100	-2.66946400	-1.91915800
H	1.04517500	-2.25075300	-2.89597100
H	2.64377200	-1.61855300	-3.31840900
C	2.95991500	-0.11102800	-0.90588100
C	2.75663000	1.08868200	0.02209100

H	2.33798700	0.81519800	0.99407400
H	2.11277100	1.84580300	-0.44027200
H	3.40326000	-0.92440800	-0.31236100
N	4.13392300	1.61419500	0.18560500
S	4.22478700	3.12971200	0.97457100
O	3.15970900	4.01006400	0.47711700
O	5.62199900	3.56382000	0.95047600
C	3.79876900	2.65980500	2.65087900
C	2.57935800	3.06350300	3.19185100
C	4.71817600	1.92999800	3.40971300
C	2.27507200	2.71849800	4.50953900
H	1.88957400	3.64192100	2.58711700
C	4.39707200	1.59411200	4.72066700
H	5.66884400	1.63611200	2.97768500
C	3.17377200	1.98274300	5.29194600
H	1.32468100	3.02895900	4.93536900
H	5.10680100	1.02378100	5.31423700
C	2.85265900	1.63497300	6.72541100
H	3.35966300	2.31932900	7.41665600
H	1.77964900	1.70264700	6.92375600
H	3.18296900	0.62171200	6.97440500
C	4.06657300	0.41660900	-1.85168900
H	4.63295700	-0.37378200	-2.34756100
H	3.60423300	1.04020000	-2.63009600
C	4.94608100	1.25067800	-0.94609900
C	6.26304700	1.50894900	-1.06890300
H	6.74503200	2.04394000	-0.25927600
C	7.14444800	1.12332400	-2.17860500
C	8.51606000	0.94654000	-1.90206100
C	6.72336900	0.94732100	-3.51158900
C	9.41557600	0.57219200	-2.89609800
H	8.86957800	1.10007600	-0.88570700
C	7.62494300	0.57260200	-4.50769100
H	5.69162200	1.14121100	-3.78237100
C	8.97344400	0.37537400	-4.20678500
H	10.46499500	0.43687800	-2.64877900
H	7.27231500	0.44928700	-5.52822900
H	9.67337000	0.08650200	-4.98543800
INT1			
C	2.40435700	-0.12355500	-0.88556200
C	1.20024500	-0.33866900	-1.50039300
H	1.17048700	-0.66343600	-2.53527000
H	0.26910500	-0.42175700	-0.94756600
C	3.73106400	-0.30931900	-1.57384600

H	4.21782000	-1.21397000	-1.18549200
H	3.61321700	-0.42805700	-2.65237900
H	4.40522000	0.53107600	-1.37983800
C	2.48279100	0.28219800	0.56734100
C	1.28803600	0.58534700	1.40190700
H	1.44050700	0.53059800	2.47679400
H	0.27414500	0.39042700	1.07038600
H	3.39634400	0.02760200	1.10056700
N	1.98610200	1.68263800	0.70980300
S	2.86296500	2.97476900	1.56569200
O	1.82101700	3.96818000	1.80717900
O	4.00484500	3.23262400	0.68919400
C	3.41944900	2.28106300	3.10129200
C	2.59648800	2.37320300	4.23138700
C	4.68611500	1.68718900	3.16597900
C	3.05210200	1.84233800	5.43424400
H	1.63546400	2.87285700	4.17045900
C	5.11762300	1.16370600	4.38159300
H	5.32772900	1.66875400	2.29149700
C	4.31328000	1.23010500	5.53122800
H	2.42360700	1.91462800	6.31701000
H	6.10156300	0.70818100	4.44347900
C	4.80691400	0.69396200	6.85001500
H	5.53266200	-0.11119600	6.71102900
H	5.30271000	1.48750600	7.42220900
H	3.98385200	0.31721400	7.46298700
Rh	1.41299100	2.01656700	-1.39494200
C	0.18953000	2.42985200	-3.13279500
C	-0.15522000	3.89052900	-2.76437200
C	2.01745200	3.89200200	-3.42100900
C	1.53323900	2.42862100	-3.52950200
H	-0.54613200	1.65661300	-3.32229800
H	2.04667900	1.65474100	-4.08857800
C	0.71719000	4.65511300	-3.79866500
H	0.77666000	5.72938400	-3.59581900
H	0.40554800	4.48534100	-4.83441000
C	0.68774300	4.08289400	-1.48182600
H	0.31093000	4.40734700	-0.51905500
C	2.02194400	4.08505400	-1.89296000
H	2.88657000	4.36405500	-1.30188100
H	-1.21364300	4.13437100	-2.69094400
H	2.94011200	4.13862100	-3.94351600
INT2			
C	1.35387700	-0.45839200	-1.32671200

C	0.57016400	0.74255500	-1.23354700
H	-0.10913600	0.96968900	-2.05010200
H	0.24828100	1.11514900	-0.26466600
C	1.23504600	-1.39600800	-2.50076800
H	0.61323000	-2.24644500	-2.19606800
H	0.73812400	-0.93402800	-3.35644000
H	2.20387400	-1.79403500	-2.81337000
C	2.37011900	-0.62363300	-0.37842900
C	2.33231000	0.04252200	0.99693200
H	3.06065100	-0.42085000	1.66732500
H	1.34666800	-0.08149700	1.45652300
H	3.10572900	-1.40593500	-0.55105700
N	2.55905100	1.49926800	0.80977200
S	4.17689200	1.99412800	0.93529400
O	4.20141300	3.41283000	1.28878300
O	4.72072500	1.61624800	-0.44442500
C	5.07853200	1.06746100	2.14771100
C	5.04002100	1.50551000	3.47758200
C	5.82400100	-0.05435900	1.76786400
C	5.75526600	0.79416700	4.43461800
H	4.47721100	2.39252900	3.74737200
C	6.53683800	-0.74466100	2.74436300
H	5.86466300	-0.35748300	0.72746400
C	6.51444900	-0.33657500	4.08782000
H	5.73300300	1.12680900	5.46823900
H	7.12748800	-1.61012200	2.45863700
C	7.31351200	-1.07247100	5.13218000
H	7.51383200	-2.10434700	4.83335900
H	8.28142100	-0.58108600	5.28915000
H	6.79650100	-1.08473900	6.09559500
Rh	2.61245500	1.48180500	-1.30726000
C	2.26688400	1.75962600	-3.65345500
C	1.57813800	3.13550300	-3.54862800
C	3.77369500	3.46307700	-3.10008500
C	3.59916900	1.95723500	-3.38801900
H	1.80431200	0.86070300	-4.03688000
H	4.40814400	1.24413200	-3.49057100
C	2.72101400	4.04226500	-4.09105800
H	2.53320200	5.10961100	-3.94054800
H	2.96113000	3.84868300	-5.14110300
C	1.67435100	3.46324800	-2.04283600
H	0.83827900	3.70387500	-1.39837900
C	3.01617000	3.66649500	-1.76882000
H	3.43850500	4.10163300	-0.87122200

H	0.59012600	3.21599300	-3.99863700
H	4.79312000	3.84116300	-3.13058300
INT3a			
C	0.99302000	-0.05943100	-2.41520400
C	0.07481900	0.54409600	-1.55519700
H	-0.91012200	0.80044000	-1.93403600
H	0.17506200	0.52760700	-0.47771300
C	0.63056800	-0.40306100	-3.84115700
H	0.50820200	-1.48972400	-3.91699900
H	-0.31548700	0.04950800	-4.14870900
H	1.41740900	-0.12044100	-4.54685700
C	2.36099500	-0.20009700	-2.01648400
C	2.74756300	-0.33947600	-0.55062000
H	3.62591500	-0.96678100	-0.41915000
H	1.92049600	-0.73289200	0.04152400
H	3.07744800	-0.58481800	-2.73271000
N	3.02957300	1.05669700	-0.06986400
S	2.36022200	1.51848700	1.52750600
O	0.93890200	1.18373300	1.41471000
O	2.81130500	2.90102500	1.70129700
C	3.05787900	0.49691000	2.80674400
C	2.51441900	-0.77255000	3.04385300
C	4.04761700	1.03105800	3.63464700
C	3.00051900	-1.52084600	4.10942500
H	1.70291800	-1.15126200	2.43311200
C	4.50753700	0.26690400	4.70541600
H	4.43187800	2.02802800	3.45661700
C	3.99936200	-1.01498500	4.95947300
H	2.58253700	-2.50500400	4.30087200
H	5.26917600	0.68062100	5.35973200
C	4.47695300	-1.81928700	6.14154000
H	5.45501000	-1.48017300	6.49155600
H	3.77591400	-1.72305800	6.97936200
H	4.54594400	-2.88370200	5.89918400
Rh	2.05404800	1.97919100	-1.81086100
C	0.85372300	2.94474300	-3.49916800
C	0.08750300	3.97341600	-2.64759100
C	2.22744200	4.70275000	-2.77861900
C	2.16497100	3.38758000	-3.58659800
H	0.39139800	2.17835500	-4.10458400
H	2.91110400	3.03261700	-4.28206800
C	0.81537200	5.27718600	-3.07964500
H	0.55773600	6.13597400	-2.45201100
H	0.66722500	5.52762500	-4.13520600

C	0.70617200	3.75774200	-1.25056200
H	0.15899300	3.49842100	-0.35326500
C	2.01891300	4.20204800	-1.33301400
H	2.68603400	4.39050900	-0.50239100
H	-0.99883200	3.93371500	-2.70709300
H	3.09803700	5.33154100	-2.95124400
C	4.14441300	2.12277800	-1.85083200
C	5.06690000	2.51938100	-2.72222100
H	6.12996200	2.44034100	-2.50692900
H	4.82807200	2.89249000	-3.71174300
C	4.39490700	1.66803700	-0.42962300
H	4.41972100	2.56283500	0.19481500
N	5.57549500	0.89455900	-0.01714900
C	6.50649300	1.59782100	0.85160200
C	6.99079700	2.86883800	0.51371500
C	6.93016100	0.98415100	2.03481500
C	7.87398700	3.52796000	1.36798000
H	6.68269700	3.33594100	-0.41618500
C	7.82935500	1.64151000	2.87668800
H	6.55234400	0.00134800	2.28960600
C	8.29859500	2.91429600	2.54867000
H	8.24158700	4.51430000	1.10287000
H	8.15881800	1.15845300	3.79170200
H	8.99389100	3.42537000	3.20737400
S	6.39253200	-0.14704100	-1.18066800
O	7.44730100	0.61392500	-1.85467500
O	5.32146200	-0.79726000	-1.94455100
C	7.19301000	-1.37787400	-0.16291200
C	8.56543100	-1.26998900	0.07204200
C	6.46125700	-2.46882400	0.31355200
C	9.20243900	-2.26364900	0.81160400
H	9.11748200	-0.42639700	-0.32580900
C	7.11622700	-3.44906700	1.05364500
H	5.40411100	-2.56354400	0.09205200
C	8.49388500	-3.36543900	1.31309500
H	10.26994700	-2.18483800	0.99655200
H	6.55410500	-4.30218100	1.42330100
C	9.20186000	-4.45537100	2.07833400
H	10.06493100	-4.06609800	2.62511200
H	8.53364100	-4.94560000	2.79163600
H	9.57178100	-5.22834000	1.39378500
INT3b			
C	0.14945300	-1.02170600	-0.97884700
C	-0.93987600	-0.16490300	-0.96958700

