Electronic Supplementary Material (ESI) for RSC Advances.

N, *N*-bis-(dimethylfluorosilylmethyl)amides of *N*-organosulfonylproline and sarcosine: synthesis, structure, stereodynamic behaviour and *in silica* studies

Supporting materials

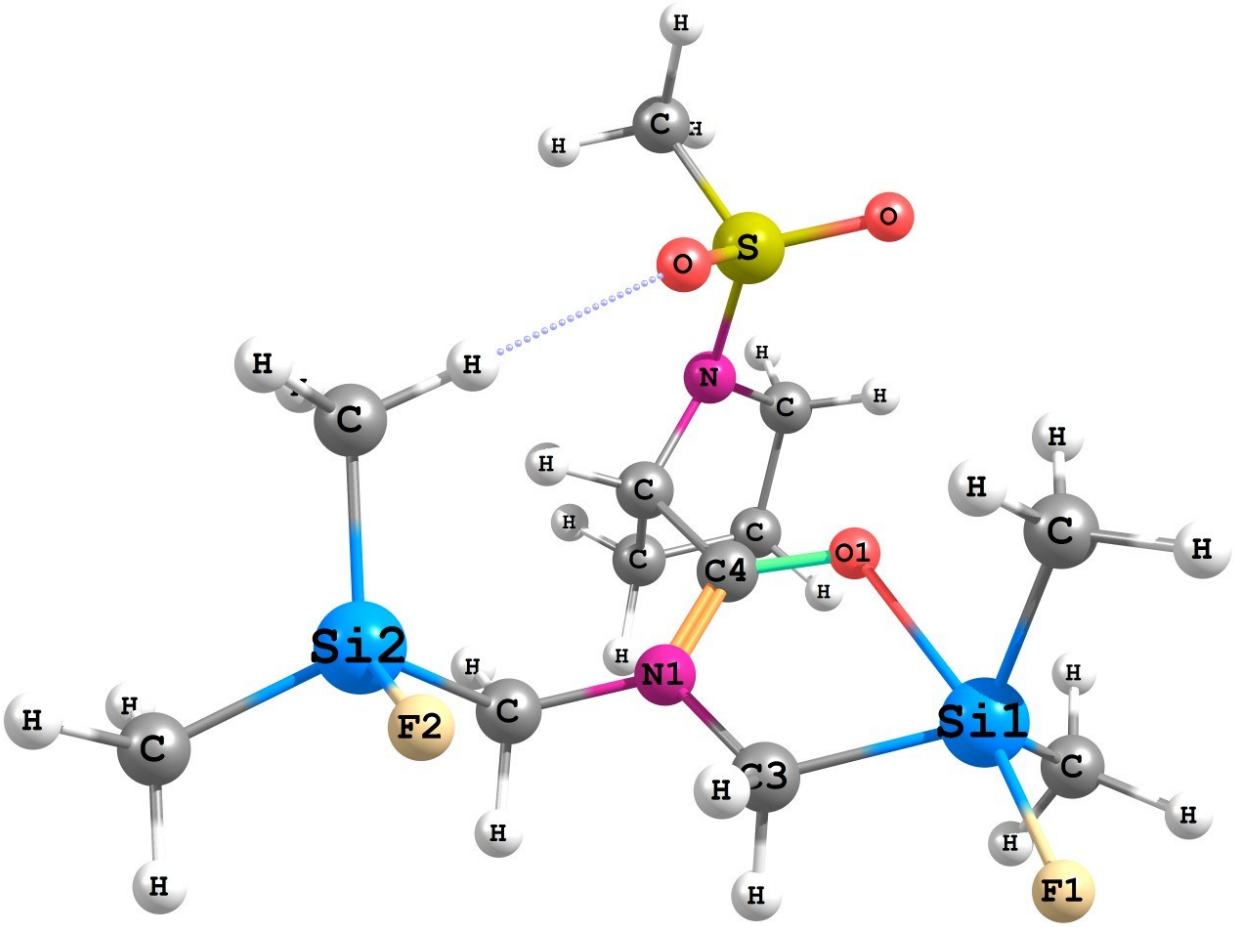

Figure 1s. General view of conformer **9a-cyclic**

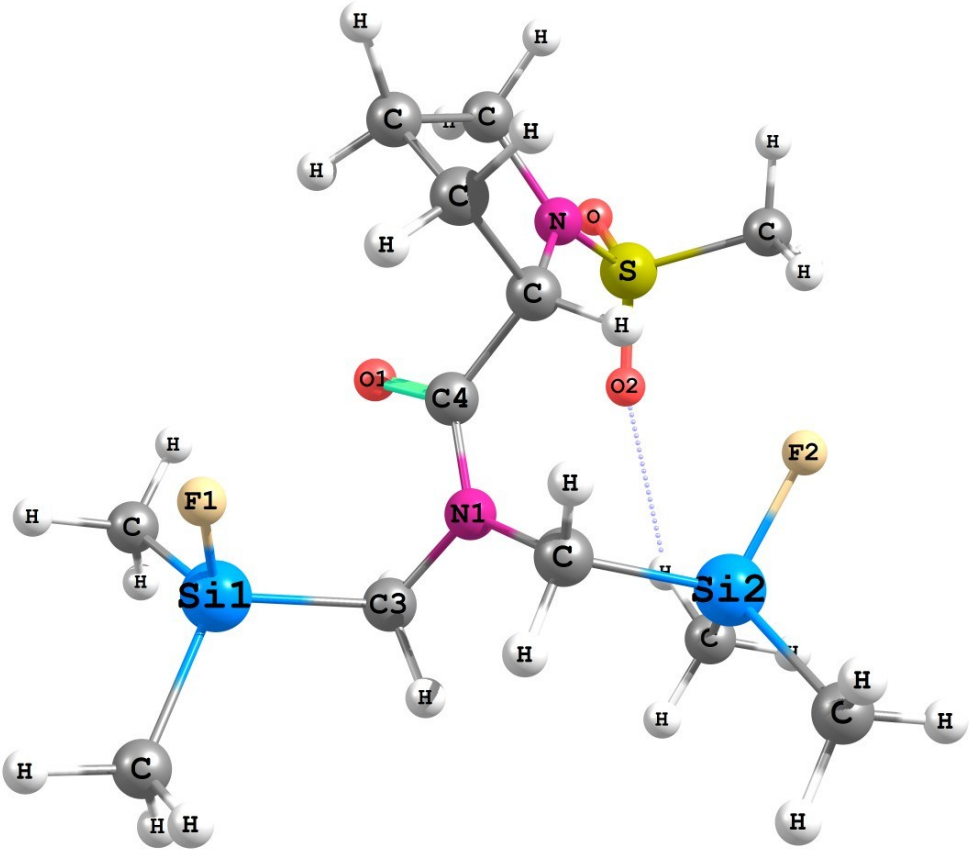

