

Electronic Supplementary Information

Synthesis of Spirocyclic Heterocycles from α,β -Unsaturated *N*-Acylimminium Ions

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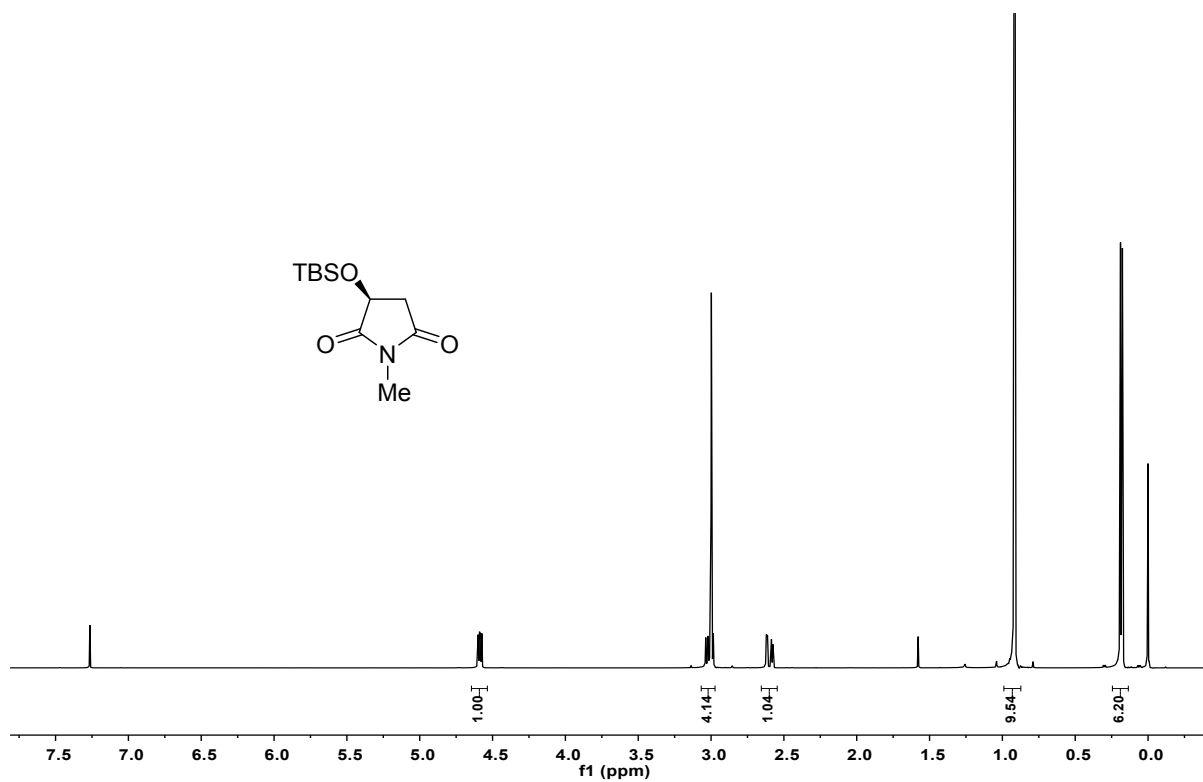


Figure S1 ¹H NMR spectrum of **2e**

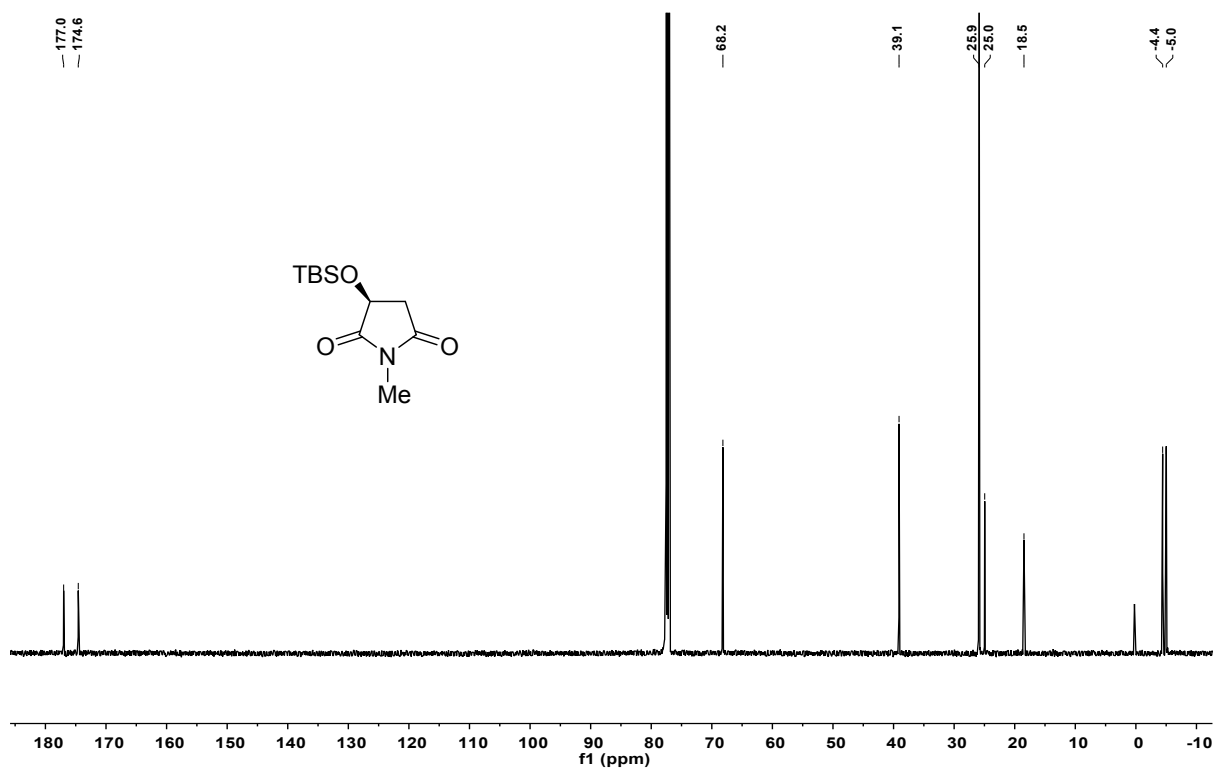


Figure S2 ¹³C NMR spectrum of **2e**

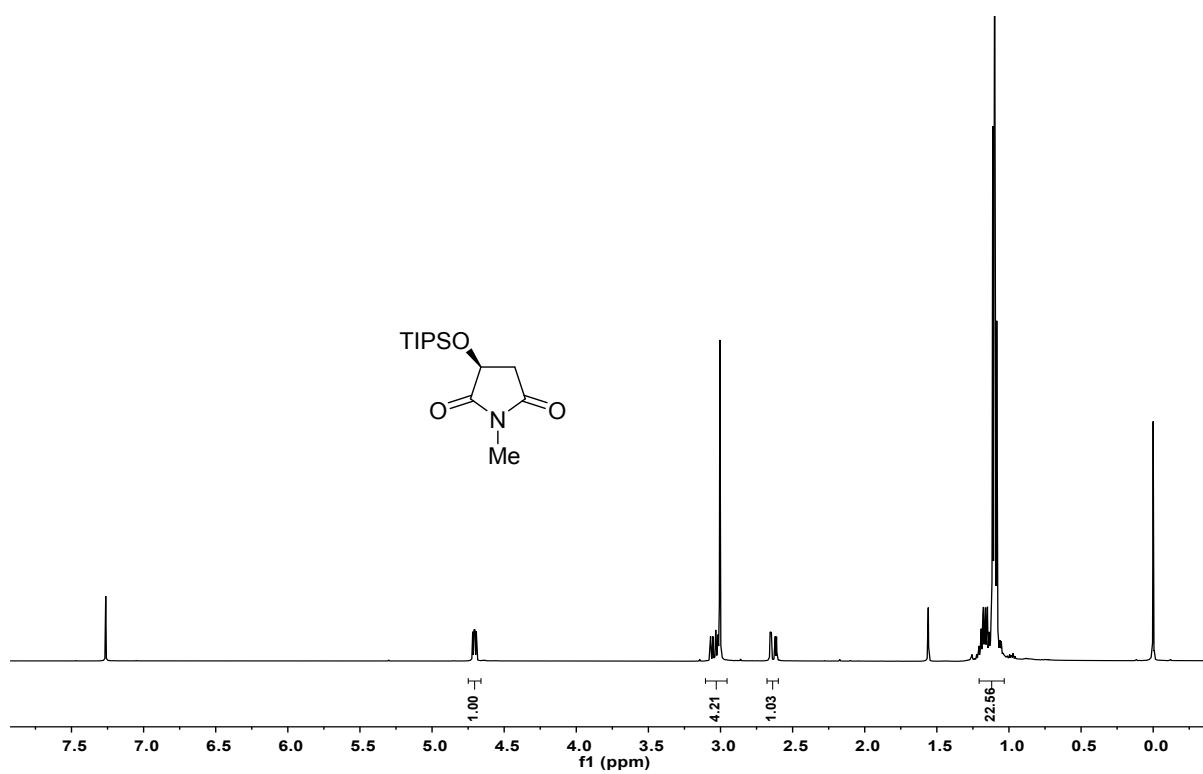


Figure S3 ¹H NMR spectrum of **3e**

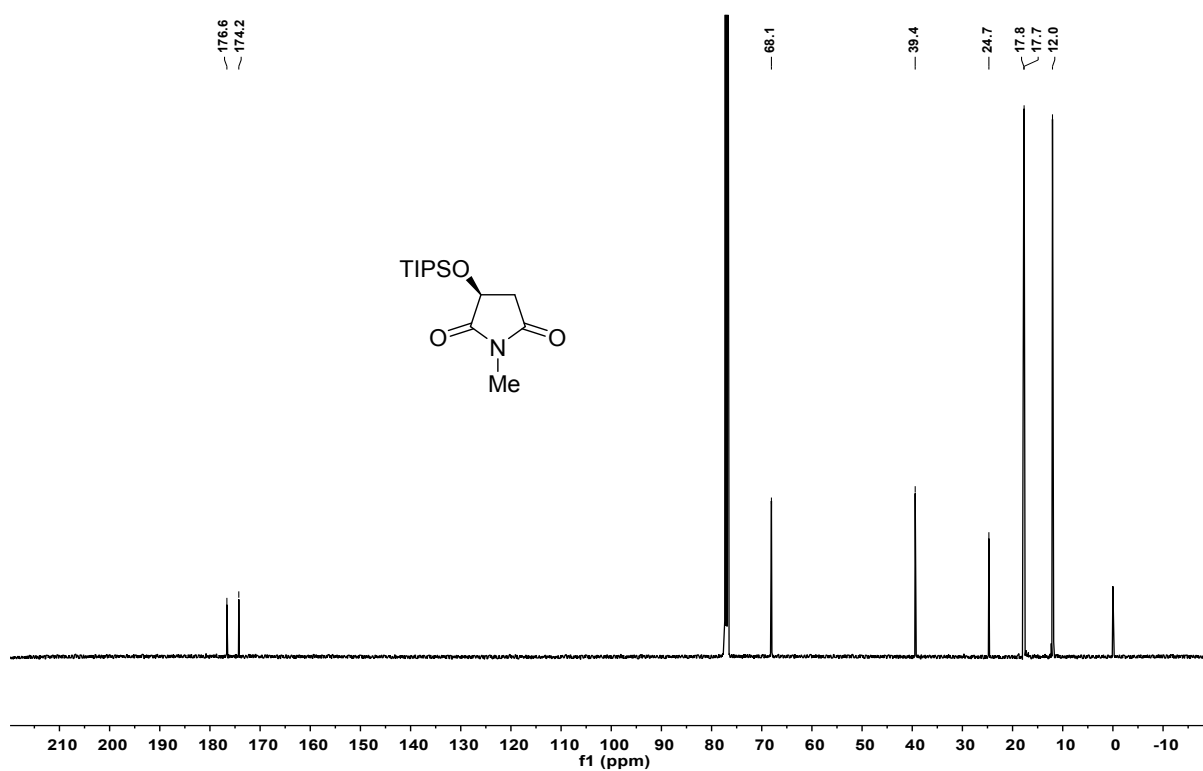


Figure S4 ¹³C NMR spectrum of **3e**

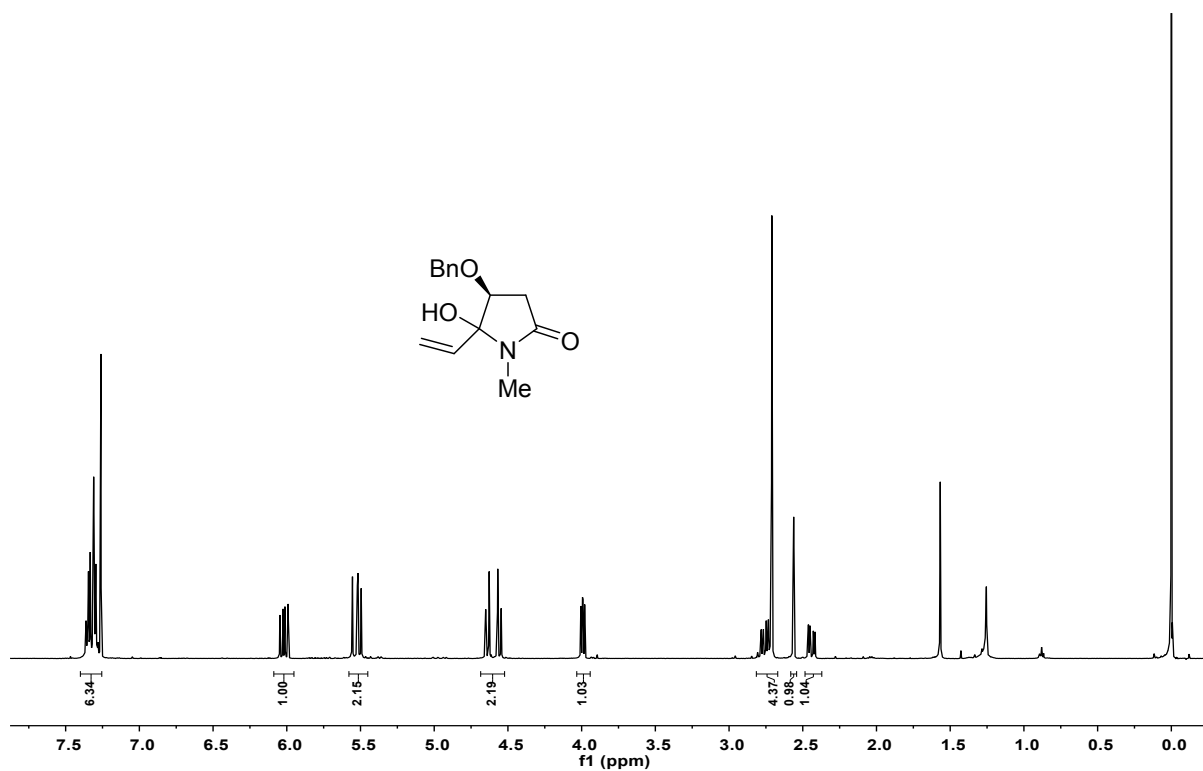


Figure S5 ¹H NMR spectrum of **4e**

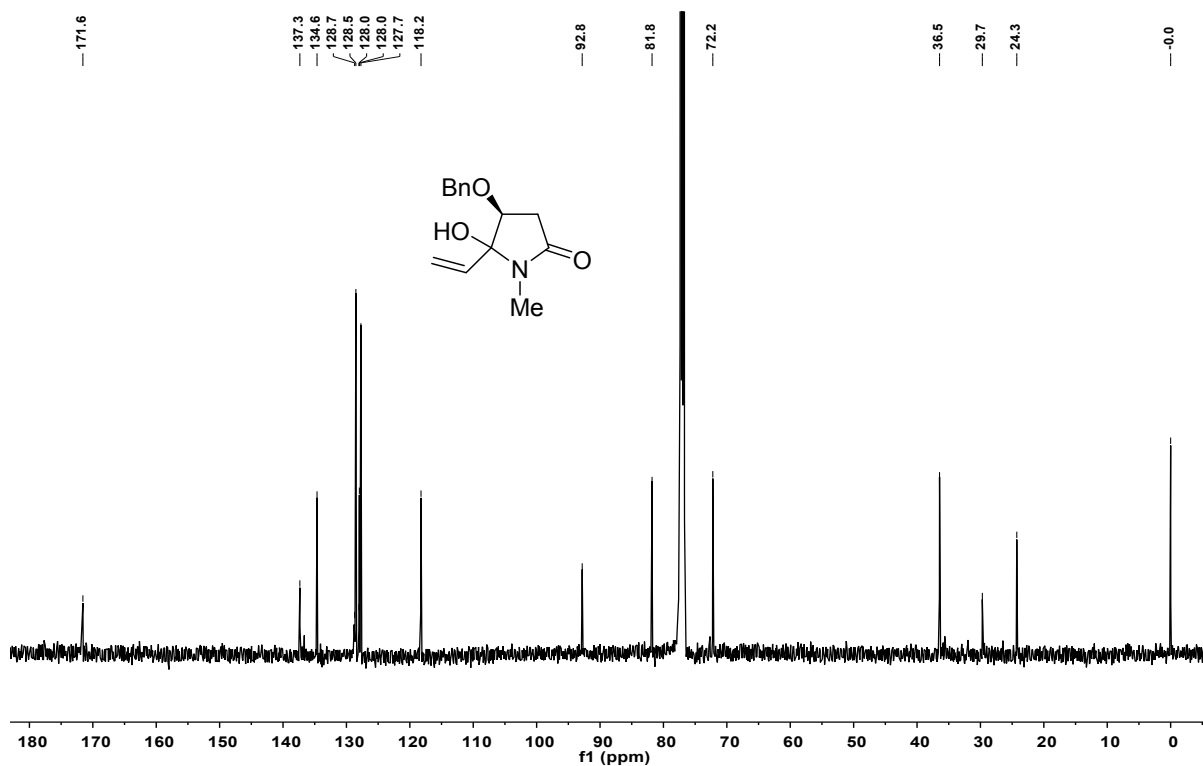


Figure S6 ¹³C NMR spectrum of **4e**

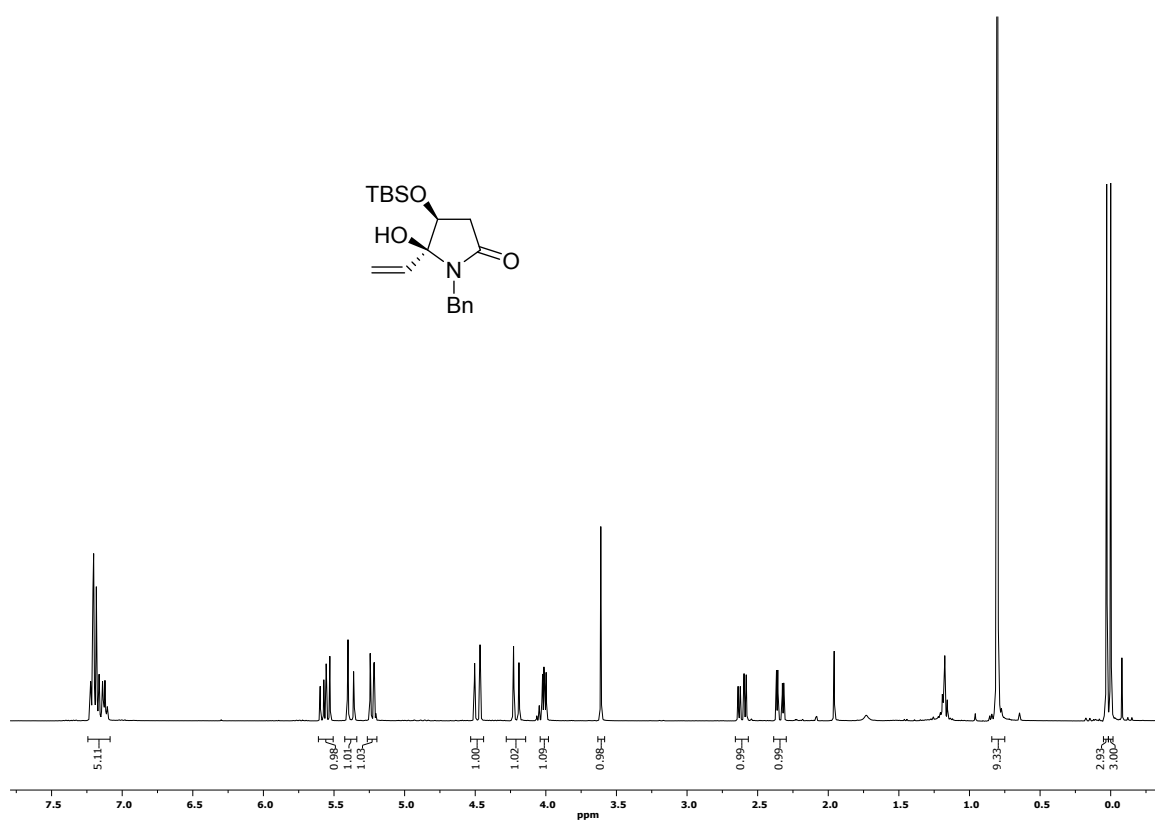


Figure S7 ¹H NMR spectrum of **5d** (major isomer)

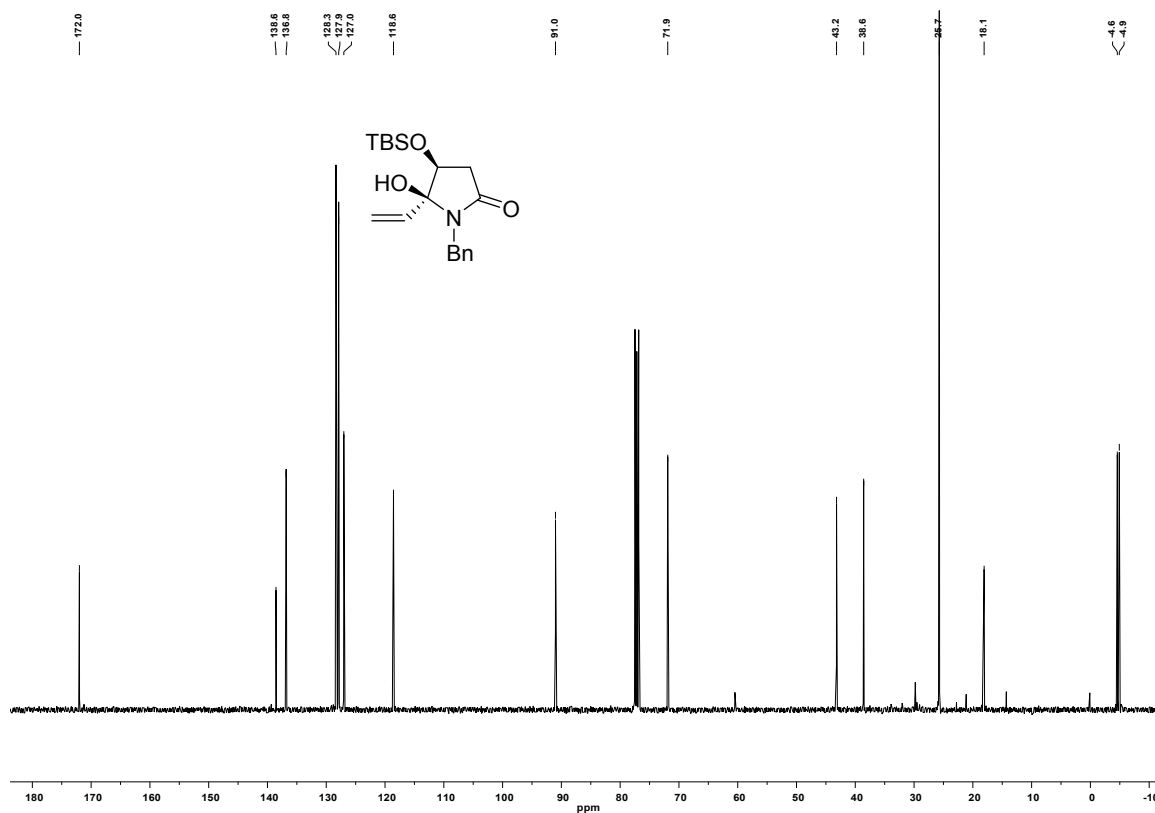


Figure S8 ¹³C NMR spectrum of **5d** (major isomer)

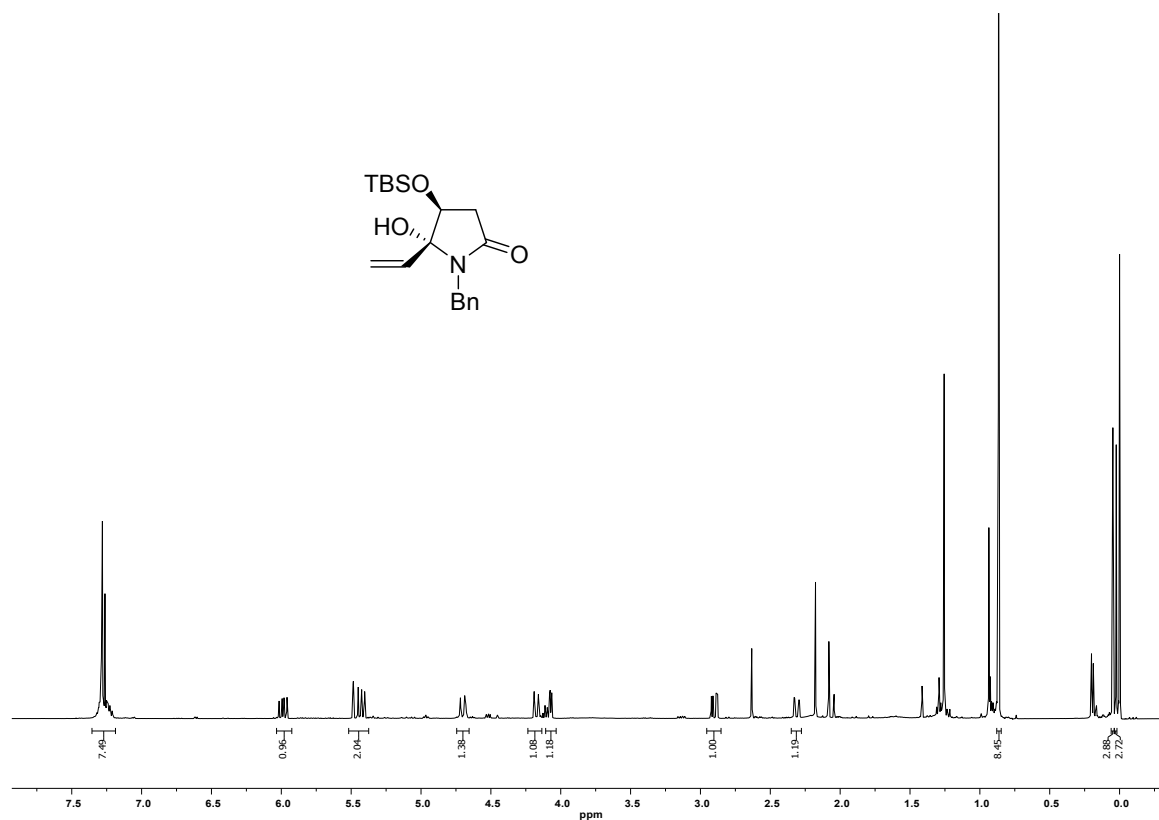


Figure S9 ¹H NMR spectrum of **5d** (minor isomer)

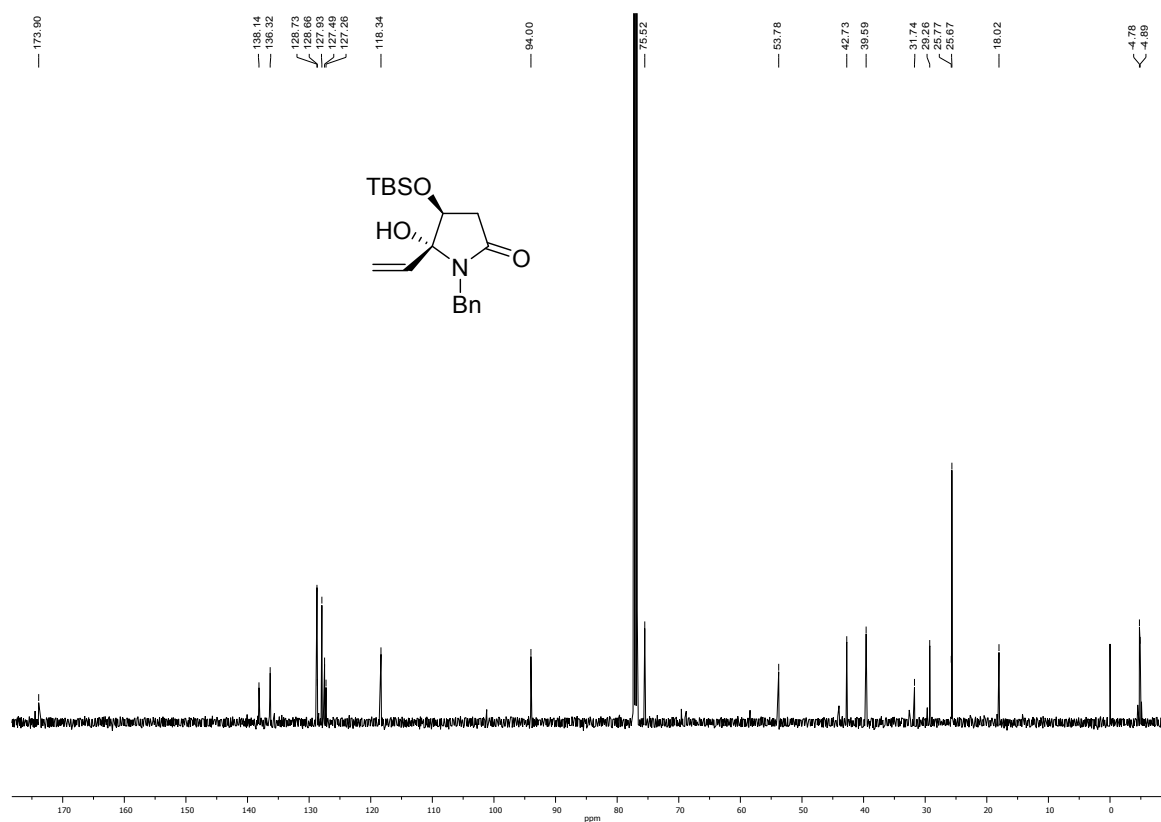


Figure S10 ¹³C NMR spectrum of **5d** (minor isomer)

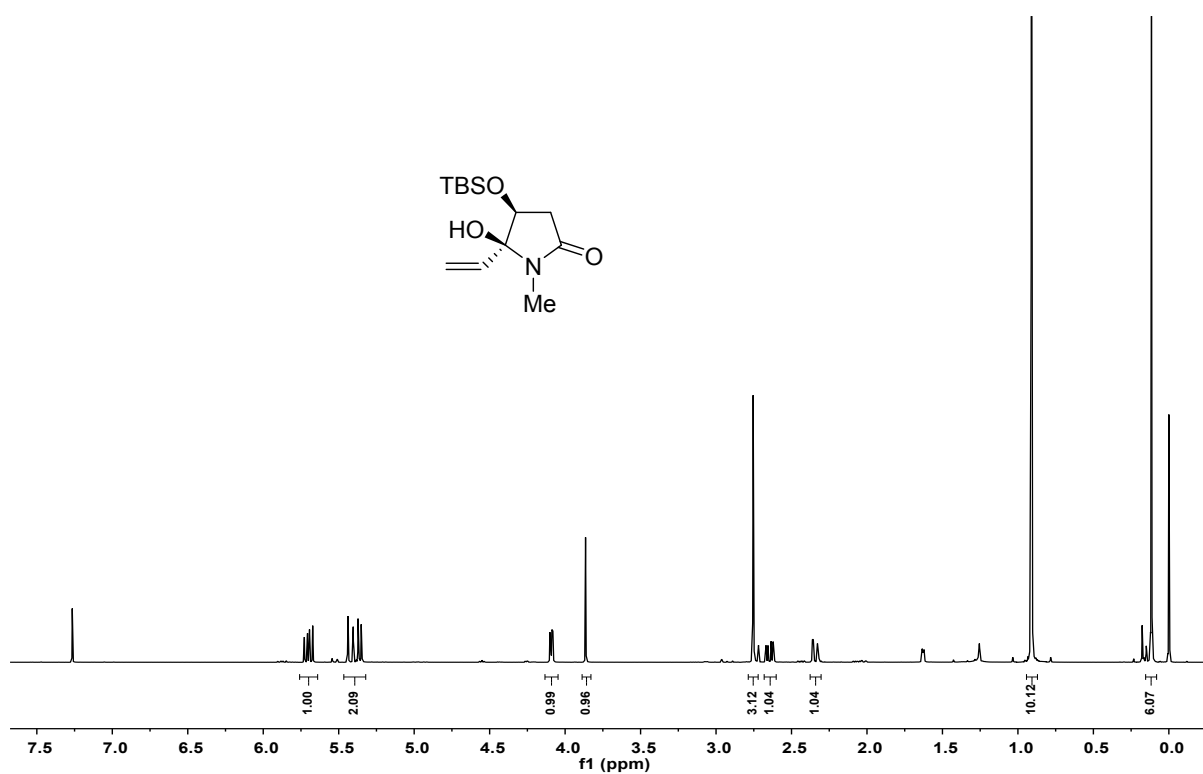


Figure S11 ¹H NMR spectrum of **5e** (major isomer)

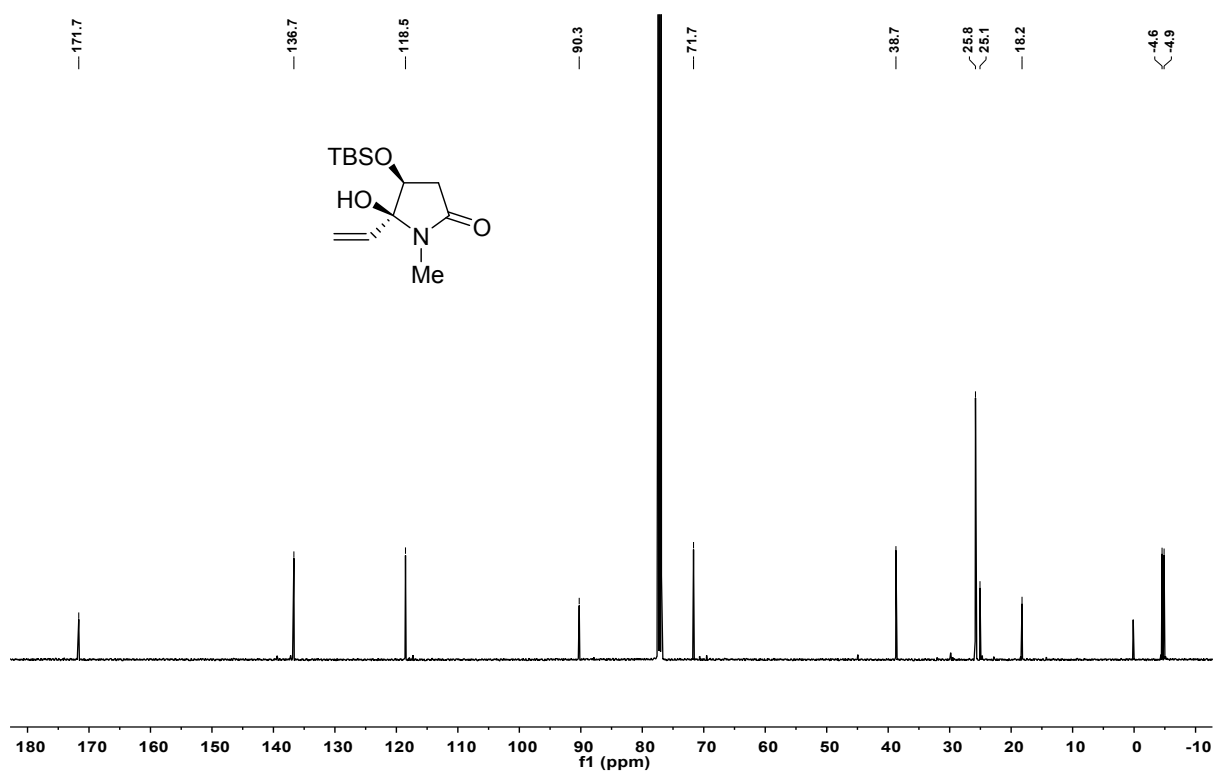


Figure S12 ¹³C NMR spectrum of **5e** (major isomer)

