Appendix

NMR Spectroscopic Investigations on Asymmetric Aminocatalysis

Dissertation

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Table of Contents

Remote-Stereocontrol in Dienamine Catalysis: Z-Dienamine Preferences and Electrophile-Catalyst Interaction Revealed by NMR and Computational Studies

Computational studies

Two points extrapolation formula to approach SCS-MP2/CBS total energy is defined in the equations 1-3.

$$E_{\mathrm{SCF}}^{X} = E_{\mathrm{SCF}}^{\infty} + Ae^{-\alpha\sqrt{X}}$$

eq. 1

$$E_{\mathrm{corr,MP2}}^{\infty} = \frac{X^{\beta} E_{\mathrm{corr,MP2}}^{X} - (X-1)^{\beta} E_{\mathrm{corr,MP2}}^{X-1}}{X^{\beta} - (X-1)^{\beta}}$$

eq.2

$$E_{\mathrm{MP2}}^{\infty} = E_{\mathrm{corr,MP2}}^{\infty} + E_{\mathrm{SCF}}^{\infty}$$

eq. 3

For the basis set def2-TZVPP (X=3) and def2-QZVPP(-g,-f) (X=4), the used alpha equals 7.88 and beta equals 2.97.

Since low vibrations can cause significant error in the calculation of entropy, the harmonic approximation is corrected using the procedure by Grimme,[3] (for reference see thesis) which employs a weighted partition function between harmonic and free rotor approximations.

Optimized Geometry

All minima and transition states were optimized in the gas-phase at M06-2X/def2SVP with the DFT-D3 empirical dispersion from Grimme.[3] The frequency analysis was also performed at the same level as the geometry optimization. Subsequently single point calculation at SCS-MP2/CBS level of theory and solvent correction (COSMO-SAC) were added to the free energies from DFT calculation.

The used solvent in the experiment was toluene, which is considered as non-interacting solvent. Furthermore, its dielectric constant is similar to the gas-phase. Since the dienamine is neutral, it does not "suffer" from charge separation. In addition, any potential interactions with the solvent were considered to be very similar for the *E-* and *Z-* dienamines. Solvation studies were conducted for the ground states of the dienamines in continuum. However, both structures (*E-* and *Z-*dienamines) relaxed only marginally. Therefore, further simulation in solvent were considered to be unnecessary. Moreover, vibrational analysis (especially in the transition state) in the solution phase is questionable since the partition function (vibration) is developed rather for gas-phase.

Dienamines *E*-1A

***sc-exo* conformation 0; ΔG298(MP2/CBS) = -1020.36150269**

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***ap* conformation 0; ΔG298(MP2/CBS) = -1020.36267466**

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_ap_ conformation 1; ΔG298(MP2/CBS) = -1020.36088838

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Dienamines Z-1A

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_ap_ conformation 0; ΔG298(MP2/CBS) = -1020.36170789

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021.4457659\RMSD=3.731e-09\RMSF=6.450e-06\Dipole=0.3431898,0.7913397,-

0.2929208\Quadrupole=5.0929019,-3.3327772,-1.7601247,-3.4694637,1.7193

386,1.7922108\PG=C01 [X(C23H27N1O1)]\\@

_ap_ conformation 1; ΔG298(MP2/CBS) = -1020.35969678

1\1\GINC-WORKER\FOpt\RM062X\def2SVP\C23H27N1O1\JHIOE\29-Sep-2015\0\\#p

 opt freq def2svp m062x empiricaldispersion=gd3 int=ultrafine\\title\\

0,1\C,0.0890509369,-0.5037993054,-1.6227947522\C,-0.3430658306,-1.8256

712011,-2.2857938914\C,0.9647260333,-2.475752892,-2.7450675459\C,1.966

6825275,-2.0256126884,-1.6824570538\H,-0.0584586359,0.3384487535,-2.31

92486881\H,-0.8397073882,-2.4668229032,-1.5449955351\H,-1.0576193947,-

1.6517010629,-3.0984886487\H,1.9557700726,-2.6908101574,-0.797622825\H

,2.9997967848,-1.9773463701,-2.058800408\N,1.5041406558,-0.6890838316,

-1.359497911\C,2.3381830761,0.3072263998,-0.9401616193\H,1.9022249407,

1.3108381082,-0.9781834667\C,3.6091719259,0.1587261469,-0.4913307676\H

,4.0373612937,-0.842507034,-0.4063731156\C,4.4092194936,1.30931639,-0.

1021500338\H,3.8988018608,2.2761926231,-0.1790390048\C,5.6782717462,1.

3130680904,0.342373531\H,6.1186628309,2.2804054873,0.6016974632\C,-0.7

759722807,-0.1687963077,-0.3541769949\C,-0.5874777704,-1.2684776584,0.