Figure 2s. General view of conformer **9a-acyclic**

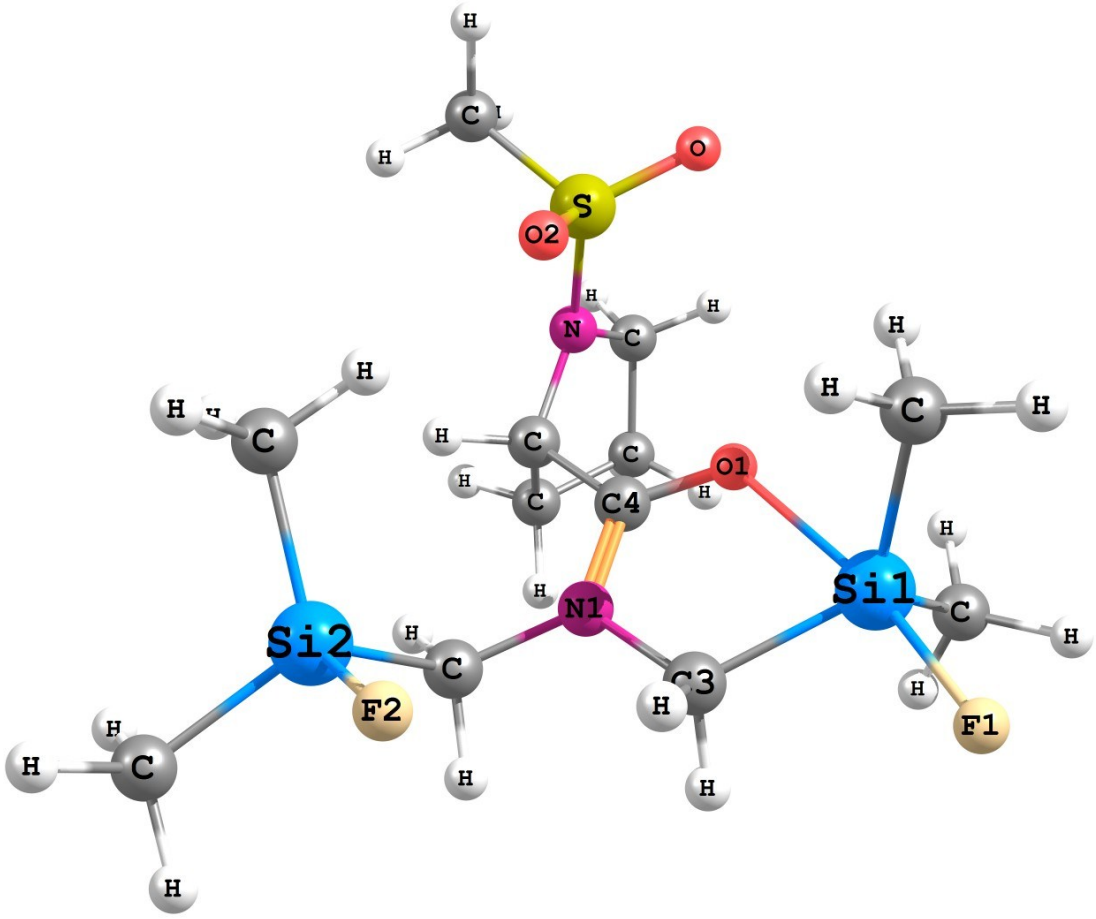

Figure 3s. General view of conformer **9a-cyclic-CDCl$_3$**

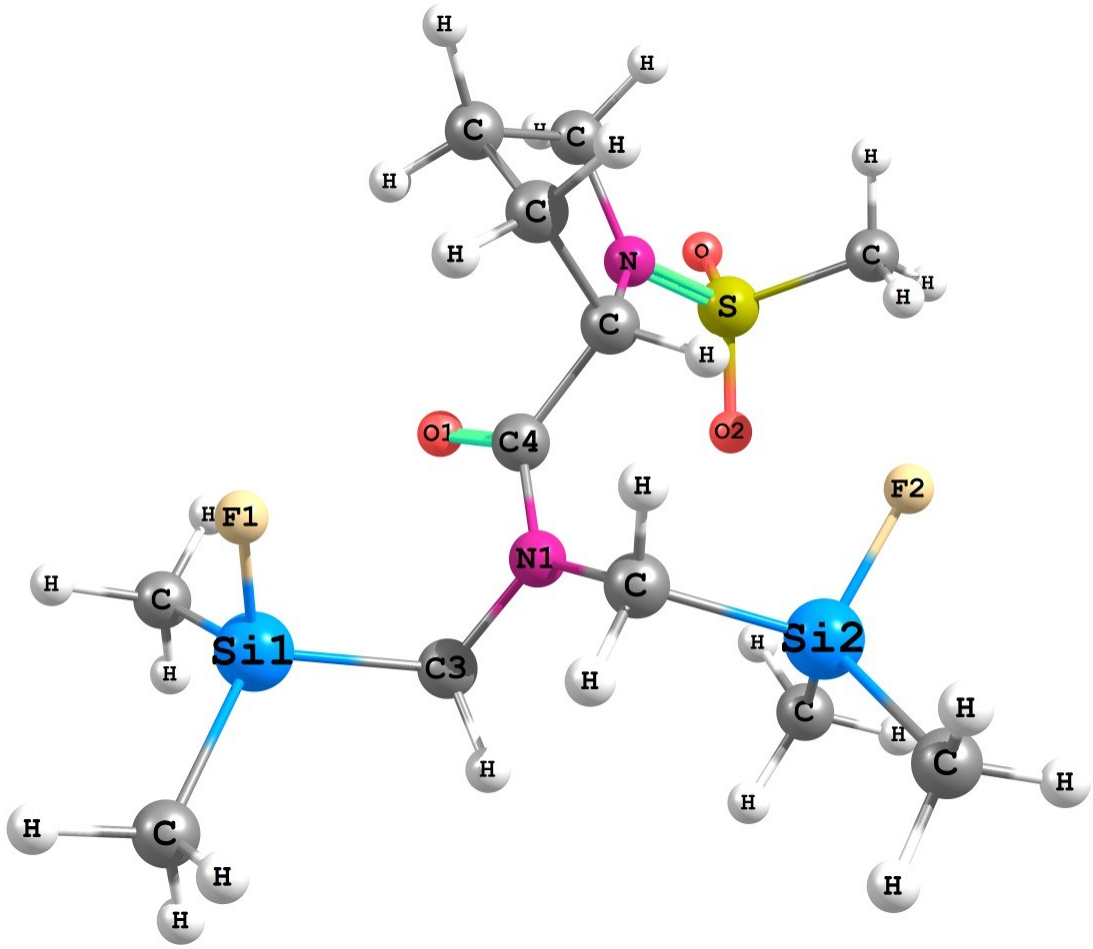

Figure 4s. General view of conformer **9a-cyclic-$CDCl_3$**

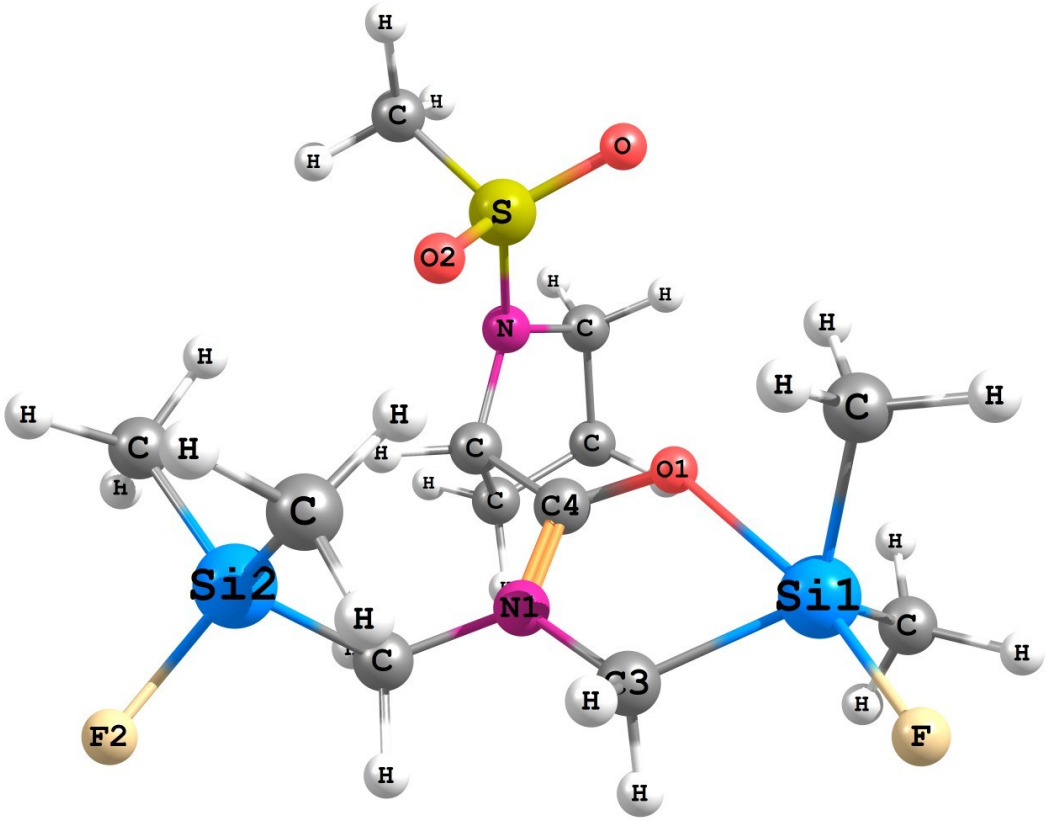

Figure 5s. General view of conformer **9a-cyclic2**

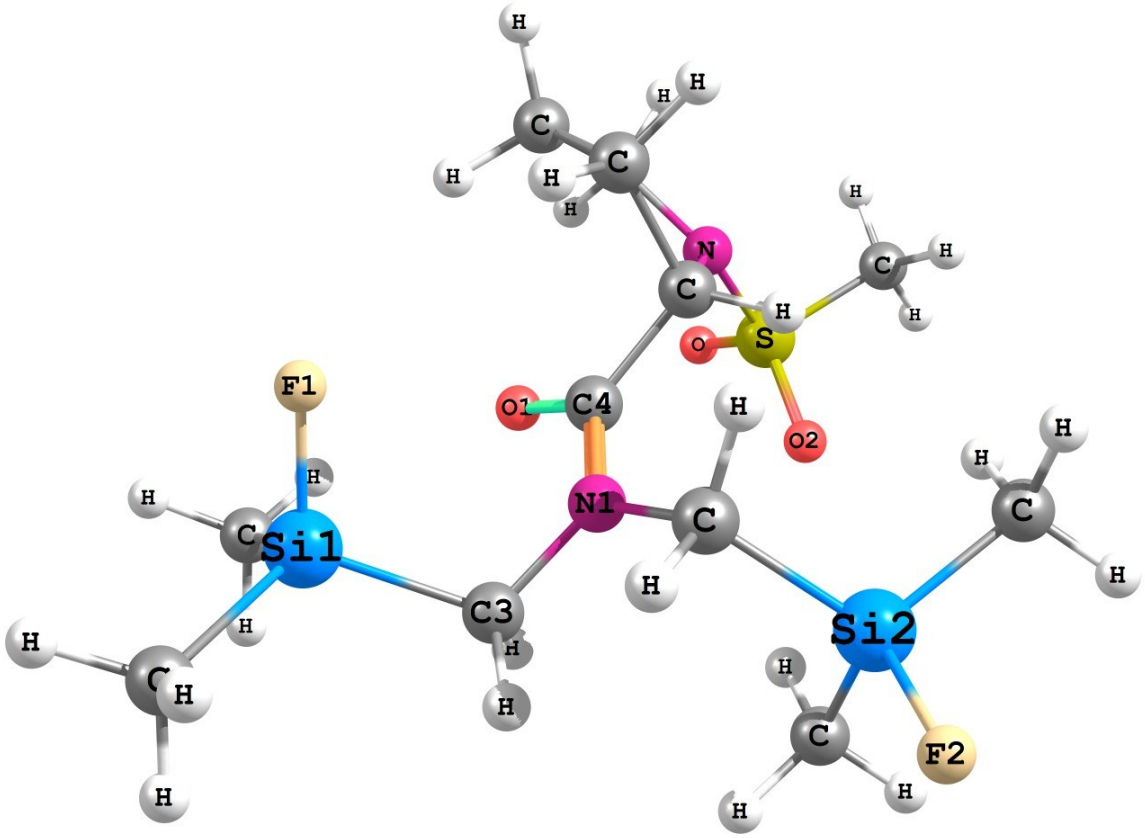