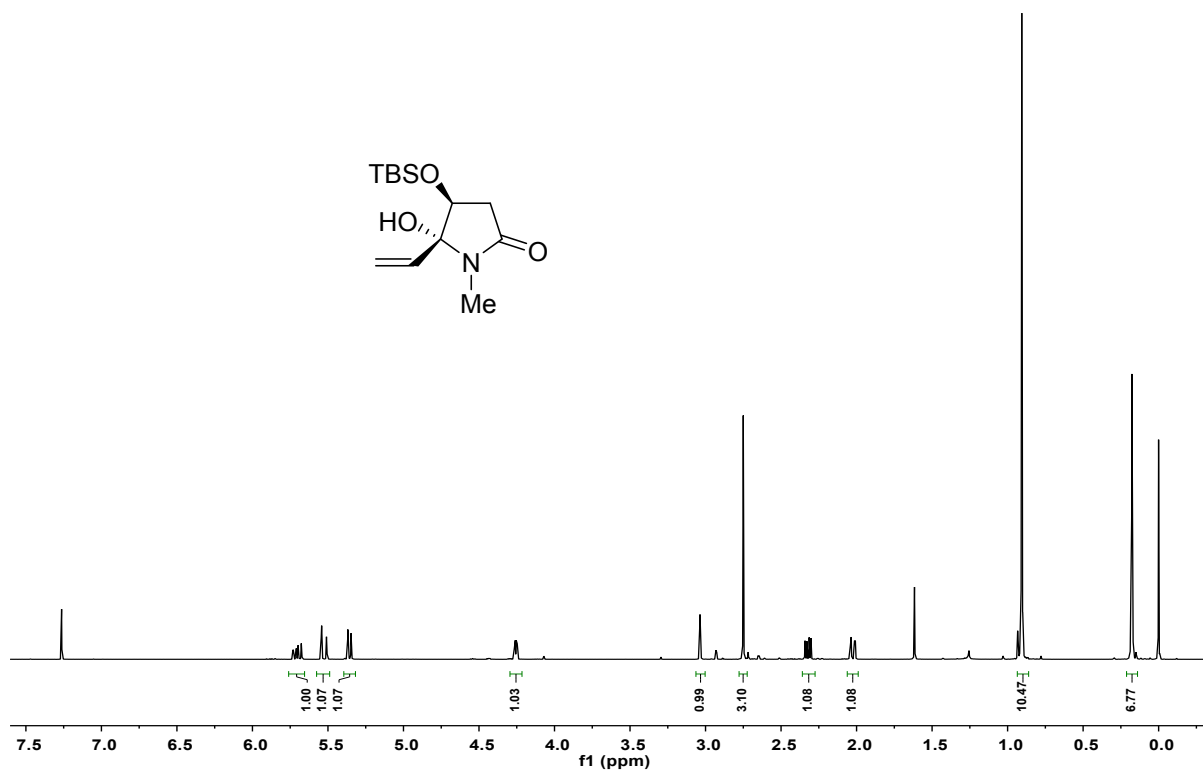


Figure S13 ¹H NMR spectrum of **5e** (minor isomer)

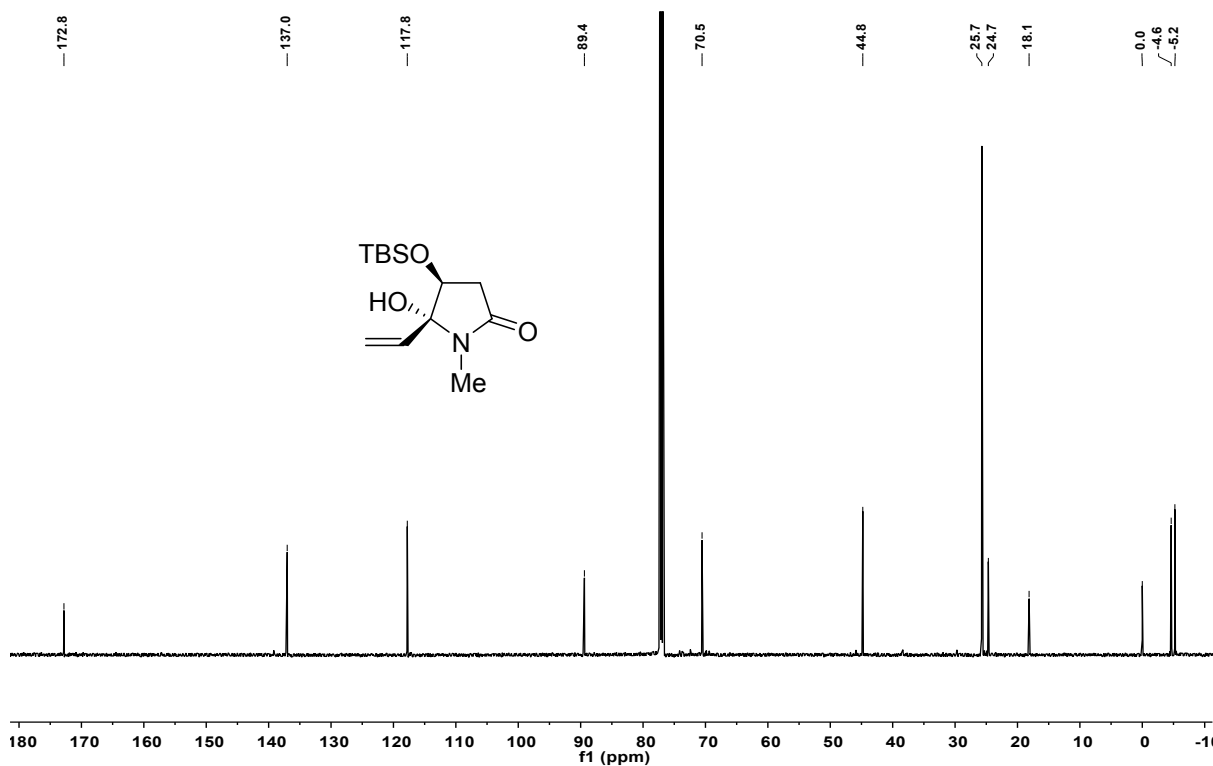


Figure S14 ¹³C NMR spectrum of **5e** (minor isomer)

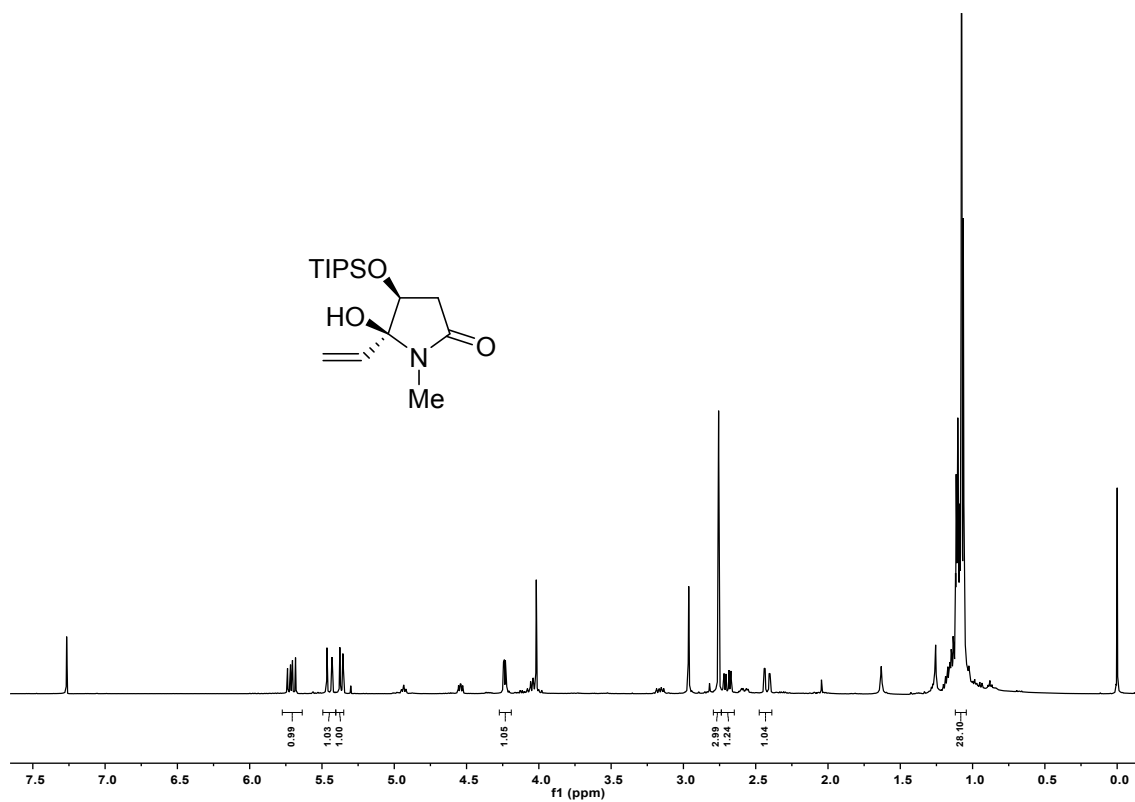


Figure S15 ¹H NMR spectrum of **6e** (major isomer + impurities)

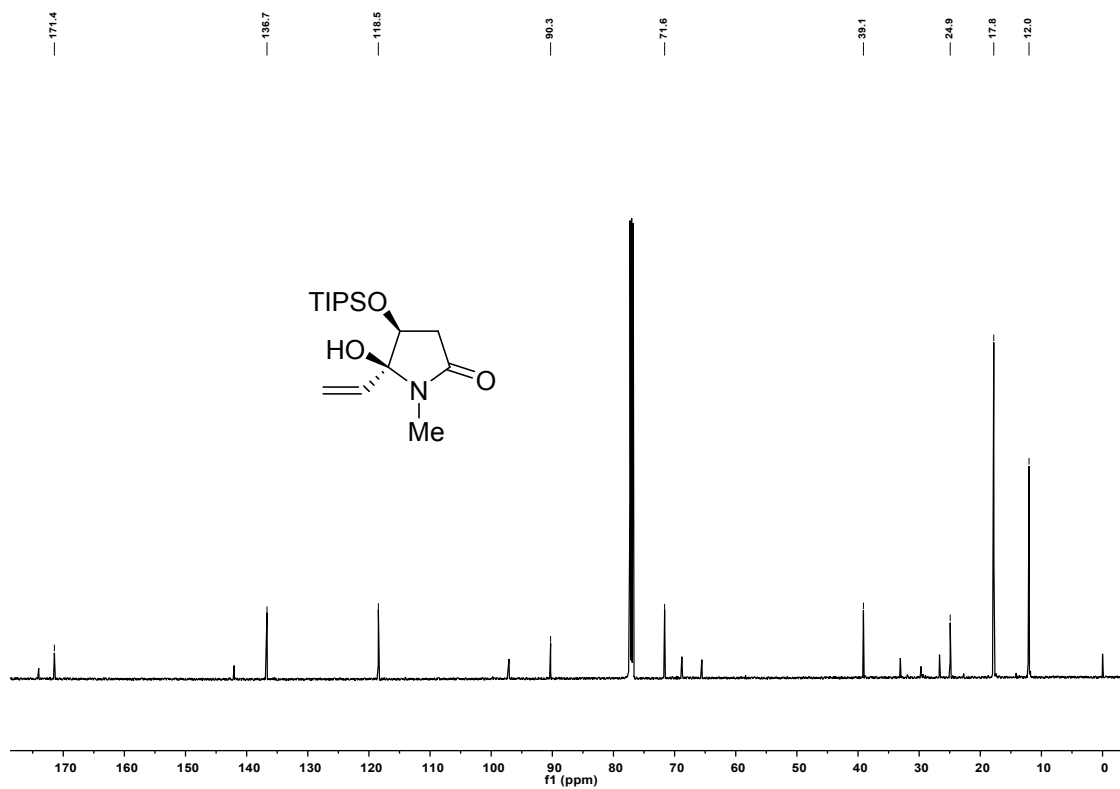


Figure S16 ¹³C NMR spectrum of **6e** (major isomer+ impurities)

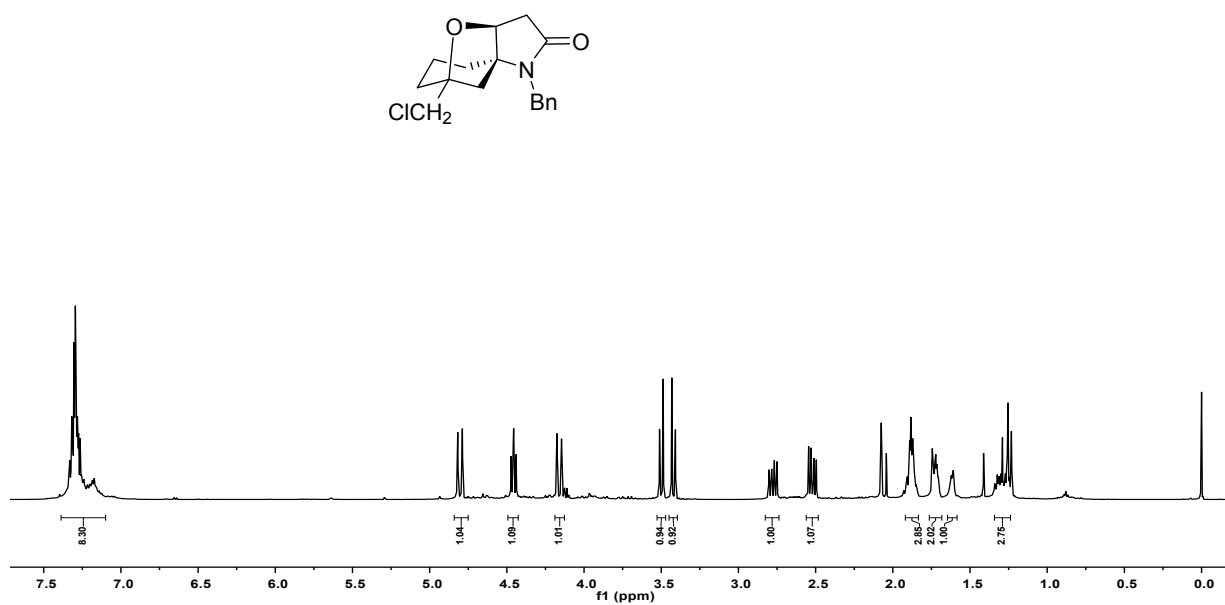


Figure S17 ^1H NMR spectrum of **8d**

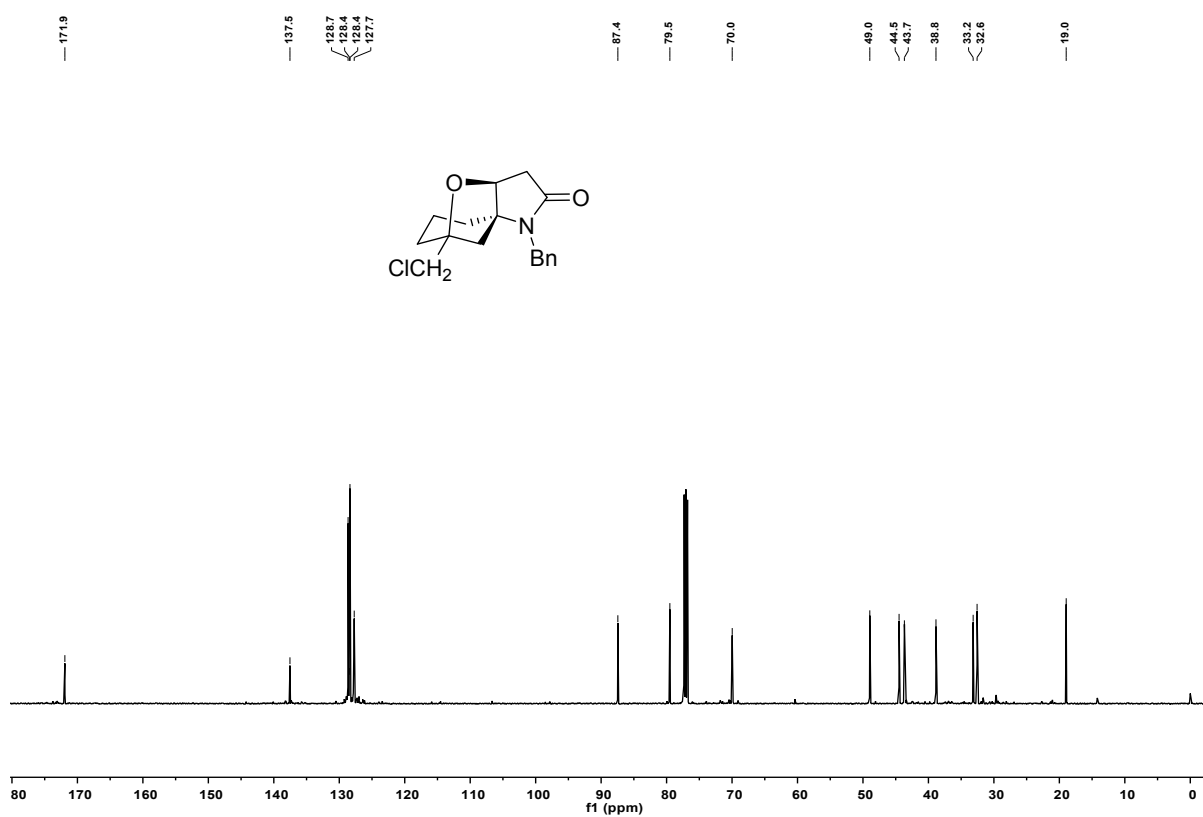


Figure S18 ^{13}C NMR spectrum of **8d**

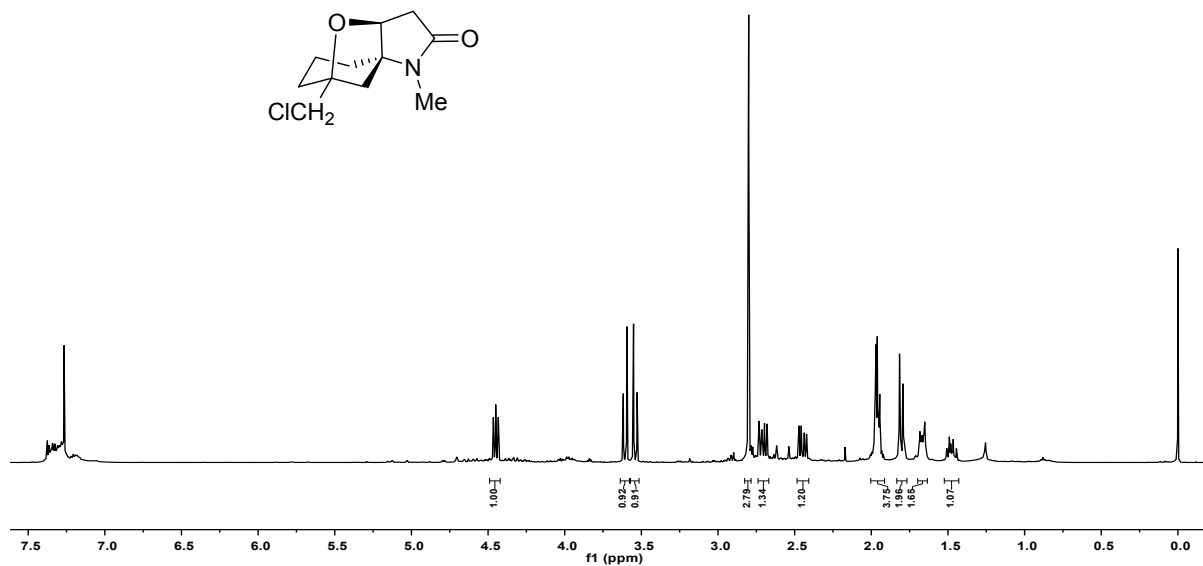


Figure S19 ¹H NMR spectrum of **8e**

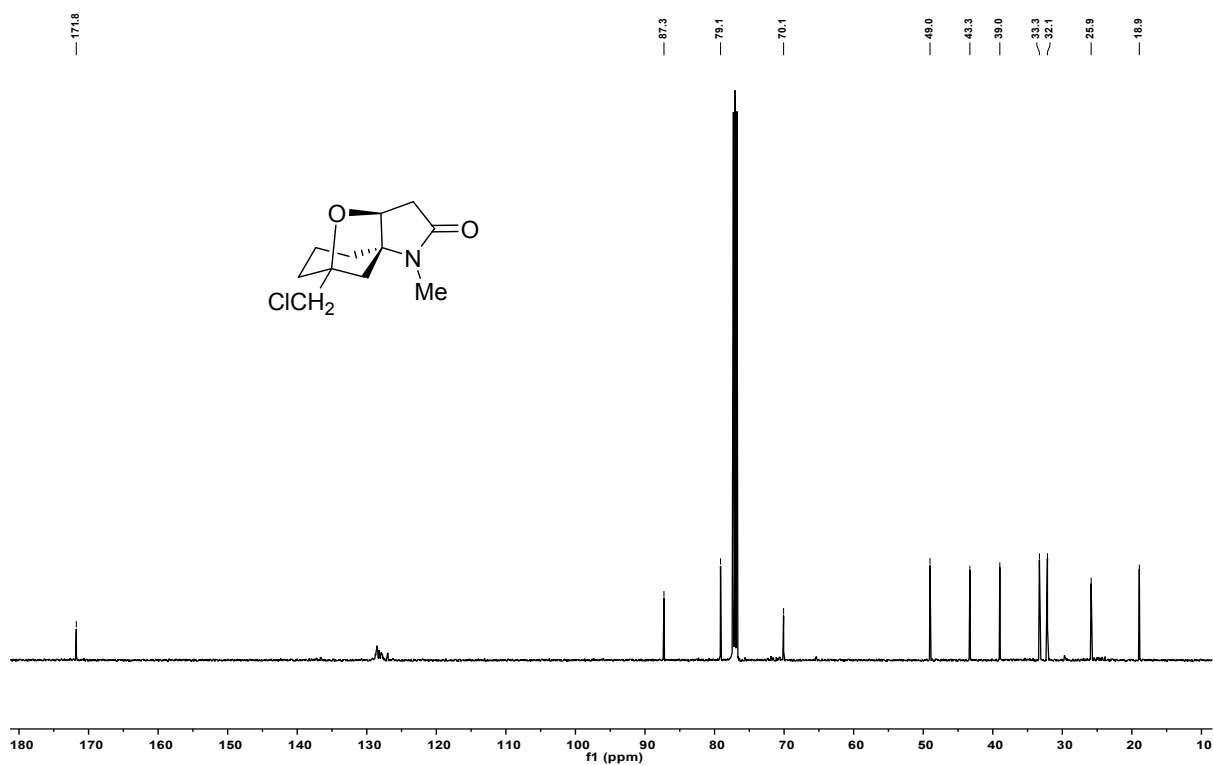


Figure S20 ¹³C NMR spectrum of **8e**

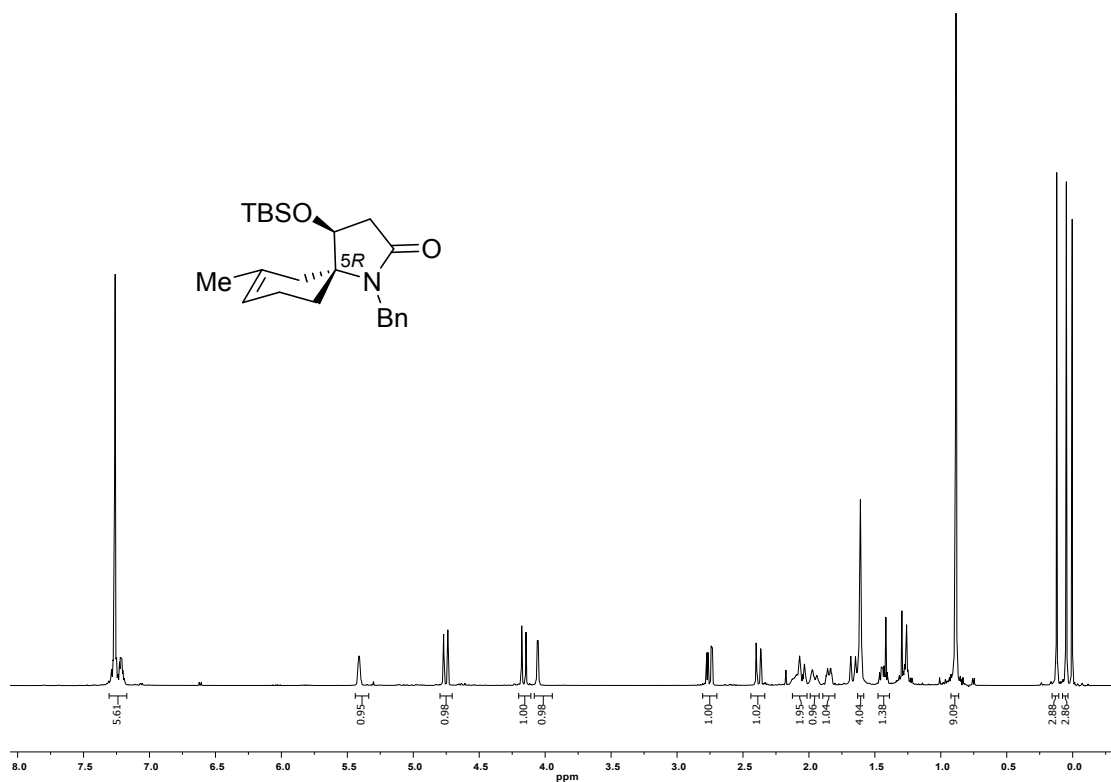


Figure S21 ^1H NMR spectrum of **16**

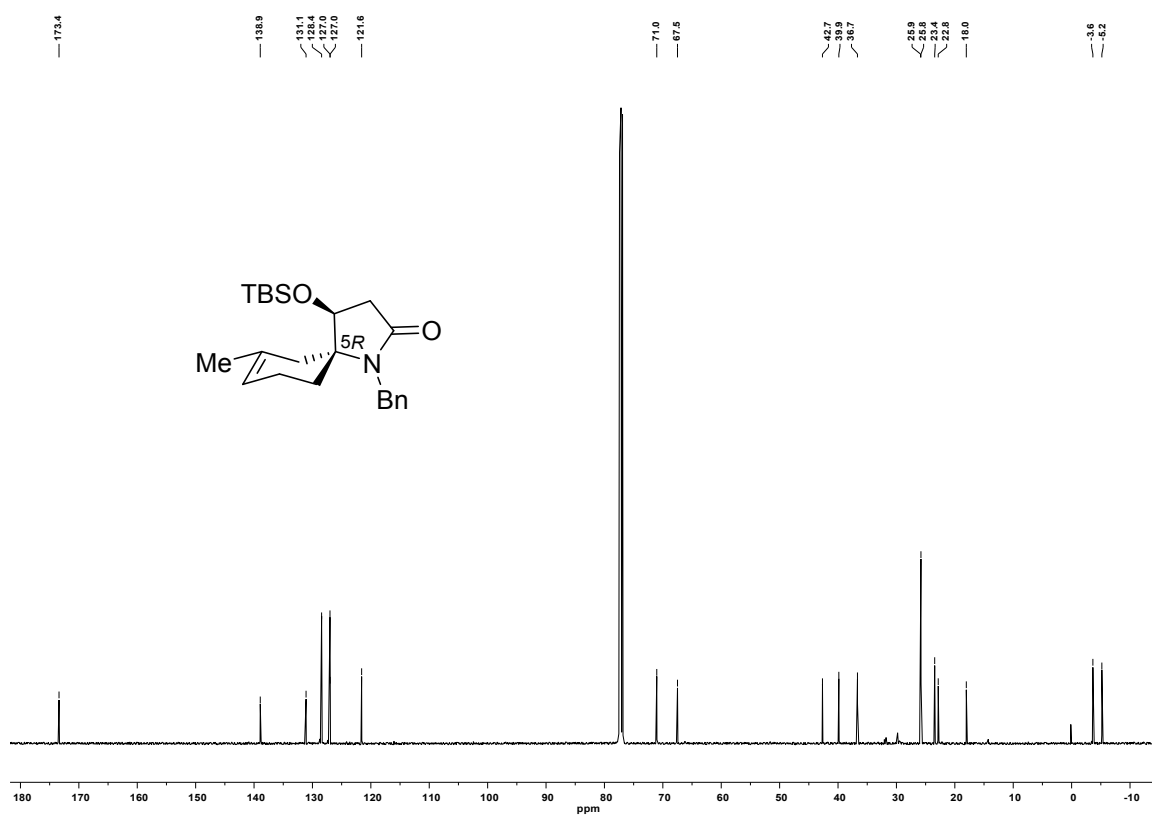


Figure S22 ^{13}C NMR spectrum of **16**

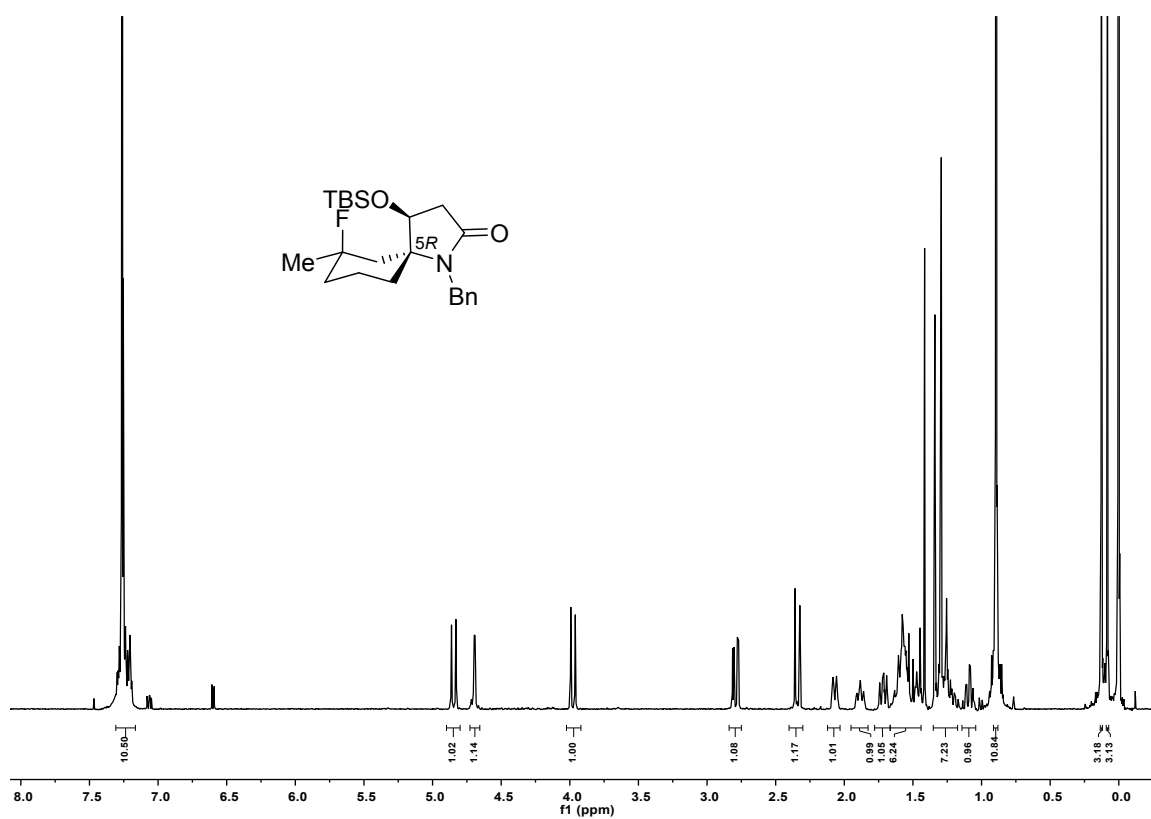


Figure S23 ¹H NMR spectrum of 16a

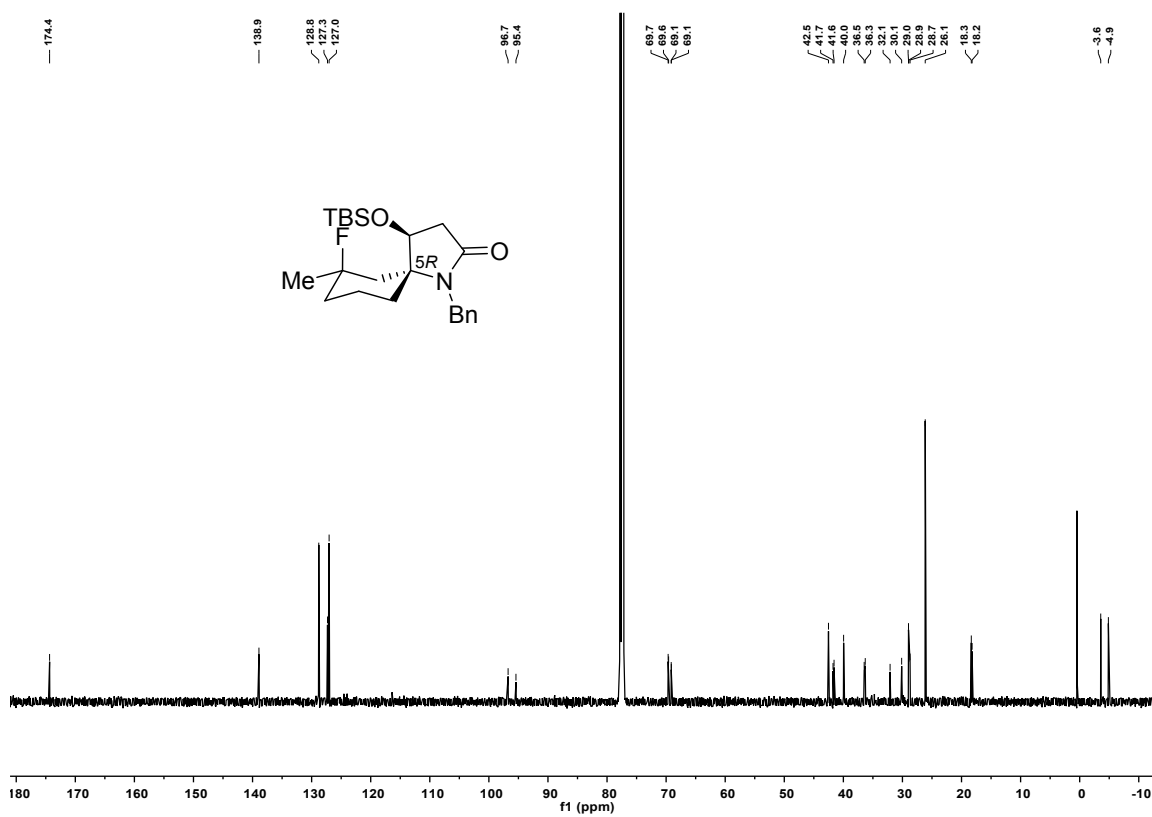


Figure S24 ¹³C NMR spectrum of 16a

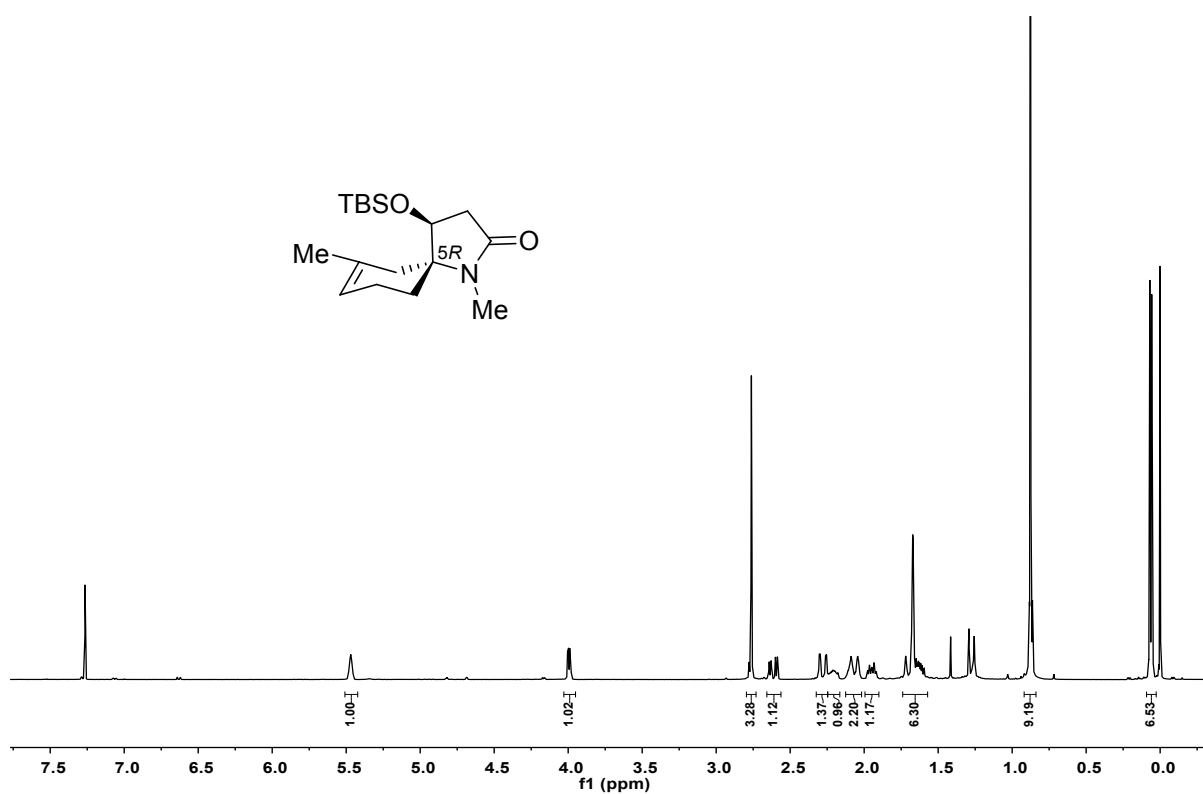


Figure S25 ¹H NMR spectrum of **17** (major isomer)