H	-1.71118600	-0.27917100	-1.72387300
H	-1.23351900	0.39996900	-0.08955100
C	0.24689200	-2.11149000	-2.02344500
H	-0.00770800	-3.08080000	-1.57359200
H	-0.45005400	-1.93781800	-2.84600400
H	1.25328400	-2.21235000	-2.44070000
C	0.97999200	-1.21419800	0.30236200
C	1.15211700	0.10807100	1.05500700
H	1.74626500	-0.06071800	1.96296900
H	0.18135700	0.50418300	1.37974100
H	0.43561700	-1.92977100	0.93381000
N	1.84383400	0.98674000	0.10218500
S	2.17384400	2.53622200	0.68025100
O	0.89644600	3.21208700	0.97903000
O	3.10485700	3.14193600	-0.28449300
C	3.05371100	2.38990900	2.24129900
C	2.33961400	2.29204300	3.44018500
C	4.44753200	2.48566300	2.24497700
C	3.03498100	2.25629500	4.64632300
H	1.25511900	2.27943400	3.42678400
C	5.12586100	2.45792600	3.46475500
H	4.98419800	2.60224700	1.30943300
C	4.43599800	2.34196200	4.68034900
H	2.48099400	2.18312700	5.57836700
H	6.20901200	2.54678600	3.47160600
C	5.17259700	2.35684900	5.99764500
H	5.13173000	3.35374800	6.45255600
H	4.72889500	1.65854800	6.71386700
H	6.22765600	2.09855200	5.87296200
Rh	0.71625800	1.08528200	-1.75421700
C	-0.60529000	1.67930800	-3.39382400
C	-0.17566900	3.15689700	-3.53844400
C	1.52500300	1.91547600	-4.37018600
C	0.44203200	0.90904500	-3.91288100
H	-1.63448300	1.37374800	-3.25645200
H	0.38591200	-0.11634200	-4.25893700
C	0.62697200	3.08351000	-4.86870700
H	1.19242100	3.99759800	-5.07939100
H	0.00725500	2.81688500	-5.73130400
C	0.98028800	3.26029300	-2.52830600
H	1.00551300	3.90286300	-1.65791900
C	2.01368900	2.50057500	-3.03086800
H	3.01682900	2.43890400	-2.63264500
H	-0.96726200	3.89885400	-3.44534900

H	2.29486100	1.52808400	-5.03623200
C	2.36209800	-1.81431200	0.06412900
C	3.32637700	-0.97602000	-0.66110500
H	2.97197000	-0.39671600	-1.50855300
C	2.65711700	-3.06596400	0.45346200
H	1.89953100	-3.68433800	0.92545900
N	4.63347800	-0.97669100	-0.49442200
C	5.36650400	-1.57162100	0.59966700
C	5.34234000	-0.95782300	1.85332300
C	6.11668200	-2.73076300	0.37192700
C	6.06218400	-1.53225100	2.90047100
H	4.77841200	-0.04468300	2.00108200
C	6.83190500	-3.29368100	1.42907100
H	6.12939400	-3.18859000	-0.61156700
C	6.80389900	-2.69698600	2.69201300
H	6.04439100	-1.06085200	3.87772500
H	7.40799800	-4.19861000	1.26472300
H	7.36177900	-3.13905800	3.51147100
S	5.60441000	0.17696300	-1.59005400
O	6.23661200	1.09342400	-0.65339500
O	4.62451400	0.58242000	-2.59390900
C	6.81858500	-0.88042800	-2.32655300
C	8.11360500	-0.89630000	-1.79978700
C	6.46664800	-1.64753500	-3.44380300
C	9.06828200	-1.70558900	-2.40971900
H	8.36391700	-0.28039200	-0.94366500
C	7.43714700	-2.45287800	-4.02863100
H	5.46391100	-1.59882100	-3.85404300
C	8.75015000	-2.49453200	-3.52626200
H	10.07939600	-1.72155300	-2.01410500
H	7.17828800	-3.05057700	-4.89773800
C	9.79938400	-3.34302700	-4.19689800
H	9.37347800	-4.26960000	-4.59165700
H	10.24300000	-2.80335900	-5.04241800
H	10.60976700	-3.59860500	-3.50990500
H	3.62595000	-3.52245400	0.29751100
INT4a			
C	0.03104200	-1.17616300	-0.81476100
C	-0.87373100	-0.22162900	-0.39733600
H	-1.86662600	-0.20921600	-0.83626100
H	-0.77174000	0.34608800	0.52181000
C	-0.37913200	-2.18568400	-1.85853300
H	-0.53414800	-3.15950100	-1.37505400
H	-1.31960100	-1.90636700	-2.33806300

H	0.38479600	-2.32644500	-2.62625100
C	1.34197200	-1.47406800	-0.06929300
C	1.72133500	-0.36238300	0.91430500
H	2.48133100	-0.70457400	1.62330500
H	0.88818800	0.06279100	1.46877200
H	1.23967900	-2.44681500	0.42846000
N	2.28671700	0.63198800	-0.04055000
S	2.49834000	2.27859300	0.54106500
O	1.10205900	2.64649000	0.82559300
O	3.27129700	2.94724000	-0.50251500
C	3.38724000	2.35090100	2.07933700
C	2.71198900	2.08621500	3.27761800
C	4.71716700	2.78289200	2.06916500
C	3.39794400	2.23028700	4.47878500
H	1.66479600	1.80550600	3.27217200
C	5.37728300	2.93067000	3.28759000
H	5.22587000	2.98434100	1.13439800
C	4.73638600	2.65844800	4.50581900
H	2.88172600	2.02734000	5.41275600
H	6.40998000	3.26671600	3.28786600
C	5.45168000	2.85944300	5.81761100
H	5.27123500	3.87130100	6.20041300
H	5.10054500	2.15730200	6.57883800
H	6.53270400	2.74058300	5.70807000
Rh	0.53200100	1.02368800	-1.64324900
C	-1.01569900	1.65664800	-2.96241800
C	-0.49611800	3.07220000	-3.29801500
C	0.86359000	1.63186600	-4.40340900
C	-0.16461300	0.76072200	-3.64855900
H	-2.02245000	1.45522200	-2.61568800
H	-0.38239000	-0.26743400	-3.91172300
C	-0.01436100	2.86364900	-4.76148500
H	0.57039700	3.70645700	-5.14501400
H	-0.82965900	2.62690100	-5.45297900
C	0.85656200	3.08096300	-2.55991700
H	1.13857900	3.76310800	-1.76852500
C	1.68819000	2.20708400	-3.23504400
H	2.75574200	2.09012500	-3.08464700
H	-1.16928300	3.89994100	-3.08157800
H	1.42367300	1.14131800	-5.19807600
C	2.55132400	-1.47039900	-1.01108700
C	3.30691200	-0.14113900	-0.87549100
H	3.39679000	0.37966500	-1.82368500
C	2.92656700	-2.44659100	-1.83538100

H	2.39650100	-3.39199300	-1.88811800
N	4.66047100	-0.25764700	-0.35850900
C	5.07998300	-1.18941800	0.66703400
C	5.21884700	-0.76235600	1.99379200
C	5.39661100	-2.51569100	0.33571900
C	5.63188600	-1.65935500	2.98039200
H	5.02035800	0.27046300	2.24438600
C	5.80660900	-3.40821100	1.32551000
H	5.33131300	-2.84111300	-0.69434600
C	5.91984100	-2.98444400	2.65097200
H	5.73581100	-1.31638500	4.00518300
H	6.04590200	-4.43281700	1.05778700
H	6.24147200	-3.68036500	3.41979900
S	5.90269000	0.64308600	-1.17038500
O	6.60624500	1.42800800	-0.15475200
O	5.23276600	1.28245600	-2.31049300
C	7.04700700	-0.57249300	-1.80529700
C	8.18224300	-0.90372500	-1.06367200
C	6.80521200	-1.14819500	-3.05610100
C	9.07630700	-1.83768500	-1.58275500
H	8.36334400	-0.42819000	-0.10665900
C	7.71059200	-2.08044200	-3.55554400
H	5.94068800	-0.84599700	-3.63753200
C	8.85859500	-2.44001700	-2.83064400
H	9.96231500	-2.09795900	-1.01063600
H	7.53316200	-2.52543000	-4.53071200
C	9.85393200	-3.42019700	-3.39940700
H	9.36850100	-4.15805400	-4.04408500
H	10.60341900	-2.89909800	-4.00739000
H	10.38924700	-3.95264100	-2.60873600
H	3.79700500	-2.34166200	-2.47639800
INT5a			
C	0.31548200	-1.02436300	-0.52925600
C	-0.42159100	0.15680300	-0.45438000
H	-1.34503400	0.23786000	-1.01949300
H	-0.28230500	0.89216000	0.32897600
C	-0.17307200	-2.20966500	-1.32770400
H	-0.55514100	-2.96440500	-0.63047200
H	-0.99434200	-1.94654900	-1.99895700
H	0.62937200	-2.68182900	-1.90253600
C	1.63677700	-1.07148700	0.02629500
C	2.00058000	-0.18791000	1.21265600
H	2.70997600	-0.66002600	1.89494500
H	1.11391400	0.11978500	1.76902400

H	2.21111800	-1.98365300	-0.10597500
N	2.62251700	1.03389700	0.58611800
S	2.19603000	2.63647200	1.26248400
O	0.74313700	2.56059500	1.44435500
O	2.81267800	3.58969600	0.34079700
C	2.96828300	2.77566200	2.85758300
C	2.36502900	2.17710000	3.96973500
C	4.14377400	3.52327000	2.98120900
C	2.97391400	2.30786300	5.21388400
H	1.42301800	1.64900900	3.87106600
C	4.72487800	3.65166600	4.23948000
H	4.57028800	4.01027800	2.11172500
C	4.16379000	3.03675000	5.37002600
H	2.51043900	1.84917100	6.08225300
H	5.62492400	4.24979200	4.35052800
C	4.82909500	3.14533900	6.71741700
H	5.54216400	2.32350900	6.85580900
H	5.38423400	4.08185500	6.81687000
H	4.10087200	3.08791400	7.53055100
Rh	1.78989000	0.61760200	-1.40791900
C	0.87432500	0.18898400	-3.43447400
C	0.24103000	1.57341500	-3.68830000
C	2.47274300	1.82035800	-3.96745400
C	2.24378000	0.33471900	-3.61655400
H	0.32453200	-0.74109400	-3.40518300
H	2.97045000	-0.45641500	-3.74284200
C	1.19036200	2.10812800	-4.79631100
H	1.04585300	3.17251200	-5.00586600
H	1.13830500	1.53272800	-5.72628800
C	0.74376400	2.38625200	-2.47809900
H	0.11898700	2.89542900	-1.75600200
C	2.11067400	2.52592900	-2.64182400
H	2.76293600	3.17290800	-2.07012800
H	-0.83260200	1.58464100	-3.86877200
H	3.43915200	2.06923800	-4.40179500
C	4.00592900	0.80418400	0.11757600
C	3.93056500	0.53220200	-1.34462700
H	4.36849600	1.29902100	-1.98396300
H	4.30742400	-0.45067600	-1.63053900
C	4.99399200	0.69784100	1.02951500
H	4.76756200	0.83080600	2.08213900
N	6.33025800	0.40892700	0.80663400
C	6.93818000	0.34200700	-0.49565900
C	7.32536200	-0.88963300	-1.03609200

C	7.16178300	1.52964700	-1.20313400
C	7.92897700	-0.92686300	-2.29397100
H	7.16478800	-1.79699100	-0.46546300
C	7.75263000	1.48042400	-2.46559800
H	6.87371800	2.47758900	-0.75982600
C	8.13832600	0.25325400	-3.01123700
H	8.23467900	-1.88056200	-2.71313200
H	7.92603600	2.40069000	-3.01517100
H	8.60801600	0.21790200	-3.98952500
S	7.32112100	0.02564000	2.19839600
O	7.87368200	-1.30827200	1.97589800
O	6.46605500	0.31844400	3.35196600
C	8.64698200	1.21182700	2.11672600
C	9.87382600	0.82959800	1.57081600
C	8.44710100	2.49686100	2.62961500
C	10.91002900	1.76036400	1.53265700
H	10.01245700	-0.17856100	1.19765000
C	9.49568000	3.40976100	2.58092100
H	7.49327500	2.76431100	3.07140300
C	10.74175900	3.05856700	2.03508900
H	11.86806700	1.46995400	1.11118500
H	9.35167900	4.40987500	2.98044400
C	11.88203600	4.04572400	2.02299900
H	11.52342400	5.07206900	1.90467800
H	12.43980800	4.00221000	2.96640300
H	12.58833100	3.83256200	1.21643900

INT6a

C	1.35738100	-0.58305600	-0.67380300
C	0.35766500	-0.00304400	0.06066600
H	-0.64020000	-0.43155500	0.06306800
H	0.54002200	0.81539500	0.74594700
C	1.10572300	-1.86293300	-1.43793600
H	1.48791000	-2.70354100	-0.84579600
H	0.04207900	-2.04232600	-1.61640700
H	1.64287600	-1.89382000	-2.39066200
C	2.66491900	0.07838400	-0.82809900
C	3.47260500	0.48176800	0.40852300
H	4.31423700	-0.20595900	0.53558300
H	2.87167600	0.41386800	1.31769700
H	3.29589600	-0.40147400	-1.57674800
N	4.07943100	1.85050800	0.34174900
S	3.04470800	3.03212200	0.96447200
O	1.67108100	2.78310600	0.36291600
O	3.63719900	4.34800400	0.74108400