Figure 6s. General view of conformer **9a-acyclic2**

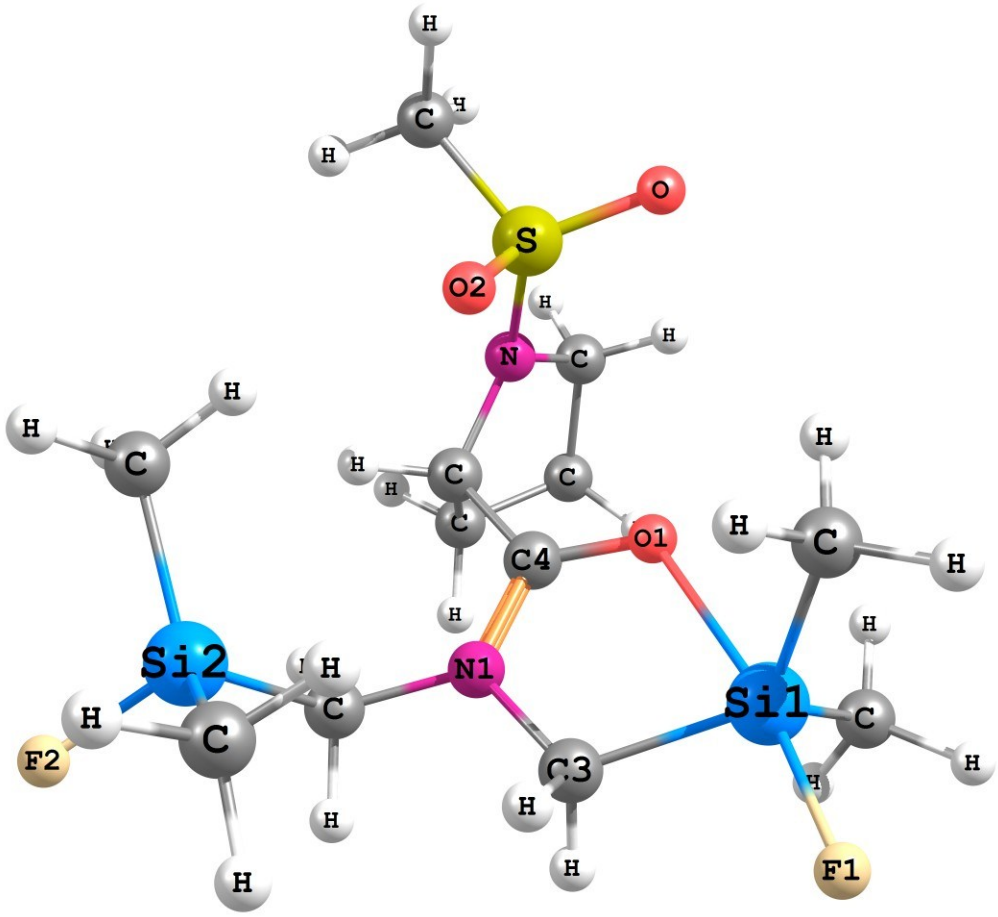

Figure 7s. General view of conformer **9a-cyclic2-$CDCl_3$**

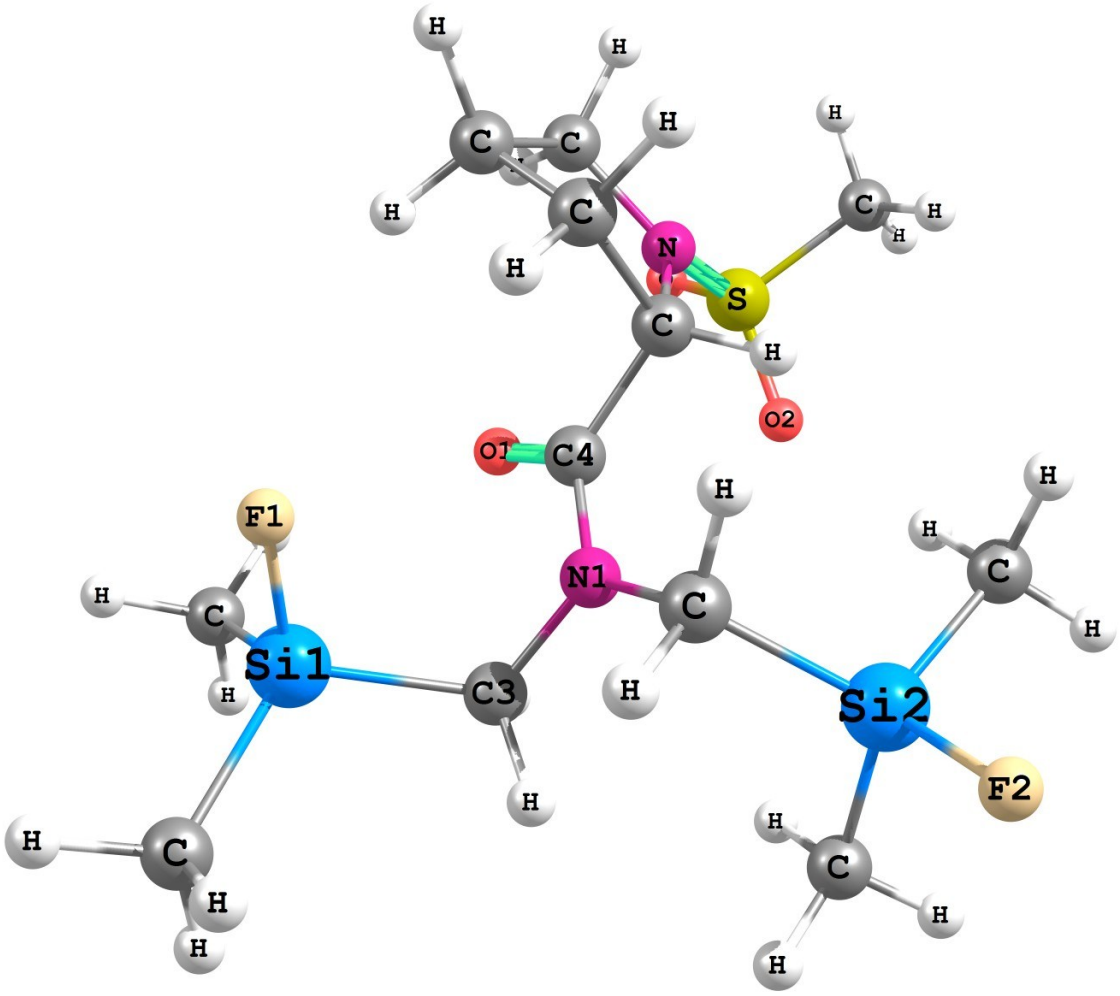

Figure 8s. General view of conformer **9a-cyclic2-CDCl$_3$**

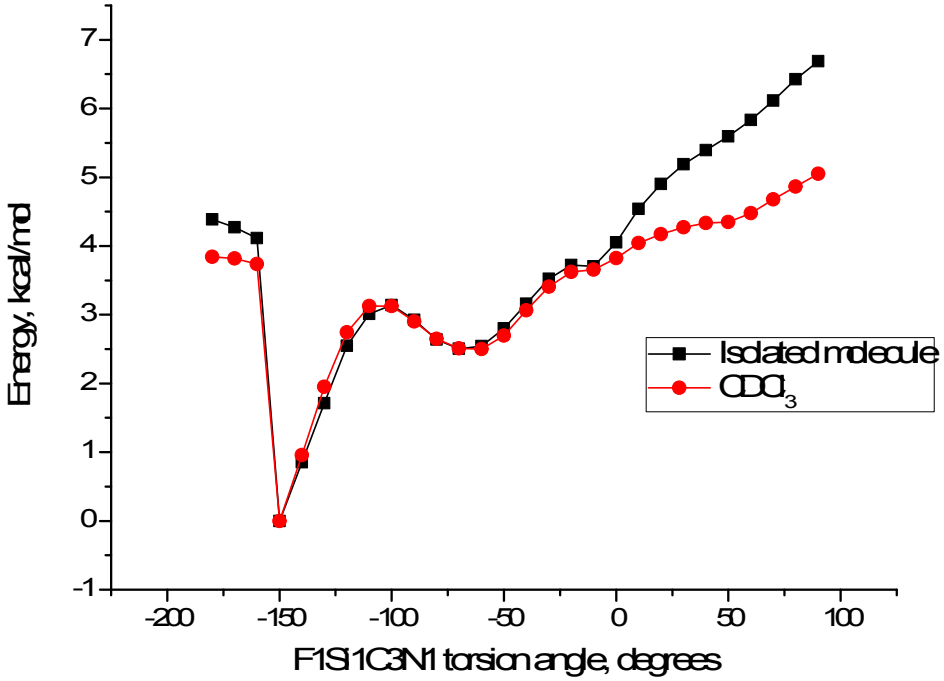

Figure 9s. The plot of total energy *vs* value of F1Si1C3N1 torsion angle. The