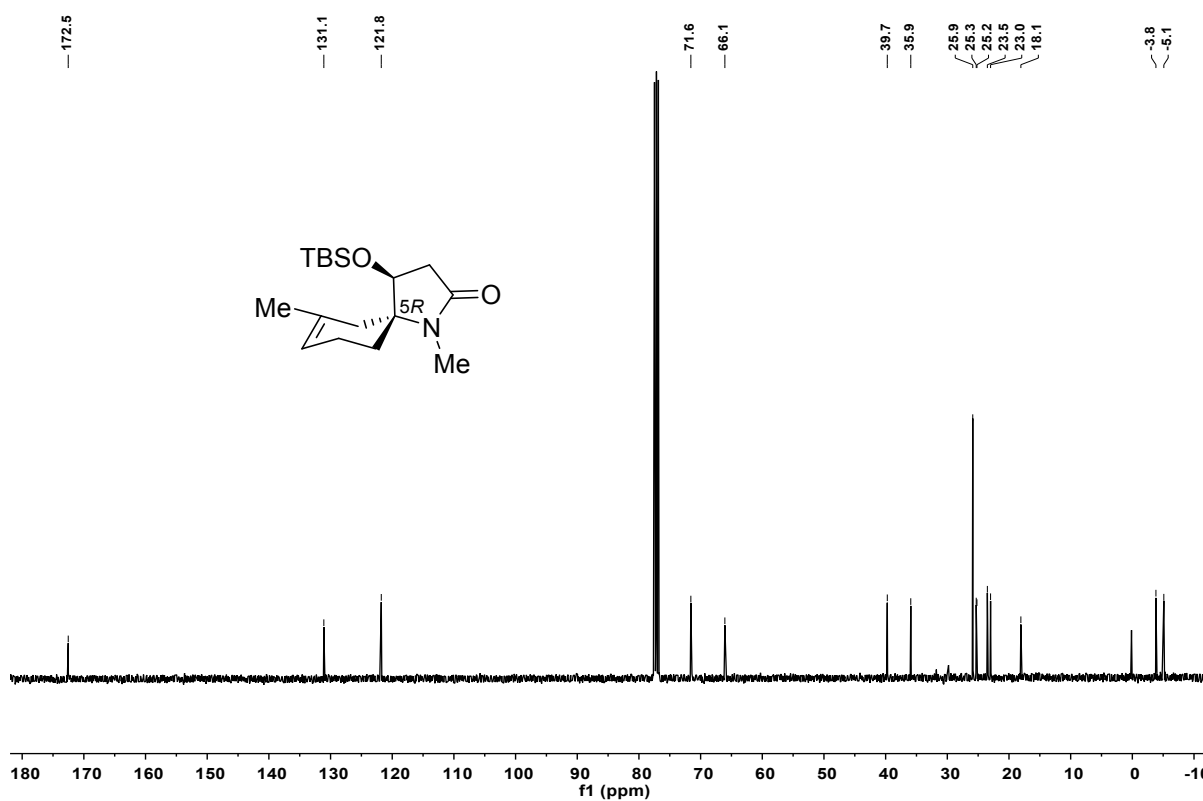


Figure S26 ¹³C NMR spectrum of **17** (major isomer)

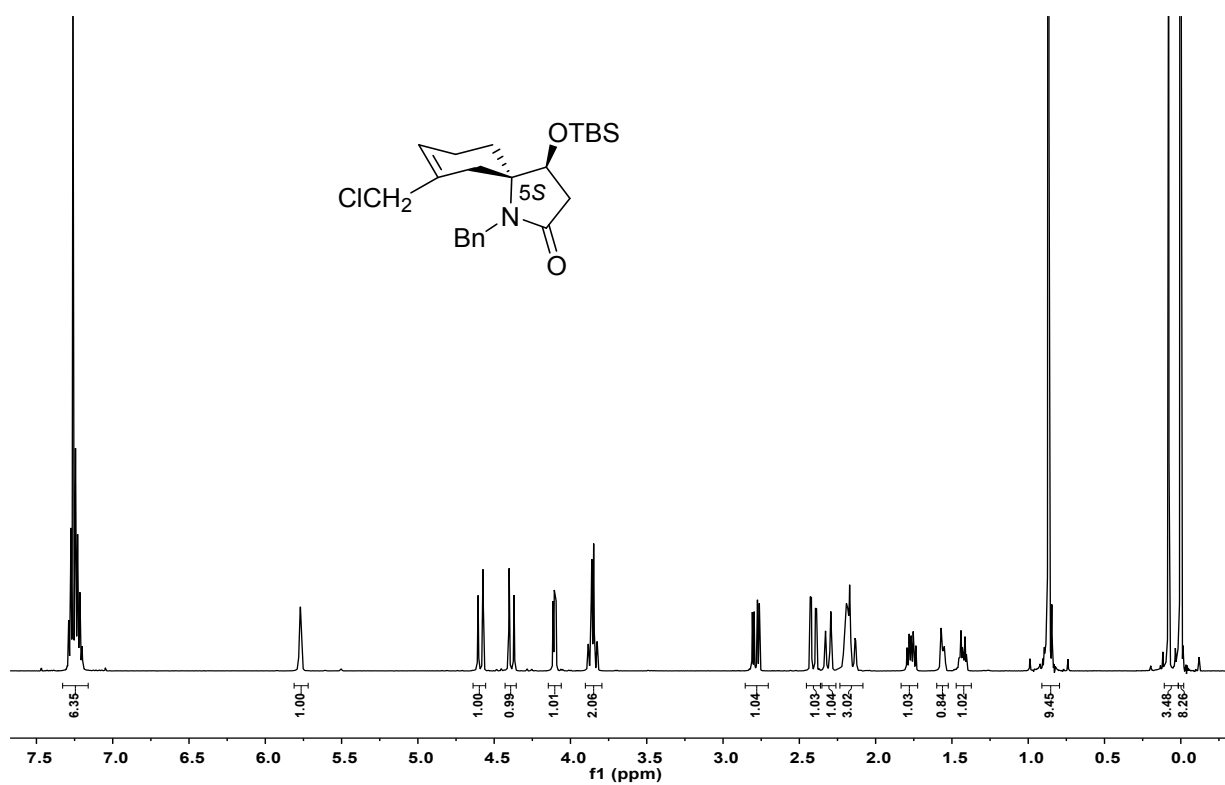


Figure S27 ¹H NMR spectrum of (5S)-18 (major isomer)

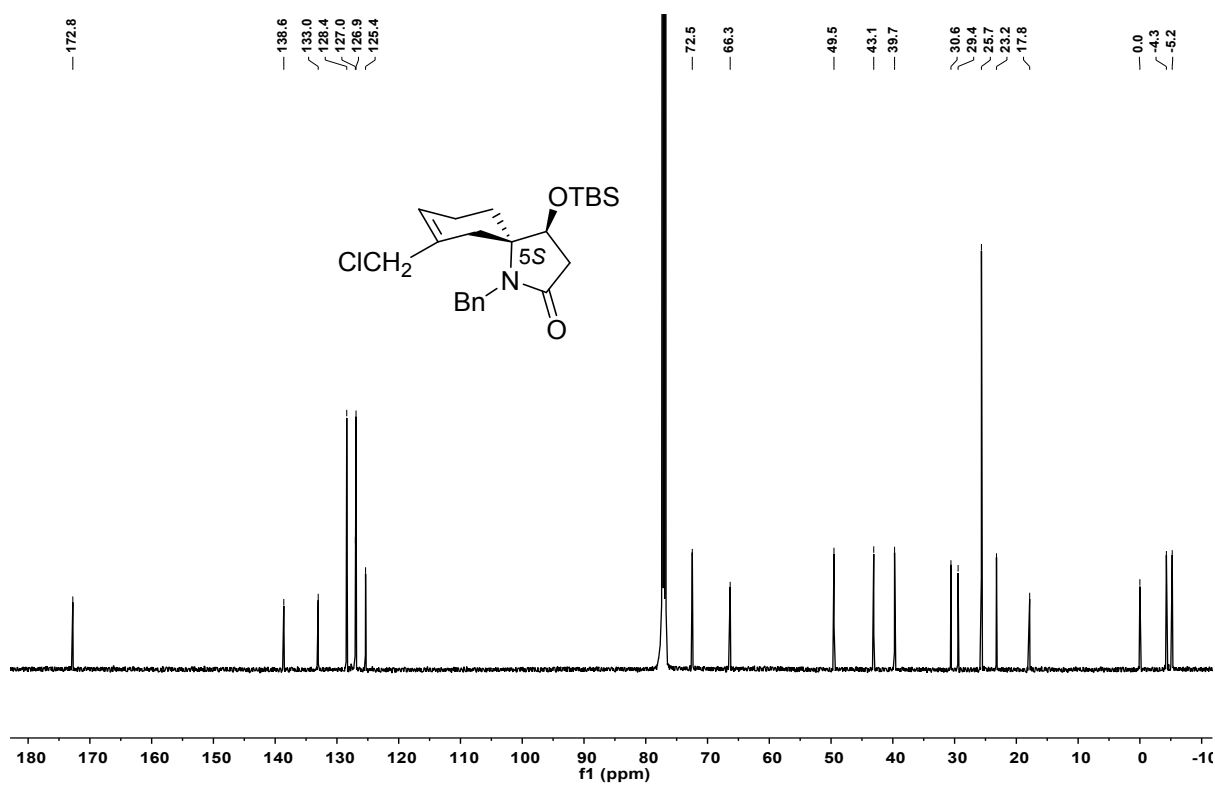


Figure S28 ¹³C NMR spectrum of (5S)-18 (major isomer)

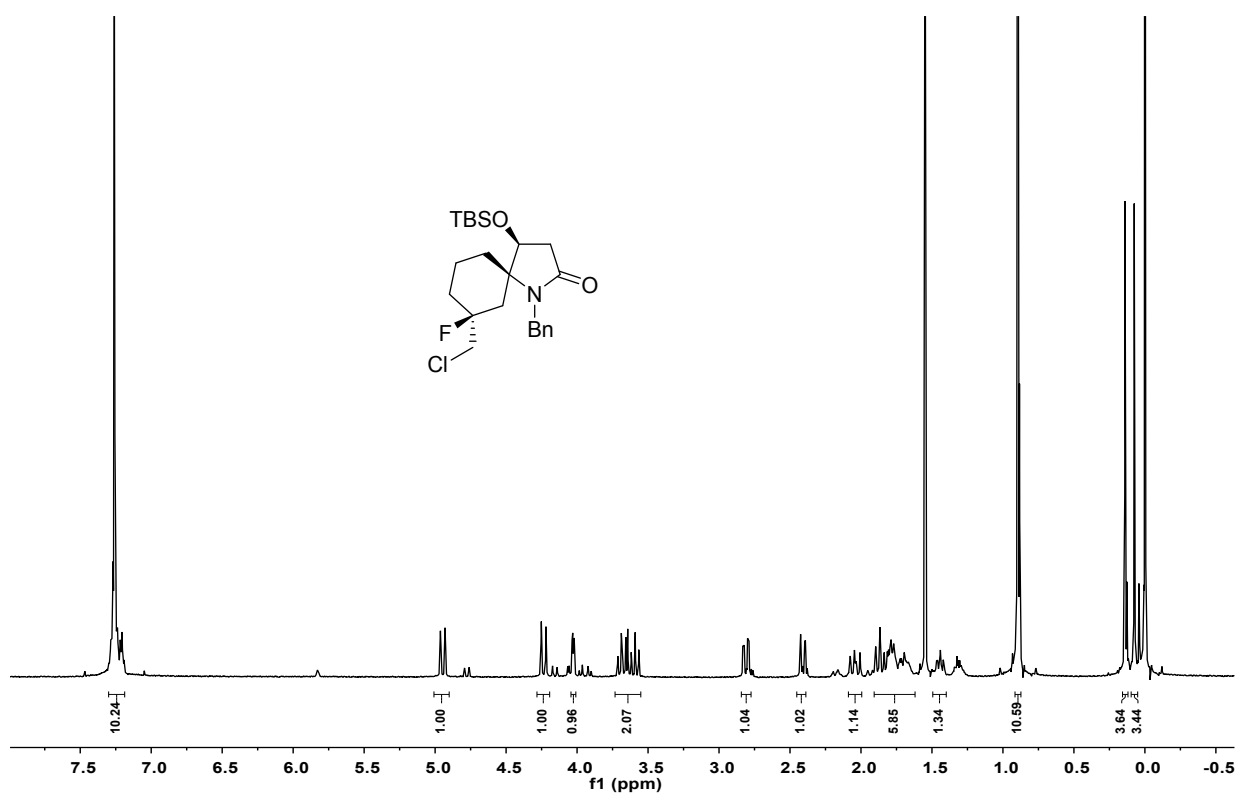


Figure S31 ¹H NMR spectrum of **19** (major isomer, dr = 88:12)

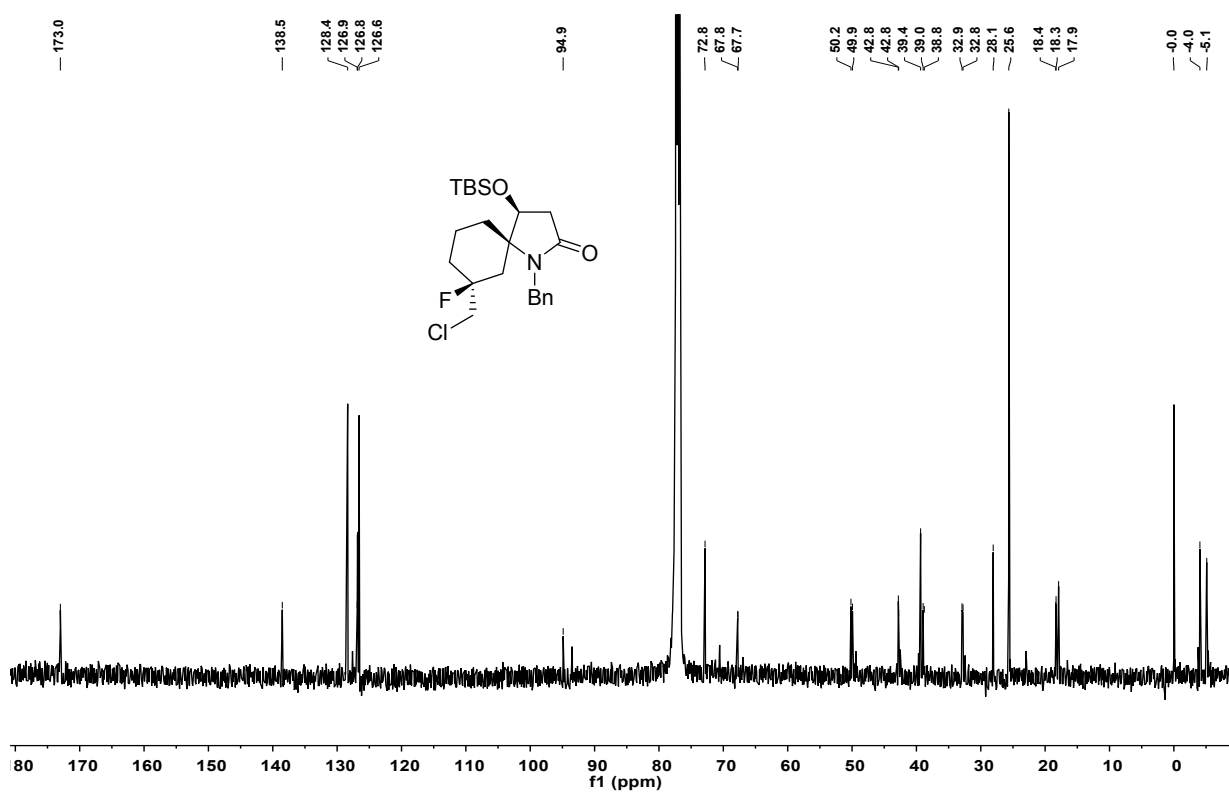


Figure S32 ¹³C NMR spectrum of **19** (major isomer, dr = 88:12)

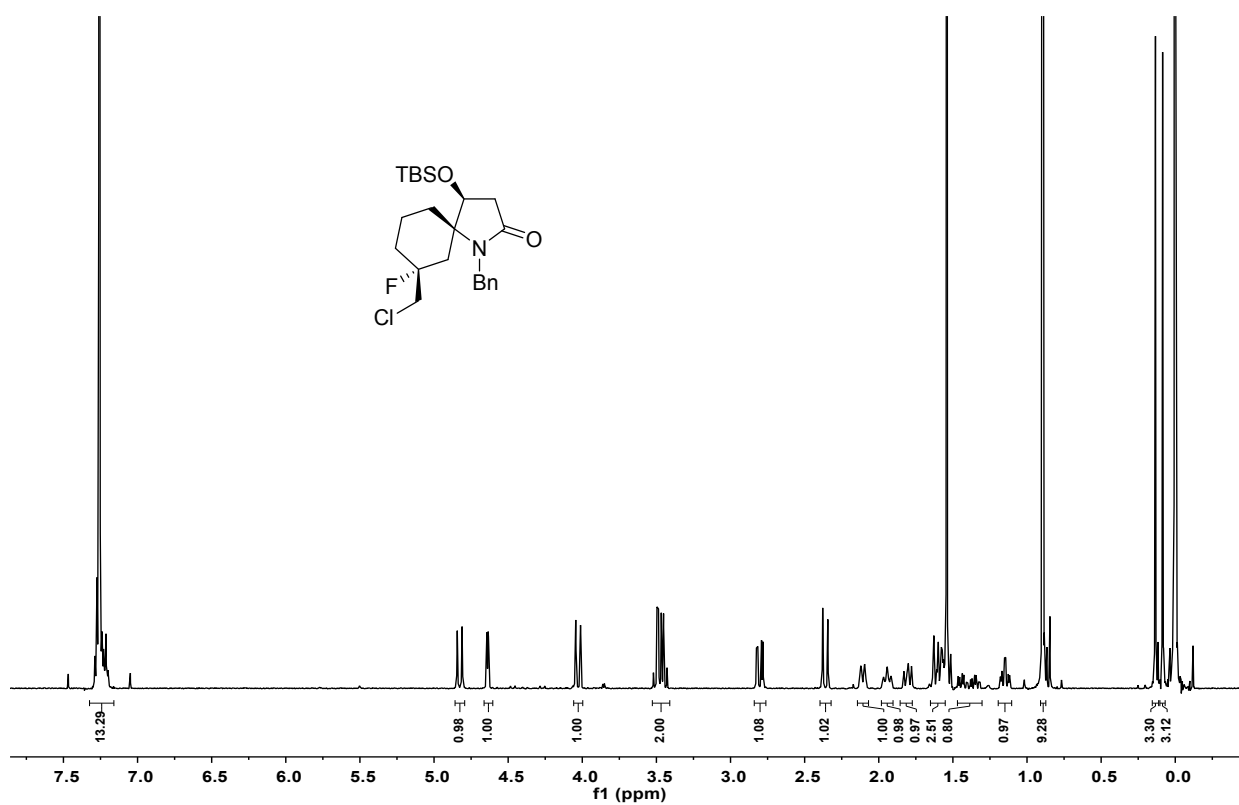


Figure S33 ¹H NMR spectrum of **19** (minor isomer)

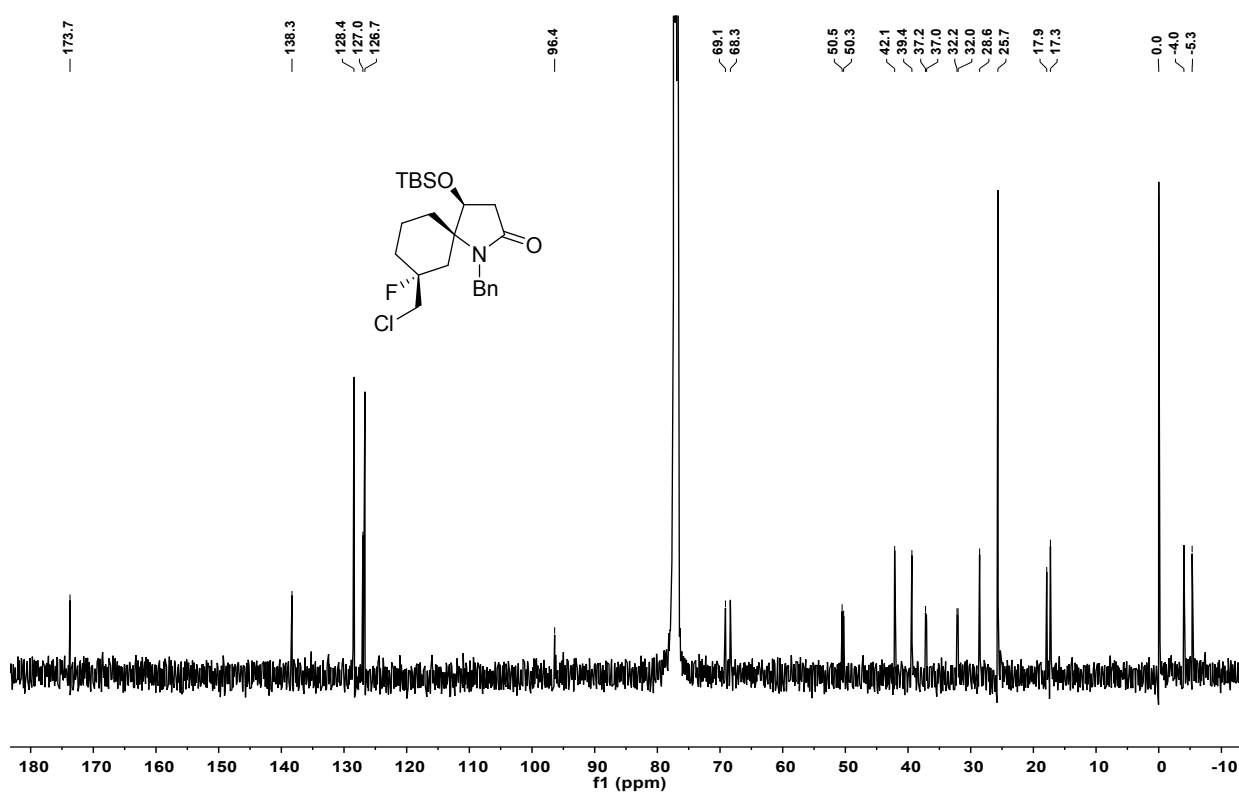


Figure S34 ¹³C NMR spectrum of **19** (minor isomer)

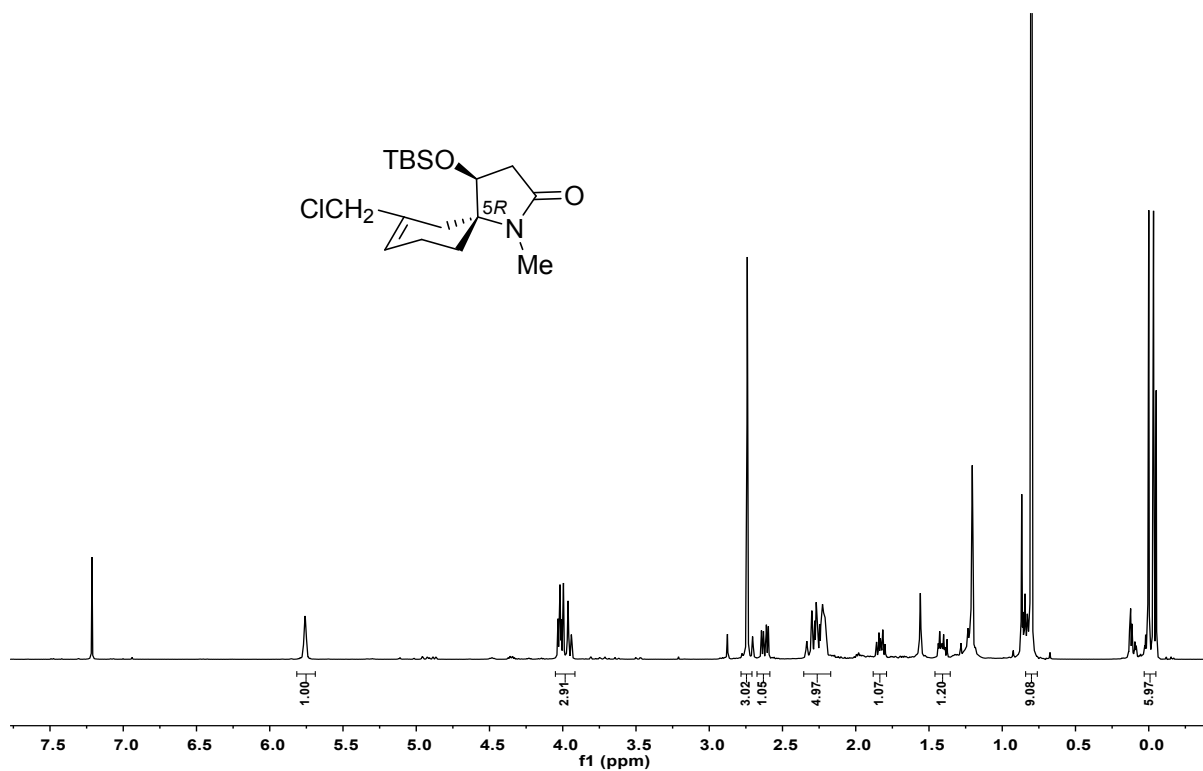


Figure S35 ¹H NMR spectrum of **20** (major isomer)

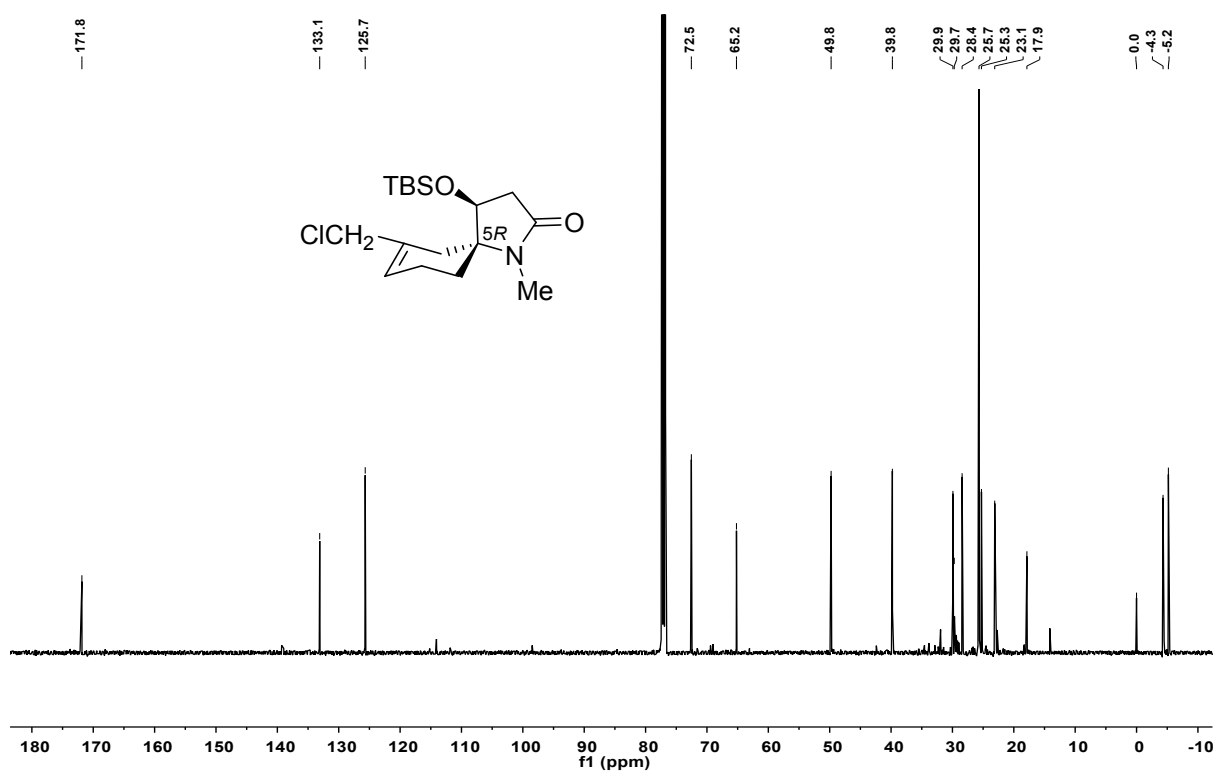


Figure S36 ¹³C NMR spectrum of **20** (major isomer)

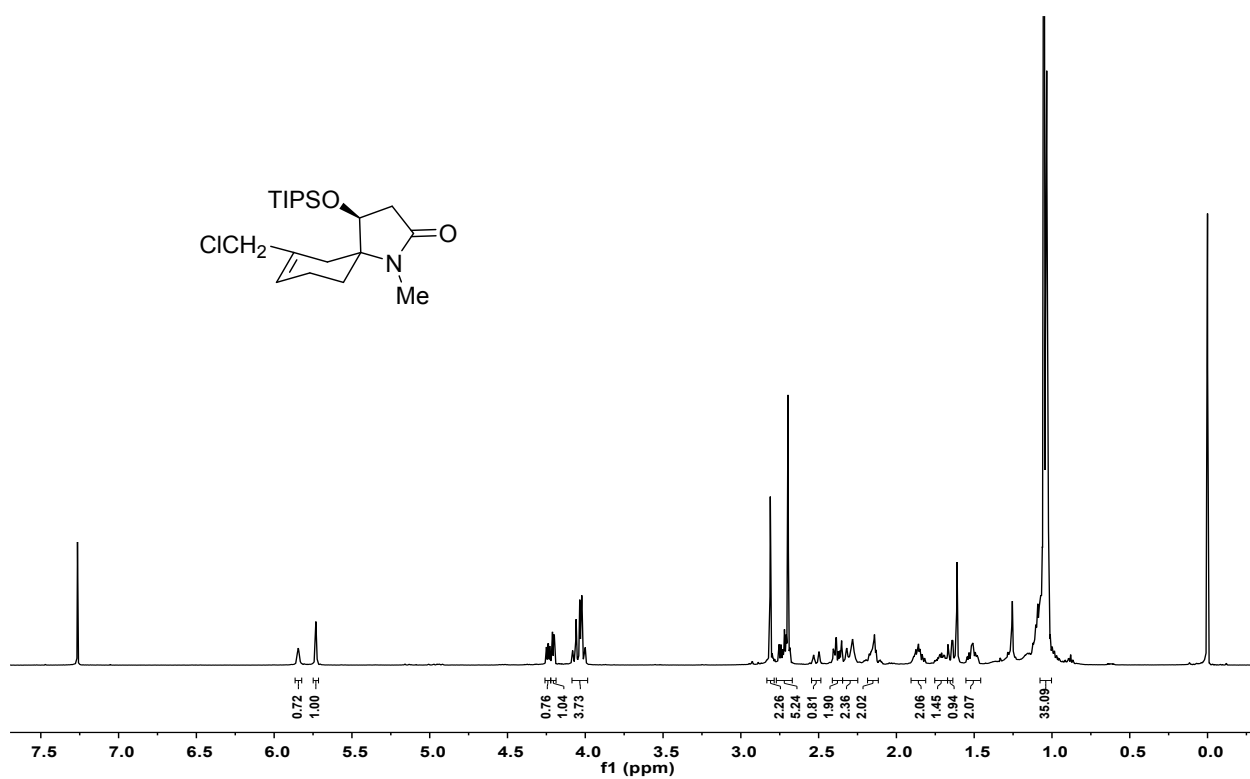


Figure S37 ¹H NMR spectrum of a mixture of **21** (dr = 54:46)

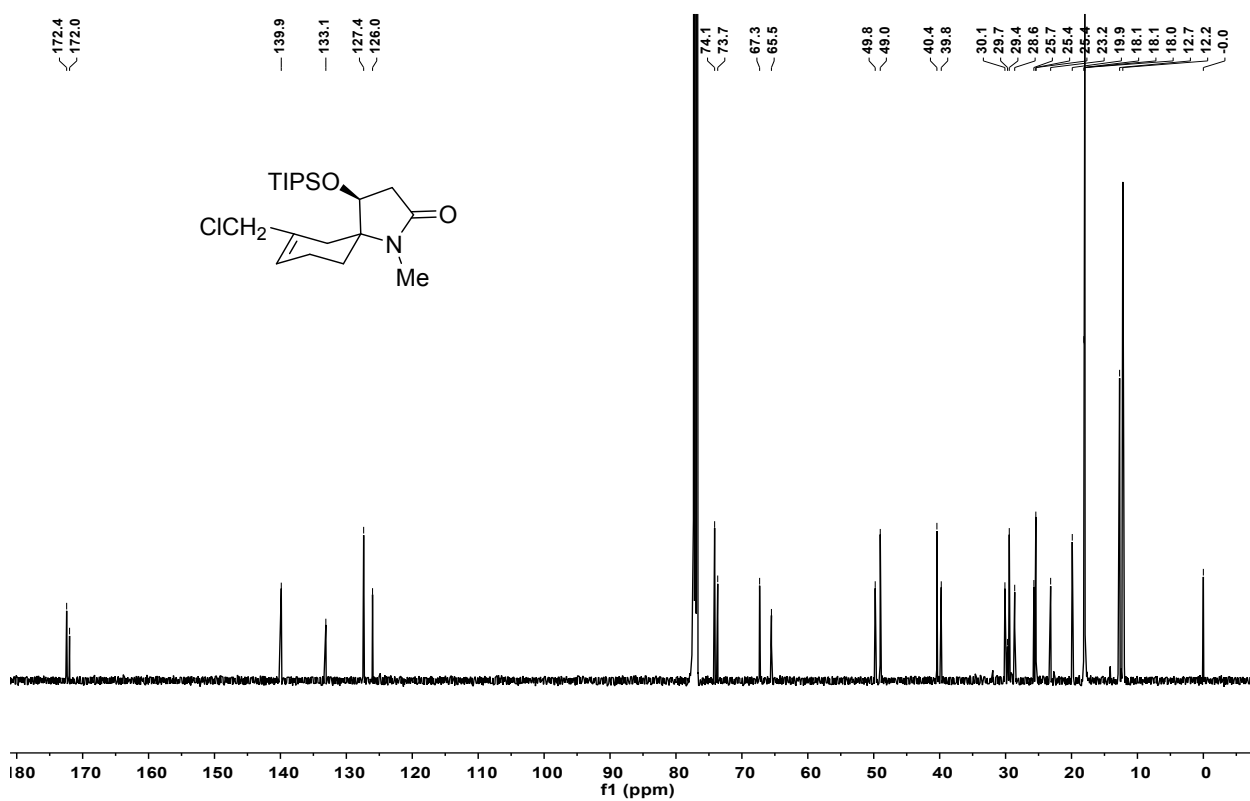


Figure S38 ¹³C NMR spectrum of a mixture of **21** (dr = 54:46)

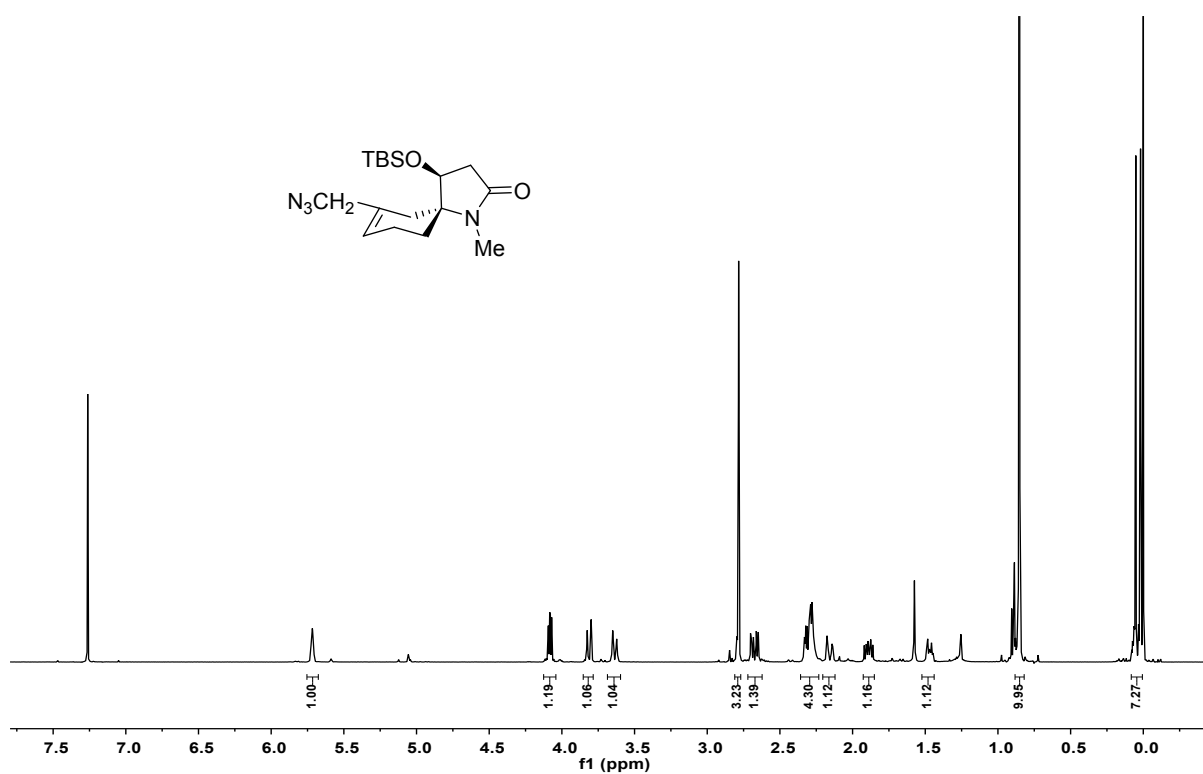


Figure S39 ^1H NMR spectrum of **26** (major isomer, dr = 95:5)