C	2.91832800	2.65684000	2.69904700
C	1.65996300	2.56483500	3.29654800
C	4.09497000	2.56647800	3.45247700
C	1.58637400	2.36133700	4.67379300
H	0.76109100	2.66154500	2.69853700
C	3.99493300	2.35733700	4.82285600
H	5.06422400	2.65082600	2.97329500
C	2.74409600	2.25077400	5.45631900
H	0.61173000	2.29152600	5.14756800
H	4.90244100	2.27965100	5.41475700
C	2.65941200	2.01028300	6.94223800
H	3.34221400	2.66782800	7.48896200
H	1.64800200	2.17680400	7.31990200
H	2.94120600	0.97885200	7.18490000
Rh	1.59740300	1.72212500	-1.62099400
C	0.65079100	3.53138400	-2.83392400
C	1.14539800	3.00497900	-4.19802500
C	-0.55850700	1.66153100	-3.55269800
C	-0.38387900	2.72032000	-2.44139800
H	0.98333200	4.44554600	-2.35861500
H	-1.04506100	2.85796900	-1.59509500
C	-0.20168600	2.51693600	-4.80263300
H	-0.07698400	1.92303500	-5.71388400
H	-0.91338600	3.32959300	-4.97814900
C	1.78337500	1.64174200	-3.83807000
H	2.76008700	1.31381900	-4.16692700
C	0.73000800	0.81933800	-3.43794400
H	0.74099700	-0.26020000	-3.39221300
H	1.76535500	3.68190300	-4.78319100
H	-1.49509100	1.10611400	-3.54870200
N	6.63403600	1.93603000	-2.33976500
C	6.23864500	2.51356100	-3.59381200
C	5.92161200	1.68371900	-4.67607300
C	6.19456100	3.90689100	-3.73048800
C	5.53608900	2.25506400	-5.89033700
H	6.00231400	0.60857900	-4.56202200
C	5.79734700	4.46864600	-4.94417400
H	6.46124600	4.53532700	-2.88687900
C	5.46648200	3.64484200	-6.02351500
H	5.30196100	1.61435000	-6.73515300
H	5.76003900	5.54849100	-5.05022600
H	5.17028000	4.08492400	-6.97097300
S	8.28003700	1.31974800	-2.22613600
O	8.48223900	0.52739600	-3.43507200

O	8.36875800	0.73897000	-0.88605500
C	9.30659500	2.77203200	-2.31157600
C	9.84403700	3.15905700	-3.54131700
C	9.57145700	3.49105600	-1.14170000
C	10.65348600	4.29200800	-3.59212600
H	9.64440900	2.57317200	-4.43123100
C	10.38143900	4.61958500	-1.21724400
H	9.16760900	3.15938900	-0.19139600
C	10.93556500	5.03798700	-2.43848400
H	11.07921400	4.59726200	-4.54372000
H	10.59653200	5.18096300	-0.31237500
C	11.84265100	6.24153200	-2.49828700
H	12.87619700	5.95713600	-2.26615000
H	11.84408400	6.69434600	-3.49321800
H	11.54535600	7.00410700	-1.77293100
C	3.53196900	2.71234100	-1.94165300
H	3.86768100	2.70815100	-2.96975300
H	3.18602200	3.71356500	-1.67606100
C	4.54370400	2.18840800	-1.00551500
C	5.85349600	1.88339000	-1.20090400
H	6.39981100	1.50789000	-0.34316200
INT7a			
C	2.05973500	-1.51315900	0.67553000
C	0.84118300	-1.40017400	0.05285600
H	0.51925300	-2.17627900	-0.63385600
H	0.05875600	-0.73130500	0.39739900
C	2.95462200	-2.69342900	0.37989700
H	3.07236400	-3.29901100	1.28798300
H	2.52504800	-3.33422900	-0.39297600
H	3.95843600	-2.39400700	0.06650500
C	2.44075900	-0.63799500	1.87246800
C	1.78256600	0.73628200	1.81238100
H	1.94276900	1.27576400	2.75274000
H	0.72414700	0.76180500	1.56812900
H	2.16978000	-1.17586900	2.78911800
N	2.57601900	1.37336800	0.70230400
S	2.14499100	3.11706800	0.52674300
O	0.69330900	3.05843000	0.35832900
O	3.01285500	3.61591300	-0.54252700
C	2.54213800	3.91353800	2.06404600
C	1.52895300	4.05929300	3.02099300
C	3.83365400	4.40917600	2.28222700
C	1.82687500	4.70213100	4.21827000
H	0.52651800	3.70087300	2.81514300

C	4.10316300	5.04474600	3.49109800
H	4.61220700	4.31976700	1.53420800
C	3.11382700	5.20305200	4.47446100
H	1.04526600	4.82699300	4.96202700
H	5.10310000	5.43034900	3.66691300
C	3.41686100	5.92823500	5.76054400
H	3.27318900	7.00821100	5.63381000
H	2.75834400	5.60384200	6.57045600
H	4.45317700	5.77322900	6.07254600
Rh	2.06175600	0.16287000	-1.14156300
C	1.08327700	-0.54627000	-2.93659900
C	1.11197200	0.77386200	-3.73396600
C	3.24261300	-0.00045900	-3.70871600
C	2.40232700	-1.02789300	-2.91805100
H	0.17892300	-1.11004700	-2.74406400
H	2.72279400	-2.04095300	-2.70421500
C	2.21285800	0.44949100	-4.78222700
H	2.53821000	1.33001100	-5.34625500
H	1.92910600	-0.35337100	-5.47061000
C	1.89646800	1.69027500	-2.77346300
H	1.54512800	2.63430900	-2.37910700
C	3.20087800	1.21211500	-2.75633600
H	4.06542600	1.71165100	-2.33818300
H	0.15129500	1.14908500	-4.08242100
H	4.22797100	-0.32808700	-4.03739100
C	3.93075900	-0.22480100	1.89028800
C	3.97509700	0.98073000	0.97386300
N	6.38331500	1.29866100	0.70654000
C	6.86996900	-0.05261100	0.69492500
C	7.61271900	-0.53974200	1.77666500
C	6.61465800	-0.87692600	-0.41089500
C	8.09439500	-1.84957600	1.74936500
H	7.81646500	0.11303800	2.61689700
C	7.08560500	-2.18989600	-0.42177800
H	6.05303100	-0.48222800	-1.25190500
C	7.82854600	-2.67786600	0.65739200
H	8.67533500	-2.22263900	2.58701500
H	6.89139200	-2.82552200	-1.28080100
H	8.20251900	-3.69690200	0.64318800
S	7.53476600	2.58985200	0.50859000
O	8.68265500	2.22004500	1.32845100
O	6.75473100	3.80778400	0.74580000
C	8.01931100	2.55434600	-1.20743900
C	9.06689000	1.71855700	-1.60596800

C	7.34746500	3.36555200	-2.12681700
C	9.43249900	1.69421600	-2.94928900
H	9.59544300	1.11890900	-0.87356200
C	7.73173300	3.32487800	-3.46564600
H	6.56383900	4.03670600	-1.79206300
C	8.77627300	2.49357400	-3.89851700
H	10.25035300	1.05228100	-3.26453500
H	7.22373000	3.96318000	-4.18330300
C	9.21436500	2.48916800	-5.34204100
H	9.55889900	1.49897500	-5.65360700
H	8.40582300	2.79896400	-6.00946100
H	10.04836900	3.18496300	-5.49385900
H	4.61418400	-1.01527500	1.58284400
C	5.03882900	1.63607700	0.47434200
H	4.88633600	2.53956400	-0.09999800
H	4.22033100	0.06460100	2.90821900

INT8a

C	0.89788200	-0.05307200	-2.09887300
C	0.02591700	0.62861900	-1.25541200
H	-0.98428200	0.83552300	-1.59517100
H	0.20086400	0.75302700	-0.19448400
C	0.45680200	-0.54124300	-3.45904400
H	0.34448100	-1.63101100	-3.42260300
H	-0.51075100	-0.12638900	-3.75189900
H	1.19600900	-0.32072300	-4.23520100
C	2.29353000	-0.14544800	-1.76872200
C	2.76401800	-0.14434300	-0.31959700
H	3.66227200	-0.74240600	-0.15861200
H	1.98594000	-0.51813000	0.34826800
H	2.94682900	-0.62149800	-2.49346700
N	3.02633300	1.29562500	0.02344100
S	2.45800400	1.83170400	1.64351100
O	0.99709400	1.80479500	1.53155100
O	3.17942600	3.08214900	1.88216800
C	2.94359400	0.59244700	2.82645800
C	2.01669100	-0.39194600	3.19092600
C	4.20727100	0.65628100	3.42103400
C	2.38047400	-1.33462100	4.14764700
H	1.02332300	-0.39778400	2.75657900
C	4.54673700	-0.29682200	4.37599100
H	4.90446000	1.43965400	3.15326700
C	3.64636100	-1.30571100	4.75427800
H	1.66495900	-2.09847400	4.43766800
H	5.52604500	-0.25173700	4.84329600

C	4.01591900	-2.30951300	5.81588700
H	3.75839900	-1.92625900	6.81078600
H	3.48031800	-3.25269200	5.68075400
H	5.08918800	-2.51737500	5.81499000
Rh	2.00579800	2.03060900	-1.77754800
C	0.76744900	2.84411600	-3.51327800
C	0.05482100	3.97229100	-2.74321100
C	2.20111200	4.63637600	-3.02925400
C	2.08289700	3.24702100	-3.69252400
H	0.26668800	2.02967700	-4.01785000
H	2.79829200	2.80952900	-4.37314000
C	0.78887400	5.20811800	-3.33520600
H	0.57223300	6.13261800	-2.79105800
H	0.60344200	5.35165000	-4.40466500
C	0.72425600	3.88663800	-1.35567000
H	0.21262100	3.72818700	-0.41489600
C	2.04059700	4.29091900	-1.53373500
H	2.74797100	4.55334300	-0.75748900
H	-1.03351100	3.95114900	-2.75713700
H	3.07632900	5.22366800	-3.29794400
C	4.08889300	2.10605200	-1.90660600
C	4.99916800	2.25616600	-2.86405700
H	6.06238800	2.19884200	-2.63362500
H	4.75781400	2.44178700	-3.90498600
C	4.38302700	1.87980000	-0.44323400
H	4.40124900	2.85446200	0.04978600
C	5.64118200	1.13503200	-0.04986100
C	6.46435000	1.68381200	0.94632400
C	6.05998700	-0.04190700	-0.69310200
C	7.65592600	1.05875300	1.31552900
H	6.17549600	2.61797500	1.42170500
C	7.24462100	-0.67446800	-0.31595600
H	5.48246000	-0.44532100	-1.51880700
C	8.04277600	-0.12853500	0.69190000
H	8.28555100	1.50447300	2.07967500
H	7.55402400	-1.58393400	-0.82188000
H	8.97050200	-0.61605700	0.97531800
INT8b			
C	1.84606100	-1.51429500	0.53985400
C	0.56358700	-1.41995400	0.05880200
H	0.20755400	-2.14924600	-0.66105600
H	-0.20836400	-0.83185600	0.54530300
C	2.76403100	-2.60951400	0.04788300
H	2.98180000	-3.30346500	0.87024400