values of total energy were calculated by relaxed potential energy scan at 10° scanstep and the lowest value taken as reference.

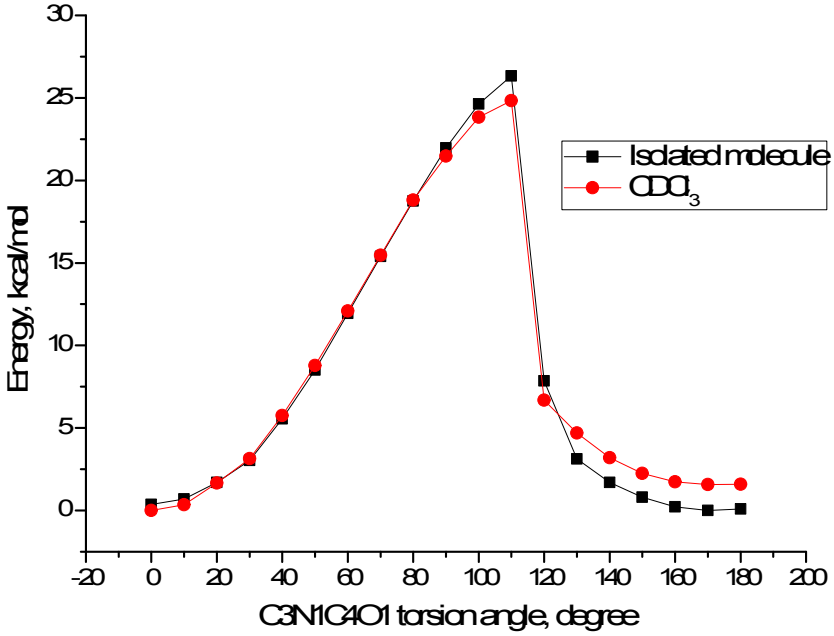

Figure 10s. The plot of total energy vs value of C3N1C4O1 torsion angle. The values of total energy were calculated by relaxed potential energy scan at 10? scanstep and the lowest value taken as reference.