6942613177\C,0.6322183342,-1.4379303154,1.3684589858\C,-1.6022014367,-2.2050937944,0.9227474092\C,0.8172495995,-2.499511016,2.2525577533\C,-1.4195768746,-3.2636429673,1.8132041131\H,-2.5412513732,-2.1166419711,0.3763602426\C,-0.2090363452,-3.4149744039,2.4838578947\H,-0.062544655,-4.2435688539,3.1782922747\C,-0.4555008424,1.2494839499,0.1461154629\C,-0.0481399105,1.5611538362,1.4447388031\C,-0.6380669065,2.3063024223,-0.7606456883\C,0.2312942251,2.8811497921,1.8089774656\C,-0.365742987,3.6216009354,-0.400249421\H,-1.0173300204,2.0911251695,-1.7616211281\C,0.0876525201,3.9134379568,0.8879099798\H,0.3115089152,4.9422891928,1.1732614072\O,-2.0945950697,-0.1871478326,-0.8766534534\H,1.4557306517,-0.7416955752,1.2007699951\H,0.0555555037,0.775880527,2.1915873752\C,6.5648104333,0.1179390541,0.5227643307\H,7.4893913662,0.2193205735,-0.0674458678\H,6.8740889345,0.0080043737,1.5746075153\H,6.0755337169,-0.815972909,0.2184306223\H,1.2716562254,-2.075271687,-3.7226040671\H,0.8915563143,-3.5676947869,-2.8308443867\H,-2.2288549762,-3.9776883101,1.973874894\H,1.7755475635,-2.6092549264,2.7629043951\H,-0.5112403322,4.4235728655,-1.1256412695\H,0.5617596532,3.0968277149,2.8260401686\C,-3.1061580603,0.3801382079,-0.0770836732\H,-3.0997871464,1.4804366683,-0.1308234941\H,-4.0640305774,0.0090768513,-0.4647034115\H,-3.0099629114,0.0870440908,0.9814570228\\Version=ES64L-G09RevD.01\State=1-A\HF=-1021.441716\RMSD=4.033e-09\RMSF=5.859e-06\Dipole=-0.7787246,-0.1500208,0.044913\Quadrupole=-4.4519042,5.1671339,-0.7152296,-2.3069229,1.7225567,-0.5995051\PG=C01 [X(C23H27N1O1)]\\@