H	2.30157800	-3.18373600	-0.75753400
H	3.72400000	-2.22710200	-0.30997200
C	2.28974800	-0.73905400	1.78425600
C	1.61069700	0.62448800	1.88453200
H	1.82497500	1.08673400	2.85509200
H	0.53796400	0.64955700	1.71341700
H	2.08707600	-1.35711700	2.66716000
N	2.31981100	1.36143300	0.77944600
S	1.89010800	3.10717500	0.77613400
O	0.42836400	3.07043900	0.76178700
O	2.64985400	3.69082500	-0.32960100
C	2.45917100	3.77762000	2.32016000
C	1.56689400	3.85077400	3.39695000
C	3.77197700	4.25183700	2.42722800
C	2.01050900	4.39494600	4.59865400
H	0.54214000	3.51543900	3.28144400
C	4.19106000	4.78894200	3.64065500
H	4.44049700	4.22107600	1.57562900
C	3.32400200	4.87044300	4.74236700
H	1.32193000	4.46320000	5.43583100
H	5.20680300	5.16267100	3.73103400
C	3.78050700	5.49249200	6.03708900
H	3.58207500	6.57119100	6.03357900
H	3.25307600	5.06717500	6.89491100
H	4.85469700	5.35938800	6.18981000
Rh	1.61215200	0.28397700	-1.10961900
C	0.43402700	-0.32467600	-2.82094500
C	0.27598300	1.05582000	-3.48964000
C	2.43326300	0.43458600	-3.81251600
C	1.76951700	-0.71375000	-3.02065100
H	-0.40259500	-0.96526600	-2.57170100
H	2.17337300	-1.71701800	-2.95045400
C	1.24270800	0.89973500	-4.69716600
H	1.43710000	1.84498800	-5.21474700
H	0.91560100	0.13985900	-5.41436100
C	1.12778500	1.93873800	-2.55667500
H	0.77299100	2.81091700	-2.02347000
C	2.44723000	1.55468900	-2.75358000
H	3.32631300	2.07742900	-2.40215000
H	-0.74352600	1.39008700	-3.67383400
H	3.38370600	0.20692500	-4.29247400
C	3.76684500	-0.28985700	1.74428900
C	3.73688700	0.95037800	0.87659000
H	4.46044500	-1.03860600	1.35966200

C	4.74448600	1.56218300	0.22455800
H	4.48434300	2.40958000	-0.40075800
H	4.08936900	-0.04847300	2.76501600
C	6.17197800	1.21938200	0.22229900
C	6.95064400	1.70845500	-0.84698600
C	6.82219700	0.46360000	1.21855100
C	8.30973400	1.42381500	-0.94086000
H	6.47591900	2.31629300	-1.61313200
C	8.18454900	0.18495200	1.12643400
H	6.27959200	0.12020700	2.09101800
C	8.93237800	0.65485300	0.04494600
H	8.88458600	1.80717600	-1.77829900
H	8.66648000	-0.39287800	1.90937500
H	9.99334500	0.43517200	-0.02177700
INT9a			
C	-0.03445900	-1.09073600	-0.44210200
C	-1.00759800	-0.11550000	-0.40031400
H	-1.88431600	-0.21541700	-1.03251800
H	-1.10535800	0.59464300	0.41466500
C	-0.18806900	-2.27895900	-1.35864000
H	-0.43391600	-3.16540500	-0.75857600
H	-1.00062000	-2.13411100	-2.07321500
H	0.73394400	-2.50697500	-1.89803300
C	1.06493700	-1.20450900	0.62326100
C	1.33502700	0.12437400	1.33287500
H	1.94330200	-0.02459400	2.23172800
H	0.45440600	0.70378800	1.60184500
H	0.77273200	-1.99549400	1.32550000
N	2.11168300	0.82396700	0.26807000
S	2.50179000	2.51373900	0.60754800
O	1.16623100	3.12343500	0.62777600
O	3.49255600	2.87161300	-0.40892100
C	3.19318200	2.68349700	2.23856600
C	2.32454900	2.82030100	3.32925700
C	4.57876300	2.77313000	2.39687300
C	2.86400900	3.02301900	4.59521500
H	1.25055300	2.80124900	3.18285800
C	5.09325300	2.98536300	3.67263300
H	5.23586300	2.68722200	1.54032500
C	4.25230500	3.11202300	4.78893700
H	2.19660300	3.13244600	5.44513500
H	6.16889900	3.05977000	3.80213600
C	4.82168200	3.37871200	6.15889600
H	4.88349500	4.45799400	6.34422600

H	4.19467100	2.94949200	6.94501900
H	5.83127400	2.97230000	6.26090900
Rh	0.62446700	0.94841600	-1.55390200
C	-0.77012600	1.48636600	-3.09335900
C	-0.11848100	2.80735800	-3.55470400
C	1.21622400	1.14413500	-4.32721600
C	0.06102000	0.45388900	-3.56985900
H	-1.80963500	1.40156300	-2.80023100
H	-0.20640400	-0.58705400	-3.70547000
C	0.47249600	2.37107400	-4.92538000
H	1.15160600	3.11453600	-5.35582300
H	-0.29450500	2.09604200	-5.65662300
C	1.16196800	2.83446600	-2.69558500
H	1.42660200	3.60758400	-1.98659100
C	1.97487400	1.81943900	-3.16750700
H	3.01346200	1.65773100	-2.90784400
H	-0.74481000	3.69669800	-3.51357800
H	1.80436900	0.51396700	-4.99262500
C	2.44369700	-1.49580100	0.03153200
C	3.19306600	-0.17391100	-0.17551200
C	2.96151100	-2.69985200	-0.20311000
H	2.40009500	-3.60822500	-0.00743400
H	3.97059500	-2.82202300	-0.58456900
C	4.54878700	-0.11254900	0.51599100
C	5.62443800	0.47453000	-0.16612400
C	4.78138400	-0.67853600	1.77902200
C	6.89847300	0.50975400	0.40243700
H	5.46311300	0.91065800	-1.14739400
C	6.05107900	-0.63384300	2.35364300
H	3.98064500	-1.18607900	2.30707700
C	7.11322800	-0.04096300	1.66711100
H	7.72123600	0.95839400	-0.14575000
H	6.21434700	-1.07767300	3.33096700
H	8.10488400	-0.02235400	2.10894000
H	3.35629900	0.02159500	-1.23621300
NBD			
C	2.10171300	-1.51909100	-0.53830600
C	3.45931700	-0.98658000	-1.04669300
C	3.47505700	-0.80714500	1.19170600
C	2.11095800	-1.41223300	0.79339600
H	1.29372800	-1.85493600	-1.17771000
H	1.31220400	-1.64089700	1.48922000
C	4.35716300	-1.51346100	0.11568500
H	5.38211600	-1.13187400	0.07792900

H	4.35581300	-2.60428700	0.20320000
C	3.52216000	0.51968200	-0.71146400
H	3.50249200	1.31531800	-1.44701600
C	3.53177100	0.62639100	0.62022100
H	3.52160300	1.52905300	1.21986000
H	3.73195300	-1.26298700	-2.06672500
H	3.76188900	-0.91827700	2.23888600
Rh[NBD ₂] ⁺			
Rh	1.28932600	0.62016400	0.06344700
C	2.03952300	-1.43862200	-0.59803000
C	3.40539400	-0.94813800	-1.12536000
C	3.50342500	-0.83358800	1.13553200
C	2.09594000	-1.36937600	0.78014400
H	1.28691600	-1.93081800	-1.20214700
H	1.40284000	-1.81071300	1.48700100
C	4.33369700	-1.50161100	-0.00210000
H	5.35890000	-1.12428700	-0.06605000
H	4.33758000	-2.59463500	0.05263400
C	3.41998200	0.55180800	-0.75885800
H	3.56895600	1.35810000	-1.46695100
C	3.47957300	0.62449100	0.61941900
H	3.70191800	1.49881400	1.22028900
H	3.63358700	-1.19010500	-2.16197200
H	3.82246000	-0.97228900	2.16692300
C	0.53557900	2.54632900	-0.90712600
C	-0.84030100	1.98782100	-1.33121400
C	-0.90666200	2.23578000	0.92027700
C	0.49816800	2.69838600	0.46540300
H	1.28153400	2.93218800	-1.59129900
H	1.20179700	3.24434800	1.08313800
C	-1.74954600	2.71952500	-0.29825300
H	-2.77733000	2.34378500	-0.28777800
H	-1.74785400	3.80721700	-0.41824600
C	-0.85622800	0.56586600	-0.73013100
H	-1.01677500	-0.34169900	-1.29936200
C	-0.89682800	0.71380600	0.64233300
H	-1.11269400	-0.05286800	1.37727700
H	-1.08226100	2.06363500	-2.38994200
H	-1.21095500	2.53817200	1.92064000
TS1			
C	1.71827100	-0.38220600	-0.86675000
C	0.43494100	-0.12697400	-1.39318500
H	0.23532100	-0.38625400	-2.42780100
H	-0.44131200	-0.02558000	-0.75921600

C	2.81547100	-1.01176700	-1.69073800
H	2.87368700	-2.07844500	-1.44500200
H	2.60992500	-0.93947300	-2.76063000
H	3.79325900	-0.56944400	-1.48190200
C	1.98651600	0.00386600	0.47556000
C	0.91934600	0.37560300	1.45618000
H	1.24412200	0.23918600	2.48973500
H	-0.04182800	-0.12688900	1.31496900
H	3.01634700	0.04866700	0.81837400
N	0.90837900	1.76126000	0.99876600
S	1.13367200	2.96369900	2.23368300
O	-0.07563800	2.84202300	3.04892300
O	1.47227000	4.20071900	1.52685200
C	2.53031200	2.45964700	3.22675600
C	2.29769400	1.81952500	4.44887200
C	3.83177500	2.74277900	2.79781500
C	3.38667000	1.44581000	5.23375600
H	1.28086400	1.64480500	4.78395300
C	4.90492500	2.36069600	3.59742000
H	4.00141400	3.28000200	1.87118400
C	4.70319100	1.70787900	4.82536600
H	3.20968800	0.95347500	6.18563200
H	5.91698900	2.58663700	3.27368500
C	5.87179500	1.33587700	5.70202500
H	6.77352100	1.14845800	5.11307900
H	6.10059500	2.15031900	6.39998800
H	5.65763700	0.44619800	6.30007400
Rh	1.31330800	1.87881200	-1.02862100
C	0.94387000	2.49622300	-3.11038200
C	0.84639800	4.01926200	-2.87094100
C	3.04570400	3.49422000	-2.71680400
C	2.29820100	2.17231000	-2.99938700
H	0.16427500	1.90410000	-3.57336600
H	2.78359100	1.27216800	-3.35389800
C	2.17289800	4.48896300	-3.53431300
H	2.40765500	5.53774200	-3.32547600
H	2.20450900	4.30507200	-4.61289500
C	1.22669400	4.13744000	-1.38096300
H	0.61925800	4.56093100	-0.59227700
C	2.57141800	3.82347900	-1.29303700
H	3.19789000	3.94588100	-0.41994100
H	-0.08680300	4.49432600	-3.16760500
H	4.12173100	3.48428100	-2.88216500

TS2a

C	0.92243500	-0.08656400	-2.29843900
C	0.05810900	0.62997500	-1.45856600
H	-0.89562300	0.96526200	-1.85491100
H	0.12772200	0.60266500	-0.37882400
C	0.54401800	-0.43181500	-3.72034700
H	0.31732000	-1.50310600	-3.77052900
H	-0.35162200	0.09902500	-4.05214300
H	1.36035600	-0.24147500	-4.42324200
C	2.25153600	-0.34853400	-1.86472900
C	2.59516200	-0.42595900	-0.38226700
H	3.49754700	-1.02101300	-0.21954900
H	1.77768200	-0.88501700	0.18431200
H	2.94822400	-0.80631800	-2.55835900
N	2.83246600	0.98495700	0.00975800
S	2.20893500	1.58524300	1.46853700
O	0.73519700	1.51253700	1.48297900
O	2.86401100	2.89803400	1.61892200
C	2.77879000	0.50386000	2.77911500
C	2.05990300	-0.65824900	3.08046100
C	3.87332000	0.89033800	3.55395600
C	2.47386400	-1.45528300	4.14362600
H	1.16966100	-0.91495800	2.51705400
C	4.26460600	0.08454400	4.62289700
H	4.38587700	1.82052900	3.33822500
C	3.57910900	-1.09883200	4.93307100
H	1.91636700	-2.35750200	4.37964300
H	5.10517200	0.39166100	5.23941300
C	3.98382700	-1.94473600	6.11467600
H	5.03001500	-1.78267400	6.38718900
H	3.37472900	-1.69781200	6.99251800
H	3.84112000	-3.01025800	5.91257000
Rh	2.08618000	1.88731600	-1.75039500
C	0.74930700	2.97280000	-3.39830600
C	0.09064600	3.97450200	-2.43443500
C	2.23155900	4.64743000	-2.71650600
C	2.04965400	3.37897600	-3.57668000
H	0.22302700	2.21490900	-3.96030500
H	2.73319400	3.01892000	-4.32981100
C	0.81814800	5.27908500	-2.86709600
H	0.64348800	6.11231700	-2.17942500
H	0.58831300	5.58537600	-3.89302200
C	0.81436000	3.68423500	-1.10440800
H	0.33040200	3.42233800	-0.17220600
C	2.13077900	4.09896100	-1.27634700