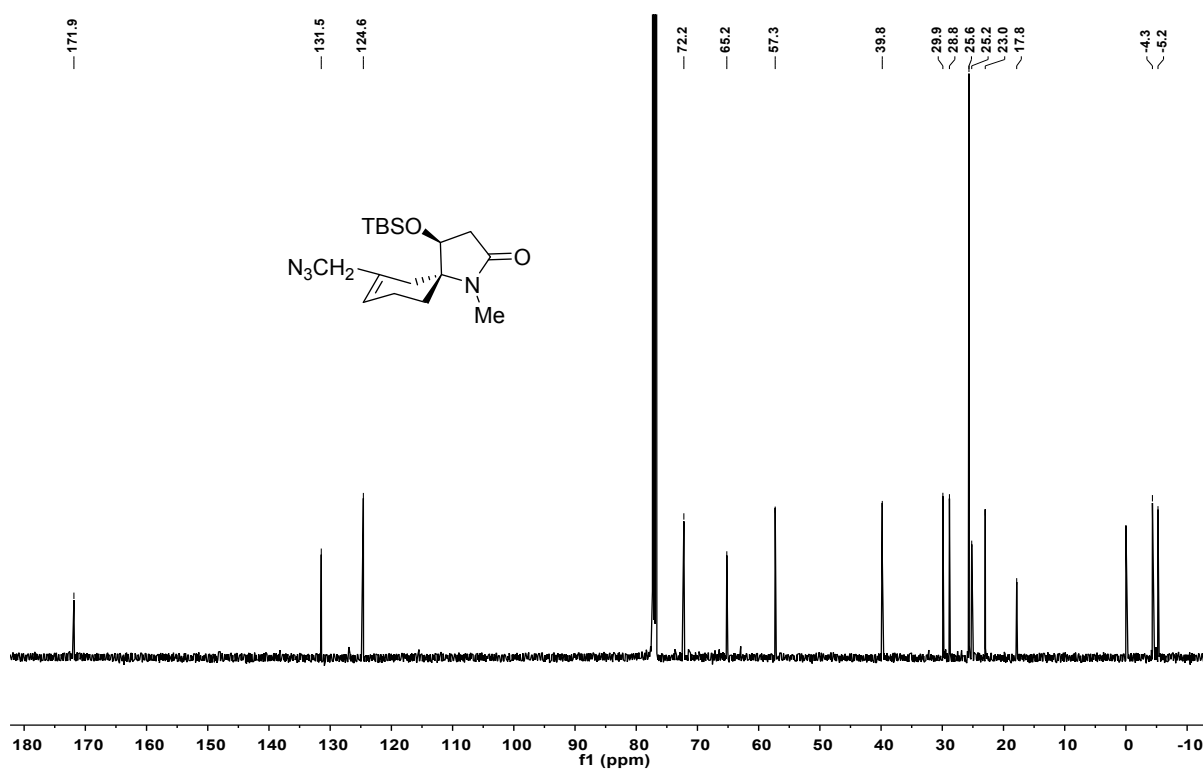


Figure S40 ^{13}C NMR spectrum of **26** (major isomer, dr = 95:5)

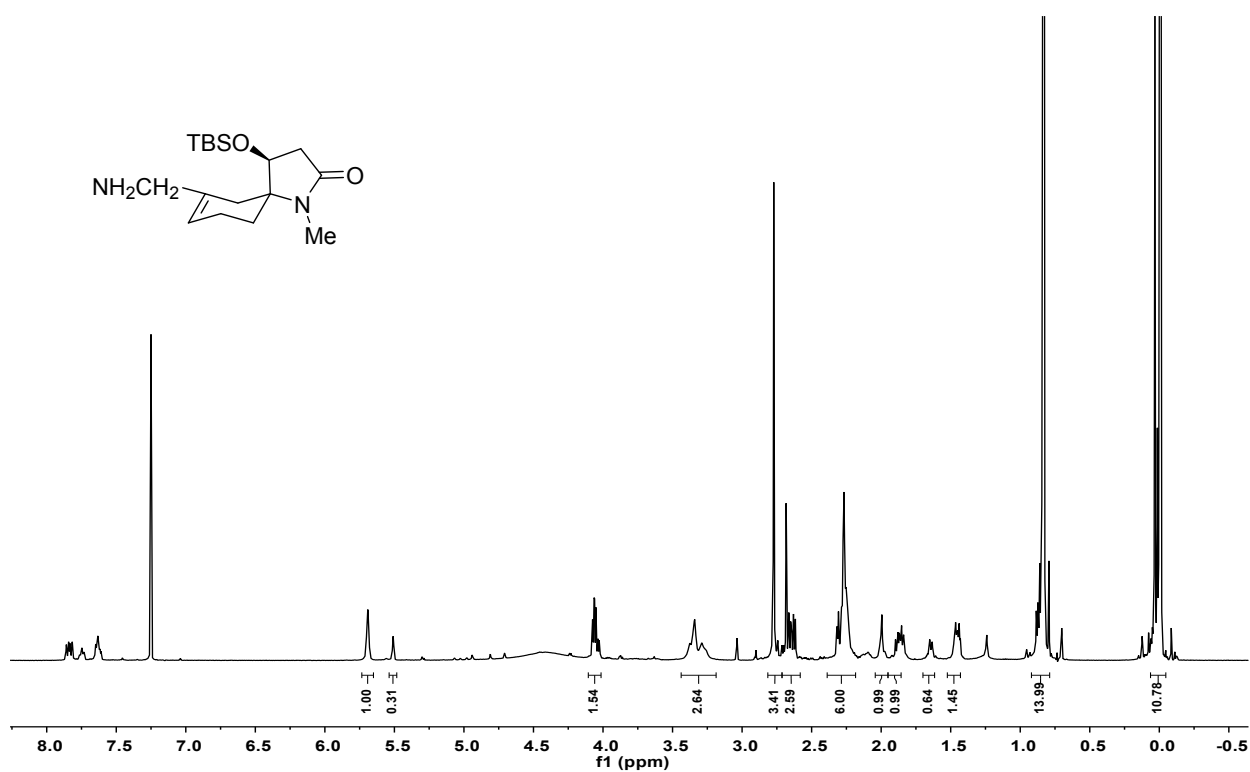


Figure S41 ¹H NMR spectrum of **27** (dr = 79:21)

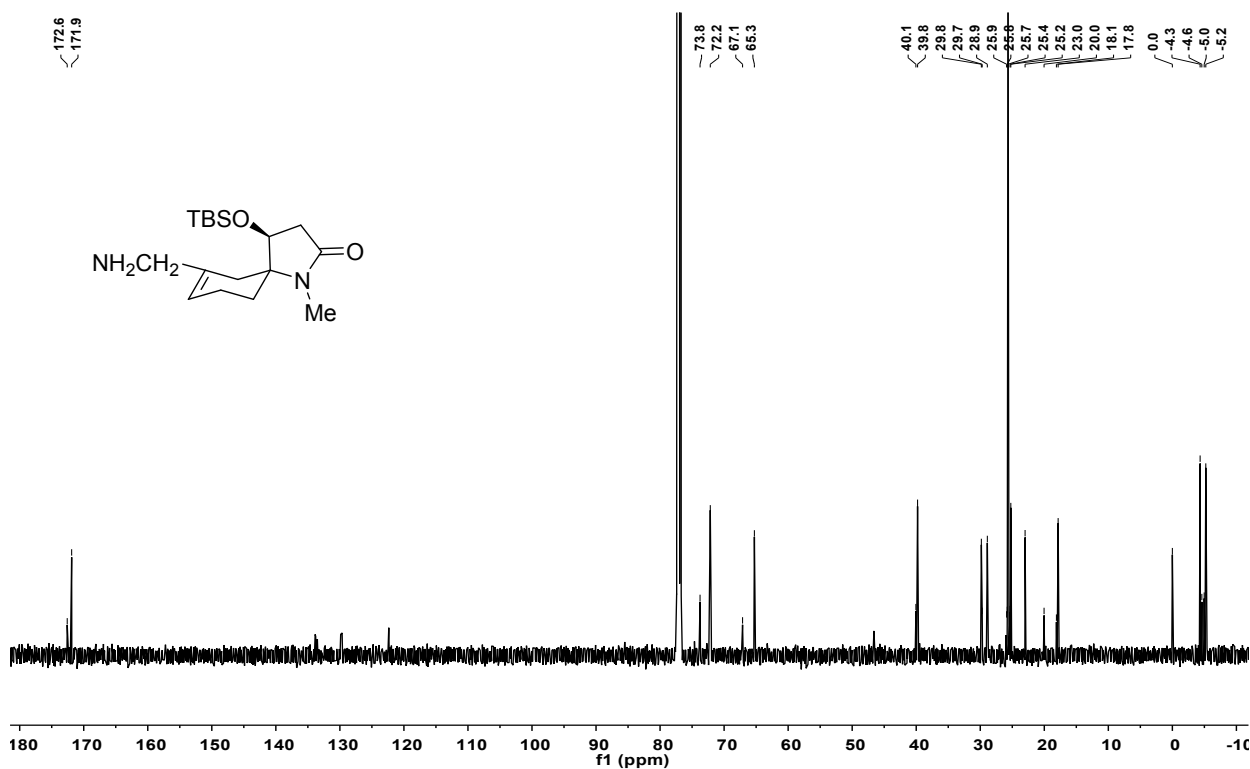


Figure S42 ¹³C NMR spectrum of **27** (dr = 79:21)

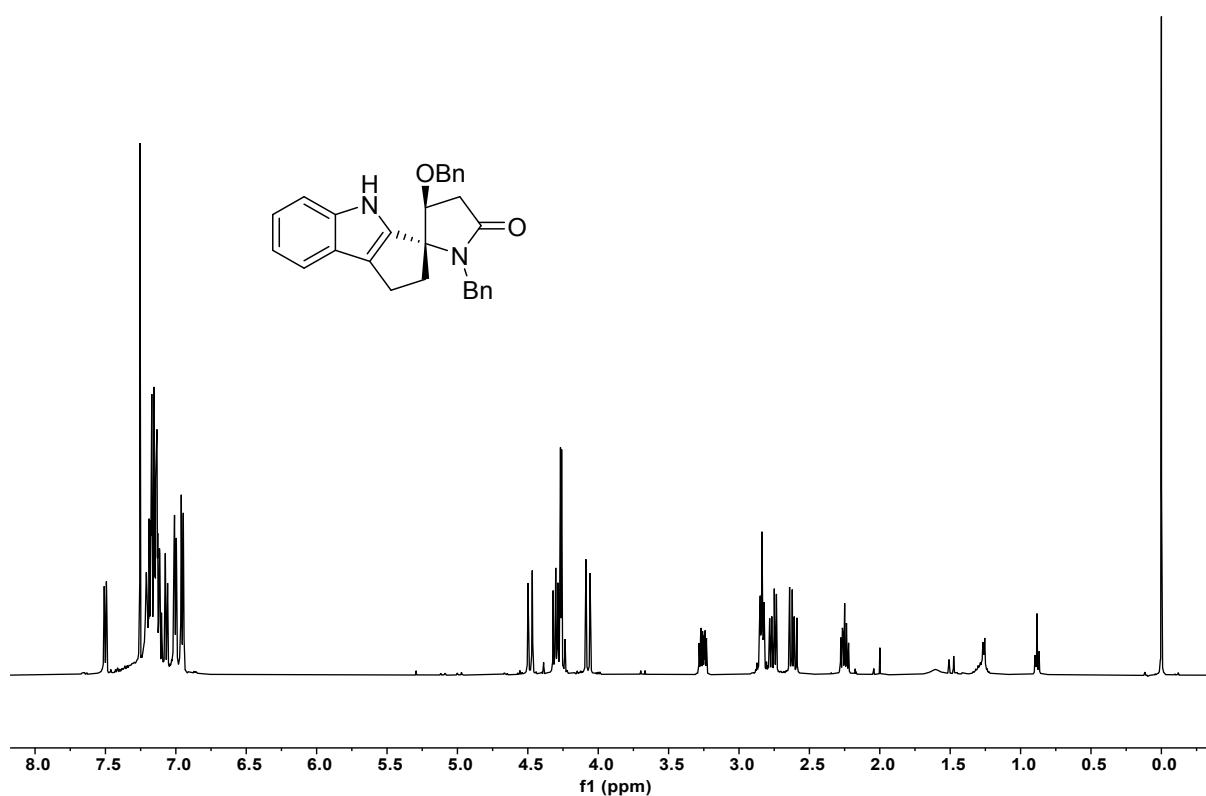


Figure S43 ¹H NMR spectrum of **29** (major isomer + impurity peaks at high field)

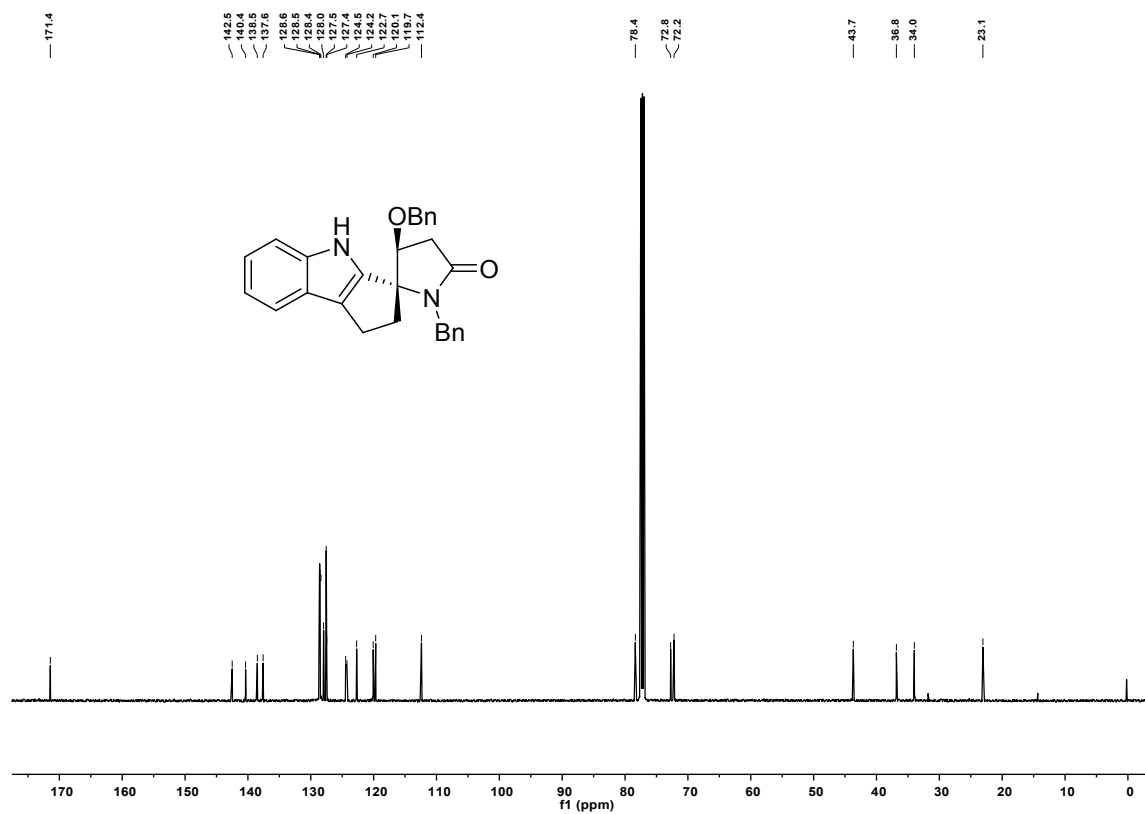


Figure S44 ¹³C NMR spectrum of **29** (major isomer + impurity peaks at high field)

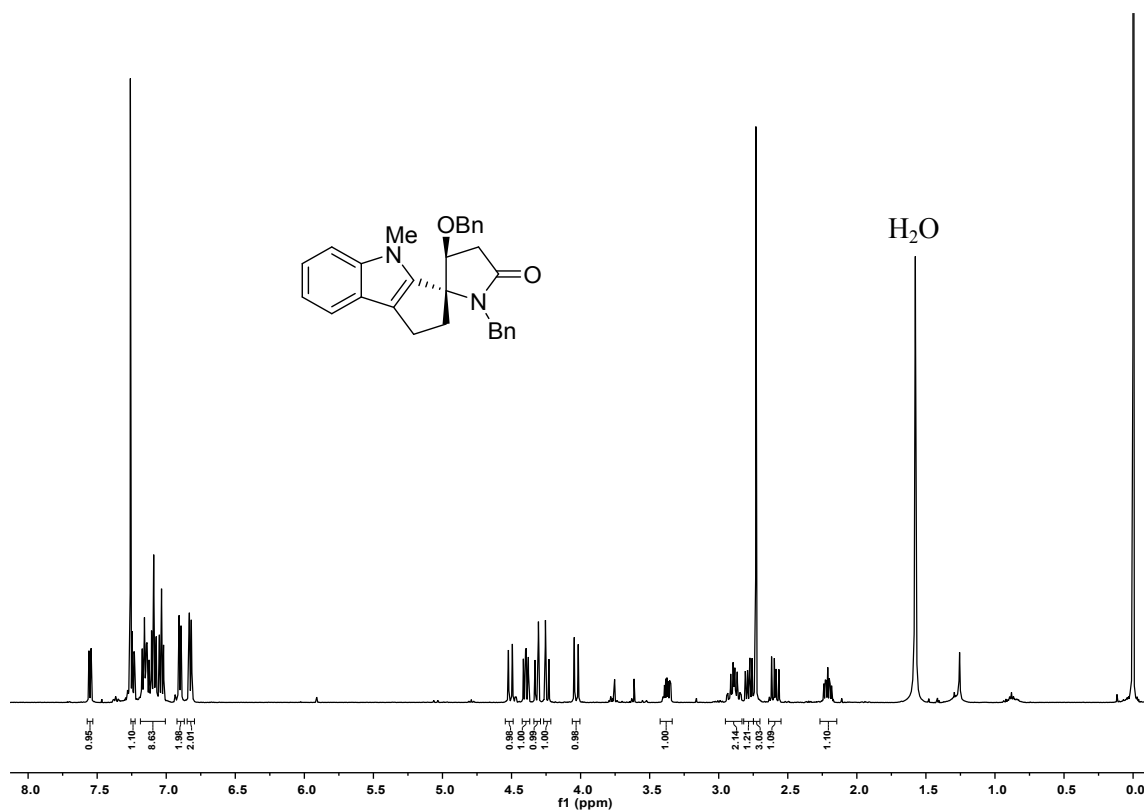


Figure S45 ¹H NMR spectrum of **30** (major isomer)

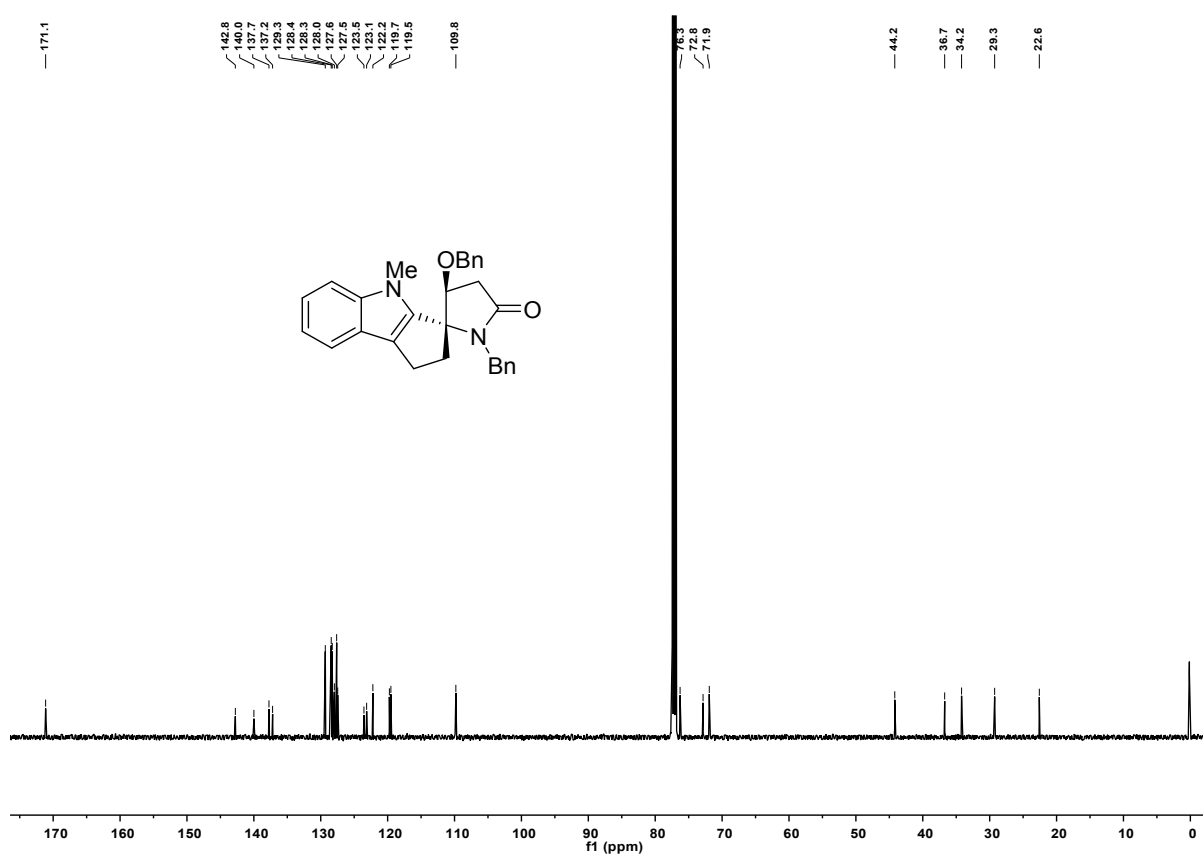
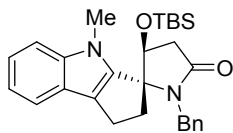


Figure S46 ¹³C NMR spectrum of **30** (major isomer)



Chemical structure of the compound is shown above the spectrum. The structure is a complex molecule featuring a benzene ring fused to a pyrrole ring, which is further substituted with a methyl group (Me), a benzyl group (Bn), and a tert-butyldimethylsilyl (OTBS) group. The spectrum displays peaks corresponding to the chemical shifts of the various atoms in the molecule, with the x-axis labeled 'f1 (ppm)' ranging from 180 to 0.

Peak list (ppm):

Peak Label	Chemical Shift (ppm)
171.9	171.9
142.4	142.4
139.7	139.7
138.6	138.6
128.6	128.6
128.2	128.2
127.4	127.4
124.7	124.7
124.2	124.2
122.4	122.4
119.8	119.8
119.4	119.4
112.2	112.2
74.2	74.2
73.3	73.3
43.7	43.7
39.5	39.5
33.4	33.4
25.7	25.7
22.9	22.9
17.9	17.9
-5.3	-5.3
-5.3	-5.3

S25

Gaussian Archive Entries for Table 2

Entry 1

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TS1

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Syn-spiro

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 654668522,0.3574200455\H,-0.9387467485,1.5873027842,-0.8758004571\H,-2
 .3547899532,2.0413367212,0.1123951602\N,-0.8754709375,0.9524275262,1.1
 286343932\O,0.6413138681,2.2727410157,2.2468613349\O,-0.3140646675,-2.
 3588443773,2.0442696242\C,-0.443821111,-3.4101812312,3.0453152301\H,0.
 0360207675,-4.2910327214,2.6233219467\H,0.0903311075,-3.0600657543,3.9
 266801699\H,-1.5001833925,-3.5830989954,3.2535444745\\Version=AM64L-G0
 9RevB.01\HF=-634.7668385\RMSD=0.000e+00\RMSF=9.147e-06\Dipole=-0.92660
 45,-4.1388363,-0.0960121\Quadrupole=-6.9073562,5.0699813,1.8373749,3.3
 426901,-6.1087839,-23.4382682\PG=C01 [X(C11H18N1O2)]\\@
 Sum of electronic and thermal Free Energies= -634.515609 Hartree

E₃ (anti)

1\1\GINC-SPARTAN-RC046\FOpt\RM062X\6-31+G(d)\C11H18N1O2(1+)\UWILLE\05-
 Jun-2020\0\#p M062X/6-31+G* scrf=(cpcm,solvent=dichloromethane) scf=(
 qc,direct) freq=noraman nosymm geom=checkpoint guess=check opt=(readfc
 ,maxcycle=500)\geom&freq\1,1\C,-2.3848505654,-2.4467684717,-0.397074
 6665\C,-0.1145409216,-1.3497773728,0.0299986675\C,-3.6122444371,-0.416
 4967423,0.4331733551\C,-3.119772392,-1.6413974355,0.635250609\H,0.9600
 337897,-1.5912971514,0.067219263\H,-2.4457779478,-1.9444532852,-1.3703
 14214\H,-2.8593731166,-3.4291251085,-0.5062899071\H,-4.1231207589,0.13
 03820889,1.2208151048\H,-3.5387360012,0.0672863166,-0.5397444191\H,-3.
 2447776955,-2.107723842,1.6144801749\H,-0.284539659,-0.7446323484,-0.8
 647743129\C,-0.3269170344,-0.5506759889,1.2545219897\C,-0.3003577044,-
 1.1550671183,2.6449806833\C,-0.2287166271,0.0569083966,3.5826302459\H,
 -1.248546907,-1.6975395398,2.7872594751\H,-0.9483595122,0.0488165714,4
 .4024927604\H,0.7808642315,0.155983532,3.99795915\C,-0.4821520381,1.23

76792455,2.6870674054\C,-0.5635121849,1.6601688485,0.1719508623\H,-0.7
 223676151,2.6562515347,0.5816261991\H,0.3569009839,1.6365166781,-0.412
 2825971\H,-1.4173423437,1.3652917977,-0.4398894692\N,-0.4469590365,0.7
 402540736,1.3035649062\O,-0.6749194555,2.3877873833,2.9260524638\O,0.7
 858387924,-2.0293435294,2.6964874321\C,0.7558370002,-2.8804762928,3.83
 89470985\H,1.6336327365,-3.5213579339,3.7700654707\H,0.8016930142,-2.2
 949282,4.7642947264\H,-0.1540844776,-3.4921065625,3.8341002978\C,-0.91
 04706629,-2.6667194774,-0.0307623359\H,-0.440071774,-3.2948500388,-0.7
 918316907\H,-0.81768368,-3.2030460273,0.9205042618\\Version=AM64L-G09R
 evB.01\HF=-634.7382022\RMSD=0.000e+00\RMSF=6.661e-06\Dipole=0.5492051,
 -0.4153429,-0.3066333\Quadrupole=-8.1513051,-2.6991341,10.8504392,2.08
 56339,-1.1537434,-11.771879\PG=C01 [X(C11H18N1O2)]\\@
 Sum of electronic and thermal Free Energies= -634.497762 Hartree

TS2

1\1\GINC-SPARTAN-RC039\FTS\RM062X\6-31+G(d)\C11H18N1O2(1+)\UWILLE\12-J
 un-2020\0\#p M062X/6-31+G* scf=(cpcm,solvent=dichloromethane) scf=(q
 c,direct) freq=norman nosymm opt=(ts,noeigentest,calcfc,maxcycle=500)
 \\geom&freq\\1,1\C,-2.4594522335,-2.8432376847,-0.5285134946\C,-0.4141
 463187,-1.4474534287,0.0505614812\C,-2.8906479472,-0.7054052447,0.6709
 371229\C,-3.0800942247,-2.0818455107,0.5510365503\H,0.6449143592,-1.47
 48315876,0.3305721882\H,-2.5360900408,-2.3340125409,-1.4929695701\H,-2
 .8332172698,-3.8648772724,-0.5954677444\H,-3.4091034189,-0.1946335648,
 1.4790401537\H,-2.81227195,-0.1395318014,-0.2576554338\H,-3.4993721266
 ,-2.6330300499,1.3929255686\H,-0.4982705393,-0.903193511,-0.895989801\
 C,-1.1191262181,-0.6846852837,1.1540721634\C,-1.002413119,-1.252077568
 3,2.5913086317\C,-1.2863968026,-0.0344417292,3.4734028828\H,-1.6958664
 005,-2.0806612602,2.7725141639\H,-2.3432907601,0.0457272464,3.74974948
 25\H,-0.6958972401,-0.0246864199,4.3914302777\C,-0.9159899797,1.137886
 536,2.5921505453\C,-0.5335848352,1.556302,0.1671940079\H,0.3909772164,
 1.2632397406,-0.3351063142\H,-1.3607272871,1.5429713042,-0.5499422455\
 H,-0.4271251917,2.5625679488,0.5713815626\N,-0.810604416,0.6675804755,
 1.282062316\O,-0.7348481299,2.2902049102,2.9135198411\O,0.3257601668,-
 1.6981385905,2.7165773999\C,0.5319333551,-2.5291288089,3.8507752684\H,
 1.5823349643,-2.8186396447,3.8368756265\H,0.3161559817,-1.9960746556,4
 .7836706276\H,-0.0990826216,-3.4243675961,3.7892045887\C,-0.9376156455
 ,-2.8620951995,-0.108382187\H,-0.4041967405,-3.3812305326,-0.907551177
 6\H,-0.8017835863,-3.4403416753,0.8112685173\\Version=AM64L-G09RevB.01
 \HF=-634.7194379\RMSD=0.000e+00\RMSF=1.150e-05\Dipole=-1.9471529,-2.76
 27969,-1.7415209\Quadrupole=4.8484824,-1.9504869,-2.8979955,13.3472985
 ,-5.8854325,-14.4782181\PG=C01 [X(C11H18N1O2)]\\@
 Frequencies -223.3886 cm⁻¹
 Sum of electronic and thermal Free Energies= -634.475888 Hartree

Anti-cycl

1\1\GINC-SPARTAN-BM095\FOpt\RM062X\6-31+G(d)\C11H18N1O2(1+)\UWILLE\27-
 Aug-2020\0\#p M062X/6-31+G* nosymm opt=(calcfc,maxcycle=500) freq=nor
 aman scf=(cpcm,solvent=dichloromethane)\\geom&freq\\1,1\C,-2.49620321
 86,-2.8461605877,-0.5070800579\C,-0.4275402802,-1.4508235052,0.0971466
 067\C,-2.8065270648,-0.7302645324,0.7777689149\C,-3.0537191486,-2.1220
 898129,0.6051514525\H,0.6293686056,-1.4834737017,0.3785541295\H,-2.530
 7368055,-2.3015586678,-1.4529192463\H,-2.8552476656,-3.869593872,-0.60
 06775003\H,-3.3542685835,-0.2664088779,1.5974508695\H,-2.8575929075,-0
 .1570665743,-0.1506130325\H,-0.5088996331,-0.9302304575,-0.8632326669\

C,-1.162212134,-0.6686195591,1.1773483488\C,-0.9729535614,-1.198287172
6,2.6266372751\C,-1.1928206637,0.0468526262,3.4886505833\H,-1.67649028
23,-2.0060893525,2.8653076785\H,-2.2357581872,0.1577710013,3.805057176
2\H,-0.567125139,0.0629010126,4.3830280741\C,-0.8336514193,1.191973402
7,2.5648548523\C,-0.574798349,1.5600972707,0.1264690185\H,0.3428231672
,1.2736623768,-0.3935251788\H,-1.4175235112,1.5107580566,-0.5713657478
\H,-0.4786882069,2.5813328585,0.4950921887\N,-0.8059646734,0.702659946
7,1.2737693838\O,-0.6093327214,2.346813319,2.869653208\O,0.3475287522,
-1.6742426669,2.7156040483\C,0.5789328573,-2.471673446,3.8675959106\H,
1.6225503379,-2.78297986,3.8269757808\H,0.4068242423,-1.9062469963,4.7
906263217\H,-0.0706336972,-3.3559027377,3.8580367143\C,-0.9618387044,-
2.8622013937,-0.0333318006\H,-0.449192928,-3.4135737245,-0.8248656026\H,
-0.8483268651,-3.4280193383,0.8962744972\H,-3.4603292818,-2.69516082
41,1.4391790308\\Version=AM64L-G09RevB.01\HF=-634.7197464\RMSD=4.843e-
09\RMSF=5.302e-06\Dipole=-2.4275059,-3.4729289,-2.0291503\Quadrupole=6
.5558033,-1.5848906,-4.9709127,15.506929,-5.9423232,-15.0860198\PG=C01
[X(C11H18N1O2)]\\@
Sum of electronic and thermal Free Energies= -634.476158 Hartree

Anti-spiro

1\1\GINC-SPARTAN-RC185\FOpt\RM062X\6-31+G(d)\C11H18N1O2(1+)\UWILLE\05-
Jun-2020\0\#p M062X/6-31+G* scrf=(cpcm,solvent=dichloromethane) nosym
m scf=(qc,direct) geom=checkpoint guess=check opt=(readfc,maxcycle=500
) freq=noraman\\geom&freq\\1,1\C,-1.508341027,-3.223023283,0.098561798
2\C,-0.3910649384,-0.9183649025,-0.0099396627\C,-2.7370817773,-1.11683
26661,0.8183554399\C,-2.3304311401,-2.5584650323,1.1819451843\H,0.5810
67967,-0.4382848209,0.1441297657\H,-2.1225899416,-3.2273661283,-0.8087
900591\H,-1.3001797635,-4.2657163168,0.3551450274\H,-3.5280695263,-0.7
324175766,1.4672652319\H,-3.0715141733,-1.0850567799,-0.2213915445\H,-
3.1270608398,-3.168545253,1.6073748451\H,-0.7795876354,-0.5322070308,-
0.9604346686\C,-1.3915667055,-0.4364536781,1.0708764779\C,-1.152206097
,-0.9161494799,2.4948531358\C,0.1072389101,-0.2115490807,2.9207782118\H,
-1.9845591609,-0.5893930596,3.1270424029\H,0.2461592721,-0.094272574
3,3.9951989304\H,1.0154042964,-0.6241801009,2.4692780615\C,-0.21579606
4,1.1577862579,2.2552165425\C,-1.5387220062,2.0172587433,0.3546578067\H,
-1.5322982249,2.9827432615,0.8615250983\H,-0.807899411,2.03861923,-0
.4619581239\H,-2.5349126122,1.8293781528,-0.0501341694\N,-1.2200863147
,0.985148068,1.3271217725\O,0.3303811912,2.2112738898,2.5160520056\O,-
1.3135737977,-2.3602573987,2.3521869961\C,-1.5634666968,-3.1087491029,
3.5802363377\H,-1.5899549054,-4.1592869608,3.2992102133\H,-0.720655000
5,-2.9024498177,4.237343479\H,-2.5086112926,-2.7736437124,4.0104577009
\C,-0.2017762205,-2.4412884738,-0.1012086986\H,0.2404422641,-2.6957304
085,-1.0677305204\H,0.5129493617,-2.760279965,0.6637519517\\Version=AM
64L-G09RevB.01\HF=-634.7393991\RMSD=0.000e+00\RMSF=6.185e-06\Dipole=-1
.9257527,-3.7151501,0.265043\Quadrupole=-2.739426,-0.1633024,2.9027283
,11.4741221,-13.0775075,-25.2864056\PG=C01 [X(C11H18N1O2)]\\@
Sum of electronic and thermal Free Energies= -634.488366 Hartree

Entry 2

E₃ (syn)

1\1\GINC-SPARTAN-BM095\FOpt\RM062X\6-31+G(d)\C13H24N1O2Si1(1+)\UWILLE\
28-Aug-2020\0\#p M062X/6-31+G* nosymm opt=(calcfc,maxcycle=500) freq=
noraman scrf=(cpcm,solvent=dichloromethane)\\geom&freq\\1,1\C,-2.82957
06682,-1.855875981,-0.1100366398\C,-1.3933071074,-2.3030279044,-0.0751