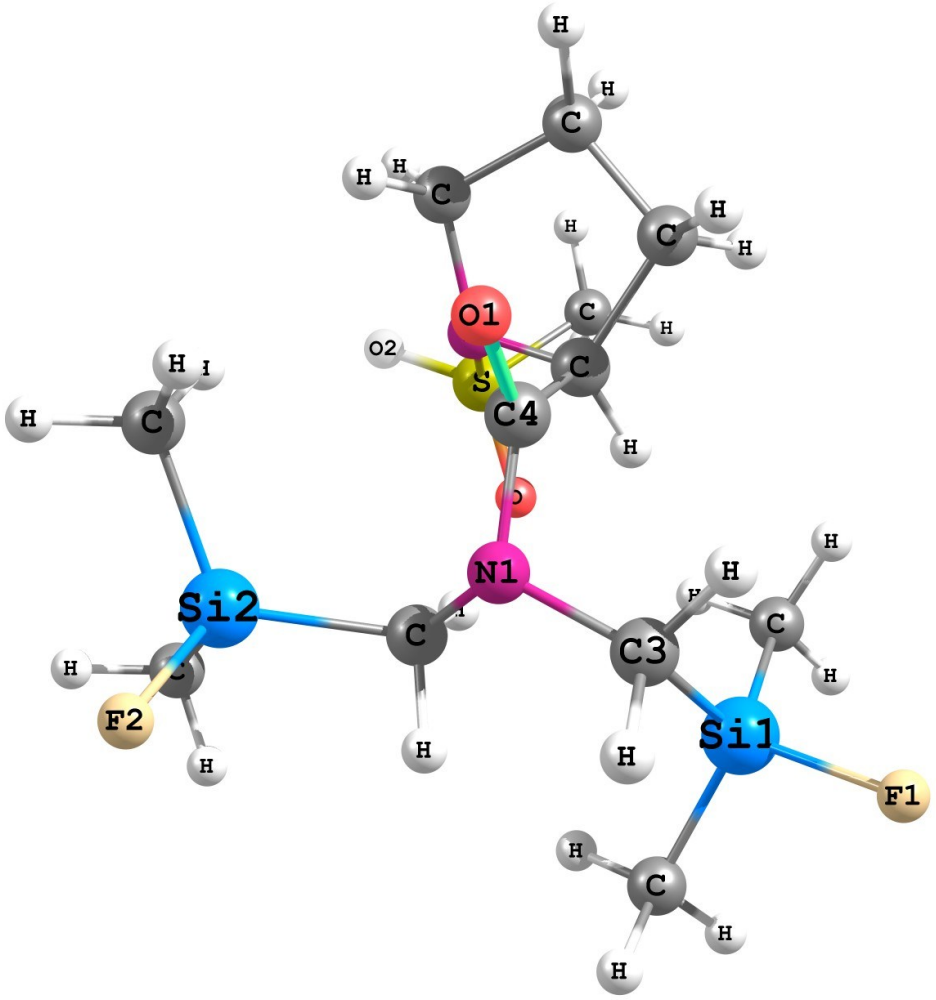

Figure 9s. General view of transition state **9a-ts**

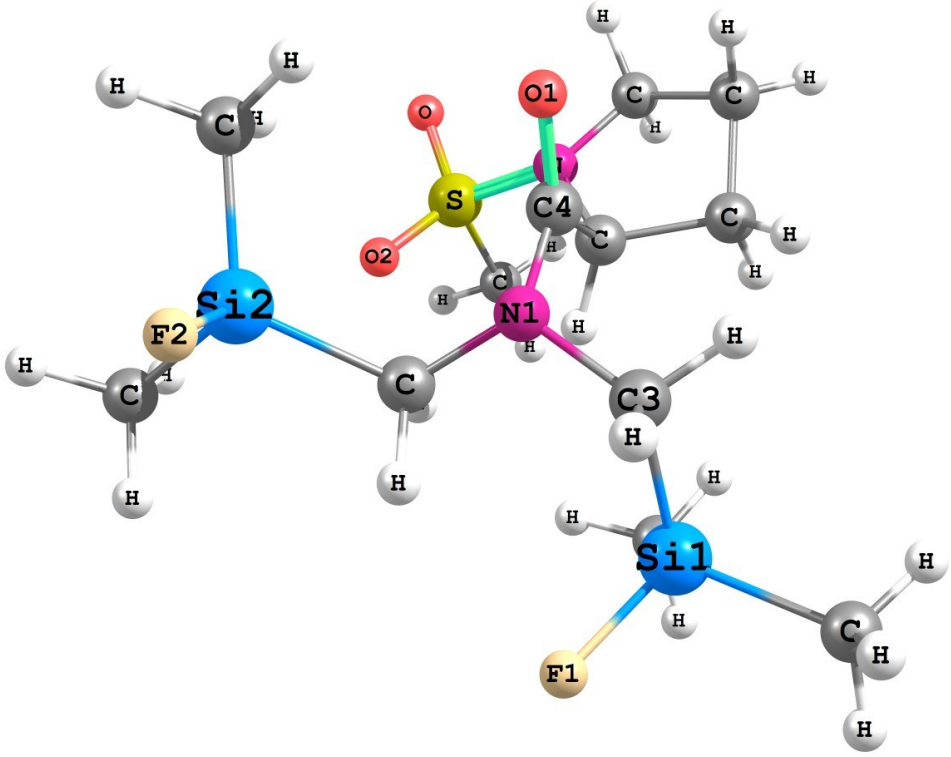

Figure 10s. General view of transition state **9a-ts-CDCl$_3$**

Coodinates and energies (a.u.) of the calculated structure (Table 2)

9a-cyclic

symmetry c1

Si	0.989330000	-2.880851000	-0.341339000
Si	2.762061000	2.030228000	-0.087038000
F	2.368514000	-3.765250000	-0.637874000
F	3.666919000	1.032815000	-1.008515000
O	-0.694672000	-1.335977000	0.278447000
O	-1.293564000	1.151638000	-1.693488000
O	-3.374221000	-0.289919000	-1.540480000
S	-2.590356000	0.849447000	-1.108016000
N	1.184384000	-0.210820000	0.743910000
N	-2.364435000	0.803754000	0.536729000
C	0.097147000	-3.994325000	0.868467000
C	0.247944000	-2.706720000	-2.042986000
C	1.951903000	-1.390240000	0.364554000
C	-0.149125000	-0.296898000	0.658858000
C	1.931263000	0.941896000	1.234095000
C	3.923431000	3.209782000	0.769221000
C	1.539251000	2.884008000	-1.189991000
C	-1.020851000	0.881364000	1.093438000
C	-1.327223000	0.791933000	2.595022000
C	-2.457576000	-0.238245000	2.653820000
C	-3.273872000	0.010461000	1.381093000
C	-3.619281000	2.290460000	-1.320335000
H	0.259997000	-5.039923000	0.591477000
H	-0.974728000	-3.792771000	0.885750000
H	0.488200000	-3.860828000	1.882485000
H	0.384534000	-3.639552000	-2.598243000
H	0.752513000	-1.913382000	-2.603178000
H	-0.814418000	-2.462795000	-2.001501000
H	2.511643000	-1.747512000	1.240075000
H	2.700164000	-1.106540000	-0.382663000
H	2.711091000	0.564824000	1.908337000
H	1.294257000	1.575427000	1.858838000

H	4.455539000	3.824275000	0.037193000
H	4.670428000	2.673394000	1.361261000
H	3.382437000	3.886588000	1.438459000
H	2.057717000	3.347683000	-2.034766000
H	1.020950000	3.681255000	-0.645850000
H	0.784708000	2.197069000	-1.583242000
H	-0.559845000	1.828621000	0.811600000
H	-0.455540000	0.501124000	3.185712000
H	-1.670341000	1.770117000	2.944471000
H	-2.042300000	-1.247248000	2.628468000
H	-3.061616000	-0.140519000	3.557642000
H	-3.550762000	-0.919792000	0.882719000
H	-4.182268000	0.588782000	1.583154000
H	-3.828648000	2.374118000	-2.387307000
H	-3.077609000	3.164803000	-0.962828000
H	-4.546842000	2.144929000	-0.766862000

Zero-point correction= 0.387268 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1983.520420

9a-acyclic

symmetry c1

Si	-0.342302000	2.969227000	0.245321000
Si	3.583671000	-0.714940000	-0.337303000
F	-1.823256000	2.515455000	0.800915000
F	3.231200000	-1.051929000	1.226165000
O	0.607771000	-1.643575000	-0.621419000
O	-1.953656000	0.139889000	-1.562221000
O	-3.420183000	-1.927250000	-1.591509000
S	-2.825949000	-0.808538000	-0.885450000
N	1.048678000	0.473367000	-0.022274000
N	-2.012471000	-1.407187000	0.408086000
C	0.049487000	4.578004000	1.104015000
C	-0.424946000	3.090936000	-1.600944000
C	0.883007000	1.640866000	0.837474000
C	0.308333000	-0.657100000	0.037509000