H	2.84332800	4.27412500	-0.48211200
H	-0.99765400	3.96702600	-2.40190700
H	3.10352000	5.25867500	-2.94078800
C	4.17748000	2.00360300	-1.98955800
C	4.96620200	2.22532900	-3.05463000
H	6.05147800	2.24916600	-2.98373400
H	4.57549700	2.40077500	-4.05048200
C	4.82050400	1.86541200	-0.68438400
H	4.57109400	2.59779200	0.08143100
N	5.92936200	1.17206600	-0.39143400
C	6.80201500	1.64038200	0.66744100
C	7.60815400	2.75441600	0.40934400
C	6.84589800	0.99210700	1.90372600
C	8.45918400	3.22961600	1.40699600
H	7.57089800	3.23135400	-0.56473100
C	7.70014700	1.47673000	2.89423900
H	6.21735800	0.12927200	2.08747800
C	8.50519800	2.59162600	2.64834800
H	9.08400600	4.09544800	1.21310700
H	7.73736000	0.98067000	3.85901900
H	9.16808100	2.96279500	3.42367300
S	6.59554400	-0.14923600	-1.47969200
O	7.59784900	0.50541900	-2.31502300
O	5.42257600	-0.82448500	-2.02625800
C	7.41864500	-1.23389400	-0.33967600
C	8.79249500	-1.08154100	-0.12801600
C	6.69838600	-2.27684500	0.25048700
C	9.44241000	-1.98348000	0.70819800
H	9.33553500	-0.28034300	-0.61589500
C	7.37041700	-3.16485400	1.08511700
H	5.64153800	-2.40191200	0.04344200
C	8.74782000	-3.03550200	1.32700900
H	10.50964400	-1.87423700	0.87759400
H	6.82102900	-3.98092800	1.54525600
C	9.47482800	-4.02631400	2.19977100
H	10.28607000	-3.54945300	2.75673700
H	8.80013800	-4.50625700	2.91320800
H	9.92306000	-4.81845100	1.58782800
TS2a'			
C	1.67518500	-0.18244300	-2.13441900
C	0.59923600	0.44391600	-1.49951600
H	-0.33976600	0.54438600	-2.03532600
H	0.53741600	0.57931100	-0.42749100
C	1.54859300	-0.75950600	-3.52511100

H	1.53416500	-1.85296200	-3.44965900
H	0.61867800	-0.45976400	-4.01414800
H	2.39664100	-0.49111000	-4.16245900
C	2.96666200	-0.13387500	-1.52896300
C	3.10725300	-0.00548400	-0.01929800
H	4.06075300	-0.41842400	0.33446200
H	2.31508600	-0.55135500	0.50302900
H	3.80061000	-0.55972600	-2.07931400
N	3.03818300	1.45707600	0.24477500
S	2.14603600	2.01211600	1.60309800
O	0.71433000	2.09135000	1.25991300
O	2.83949900	3.23143300	2.03521900
C	2.30111300	0.71632300	2.83683500
C	1.13327900	0.11842200	3.31882100
C	3.55368900	0.34371000	3.33198200
C	1.23129100	-0.86183400	4.30452800
H	0.16947100	0.42667300	2.93032700
C	3.63037200	-0.64322200	4.31080300
H	4.45751200	0.81698800	2.96774700
C	2.47485900	-1.25910400	4.81697400
H	0.32420300	-1.32480100	4.68276600
H	4.60417700	-0.93575400	4.69374600
C	2.56678500	-2.29986300	5.90450000
H	2.48488100	-1.83247600	6.89335200
H	1.76117900	-3.03488200	5.82540600
H	3.52178900	-2.83119700	5.87259700
Rh	2.43087900	2.02160400	-1.70594500
C	1.29524700	2.60344000	-3.69463500
C	0.24478500	3.52356400	-3.04618000
C	2.21090900	4.64237400	-3.00026800
C	2.49191400	3.28169000	-3.67132600
H	1.07430100	1.69852200	-4.24217700
H	3.38485400	3.01406600	-4.21460700
C	0.77162300	4.90593700	-3.52853500
H	0.27907200	5.74733600	-3.03135500
H	0.72342400	5.03270900	-4.61526500
C	0.69125800	3.56414300	-1.57125100
H	0.09413300	3.27934500	-0.71535700
C	1.89432600	4.24773300	-1.54233100
H	2.40643700	4.64494800	-0.67897400
H	-0.79739200	3.26638200	-3.22928900
H	2.97012600	5.41000500	-3.12987100
C	4.46742600	2.52767200	-1.60491200
C	5.40970900	2.80243600	-2.51575100

H	6.45793900	2.91795800	-2.23926300
H	5.20922600	2.91276800	-3.57539100
C	4.95028100	2.24179800	-0.23035200
H	5.28858900	1.22364300	-0.05188900
N	5.55781900	3.09606700	0.60828300
C	6.40704800	2.58380800	1.66648500
C	6.06538400	2.76754400	3.01096300
C	7.59066700	1.92672200	1.30852500
C	6.92465600	2.28005300	3.99787100
H	5.14708700	3.28210300	3.26422400
C	8.43115600	1.43078900	2.30466200
H	7.85257700	1.81728800	0.26020300
C	8.10119700	1.61201200	3.64971400
H	6.66789300	2.42217500	5.04294600
H	9.34705300	0.91758200	2.02928000
H	8.76185100	1.23636700	4.42496000
S	5.45967900	4.92171900	0.53579600
O	5.30267500	5.33804800	1.91966400
O	4.48067300	5.23563100	-0.49625700
C	7.08692300	5.37704100	-0.02102500
C	8.10003500	5.56264700	0.92488300
C	7.30551300	5.61065200	-1.38208300
C	9.35658400	5.97061500	0.48581700
H	7.90094600	5.40692400	1.97877300
C	8.56915200	6.02179500	-1.79522600
H	6.49676900	5.48942000	-2.09312700
C	9.61243500	6.20829400	-0.87369900
H	10.14957200	6.11793900	1.21317600
H	8.74721000	6.21307300	-2.84961000
C	10.96499500	6.69182600	-1.33150900
H	11.76143400	6.34649200	-0.66720300
H	11.18967900	6.35305400	-2.34642700
H	10.99748900	7.78814800	-1.33861000
TS2b			
C	-0.27533800	-0.73933800	-0.60280100
C	-0.83905400	0.58264300	-0.62754100
H	-1.74243700	0.71237600	-1.21720900
H	-0.76463500	1.24223900	0.23270000
C	-0.93599400	-1.86149200	-1.37812400
H	-1.56080800	-2.46867800	-0.71137800
H	-1.58915300	-1.47129200	-2.16167900
H	-0.19999900	-2.52680700	-1.83577600
C	0.71948200	-1.05095900	0.35970100
C	1.42504600	0.02863700	1.12290700

H	2.30126900	-0.39192100	1.62990500
H	0.72853900	0.35537100	1.91721900
H	0.71315400	-2.03438800	0.81648800
N	1.82030800	1.12340900	0.21831300
S	1.74649300	2.63212500	0.96192500
O	0.41378700	2.82050800	1.57576800
O	2.22481200	3.61099600	-0.02521400
C	2.93495000	2.55267500	2.30180900
C	2.47858400	2.51879800	3.62102900
C	4.30232600	2.58076200	2.01133300
C	3.40807400	2.50090600	4.66008400
H	1.41296600	2.52753300	3.82198800
C	5.21470400	2.56079700	3.06446600
H	4.64712300	2.61879300	0.98419000
C	4.78609200	2.52490100	4.40155300
H	3.05645200	2.48019700	5.68805200
H	6.27856500	2.58808200	2.84444300
C	5.78315000	2.55302500	5.53409500
H	5.97868300	3.58448600	5.85148200
H	5.41340400	2.01023200	6.40866300
H	6.74204900	2.11821000	5.23806300
Rh	0.98684600	0.91801100	-1.66515000
C	-0.20618600	1.07819800	-3.59026600
C	-0.15337100	2.61602900	-3.71840300
C	1.93014700	1.85229900	-4.18636000
C	1.06110400	0.60642200	-3.89160800
H	-1.11936900	0.50054600	-3.53351300
H	1.33683200	-0.41607100	-4.12321300
C	0.87309600	2.76107500	-4.87837600
H	1.22041100	3.78976700	-5.01813600
H	0.50784000	2.35604200	-5.82789900
C	0.72906800	3.00098200	-2.51984000
H	0.46406300	3.67843000	-1.71909300
C	2.00999200	2.53162500	-2.80322700
H	2.91382800	2.78716900	-2.26771800
H	-1.11139700	3.12673000	-3.80104600
H	2.88012900	1.67017100	-4.68357600
C	2.44869400	-2.38961400	-0.65471100
C	3.33844600	-1.54672000	-1.24787000
H	3.05948400	-1.01397200	-2.15348600
C	2.08167500	-3.63935200	-0.45156200
H	1.23451400	-3.91724800	0.17250500
N	4.55929600	-1.19866300	-0.75936100
C	5.16482500	-1.84292900	0.37836400

C	5.26397200	-1.16052000	1.59476600
C	5.64723400	-3.14953700	0.24380400
C	5.84634200	-1.80422900	2.68737100
H	4.89999200	-0.14296100	1.67695500
C	6.22012100	-3.78388300	1.34511400
H	5.57693300	-3.65374900	-0.71464900
C	6.32032900	-3.11222600	2.56611000
H	5.92445500	-1.27994700	3.63451100
H	6.59220000	-4.79885800	1.24777200
H	6.76940200	-3.60802200	3.42108500
S	5.45074000	0.10088300	-1.58305400
O	5.84971100	1.05102900	-0.55100500
O	4.57129600	0.48251600	-2.69298300
C	6.89315800	-0.72135100	-2.21229600
C	8.07899500	-0.67426500	-1.47471900
C	6.82168500	-1.38066900	-3.44434700
C	9.20873000	-1.30730200	-1.98704000
H	8.11543800	-0.14258500	-0.53094600
C	7.96330300	-2.00565600	-3.93402300
H	5.89866700	-1.38511500	-4.01369200
C	9.17262900	-1.97920800	-3.21814200
H	10.13619800	-1.27372000	-1.42308400
H	7.92053300	-2.51518600	-4.89236100
C	10.41057000	-2.63052900	-3.77984300
H	10.16715700	-3.53740300	-4.34032500
H	10.92274800	-1.94925200	-4.47009900
H	11.12032500	-2.89202600	-2.99105900
H	2.61452100	-4.46843400	-0.91618000
TS3a			
C	1.12482900	0.02344800	-2.48670100
C	0.02957000	0.39155200	-1.71644300
H	-0.92679900	0.55535200	-2.20205100
H	-0.00344200	0.30149400	-0.63639800
C	1.00873600	-0.16396400	-3.98354300
H	1.08773500	-1.23062400	-4.22407600
H	0.04733900	0.18716700	-4.36574500
H	1.81142300	0.34531000	-4.52610800
C	2.45073100	-0.14162000	-1.89707800
C	2.54539700	-0.35209500	-0.39178900
H	3.35499400	-1.03338400	-0.13764200
H	1.60375000	-0.71730500	0.01679200
H	3.17864300	-0.67719400	-2.49398600
N	2.79854900	1.01365400	0.14761000
S	2.17875700	1.41824400	1.73929700