Dienamines *E*-1B

***sc-exo* conformation 0; ΔG298(MP2/CBS) = -1389.1384124**

1\1\GINC-WORKER\FOpt\RM062X\def2SVP\C25H33N1O1Si1\JHIOE\17-Jun-2015\0\

\#p m062x/def2svp empiricaldispersion=gd3 int=ultrafine opt freq scf=t

ight\\title\\0,1\C,-0.4253573104,-1.1468614747,-1.7287493057\C,-0.0954

927554,-0.2892549617,-2.959714076\C,-1.360347066,0.5472964834,-3.21351

24471\C,-2.5068797244,-0.321473654,-2.6867864604\H,0.0014288261,-2.159

5032338,-1.7986502393\H,0.7986247089,0.3319002624,-2.8098206313\H,0.10

10022369,-0.9528674355,-3.81481086\H,-1.3171883046,1.490921217,-2.6536

575383\H,-1.4856202092,0.7951714335,-4.2753599689\H,-3.2727416653,0.28

13540625,-2.1680008063\H,-3.0226920925,-0.883011482,-3.4886462188\N,-1

.8699240769,-1.2494874834,-1.7749857715\C,-2.5842683815,-2.2119812495,

-1.1220839239\H,-1.9721236699,-2.9281447027,-0.5686420972\C,-3.9349549

291,-2.3275656758,-1.1032276625\H,-4.5623938931,-1.6037446273,-1.62998

88338\C,-4.5992986619,-3.4021462133,-0.3841964987\H,-3.9421153008,-4.1

11585784,0.1365415047\C,-5.9264419208,-3.5880353643,-0.3039983258\H,-6

.5825946499,-2.8802720972,-0.8243059234\C,0.0894754788,-0.5777589034,-

0.3623286748\C,1.6230355292,-0.5902101051,-0.2739319538\C,2.2489006236

,0.0998914446,0.7737767251\C,2.4304510163,-1.3358689229,-1.139491836\C

,3.6278738984,0.0468322844,0.9558534366\H,2.1153659302,-1.8945475376,2

.6432829913\C,3.8142492159,-1.3920422136,-0.9617627916\H,1.9945569947,

-1.8850331017,-1.9734531221\C,4.4188178148,-0.704109498,0.0862179531\H

,5.5000427115,-0.7489468518,0.2238725392\C,-0.5023866684,0.8178034405,

-0.1623608082\C,0.1879263537,1.9847178082,-0.5101562011\C,-1.831871592

,0.9255231376,0.2657743414\C,-0.4357040216,3.230464919,-0.4342586999\H

,-0.5001646346,-0.3776636039,4.306481667\C,-2.4560678695,2.1693224419,

0.3386005833\H,-2.3828703507,0.0183289283,0.5236738334\C,-1.7607267441

,3.3267388948,-0.0129966313\H,-2.2494765818,4.3004774784,0.044552328\O

,-0.4342477731,-1.4768825269,0.5840328152\Si,-0.361396437,-1.725282078

4,2.2459524843\C,-1.7986471229,-2.8879955176,2.5401799177\H,-2.7329553

056,-2.4492560156,2.1565630083\H,-1.6356603073,-3.8432627922,2.0180630

906\H,-1.9303441831,-3.1046789653,3.6109268199\C,1.248791597,-2.566368

3951,2.7122400787\H,1.1886402071,-2.9486262858,3.7431789498\H,1.430210

1751,-3.4207037702,2.0425613385\H,1.6416282128,0.6972444379,1.45596910

31\C,-0.6123634542,-0.1471658375,3.2350610606\H,0.105440592,0.64715813

5,2.9861443663\H,1.2226650737,1.9243414306,-0.8515460179\C,-6.58867843

83,-4.7000144214,0.4497506717\H,-7.2618863489,-4.3143221663,1.23234610

83\H,-7.2051602451,-5.3283003211,-0.2132561219\H,-5.8434853852,-5.3473

641484,0.9334164492\H,4.0864512989,0.5949582473,1.7804423331\H,4.42039

35246,-1.9805664089,-1.6521140768\H,0.1189658738,4.1291589254,-0.70851

13456\H,-3.4940740144,2.2333620711,0.6692856063\H,-1.6226297547,0.2572

167739,3.077677415\\Version=ES64L-G09RevD.01\State=1-A\HF=-1390.648053

\RMSD=9.278e-09\RMSF=4.568e-06\Dipole=1.1204393,0.7302866,-0.1126768\Q

uadrupole=-0.103904,-1.1127887,1.2166927,-4.8487837,-1.6455527,-1.1933

204\PG=C01 [X(C25H33N1O1Si1)]\\@

ap conformation 0; ΔG298(MP2/CBS) = -1389.1382374

1\1\GINC-WORKER\FOpt\RM062X\def2SVP\C25H33N1O1Si1\JHIOE\19-Jun-2015\0\

\#p m062x/def2svp empiricaldispersion=gd3 int=ultrafine opt freq scf=t

ight\\title\\0,1\C,0.1938935362,0.438098252,2.1929231801\C,1.428387240

9,0.6559766035,3.0805637837\C,2.1612737172,-0.6923957568,3.08662136\C,

1.045768284,-1.7262538875,2.9060674683\H,-0.6635809586,1.0059202793,2.

587214409\H,2.0431098875,1.4887224767,2.7171384597\H,1.0895426467,0.90

80654123,4.0959224054\H,2.8705998906,-0.7516241671,2.2500141874\H,2.72
49243944,-0.85604662,4.0141534039\H,1.3583977339,-2.563502094,2.257435
8257\H,0.7108462238,-2.1662484374,3.8646155967\N,-0.0452545553,-0.9850
171095,2.3019815586\C,-1.2240656436,-1.5950134996,1.9797654893\H,-2.01
14784365,-0.9186921245,1.6340722638\C,-1.48017104,-2.9243453891,2.0484
098783\H,-0.7096747507,-3.6214346934,2.3877315324\C,-2.7743293531,-3.4
737921725,1.6800354282\H,-3.5238741108,-2.7509702903,1.33133152\C,-3.1
122005426,-4.7719608049,1.7269618596\H,-2.3616572191,-5.4918105268,2.0
742966008\C,0.3966393412,0.9651484375,0.7203335345\C,1.5868754435,0.23
58656761,0.1020601127\C,1.5314617225,-1.1397542991,-0.1784665389\C,2.8
041272496,0.8991802448,-0.0755541173\C,2.6621205202,-1.8214931036,-0.6
218875284\H,3.0283640339,4.1589886663,-0.2529698091\C,3.9368277412,0.2
165430278,-0.5229774313\H,2.8736174641,1.9579784852,0.1699215355\C,3.8
718541087,-1.147178053,-0.7949325074\H,4.7569100745,-1.6839365383,-1.1
395453967\C,-0.9147894198,0.8171646825,-0.0712014244\C,-1.0466836525,0
.1122368451,-1.2702692499\C,-2.0413828626,1.4921424772,0.4237502862\C,
-2.2734671216,0.0546883853,-1.9352701044\H,0.6711207148,4.0044984803,-
2.5998519518\C,-3.2650703931,1.4394148645,-0.2370829864\H,-1.951980256
5,2.0846865178,1.336368545\C,-3.3884674757,0.7093615598,-1.4202957929\
H,-4.3460596907,0.6605258514,-1.9404995102\O,0.6728432134,2.3363914607
,0.8915122956\Si,0.5707934497,3.6580013285,-0.158659012\C,-0.904718319
7,4.7122513833,0.3216826442\H,-1.8537225374,4.2477656924,0.0191911973\
H,-0.9262258755,4.8721183514,1.4103890387\H,-0.8381191837,5.6979678675
,-0.1639463877\C,2.1329853043,4.6493314154,0.1560221385\H,2.0558553234
,5.6440397277,-0.3084883997\H,2.2830427202,4.7900950272,1.2369490539\H
,0.600386217,-1.6910452254,-0.0343620792\C,0.4590440267,3.1361848495,-
1.9562943265\H,-0.5430055171,2.758325501,-2.2056692958\H,1.1924673769,