C	2.186750000	0.439299000	-0.935469000
C	5.208422000	0.208980000	-0.321390000
C	3.709203000	-2.299635000	-1.294663000
C	-0.885657000	-0.693828000	0.993299000
C	-0.558114000	-1.574486000	2.209649000
C	-0.893596000	-2.985207000	1.723179000
C	-2.140916000	-2.796738000	0.862198000
C	-4.150674000	0.150753000	-0.174218000
H	-0.717509000	5.327911000	0.889978000
H	1.010389000	4.979445000	0.766623000
H	0.099313000	4.451514000	2.189582000
H	-1.137999000	3.861378000	-1.908260000
H	-0.750560000	2.133535000	-2.016437000
H	0.551721000	3.347856000	-2.023175000
H	1.866297000	2.113670000	0.939168000
H	0.630264000	1.336208000	1.859044000
H	2.555015000	1.461472000	-1.056426000
H	1.840698000	0.096457000	-1.916434000
H	6.022429000	-0.425537000	0.041241000
H	5.160166000	1.093787000	0.320426000
H	5.474256000	0.541833000	-1.330666000
H	4.476798000	-2.956605000	-0.875335000
H	3.977287000	-2.093913000	-2.336535000
H	2.745139000	-2.811200000	-1.285957000
H	-1.196938000	0.307541000	1.290557000
H	0.482667000	-1.469176000	2.524566000
H	-1.205696000	-1.285713000	3.043597000
H	-0.078397000	-3.358235000	1.101898000
H	-1.062494000	-3.683875000	2.545356000
H	-2.175842000	-3.478277000	0.012017000
H	-3.060811000	-2.920904000	1.447543000
H	-4.733189000	0.554252000	-1.003360000
H	-3.713137000	0.960272000	0.410395000
H	-4.768054000	-0.505670000	0.438494000

Zero-point correction= 0.387092 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1983.516415

9a-cyclic-$CDCl_3$

symmetry c1

Si	0.919167000	-2.865124000	-0.316333000
Si	2.794508000	2.005700000	-0.092339000
F	2.281831000	-3.799655000	-0.651145000
F	3.703757000	0.994487000	-1.009652000
O	-0.649813000	-1.369147000	0.278396000
O	-1.306221000	1.010470000	-1.748266000
O	-3.505057000	-0.211917000	-1.508373000
S	-2.605698000	0.858627000	-1.106637000
N	1.213444000	-0.229421000	0.742655000
N	-2.329798000	0.768994000	0.512465000
C	0.051129000	-3.999762000	0.894287000
C	0.186956000	-2.708242000	-2.029228000
C	1.962532000	-1.420006000	0.365055000
C	-0.114878000	-0.315165000	0.656615000
C	1.966628000	0.921038000	1.231322000
C	3.950191000	3.197740000	0.744742000
C	1.564708000	2.826870000	-1.212200000
C	-0.989263000	0.865000000	1.068125000
C	-1.288042000	0.822804000	2.575463000
C	-2.461638000	-0.152085000	2.669427000
C	-3.300196000	0.147296000	1.427070000
C	-3.491023000	2.388642000	-1.309053000
H	0.221981000	-5.044473000	0.618941000
H	-1.023165000	-3.810743000	0.921228000
H	0.446227000	-3.856470000	1.905622000
H	0.348019000	-3.632464000	-2.592065000
H	0.673933000	-1.896047000	-2.578690000
H	-0.881909000	-2.490813000	-1.992719000
H	2.521406000	-1.782201000	1.238078000
H	2.706538000	-1.150911000	-0.391227000
H	2.743740000	0.541179000	1.905443000

H	1.332724000	1.558207000	1.854074000
H	4.478337000	3.805843000	0.004635000
H	4.695273000	2.671017000	1.347511000
H	3.398512000	3.876900000	1.402502000
H	2.078720000	3.297115000	-2.055863000
H	1.029105000	3.614353000	-0.671096000
H	0.827127000	2.120568000	-1.603137000
H	-0.523198000	1.803669000	0.765701000
H	-0.424916000	0.510291000	3.166493000
H	-1.584937000	1.823316000	2.901964000
H	-2.097108000	-1.180427000	2.627346000
H	-3.033703000	-0.028984000	3.590191000
H	-3.726366000	-0.754572000	0.985597000
H	-4.110841000	0.851822000	1.643213000
H	-3.724814000	2.488847000	-2.369335000
H	-2.851869000	3.205327000	-0.976215000
H	-4.408808000	2.343033000	-0.723040000

Zero-point correction= 0.387151 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1983.537649

9a-acyclic-$CDCl_3$

symmetry c1

Si	-0.097906000	2.961269000	0.234408000
Si	3.636395000	-0.868682000	-0.305370000
F	-1.618705000	2.631315000	0.788661000
F	3.173392000	-1.276252000	1.218800000
O	0.553695000	-1.674604000	-0.783499000
O	-2.226378000	0.214578000	-1.669500000
O	-3.838009000	-1.719669000	-1.461724000
S	-3.036264000	-0.673161000	-0.846489000
N	1.115890000	0.384667000	-0.078932000
N	-2.029976000	-1.400626000	0.214125000
C	0.424425000	4.539425000	1.069153000
C	-0.188497000	3.048412000	-1.614257000
C	0.994090000	1.522827000	0.830704000

C	0.302273000	-0.693406000	-0.093936000
C	2.291755000	0.324594000	-0.941770000
C	5.271372000	0.012891000	-0.143059000
C	3.774560000	-2.422772000	-1.310756000
C	-0.921602000	-0.667863000	0.822652000
C	-0.651740000	-1.471196000	2.109933000
C	-1.143971000	-2.875596000	1.764940000
C	-2.401707000	-2.613318000	0.949417000
C	-4.131168000	0.357522000	0.109850000
H	-0.271691000	5.350389000	0.836772000
H	1.419543000	4.842548000	0.728771000
H	0.459448000	4.421684000	2.156078000
H	-0.835460000	3.870980000	-1.932072000
H	-0.595797000	2.113982000	-2.009983000
H	0.803677000	3.210409000	-2.046689000
H	2.002602000	1.914699000	0.999328000
H	0.665570000	1.194697000	1.822301000
H	2.693314000	1.336423000	-1.037507000
H	1.981556000	0.001243000	-1.940337000
H	6.045260000	-0.654049000	0.247969000
H	5.193603000	0.876207000	0.524530000
H	5.606188000	0.374336000	-1.121284000
H	4.512659000	-3.107608000	-0.883334000
H	4.089145000	-2.183547000	-2.332055000
H	2.803581000	-2.919582000	-1.360679000
H	-1.218367000	0.355858000	1.054161000
H	0.401494000	-1.444862000	2.396690000
H	-1.242081000	-1.049178000	2.928804000
H	-0.406386000	-3.384765000	1.141386000
H	-1.343283000	-3.484896000	2.648234000
H	-2.644486000	-3.417162000	0.254824000
H	-3.267265000	-2.436553000	1.602993000
H	-4.830664000	0.818395000	-0.588147000
H	-3.538931000	1.124897000	0.608896000
H	-4.668638000	-0.265589000	0.824687000

Zero-point correction= 0.386543 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1983.531985