164408\C,-0.4228030308,-1.8293054871,-0.8604927322\C,-2.8380466885,-0.0996348329,1.8019604627\C,-3.3684759482,-1.4577865749,1.2688929247\H,0.5928821417,-2.2124564261,-0.8039010491\H,-1.1592726179,-3.0835680668,0.6508866168\H,-2.9591484097,-1.0370833068,-0.8300108911\H,-3.4440257165,-2.6907771775,-0.4710335361\H,-3.2188736723,0.0322815973,2.8225581034\H,-3.2235824898,0.7146862451,1.1835694778\H,-3.1465524272,-2.2427015184,1.9957217626\H,-4.4552925525,-1.3461791444,1.2205120691\H,-0.6150477193,-1.0568669782,-1.6041615539\C,-1.3640310273,-0.0141043108,1.8904975319\C,-0.5277704163,-0.7521995718,2.9174488396\C,0.9002167892,-0.6193863067,2.3723847235\H,-0.6310334905,-0.1484794427,3.8374206966\H,1.6685317632,-0.423994077,3.1217962569\H,1.1604476272,-1.5278350213,1.8144238489\C,0.810251893,0.5168046315,1.3933313943\C,-1.0529237059,1.7104985611,0.1349071976\H,-0.1674561783,2.2475710393,-0.2012992624\H,-1.4942981865,1.1630067453,-0.7003436259\H,-1.7742190354,2.4069055344,0.5613267994\N,-0.6189716335,0.7622998116,1.1615954785\O,1.6476039982,1.1479274348,0.8275904804\O,-0.9953811243,-2.0408453168,3.1024971567\Si,-0.6033249257,-3.0193145501,4.445400517\C,-0.7938882995,-1.9861477061,5.9939052294\H,-1.7872058488,-1.5275604024,6.0521026353\H,-0.6679041475,-2.623741183,6.8768026249\H,-0.0409217799,-1.1924240119,6.0579295135\C,-1.8443357784,-4.4042288612,4.3259007518\H,-1.7675094154,-4.9052821831,3.3545469658\H,-1.6721672037,-5.1523235299,5.1069886823\H,-2.8653346394,-4.0239600598,4.4365092549\C,1.1566806141,-3.6268309044,4.2533454841\H,1.3783531019,-4.3735082684,5.0248918563\H,1.3064153046,-4.0992513176,3.2762588353\H,1.8868416517,-2.8172471771,4.3619798194\\Version=AM64L-G09RevB.01\HF=-1004.06842\RMSD=9.046e-09\RMSF=4.034e-06\Dipole=-1.1829598,1.7366691,0.0431017\Quadrupole=-5.5577907,-6.7701627,12.3279534,-2.8481231,-5.2809669,-11.1507253\PG=C01 [X(C13H24N1O2Si1)]\\@
Sum of electronic and thermal Free Energies= -1003.763396 Hartree

TS1

1\1\GINC-SPARTAN-BM089\FTS\RM062X\6-31+G(d)\C13H24N1O2Si1(1+)\UWILLE\28-Aug-2020\0\\#p M062X/6-31+G* nosymm scf=(qc,direct) freq=normal opt=(ts,noeigentest,calcf,maxcycle=500) scrf=(cpcm,solvent=dichloromethane)\geom&freq\\1,1\C,-2.2378843774,-2.9901766393,-0.1470734601\C,-0.823089696,-2.6203200444,0.068890934\C,-0.3749954229,-1.3464910713,-0.1940815353\C,-2.7900900618,-0.788783987,0.9883857821\C,-3.054080004,-2.2888054982,0.9811496482\H,0.6677662723,-1.0990181315,-0.0136659548\H,-0.173373599,-3.3167630936,0.5895385603\H,-2.5951979298,-2.6156459388,-1.1122239421\H,-2.389132616,-4.069495496,-0.0960235193\H,-3.382551474,-0.3150134614,1.784034574\H,-3.1167611498,-0.3440055548,0.0423011458\H,-2.8052856174,-2.7330855964,1.9483345354\H,-4.1154478523,-2.4663134865,0.7926373033\H,-0.8773458489,-0.7702004697,-0.9694298148\C,-1.3590372248,-0.4025916701,1.2726284347\C,-0.6911390721,-0.8324256138,2.5907028295\C,0.530159249,0.085443973,2.6814953829\H,-1.4250838791,-0.5427087728,3.362098862\H,0.7814328736,0.4066208144,3.6935228859\H,1.407325117,-0.4056606699,2.2429507122\C,0.1446546686,1.271146709,1.8289691509\C,-1.6002976138,1.8125490155,0.1216089047\H,-1.0414128989,2.7468429541,0.1578737478\H,-1.541046568,1.3963796867,-0.8889952949\H,-2.6438447885,1.9971774512,0.3841032159\N,-0.9898638157,0.9040253249,1.0798597367\O,0.6613608747,2.3594889242,1.7626943564\O,-0.4258280654,-2.1918776161,2.6464749719\Si,-0.3007616494,-3.0901420889,4.0914080386\C,-0.0807512326,-4.8316356533,3.4623159842\H,-0.0138243297,-5.5429853723,4.292330043\H,-0.9310243909,-5.1225353663,2.8346701728\H,0.8338535438,-4.920194300

1,2.8659757823\C,1.1731068157,-2.4689145901,5.0609792392\H,2.072342192
 5,-2.4379934229,4.4361890644\H,0.9998806376,-1.4661258199,5.46734844\H
 ,1.3735576206,-3.1358165587,5.9075806249\C,-1.8842422645,-2.8756419666
 ,5.0665735131\H,-2.7627951686,-3.1694052828,4.4818274655\H,-1.85178048
 95,-3.5101842294,5.9599306605\H,-2.0253787945,-1.8437306599,5.40661254
 8\\Version=AM64L-G09RevB.01\HF=-1004.0553264\RMSD=0.000e+00\RMSF=9.612
 e-06\Dipole=-1.7360305,-0.8822341,-1.5649216\Quadrupole=-1.768213,-3.0
 703641,4.8385771,2.5842453,-4.2554875,-14.009375\PG=C01 [X(C13H24N1O2Si1)]\\@
 Frequencies -298.1872 cm⁻¹
 Sum of electronic and thermal Free Energies= -1003.747034 Hartree

Syn-spiro

1\I\GINC-SPARTAN-BM094\FOpt\RM062X\6-31+G(d)\C13H24N1O2Si1(1+)\UWILLE\
 27-Aug-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) opt=(calcfc,max
 cycle=500) freq=noraman scrf=(cpcm,solvent=dichloromethane)\geom&freq
 \1,1\C,-2.1541377708,-3.0429221993,0.305757989\C,-0.7225842749,-2.596
 938494,0.553757236\C,-0.4650907894,-1.2090473102,0.0086956967\C,-2.796
 966203,-0.5774092566,0.675513491\C,-3.1742744132,-2.0534227735,0.89293
 53118\H,0.594969749,-0.9447074544,0.0685961489\H,0.027853075,-3.342542
 3411,0.293432721\H,-2.2643059148,-3.1177391048,-0.782632324\H,-2.32371
 95689,-4.0489452693,0.7045436882\H,-3.4056934485,0.0618509575,1.324518
 2297\H,-2.9907033812,-0.2801788748,-0.3617326355\H,-3.2695084994,-2.23
 78799985,1.9692837186\H,-4.1609412869,-2.250995567,0.4665871169\H,-0.8
 013415683,-1.1178111351,-1.0267744682\C,-1.3124754014,-0.3673972701,0.
 9835882931\C,-0.9047448022,-0.9534857638,2.3518732369\C,0.2403079377,-
 0.07883535,2.8357914905\H,-1.7374821621,-0.9999241137,3.0582505648\H,0
 .2419999496,0.1052256292,3.9107207344\H,1.2133816877,-0.4945526679,2.5
 515073923\C,0.0320958716,1.2280528346,2.0696630393\C,-1.2191947677,1.9
 999219448,0.0810741357\H,-0.7382906034,2.9380534442,0.3593391837\H,-0.
 8468861154,1.6795219345,-0.8981828195\H,-2.300296704,2.1503917969,0.02
 49099748\N,-0.8961336149,1.0165153074,1.0972501906\O,0.61374535,2.2779
 765936,2.2910948599\O,-0.5221900291,-2.3396441571,2.0307620189\Si,-0.4
 326842171,-3.6471855313,3.2910965187\C,0.3720872913,-5.0451097297,2.37
 43993999\H,0.561697026,-5.8500070097,3.0942137982\H,-0.2595104731,-5.4
 588429587,1.5818589485\H,1.3355219927,-4.7478249804,1.9484638251\C,0.6
 099435079,-2.8754216205,4.6169179133\H,1.5787721692,-2.5376133509,4.23
 69658434\H,0.1022419494,-2.0364899916,5.1029981714\H,0.7966506905,-3.6
 330028472,5.3871897076\C,-2.1773922313,-3.976189219,3.8394759554\H,-2.
 6582049114,-3.0846687406,4.255206361\H,-2.8050444324,-4.3807034843,3.0
 402762446\H,-2.1378772927,-4.7248886574,4.6402256173\\Version=AM64L-G0
 9RevB.01\HF=-1004.102839\RMSD=0.000e+00\RMSF=5.631e-06\Dipole=-0.97344
 52,-3.3806712,-0.5085673\Quadrupole=-11.3864962,7.8816831,3.5048132,2.
 6912616,-6.0007467,-30.8682548\PG=C01 [X(C13H24N1O2Si1)]\\@
 Sum of electronic and thermal Free Energies= -1003.785132 Hartree

E₃ (anti)

1\I\GINC-SPARTAN-BM098\FOpt\RM062X\6-31+G(d)\C13H24N1O2Si1(1+)\UWILLE\
 09-Sep-2020\0\#p M062X/6-31+G* nosymm opt=(calcfc,maxcycle=500) freq=
 noraman scrf=(cpcm,solvent=dichloromethane)\geom&freq\1,1\C,-2.47984
 75603,-2.3597175724,-0.2591455683\C,-0.1418321418,-1.3548593707,0.0322
 01148\C,-3.6120578871,-0.2535580392,0.520950119\C,-3.1580738321,-1.487
 0469251,0.7569659125\H,0.9175708155,-1.6528045548,0.084446905\H,-2.544
 5142199,-1.8951731005,-1.2508320794\H,-2.9956939472,-3.3256820446,-0.3

167711553\H,-4.0833304221,0.3396254307,1.2997924051\H,-3.5462614099,0.1925066955,-0.4703278133\H,-0.2853733404,-0.8176034064,-0.9091467516\C,-0.2960532081,-0.4484862291,1.1883946374\C,-0.2521749151,-0.934296599,2.6289667829\C,-0.0896293421,0.3568411266,3.442944883\H,-1.2357368226,-1.3862693854,2.834517845\H,-0.7633908227,0.4503254384,4.2958638163\H,0.9443957706,0.4459327943,3.7950841298\C,-0.3436539549,1.4628263465,2.4576349303\C,-0.4833900727,1.6681400879,-0.0803246841\H,-0.6733354564,2.6902495222,0.2434556496\H,0.4508362999,1.6199362356,-0.641190075\H,-1.3149860248,1.3052879951,-0.6854270463\N,-0.3696897604,0.8456233309,1.124624174\O,-0.4968937329,2.6351150834,2.6011549485\O,0.7863131712,-1.8518851155,2.7544095734\C,-1.0078531021,-2.6262898646,0.0843609586\H,-0.5902144072,-3.3313545213,-0.6392191168\H,-0.9170879393,-3.0975688346,1.069447296\Si,0.787905401,-3.0595621627,3.9672100281\C,2.5047977548,-3.7736520355,3.8764136893\H,2.6255329753,-4.5771219148,4.6108874881\H,2.6991775121,-4.1911741083,2.8827895776\H,3.2595271296,-3.0076431415,4.0821078631\C,-0.5333674648,-4.3197985678,3.5534414605\H,-1.5264432868,-3.8666205665,3.4489858577\H,-0.2991871424,-4.8565922777,2.6280367678\H,-0.5987469474,-5.0584721915,4.3610065711\C,0.4186356268,-2.236522534,5.60784295\H,1.1227551809,-1.4245746751,5.8202435608\H,-0.6001010748,-1.8332253106,5.646754399\H,0.5059741566,-2.9731293872,6.4149327336\H,-3.2747578561,-1.9123513108,1.7559651994\\Version=AM64L-G09RevB.01\\HF=-1004.0700884\RMSD=5.025e-09\RMSF=2.883e-06\Dipole=-0.0283442,0.4309387,-1.3864629\Quadrupole=-9.5715863,-2.3050557,11.876642,0.9706161,-0.1216571,-13.882988\PG=C01 [X(C13H24N1O2Si1)]\\@
Sum of electronic and thermal Free Energies= -1003.765709 Hartree

TS2

1\1\GINC-SPARTAN-BM087\FTS\RM062X\6-31+G(d)\C13H24N1O2Si1(1+)\UWILLE\09-Sep-2020\0\#p M062X/6-31+G* nosymm opt=(ts,noeigentest,calcfc,maxcycle=500) freq=norman scrf=(cpcm,solvent=dichloromethane)\geom&freq\\1,1\C,-3.0798788554,-2.6983120413,0.0335641521\C,-0.721211614,-1.7493108084,0.2042787125\C,-2.8728379575,-0.3789636355,0.9129500555\C,-3.3778067263,-1.6780647928,1.0301098217\H,0.3293900187,-1.9829339429,0.4099071047\H,-3.1552249337,-2.3190464672,-0.9889664585\H,-3.6681198841,-3.6066570451,0.1628736086\H,-3.171447342,0.3396263214,1.673284127\H,-2.8126622374,0.0257888652,-0.0976983099\H,-3.795038498,-1.999135024,1.9848602182\H,-0.7842285353,-1.3455742162,-0.8117967422\C,-1.1171275304,-0.6900277113,1.2132218532\C,-0.9298233811,-1.0471342633,2.7156870094\C,-0.8608549189,0.3276594151,3.383564018\H,-1.7603137621,-1.6557560305,3.0925332746\H,-1.8456398063,0.6861978333,3.7037466271\H,-0.1931981302,0.3426781826,4.2459586317\C,-0.3430499795,1.2301631868,2.2856089155\C,-0.1755300355,1.175721916,-0.1965738763\H,0.6247259708,0.6239000343,-0.6954307472\H,-1.0553650458,1.210240269,-0.8471695561\H,0.1562802578,2.1931428772,0.0091937725\N,-0.5053375829,0.5593490109,1.0760833632\O,0.1304646764,2.3404651064,2.3885706262\O,0.2937552448,-1.7231295521,2.8204558494\C,-1.5565862404,-3.0086487432,0.3247683392\H,-1.249604805,-3.7502522592,-0.4162164656\H,-1.4457832802,-3.4636930354,1.3139908099\Si,0.6245217532,-2.8381312649,4.0630955683\C,0.2616260346,-2.0446866161,5.7210799308\H,-0.7850359112,-1.7293257058,5.8065966359\H,0.4499450753,-2.7697293932,6.521450209\H,0.9010302798,-1.1740154115,5.9031718965\C,2.4301143902,-3.2404239564,3.8406686613\H,2.7591709032,-3.9645290321,4.5939807387\H,2.6134867752,-3.6736453421,2.8516361476\H,3.0461406462,-2.3408187323,3.9417663878\C,-0.4661395526,-4.343367753,3.8205231801\H,-0.2307714401,-4.8598024256,2.8835281936\H,-0.301252448,-5.0519191108,4.6407645118\H,-1.5337970624,-4.0925450961,3.8208831642\\Version=AM6

4L-G09RevB.01\HF=-1004.0512105\RMSD=4.068e-09\RMSF=5.825e-06\Dipole=-3.4113446,-1.7732512,-2.2243294\Quadrupole=5.4277449,-5.8207196,0.3929747,10.666385,-9.1061703,-16.4187244\PG=C01 [X(C13H24N1O2Si1)]\@
Frequencies -159.6848 cm⁻¹
Sum of electronic and thermal Free Energies= -1003.741551 Hartree

Anti-cycl

1\1\GINC-SPARTAN-BM096\FOpt\RM062X\6-31+G(d)\C13H24N1O2Si1(1+)\UWILLE\07-Sep-2020\0\#p M062X/6-31+G* nosymm opt=(calcfc,maxcycle=500) freq=noraman scrf=(cpcm,solvent=dichloromethane)\geom&freq\1,1\C,-2.4702811126,-2.0033265985,-0.3737537077\C,-0.3499707829,-0.788615578,0.4020494276\C,-2.7220619612,0.0120477583,1.0692915572\C,-3.0351441432,-1.3403647178,0.7780741248\H,0.6904727815,-0.9109081085,0.7195622209\H,-2.4586380984,-1.3824030378,-1.272227981\H,-2.8853377979,-2.992126586,-0.5624475135\H,-3.2635978423,0.4472306407,1.9081560315\H,-2.6893678318,0.659818023,0.1906274995\H,-0.3581627772,-0.1776910053,-0.5067715924\C,-1.072039534,-0.0629408408,1.5265463318\C,-0.9540685138,-0.7214860393,2.9353551424\C,-1.1638322405,0.4603563084,3.8845337361\H,-1.7104355164,-1.5037634077,3.0739739864\H,-2.2160816007,0.5935955389,4.1598971042\H,-0.5795579326,0.3691000788,4.8014094206\C,-0.7121595508,1.6568841902,3.0748539712\C,-0.3375206167,2.2081561878,0.6854847957\H,0.5780361696,1.91126855,0.1679282618\H,-1.1589691051,2.2682835885,-0.0366680307\H,-0.1951179588,3.1867989399,1.1435020164\N,-0.6549376763,1.2720318322,1.7477613511\O,-0.4445083695,2.7704439395,3.479793818\O,0.3437555041,-1.239272201,3.0495110359\C,-0.957769222,-2.1480032731,0.122418217\H,-0.4458554659,-2.6527052669,-0.7001322745\H,-0.9050944488,-2.8027804781,0.9977735847\Si,0.7259539967,-2.5493943526,4.0634935234\C,-0.1192506992,-4.0873625577,3.4013456832\H,-1.2055928149,-3.9648800389,3.3124837811\H,0.2802242756,-4.3726080736,2.4218286869\H,0.05528408,-4.9246208067,4.0873585518\C,0.1226888226,-2.1861205604,5.7994740651\H,0.3453472797,-3.0390149422,6.4511200514\H,0.6157392978,-1.3046154862,6.223496081\H,-0.9613905175,-2.0242887315,5.8302450082\H,-3.5050758826,-1.954955079,1.5469707451\C,2.5821813445,-2.6789845871,3.962459009\H,3.0595908932,-1.7642664187,4.3289505622\H,2.9413901097,-3.5169860418,4.5698721649\H,2.9060166986,-2.846458051,2.9296686914\Version=AM64L-G09RevB.01\HF=-1004.0511376\RMSD=2.762e-09\RMSF=5.092e-06\Dipole=-3.0831158,-2.0839699,-3.3109866\Quadrupole=8.5378754,-6.0282053,-2.5096701,7.7418961,-6.9742,-18.7791496\PG=C01 [X(C13H24N1O2Si1)]\@
Sum of electronic and thermal Free Energies= -1003.742379 Hartree

Entry 3

E₃ (syn)

1\1\GINC-SPARTAN-BM096\FOpt\RM062X\6-31+G(d)\C12H20N1O2(1+)\UWILLE\31-Aug-2020\0\#p M062X/6-31+G* nosymm opt=(calcfc,maxcycle=500) freq=noraman scrf=(cpcm,solvent=dichloromethane)\geom&freq\1,1\C,-2.0583756049,-2.6315515949,-0.3553407572\C,-0.587196332,-2.7118523361,-0.0182541097\C,0.2875460715,-1.7895821203,-0.4397415385\C,-2.8989334157,-0.752321332,1.2223319749\C,-2.9382909091,-2.2551565196,0.846927787\H,1.3465743528,-1.8569810756,-0.1992314755\H,-2.2267849287,-1.921828276,-1.1746276586\H,-2.3901083498,-3.6149614967,-0.7123064689\H,-3.5438231986,-0.6115808519,2.1018301447\H,-3.3149002974,-0.1582888369,0.4050283227\H,-2.6771736038,-2.8575718968,1.7184479334\H,-3.9849243709,-2.4626985844,0.6067241137\H,-0.0194355008,-0.9593576462,-1.0735204189\C,-1.57761080

22,-0.2105476822,1.6137984266\C,-0.8021665393,-0.6270419828,2.84575186
 77\C,0.5886391325,-0.0212021152,2.6226126768\H,-1.3050475809,-0.108435
 2826,3.683277534\H,1.0605748187,0.4094052632,3.5063851455\H,1.25186333
 46,-0.7800833187,2.1876714061\C,0.3483344282,1.0383797392,1.5850425935
 \C,-1.4901729488,1.6053083625,-0.0807681947\H,-0.7727650071,2.40971430
 19,-0.2345374256\H,-1.5580878244,0.994557532,-0.9826353887\H,-2.465281
 3985,2.0170961656,0.178578746\N,-0.9906777281,0.7958453837,1.033299971
 5\O,1.0323754443,1.9287191277,1.1870558567\O,-0.8578863045,-2.00241516
 11,3.0201678216\C,-0.3048533811,-2.4280390992,4.2608262364\H,-0.444270
 0478,-3.5078307368,4.3052558056\H,0.7652106278,-2.1963976146,4.3125209
 052\H,-0.8272279497,-1.9511992577,5.0985209202\C,-0.1552317303,-3.9184
 812699,0.7725497956\H,-0.1774236033,-4.8057993345,0.1275405485\H,0.858
 3062189,-3.7991882099,1.1653590113\H,-0.8292191014,-4.1080627132,1.613
 355301\\Version=AM64L-G09RevB.01\HF=-674.0353616\RMSD=7.387e-09\RMSF=4
 .310e-06\Dipole=-1.4836823,0.8868398,1.0252084\Quadrupole=-0.9904996,-
 8.0212947,9.0117943,-1.5988885,-3.8715593,-7.3122147\PG=C01 [X(C12H20N
 1O2)]\@
 Sum of electronic and thermal Free Energies= -673.767055 Hartree

TS1

1\1\GINC-SPARTAN-BM120\FTS\RM062X\6-31+G(d)\C12H20N1O2(1+)\UWILLE\31-A
 ug-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) freq=noraman opt=(t
 s,noeigentest,calcf, maxcycle=500) scrf=(cpcm,solvent=dichloromethane)
 \geom&freq\1,1\C,-2.2329122105,-2.949101912,-0.1873567697\C,-0.78629
 69211,-2.6851089611,0.0728445774\C,-0.2979670139,-1.4264145751,-0.1554
 466871\C,-2.8001976045,-0.782586913,1.0032340915\C,-3.0441785505,-2.28
 744153,0.9552360846\H,0.7423693308,-1.192322933,0.0586547104\H,-2.5449
 273749,-2.5091521387,-1.1408262039\H,-2.4423041021,-4.0216784167,-0.20
 99874281\H,-3.4406609854,-0.3332225308,1.7778334021\H,-3.0913816953,-0
 .326210194,0.051724399\H,-2.7918339052,-2.7517793184,1.9127455897\H,-4
 .1080264432,-2.4581719447,0.7713539707\H,-0.8011810003,-0.7902630014,-
 0.8798912482\C,-1.4094355354,-0.3465061822,1.3690162545\C,-0.758564844
 7,-0.7342334361,2.6946508407\C,0.480376061,0.16407993,2.7666060502\H,-
 1.4886504632,-0.4176811124,3.4614404882\H,0.7285061443,0.5302619781,3.
 7637273915\H,1.3522106897,-0.3584533613,2.3530331675\C,0.1213495254,1.
 3139248545,1.8592879368\C,-1.5921360399,1.7934562099,0.092372334\H,-1.
 0149102922,2.7169172174,0.0947323659\H,-1.523064407,1.3252433592,-0.89
 40226995\H,-2.6354839867,2.0079855411,0.3297110199\N,-1.0157656898,0.9
 20057012,1.1050173692\O,0.6432585247,2.3916014844,1.7440861661\C,0.034
 199164,-3.7898803407,0.6439815176\H,1.0002390146,-3.4433711673,1.01353
 19675\H,-0.5049986946,-4.3072598012,1.4436314029\H,0.1987797376,-4.521
 5072305,-0.1594545974\O,-0.5320495799,-2.1003468433,2.7866725085\C,-0.
 1197568941,-2.5154990218,4.0827386294\H,-0.0077404313,-3.5989227621,4.
 0381409834\H,0.8409857545,-2.0617687218,4.3520923197\H,-0.8753055308,-
 2.2518997469,4.8325243648\\Version=AM64L-G09RevB.01\HF=-674.0276515\RM
 SD=0.000e+00\RMSF=1.278e-05\Dipole=-1.3287569,-1.0937902,-0.107339\Qua
 drupole=-0.7089368,-3.5790959,4.2880327,0.5141822,-3.5300978,-9.501595
 5\PG=C01 [X(C12H20N1O2)]\@
 Frequencies -248.4672 cm⁻¹
 Sum of electronic and thermal Free Energies= -673.757529 Hartree

Syn-spiro

1\1\GINC-SPARTAN-BM125\FOpt\RM062X\6-31+G(d)\C12H20N1O2(1+)\UWILLE\31-

Aug-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) opt=(calcfc,maxcyc
le=500) freq=noraman scrf=(cpcm,solvent=dichloromethane)\geom&freq\1
,1\C,-1.0477119939,-1.9883706697,-0.3671250258\C,0.0299914103,-1.43093
57533,0.5529611914\C,-0.2620772226,0.0063856591,0.9373480815\C,-2.7195
59604,-0.4705035762,0.8743562219\C,-2.4764421998,-1.8202798018,0.17712
6228\H,0.5630738893,0.430130952,1.52038892\H,-0.93055134,-1.4361576755
, -1.3076635876\H,-0.8465156796,-3.0396457941,-0.6006809496\H,-3.642965
0437,-0.5161873691,1.4623665813\H,-2.834212065,0.3298173292,0.13453211
16\H,-2.6905774414,-2.6302495422,0.8846519023\H,-3.1890790375,-1.94913
25409,-0.6410584166\H,-0.4202799304,0.6200747957,0.0468805347\C,-1.537
504567,-0.1412200331,1.7884705773\C,-1.1851417623,-1.313105512,2.72362
70655\C,-0.6642853728,-0.6873533024,4.0037133712\H,-2.014167624,-2.005
0983625,2.882739712\H,-0.9765598946,-1.2063707305,4.9105825339\H,0.428
9979546,-0.6163466785,4.0009938767\C,-1.2419734361,0.7283289939,3.9593
641629\N,-1.7624016307,0.9462032391,2.7200467102\O,-1.223735421,1.5284
010205,4.8802022081\O,-0.1489568519,-2.0471860812,1.9689393563\C,-0.10
91594002,-3.4912945494,2.1485188335\H,0.7778247528,-3.8461150097,1.629
6506794\H,-0.0183747753,-3.6622003698,3.2199167468\H,-1.0212216981,-3.
9328324559,1.7451813016\C,1.4478078471,-1.7157457703,0.1247155082\H,1.
5988388066,-2.7635490264,-0.1470370763\H,1.6531165416,-1.1116485287,-0
.7641211368\H,2.1546641423,-1.4286261648,0.9074736078\C,-2.2686645094,
2.2340823442,2.2847433083\H,-2.2882739274,2.8950071686,3.1514411447\H,
-1.6173994276,2.6649939077,1.5165645516\H,-3.2806744483,2.1313923679,1
.8845136543\Version=AM64L-G09RevB.01\HF=-674.0688424\RMSD=0.000e+00\R
MSF=7.329e-06\Dipole=0.7191179,-3.0774648,-2.4953165\Quadrupole=1.2821
205,13.3417241,-14.6238446,2.4392896,0.1196005,-21.812431\PG=C01 [X(C1
2H20N1O2)]\@
Sum of electronic and thermal Free Energies= -673.791867 Hartree

E₃ (*anti*)

1\1\GINC-SPARTAN-BM065\FOpt\RM062X\6-31+G(d)\C12H20N1O2(1+)\UWILLE\22-
Aug-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) opt=(calcfc,maxcyc
le=500) freq=noraman scrf=(cpcm,solvent=dichloromethane)\geom&freq\1
,1\C,-2.4339296279,-2.4381530102,-0.3350915552\C,-0.1574121029,-1.3080
829836,-0.0080013989\C,-3.412815971,-0.4362124519,0.7704079586\C,-3.15
52328179,-1.7499033914,0.7977148444\H,0.9211222563,-1.5382700667,0.007
2562425\H,-2.5394326001,-1.8595641357,-1.2602557787\H,-2.8801598652,-3
.424001524,-0.5118296301\H,-3.8928381335,0.0703315484,1.6048757199\H,-
3.1823150147,0.1658552641,-0.1065829879\H,-0.3453266133,-0.7186693505,
-0.9099965259\C,-0.3383852448,-0.4826023462,1.2051032833\C,-0.33783195
76,-1.0617680336,2.6076639802\C,-0.2475333831,0.1644891306,3.524852249
7\H,-1.2896446593,-1.5926182922,2.7572020191\H,-1.0123380728,0.2122197
213,4.3018375449\H,0.7397936712,0.218837278,3.9973542216\C,-0.38537709
27,1.3417602766,2.5998595907\C,-0.3717874378,1.7221381883,0.0796271153
\H,-0.495620813,2.7317010545,0.4676990099\H,0.5756907006,1.6373947183,
-0.4540311422\H,-1.2054706374,1.4687429099,-0.5760100858\N,-0.36195221
15,0.8156192907,1.2286359321\O,-0.4909488964,2.5082596807,2.813765621\
O,0.7436524008,-1.9447279727,2.6747598273\C,0.7055026329,-2.7791069615
,3.8289721781\H,1.5803345461,-3.4252458874,3.7718584641\H,0.751519511,
-2.1812079206,4.7464149304\H,-0.2070751236,-3.3872727139,3.8317408717\
C,-0.937195434,-2.6325302393,-0.0395653542\H,-0.4948669094,-3.24292788
36,-0.8315352321\H,-0.781040353,-3.1794555707,0.8973826787\C,-3.553097
2711,-2.6239431099,1.9582651058\H,-2.7379503754,-3.2908742047,2.265801

2885\H,-3.8730973526,-2.0363526184,2.8232086247\H,-4.383393937,-3.2748
 771728,1.6585100784\\Version=AM64L-G09RevB.01\HF=-674.0377431\RMSD=0.0
 00e+00\RMSF=5.103e-06\Dipole=0.7408243,-0.3146604,-0.4174596\Quadrupol
 e=-7.2864912,-2.7097421,9.9962334,4.1501139,-2.6776622,-11.5710102\PG=
 C01 [X(C12H20N1O2)]\\@
 Sum of electronic and thermal Free Energies= -673.770512 Hartree

TS2

1\1\GINC-SPARTAN-BM106\FTS\RM062X\6-31+G(d)\C12H20N1O2(1+)\UWILLE\24-A
 ug-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) freq=noraman opt=(t
 s,noeigentest,calcfc,maxcycle=500) scrf=(cpcm,solvent=dichloromethane)
 \geom&freq\1,1\C,-2.4858819058,-2.8243281199,-0.4525421341\C,-0.4205
 386902,-1.4427354163,0.0454570686\C,-3.0075556559,-0.6785651412,0.6509
 030648\C,-3.1643293507,-2.0466241864,0.6182239169\H,0.6525140904,-1.48
 72612907,0.274885362\H,-2.6016423,-2.3408533533,-1.4271537116\H,-2.869
 8539508,-3.8456552826,-0.5094249076\H,-3.486797846,-0.0998557699,1.437
 6935886\H,-2.8099899847,-0.1513438314,-0.2800504\H,-0.5341890161,-0.89
 78105728,-0.8973311993\C,-1.0241487949,-0.6568966031,1.177907359\C,-0.
 9518440879,-1.2161689669,2.6100280564\C,-1.2350244115,0.0075487582,3.4
 831246148\H,-1.6571131508,-2.0347622931,2.7799574797\H,-2.2882171457,0
 .0806240318,3.775044898\H,-0.6293397073,0.0328893986,4.391040843\C,-0.
 8946382558,1.1753399486,2.5879677638\C,-0.5053148566,1.5606348222,0.14
 52903398\H,0.4190617583,1.265399298,-0.354794136\H,-1.3371637708,1.531
 3899496,-0.5648003479\H,-0.4037288706,2.57061586,0.5404524169\N,-0.772
 9215999,0.6785635457,1.2707601001\O,-0.7470918013,2.3362014514,2.87379
 202\O,0.37024384,-1.680391895,2.7474418985\C,0.5484223399,-2.525082511
 2,3.8773012248\H,1.5948226012,-2.8287202373,3.8753544955\H,0.326171221
 1,-1.9955934471,4.8108038284\H,-0.0943693802,-3.4104788878,3.798262008
 4\C,-0.975264747,-2.852677083,-0.0838138559\H,-0.4398520617,-3.3834205
 15,-0.8742660116\H,-0.8178525722,-3.4129349569,0.845238653\C,-3.829989
 6252,-2.8021367793,1.713485097\H,-4.7520491972,-3.2331286126,1.2987272
 366\H,-3.219288785,-3.6536494995,2.0381755835\H,-4.0972343292,-2.17672
 28119,2.5673157858\\Version=AM64L-G09RevB.01\HF=-674.0282118\RMSD=0.00
 0e+00\RMSF=4.202e-06\Dipole=-1.392879,-2.104717,-1.2269035\Quadrupole=
 4.1957438,-3.0380627,-1.1576811,13.7260219,-7.8307995,-15.1763094\PG=C
 01 [X(C12H20N1O2)]\\@
 Frequencies -287.8558 cm⁻¹
 Sum of electronic and thermal Free Energies= -673.757525 Hartree

Anti-cycl

1\1\GINC-SPARTAN-BM123\FOpt\RM062X\6-31+G(d)\C12H20N1O2(1+)\UWILLE\21-
 Aug-2020\0\#p M062X/6-31+G* nosymm opt=(calcfc,maxcycle=500) freq=nor
 aman scrf=(cpcm,solvent=dichloromethane)\geom&freq\1,1\C,-2.45603488
 35,-2.871894193,-0.4470869177\C,-0.4148989737,-1.4429328603,0.10027025
 24\C,-2.7617505667,-0.7296027819,0.7852120311\C,-3.1058194676,-2.13172
 09887,0.6298460735\H,0.6424573176,-1.4532059569,0.3770788561\H,-2.5277
 279319,-2.338053331,-1.3998905465\H,-2.8256402197,-3.8931641289,-0.543
 2204046\H,-3.3422003533,-0.2255563661,1.5600917799\H,-2.8333918053,-0.
 1983711259,-0.1695886905\H,-0.5106698227,-0.9284668876,-0.8629687279\C
 ,-1.1806316374,-0.670719702,1.1701664386\C,-0.9701205726,-1.2014994732
 ,2.6168166198\C,-1.1854211133,0.0404047674,3.4843947073\H,-1.668665784
 7,-2.0131836335,2.8624943208\H,-2.2287620059,0.1548325159,3.7993605256
 \H,-0.5619635542,0.0494092029,4.3805008123\C,-0.8209599425,1.189363616
 7,2.5646206037\C,-0.5864484037,1.573540617,0.1326696148\H,0.3148069368

,1.2812799724,-0.412331543\H,-1.4452185115,1.5420606239,-0.5470210517\H,-0.4685485154,2.5911737846,0.5056248018\N,-0.8017422714,0.7115837393,1.2783053414\O,-0.5912745377,2.3424710438,2.8855640176\O,0.3510135572,-1.6775638241,2.7031806127\C,0.582517787,-2.4777151576,3.8518809038\H,1.6259016859,-2.7902715925,3.8109758656\H,0.4108189314,-1.9158827605,4.7774245388\H,-0.0676247144,-3.3620031437,3.8406108036\C,-0.9327550477,-2.8661004318,-0.029021762\H,-0.4076998416,-3.4052251386,-0.8203164045\H,-0.7917205364,-3.4261257852,0.9015381592\C,-3.9460806096,-2.8306097449,1.603105611\H,-4.9232375226,-2.9291327177,1.0924444707\H,-3.6049868473,-3.8563491766,1.7778860922\H,-4.1075060514,-2.2793617918,2.5298378542\\Version=AM64L-G09RevB.01\HF=-674.0343833\RMSD=7.849e-09\RMSF=1.267e-05\Dipole=-3.0539228,-3.7904591,-1.9863833\Quadrupole=13.1081008,-3.154631,-9.9534699,22.1127986,-8.920379,-17.8962155\PG=C01 [X(C12H20N1O2)]\\@
Sum of electronic and thermal Free Energies= -673.763403 Hartree