2.3498060155,-2.1920582954\H,-0.1860428974,-0.386058171,-1.7129760225\
C,-4.4499436419,-5.3210679065,1.3375445014\H,-4.3638830259,-6.05367269
49,0.5188942083\H,-4.932603291,-5.8447560598,2.1783944993\H,-5.1244898
804,-4.5193087123,1.0053883834\H,4.8765986615,0.7565126845,-0.64931219
68\H,2.5961704236,-2.8906674432,-0.8303520152\H,-4.1251304311,1.972384
4065,0.1718049246\H,-2.3502294124,-0.5050205262,-2.8685681401\\Version
=ES64L-G09RevD.01\State=1-A\HF=-1390.6492242\RMSD=6.861e-09\RMSF=4.469
e-06\Dipole=0.3737751,0.6844367,-0.3215745\Quadrupole=3.6898433,-2.060
3999,-1.6294433,-5.3021392,2.7111964,2.1819837\PG=C01 [X(C25H33N1O1Si1
)]\\@

_ap_ conformation 1; ΔG298(MP2/CBS) = -1389.1359214

1\1\GINC-WORKER\FOpt\RM062X\def2SVP\C25H33N1O1Si1\JHIOE\23-Jul-2015\0\
\#p freq def2svp m062x opt empiricaldispersion=gd3 int=ultrafine\\titl
e\\0,1\C,-0.1629891849,-0.5506332337,2.224284985\C,-1.3912581506,-0.86
70391748,3.0983639054\C,-1.490697114,0.3099894948,4.0721098506\C,-0.97
00283865,1.4872054093,3.2483190073\H,0.7138894127,-1.1216524788,2.5753
451242\H,-2.2906518849,-0.9112832882,2.4682567677\H,-1.2924178555,-1.8
392275295,3.5946610995\H,-1.7695367114,1.9475369222,2.6363170715\H,-0.
5191295728,2.2784351861,3.8666411766\N,0.0534497028,0.8698472865,2.426
5782185\C,1.1458299407,1.5494273241,1.9672609365\H,1.9483751323,0.9134
224024,1.5804066647\C,1.307764144,2.8947513332,1.9454070034\H,0.504881
7291,3.5538030213,2.2880383293\C,2.5319418475,3.5107046895,1.460993865
4\H,3.3069839046,2.8219012923,1.0993485158\C,2.776082181,4.8296669694,
1.4141954762\H,2.0009975454,5.5148780719,1.777393038\C,-0.382755745,-0
.9953957238,0.7304951257\C,-1.571994736,-0.2378955126,0.1348074982\C,-
1.5345591853,1.1535728729,-0.0542038951\C,-2.7591960286,-0.9111988435,
-0.1678856853\C,-2.6474674483,1.8367424084,-0.5405254447\H,-3.00367234

1,-4.1574967586,-0.4097814463\C,-3.8723785363,-0.2278375619,-0.6605371061\H,-2.8220322186,-1.9834967501,0.0103206707\C,-3.8218219371,1.149938299,-0.8493734367\H,-4.690809609,1.6875866096,-1.2314944558\C,0.9178040557,-0.8217834009,-0.0744893442\C,1.0355599529,-0.0559855518,-1.2372211576\C,2.0475954676,-1.5257720305,0.3696443586\C,2.2519867115,0.0267179099,-1.9182566411\H,-0.5680992385,-3.9640343172,-2.6794148247\C,3.2604846966,-1.4492661722,-0.3086846435\H,1.9698960767,-2.1578685216,1.2562992391\C,3.3696712177,-0.6625478958,-1.4564943864\H,4.3187650514,-0.5950282021,-1.9900443914\O,-0.670102902,-2.3713662455,0.8483979019\Si,-0.5462848717,-3.6680787081,-0.2299854096\C,0.9053390593,-4.7470694322,0.2704122782\H,1.8673829505,-4.2938253277,-0.0066270584\H,0.9008808708,-4.9189985161,1.3575163753\H,0.8356679301,-5.7264931753,-0.2273251795\C,-2.1218577241,-4.6582524373,0.0154551161\H,-2.0328357117,-5.6434743584,-0.4667888933\H,-2.3050756891,-4.8198437923,1.088271132\H,-0.6279240863,1.7169439989,0.1728231529\C,-0.3753016566,-3.1093678239,-2.0118984559\H,0.6350049827,-2.7285646843,-2.2207116485\H,-1.0987293094,-2.3161164142,-2.2552475927\H,0.172571392,0.4742713315,-1.6361084815\C,4.0396402476,5.4462537849,0.8984957176\H,3.8434665863,6.1208034282,0.0495000873\H,4.53927815,6.0515471658,1.6718829387\H,4.7467699858,4.6748757338,0.5622560899\H,-0.8269745118,0.1523382833,4.9351485079\H,-2.5094688928,0.4676363548,4.4493692512\H,-4.7855408802,-0.7800027347,-0.8884862331\H,-2.5915023127,2.9175117404,-0.6808503443\H,4.1235151659,-2.0066470355,0.0593878365\H,2.3185514518,0.6338128284,-2.822236188\\Version=ES64L-G09RevD.01\State=1-A\HF=-1390.6453566\RMSD=5.498e-09\RMSF=2.803e-06\Dipole=-0.2569509,-0.6532707,-0.1994795\Quadrupole=3.0495037,-2.1143347,-0.935169,-4.8006065,-2.5411649,-1.8075741\PG=C01 [X(C25H33N1O1Si1)]\\@