9a-cyclic2

symmetry c1

Si	2.555795000	-1.783677000	-0.394770000
Si	0.743110000	3.147311000	0.100946000
F	4.185714000	-1.656745000	-0.718109000
F	1.582002000	4.415408000	0.706361000
O	0.311435000	-1.575738000	0.289564000
O	-1.461752000	0.630106000	-1.473029000
O	-2.370467000	-1.698240000	-1.890983000
S	-2.404432000	-0.440721000	-1.171830000
N	1.169569000	0.408728000	0.873291000
N	-2.298832000	-0.696144000	0.463145000
C	2.517430000	-3.297259000	0.702217000
C	1.835749000	-1.947810000	-2.107128000
C	2.475057000	-0.067681000	0.442250000
C	0.144737000	-0.439510000	0.747321000
C	1.081404000	1.773139000	1.386760000
C	-1.044288000	3.665726000	0.054973000
C	1.393279000	2.731685000	-1.585633000
C	-1.246115000	-0.034428000	1.226359000
C	-1.510650000	-0.591781000	2.631013000
C	-1.910020000	-2.045292000	2.365097000
C	-2.671223000	-2.001910000	1.035554000
C	-4.047716000	0.221776000	-1.365566000
H	3.279652000	-4.008484000	0.371410000
H	1.541386000	-3.783899000	0.680665000
H	2.744547000	-3.032846000	1.740064000
H	2.431715000	-2.662397000	-2.683240000
H	1.880923000	-0.989831000	-2.634997000
H	0.795950000	-2.276251000	-2.091295000
H	3.154704000	-0.085806000	1.304837000
H	2.903919000	0.647396000	-0.268180000

H	2.049153000	2.003153000	1.844741000
H	0.358067000	1.831682000	2.206086000
H	-1.146950000	4.592098000	-0.518465000
H	-1.447784000	3.846777000	1.055632000
H	-1.638939000	2.895430000	-0.444382000
H	1.171154000	3.545935000	-2.281939000
H	0.896336000	1.829631000	-1.956558000
H	2.474051000	2.570643000	-1.590935000
H	-1.380880000	1.045324000	1.178356000
H	-0.641029000	-0.499612000	3.285810000
H	-2.338016000	-0.033822000	3.078827000
H	-1.016841000	-2.660807000	2.251360000
H	-2.515335000	-2.461540000	3.172463000
H	-2.375925000	-2.813692000	0.368939000
H	-3.756274000	-2.038706000	1.182482000
H	-4.191172000	0.405404000	-2.430911000
H	-4.124115000	1.147972000	-0.797883000
H	-4.766257000	-0.518089000	-1.013109000

Zero-point correction= 0.387603 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1983.521917

9a-acyclic2

symmetry c1

Si	-0.013601000	3.177921000	0.199499000
Si	3.353550000	-1.030181000	-0.363123000
F	0.796191000	4.491015000	0.752105000
F	2.902746000	-1.619526000	1.096538000
O	0.412857000	-1.455692000	-0.638217000
O	-2.265583000	0.542565000	-1.149603000
O	-2.911182000	-1.806331000	-1.851413000
S	-2.849215000	-0.760332000	-0.850349000
N	1.059929000	0.529169000	0.175726000
N	-2.100898000	-1.303607000	0.519943000
C	0.103851000	3.128971000	-1.651653000
C	-1.771212000	3.340474000	0.789115000

C	0.905393000	1.714134000	1.013988000
C	0.208660000	-0.514671000	0.120154000
C	2.209437000	0.455554000	-0.721902000
C	5.102453000	-0.407166000	-0.143899000
C	3.281964000	-2.377496000	-1.638199000
C	-0.980944000	-0.554856000	1.080298000
C	-0.632020000	-1.418857000	2.299374000
C	-0.839607000	-2.846903000	1.788043000
C	-2.007989000	-2.746660000	0.800509000
C	-4.522532000	-0.472719000	-0.303427000
H	-0.383044000	4.008009000	-2.084288000
H	-0.415507000	2.239145000	-2.021711000
H	1.138080000	3.106400000	-2.003783000
H	-2.195945000	4.290567000	0.451161000
H	-1.842658000	3.310169000	1.880323000
H	-2.373816000	2.532778000	0.363117000
H	1.907308000	2.063452000	1.286014000
H	0.440579000	1.445318000	1.966476000
H	2.771765000	1.386759000	-0.620308000
H	1.864100000	0.391245000	-1.760908000
H	5.789466000	-1.226655000	0.086888000
H	5.167552000	0.324961000	0.666553000
H	5.460809000	0.075469000	-1.059768000
H	3.929764000	-3.213800000	-1.359100000
H	3.624796000	-2.001222000	-2.608060000
H	2.256672000	-2.733074000	-1.749450000
H	-1.314571000	0.443823000	1.360323000
H	0.387176000	-1.243834000	2.650478000
H	-1.328822000	-1.185417000	3.109999000
H	0.055266000	-3.178792000	1.261037000
H	-1.045667000	-3.549215000	2.598162000
H	-1.817135000	-3.305965000	-0.116514000
H	-2.949961000	-3.093805000	1.240136000
H	-5.084218000	-0.118383000	-1.168413000
H	-4.511624000	0.277695000	0.485770000

H	-4.939329000	-1.414172000	0.054177000

Zero-point correction= 0.387208 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1983.515487

9a-cyclic2-$CDCl_3$

symmetry c1

Si	-1.238124000	2.782900000	-0.331161000
Si	-2.440484000	-2.331036000	-0.003850000
F	-2.698138000	3.566485000	-0.642828000
F	-3.371510000	-3.344785000	0.892614000
O	0.487434000	1.464266000	0.259758000
O	1.257251000	-0.971083000	-1.706772000
O	3.311884000	0.497652000	-1.644429000
S	2.565295000	-0.648070000	-1.148439000
N	-1.243745000	0.153326000	0.785211000
N	2.363366000	-0.520262000	0.479246000
C	-0.447554000	4.033588000	0.814560000
C	-0.557051000	2.641948000	-2.066182000
C	-2.112763000	1.262603000	0.422683000
C	0.067671000	0.371089000	0.671677000
C	-1.862909000	-1.066470000	1.298370000
C	-1.046783000	-3.333988000	-0.709055000
C	-3.518340000	-1.586991000	-1.320360000
C	1.060414000	-0.702973000	1.100285000
C	1.414381000	-0.550696000	2.588264000
C	2.500995000	0.524449000	2.580738000
C	3.310289000	0.233545000	1.316837000
C	3.606885000	-2.076979000	-1.343069000
H	-0.726199000	5.047274000	0.512705000
H	0.640117000	3.947911000	0.812319000
H	-0.797294000	3.887275000	1.841945000
H	-0.778471000	3.553632000	-2.629208000
H	-1.027943000	1.806317000	-2.594231000
H	0.520546000	2.472413000	-2.066905000
H	-2.667527000	1.588844000	1.312262000

H	-2.860433000	0.920300000	-0.299647000
H	-2.740082000	-0.762971000	1.880340000
H	-1.200879000	-1.561730000	2.013769000
H	-1.435640000	-4.069659000	-1.419665000
H	-0.507932000	-3.874607000	0.075111000
H	-0.337782000	-2.689965000	-1.239468000
H	-3.900059000	-2.375950000	-1.975675000
H	-2.946715000	-0.890271000	-1.941400000
H	-4.372590000	-1.052488000	-0.896561000
H	0.669280000	-1.694512000	0.872485000
H	0.550124000	-0.281798000	3.198974000
H	1.809756000	-1.502809000	2.952529000
H	2.046699000	1.514340000	2.506496000
H	3.119693000	0.497603000	3.478903000
H	3.633688000	1.144532000	0.811317000
H	4.189504000	-0.384256000	1.529518000
H	3.793739000	-2.196905000	-2.410577000
H	3.084089000	-2.944530000	-0.942580000
H	4.543641000	-1.903143000	-0.813799000

Zero-point correction= 0.387487 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1983.537676