Anti-spiro

1\1\GINC-SPARTAN-BM086\FOpt\RM062X\6-31+G(d)\C12H20N1O2(1+)\UWILLE\01-Sep-2020\0\#p M062X/6-31+G* nosymm opt=(calcfc,maxcycle=500) freq=normal aman scrf=(cpcm,solvent=dichloromethane)\geom&freq\1,1\C,-1.5275446562,-3.2258706585,0.1214378132\C,-0.389832832,-0.9340109777,0.012483936\C,-2.7397729881,-1.1132062338,0.8211556927\C,-2.389828137,-2.5727592111,1.186068646\H,0.5844450999,-0.4599931519,0.1715429931\H,-2.1247011229,-3.2324760683,-0.7982655959\H,-1.329114674,-4.2701449526,0.3843079923\H,-3.5339077769,-0.7157451828,1.4604474457\H,-3.0654742897,-1.0797761699,-0.2220949046\H,-0.7676368741,-0.550575628,-0.9435088553\C,-1.3955069599,-0.4430356534,1.0822327631\C,-1.16583902,-0.9162758005,2.5092070191\C,0.0896465148,-0.2011608723,2.9373893945\H,-2.000959018,-0.5848816324,3.1366315283\H,0.221839683,-0.0751690819,4.0118669203\H,1.0021423638,-0.6159284588,2.4960713853\C,-0.2293256439,1.1619636235,2.2605294052\C,-1.5455427553,2.0049885646,0.3474331195\H,-1.5313911918,2.9752076129,0.8450705424\H,-0.8195605378,2.0151489447,-0.4737229361\H,-2.5450555695,1.8185788981,-0.0501612142\N,-1.2264492632,0.9810299241,1.3276977026\O,0.3139675163,2.2186772532,2.5173492306\O,-1.3137865563,-2.3533405392,2.3768085835\C,-1.3950943156,-3.1056948792,3.6191742654\H,-1.4157016926,-4.1594757785,3.3529514213\H,-0.483791852,-2.8708920629,4.1675364347\H,-2.2847103135,-2.8037128562,4.173326898\C,-0.2128852281,-2.4576037622,-0.0671576586\H,0.2343299762,-2.7220476642,-1.0288973839\H,0.4918529919,-2.7791693812,0.7054482349\C,-3.5462151171,-3.3902325031,1.6893595105\H,-4.2617225294,-3.4458593373,0.8614993085\H,-3.2599310114,-4.4122587292,1.9467142421\H,-4.0546878497,-2.9145437142,2.5316811197\\Version=AM64L-G09RevB.01\HF=-674.0409572\RMSD=8.499e-09\RMSF=8.771e-06\Dipole=-1.8186153,-3.5724029,0.1544395\Quadrupole=-1.1251913,0.0959905,1.0292008,13.5643396,-13.0144139,-25.6418097\PG=C01 [X(C12H20N1O2)]\\@
Sum of electronic and thermal Free Energies= -673.764116 Hartree

Entry 4

E₃ (syn)

1\1\GINC-SPARTAN-BM090\FOpt\RM062X\6-31+G(d)\C18H24N1O2(1+)\UWILLE\14-Sep-2020\0\#p M062X/6-31+G* nosymm opt=(calcfc,maxcycle=500) freq=normal aman scrf=(cpcm,solvent=dichloromethane)\geom&freq\1,1\C,-3.48472086

58,-0.3710228362,3.2565943789\C,-3.1062630158,-1.6104429972,2.48076085
52\C,-3.0103799566,-1.5997854573,1.1446996918\C,-1.3389915459,1.071593
039,3.1465429762\C,-2.3082452327,0.2488435557,4.026649606\H,-2.7444912
552,-2.4959990822,0.587401504\H,-3.9206722021,0.3780815737,2.584547869
8\H,-4.2575445787,-0.6362601798,3.9897471542\H,-0.5422394023,1.4591800
228,3.799832526\H,-1.8675505297,1.9313398682,2.7316006059\H,-1.7546872
383,-0.5168505109,4.5727455503\H,-2.695677203,0.9591126865,4.762896449
5\H,-3.2394191194,-0.706893733,0.5667937454\C,-0.617637605,0.353437731
7,2.0696220672\C,0.3359437371,-0.8035573598,2.2998412027\C,0.577398530
5,-1.3582131808,0.8915200236\H,1.2621056111,-0.3258846343,2.6722579317
\H,1.5908783605,-1.7034803055,0.6865103425\H,-0.1367225986,-2.16937756
8,0.696548075\C,0.2217431622,-0.201853512,0.0051462761\C,-1.1303760649
,1.9464683643,0.1887256019\H,-1.1055192713,2.7549638445,0.9195373229\H
,-0.4431202046,2.1926784155,-0.6232734981\N,-0.5489573752,0.7408150465
,0.8256351079\O,0.4497510093,0.0198663599,-1.1439251104\O,-0.162094997
,-1.6920281899,3.2391148998\C,0.7784834131,-2.6923968909,3.6139647996\H
,0.2998419082,-3.2866875394,4.3919745906\H,1.0242026301,-3.3374114921
,2.7626014156\H,1.6935060452,-2.2337497816,4.007286688\C,-2.9034721182
,-2.8615592401,3.292445609\H,-2.4255042348,-3.6506712716,2.705302789\H
,-2.2885141942,-2.66932491,4.1770698861\C,-2.5251974688,1.6819269648,-
0.3268880372\C,-2.7098327328,0.9665086604,-1.5145538552\C,-3.637626685
9,2.1198321931,0.3943105494\C,-3.9959330483,0.6615476432,-1.9542199761
\H,-1.8470003368,0.6460800513,-2.0925284748\C,-4.9253687551,1.81481192
58,-0.0462673752\H,-3.5052298624,2.7063687819,1.3007661973\C,-5.104995
667,1.0767676515,-1.2150891929\H,-4.1326867151,0.1031004479,-2.8752742
901\H,-5.7850350609,2.1549523544,0.5232170982\H,-6.1070520418,0.834943
3713,-1.5562183635\H,-3.8752318632,-3.2300496414,3.644681996\\Version=
AM64L-G09RevB.01\HF=-904.9993729\RMSD=5.016e-09\RMSF=3.242e-06\Dipole=
2.072843,0.3940018,1.8566027\Quadrupole=-0.9624678,-5.3058422,6.268310
1,-7.4805101,-0.9803993,0.1370227\PG=C01 [X(C18H24N1O2)]\\@
Sum of electronic and thermal Free Energies= -904.653687 Hartree

TS1

1\1\GINC-SPARTAN-BM092\FTS\RM062X\6-31+G(d)\C18H24N1O2(1+)\UWILLE\16-S
ep-2020\0\#p M062X/6-31+G* scf=(qc,direct) nosymm freq=noraman opt=(t
s,noeigentest,calcf, maxcycle=500) scrf=(cpcm,solvent=dichloromethane)
\\geom&freq\\1,1\C,-4.2403865783,-2.3764818888,1.8368587446\C,-3.18604
1363,-2.7738785894,0.8556466505\C,-2.6662897897,-1.8107568339,0.035198
6946\C,-2.8553436254,-0.3528147764,2.4809272243\C,-3.5418430791,-1.616
5960318,2.9911514409\H,-1.8691468214,-2.0509720706,-0.6660516753\H,-4.
9764221633,-1.7106077543,1.3727526344\H,-4.7600309673,-3.2510791835,2.
2374212876\H,-2.442354096,0.206952393,3.3345415257\H,-3.5944654131,0.2
97085529,2.0024271058\H,-2.8266793848,-2.2717161968,3.4961980132\H,-4.
2983671853,-1.3203896343,3.7227189694\H,-3.2641141715,-0.9315554991,-0
.1897192574\C,-1.6849654915,-0.5480061148,1.5595492702\C,-0.4548752376
,-1.3581839367,1.9657268065\C,0.5604819168,-1.055855866,0.8601782696\H
,-0.1216732763,-0.887147513,2.9088745928\H,1.5962371055,-0.9758881082,
1.1926627375\H,0.4978540047,-1.8143474154,0.0699394297\C,0.0829828695,
0.2640998931,0.3135997893\C,-1.9583957198,1.7174265087,0.4683397347\H,
-2.4291542187,2.1062680138,1.3736621641\H,-1.1873947616,2.4250650744,0
.1557484221\N,-1.2300009776,0.4865496101,0.8154395643\O,0.6462514151,1
.0453323089,-0.4070352861\O,-0.7483469385,-2.6964374533,2.1794122229\C
,0.3308340852,-3.4246177883,2.7514178941\H,-0.0301197741,-4.4422890367

,2.9011810489\H,1.1946402908,-3.4411341396,2.0771205065\H,0.623805602,
-2.990774643,3.714999679\C,-2.70769419,-4.1851329124,0.8816831423\H,-1
.7871092569,-4.324535813,0.3132063346\H,-2.5642567127,-4.5316928282,1.
9101065015\C,-2.9670955341,1.4920174625,-0.6353539827\C,-2.5255573931,
1.1130159655,-1.9080475175\C,-4.3351356863,1.6225580429,-0.3919420178\
C,-3.445383797,0.8473835648,-2.9185727431\H,-1.4589273452,1.0203619482
,-2.1023703782\C,-5.2580359902,1.3602000575,-1.4063214723\H,-4.6858061
492,1.9338154609,0.5897956529\C,-4.8144303283,0.9661775116,-2.66717827
3\H,-3.095985256,0.549912019,-3.9026817661\H,-6.3207245771,1.462998819
5,-1.2083893176\H,-5.5320143813,0.7584673203,-3.4552334353\H,-3.499034
6584,-4.8066404763,0.4397130683\\Version=AM64L-G09RevB.01\HF=-904.9919
01\RMSD=0.000e+00\RMSF=7.214e-06\Dipole=-0.1393302,-1.5621504,2.385683
3\Quadrupole=9.2900241,-6.6436526,-2.6463715,3.4718788,-7.1447381,-6.9
512432\PG=C01 [X(C18H24N1O2)]\@
Frequencies -239.3573 cm⁻¹
Sum of electronic and thermal Free Energies= -904.646289 Hartree

Syn-spiro

1\1\GINC-SPARTAN-BM092\FOpt\RM062X\6-31+G(d)\C18H24N1O2(1+)\UWILLE\15-
Sep-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) opt=(calcfc,maxcyc
le=500) freq=noraman scrf=(cpcm,solvent=dichloromethane)\geom&freq\1
,1\C,0.978077664,-1.9159320144,-0.4443420094\C,1.891663043,-0.91170813
91,0.2440925865\C,1.4952270177,0.5140860694,-0.0873097697\C,-0.9102218
831,-0.1742228016,-0.1993814989\C,-0.5184168078,-1.6619261898,-0.19776
60766\H,2.2138923008,1.2265367292,0.3320752135\H,1.2112746143,-1.82614
57288,-1.5124609634\H,1.2477073542,-2.9383383841,-0.156768326\H,-1.904
3518659,-0.0490445536,0.242977563\H,-0.9573401917,0.2150519234,-1.2233
834824\H,-0.8037371661,-2.1029126779,0.7647289869\H,-1.1011715765,-2.1
985159216,-0.9504167336\H,1.4406750243,0.6581940289,-1.1693910729\C,0.
1190275602,0.6348138646,0.5944778375\C,0.3798107127,0.0275758351,1.986
3934596\C,0.6969310397,1.1944531085,2.9025873954\H,-0.4395197522,-0.59
7625858,2.3465514588\H,0.2914349102,1.0922167711,3.9095484378\H,1.7765
651047,1.3661021431,2.974924333\C,0.0654520759,2.3835631931,2.17916571
53\C,-0.7723609614,2.925261138,-0.0861536016\H,-0.5631200284,3.9296497
731,0.2947221275\H,-0.2007929821,2.7928639789,-1.011943008\N,-0.265161
0479,1.9975946396,0.9149006375\O,-0.1023623627,3.4959141884,2.65089944
89\O,1.5348054325,-0.8623715969,1.7560055401\C,1.5939680463,-2.0721583
678,2.5641185035\H,2.558239264,-2.534547021,2.3680605267\H,1.530538261
6,-1.746834161,3.6011521467\H,0.7646085106,-2.7277629396,2.2958546955\
C,3.3651484397,-1.2179343594,0.1491581997\H,3.6729563606,-1.0426200827
,-0.8861187152\H,3.9432523891,-0.5547684464,0.7976819252\C,-2.25517202
18,2.7589092316,-0.3515792212\C,-2.7362159551,2.6311978362,-1.65480283
92\C,-3.1581500516,2.7385887682,0.7159891878\C,-4.1038221766,2.4804376
626,-1.8925028363\H,-2.0392501641,2.6407696361,-2.4903806423\C,-4.5226
357601,2.5856691505,0.4821245073\H,-2.7878200877,2.8394411093,1.734297
9662\C,-4.9987161159,2.4544391165,-0.8245297345\H,-4.4670713825,2.3775
981702,-2.9109420441\H,-5.2157726849,2.5702948187,1.3182383101\H,-6.06
23798341,2.3329042299,-1.0071831695\H,3.588445784,-2.2606581104,0.3876
313648\\Version=AM64L-G09RevB.01\HF=-905.0334402\RMSD=0.000e+00\RMSF=4
.830e-06\Dipole=3.2438092,-4.9084945,0.0368347\Quadrupole=9.3134901,-1
3.9803475,4.6668574,-6.0115397,6.5474595,-17.0915858\PG=C01 [X(C18H24N1O2)]\@
Sum of electronic and thermal Free Energies= -904.680865 Hartree

E₃ (*anti*)

1\1\GINC-SPARTAN-BM093\FOpt\RM062X\6-31+G(d)\C18H24N1O2(1+)\UWILLE\12-Sep-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) opt=(calcf, maxcyc le=500) freq=noraman scrf=(cpcm,solvent=dichloromethane)\geom&freq\1,1\C,-2.1399416758,-3.0002513474,-0.2433972877\C,-0.0291573771,-1.5812021997,0.0587843331\C,-3.3958846523,-1.00077541,0.5313025543\C,-3.0105839322,-2.2657474382,0.7459319614\H,1.0673615846,-1.6761939341,0.1387195264\H,-2.2421510788,-2.556311897,-1.2408379157\H,-2.4612060872,-4.0462851419,-0.3147504473\H,-3.9879599317,-0.4509236454,1.2606071295\H,-3.157316096,-0.4893570493,-0.3988763982\H,-0.2388192094,-1.132578115,-0.9158175995\C,-0.3623402408,-0.6339386646,1.1460986901\C,-0.4847000052,-1.0548869071,2.6037774253\C,-0.7085162869,0.2566768035,3.3628230454\H,-1.3317797878,-1.7410986327,2.7203361134\H,-1.6996337872,0.3297788772,3.8192363399\H,0.044736695,0.4163838827,4.1392991195\C,-0.5794582755,1.3310675003,2.3196632674\C,-0.2020344375,1.4618269694,-0.2044195951\H,0.139951498,2.4404552899,0.1380281869\H,0.5934230604,1.0006446039,-0.7917711259\N,-0.3740421949,0.6602104236,1.0283535557\O,-0.6279355089,2.5189863043,2.395541791\O,0.7276251215,-1.6996496014,2.8897915807\C,0.6863829457,-2.4496616297,4.1006801312\H,1.6689272771,-2.9056010433,4.2139510254\H,0.4836117555,-1.7997887268,4.9593881923\H,-0.0816487886,-3.2297971124,4.0409569153\C,-0.6548961404,-2.9788977861,0.1588312188\H,-0.0945261305,-3.6275852278,-0.5199938476\H,-0.5075261702,-3.3868416298,1.165621315\C,-3.4057254016,-3.0350374322,1.9791816632\H,-2.5572619188,-3.5793738629,2.4129489577\H,-3.8387831741,-2.3866412,2.7461323365\H,-4.1499574525,-3.79539659,1.7122052555\C,-1.4990799425,1.5596950116,-0.9721786669\C,-1.6413793867,0.924584419,-2.2072539241\C,-2.575582848,2.268862121,-0.4296004931\C,-2.8596062362,0.9772068497,-2.8859191252\H,-0.8010127855,0.3926948087,-2.6478963422\C,-3.7923832144,2.3158479595,-1.1041848523\H,-2.4624818851,2.7818706868,0.5226350568\C,-3.9378551942,1.6643368972,-2.3306984008\H,-2.9635789516,0.4813337525,-3.8461696966\H,-4.626341646,2.8625951386,-0.67462363\H,-4.8875944556,1.7001977752,-2.8557647695\Version=AM64L-G09RevB.01\HF=-905.002243\RMSD=0.000e+00\RMSF=5.720e-06\Dipole=1.1079212,-1.456333,0.9155987\Quadrupole=-4.4355087,-6.4526798,10.8881885,0.5693336,-1.679539,-9.2238745\PG=C01 [X(C18H24N1O2)]\@
Sum of electronic and thermal Free Energies= -904.658046 Hartree

TS2

1\1\GINC-SPARTAN-BM086\FTS\RM062X\6-31+G(d)\C18H24N1O2(1+)\UWILLE\14-Sep-2020\0\#p M062X/6-31+G* scf=(qc,direct) nosymm freq=noraman opt=(t s, noeigentest, calcf, maxcycle=500) scrf=(cpcm,solvent=dichloromethane)\geom&freq\1,1\C,-2.3524481826,-3.1292242409,-0.3640161937\C,-0.3755908989,-1.6065874796,0.07956773\C,-3.0334529278,-0.9518909312,0.5685194693\C,-3.1032850579,-2.3241670808,0.6370357798\H,0.693583558,-1.5789202206,0.3302726727\H,-2.4649799346,-2.7133030571,-1.3700449119\H,-2.6779107671,-4.1723323553,-0.3660881231\H,-3.5571930778,-0.3440282434,1.3041674014\H,-2.8399310132,-0.4813527135,-0.3926456672\H,-0.4979723742,-1.1424556021,-0.9041038708\C,-1.0404300093,-0.7656086883,1.1334640427\C,-1.0059898711,-1.2197115129,2.6039748196\C,-1.387308828,0.0446906413,3.3749149093\H,-1.6737571015,-2.0616948322,2.8043136452\H,-2.4572006512,0.0920422474,3.6059097449\H,-0.8332149854,0.1599545298,4.3084351052\C,-1.0475930752,1.1605670072,2.4179908846\C,-0.4790818816,1.415988734,-0.0108117527\H,0.3571228093,0.9429148206,-0.531251549\H,-0.12596506

24,2.3578500563,0.4152939809\N,-0.8383758465,0.5815710121,1.1433516161
\O,-0.960054418,2.3438662016,2.6262185269\O,0.3320582986,-1.5994574566
,2.8237287148\C,0.505851335,-2.3671099422,4.0082578238\H,1.5656402082,
-2.6140805756,4.0640175327\H,0.2185957141,-1.797181528,4.8991829093\H,
-0.0870576272,-3.2886581091,3.9577536726\C,-0.8552378247,-3.049438176,
0.0451924219\H,-0.2687236903,-3.6073754525,-0.6885378837\H,-0.69571154
97,-3.5308127485,1.0173083548\C,-3.7440123796,-3.0445386254,1.77079160
05\H,-4.6257089382,-3.5654807448,1.3722158696\H,-3.0861397811,-3.82748
2713,2.1681680691\H,-4.0706903238,-2.3787627547,2.5719228608\C,-1.6500
17184,1.6447594834,-0.940440543\C,-1.6240908595,1.1605338382,-2.248870
71\C,-2.7862660738,2.3162460301,-0.4757774555\C,-2.7297197182,1.330318
4961,-3.0847080731\H,-0.738364879,0.6489675945,-2.6198100335\C,-3.8910
23671,2.4813269337,-1.3065329733\H,-2.8057441451,2.7026676475,0.541454
3814\C,-3.8657206917,1.983931212,-2.6119644467\H,-2.7014210461,0.94895
61949,-4.1009549169\H,-4.7714612161,2.9999476819,-0.9388304779\H,-4.72
84433597,2.1115464219,-3.2590349579\\Version=AM64L-G09RevB.01\HF=-904.
9927927\RMSD=0.000e+00\RMSF=5.395e-06\Dipole=-0.6734208,-3.4484228,0.3
35281\Quadrupole=4.5346884,-5.6251551,1.0904667,11.1629064,-5.2992747,
-14.0287304\PG=C01 [X(C18H24N1O2)]\\@
Frequencies -278.3350 cm⁻¹
Sum of electronic and thermal Free Energies= -904.645701 Hartree

Anti-cycl

1\1\GINC-SPARTAN-BM092\FOpt\RM062X\6-31+G(d)\C18H24N1O2(1+)\UWILLE\11-
Sep-2020\0\#p M062X/6-31+G* nosymm opt=(calcfc,maxcycle=500) freq=nor
aman scrf=(cpcm,solvent=dichloromethane)\geom&freq\1,1\C,-0.81362932
57,-3.5235749633,1.1678934253\C,-0.1198304397,-1.1581709605,1.82020779
14\C,-2.0768695368,-1.5837096096,0.2529019923\C,-2.098308373,-2.922846
3036,0.817413322\H,0.2798226374,-0.5262752805,2.6176447655\H,-0.108373
9119,-3.4576279919,0.3326643227\H,-0.9061093291,-4.5525768449,1.517027
793\H,-3.062021309,-1.2276760935,-0.0554384911\H,-1.366726084,-1.52644
33968,-0.5796304268\H,0.58066496,-1.1299123037,0.9772522937\C,-1.46633
91971,-0.5907947421,1.3846895919\C,-2.4958646886,-0.4413755831,2.54060
68308\C,-3.4032565272,0.6931107565,2.060626279\H,-3.0460508036,-1.3749
12925,2.7232021127\H,-4.255530438,0.33002732,1.4756728299\H,-3.7924731
536,1.3050209547,2.8765786785\C,-2.4992613872,1.5126045492,1.160955167
7\C,-0.3491619722,1.241763054,-0.0306194033\H,-0.5020446917,2.32282059
45,-0.089268303\H,0.6263694425,1.0665057025,0.4321052225\N,-1.39896295
77,0.7494032053,0.855230011\O,-2.6953273879,2.6467680082,0.759715034\O
,-1.7826246088,-0.0833712191,3.6990195261\C,-2.5396943824,-0.233598280
4,4.8897885462\H,-1.8908906967,0.0637808227,5.7134920417\H,-3.43146269
17,0.4037944566,4.8852433608\H,-2.8444753701,-1.28017387,5.0201007793\
C,-0.2586255015,-2.5904359975,2.3116172556\H,0.7130517732,-3.005089958
3,2.5887501184\H,-0.9036943418,-2.6481620558,3.1949220963\C,-3.3501492
788,-3.5992501464,1.1569894645\H,-3.2658537496,-4.1776434279,2.0831682
627\H,-4.2233267238,-2.9467641276,1.1500412897\C,-0.4125980195,0.62095
61124,-1.4103281848\C,-1.5567396104,0.8044343324,-2.1953472537\C,0.634
3336827,-0.1613592664,-1.8995582034\C,-1.6551084795,0.2041987856,-3.44
73187871\H,-2.3724266646,1.4177568077,-1.8164904159\C,0.5386631149,-0.
7629719743,-3.1572232068\H,1.5299935106,-0.3037047277,-1.2976987893\C,
-0.6068928305,-0.5843520355,-3.929668238\H,-2.5463453162,0.3531426994,
-4.0501211314\H,1.3585997373,-1.3709588481,-3.5281494144\H,-0.68446890
67,-1.0525251328,-4.9064556521\H,-3.478591752,-4.3508626357,0.35450805

59\\Version=AM64L-G09RevB.01\\HF=-904.9999266\\RMSD=4.004e-09\\RMSF=5.810
e-06\\Dipole=-0.6356519,-5.5756589,1.3500841\\Quadrupole=2.1154715,-0.72
59085,-1.389563,25.32574,-12.1222398,-10.9924822\\PG=C01 [X(C18H24N1O2)
]\\@
Sum of electronic and thermal Free Energies= -904.654317 Hartree

Entry 5 (numbers in italics from single point calculation at M062X/6-311++G** level)
E₃ (syn)

1\\1\\GINC-SPARTAN-BM064\\FOpt\\RM062X\\6-31+G(d)\\C14H26N1O2Si1(1+)\\UWILLE\\
26-Aug-2020\\0\\#p M062X/6-31+G* nosymm opt=(calcfc,maxcycle=500) freq=
noraman scrf=(cpcm,solvent=dichloromethane)\\geom&freq\\1,1\\C,-1.81951
55785,-2.3566863861,-0.5760929462\\C,-0.3567321073,-2.2999420268,-0.188
5010022\\C,0.4245166614,-1.2644926413,-0.5198374543\\C,-3.0873058414,-1.
0043366216,1.2572714915\\C,-2.8009251336,-2.3867816875,0.6066301729\\H,1
.4832165872,-1.2482920429,-0.2698157542\\H,-2.0676727597,-1.5231818937,
-1.2453318842\\H,-1.97953331,-3.2768748307,-1.1533243634\\H,-3.732854857
9,-1.1730513454,2.1278245496\\H,-3.6195295803,-0.3637318071,0.549424501
5\\H,-2.4584449033,-3.08067294,1.3768529203\\H,-3.7742464745,-2.74125639
54,0.2562831058\\H,0.0436726799,-0.4155658182,-1.0854780725\\C,-1.875088
8916,-0.3202530622,1.7507954937\\C,-1.1126646392,-0.7318058946,2.992496
7068\\C,0.2363402673,-0.0195672932,2.8259523188\\H,-1.6749502837,-0.2623
371575,3.8207750583\\H,0.6634662455,0.3917103262,3.7415250236\\H,0.95341
62557,-0.7100332319,2.3626187602\\C,-0.0580434453,1.0727538988,1.835941
0116\\C,-1.8785144946,1.5412405321,0.1115953453\\H,-1.1699485118,2.34812
28313,-0.068763488\\H,-1.9629386251,0.915287893,-0.7778773441\\H,-2.8516
786029,1.9498770578,0.3849097564\\N,-1.3550014744,0.7487903408,1.226226
1369\\O,0.5636618711,2.0322968552,1.5011877766\\O,-1.0817660092,-2.10762
06627,3.1236235482\\C,0.1961278635,-3.512249031,0.5142371965\\H,1.249465
6634,-3.3744591076,0.7743508529\\H,-0.3571759962,-3.7273979024,1.433212
351\\H,0.1111111491,-4.3920455166,-0.135680506\\Si,-0.6220463157,-2.9190
993492,4.5544728286\\C,-1.3138144763,-4.63543839,4.3275308388\\H,-0.8818
75031,-5.1221866807,3.4463593008\\H,-1.0822964592,-5.2570530549,5.19946
27501\\H,-2.4019541471,-4.6083791147,4.2074564787\\C,-1.3818443795,-2.01
20266916,6.0044289405\\H,-1.1927660493,-2.57498325,6.9257891346\\H,-0.95
26008625,-1.0129762959,6.1418336209\\H,-2.4670897955,-1.91117986,5.8915
495052\\C,1.2467938522,-2.9280586885,4.653500005\\H,1.6594002887,-1.9253
41756,4.8098720022\\H,1.5737639675,-3.552953265,5.4927393594\\H,1.682959
0941,-3.3415363823,3.7371066921\\Version=AM64L-G09RevB.01\\HF=-1043.367
5811\\RMSD=4.792e-09\\RMSF=3.478e-06\\Dipole=-1.8873051,1.1744096,-0.1272
994\\Quadrupole=-1.8826672,-9.3289259,11.2115931,-0.2187112,-6.8773668,
-11.6803497\\PG=C01 [X(C14H26N1O2Si1)]\\@
Sum of electronic and thermal Free Energies= -1043.035397 Hartree
Sum of electronic and thermal Free Energies= -1043.262145 Hartree

TS1

1\\1\\GINC-SPARTAN-BM115\\FTS\\RM062X\\6-31+G(d)\\C14H26N1O2Si1(1+)\\UWILLE\\0
3-Sep-2020\\0\\#p M062X/6-31+G* nosymm opt=(ts,noeigentest,calcfc,maxcy
cle=500) freq=noraman scrf=(cpcm,solvent=dichloromethane)\\geom&freq\\
1,1\\C,-1.9571553704,-2.9386550825,-0.5123214753\\C,-0.5748828409,-2.574
7030484,-0.0790990362\\C,-0.1861788739,-1.264903038,-0.1536981602\\C,-2.
8356163714,-0.9498198277,0.7878637397\\C,-2.934317261,-2.4591293005,0.5
899938039\\H,0.8016643987,-0.9617432533,0.1850467595\\H,-2.2156802468,-2
.4405434607,-1.4530335585\\H,-2.058124498,-4.0188387583,-0.6470018127\\H

, -3.5886563334, -0.6262974284, 1.5228660179\H, -3.0695392271, -0.434002325
 2, -0.1492656523\H, -2.7325489185, -2.9862591313, 1.5267444869\H, -3.954850
 458, -2.7013454029, 0.2822775319\H, -0.676639617, -0.6092423685, -0.8694557
 223\C, -1.5333767574, -0.4400794929, 1.3356633783\C, -0.984752295, -0.89673
 25173, 2.6907782375\C, 0.1773740351, 0.0698067241, 2.9374152307\H, -1.80679
 4815, -0.6514063566, 3.3872958956\H, 0.3217259156, 0.3544877959, 3.98148877
 9\H, 1.113179252, -0.3569167816, 2.5553872089\C, -0.1940678329, 1.274249620
 7, 2.1095586307\C, -1.7931097102, 1.7950636872, 0.247774375\H, -1.308794833
 6, 2.7595648692, 0.3932639976\H, -1.5930686509, 1.4381276691, -0.7670201057
 \H, -2.8692538542, 1.8942997229, 0.4006215769\N, -1.2299886583, 0.874003622
 7, 1.2250121752\O, 0.2482630387, 2.3926879116, 2.139880292\O, -0.6881704588
 , -2.2465039655, 2.7496404505\Si, -0.2968257227, -3.0299918131, 4.214067996
 5\C, -0.6258526203, -4.8401865694, 3.8987637283\H, -0.6018119762, -5.391079
 0457, 4.8458054826\H, -1.6112439345, -4.9919727411, 3.4448640392\H, 0.13197
 98237, -5.2795165493, 3.2418338345\C, 1.5108929419, -2.7221952793, 4.592078
 9994\H, 2.1377134467, -2.995592271, 3.7357506189\H, 1.7114015467, -1.675415
 1379, 4.8441563068\H, 1.8232625114, -3.3342217071, 5.4462199604\C, -1.39877
 69504, -2.3325698687, 5.5585476624\H, -2.4601785052, -2.4341681719, 5.30574
 18465\H, -1.2239547151, -2.8806150751, 6.4915839309\H, -1.1913450774, -1.27
 52859157, 5.760527147\C, 0.2839922392, -3.653122543, 0.4850957641\H, 1.1602
 816094, -3.2624460749, 1.0055387959\H, -0.292171834, -4.2980581723, 1.15461
 73702\H, 0.6166854594, -4.2770821482, -0.3564455284\\Version=AM64L-G09Rev
 B.01\HF=-1043.3591911\RMSD=3.340e-09\RMSF=3.616e-06\Dipole=-1.5078449,
 -0.4568744, -1.4977671\Quadrupole=-1.9494738, -2.7453944, 4.6948682, 1.179
 7625, -3.9447825, -13.663663\PG=C01 [X(C14H26N1O2Si1)]\\@

Frequencies -241.4701 cm⁻¹

Frequencies -243.536 cm⁻¹

Sum of electronic and thermal Free Energies= -1043.022071 Hartree

Sum of electronic and thermal Free Energies= -1043.250308 Hartree

Syn-spiro

1\1\GINC-SPARTAN-BM110\FOpt\RM062X\6-31+G(d)\C14H26N1O2Si1(1+)\UWILLE\
 26-Aug-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) opt=(calcfc,max
 cycle=500) freq=norman scrf=(cpcm,solvent=dichloromethane)\geom&freq
 \1,1\C, -1.4007880766, -3.085327245, -0.0052036087\C, -0.1328060113, -2.37
 82677084, 0.45938392\C, -0.1634779086, -0.9128015074, 0.0679428451\C, -2.63
 84040858, -0.8687665907, 0.4193680383\C, -2.6891118263, -2.4043710964, 0.48
 38475991\H, 0.7916927337, -0.4268609743, 0.296166687\H, -1.3566981709, -3.0
 812823787, -1.1013481602\H, -1.3814997924, -4.1382866321, 0.299653388\H, -3
 .4546287402, -0.4442511095, 1.014630262\H, -2.762306819, -0.5207062198, -0.
 6127379174\H, -2.8814630976, -2.704214347, 1.5191948558\H, -3.5376767635, -
 2.7738085064, -0.0976204193\H, -0.37077265, -0.8032774503, -0.9998590178\C
 , -1.2942455411, -0.3720488436, 0.9511826782\C, -0.9332955899, -0.971588136
 4, 2.3246043213\C, -0.0805887262, 0.0895003001, 3.0043808531\H, -1.81789584
 01, -1.2465129869, 2.9054048011\H, -0.2417928018, 0.1789302508, 4.078969702
 3\H, 0.9874466185, -0.0800165038, 2.8262169215\C, -0.4913502794, 1.38060183
 3, 2.2969494536\C, -1.65653983, 2.0273705862, 0.2133356936\H, -1.4174848014
 , 3.0197553795, 0.5965576335\H, -1.1328612398, 1.8698617093, -0.7359585565\
 H, -2.7344527896, 1.9539462002, 0.0473819605\N, -1.2272994438, 1.0554583522
 , 1.2004827275\O, -0.1959247225, 2.5094899248, 2.656145886\O, -0.2129852929
 , -2.2186738245, 1.9983245562\C, 1.1529634383, -3.0781984653, 0.093310065\H
 , 1.2999577021, -2.9398662779, -0.9825079075\H, 2.0036140822, -2.6288695281
 , 0.6125509811\H, 1.1195931734, -4.1503687977, 0.2880690245\Si, -0.15408063
 81, -3.5097947464, 3.2909554563\C, 0.2649964914, -2.5443455571, 4.822409815

4\H,1.1813179655,-1.9568568345,4.7111962545\H,-0.5470433193,-1.8902464
602,5.1530397209\H,0.4358712714,-3.2772238631,5.620425495\C,1.17421398
9,-4.7258384477,2.8432051267\H,1.3488254086,-5.3153297091,3.7525083689
\H,0.8783625585,-5.4244034844,2.0563277135\H,2.1196388986,-4.248238094
9,2.5732527831\C,-1.8428583728,-4.2823293741,3.3865691788\H,-2.6265677
556,-3.5693231502,3.6614863128\H,-2.1332236492,-4.8014961404,2.4687036
069\H,-1.7943787754,-5.032935054,4.1860374599\\Version=AM64L-G09RevB.0
1\HF=-1043.4002432\RMSD=0.000e+00\RMSF=8.145e-06\Dipole=-0.1865198,-3.
347496,-0.8430122\Quadrupole=-9.2872441,6.586456,2.7007882,1.0766839,-
1.9190281,-30.6317615\PG=C01 [X(C14H26N1O2Si1)]\\@
Sum of electronic and thermal Free Energies= -1043.055043 Hartree
Sum of electronic and thermal Free Energies= -1043.282467 Hartree

E₃ (*anti*)

1\1\GINC-SPARTAN-BM091\FOpt\RM062X\6-31+G(d)\C14H26N1O2Si1(1+)\UWILLE\
25-Aug-2020\0\#p M062X/6-31+G* nosymm opt=(calcfc,maxcycle=500) freq=
noraman scrf=(cpcm,solvent=dichloromethane)\\geom&freq\\1,1\C,-2.72718
6111,-2.3208978595,-0.1039924304\C,-0.3291979242,-1.4143205294,-0.0124
160033\C,-3.4380668497,-0.1345665105,0.849680632\C,-3.2982819975,-1.45
84014653,0.9951457045\H,0.7196003976,-1.7538914943,-0.0339812144\H,-2.
8400174337,-1.822754136,-1.0738462547\H,-3.2797532407,-3.2667077525,-0
.155537431\H,-3.8113329685,0.4928270354,1.6561939805\H,-3.2165000636,0
.3570810624,-0.0957782591\H,-0.5129518656,-0.8849780037,-0.9519826508\
C,-0.3564050888,-0.4781097331,1.1310321218\C,-0.3218376609,-0.93891581
96,2.5817211002\C,-0.1177194916,0.3575345784,3.3764024708\H,-1.2991061
937,-1.3847569859,2.8131286584\H,-0.8762266734,0.5396720543,4.14094063
19\H,0.8691531247,0.3655777236,3.8506890968\C,-0.1569760681,1.45646295
1,2.3516239199\C,-0.2092710507,1.6068703527,-0.1927854207\H,-0.1842694
271,2.6548626174,0.1007971308\H,0.6867911182,1.3525929968,-0.760349132
8\H,-1.1046039272,1.4048954152,-0.7820173759\N,-0.2446954746,0.8120096
686,1.0355241793\O,-0.123735747,2.6422166368,2.45990118\O,0.7235772587
, -1.8563382257,2.6916511882\C,-1.2398342413,-2.645480047,0.1178627859\
H,-0.9156919317,-3.3654080457,-0.6385947665\H,-1.0799440685,-3.1265799
134,1.0898306699\C,-3.6949785371,-2.1710310644,2.2616791495\H,-2.92578
37854,-2.8813234113,2.5902149778\H,-3.8987797697,-1.4724432829,3.07802
04724\H,-4.5995702917,-2.7644058102,2.081314229\Si,0.7914336702,-3.052
7838692,3.9126009677\C,2.6084188855,-3.4240257243,4.0849997123\H,2.769
9014195,-4.2041425067,4.836843588\H,3.023527999,-3.7793589331,3.135801
3317\H,3.165068372,-2.5327775497,4.3921089569\C,-0.1658129742,-4.55660
44091,3.3418854121\H,-1.2404022159,-4.3635941386,3.2497332183\H,0.2053
170152,-4.9211353599,2.3778901812\H,-0.0438964564,-5.3632269001,4.0746
420035\C,0.0335955869,-2.3343305846,5.4673140972\H,0.5789139482,-1.451
080225,5.8174735998\H,-1.0188065493,-2.0595958939,5.3260464921\H,0.067
0197434,-3.0838895883,6.2665112088\\Version=AM64L-G09RevB.01\HF=-1043.
3690875\RMSD=1.875e-09\RMSF=5.227e-06\Dipole=0.014402,0.3266011,-1.406
4365\Quadrupole=-8.2217732,-2.8364925,11.0582657,2.7002227,-2.1542345,
-13.9461245\PG=C01 [X(C14H26N1O2Si1)]\\@
Sum of electronic and thermal Free Energies= -1043.037146 Hartree
Sum of electronic and thermal Free Energies= -1043.264205 Hartree