Dienamines *Z*-1B

***sc-exo* conformation 0; ΔG298(MP2/CBS) = -1389.1383237**

1\1\GINC-LOGIN\FOpt\RM062X\def2SVP\C25H33N1O1Si1\JHIOE\17-Jun-2015\0\\

#p m062x/def2svp empiricaldispersion=gd3 int=ultrafine opt freq scf=ti

ght\\title\\0,1\C,0.3132468792,-1.1582681337,1.7181446899\C,0.12471999

62,-0.2833977452,2.9652705846\C,1.4799227428,0.4127903155,3.1780398196

\C,2.5102931167,-0.5471511091,2.5719717415\H,-0.208825988,-2.123007457

2,1.8058523592\H,-0.706346129,0.4273485182,2.8543978331\H,-0.10908683,

-0.9317963658,3.8222112482\H,1.50859689,1.3743471713,2.650645288\H,1.6

783359033,0.6102070141,4.2393330914\H,3.2897789386,-0.0070590854,2.006

3101278\H,3.0267716356,-1.1591751678,3.3351677814\N,1.7400575399,-1.41

03606964,1.7003909851\C,2.3234373556,-2.4365522583,1.0167754846\H,1.61

74029189,-3.0873514083,0.4954324097\C,3.6546043868,-2.6846491689,0.935

1470755\H,4.3623256461,-2.0173818063,1.4305916522\C,4.1610021902,-3.82

396863,0.1864835048\H,3.3927470354,-4.4475926227,-0.2852377767\C,5.443

4641326,-4.1878421547,0.008010526\H,5.6355330848,-5.080599444,-0.59451

49247\C,-0.1963225619,-0.5354874915,0.3728251612\C,-1.7210932197,-0.35

08766984,0.3541898859\C,-2.5724721142,-1.141295434,1.1354433289\C,-2.3

062194202,0.5246479786,-0.5716261814\C,-3.958177672,-1.0637393673,0.99

25766932\H,-2.7942742366,-1.8905430717,-1.9165683226\C,-3.6892611803,0

.6040033179,-0.718873935\H,-1.6668812529,1.1555925852,-1.1900331697\C,

-4.5233020796,-0.1945076286,0.0625983094\H,-5.6067915215,-0.137169779,

-0.0505382873\C,0.5705670889,0.7619914963,0.1150901316\C,0.1065817924,

2.0094709793,0.5501786899\C,1.8411153126,0.684827254,-0.4681277972\C,0

.8911116576,3.1530232193,0.4021601391\H,-0.9774075259,0.3332940961,-3.

1547834582\C,2.6279922551,1.826723825,-0.611734886\H,2.2166575394,-0.2

877635517,-0.7923827681\C,2.1562124594,3.0650597845,-0.1770602919\H,2.7712004153,3.95898635,-0.2912974071\O,0.1559395705,-1.505185166,-0.5851136399\Si,-0.2966978874,-1.8766972541,-2.1638512924\C,0.975319032,-3.1652082651,-2.6388585971\H,1.9939707478,-2.7704750473,-2.5033996874\H,0.8616533756,-3.4793697523,-3.6871435557\H,0.8741214849,-4.0585307703,-2.0039831138\C,-2.0193230194,-2.6177995357,-2.200608588\H,-2.0787345831,-3.4683495129,-1.50463696\H,-2.2497351485,-2.9900482962,-3.2110855344\H,-2.1669382039,-1.8380274057,1.868375225\C,-0.1706589003,-0.395699181,-3.3115524163\H,0.7917412711,0.1217713966,-3.1849231078\H,-0.2363993157,-0.7436739237,-4.3545210271\H,-0.877214564,2.0927325629,1.0157392364\C,6.6526458256,-3.4904436363,0.5545863327\H,7.2375657839,-4.160562925,1.2048362611\H,7.3272512617,-3.1721221694,-0.2563141873\H,6.3920251378,-2.600266897,1.1410055751\H,3.6178976543,1.7456285404,-1.0636376753\H,0.510624143,4.1166851233,0.7444057328\H,-4.115883928,1.2926916385,-1.4498457407\H,-4.5982176597,-1.6924356028,1.6134003944\\Version=ES64L-G09RevD.01\State=1-A\HF=-1390.6472901\RMSD=8.488e-09\RMSF=2.442e-06\Dipole=-1.1702337,0.8601745,0.1977538\Quadrupole=0.8576934,-1.9039801,1.0462868,5.684248,-0.9664522,1.073499\PG=C01 [X(C25H33N1O1Si1)]\\@

_ap_ conformation 0; ΔG298(MP2/CBS) = -1389.1371858

1\1\GINC-WORKER\FOpt\RM062X\def2SVP\C25H33N1O1Si1\JHIOE\19-Jun-2015\0\

\#p m062x/def2svp empiricaldispersion=gd3 int=ultrafine opt freq scf=t

ight\\title\\0,1\C,0.1224863594,0.4316760277,2.1595227824\C,1.316360812,0.8601521607,3.0256464456\C,2.2948896511,-0.3209349508,2.9720464172\C,1.3937589785,-1.5456048615,2.7868630246\H,-0.8168580809,0.8135804013,2.5893464732\H,1.7486164521,1.8054460971,2.6749673622\H,0.9642050994,1.0145033951,4.0559381842\H,2.9766821178,-0.2202038181,2.1165105341\H,