O	0.75872500	1.07659700	1.62276700
O	2.63216400	2.79393600	1.95076400
C	2.90149500	0.35760500	2.97510400
C	2.45523600	-0.96176600	3.10367600
C	3.82048700	0.90508400	3.87444600
C	2.97365100	-1.74944900	4.12855500
H	1.69186300	-1.35744000	2.44322300
C	4.31211100	0.10317300	4.90081200
H	4.12225600	1.94128700	3.77844500
C	3.90770700	-1.23398600	5.04072300
H	2.62731000	-2.77297600	4.23767500
H	5.01264000	0.52730800	5.61482800
C	4.46414400	-2.08888800	6.15130000
H	5.50794200	-2.35723200	5.94863100
H	4.44975900	-1.55517400	7.10648700
H	3.89803500	-3.01564800	6.26961800
Rh	1.69105500	2.12503800	-1.61420700
C	0.50826800	3.23656500	-3.10621600
C	-0.08787500	4.27291400	-2.13616900
C	2.09867900	4.82481800	-2.39771000
C	1.85987000	3.57800300	-3.26788100
H	-0.06634100	2.56427100	-3.72918200
H	2.53723700	3.21127900	-4.02673700
C	0.72614500	5.53718100	-2.51194900
H	0.60768900	6.34990700	-1.78805400
H	0.51321100	5.90276700	-3.52246700
C	0.62181200	3.81663000	-0.84738200
H	0.12159800	3.59206200	0.08721200
C	1.99231500	4.16678300	-1.00836400
H	2.70472700	4.30266800	-0.20479900
H	-1.17391000	4.33864300	-2.10199600
H	3.00275000	5.39437900	-2.60474900
C	3.84682800	1.50536600	-1.83199900
C	4.68143500	1.69076700	-2.85258900
H	5.74791800	1.85200200	-2.71080100
H	4.34248100	1.62345700	-3.88242200
C	4.12221100	1.55334300	-0.34373700
H	4.12674500	2.59335800	-0.01996100
N	5.34998900	0.97643100	0.25259200
C	6.22769900	1.95493300	0.88011700
C	6.65432100	3.09484500	0.18539200
C	6.65945400	1.73930800	2.19202400
C	7.48171100	4.02519900	0.81290300
H	6.34827900	3.24940900	-0.84445000

C	7.49949500	2.66716100	2.81055300
H	6.33688400	0.84824200	2.71633500
C	7.90686200	3.81296400	2.12621500
H	7.80585100	4.90787100	0.27044000
H	7.83238800	2.49469900	3.82957900
H	8.55595000	4.53548100	2.61102300
S	6.25034300	-0.25902900	-0.61161700
O	7.23128600	0.37832900	-1.49579100
O	5.24528800	-1.17879600	-1.16241900
C	7.14361800	-1.09898700	0.68448800
C	8.52345000	-0.91043200	0.78212600
C	6.47128200	-1.99034500	1.52487200
C	9.23283200	-1.62090400	1.74782300
H	9.02455300	-0.22504600	0.10835500
C	7.19905500	-2.68734400	2.48500500
H	5.40223700	-2.14348400	1.42797800
C	8.58783400	-2.51886100	2.61074100
H	10.30676800	-1.47890400	1.82817200
H	6.68473600	-3.38629200	3.13882600
C	9.37402700	-3.31171900	3.62472700
H	10.23546400	-2.74815800	3.99337400
H	8.75663200	-3.59685600	4.48093900
H	9.75788000	-4.23640700	3.17699600
TS3a'			
C	1.19654400	-0.08878800	-2.30142100
C	0.09775500	0.40580900	-1.63578300
H	-0.86220000	0.43625500	-2.14157200
H	0.07755000	0.61931400	-0.57279200
C	1.09381300	-0.61890000	-3.71449500
H	1.25217600	-1.70389800	-3.71625500
H	0.10840300	-0.42943100	-4.14631100
H	1.85329300	-0.18305000	-4.37170400
C	2.53710100	-0.06460900	-1.70064100
C	2.63541100	0.06541100	-0.18513700
H	3.43665700	-0.55612400	0.23222000
H	1.70120400	-0.21888500	0.29686500
H	3.23115900	-0.75289400	-2.16726100
N	2.90056500	1.51452300	0.05624100
S	2.26553500	2.09738300	1.59608600
O	0.81606500	1.98213900	1.39935200
O	2.90016500	3.38854300	1.82892600
C	2.72712300	0.90034000	2.84259700
C	1.76919600	-0.03388900	3.25470000
C	4.00313900	0.92577300	3.41233500

C	2.10864300	-0.95916100	4.23759400
H	0.77289100	-0.01593400	2.82789200
C	4.31979200	-0.01183600	4.39206300
H	4.72896300	1.67201200	3.11527600
C	3.38509600	-0.96649600	4.82153300
H	1.36627700	-1.68199400	4.56378600
H	5.31025900	0.00647000	4.83757400
C	3.72973200	-1.95141600	5.90964900
H	3.46759500	-1.54366900	6.89350300
H	3.18137100	-2.88966000	5.79010700
H	4.79953900	-2.17596400	5.92422700
Rh	1.83128700	2.19006400	-1.88693300
C	0.80444000	2.87137500	-3.69067400
C	-0.12701800	3.88554300	-2.98847200
C	1.93147400	4.83835700	-3.03619600
C	2.07638300	3.46316400	-3.70047000
H	0.47150900	2.04054300	-4.29880400
H	2.95653200	3.13447700	-4.23548300
C	0.49168800	5.22717800	-3.45470600
H	0.10632000	6.08959300	-2.90074700
H	0.38799400	5.39904200	-4.53176700
C	0.42791100	3.78512400	-1.55033500
H	-0.16310100	3.60219800	-0.66090700
C	1.71592400	4.36743700	-1.58924700
H	2.31088500	4.69467500	-0.74550300
H	-1.19754300	3.72857600	-3.11146000
H	2.74492000	5.53779900	-3.19960000
C	3.98475400	1.45826900	-1.98093100
C	4.82742600	1.29062000	-2.99674700
H	5.89696200	1.46195300	-2.88371000
H	4.49081500	1.01308400	-3.99141000
C	4.36309400	1.70302000	-0.52746200
H	4.91490100	0.84892600	-0.11859800
N	5.16870900	2.84029000	-0.17585400
C	6.06269600	2.71482300	0.95871600
C	5.95647600	3.57111800	2.06148500
C	7.07672700	1.74771300	0.91994100
C	6.86090600	3.44657200	3.11975800
H	5.16532300	4.30903100	2.08929900
C	7.95553700	1.61144600	1.99339700
H	7.18572500	1.11346900	0.04461500
C	7.85268200	2.46458000	3.09531600
H	6.77665200	4.11452200	3.97164500
H	8.73432900	0.85586800	1.95736900

H	8.54714300	2.36916900	3.92433800
S	5.21258900	4.39645400	-0.97098900
O	4.55596100	5.38150600	-0.10862100
O	4.73080400	4.19345600	-2.33789100
C	6.95807300	4.77085700	-1.03576200
C	7.49186300	5.71462700	-0.15601500
C	7.74323800	4.17962500	-2.02887500
C	8.83975000	6.04747400	-0.26462500
H	6.85850600	6.18141500	0.58912200
C	9.08829500	4.52515700	-2.11871500
H	7.30477200	3.48112900	-2.73314400
C	9.65875600	5.46067700	-1.24081500
H	9.26158200	6.78010400	0.41753400
H	9.70470500	4.07015900	-2.88882600
C	11.10914000	5.85421000	-1.36728800
H	11.55024800	6.07476500	-0.39123800
H	11.69970600	5.06629200	-1.84200100
H	11.21192200	6.75685900	-1.98177500
TS3b			
C	0.00819900	-1.00710600	-0.91124500
C	-1.02610800	-0.09487500	-0.79245100
H	-1.86884700	-0.15620600	-1.47342800
H	-1.20277100	0.48077600	0.11100500
C	-0.04872200	-2.08124200	-1.97349600
H	-0.31430100	-3.04259100	-1.51301300
H	-0.80889000	-1.85776200	-2.72463800
H	0.91039300	-2.22714800	-2.47746400
C	0.97308900	-1.25082300	0.26243300
C	1.23851000	0.03326700	1.04843000
H	1.87434600	-0.18569300	1.91634500
H	0.31356400	0.48068200	1.42868600
H	0.51430000	-2.01145400	0.90864800
N	1.92456500	0.88699700	0.06675600
S	2.29933700	2.45490000	0.61146000
O	1.01791200	3.13401700	0.88292900
O	3.22631700	3.01203100	-0.38317500
C	3.17236600	2.36537600	2.17680500
C	2.45475200	2.23665000	3.37141100
C	4.55858200	2.54279400	2.18672000
C	3.14347800	2.24906100	4.58148400
H	1.37286800	2.16313200	3.35415000
C	5.22758600	2.56398300	3.41066700
H	5.09490700	2.66815000	1.25283200
C	4.53725600	2.41676400	4.62271900

H	2.58893800	2.15025100	5.51066400
H	6.30425100	2.70960100	3.42306300
C	5.26492500	2.48449600	5.94293500
H	5.24043700	3.50464600	6.34471000
H	4.80387500	1.83238100	6.69044900
H	6.31586100	2.20142200	5.83864700
Rh	0.61845600	1.09054600	-1.71408800
C	-0.78058900	1.76633900	-3.23952000
C	-0.25595700	3.20572400	-3.43984300
C	1.27385700	1.83556300	-4.39404200
C	0.16255200	0.91702300	-3.83369000
H	-1.81480100	1.53748100	-3.01583900
H	0.00505100	-0.10401600	-4.15991600
C	0.42546300	3.06381600	-4.83065600
H	1.03716900	3.93172200	-5.09921400
H	-0.28176600	2.83811300	-5.63563100
C	0.98497100	3.22661500	-2.52968900
H	1.12877100	3.87237300	-1.67379600
C	1.91628100	2.39032500	-3.10667800
H	2.94453000	2.26109100	-2.79586600
H	-0.97839200	4.00643100	-3.28985500
H	1.95236200	1.38713200	-5.11861100
C	2.33410100	-1.78089600	-0.16682900
C	3.27071100	-0.79105100	-0.75288800
H	2.98977000	-0.27385900	-1.66303900
C	2.66061900	-3.07589700	-0.06665900
H	1.94253200	-3.79699600	0.31196900
N	4.58090600	-0.80846900	-0.50822000
C	5.22767500	-1.44072700	0.62226400
C	5.07980100	-0.90015900	1.90039800
C	6.01583300	-2.57764800	0.41034400
C	5.71171100	-1.51839000	2.97943500
H	4.49064300	-0.00415200	2.04500700
C	6.64612700	-3.18441700	1.49649000
H	6.12489300	-2.98696900	-0.58808700
C	6.49374700	-2.65751400	2.78099600
H	5.59531700	-1.09981500	3.97382900
H	7.25099600	-4.07146800	1.33769300
H	6.98427100	-3.13395400	3.62398500
S	5.62174300	0.32624700	-1.51055800
O	6.22856700	1.22689600	-0.54073700
O	4.71854300	0.76289300	-2.57339900
C	6.86614800	-0.73453600	-2.19800800
C	8.13410800	-0.76231100	-1.61006500

C	6.56799500	-1.48636900	-3.33988900
C	9.11475900	-1.56842400	-2.18139300
H	8.34310300	-0.15827800	-0.73467400
C	7.56324300	-2.28932200	-3.88699900
H	5.58679600	-1.42851200	-3.79822300
C	8.84939000	-2.34251100	-3.32209400
H	10.10501100	-1.59397000	-1.73620900
H	7.34504100	-2.87557500	-4.77486900
C	9.92984100	-3.18536400	-3.94944900
H	9.51365400	-4.05784700	-4.45994300
H	10.48311900	-2.60296900	-4.69627200
H	10.65246000	-3.53065300	-3.20551900
H	3.62384100	-3.46605000	-0.36993200
TS4a			
C	0.43478900	-0.96446800	-0.51331400
C	-0.21572300	0.29965600	-0.49475100
H	-1.06881100	0.44430600	-1.15116000
H	-0.19856000	0.94484900	0.37578800
C	-0.05042700	-2.09903700	-1.38432800
H	-0.62829800	-2.79118600	-0.76063200
H	-0.71898000	-1.75888800	-2.17824000
H	0.77323800	-2.66708700	-1.82534500
C	1.64325900	-1.09142900	0.19000900
C	2.02765000	-0.17162400	1.33761800
H	2.82072000	-0.61613800	1.94656900
H	1.16102200	-0.00178500	1.98664000
H	2.21906300	-2.00387600	0.05682200
N	2.51141600	1.07465200	0.70040700
S	2.02841100	2.57338500	1.36612500
O	0.55864900	2.71874900	1.28440100
O	2.88008400	3.56365400	0.69351300
C	2.44971200	2.47830900	3.09895000
C	1.46943400	2.09779400	4.02170200
C	3.73834200	2.82066700	3.51677300
C	1.80368400	2.03354900	5.37191900
H	0.45823700	1.89174600	3.68887100
C	4.05371600	2.74228200	4.87022900
H	4.47795300	3.16318300	2.80351200
C	3.09841800	2.34304400	5.81734900
H	1.04333000	1.74945300	6.09388800
H	5.05905400	2.99677300	5.19087500
C	3.46064000	2.23884800	7.27738500
H	3.93768400	1.27408300	7.48888100
H	4.16795000	3.02008900	7.56946200