TS2

1\1\GINC-SPARTAN-BM124\FTS\RM062X\6-31+G(d)\C14H26N1O2Si1(1+)\UWILLE\
6-Aug-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) freq=noraman opt

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=(ts,noeigentest,calcfc,maxcycle=500) scrf=(cpcm,solvent=dichloromethane)\
\geom&freq\1,1\C,-2.6691344149,-2.7754497079,-0.3683164142\C,-0.5063960206,-1.5306001044,0.0797524608\C,-3.0324797353,-0.5404997434,0.6090714537\C,-3.2939881745,-1.8926319086,0.6523026126\H,0.5551862059,-1.6446543303,0.3368663237\H,-2.7376649098,-2.3353905686,-1.3678010673\H,-3.1290854288,-3.7666634831,-0.3773172814\H,-3.468755339,0.1194950994,1.3555421949\H,-2.7977749369,-0.0855765926,-0.3508766796\H,-0.5569042967,-1.0393929763,-0.8972640368\C,-1.0643911431,-0.6294763504,1.1468200689\C,-1.0318673241,-1.0857141873,2.6219349468\C,-1.2831129907,0.2161006703,3.3848357311\H,-1.7843085951,-1.8518964941,2.8316957618\H,-2.3439878401,0.3716950402,3.6113182163\H,-0.7205378336,0.2718697925,4.3177843153\C,-0.830733252,1.2876477095,2.4214126125\C,-0.3606780022,1.4616655484,-0.0316233731\H,0.5684601122,1.0836814815,-0.4630386635\H,-1.1617585033,1.4096071966,-0.7752274881\H,-0.2267998218,2.4958898848,0.2833938853\N,-0.7177834533,0.6896596297,1.1483999115\O,-0.6007441726,2.4524246252,2.6303385961\O,0.270979192,-1.5623104732,2.8321349569\C,-1.1695640276,-2.8975464724,0.0241867362\H,-0.6676038037,-3.5176506855,-0.7222033684\H,-1.0707833249,-3.4104821702,0.987913599\C,-4.022863101,-2.5356259189,1.7787834131\H,-4.9782256508,-2.9037109826,1.3788093945\H,-3.4896211967,-3.4213886226,2.144594948\H,-4.2368046739,-1.8510307237,2.6015716235\Si,0.6658943695,-2.7025588724,4.0347271038\C,-0.051186601,-4.3680271471,3.5624797261\H,-1.1470382077,-4.3685783298,3.5400325979\H,0.3193505904,-4.700884938,2.5869607337\H,0.2548297996,-5.1140905357,4.305967488\C,2.5292317731,-2.7282151008,4.0285821539\H,2.9354935663,-1.7406482409,4.27036839\H,2.9067321163,-3.4423275716,4.7685009618\H,2.9105641617,-3.0261316488,3.0460511319\C,-0.0490171779,-2.1344835846,5.6707342359\H,0.1512171654,-2.8886913427,6.4405312594\H,0.3981175777,-1.1913182385,6.0032361024\H,-1.1365248367,-2.0025858315,5.6186211051\
Version=AM64L-G09RevB.01\HF=-1043.3600037\RMSD=0.000e+00\RMSF=6.649e-06\
Dipole=-2.2120936,-1.4636707,-2.1745684\Quadrupole=4.7533685,-4.8104279,0.0570594,12.1470616,-7.3600622,-16.7895733\PG=C01 [X(C14H26N1O2Si1)]\
Frequencies -284.2839 cm-1
Frequencies -289.1846 cm-1
Sum of electronic and thermal Free Energies= -1043.025047 Hartree
Sum of electronic and thermal Free Energies= -1043.252276 Hartree

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Anti-cycl

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1\1\GINC-SPARTAN-BM064FOpt\RM062X\6-31+G(d)\C14H26N1O2Si1(1+)\UWILLE\
26-Aug-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) opt=(calcfc,maxcycle=500) freq=noraman scrf=(cpcm,solvent=dichloromethane)\
\geom&freq\1,1\C,-2.5593626902,-2.8636314684,-0.3545604794\C,-0.4704704794,-1.4817511703,0.1417092149\C,-2.8013950872,-0.6366135295,0.7287912828\C,-3.1960515728,-2.0304594266,0.6612995416\H,0.5786531201,-1.5174947648,0.4473612103\H,-2.599318962,-2.3905079631,-1.3407582828\H,-2.9654538257,-3.8749639592,-0.3909229958\H,-3.3762969092,-0.0589295696,1.4543853036\H,-2.8305650011,-0.1681660482,-0.2606414955\H,-0.5213442634,-1.0246567947,-0.8532590712\C,-1.2231965667,-0.6141440033,1.1432961556\C,-1.0522577199,-1.0525825552,2.6310114411\C,-1.2712321548,0.2532011282,3.3978468532\H,-1.7854344664,-1.8231412396,2.9060554828\H,-2.3253782568,0.4174886628,3.6497027176\H,-0.6882092522,0.3013096539,4.3187259375\C,-0.8317285903,1.3223524732,2.4177532912\C,-0.5087005744,1.5278878021,-0.0264452713\H,0.401318232,1.1695843072,-0.5149357633\H,-1.3433263067,1.47

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31682736,-0.7342568569\H,-0.3705578038,2.5657523896,0.2777067096\N,-0.7932096183,0.7568515198,1.1678618417\O,-0.5665490009,2.4857912327,2.6675112402\O,0.2580602081,-1.5235664381,2.8008469056\C,-1.0443854489,-2.8878570298,0.0877384473\H,-0.5268061201,-3.4965049245,-0.6569883757\H,-0.9432048742,-3.3943921246,1.0533326326\C,-4.0754305762,-2.63279667,1.6653050527\H,-5.0460263841,-2.7398021668,1.14411609\H,-3.7702680133,-3.653377114,1.9202706231\H,-4.2356648454,-2.0116477251,2.5471007929\Si,0.6931308215,-2.6405768961,4.0022855157\C,-0.2034223792,-4.2574554505,3.6801389883\H,-1.2919646055,-4.1316354767,3.6389627573\H,0.1282352774,-4.7217742911,2.7449443032\H,0.0089966915,-4.9612125256,4.4936576289\C,0.2117324038,-1.9751790752,5.6869282053\H,0.5031605366,-2.6930548019,6.4625937064\H,0.7141793483,-1.0262631046,5.9043335472\H,-0.8703681251,-1.8202212612,5.7731168628\C,2.538497073,-2.8188738596,3.81179044\H,3.0442653563,-1.8652320833,3.9958751486\H,2.9299362371,-3.5536470722,4.5237247709\H,2.7960547285,-3.1547639696,2.8016599792\Version=AM64L-G09RevB.01\HF=-1043.3658823\RMSD=0.000e+00\RMSF=3.249e-06\Dipole=-3.8277486,-3.1051088,-2.8579759\Quadrupole=13.7122151,-5.4108053,-8.3014098,20.4137678,-8.4636514,-19.3868506\PG=C01 [X(C14H26N1O2Si1)]\@
Sum of electronic and thermal Free Energies= -1043.030679 Hartree
Sum of electronic and thermal Free Energies= -1043.256922 Hartree

Anti-spiro

1\1\GINC-SPARTAN-BM089\FOpt\RM062X\6-31+G(d)\C14H26N1O2Si1(1+)\UWILLE\02-Sep-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) opt=(calcfc,max cycle=500) freq=norman scrf=(cpcm,solvent=dichloromethane)\geom&freq\1,1\C,-1.6734307022,-3.1929109257,0.1939878492\C,-0.3443739294,-1.0199671966,0.0572263148\C,-2.7706709521,-0.9631303525,0.6270026352\C,-2.5640287477,-2.4061633096,1.1440986325\H,0.6426492449,-0.6023658984,0.2831645782\H,-2.1712560529,-3.1842639702,-0.7827287597\H,-1.6045711574,-4.2391474004,0.5062292002\H,-3.5876559493,-0.4584884537,1.1517623038\H,-2.9937687049,-0.995983206,-0.4424874697\H,-0.5916960435,-0.6947754587,-0.9614177787\C,-1.4141080539,-0.3736510043,0.9726169372\C,-1.3630115944,-0.7497401462,2.4485393769\C,-0.0944028812,-0.0829814397,2.930134957\H,-2.2143593392,-0.2870139619,2.9578514439\H,-0.0398797688,0.1322523074,3.9960810509\H,0.8212573434,-0.5890287092,2.6067643756\C,-0.2468289692,1.2387260626,2.127938712\C,-1.3271283819,2.011067577,0.0436913573\H,-1.2692376042,3.0149458036,0.4657753607\H,-0.5467433616,1.8988976283,-0.7177027013\H,-2.3075838261,1.8682713684,-0.4147806649\N,-1.1627815138,1.0507851471,1.1209155966\O,0.3492769652,2.2735409007,2.3611921712\O,-1.6538240818,-2.1791255682,2.4138549594\C,-0.2828371746,-2.5536700606,0.1130000155\H,0.2500689846,-2.9309716398,-0.7638931665\H,0.3018777977,-2.8588005049,0.9880627895\C,-3.8458010085,-3.0832464692,1.5552338166\H,-4.4727206094,-3.1531400636,0.6598617465\H,-3.6878259587,-4.0993430786,1.924466657\H,-4.3862906517,-2.494291727,2.3011383179\Si,-1.4977336817,-3.2986480246,3.8364089093\C,-3.0775106575,-3.1529695809,4.8067928799\H,-3.8817374147,-3.7732610127,4.4029599768\H,-2.8797988524,-3.482932887,5.8333817486\H,-3.4240000902,-2.1149986446,4.8556664552\C,-0.0283163642,-2.6567231489,4.7719654691\H,-0.2380790697,-1.7239884034,5.3016558143\H,0.2121538417,-3.4139420833,5.5287370176\H,0.8566251759,-2.5292380237,4.1415837791\C,-1.1601787465,-4.9746824088,3.1056056526\H,-0.9308549278,-5.6411244446,3.9466186914\H,-2.0025980768,-5.4146024969,2.5658258819\H,-0.2822510735,-4.961234311,2.4517338495\Version=AM64L-G09RevB.01\HF=-1043.3747315\RMSD=0.000e+00\RMSF=7.168e-06\Dipole=-1.7298824,-2.918022,-0.2735604\Quadrupole=-4.8488918,-0.8376832,5.686575,13.6678799,-14.8595285,-31.4801587\PG=C01 [X(C14H26N1O2Si1)]\@

Sum of electronic and thermal Free Energies= -1043.029818 Hartree
Sum of electronic and thermal Free Energies= -1043.257223 Hartree

Entry 6

E₃ (syn)

1\1\GINC-SPARTAN-BM102\FOpt\RM062X\6-31+G(d)\C17H32N1O2Si1(1+)\UWILLE\03-Sep-2020\0\#p M062X/6-31+G* nosymm opt=(calcf, maxcycle=500) freq=noraman scrf=(cpcm, solvent=dichloromethane)\geom&freq\1,1\C,-1.8951242479,-2.3117487196,-0.5816423405\C,-0.4141829259,-2.2064944196,-0.2772953173\C,0.3375262175,-1.1997958487,-0.7398574366\C,-3.1258958607,-0.9786167618,1.3069612523\C,-2.8215418414,-2.3554261669,0.644917319\H,1.4088186837,-1.1601474883,-0.5545691738\H,-2.2034111173,-1.5053910824,-1.2587691202\H,-2.052576005,-3.2495186403,-1.1311552909\H,-3.7312831568,-1.1662022588,2.2009662716\H,-3.6982926843,-0.3518617193,0.6181636684\H,-2.4278936899,-3.0355824312,1.4035345674\H,-3.7985428408,-2.7400540795,0.3393537641\H,-0.0813144278,-0.3988062497,-1.3464799261\C,-1.8987447374,-0.2825439477,1.7365182215\C,-1.1046618517,-0.6450841217,2.9746983954\C,0.2697317242,-0.0187647371,2.6974585803\H,-1.6059437137,-0.0778864873,3.7801125207\H,0.7654316669,0.4284974781,3.5601891084\H,0.930230287,-0.7700840559,2.2446885752\C,-0.0239692437,1.0271123554,1.6566650877\C,-1.9138183515,1.4933904149,0.0061494666\H,-1.1862569722,2.2622457551,-0.2497371337\H,-2.0691907869,0.8298559477,-0.8451052511\H,-2.8555624062,1.9525344191,0.3080416077\N,-1.3650668772,0.7363366318,1.1330261703\O,0.6273439701,1.929564957,1.2329230637\O,-1.1533230619,-2.0054013393,3.2126453124\C,0.1908265608,-3.344908413,0.5031306799\H,1.2728392356,-3.2237517696,0.60683774\H,-0.2432440479,-3.412803067,1.5054670628\H,-0.0058002377,-4.2983863842,-0.0025065125\Si,-0.5836977015,-2.8303041025,4.5972586439\C,-1.1216693601,-4.5869478535,4.2630793303\H,-0.7607248304,-4.9233715475,3.2852267993\H,-0.7144040173,-5.2668561579,5.0191421381\H,-2.2130691204,-4.6808595926,4.273771052\C,-1.3965551973,-2.1234466019,6.1574515412\C,1.283494832,-2.6801872803,4.6509957573\H,1.6245089081,-1.6486358238,4.7882981411\H,1.6828460918,-3.2717219299,5.4835033513\H,1.7245534377,-3.0683696998,3.725566891\C,-0.7237890627,-0.8192142005,6.6129362788\H,-0.7956330939,-0.0187924613,5.8659721493\H,-1.2081776844,-0.4492336805,7.5272192021\H,0.3380402081,-0.969697407,6.8386274516\C,-1.2383941932,-3.1673106849,7.2785805361\H,-1.6569925517,-2.7722864788,8.2143657191\H,-1.7668102836,-4.0988999617,7.0466387283\H,-0.1855901356,-3.4118829986,7.4686888898\C,-2.8937167391,-1.881133678,5.9128677155\H,-3.07332618,-1.1070973933,5.1569045221\H,-3.4069007904,-2.7924805168,5.5829469328\H,-3.3756779263,-1.5477882992,6.8423952564\Version=AM64L-G09RevB.01\HF=-1161.244391\RMSD=4.724e-09\RMSF=5.760e-06\Dipole=-1.6429411,1.3016532,-1.2664621\Quadrupole=-2.055144,-9.6533511,11.7084951,-0.6280458,-6.1642008,-11.0648553\PG=C01 [X(C17H32N1O2Si1)]\@

Sum of electronic and thermal Free Energies= -1160.829282 Hartree

TS1

1\1\GINC-SPARTAN-BM110\FTS\RM062X\6-31+G(d)\C17H32N1O2Si1(1+)\UWILLE\04-Sep-2020\0\#p M062X/6-31+G* nosymm opt=(ts, noeigentest, calcf, maxcycle=500) freq=noraman scrf=(cpcm, solvent=dichloromethane)\geom&freq\1,1\C,-2.2723913265,-2.9446276485,-0.2864503268\C,-0.8240467887,-2.6661199338,-0.057146948\C,-0.356111091,-1.3991966655,-0.2726556017\C,-2.8300210339,-0.840669902,1.0052087543\C,-3.0435974117,-2.349177586,0.917

5926553\H,0.6864100564,-1.1560305736,-0.0813834616\H,-2.6253084535,-2.466054553,-1.2062498403\H,-2.4648307268,-4.0188306069,-0.3501253273\H,-3.4425908924,-0.4282653336,1.8222353646\H,-3.179910521,-0.3642685253,0.0836024218\H,-2.7300806945,-2.8427975859,1.8424812828\H,-4.1114655521,-2.5397748545,0.7820948357\H,-0.8884129989,-0.752628106,-0.9660203286\C,-1.4329136378,-0.3839007399,1.3152371176\C,-0.7271901014,-0.7603186151,2.62188135\C,0.524975004,0.122140923,2.6054324513\H,-1.4233516524,-0.3668492791,3.3833031782\H,0.8396642324,0.4917083835,3.582235265\H,1.362603372,-0.4159366899,2.1449774866\C,0.1184442981,1.2752552544,1.7216616543\C,-1.7062034038,1.7714444233,0.0751144898\H,-1.1388457251,2.7008952175,0.0590056333\H,-1.685988566,1.3178889317,-0.9204864695\H,-2.7373905805,1.972129289,0.3707597292\N,-1.0683538839,0.8912530533,1.0442570261\O,0.6415347808,2.3488596794,1.5741108155\O,-0.5290730159,-2.120581646,2.789607936\Si,-0.1522625815,-2.841497987,4.2930393117\C,-0.0552535284,-4.6683254001,3.9138013528\H,0.2039575214,-5.2191399203,4.8246995532\H,-1.0068640748,-5.0639049682,3.540834393\H,0.7226785892,-4.8735113292,3.1714104588\C,1.5117395622,-2.2095488505,4.884309714\H,2.2754032714,-2.3606548914,4.1129558218\H,1.5015609059,-1.1495800831,5.1571371805\H,1.8215979821,-2.7724131578,5.7732873883\C,-1.5260713098,-2.4704189357,5.5551600099\C,0.0197388211,-3.767451601,0.4816147865\H,0.9689430771,-3.4084910526,0.8832604423\H,-0.5199949389,-4.3315803202,1.2469713288\H,0.2203953824,-4.4599476031,-0.3481738532\C,-1.4787108609,-3.5657721866,6.6365077242\H,-2.215447953,-3.3439409264,7.4209279129\H,-1.7181575443,-4.5535692377,6.2269640545\H,-0.4951540783,-3.6286532313,7.1194851059\C,-1.3246288512,-1.1108390433,6.2436893432\H,-0.3778809575,-1.0761302697,6.794570251\H,-1.3300864895,-0.2680938894,5.541639942\H,-2.134539163,-0.9354948233,6.9652844914\C,-2.9035177501,-2.5139573907,4.8770188338\H,-3.0297042064,-1.7139204492,4.1373193607\H,-3.0781126432,-3.4700455331,4.3678797098\H,-3.6960614277,-2.3897426797,5.6277590289\Version=AM64L-G09RevB.01\HF=-1161.2363753\RMSD=4.020e-09\RMSF=7.147e-06\Dipole=-1.3547267,-0.2189324,-2.2639762\Quadrupole=-2.6205619,-3.4669884,6.0875503,0.7541448,-3.5927742,-12.2634432\PG=C01 [X(C17H32N1O2Si1)]\@\

Frequencies -245.5884 cm⁻¹

Sum of electronic and thermal Free Energies= -1160.816363 Hartree

Syn-spiro

1\1\GINC-SPARTAN-BM106\FOpt\RM062X\6-31+G(d)\C17H32N1O2Si1(1+)\UWILLE\04-Sep-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) opt=(calcfc,max cycle=500) freq=noraman scrf=(cpcm,solvent=dichloromethane)\geom&freq \\1,1\C,-2.0076046023,-2.9477530886,-0.0801639213\C,-0.6079009534,-2.5303387458,0.3481102082\C,-0.3441606398,-1.079101665,-0.0087745897\C,-2.7378452689,-0.5356592133,0.4540826126\C,-3.100279046,-2.0298806373,0.4893810444\H,0.7007507706,-0.8133753113,0.1860699665\H,-2.010044494,-2.9206286587,-1.1768995836\H,-2.1947756103,-3.9903285341,0.2050736475\H,-3.4233943588,0.0284961995,1.0965179155\H,-2.8340375231,-0.1408992353,-0.5642195727\H,-3.2933823146,-2.3159971577,1.5294673909\H,-4.0377481098,-2.2007113607,-0.0460596699\H,-0.5624358678,-0.9010412314,-1.0651325626\C,-1.2987971998,-0.3365931902,0.9294517983\C,-1.0090332192,-1.0282271522,2.2733741201\C,0.0929225396,-0.1947253935,2.9112229554\H,-1.8965655634,-1.0927335705,2.9022587883\H,0.0237068302,-0.1115831788,3.9964296047\H,1.0904661087,-0.5653227683,2.6517080239\C,-0.0890426898,1.1761938781,2.2590953527\C,-1.1977604367,2.107359518,0.2532782125\H,-0.7566268911,3.022287214,0.6493811491\H,-0.7497968351,1.8827649658,-0.720

9520426\H,-2.2747609496,2.2489253263,0.1316403307\N,-0.9290638689,1.04
02453337,1.1981875424\O,0.4455532779,2.2107146573,2.62569755\O,-0.6318
070404,-2.4062914241,1.9007416877\Si,-0.5614660588,-3.6843141297,3.215
9118555\C,0.0297508368,-5.2605942037,2.422893495\H,0.0436248517,-6.008
0914087,3.2261778539\H,-0.6267577698,-5.6448550979,1.6379456031\H,1.04
9638758,-5.1787609954,2.0399426306\C,0.7148222726,-2.9984756397,4.3884
464064\H,1.5878440638,-2.6182097072,3.8494524632\H,0.3311572184,-2.213
0166898,5.0463000998\H,1.0541812707,-3.8241632633,5.0251864205\C,-2.24
25671127,-3.9631492934,4.0524259186\C,0.5037439309,-3.4520510262,-0.09
28858999\H,1.4254413016,-3.2464902519,0.4592134231\H,0.2426244766,-4.5
061639414,-0.0118317702\H,0.6928882749,-3.237092641,-1.1494601335\C,-1
.8650759189,-4.7498510544,5.3327483463\H,-1.3040488117,-4.1327370968,6
.0427901363\H,-2.7894022566,-5.0695644879,5.829999539\H,-1.281673056,-
5.6550427565,5.1270233687\C,-3.1623915657,-4.8474142139,3.1962402462\H
,-3.4471801284,-4.3694464474,2.2525451406\H,-2.7006445425,-5.812452203
5,2.9617736715\H,-4.0882022628,-5.0514989181,3.7497104058\C,-3.0030747
498,-2.7054634235,4.4999295611\H,-2.3664959163,-1.9983213481,5.0456146
75\H,-3.4767276688,-2.1796444484,3.6642842643\H,-3.8118790516,-3.00279
79982,5.1800064501\\Version=AM64L-G09RevB.01\HF=-1161.2722903\RMSD=0.0
00e+00\RMSE=5.171e-06\Dipole=-0.4833976,-2.5604326,-1.4922267\Quadrupo
le=-10.5501827,9.6862869,0.8638959,4.199231,-8.1087858,-31.13843\PG=C0
1 [X(C17H32N1O2Si1)]\\@
Sum of electronic and thermal Free Energies= -1160.843192 Hartree

E₃ (*anti*)

1\1\GINC-SPARTAN-BM098\FOpt\RM062X\6-31+G(d)\C17H32N1O2Si1(1+)\UWILLE\
04-Sep-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) freq=noraman op
t=(calcfc,maxcycle=500) scrf=(cpcm,solvent=dichloromethane)\geom&freq
\1,1\C,-2.3655453887,-2.490406489,-0.3675730569\C,-0.1325493722,-1.30
78204228,0.0518490511\C,-3.4471664332,-0.4369705983,0.5295280378\C,-3.
1689699639,-1.7394783086,0.6656703265\H,0.9461546578,-1.5166800567,0.1
477027722\H,-2.4108222964,-1.9736311786,-1.3332577572\H,-2.790146032,-
3.4912245357,-0.510306099\H,-3.9856788651,0.1155874212,1.2963064605\H,
-3.1719924999,0.1076675641,-0.3715855323\H,-0.2716426135,-0.7705405929
,-0.8906328719\C,-0.4028043045,-0.4267625512,1.2075755861\C,-0.4558597
872,-0.9411426907,2.6378743649\C,-0.419513497,0.3359985419,3.488670888
7\H,-1.4180642737,-1.4595853833,2.7642048503\H,-1.1956759914,0.3980899
712,4.2534338772\H,0.560022986,0.4419537897,3.9680760355\C,-0.57216388
89,1.4603849279,2.502092462\C,-0.4283303252,1.7160046902,-0.0309291964
\H,-0.6002357321,2.7406916082,0.2944324304\H,0.5497802281,1.630125996,
-0.5062430535\H,-1.2158795356,1.4049678925,-0.7183330701\N,-0.46022192
06,0.8698890658,1.1629015307\O,-0.7384170527,2.6302003353,2.6525979254
\O,0.6254881872,-1.8020993923,2.8018431789\C,-0.8920320338,-2.64478788
04,0.0446771161\H,-0.386103842,-3.2983149149,-0.6716154345\H,-0.801076
4217,-3.1304845963,1.0239195141\Si,0.7866946416,-2.9156357948,4.085927
9135\C,2.2067456748,-4.0206681677,3.5205894366\C,-0.8272284775,-3.8497
31216,4.281799387\H,-1.6658566535,-3.1787959674,4.5036561954\H,-1.0815
581089,-4.4435860301,3.3967052553\H,-0.7407457491,-4.5403325596,5.1291
528648\C,1.1698444544,-1.9618167215,5.6527359566\H,2.0112315351,-1.274
7113212,5.5117794082\H,0.3011569063,-1.3807408503,5.9839406331\H,1.430
3408321,-2.6507472754,6.4647870485\C,3.5230397328,-3.2293408115,3.5478
363811\H,4.3459402811,-3.8589843536,3.1816607198\H,3.4760332532,-2.338
3787916,2.9101798183\H,3.7807019268,-2.9074089788,4.5636948725\C,2.317

9598065,-5.2271312395,4.4663775393\H,3.1686923954,-5.8553763268,4.1686
856175\H,2.4855933403,-4.9213516575,5.5066143577\H,1.4187583645,-5.853
8412369,4.4374364086\C,1.940698413,-4.5169421908,2.0915356979\H,1.0047
868856,-5.085397636,2.0205451071\H,1.8867595651,-3.6840506653,1.380800
1758\H,2.7544604162,-5.1815081885,1.7694841612\C,-3.6246065672,-2.5397
537314,1.8573453356\H,-2.8213498348,-3.1726721254,2.2539916727\H,-3.99
98683079,-1.9015540515,2.662478496\H,-4.4289614637,-3.2215636831,1.555
1994032\\Version=AM64L-G09RevB.01\HF=-1161.2490908\RMSD=0.000e+00\RMSF
=2.333e-06\Dipole=-0.6475203,1.2617521,-1.6476736\Quadrupole=-8.412269
2,-2.8096905,11.2219597,2.8747215,-1.8350374,-13.9571014\PG=C01 [X(C17
H32N1O2Si1)]\\@
Sum of electronic and thermal Free Energies= -1160.833663 Hartree

TS2

1\1\GINC-SPARTAN-BM114\FTS\RM062X\6-31+G(d)\C17H32N1O2Si1(1+)\UWILLE\0
6-Sep-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) opt=(ts,noeigent
est,calcfc,maxcycle=500) freq=noraman scrf=(cpcm,solvent=dichlorometha
ne)\geom&freq\1,1\C,-1.9457459462,-2.8657186439,-0.5323371527\C,-0.2
104955492,-1.1981387842,0.2573017524\C,-2.9431464862,-0.8276115874,0.4
403485459\C,-2.8898289033,-2.2038484264,0.4072062607\H,0.8042516458,-1
.0795921661,0.6611718186\H,-1.9738807842,-2.395438574,-1.5199723014\H,
-2.162300684,-3.9318573021,-0.6338397917\H,-3.6159931568,-0.3312719756
,1.1364926689\H,-2.6905818045,-0.2724751858,-0.4602989476\H,-0.2443209
78,-0.6738041407,-0.7031721328\C,-1.0989784569,-0.5140974919,1.2601921
169\C,-1.1666662205,-1.0603241561,2.7029652817\C,-1.7487185397,0.11541
59554,3.4906194695\H,-1.7885054857,-1.9560681806,2.7706866251\H,-2.835
0910604,0.0385821198,3.612536818\H,-1.2982588355,0.2232166637,4.478795
9253\C,-1.441545869,1.3194299105,2.6325702655\C,-0.747928114,1.7539199
743,0.2672219346\H,0.2804629712,1.6060008009,-0.0685114653\H,-1.436873
1987,1.590543904,-0.5671572033\H,-0.8704459086,2.7689911643,0.64306631
39\N,-1.058233273,0.8448102149,1.3597711363\O,-1.4972472568,2.49003549
21,2.9143823928\O,0.1594414766,-1.3390969699,3.0587285142\C,-0.5259323
784,-2.6739742366,0.0728621868\H,0.2025678165,-3.1235542219,-0.6062975
16\H,-0.4430936817,-3.2042887957,1.0297136558\Si,0.6159569033,-2.43790
33183,4.2778528738\C,-0.5501543414,-3.909258538,4.2256978827\H,-0.2206
823669,-4.6563285526,4.9576819772\H,-1.5752073762,-3.6296001276,4.4957
851722\H,-0.5708740152,-4.3989574107,3.2453431268\C,2.3878031877,-2.89
90197122,3.8164660633\C,0.505399062,-1.591201857,5.945855291\H,-0.5368
802417,-1.4008965602,6.2260755568\H,0.9411579921,-2.2261384076,6.72602
29426\H,1.0411504543,-0.635804448,5.9488933226\C,-3.5984118197,-3.0568
731468,1.3994843229\H,-4.3814138477,-3.6051752886,0.8566546443\H,-2.93
21217793,-3.8208912963,1.8189814489\H,-4.0721506301,-2.4837274302,2.19
876171\C,2.9518227923,-3.8877178221,4.8487765654\H,2.3711742616,-4.817
3351899,4.8870552862\H,3.9837301031,-4.1553088672,4.582644904\H,2.9740
918114,-3.4588023705,5.8576757158\C,3.2595859483,-1.6340516662,3.79259
32855\H,2.8841053191,-0.8986307721,3.0714570841\H,3.3057732215,-1.1528
852885,4.7769797873\H,4.2876129427,-1.8933742493,3.5032943126\C,2.4056
083224,-3.5517479893,2.4266740508\H,1.8035680964,-4.4683227182,2.39541
33401\H,2.0272119352,-2.8683604541,1.6571388373\H,3.434510726,-3.82322
78796,2.1520693235\\Version=AM64L-G09RevB.01\HF=-1161.2391163\RMSD=0.0
00e+00\RMSF=5.284e-06\Dipole=-2.5502078,-1.180142,-2.848249\Quadrupole
=2.2252931,-2.315518,0.0902249,13.3809024,-4.6735163,-17.3294791\PG=C0
1 [X(C17H32N1O2Si1)]\\@
Frequencies -287.7195 cm⁻¹

Sum of electronic and thermal Free Energies= -1160.821163 Hartree

Anti-cycl

1\1\GINC-SPARTAN-BM097\FOpt\RM062X\6-31+G(d)\C17H32N1O2Si1(1+)\UWILLE\
04-Sep-2020\0\#p M062X/6-31+G* nosymm opt=(calcf, maxcycle=500) freq=
noraman scrf=(cpcm, solvent=dichloromethane)\geom&freq\1,1\C,-2.39311
78171,-2.0361970345,-0.3519248741\C,-0.3186131991,-0.7652688563,0.4237
324173\C,-2.6664714897,-0.0001026423,1.0528082166\C,-3.0615427996,-1.3
640864064,0.7586869801\H,0.7175642834,-0.8584718775,0.759691815\H,-2.3
979485997,-1.417649354,-1.2548233036\H,-2.801650715,-3.0266762103,-0.5
556969707\H,-3.2635329825,0.4662736863,1.8382229671\H,-2.6569846191,0.
6143535718,0.1467113109\H,-0.3273585852,-0.1586133778,-0.4888244839\C,
-1.1044178856,-0.0560672993,1.5204409602\C,-0.9851643475,-0.7231632522
,2.926246871\C,-1.2043092567,0.4493832791,3.8841096594\H,-1.7401829943
, -1.5095589856,3.0569000869\H,-2.2613773929,0.5845095967,4.1411042388\
H,-0.6379186248,0.3445987848,4.8108720698\C,-0.7352867877,1.6540275122
,3.0928826534\C,-0.3505607077,2.2356763995,0.7193876862\H,0.5699104797
,1.9493371941,0.2037036971\H,-1.1662678277,2.2990752997,-0.009525274\H
, -0.2154074994,3.2120896846,1.1849688682\N,-0.6711148219,1.2905375372,
1.7710897225\O,-0.4679037486,2.7614155091,3.5267579481\O,0.3102204405,
-1.2444939317,3.0531957426\C,-0.8940449704,-2.1412985109,0.1321610858\
H,-0.3529812188,-2.6317781068,-0.679990687\H,-0.828005078,-2.792955931
1,1.0102434498\C,-3.9719837575,-2.1089484272,1.6307544832\H,-4.9276762
343,-2.124361724,1.0726489441\H,-3.6776009132,-3.1591268498,1.72953467
08\H,-4.1539998252,-1.6335299776,2.5950734491\Si,0.7086794555,-2.55053
28607,4.059337867\C,-0.1961590464,-4.088332667,3.4698680352\H,-1.27672
36664,-3.9232022695,3.379776053\H,0.1780110924,-4.4463082957,2.5046098
072\H,-0.0562058347,-4.8939703873,4.2004096929\C,0.1851587036,-2.16999
90875,5.8203094915\H,0.4788721146,-2.9922896684,6.4834808799\H,0.64592
04292,-1.2519131851,6.2000865559\H,-0.9039374153,-2.0644523218,5.89523
608\C,2.5774936672,-2.7146720555,3.8618883297\C,3.2813091221,-1.532141
42,4.5440633547\H,4.3663850856,-1.5960004855,4.3814289592\H,2.93960056
67,-0.5706859022,4.1419632414\H,3.1093332567,-1.5278091064,5.626857317
\C,2.9376568159,-2.7255008112,2.3684256637\H,2.4345670974,-3.538028820
3,1.8287932106\H,2.6689747065,-1.7793009505,1.8857654541\H,4.020432443
8,-2.8696285719,2.2461439745\C,3.0429390614,-4.0294930478,4.5064920519
\H,4.1347829685,-4.1213847316,4.4222587209\H,2.7910759091,-4.076427253
7,5.5733551037\H,2.5987762923,-4.9030418301,4.0141773654\Version=AM64
L-G09RevB.01\HF=-1161.244863\RMSE=2.625e-09\RMSF=4.371e-06\Dipole=-4.7
942221,-2.043312,-3.7732712\Quadrupole=16.7281012,-8.503479,-8.2246222
,13.2091724,-9.6883216,-21.1117695\PG=C01 [X(C17H32N1O2Si1)]\@
Sum of electronic and thermal Free Energies= -1160.827051 Hartree

Entry 7

E₃ (syn)

1\1\GINC-SPARTAN-RC009\FOpt\RM062X\6-31+G(d)\C12H19Cl1N1O2(1+)\UWILLE\
17-Jun-2020\0\#p M062X/6-31+G* scrf=(cpcm, solvent=dichloromethane) no
symm freq=noraman opt=(calcf, maxcycle=500)\geom&freq\1,1\C,-2.43477
41888,-2.4500199662,-0.3342639421\C,-0.1565260651,-1.3180548967,0.0079
502399\C,-3.4830276136,-0.4539278793,0.7501497905\C,-3.1878240006,-1.7
584167284,0.774064599\H,0.9203792157,-1.5558638585,0.0146349152\H,-2.5
296047209,-1.875919769,-1.2626395348\H,-2.8768372972,-3.4361711895,-0.