2.9069918641,-0.3965646592,3.8799911007\H,1.8424814147,-2.290153887,2.1059578715\H,1.1771395966,-2.0658262822,3.7391563493\N,0.1632633216,-1.0135888399,2.2313803598\C,-0.8848286725,-1.8295338842,1.917231969\H,-1.7965032472,-1.3075625501,1.6114415468\C,-0.8789034605,-3.185631016,1.9494555144\H,0.0260030324,-3.7170182365,2.2496774416\C,-2.0624812298,-3.9502013251,1.5893138791\H,-2.9282136518,-3.3503863495,1.2860294931\C,-2.2045002779,-5.2873569938,1.5815958295\H,-3.1744308892,-5.6895025787,1.2742208594\C,0.1804430113,1.024297487,0.6990982891\C,1.4721353336,0.5536744588,0.0350147814\C,1.6761769554,-0.7993434869,-0.2841788779\C,2.5335129201,1.4441956214,-0.1476773952\C,2.9058318733,-1.2379826686,-0.7695167655\H,2.1250843043,4.6877505065,-0.2330954884\C,3.7652124858,1.0051531498,-0.6367807473\H,2.4031650847,2.4898976122,0.1271949242\C,3.9579953849,-0.3382532647,-0.9466037911\H,4.9211993955,-0.6848881752,-1.3237634491\C,-1.0981717285,0.6459492681,-0.0686927988\C,-1.1227494266,-0.0408114849,-1.2851470901\C,-2.3203995769,1.0776913582,0.4693548532\C,-2.3322597525,-0.3178059752,-1.9261055003\H,-0.2211332042,4.140036037,-2.5347493163\C,-3.5276927201,0.8058683389,-0.1673648228\H,-2.3232198712,1.6529042046,1.3973312992\C,-3.5387093829,0.0957687409,-1.3689721554\H,-4.4821521832,-0.1244372194,-1.8703290411\O,0.1924845031,2.4182976791,0.9055410988\Si,-0.1885235384,3.7216187783,-0.1026488144\C,-1.8244301899,4.4606302251,0.4420869842\H,-2.6751884199,3.8303669334,0.1474012428\H,-1.8454363083,4.5857103793,1.5353617047\H,-1.9613930482,5.4527983282,-0.0147672846\C,1.1626892965,4.9867700074,0.2070711854\H,0.8842784205,5.9583593062,-0.2284705757\H,1.3100317556,5.1291562807,1.2881739865\H,0.8732035867,-1.5242135701,-0.1375488159\C,-0.247551101,3.2321494921,-1.9117832253\H,-1.1662981923,2.6768357443,-2.1497138479\H,0.6148017532,2.60523254,-2.1860907452\H,-0.1939241862,-0.3519470748,-

S18

1.7600133749\C,-1.1622009805,-6.2983287991,1.9534482087\H,-1.504385958

2,-6.9310618306,2.7878864304\H,-0.9496126731,-6.9764837859,1.111539926

\H,-0.2156118067,-5.8321309712,2.2547232793\H,4.5796497092,1.719798412

9,-0.7657625973\H,3.042348462,-2.2942228847,-1.0075305069\H,-4.4635098

057,1.151583663,0.2749579682\H,-2.3239881711,-0.8582591422,-2.87372938

24\\Version=ES64L-G09RevD.01\State=1-A\HF=-1390.6483634\RMSD=9.856e-09

\RMSF=2.336e-06\Dipole=0.2957942,0.7882687,-0.2962004\Quadrupole=5.351

7485,-4.0524273,-1.2993212,-4.4207516,2.1092157,2.5999968\PG=C01 [X(C2

5H33N1O1Si1)]\\@

ap conformation 1; ΔG298(MP2/CBS) = -1389.1348444

1\1\GINC-WORKER\FOpt\RM062X\def2SVP\C25H33N1O1Si1\JHIOE\28-Sep-2015\0\

\#p freq def2svp m062x opt empiricaldispersion=gd3 int=ultrafine\\titl

e\\0,1\C,0.0330187307,-0.6659553681,1.5885236899\C,0.6838446185,-1.923

0392987,2.1960369843\C,-0.4918434504,-2.7794735476,2.6734585163\C,-1.5

900366061,-2.4585432239,1.6603203378\H,0.0735265818,0.1711811563,2.306

4353524\H,1.2487053059,-2.4577392662,1.4196235277\H,1.3899493952,-1.66

5065391,2.9935884427\H,-1.5157118741,-3.0935785857,0.756645277\H,-2.60

36010322,-2.5748693652,2.0735981015\N,-1.3451323481,-1.0604351433,1.36

08233039\C,-2.3337084764,-0.1987545243,0.9816532055\H,-2.0584082459,0.

8596721865,1.030801364\C,-3.5771380868,-0.5361238079,0.558151426\H,-3.