9a-acyclic2-$CDCl_3$

symmetry c1

Si	0.969882000	3.097097000	0.195258000
Si	3.074916000	-1.708626000	-0.350355000
F	1.621042000	4.109187000	1.315715000
F	2.486288000	-2.058515000	1.144570000
O	-0.060516000	-1.496299000	-0.802987000
O	-2.368241000	0.777768000	-1.425662000
O	-3.677330000	-1.374143000	-1.630304000
S	-3.202975000	-0.257132000	-0.827139000
N	1.082391000	0.266713000	-0.008719000
N	-2.401602000	-0.827059000	0.481854000
C	1.865713000	3.385806000	-1.407792000

C	-0.840556000	3.491775000	0.074966000
C	1.300550000	1.371812000	0.922797000
C	-0.004538000	-0.533096000	-0.045783000
C	2.192233000	-0.103715000	-0.883444000
C	4.902032000	-1.403537000	-0.138793000
C	2.733565000	-3.148379000	-1.470922000
C	-1.145871000	-0.246579000	0.935389000
C	-0.919568000	-1.014070000	2.248219000
C	-1.455792000	-2.409908000	1.930886000
C	-2.677962000	-2.154373000	1.049717000
C	-4.642524000	0.544939000	-0.153340000
H	1.674139000	4.402294000	-1.764468000
H	1.513267000	2.691112000	-2.176260000
H	2.946687000	3.261318000	-1.300210000
H	-0.982417000	4.491189000	-0.347370000
H	-1.317499000	3.470497000	1.059817000
H	-1.351422000	2.771328000	-0.572370000
H	2.340170000	1.325933000	1.266715000
H	0.702849000	1.234734000	1.826744000
H	2.903156000	0.724999000	-0.891743000
H	1.822235000	-0.227855000	-1.906211000
H	5.418841000	-2.308581000	0.193677000
H	5.092508000	-0.612045000	0.592071000
H	5.348592000	-1.095801000	-1.090383000
H	3.212421000	-4.059769000	-1.101345000
H	3.125953000	-2.945461000	-2.473021000
H	1.656914000	-3.309854000	-1.551615000
H	-1.267471000	0.824105000	1.101006000
H	0.130421000	-1.025118000	2.546748000
H	-1.504331000	-0.541575000	3.042854000
H	-0.708791000	-2.971070000	1.366931000
H	-1.708962000	-2.975745000	2.828931000
H	-2.785550000	-2.899420000	0.260246000
H	-3.603324000	-2.125629000	1.636638000
H	-5.223772000	0.928293000	-0.992491000

H	-4.315980000	1.359582000	0.491869000
H	-5.224701000	-0.188249000	0.404544000

Zero-point correction= 0.386787 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1983.530703

9a-ts

symmetry c1

Si	-3.048440000	-1.382894000	-0.219959000
Si	-0.238432000	2.965528000	-0.115602000
F	-4.193360000	-2.241870000	0.577581000
F	-1.274608000	3.980023000	0.639922000
O	0.471468000	0.443413000	2.680260000
O	0.840978000	-0.759121000	-2.058339000
O	3.200290000	0.128613000	-1.832207000
S	2.139524000	-0.759417000	-1.404961000
N	-1.205915000	0.564154000	1.118809000
N	1.857137000	-0.418054000	0.197227000
C	-3.945128000	-0.343117000	-1.479099000
C	-1.939556000	-2.630622000	-1.050687000
C	-2.319879000	-0.386911000	1.236654000
C	0.002678000	0.037467000	1.650806000
C	-1.111350000	1.285372000	-0.149348000
C	-0.079503000	3.544948000	-1.879683000
C	1.378562000	3.060246000	0.794682000
C	0.739703000	-1.084352000	0.890010000
C	1.394181000	-2.100397000	1.846095000
C	2.878026000	-1.691217000	1.944464000
C	2.997463000	-0.400472000	1.124674000
C	2.768094000	-2.430950000	-1.504409000
H	-4.601060000	-0.979185000	-2.081835000
H	-3.247344000	0.154008000	-2.158769000
H	-4.565893000	0.421655000	-1.003775000
H	-2.539334000	-3.235517000	-1.738623000
H	-1.483660000	-3.313995000	-0.327438000
H	-1.149469000	-2.147566000	-1.634598000

H	-3.185003000	0.161787000	1.639457000
H	-2.085744000	-1.114633000	2.025552000
H	-2.136026000	1.570518000	-0.420245000
H	-0.730662000	0.671517000	-0.983098000
H	0.304428000	4.568544000	-1.916703000
H	-1.043114000	3.529929000	-2.397427000
H	0.613381000	2.904544000	-2.434645000
H	1.746065000	4.090801000	0.775842000
H	2.125743000	2.423311000	0.312278000
H	1.269515000	2.751597000	1.836736000
H	0.074458000	-1.536100000	0.155377000
H	0.906879000	-2.077045000	2.821109000
H	1.289839000	-3.112777000	1.447396000
H	3.186814000	-1.526127000	2.977540000
H	3.520773000	-2.474831000	1.534058000
H	2.885390000	0.475182000	1.766980000
H	3.930649000	-0.290669000	0.570219000
H	2.937149000	-2.637971000	-2.561637000
H	2.023713000	-3.118266000	-1.102424000
H	3.707880000	-2.494195000	-0.956559000

Zero-point correction= 0.385834 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1983.472504

9a-ts-$CDCl_3$

symmetry c1

Si	3.033023000	-1.479829000	0.502141000
Si	0.623820000	3.005272000	-0.178828000
F	3.929537000	-0.311721000	1.235366000
F	1.867097000	3.707534000	-1.000998000
O	-0.656465000	0.184941000	-2.341153000
O	-1.859990000	0.973540000	1.212923000
O	-4.194146000	0.230573000	0.592058000
S	-2.818482000	-0.087793000	0.933767000
N	1.199987000	0.332564000	-1.000676000
N	-2.201073000	-0.964061000	-0.304444000

C	1.889467000	-2.136234000	1.820663000
C	4.224349000	-2.782667000	-0.089806000
C	2.279384000	-0.664922000	-1.042670000
C	-0.095583000	-0.165772000	-1.338761000
C	1.212899000	1.238312000	0.153186000
C	0.482643000	3.891946000	1.452738000
C	-0.884288000	3.221484000	-1.237757000
C	-0.757372000	-1.197500000	-0.409544000
C	-0.698123000	-2.609968000	-1.024035000
C	-1.976743000	-2.689444000	-1.853896000
C	-3.006275000	-1.997828000	-0.972151000
C	-2.851984000	-1.158698000	2.358682000
H	2.490613000	-2.586259000	2.617301000
H	1.227531000	-2.914609000	1.429853000
H	1.280299000	-1.348055000	2.271628000
H	4.827252000	-3.158884000	0.741868000
H	4.904386000	-2.385204000	-0.848701000
H	3.688899000	-3.631694000	-0.526089000
H	3.148833000	-0.185805000	-1.519965000
H	2.005765000	-1.459049000	-1.747371000
H	2.259841000	1.363742000	0.452802000
H	0.691844000	0.831733000	1.034990000
H	0.289851000	4.957845000	1.300268000
H	1.395012000	3.791788000	2.047921000
H	-0.350015000	3.476136000	2.028310000
H	-1.059811000	4.288232000	-1.408297000
H	-1.758479000	2.802148000	-0.733056000
H	-0.772153000	2.722268000	-2.202207000
H	-0.278350000	-1.167471000	0.570957000
H	0.203585000	-2.786924000	-1.611854000
H	-0.722412000	-3.346548000	-0.214785000
H	-1.855648000	-2.134188000	-2.786154000
H	-2.262157000	-3.715454000	-2.091406000
H	-3.819924000	-1.538900000	-1.533158000
H	-3.432225000	-2.701449000	-0.244685000

H	-3.248253000	-0.576406000	3.190781000
H	-1.836993000	-1.489068000	2.580084000
H	-3.504918000	-2.005956000	2.150318000

Zero-point correction= 0.384932 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1983.490984