H	2.57801500	2.31697300	7.91732900
Rh	1.87081100	0.71829400	-1.29109700
C	0.71512600	0.70562500	-3.37935300
C	0.27677800	2.18097200	-3.29700700
C	2.49450600	2.17885800	-3.74244700
C	2.05923100	0.69994200	-3.65799000
H	0.04657500	-0.14327200	-3.39358700
H	2.66392400	-0.15391000	-3.93467700
C	1.21457700	2.79932800	-4.37085100
H	1.21837600	3.89344200	-4.35737100
H	1.01087800	2.43742500	-5.38388000
C	0.97540000	2.66605300	-2.01071800
H	0.48350700	3.13887900	-1.16973400
C	2.34378200	2.66168900	-2.28132200
H	3.10209100	3.16170100	-1.69187600
H	-0.79303600	2.37031800	-3.36605300
H	3.45266600	2.37306900	-4.22153900
C	4.49990900	0.57538400	-0.28657800
C	4.10908000	0.21604000	-1.54618300
H	4.44248100	0.84448600	-2.37021000
H	4.02363600	-0.84672500	-1.77632400
C	5.30838100	0.93456900	0.69662300
H	4.93235700	1.36695400	1.61324000
N	6.69587800	0.78296500	0.64730100
C	7.34741000	0.14061100	-0.46663900
C	7.53036100	-1.24681400	-0.48069200
C	7.79223300	0.92950900	-1.53273600
C	8.15857900	-1.84283500	-1.57476800
H	7.20129000	-1.83856700	0.36628100
C	8.41099800	0.32352200	-2.62645800
H	7.65714300	2.00560500	-1.49054100
C	8.59463800	-1.06129500	-2.64746300
H	8.31098400	-2.91767000	-1.58657000
H	8.75974200	0.93273600	-3.45470400
H	9.08437300	-1.53017500	-3.49555200
S	7.56317400	0.89208400	2.16093800
O	8.04681800	-0.44138200	2.51480900
O	6.65298600	1.62764100	3.04520200
C	8.95315200	1.91771400	1.73222700
C	10.20164600	1.32603500	1.53631300
C	8.77746900	3.30225400	1.63395400
C	11.28842100	2.14192000	1.22516300
H	10.31714700	0.25282900	1.63642100
C	9.87553300	4.09575400	1.32170100

H	7.80448200	3.74719900	1.81219600
C	11.14627500	3.53172100	1.11300400
H	12.26397400	1.68966900	1.07225300
H	9.74945200	5.17226600	1.24629300
C	12.33207400	4.41140800	0.80529100
H	12.06718900	5.20723800	0.10264200
H	12.70137700	4.89536100	1.71739500
H	13.15850600	3.83764600	0.37883900
TS4b			
C	0.99326700	-1.35872700	0.70436600
C	-0.02435000	-0.50577100	0.33562300
H	-0.85599900	-0.90348500	-0.23945500
H	-0.16371500	0.48214700	0.76341300
C	0.94909000	-2.82838500	0.35206600
H	0.84795300	-3.42402400	1.26694700
H	0.09532600	-3.06218800	-0.28776500
H	1.86293900	-3.16770100	-0.14777700
C	2.17105300	-0.88140100	1.44141700
C	2.16961300	0.52775700	2.01805600
H	3.04546800	0.67009700	2.66259100
H	1.27440600	0.65059200	2.64476500
H	2.59748400	-1.64557500	2.08668100
N	2.21226100	1.46128100	0.88173400
S	1.33854700	2.87568800	1.01720800
O	-0.04966200	2.60445200	1.45104500
O	1.55895200	3.59356900	-0.25015800
C	2.15993100	3.74756600	2.34402500
C	1.50510400	3.90667400	3.56664000
C	3.43858200	4.27614000	2.13352900
C	2.14795900	4.59782400	4.59303700
H	0.50548800	3.50765100	3.69892300
C	4.06225900	4.96064600	3.17167800
H	3.93684000	4.16714000	1.17622400
C	3.43032200	5.13496100	4.41460100
H	1.64071200	4.72737200	5.54509700
H	5.05513800	5.37206600	3.01221800
C	4.10564900	5.91155800	5.51760000
H	3.93013700	6.98741300	5.39599100
H	3.72354800	5.62751800	6.50170200
H	5.18859700	5.75783300	5.51074300
Rh	2.07550600	0.25837500	-0.79689900
C	1.36204000	-0.86953300	-2.70557500
C	0.66965800	0.37396700	-3.30486400
C	2.90249700	0.69660900	-3.52993800

C	2.71809700	-0.67275700	-2.84503300
H	0.85813600	-1.77853300	-2.40274400
H	3.51056300	-1.38675400	-2.66306700
C	1.65631900	0.71050700	-4.45812900
H	1.46784000	1.68893500	-4.91083600
H	1.68780700	-0.06175400	-5.23373800
C	1.05085200	1.46572100	-2.28806600
H	0.36831100	2.15483900	-1.80818100
C	2.44028400	1.66222700	-2.42083600
H	2.96539600	2.54268800	-2.07693800
H	-0.38989900	0.27431300	-3.53384300
H	3.88080100	0.88779100	-3.96644100
C	3.95460100	-0.99243900	0.36220100
C	4.15507200	0.16507500	-0.42520000
N	6.32222800	1.21597700	-0.02791900
C	7.03624700	0.02978400	0.36529200
C	7.31711400	-0.20173600	1.71612800
C	7.45294700	-0.87718700	-0.61616000
C	8.00801800	-1.35765500	2.08294900
H	7.01282600	0.52868400	2.45739400
C	8.13530900	-2.03385500	-0.23841300
H	7.24132300	-0.67127800	-1.66052800
C	8.41275000	-2.27448000	1.10949300
H	8.23429500	-1.53830800	3.12911700
H	8.45861400	-2.74057500	-0.99643100
H	8.95025200	-3.17173100	1.40033900
S	7.20918800	2.74313100	-0.09573200
O	8.03094500	2.75143000	1.10852400
O	6.17571900	3.74947500	-0.35111900
C	8.26325100	2.60699000	-1.52147700
C	9.53700000	2.04854600	-1.37848200
C	7.80827400	3.08161900	-2.75544200
C	10.35735700	1.95926500	-2.50009300
H	9.88097300	1.71279200	-0.40688400
C	8.64782700	2.98348000	-3.86126900
H	6.83056700	3.54373300	-2.83628200
C	9.93119400	2.42362100	-3.75418900
H	11.35067600	1.53187000	-2.39737300
H	8.30788100	3.36046200	-4.82170500
C	10.84658400	2.36127100	-4.95084400
H	11.52657200	1.50710300	-4.89238800
H	10.28288300	2.29090000	-5.88495300
H	11.46401000	3.26585900	-5.00938300
H	3.79631600	-1.95611700	-0.11832900

C	4.99004400	1.22902200	-0.36815400
H	4.63679600	2.21034200	-0.65917100
H	4.52473200	-1.05456200	1.28734200
TS5a			
C	1.21943300	-0.68523100	-1.14188000
C	0.23327400	-0.09664300	-0.36685900
H	-0.80367800	-0.37569400	-0.52139500
H	0.44794600	0.45773000	0.53849500
C	0.85860000	-1.71259600	-2.19568900
H	1.18492500	-2.70333400	-1.85799200
H	-0.21927400	-1.76618500	-2.36558100
H	1.35773700	-1.52334600	-3.15166200
C	2.63788600	-0.34639300	-1.02171600
C	3.27045300	-0.03450400	0.33609800
H	3.92966500	-0.86255900	0.61417900
H	2.52240400	0.06650800	1.12345400
H	3.25415700	-1.00706400	-1.62312300
N	4.12247000	1.17785700	0.28279400
S	3.25007600	2.59186000	0.71812900
O	1.80566200	2.42815200	0.28752300
O	3.98159600	3.74476000	0.19578600
C	3.22558400	2.55510600	2.49475900
C	2.01442800	2.67647400	3.17868900
C	4.44603300	2.47640200	3.17700100
C	2.03317300	2.70848700	4.57237200
H	1.08161400	2.75001000	2.63208600
C	4.43763200	2.50765900	4.56599100
H	5.37900000	2.38393200	2.63230200
C	3.23584200	2.62298000	5.28695200
H	1.09584100	2.80455700	5.11225600
H	5.37945900	2.44233000	5.10324300
C	3.25001200	2.63907600	6.79428200
H	4.00573800	3.33320100	7.17492200
H	2.28021900	2.93118700	7.20344700
H	3.49530000	1.64675300	7.19064200
Rh	1.31672800	1.56979800	-1.71815000
C	1.30170900	3.50251900	-2.61083300
C	1.23709000	3.06836800	-4.09166400
C	-0.82513200	2.66171400	-3.23372400
C	0.01247700	3.22911900	-2.07240900
H	2.04282800	4.17481600	-2.19458300
H	-0.40074600	3.63204500	-1.15597000
C	-0.23074100	3.41382900	-4.45057300
H	-0.54884100	2.99568500	-5.41187000

H	-0.43257500	4.48960200	-4.42500200
C	1.14211900	1.53801000	-3.89662500
H	1.80945100	0.81071400	-4.34181800
C	-0.13242200	1.29471900	-3.36162100
H	-0.63336700	0.33948400	-3.28711100
H	2.03383200	3.42366600	-4.74267500
H	-1.90558500	2.64874900	-3.10132400
N	6.87025200	1.48320900	-2.18839400
C	6.42546900	2.03438200	-3.43847600
C	6.56119800	1.29824100	-4.62177300
C	5.88240500	3.32721000	-3.46745800
C	6.14844200	1.85863600	-5.83155900
H	7.00009000	0.30825700	-4.58467600
C	5.45927800	3.87157300	-4.68059200
H	5.79713500	3.89156600	-2.54389900
C	5.59384200	3.14054400	-5.86455800
H	6.26126100	1.29032700	-6.74975700
H	5.04842200	4.87680600	-4.70320400
H	5.27899200	3.57272200	-6.80967000
S	8.60020100	1.29097400	-1.94881400
O	9.07343200	0.53098900	-3.10127900
O	8.72582500	0.79561300	-0.57792600
C	9.26245400	2.94302500	-2.04275400
C	9.71641000	3.43088400	-3.27040600
C	9.33279200	3.71823000	-0.88135200
C	10.24004500	4.72056900	-3.32797500
H	9.67508600	2.80484600	-4.15427900
C	9.86024600	5.00333100	-0.96266300
H	9.00257100	3.31137100	0.06796800
C	10.32189300	5.52506500	-2.18200500
H	10.59871700	5.10528800	-4.27844000
H	9.92491700	5.60947200	-0.06337200
C	10.92608400	6.90556900	-2.24766100
H	11.99325300	6.87214800	-1.99665300
H	10.83960700	7.33467100	-3.24937500
H	10.44729000	7.58678200	-1.53848400
C	3.73731100	1.21387300	-2.16185400
H	3.98220400	0.51108300	-2.95502400
H	3.56112000	2.19209100	-2.60648800
C	4.71209800	1.27729400	-1.03295200
C	6.05848700	1.37328700	-1.06970700
H	6.59744100	1.31617200	-0.13153400
TS6a			
C	0.95931000	-0.11689900	-2.23196700