8469348421,-1.590285122,0.4631731217\C,-4.5557664929,0.4821277395,0.21

06128573\H,-4.2005547751,1.5153241095,0.2978468623\C,-5.8201571541,0.2

956796954,-0.2071967391\H,-6.4119369388,1.1869142816,-0.4361600566\C,0

.811225361,-0.1656580633,0.3150669636\C,0.7913704161,-1.2523683926,-0.

7628276255\C,-0.4045730022,-1.6467586296,-1.3851251685\C,1.9641578165,

-1.9346099955,-1.1000733761\C,-0.4145519079,-2.6800728147,-2.319991796

7\H,4.9603351622,-0.8988751535,-0.3223621116\C,1.9554538895,-2.9662217511,-2.0405300559\H,2.8944079563,-1.6719939029,-0.5988288109\C,0.7656636923,-3.3438037349,-2.6556291225\H,0.7548113882,-4.1511138679,-3.3893373523\C,0.2398860302,1.1816432519,-0.162519955\C,-0.2558537655,1.4242883126,-1.4460669754\C,0.2685831196,2.2501083234,0.7468989352\C,-0.7354805083,2.6872526026,-1.7999817411\H,4.1567512564,1.9295573503,-1.8910885539\C,-0.2044479406,3.5112486479,0.3965822475\H,0.6844487774,2.093357925,1.7440320392\C,-0.7182739358,3.7334291681,-0.8820185323\H,-1.0951102141,4.7183918135,-1.1609908909\O,2.1194797998,0.0366032323,0.8022070809\Si,3.4098763886,0.9884371997,0.2644397352\C,3.6132328825,2.4561591435,1.4159993794\H,2.8457186739,3.223134135,1.2418733296\H,3.5521342765,2.1334428783,2.4664801883\H,4.5990450127,2.9213272144,1.2620893949\C,4.9258958504,-0.1046408691,0.4373498364\H,5.842933125,0.4950686157,0.3346613403\H,4.9396431407,-0.5801459013,1.4294758609\H,-1.3425738683,-1.1422729027,-1.1475595133\C,3.1924501931,1.5596866295,-1.508400773\H,2.4559903747,2.3728886533,-1.5831466681\H,2.8610524003,0.7349981163,-2.1579027045\H,-0.2589476198,0.6325979724,-2.1931666275\C,-6.5136041601,-1.0197262501,-0.3955341616\H,-7.4278009103,-1.0755616551,0.2165056219\H,-6.8278861396,-1.1563940214,-1.4427466244\H,-5.8772389895,-1.8712530057,-0.1232326595\H,-0.8195320389,-2.4594844979,3.6736658422\H,-0.2503817736,-3.8493240722,2.7195191196\H,2.8865909385,-3.4804610032,-2.2839367545\H,-1.3567397912,-2.9649373733,-2.791166513\H,-0.1710260592,4.3240146931,1.1240672136\H,-1.120514846,2.849886994,-2.8076612355\\Version=ES64L-G09RevD.01\State=1-A\HF=-1390.6445396\RMSD=7.107e-09\RMSF=4.054e-06\Dipole=0.7760269,0.0249083,-0.0221071\Quadrupole=-6.2277895,6.1310595,0.09673,0.8690519,2.0151009,0.986888\PG=C01 [X(C25H33N1O1Si1)]\\@

Dienamines *E*-1C

***sc-exo* conformation 0; ΔG298(MP2/CBS) = -2736.0628973**

1\1\GINC-WORKER\FOpt\RM062X\def2SVP\C29H29F12N1O1Si1\JHIOE\14-Jun-2015

\0\\#p m062x/def2svp empiricaldispersion=gd3 int=ultrafine opt freq sc

f=tight\\title\\0,1\C,-0.395684287,-1.197012957,-1.7514965862\C,-0.071

9592167,-0.3310590297,-2.9794348583\C,-1.3435603369,0.4956086803,-3.23

67587699\C,-2.4867037974,-0.3624492975,-2.6820289031\H,0.0416244012,-2

.2064331603,-1.8211278254\H,0.8151951584,0.3015569867,-2.8318770186\H,

0.1347341877,-0.9907791772,-3.8344996745\H,-1.2952068723,1.456725717,-

2.7071486591\H,-1.4772459784,0.7195842896,-4.3023483693\H,-3.233171314

8,0.2476719864,-2.1446174468\H,-3.0289356275,-0.916456575,-3.470202415

2\N,-1.8355098608,-1.3031590652,-1.7895068711\C,-2.5428351983,-2.26227

85887,-1.1136559314\H,-1.9230108164,-3.0152006284,-0.619939353\C,-3.89

09659134,-2.3267705708,-1.0104500139\H,-4.5202634815,-1.5569846656,-1.