5178513527\H,-4.0011538045,0.0327003718,1.5730139832\H,-3.2357248849,0.1617552368,-0.1120266354\H,-0.348263147,-0.7304952095,-0.8943202199\C,-0.3189417134,-0.4886477819,1.220663934\C,-0.2945276457,-1.0645266403,2.6243885163\C,-0.178441169,0.1628930248,3.5371329372\H,-1.2513916423,-1.5827868355,2.7927527112\H,-0.9154895786,0.2084357708,4.3404351407\H,0.8250759603,0.2209440235,3.9738233105\C,-0.3532740023,1.3377054878,2.6154406166\C,-0.4005772235,1.7147252027,0.0927682054\H,-0.5622703258,2.7188883304,0.4810804078\H,0.5526691436,1.6644364902,-0.4351525345\H,-1.220110155,1.4321167004,-0.5682185877\N,-0.3629937919,0.8077895772,1.2416629758\O,-0.4633245145,2.5031185164,2.8282547801\O,0.7744804502,-1.9604915864,2.674619418\C,0.754189896,-2.7843183178,3.8376573578\H,1.6240986889,-3.4357934591,3.7688550528\H,0.821541434,-2.1782465241,4.7482693463\H,-0.1615265091,-3.3870960919,3.862940039\C,-0.9432816494,-2.6396142262,-0.0127679947\H,-0.4948514161,-3.2629144338,-0.7908824875\H,-0.7985939004,-3.1765706848,0.9319354501\C,-3.5960337991,-2.6057209445,1.9463200439\H,-2.8074531895,-3.2909482007,2.2664108832\H,-3.92917002,-2.0045075691,2.792359965\Cl,-4.9896837606,-3.6730591497,1.4935521196\\Version=AM64L-G09RevB.01\HF=-1133.6047374\RMSD=2.997e-09\RMSF=6.304e-06\Dipole=2.5868613,1.2101156,-0.2243541\Quadrupole=-13.6049336,-4.1245602,17.7294938,-6.5962321,-0.744369,-10.1030611\PG=C01 [X(C12H19Cl1N1O2)]\\@
Sum of electronic and thermal Free Energies= -1133.349935 Hartree

TS1

1\1\GINC-SPARTAN-RC101\FTS\RM062X\6-31+G(d)\C12H19Cl1N1O2(1+)\UWILLE\18-Jun-2020\0\#p M062X/6-31+G* scrf=(cpcm,solvent=dichloromethane) nosymm freq=noraman opt=(ts,noeigentest,calcfc,maxcycle=500)\geom&freq\\1,1\C,-2.2676563596,-2.966898976,-0.2985081313\C,-0.8438961005,-2.708165238,0.0354373509\C,-0.3434345136,-1.4272247226,-0.0704923669\C,-2.8172672539,-0.8127687516,0.9299371674\C,-3.1264353802,-2.2992037966,0.8137699189\H,0.6979934354,-1.237348818,0.1805581826\H,-2.5256809285,-2.5116718405,-1.2604460237\H,-2.4828352522,-4.0367950782,-0.34309283\H,-3.4603005702,-0.3628350724,1.6998567672\H,-3.0475784285,-0.3049190902,-0.0125648905\H,-2.9621023003,-2.8073923409,1.7677314574\H,-4.1782848163,-2.423237406,0.5452825349\H,-0.7751885113,-0.7795866181,-0.8311672925\C,-1.4052636,-0.4864633966,1.3527858435\C,-0.8691010223,-0.9778610398,2.7021770224\C,0.3720372445,-0.1154297182,2.938006969\H,-1.6526096258,-0.7105526546,3.4321462345\H,0.5452482714,0.1654106325,3.9777267488\H,1.2687956912,-0.6191412139,2.5558667272\C,0.1009765677,1.1108593432,2.0999991251\C,-1.4631986086,1.7675083456,0.2598121004\H,-0.8735698286,2.6764144412,0.3724827709\H,-1.334471044,1.3779857215,-0.7550090449\H,-2.517311526,1.986771358,0.4396857081\N,-0.9731008401,0.807391394,1.2369311321\O,0.6537407674,2.1815279874,2.121072986\O,-0.6684351022,-2.3548977178,2.7101050841\C,-0.3785995479,-2.8760036864,4.00328866\H,-0.2766965199,-3.9550665002,3.8872228458\H,0.5588045932,-2.4614368171,4.3898158785\H,-1.1968129559,-2.6542913213,4.6978146073\C,-0.0155291183,-3.8359418034,0.5688879153\H,0.9178401989,-3.5013987271,1.0159019325\H,-0.5751140357,-4.4706048474,1.2561898017\Cl,0.3941270905,-4.8478274905,-0.8715654728\\Version=AM64L-G09RevB.01\HF=-1133.5911432\RMSD=3.805e-09\RMSF=7.203e-06\Dipole=-1.9278638,0.0713033,0.7200595\Quadrupole=1.6247126,-7.0480577,5.4233451,3.7479444,-4.4112621,-16.7145295\PG=C01 [X(C12H19Cl1N1O2)]\\@
Frequencies -314.4556 cm⁻¹
Sum of electronic and thermal Free Energies= -1133.331811 Hartree

Syn-spiro

1\1\GINC-SPARTAN-RC097\FOpt\RM062X\6-31+G(d)\C12H19Cl1N1O2(1+)\UWILLE\18-Jun-2020\0\#p M062X/6-31+G* scrf=(cpcm,solvent=dichloromethane) no symm freq=noraman opt=(calcfc,maxcycle=500)\geom&freq\1,1\C,-2.12454 6871,-3.1590539705,0.5192452569\C,-0.6767922171,-2.7061557131,0.619732 4296\C,-0.4924082453,-1.3077602206,0.0520260202\C,-2.7727629649,-0.680 9614134,0.8611637538\C,-3.1148242255,-2.1550198725,1.133888649\H,0.566 9785749,-1.028777177,0.0253986275\H,-2.3123616896,-3.2845401111,-0.554 4367128\H,-2.2553366354,-4.1465753743,0.9711024296\H,-3.34435972,-0.03 609213,1.5375572914\H,-3.0380169069,-0.4064279953,-0.1661208308\H,-3.1 598149977,-2.3147230764,2.21747073\H,-4.1180005212,-2.3779084258,0.763 0906835\H,-0.9040066369,-1.2437218996,-0.9580003578\C,-1.2742577439,-0 .4515625212,1.0663359772\C,-0.778788143,-0.9989355515,2.4166288887\C,0 .3619577905,-0.0949736023,2.8430779914\H,-1.5675080409,-1.0915553246,3 .165045906\H,0.3911080772,0.1068197696,3.9142354425\H,1.3330346159,-0. 4986989289,2.5359974483\C,0.0989370643,1.1887689496,2.0533321944\C,-1. 257124906,1.8942992642,0.1054904391\H,-0.7711842,2.8424962039,0.336214 6224\H,-0.9416030421,1.5598429736,-0.8886489202\H,-2.3413415148,2.0319 214021,0.1145349991\N,-0.8594886126,0.9348747217,1.1187255588\O,0.6653 617444,2.2543600959,2.2267840986\O,-0.3398863981,-2.3770939447,2.08673 16769\C,-0.5198292167,-3.3750443803,3.1422758074\H,0.0279150898,-4.260 7540193,2.8334002305\H,-0.0818295624,-2.9405781837,4.0392846246\H,-1.5 843679603,-3.5750830814,3.2686662096\C,0.3850716329,-3.6546386914,0.09 53731642\H,0.3982903173,-3.5634392027,-0.992024388\H,1.3652800438,-3.3 792797252,0.4878674138\Cl,0.117054781,-5.3907184739,0.4533383545\Vers ion=AM64L-G09RevB.01\HF=-1133.6298442\RMSD=4.403e-09\RMSF=6.430e-06\Di pole=-1.2428054,-1.9091822,0.0936212\Quadrupole=-2.7153038,-3.4247991, 6.1401029,2.6139443,-6.6977118,-21.0953083\PG=C01 [X(C12H19Cl1N1O2)]\@ Sum of electronic and thermal Free Energies= -1133.363165 Hartree

E₃ (anti)

1\1\GINC-SPARTAN-BM111\FOpt\RM062X\6-31+G(d)\C12H19Cl1N1O2(1+)\UWILLE\24-Aug-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) opt=(calcfc,max cycle=500) freq=noraman scrf=(cpcm,solvent=dichloromethane)\geom&freq \1,1\C,-2.4235982223,-2.4425970128,-0.3488563335\C,-0.1471778713,-1.3 111705771,0.0055683386\C,-3.4736982988,-0.4472945,0.735086248\C,-3.181 2739766,-1.7524276598,0.7571808143\H,0.9297250834,-1.5486872111,0.0179 879359\H,-2.5139301719,-1.8670963033,-1.2768161601\H,-2.865064918,-3.4 283608912,-0.5358799303\H,-3.9948647471,0.0384150468,1.5565879546\H,-3 .2210117479,0.1699162486,-0.1244210726\H,-0.3341141079,-0.7231037161,- 0.8973827469\C,-0.3168901099,-0.4825404247,1.2178112146\C,-0.300307482 2,-1.0591791498,2.6213372986\C,-0.190844079,0.1678915264,3.5353895764\ H,-1.2574396096,-1.5787236408,2.7838660381\H,-0.9324276804,0.212329285 5,4.3345658833\H,0.8101725389,0.2267486374,3.977717299\C,-0.3613470394 ,1.3430139413,2.6132916361\C,-0.3917425799,1.7213840175,0.0905301503\H ,-0.5557490865,2.7253817806,0.4783028104\H,0.5647938143,1.671117442,-0 .4314301536\H,-1.2070712669,1.4392363293,-0.5758580696\N,-0.3614138961 ,0.8138676491,1.23920307\O,-0.4743675417,2.5081707135,2.8259965763\O,0 .7696224341,-1.9537584865,2.6771281626\C,0.7426595016,-2.7797584598,3. 8384537852\H,1.6137270282,-3.4301316296,3.774135376\H,0.8034293151,-2. 1752743546,4.750572061\H,-0.1725359291,-3.3835427585,3.8565911083\C,-0 .9337162494,-2.6327992077,-0.0203625197\H,-0.4814391831,-3.2553747133,

-0.7968212458\H,-0.7939963682,-3.1705630775,0.9246266577\C,-3.5977752835,-2.6022902622,1.9247134253\H,-2.8128265514,-3.2907800269,2.2468120794\H,-3.933950267,-2.0029163323,2.7708690968\Cl,-4.9920665605,-3.6637231726,1.4601195455\\Version=AM64L-G09RevB.01\HF=-1133.6047327\RMSD=0.000e+00\RMSF=4.649e-06\Dipole=2.5904095,1.204276,-0.2083254\Quadrupole=-13.627768,-4.080531,17.708299,-6.5205656,-0.8871524,-10.136258\PG=C01[X(C12H19Cl1N1O2)]\\@
Sum of electronic and thermal Free Energies= -1133.350154 Hartree

TS2

1\1\GINC-SPARTAN-BM108\FTS\RM062X\6-31+G(d)\C12H19Cl1N1O2(1+)\UWILLE\24-Aug-2020\0\#p M062X/6-31+G* nosymm opt=(ts,noeigentest,calcfc,maxcycle=500) freq=noraman scrf=(cpcm,solvent=dichloromethane)\\geom&freq\\1,1\C,-2.4709218853,-2.8591288951,-0.4469011747\C,-0.4228246406,-1.4434910471,0.0592727662\C,-2.9106720825,-0.6956452345,0.682656902\C,-3.1321587303,-2.0682595144,0.6087952629\H,0.6437178844,-1.4680422083,0.311993963\H,-2.5819029599,-2.3855171392,-1.4263679844\H,-2.8458230411,-3.8836780057,-0.4886498889\H,-3.428812586,-0.1311747513,1.4557284933\H,-2.7793876943,-0.1699105745,-0.2624140445\H,-0.5295599731,-0.9107927512,-0.8915570168\C,-1.0896177595,-0.6647630461,1.1720169492\C,-0.9641285046,-1.2205959622,2.6102399445\C,-1.2347860308,0.0028749062,3.4878145463\H,-1.6568981637,-2.0471561132,2.8052682335\H,-2.2851035391,0.0827219563,3.7885825223\H,-0.623513446,0.0223173404,4.3920254615\C,-0.8889540447,1.1691025645,2.5898512438\C,-0.541225297,1.5635454854,0.1514221901\H,0.3707876083,1.2624139779,-0.3681561868\H,-1.3846864941,1.54815315,-0.546514206\H,-0.422590453,2.5718366286,0.5466776565\N,-0.7975426978,0.6827521815,1.2781583553\O,-0.7148400166,2.3258496629,2.8903582613\O,0.3621142572,-1.6735914974,2.7214740414\C,0.577195129,-2.5001127047,3.8581596787\H,1.6255675219,-2.7957073952,3.832400005\H,0.3758926001,-1.9601294592,4.7902063468\H,-0.0599911566,-3.3917422851,3.8088480275\C,-0.9525662919,-2.8605379149,-0.0658831617\H,-0.4226727949,-3.3907767147,-0.8600932616\H,-0.7914787074,-3.419716573,0.8625301334\C,-3.8619572792,-2.7982099802,1.6930643507\H,-3.3392138,-3.70660642,2.0018265285\H,-4.1019145412,-2.172025709,2.5510567883\Cl,-5.4168522797,-3.3075258174,0.9450924635\\Version=AM64L-G09RevB.01\HF=-1133.586212\RMSD=3.623e-09\RMSF=5.159e-06\Dipole=-0.0264059,-1.6094737,-1.0347218\Quadrupole=-1.0947562,-1.6120451,2.7068012,9.1063854,-8.1420316,-16.3230714\PG=C01[X(C12H19Cl1N1O2)]\\@
Frequencies -282.1036 cm⁻¹
Sum of electronic and thermal Free Energies= -1133.326331 Hartree

Anti-cycl

1\1\GINC-SPARTAN-BM065\FOpt\RM062X\6-31+G(d)\C12H19Cl1N1O2(1+)\UWILLE\22-Aug-2020\0\#p M062X/6-31+G* nosymm opt=(calcfc,maxcycle=500) freq=noraman scrf=(cpcm,solvent=dichloromethane)\\geom&freq\\1,1\C,-2.4551207848,-2.8839208864,-0.4527083342\C,-0.4179251546,-1.4466393262,0.096960977\C,-2.7784779344,-0.7352354944,0.7765511559\C,-3.0937191522,-2.1331805179,0.6191699967\H,0.6403834348,-1.4543069163,0.3716878205\H,-2.5226222771,-2.3636134453,-1.4123451502\H,-2.8207214365,-3.9077655613,-0.5363364264\H,-3.3551359521,-0.2341540268,1.5560606582\H,-2.8321932483,-0.1951803791,-0.1732685796\H,-0.5171196924,-0.9341200356,-0.8666611005\C,-1.1746334676,-0.6738984084,1.1714691917\C,-0.9682017074,-1.2062127264,2.6178061043\C,-1.2004645188,0.0320555063,3.4862285769\H,-1.6587

900934,-2.0264821738,2.8593772137\H,-2.2461807328,0.1364925363,3.79653
80241\H,-0.5809637355,0.0465672377,4.3848705945\C,-0.8412066534,1.1840
327611,2.5687939983\C,-0.5907640425,1.5680186761,0.1348028897\H,0.3113
274098,1.2733051692,-0.4071724803\H,-1.4479984028,1.5393704696,-0.5469
165949\H,-0.4716885386,2.5844271967,0.5102984518\N,-0.8112017011,0.704
3154105,1.2786751041\O,-0.6204174928,2.3376832448,2.8862954491\O,0.356
4199439,-1.6684259405,2.7038728684\C,0.5993688961,-2.4641376547,3.8544
19095\H,1.6452021373,-2.7672661032,3.8090601597\H,0.4267870776,-1.9010
121732,4.7787316571\H,-0.0430831655,-3.3538285001,3.847337051\C,-0.930
1613575,-2.8706178231,-0.0242670358\H,-0.4066003548,-3.4121927618,-0.8
151046721\H,-0.7876134698,-3.4277442392,0.907398951\C,-3.9272861639,-2
.8473874588,1.6230279882\H,-3.6524534596,-3.8941832876,1.7540216622\H,
-4.0382590911,-2.3250899761,2.5717063904\Cl,-5.5069648783,-2.776388752
2,0.7588014246\\Version=AM64L-G09RevB.01\HF=-1133.5876731\RMSD=6.101e-
09\RMSF=5.030e-06\Dipole=-1.1786537,-3.1228716,-1.4400786\Quadrupole=5
.0550645,-0.4578997,-4.5971648,17.6798941,-9.4269694,-18.7698638\PG=C0
1 [X(C12H19Cl1N1O2)]\\@
Sum of electronic and thermal Free Energies= -1133.327620 Hartree

Entry 8

E₃ (syn)

1\1\GINC-SPARTAN-BM087\FOpt\RM062X\6-31+G(d)\C14H25Cl1N1O2Si1(1+)\UWIL
LE\26-Aug-2020\0\#p M062X/6-31+G* nosymm opt=(calcfc,maxcycle=500) fr
eq=noraman scrf=(cpcm,solvent=dichloromethane)\geom&freq\1,1\C,-2.09
52131027,-2.6318006707,-0.3548177981\C,-0.6044617365,-2.6836986165,-0.
1225162138\C,0.2502218925,-1.7809532872,-0.6163421021\C,-2.8483335776,
-0.7849646125,1.3016578919\C,-2.9023332584,-2.2808456235,0.9042093653\
H,1.3215385011,-1.8566054167,-0.4438660181\H,-2.3262317814,-1.92067504
69,-1.1563448849\H,-2.4288993087,-3.617315137,-0.7025088601\H,-3.44428
72338,-0.6612234936,2.2178417026\H,-3.3116277441,-0.1797526336,0.51845
37485\H,-2.5923988248,-2.8979799676,1.7502934626\H,-3.958964528,-2.493
3262181,0.7195452127\H,-0.0898209608,-0.9550655755,-1.2375763594\C,-1.
5084149146,-0.2459253247,1.6304155624\C,-0.6763178577,-0.6802398935,2.
8247088743\C,0.6917920282,-0.0419197136,2.5619623868\H,-1.1628001865,-
0.1641328288,3.6731398677\H,1.1754205261,0.3921758328,3.4383146774\H,1
.3620419641,-0.7878522488,2.1176474305\C,0.4067368209,1.0194902244,1.5
389895518\C,-1.5032876262,1.5930422693,-0.0440315904\H,-0.7955390241,2
.4020153955,-0.2175250111\H,-1.6134583592,0.9995288561,-0.9531443607\H
,-2.465420491,1.9977544021,0.2690422638\N,-0.9504675604,0.7660805536,1
.0322858997\O,1.0643585459,1.9215553465,1.123541744\O,-0.6637034246,-2
.0553633282,2.9953334814\C,-0.0881767837,-3.8439468854,0.6787818003\H,
0.9513528849,-3.7074273639,0.9769635609\H,-0.6965874311,-4.0428136214,
1.5588353296\Si,-0.7015640876,-2.7547148961,4.5590448191\C,-0.50349422
95,-4.5817648239,4.2497304789\H,0.4224416165,-4.7970840832,3.705710692
3\H,-0.4620010909,-5.1155115159,5.2058380456\H,-1.3464976449,-4.988935
1769,3.6802057751\C,-2.3571400836,-2.3381189931,5.3230829813\H,-2.4528
219581,-2.8229944392,6.3013188793\H,-2.4858553256,-1.2610979119,5.4790
776537\H,-3.1771138567,-2.6938001529,4.6889932122\C,0.7171722087,-2.03
0497817,5.5396719349\H,0.580175015,-0.9606451782,5.7356413186\H,0.7960
924949,-2.5309935032,6.5115328014\H,1.6685735415,-2.1666262209,5.01355
34361\Cl,-0.1490160478,-5.3681046601,-0.309566644\\Version=AM64L-G09Re
vB.01\HF=-1502.937285\RMSD=9.246e-09\RMSF=4.396e-06\Dipole=-1.8094388,
3.2730923,0.891247\Quadrupole=1.9196726,-19.9793737,18.0597011,-0.5001

294,-6.3640592,-15.2209551\PG=C01 [X(C14H25Cl1N1O2Si1)]\@
Sum of electronic and thermal Free Energies= -1502.615550 Hartree

TS1

1\1\GINC-SPARTAN-BM089\FTS\RM062X\6-31+G(d)\C14H25Cl1N1O2Si1(1+)\UWILL
E\28-Aug-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) freq=noraman
opt=(ts,noeigentest,calcfc,maxcycle=500) scrf=(cpcm,solvent=dichlorome
thane)\geom&freq\1,1\C,-2.4251502934,-2.9169274231,-0.098656232\C,-0
.963810409,-2.6655522649,0.0079912373\C,-0.4747754056,-1.4004627154,-0
.2305892845\C,-2.7607918823,-0.7085105657,1.1099041207\C,-3.1117674734
,-2.1908100179,1.092461766\H,0.5945318568,-1.2163639522,-0.1551849171\
H,-2.8163740169,-2.5002913013,-1.0328089344\H,-2.6528638789,-3.9848148
363,-0.0658101863\H,-3.2733232101,-0.2194764149,1.9507630802\H,-3.1205
611937,-0.2255370328,0.1952146538\H,-2.8268873233,-2.6686563332,2.0332
487364\H,-4.1928113483,-2.2993696813,0.9772809543\H,-1.0170501207,-0.7
717926969,-0.9339100544\C,-1.2958301341,-0.4067078346,1.3088398173\C,-
0.5760220337,-0.8741305225,2.5831193052\C,0.7222245595,-0.0640931176,2
.5685890466\H,-1.2268738066,-0.4955111843,3.3908564212\H,1.0815239209,
0.2385987351,3.5531526097\H,1.5183039204,-0.6278076843,2.0674851067\C,
0.3645825825,1.1485455671,1.7426207732\C,-1.4670565326,1.822642995,0.1
754219366\H,-0.8493399828,2.7196876598,0.1782155097\H,-1.5016791175,1.
4117255374,-0.838882374\H,-2.477334869,2.0684092987,0.5080094221\N,-0.
8539570502,0.8701010884,1.0880973981\O,0.9550763863,2.1934803751,1.628
8395889\O,-0.4255646234,-2.2530863362,2.6711290693\C,-0.0685467944,-3.
7834127922,0.4402116703\H,0.9135842263,-3.443383193,0.760846471\H,-0.5
313022597,-4.4146121114,1.1970744353\Cl,0.1559092254,-4.8079858701,-1.
0321938881\Si,-0.3819537537,-3.0285577937,4.1991578018\C,0.8523389749,
-2.1279165264,5.2788632485\H,0.5102937246,-1.1216824126,5.5467300179\H
,0.9893847598,-2.682622545,6.2143894996\H,1.8305289249,-2.0452369133,4
.7925386196\C,0.1425755633,-4.7829521043,3.8454700374\H,-0.6334671534,
-5.3428945599,3.3128158063\H,1.0691610271,-4.8218288189,3.2630662685\H
,0.32356183,-5.2999840729,4.7947977929\C,-2.0971269071,-2.9563437513,4
.9466160691\H,-2.8095116042,-3.5582367008,4.3720898206\H,-2.0682315448
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\Version=AM64L-G09RevB.01\HF=-1502.9229174\RMSD=0.000e+00\RMSF=8.644e
-06\Dipole=-2.1055787,0.5651448,-0.0193397\Quadrupole=-0.642068,-7.181
8551,7.823923,2.3848588,-4.5598381,-19.033008\PG=C01 [X(C14H25Cl1N1O2Si1)]\@
Frequencies -310.2504 cm⁻¹
Sum of electronic and thermal Free Energies= -1502.596244 Hartree

Syn-spiro

1\1\GINC-SPARTAN-BM092\FOpt\RM062X\6-31+G(d)\C14H25Cl1N1O2Si1(1+)\UWILL
LE\26-Aug-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) opt=(calcfc,
maxcycle=500) freq=noraman scrf=(cpcm,solvent=dichloromethane)\geom&f
req\1,1\C,-1.8737841676,-2.9806673512,0.128934293\C,-0.4762280515,-2.
4685149512,0.4667645371\C,-0.3138390426,-1.0326534501,0.0025492189\C,-
2.7007442344,-0.6015013334,0.6287635578\C,-2.9674940019,-2.1108367546,
0.7688555328\H,0.7240601228,-0.6968658052,0.1069509871\H,-1.9552211917
,-2.9512435503,-0.9633739657\H,-1.9907801798,-4.0269054589,0.426790913
9\H,-3.3678433359,-0.0394362208,1.2915365469\H,-2.8953938561,-0.274262
6867,-0.3991804897\H,-3.0521500601,-2.364062309,1.8332527437\H,-3.9330
225426,-2.3598609831,0.3219827584\H,-0.6224314333,-0.9168448474,-1.038

383955\C,-1.2436961882,-0.2988397642,0.9821723267\C,-0.8334580335,-0.9
08675082,2.3333444728\C,0.2542197463,0.0054326797,2.8720745636\H,-1.67
66429848,-1.0167225044,3.0166508601\H,0.2263254695,0.1479912166,3.9529
624057\H,1.2561442392,-0.3378603251,2.5909666123\C,-0.0207550078,1.329
4379283,2.1555809561\C,-1.293313754,2.1093954023,0.1839671873\H,-0.895
9944693,3.066085621,0.523676564\H,-0.8678852089,1.8693148983,-0.796753
9452\H,-2.3806576389,2.1786127644,0.0998194762\N,-0.9250467197,1.10408
66151,1.1630554875\O,0.4944890965,2.4008640213,2.428552329\O,-0.385685
5103,-2.2716010811,1.9783394204\C,0.6756860943,-3.389389183,0.09049752
25\H,1.6214022782,-2.9906330926,0.4618533663\H,0.5261433005,-4.4079758
808,0.4520800803\Si,-0.0966449396,-3.5589378153,3.2606735769\C,-0.6685
665344,-2.7438754247,4.8266095974\H,-0.0962675217,-1.8500214121,5.0879
424496\H,-1.7359683485,-2.5034124955,4.8138816319\H,-0.5101350963,-3.4
748460792,5.629143934\C,1.7314151455,-3.8874215345,3.2233719425\H,1.99
9558176,-4.3774872907,4.1670010922\H,2.0332444147,-4.5533768094,2.4104
082538\H,2.3095487029,-2.9602325933,3.1569889199\C,-1.1666860882,-5.00
66028564,2.8012865134\H,-2.2219369586,-4.7271015875,2.7220424569\H,-0.
860553806,-5.5275002312,1.8901742081\H,-1.0807028442,-5.7253715901,3.6
262932816\Cl,0.7956918138,-3.4912603321,-1.6908181429\\Version=AM64L-G
09RevB.01\HF=-1502.9631134\RMSD=0.000e+00\RMSF=1.113e-05\Dipole=-1.182
7553,-2.7253805,1.0368442\Quadrupole=-10.2387866,6.5516231,3.6871635,0
.2151966,-2.8420543,-35.6811799\PG=C01 [X(C14H25ClIN1O2Si1)]\\@
Sum of electronic and thermal Free Energies= -1502.628249 Hartree

E₃ (*anti*)

1\1\GINC-SPARTAN-BM030\FOpt\RM062X\6-31+G(d)\C14H25ClIN1O2Si1(1+)\UWIL
LE\25-Aug-2020\0\#p M062X\6-31+G* nosymm opt=(calcfc,maxcycle=500) fr
eq=norman scrf=(cpcm,solvent=dichloromethane)\geom&freq\1,1\C,-2.32
24973243,-2.4465755116,-0.4281883005\C,-0.0956608282,-1.2609941617,0.0
548431303\C,-3.5403672564,-0.4521319649,0.4676571564\C,-3.1764273599,-
1.7336020577,0.5898933116\H,0.9790409429,-1.4803472297,0.1647996657\H,
-2.3538840831,-1.9058621784,-1.3805431448\H,-2.7322625418,-3.446788930
9,-0.6113593863\H,-4.1356760578,0.0493520713,1.2269878828\H,-3.2720001
033,0.1271940373,-0.4129629466\H,-0.2175521128,-0.7077075193,-0.880270
1165\C,-0.3761027351,-0.4020986057,1.2238733989\C,-0.4047705567,-0.938
6463176,2.6459701192\C,-0.355678479,0.3254519529,3.5158443932\H,-1.374
860685,-1.4447771527,2.7752713148\H,-1.0946574553,0.3593168872,4.31811
65383\H,0.6444838968,0.4437745601,3.9480658215\C,-0.5811164806,1.45821
74523,2.553929885\C,-0.5383675985,1.7606036091,0.0235148566\H,-0.86398
66423,2.7429964882,0.3618203906\H,0.4594340023,1.8265871296,-0.4126794
221\H,-1.2467074218,1.3596063724,-0.7009923663\N,-0.4953933518,0.88989
25324,1.1997159076\O,-0.7814742285,2.6189843887,2.7257334391\O,0.66174
22366,-1.8176066641,2.7909113112\C,-0.8583789036,-2.5971464794,0.01480
40906\H,-0.339647826,-3.2381866082,-0.7028691068\H,-0.7806780303,-3.09
93859651,0.9865379571\C,-3.6119442678,-2.5311918028,1.7866490493\H,-2.
801077513,-3.1249078081,2.2152133161\H,-4.0552548683,-1.9036369318,2.5
602690831\Si,0.7940728506,-2.937111669,4.0770778115\C,2.2037098344,-4.
0355399672,3.554641409\H,2.3864598299,-4.8082623726,4.3092123568\H,1.9
778186633,-4.5332896627,2.6056479035\H,3.1258357785,-3.4583256765,3.43
01744517\C,-0.8276193522,-3.8655163466,4.2155515217\H,-1.6672792464,-3
.2121297366,4.4810075626\H,-1.0736785384,-4.4031664525,3.2924602839\H,
-0.7422478822,-4.6131016455,5.0131925019\C,1.1498210831,-1.9990161788,
5.6561820751\H,2.0340386674,-1.360785631,5.5516204594\H,0.3033915478,-

1.3731239272,5.9605187648\H,1.3420894416,-2.7075439506,6.4702227378\Cl
 ,-4.8760651548,-3.7423273249,1.316603841\\Version=AM64L-G09RevB.01\HF=
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 -0.9907297\Quadrupole=-14.1179485,-4.8127574,18.9307059,-7.889677,-0.0
 337863,-12.9524166\PG=C01 [X(C14H25Cl1N1O2Si1)]\\@
 Sum of electronic and thermal Free Energies= -1502.616081 Hartree

TS2

1\1\GINC-SPARTAN-BM085\FTS\RM062X\6-31+G(d)\C14H25Cl1N1O2Si1(1+)\UWILL
 E\26-Aug-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) freq=noraman
 opt=(ts,noeigentest,calcfc,maxcycle=500) scrf=(cpcm,solvent=dichlorome
 thane)\\geom&freq\\1,1\C,-2.6385013306,-2.8449463641,-0.3163767252\C,-
 0.4978472755,-1.537517516,0.1064855034\C,-2.9306500614,-0.5756458347,0
 .6359469605\C,-3.2532892428,-1.9305351596,0.6651225636\H,0.5594660097,
 -1.617657446,0.3856481065\H,-2.7106717355,-2.4400108093,-1.3301246495\
 H,-3.0829705897,-3.8416601307,-0.2848564072\H,-3.4145862446,0.08418708
 86,1.3534766385\H,-2.7590625803,-0.1365267604,-0.3462071303\H,-0.54743
 31961,-1.0734245047,-0.8840244499\C,-1.1243516311,-0.6311441644,1.1420
 640041\C,-1.0442276332,-1.0738148746,2.6272289882\C,-1.2837149156,0.23
 36807347,3.384407274\H,-1.7900401189,-1.8419908051,2.8638210842\H,-2.3
 41414427,0.4000585515,3.618000832\H,-0.7149878371,0.2890617074,4.31365
 2238\C,-0.8261779999,1.2951982432,2.4097295866\C,-0.3914183362,1.45940
 30954,-0.0419507322\H,0.5281901062,1.0718466831,-0.4862609351\H,-1.201
 5947811,1.4135100231,-0.7771869343\H,-0.2434175723,2.4945755565,0.2642
 342498\N,-0.7398416931,0.6988805071,1.145787574\O,-0.5732700405,2.4574
 770889,2.6239773721\O,0.2602025241,-1.5443549799,2.8241585218\C,-1.125
 4909782,-2.9191002433,0.078761982\H,-0.6284542949,-3.5442476243,-0.666
 4620988\H,-1.0093076622,-3.4168216925,1.0476999973\C,-4.0652767257,-2.
 5110225077,1.7811816923\H,-3.6522640551,-3.4480357728,2.1604913534\H,-
 4.2519128857,-1.8076602139,2.5914315601\Si,0.6665046931,-2.6941757962,
 4.0141536156\C,-0.0240055188,-4.3622790547,3.5096403414\H,-1.116663423
 9,-4.3625477447,3.4201897476\H,0.40353342,-4.6987148593,2.5587310201\H
 ,0.2355262955,-5.1063836614,4.2723120005\C,2.5296667673,-2.6961596317,
 4.0227690085\H,2.9212938457,-1.7120696608,4.3001387645\H,2.9095653617,
 -3.4289666141,4.7429300316\H,2.9230251974,-2.9575855451,3.0346398736\C
 ,-0.0686015554,-2.1576289452,5.6516207576\H,0.1320374253,-2.9201404809
 ,6.4130234522\H,0.3666366454,-1.2149210571,6.0006289867\H,-1.156740694
 3,-2.0342192002,5.5920300123\Cl,-5.6539980845,-2.9016406937,1.03051049
 82\\Version=AM64L-G09RevB.01\HF=-1502.9180741\RMSD=0.000e+00\RMSF=1.33
 8e-05\Dipole=-0.9135179,-1.308151,-1.8652787\Quadrupole=-1.340541,-2.7
 093194,4.0498604,8.2070317,-7.859809,-18.04981\PG=C01 [X(C14H25Cl1N1O2Si1)]\\@
 Frequencies -266.4804 cm⁻¹
 Sum of electronic and thermal Free Energies= -1502.593967 Hartree

Anti-cycl

1\1\GINC-SPARTAN-BM086\FOpt\RM062X\6-31+G(d)\C14H25Cl1N1O2Si1(1+)\UWIL
 LE\26-Aug-2020\0\#p M062X/6-31+G* nosymm scf=(qc,direct) opt=(calcfc,
 maxcycle=500) freq=noraman scrf=(cpcm,solvent=dichloromethane)\\geom&f
 req\\1,1\C,-2.5451443573,-2.927737447,-0.3481272387\C,-0.4768118659,-1
 .5081086993,0.1390282026\C,-2.8362750233,-0.6853118661,0.7005774974\C,
 -3.1811417036,-2.0805538348,0.6519315646\H,0.5727340045,-1.526103459,0
 .4462801034\H,-2.5841313864,-2.480203428,-1.3453077553\H,-2.9358758749

, -3.9456416144, -0.3610063087\H, -3.4168049403, -0.1056812442, 1.419633539
9\H, -2.8441702689, -0.2233702755, -0.2908987197\H, -0.5325165804, -1.06501
45197, -0.8617030162\C, -1.2321490778, -0.6356456543, 1.1330175648\C, -1.06
61269885, -1.0545576968, 2.6265514705\C, -1.3192750624, 0.2546208246, 3.376
7841785\H, -1.7830312341, -1.8394533977, 2.9050631813\H, -2.3783771648, 0.4
005742274, 3.6188763368\H, -0.7441611679, 0.3260674014, 4.3010186509\C, -0.
8933245871, 1.3190819785, 2.3865419901\C, -0.5489125888, 1.4961054542, -0.0
611200568\H, 0.3737903179, 1.1458614295, -0.5310627942\H, -1.372804203, 1.4
163936309, -0.7789380017\H, -0.4334663825, 2.5400310553, 0.2309946944\N, -0.
8363990688, 0.7358244007, 1.1399635709\O, -0.6482466376, 2.4883304689, 2.6
17649519\O, 0.2520345796, -1.493868929, 2.8044473502\C, -1.0293724122, -2.9
215392738, 0.1082718068\H, -0.5041577593, -3.53511016, -0.6272766366\H, -0.
9232036215, -3.4127096601, 1.0810216242\C, -4.0409780773, -2.6961576581, 1.
6999732154\H, -3.7848678585, -3.7329546532, 1.9203137724\H, -4.1486170547,
-2.0972477154, 2.6032120394\Si, 0.7149788003, -2.5863549499, 4.0207006634\
C, -0.1571046411, -4.2211728338, 3.7250242996\H, -1.2476825542, -4.11409222
94, 3.6848743619\H, 0.1800902455, -4.6952667812, 2.7967715533\H, 0.06808886
05, -4.9082699108, 4.5492237433\C, 0.2320876125, -1.9013470191, 5.696369631
5\H, 0.7154721535, -0.9379188862, 5.8919760281\H, -0.8524679164, -1.7688563
749, 5.7893905161\H, 0.5458184944, -2.5980677935, 6.4825073454\C, 2.5613048
759, -2.7333584034, 3.8175034343\H, 3.0510022063, -1.7683882761, 3.98503605
87\H, 2.9713136334, -3.4516594165, 4.5357273287\H, 2.8165027534, -3.0780490
618, 2.8097567269\Cl, -5.6154712387, -2.6747321088, 0.8251270433\\Version=
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=-1.9483552, -2.6642191, -2.2024699\Quadrupole=4.7234752, -2.3879436, -2.3
355316, 16.164024, -8.6669485, -20.1779553\PG=C01 [X(C14H25Cl1N1O2Si1)]\\@
Sum of electronic and thermal Free Energies= -1502.594174 Hartree