C	0.12742000	0.71694800	-1.44400100
H	-0.78304700	1.10396400	-1.89147800
H	0.12467600	0.68126600	-0.36062800
C	0.59166600	-0.50842300	-3.64372700
H	0.21775200	-1.53891400	-3.63214600
H	-0.20801500	0.11272500	-4.05295200
H	1.45096400	-0.48062900	-4.31967500
C	2.23013300	-0.44806300	-1.72334600
C	2.54120200	-0.42981300	-0.23220900
H	3.45329200	-0.99940300	-0.02214200
H	1.72489200	-0.89355700	0.33679900
H	2.92224500	-0.96741300	-2.38097000
N	2.75026400	0.99542700	0.08157000
S	2.13034100	1.65212300	1.49132800
O	0.64898500	1.66740900	1.51772000
O	2.83117200	2.94373500	1.62871800
C	2.65728900	0.51321800	2.76877200
C	1.68582600	-0.17239100	3.50217400
C	4.01724300	0.34715300	3.04515600
C	2.08968100	-1.03638500	4.51841600
H	0.63591400	-0.01545600	3.28247100
C	4.40006100	-0.52307700	4.06139300
H	4.76352000	0.89060600	2.47743300
C	3.44673600	-1.22567300	4.81634900
H	1.33677300	-1.56850400	5.09307000
H	5.45624000	-0.65611800	4.27940100
C	3.87151400	-2.13637700	5.94113800
H	3.94545400	-1.57829500	6.88247700
H	3.15098900	-2.94361300	6.09748800
H	4.85146900	-2.58224800	5.74943900
Rh	2.11215800	1.85163000	-1.73110700
C	0.79271800	2.98587500	-3.43822300
C	0.11988800	3.95458200	-2.44747300
C	2.25895900	4.64634000	-2.69754600
C	2.08350900	3.41060500	-3.59974700
H	0.27992000	2.22667200	-4.01183000
H	2.79991400	3.06265400	-4.32787700
C	0.84218000	5.27670400	-2.83657200
H	0.66157000	6.08851700	-2.12541500
H	0.61465500	5.61211500	-3.85369900
C	0.83268900	3.64152700	-1.11802400
H	0.34251300	3.38379100	-0.18709900
C	2.15185300	4.06006800	-1.27190200
H	2.83610500	4.24200600	-0.45387400

H	-0.96856400	3.94156000	-2.42436200
H	3.12837800	5.26933900	-2.90013100
C	4.31118300	1.91449400	-2.15863400
C	4.84200500	1.68090300	-3.36782400
H	5.88407100	1.91835600	-3.58540300
H	4.25388900	1.31917800	-4.20642900
C	4.93687200	2.17600800	-0.93959500
H	4.58646900	3.01743400	-0.34798100
C	6.00819100	1.42831400	-0.34828900
C	6.61051900	1.95227000	0.82419700
C	6.54669600	0.25637700	-0.93387000
C	7.73700900	1.34836700	1.36543400
H	6.18849500	2.84220600	1.28242700
C	7.66870200	-0.34562600	-0.38159100
H	6.07009900	-0.16709400	-1.81096300
C	8.26602500	0.19998800	0.76276800
H	8.20616000	1.76425800	2.25113900
H	8.08141300	-1.24266600	-0.83174700
H	9.14318800	-0.27660700	1.19010300
TS6b			
C	1.00094100	-1.26904800	0.75032700
C	-0.02418400	-0.43553800	0.37171800
H	-0.83822200	-0.84163800	-0.22240600
H	-0.16997500	0.56372500	0.77246600
C	0.99361900	-2.74138000	0.40636600
H	0.84484200	-3.32899100	1.31994300
H	0.18115900	-2.99180300	-0.27918400
H	1.94013500	-3.07272300	-0.03420600
C	2.15258300	-0.77343700	1.52393000
C	2.10234800	0.61933100	2.13682600
H	2.91611200	0.74658100	2.86036800
H	1.15440100	0.73417700	2.68077400
H	2.60079300	-1.54686000	2.14170500
N	2.25648400	1.56192600	1.01645500
S	1.33498200	2.95611600	1.06040100
O	-0.09015100	2.65333300	1.32482500
O	1.67851900	3.69040600	-0.16829500
C	1.97680100	3.81847900	2.48650700
C	1.13288600	4.07477500	3.56856900
C	3.30496400	4.25896000	2.48369500
C	1.63401500	4.77820800	4.66318300
H	0.10292000	3.73692300	3.54130600
C	3.78534800	4.95684800	3.58648700
H	3.94547400	4.06036700	1.63110900

C	2.96038600	5.23090600	4.69102100
H	0.98121700	4.98285300	5.50703900
H	4.81565300	5.30181300	3.59173500
C	3.48453700	6.02095400	5.86409700
H	3.40026800	7.09758600	5.67240400
H	2.92205100	5.80663500	6.77650800
H	4.54056400	5.80707200	6.05225000
Rh	2.19024600	0.32514700	-0.65621800
C	1.50630400	-0.85483500	-2.59363700
C	0.73424000	0.35051100	-3.16843400
C	2.94107400	0.79744200	-3.43189700
C	2.84339800	-0.58570100	-2.75754800
H	1.06044400	-1.78888100	-2.27738500
H	3.67655500	-1.25663700	-2.59289300
C	1.67914400	0.74675600	-4.33881900
H	1.42889700	1.71550300	-4.78189500
H	1.74020100	-0.01758200	-5.12022600
C	1.07208000	1.46407300	-2.15878000
H	0.35707700	2.11370900	-1.67073100
C	2.44142200	1.73782600	-2.31565700
H	2.92661500	2.63627400	-1.95950600
H	-0.32230300	0.19249700	-3.37767900
H	3.89909600	1.04463600	-3.88419700
C	4.01924900	-0.76629800	0.51601900
C	4.24936700	0.30822600	-0.38605800
H	4.00778000	-1.78845800	0.14163200
C	5.23761500	1.12758100	-0.74756600
H	4.99030600	2.02209700	-1.31273000
H	4.47533500	-0.64941000	1.49765600
C	6.67102300	0.94923000	-0.47110600
C	7.53011700	2.03767500	-0.71517500
C	7.22486600	-0.24378000	0.02977700
C	8.89165500	1.94739600	-0.43846600
H	7.11999500	2.96213900	-1.11330000
C	8.58688900	-0.33230200	0.30452600
H	6.59567800	-1.11621300	0.17843400
C	9.42424300	0.76294000	0.07519200
H	9.53765300	2.79920800	-0.62721800
H	9.00005200	-1.26120500	0.68565000
H	10.48680200	0.68865800	0.28434300
TS6b'			
C	1.04960300	-1.31973600	0.72756400
C	0.00538300	-0.44541500	0.55058300
H	-0.88677700	-0.79148700	0.03566800

H	-0.06224300	0.52220500	1.03912000
C	0.96019100	-2.76219300	0.28336800
H	0.89208400	-3.40954600	1.16567800
H	0.07101900	-2.94469600	-0.32402900
H	1.84390400	-3.08358000	-0.27796900
C	2.30227000	-0.90753800	1.37956500
C	2.38079400	0.41888600	2.12162200
H	3.29439800	0.46098800	2.72588300
H	1.52741800	0.48876400	2.81053400
H	2.82168100	-1.73927500	1.84677200
N	2.39762900	1.47177100	1.09141900
S	1.47938500	2.83638100	1.38357900
O	0.08380400	2.49526600	1.74380700
O	1.69808600	3.70815400	0.21674600
C	2.24778100	3.53632200	2.83837200
C	1.47453200	3.73111300	3.98420200
C	3.59452400	3.91654800	2.80187300
C	2.06419300	4.31122000	5.10677700
H	0.43087400	3.43753100	3.98571400
C	4.16365300	4.49017200	3.93365300
H	4.18711200	3.76426100	1.90620600
C	3.41038800	4.70089600	5.10159200
H	1.46587700	4.46624000	6.00006700
H	5.20909900	4.78549100	3.91232100
C	4.03395400	5.35585400	6.30863900
H	4.05316500	6.44595100	6.18958600
H	3.47323800	5.13537400	7.22044200
H	5.06779400	5.02838900	6.45268500
Rh	2.12481800	0.38611200	-0.66806700
C	1.18790600	-0.69075200	-2.55583400
C	0.28458500	0.50538000	-2.92018900
C	2.39966800	1.07784700	-3.49968300
C	2.46936300	-0.34230600	-2.90861100
H	0.83691000	-1.66576300	-2.24501200
H	3.34569900	-0.97687000	-2.92131600
C	1.01210800	1.01314900	-4.19839200
H	0.65457000	1.99104300	-4.53519100
H	0.97701000	0.29735800	-5.02616300
C	0.73590500	1.57855600	-1.90801100
H	0.08233300	2.15927800	-1.26917400
C	2.04359500	1.92883700	-2.26664600
H	2.56242800	2.82074200	-1.95337000
H	-0.78443700	0.30537200	-2.96910100
H	3.26617800	1.40455500	-4.07030100

C	4.01870300	-0.83804600	0.09233600
C	4.21166200	0.34089400	-0.69065500
H	3.89862100	-1.80058500	-0.40171100
C	5.28220500	1.02754500	-1.09466500
H	6.22022500	0.47807200	-0.97054600
H	4.58753600	-0.87873700	1.01761900
C	5.45410800	2.35553300	-1.70754100
C	4.74136600	3.48566000	-1.26994600
C	6.43776600	2.51646400	-2.70052900
C	4.98399600	4.73542900	-1.84024400
H	4.00739700	3.38903800	-0.47757200
C	6.66945300	3.76459400	-3.27535300
H	7.01926400	1.65683400	-3.02404100
C	5.94078400	4.87760200	-2.84832400
H	4.42803000	5.59916900	-1.48825400
H	7.42482400	3.87069000	-4.04795400
H	6.12832700	5.85220900	-3.28839800
TS7a			
C	1.18288100	0.00105800	-2.40966600
C	0.07787200	0.36147300	-1.65010500
H	-0.88173600	0.48534600	-2.14089200
H	0.04659200	0.30307700	-0.56765600
C	1.07228200	-0.23078900	-3.90100000
H	1.16138200	-1.30307200	-4.11175100
H	0.10768600	0.09869300	-4.29386100
H	1.86900500	0.27284500	-4.45764400
C	2.51375200	-0.11337400	-1.81577400
C	2.60937200	-0.28909800	-0.30555000
H	3.45218500	-0.91360800	-0.00181900
H	1.69272400	-0.71789000	0.09954400
H	3.23793300	-0.64616400	-2.42119000
N	2.76300800	1.10105200	0.20276100
S	2.12541400	1.47460800	1.80201600
O	0.70063400	1.16645300	1.65299000
O	2.60651300	2.83448100	2.05284300
C	2.81567600	0.34871000	2.99520000
C	2.21670800	-0.90372500	3.17668200
C	3.89237700	0.75971400	3.78568600
C	2.73361000	-1.76128800	4.14245200
H	1.34053100	-1.18410200	2.60290200
C	4.38642400	-0.11230500	4.75122500
H	4.31191000	1.75035800	3.66403900
C	3.82699200	-1.38557400	4.93987800
H	2.26832700	-2.73079800	4.29429900

H	5.21397800	0.20612400	5.37829100
C	4.39056400	-2.33014900	5.97059400
H	5.18702600	-2.94516300	5.53390600
H	4.82320100	-1.78843300	6.81574900
H	3.62505200	-3.01033100	6.35270600
Rh	1.69157600	2.13426900	-1.59840700
C	0.49347800	3.19342600	-3.12513200
C	-0.10588300	4.25423700	-2.18385000
C	2.07775200	4.80837600	-2.46572100
C	1.84186200	3.53566400	-3.29989400
H	-0.07908300	2.49565200	-3.72137800
H	2.52083600	3.14797300	-4.04724100
C	0.70150600	5.51074500	-2.59845600
H	0.58090600	6.34408400	-1.89888400
H	0.48442600	5.84515100	-3.61878200
C	0.60824100	3.84172400	-0.88291800
H	0.10981200	3.63816800	0.05753200
C	1.97589100	4.19497100	-1.05496800
H	2.68886900	4.36322700	-0.25790100
H	-1.19210400	4.31559800	-2.14918800
H	2.97903800	5.37513500	-2.69132800
C	3.87636600	1.57091700	-1.74484300
C	4.75972200	1.72578300	-2.72856400
H	5.80383900	1.95664600	-2.51949100
H	4.49075100	1.62360900	-3.77588800
C	4.11023100	1.65655100	-0.25340400
H	4.08440300	2.70552400	0.04431000
C	5.37565200	1.03746600	0.31420100
C	6.05582100	1.73021000	1.32764600
C	5.93512800	-0.15374800	-0.17578800
C	7.24586800	1.23405900	1.85991200
H	5.65304400	2.67179000	1.69194900
C	7.11971400	-0.65649400	0.36305800
H	5.47174300	-0.67676200	-1.00632000
C	7.77561300	0.03352000	1.38432100
H	7.76344300	1.78976000	2.63594800
H	7.53928700	-1.57864200	-0.02734200
H	8.70388600	-0.35332200	1.79338400