465525075\C,-4.5541637129,-3.4015451994,-0.2879210081\H,-3.8995961972,

-4.164161646,0.154542159\C,-5.8802438747,-3.5227101348,-0.1226377633\H

,-6.5301737874,-2.7596599788,-0.5668006851\C,0.1145602487,-0.629314072

2,-0.379507306\C,1.6453053871,-0.6065821651,-0.2930252221\C,2.24684654

33,0.0442217455,0.78659119\C,2.4723437465,-1.2821070391,-1.19579176\C,

3.6284111281,0.0206292765,0.9626203619\H,2.0260121603,-1.641815317,2.9

449286779\C,3.8540936645,-1.3016330437,-1.0152566307\H,2.0598613471,-1

.7955037921,-2.0635360919\C,4.4482623785,-0.6515054304,0.0633326504\H,

5.5305106053,-0.660078341,0.1946387109\C,-0.5019801037,0.7526296397,-0

.1839127559\C,0.1606087985,1.937915051,-0.5080783231\C,-1.8404001373,0

.8180670609,0.213311622\C,-0.5098089712,3.1596727959,-0.4459269673\H,-

0.7007108566,-0.2645595724,4.225222714\C,-2.4976269633,2.0430079612,0.

2768974336\H,-2.3758625492,-0.1033624759,0.4577125374\C,-1.8433240535,3.2271679641,-0.0532176909\H,-2.3616542695,4.1844127924,-0.0010495197\O,-0.3798838255,-1.5301584707,0.5706566615\Si,-0.3962268641,-1.6998920861,2.2552840254\C,-1.7812571978,-2.9263242862,2.5121437157\H,-2.7163230313,-2.5490977783,2.0690315125\H,-1.541452867,-3.8869769769,2.0315069226\H,-1.9557705694,-3.1151582309,3.5818517782\C,1.2392348081,-2.4021533691,2.8449547742\H,1.1015925476,-2.8706779279,3.8319001942\H,1.5946527132,-3.1779820121,2.1497828759\H,1.6295053204,0.591693055,1.5033611401\C,-0.7818799526,-0.0879229304,3.1407837889\H,-1.8047740083,0.2570886706,2.9314662556\H,-0.0930193178,0.7329079764,2.8910665686\H,1.2059246934,1.9238380304,-0.8234047152\C,-3.944085464,2.0436534518,0.6961861755\F,-4.4416113176,3.2756955747,0.7759058978\F,-4.6965444938,1.3589571653,-0.1707049546\F,-4.1010782646,1.4626894258,1.8881292703\C,0.2138185684,4.4023731111,-0.8926487069\F,0.2426885733,4.4820716202,-2.2265750624\F,-0.3725528555,5.5087945526,-0.440487296\F,1.4798625615,4.4072394755,-0.4751624788\C,4.7203627541,-2.0780650775,-1.9745031979\F,4.1494054761,-2.1834934353,-3.1751159869\F,5.9088428855,-1.4978079388,-2.135258569\F,4.942227309,-3.3166601487,-1.5319612033\C,4.2059888267,0.7358030953,2.1564251719\F,3.8467886367,2.0192707311,2.1699827611\F,3.7607620014,0.1975895039,3.2971622201\F,5.53467947,0.6811350741,2.1762959262\C,-6.5496171136,-4.6301195957,0.6303228629\H,-7.1467554382,-4.2417618961,1.4707576376\H,-7.2429587502,-5.1935677708,-0.0143009413\H,-5.8113763914,-5.3364996068,1.0352134129\\Version=ES64L-G09RevD.01\State=1-A\HF=-2737.413738\RMSD=6.987e-09\RMSF=2.018e-06\Dipole=0.1280206,-0.3426442,-0.1792747\Quadrupole=-7.4667304,-1.812373,9.2791034,-2.39229,1.0194018,-3.8586965\PG=C01 [X(C29H29F12N1O1Si1)]\\@

sc-exo conformation 1; ΔG298(MP2/CBS) = -2736.0635041

1\1\GINC-WORKER\FOpt\RM062X\def2SVP\C29H29F12N1O1Si1\JHIOE\10-Jul-2015

\0\\#p freq m062x/def2svp empiricaldispersion=gd3 opt int=ultrafine\\t

itle\\0,1\C,-0.2352693208,-1.3236793617,-1.820262437\C,0.3231703144,-0

.5465123276,-3.0234845071\C,-0.8574842609,0.2601173009,-3.6097213606\C

,-2.1198111177,-0.261105146,-2.8994858462\H,0.1397623873,-2.358548144,

-1.7830915522\H,1.1756077761,0.0892835072,-2.7469616268\H,0.6985502672

,-1.2662197196,-3.7629026655\H,-2.6003884641,0.5316832807,-2.293079518

2\H,-2.8855613089,-0.6346821892,-3.5987072922\N,-1.6569818685,-1.35821

94381,-2.0745845286\C,-2.5285406007,-2.1230741381,-1.3393859936\H,-2.0

576045465,-2.9595682041,-0.8152475189\C,-3.858273509,-1.9098934434,-1.

2175899996\H,-4.3235522692,-1.0394178998,-1.6879510875\C,-4.7121833552

,-2.7785256391,-0.4222595947\H,-4.2342642804,-3.6653435932,0.014523117

8\C,-6.0133639755,-2.5626620284,-0.1754774599\H,-6.4812264846,-1.67122

61205,-0.6092679344\C,0.1083568449,-0.7246065429,-0.4072598734\C,1.616

1149615,-0.5481793834,-0.2014965253\C,2.1338202668,0.4685512406,0.6026

954688\C,2.4963971983,-1.5308465887,-0.6687295236\C,3.4870991522,0.492

3368492,0.9408351045\H,2.4520425306,-1.8616896936,2.3054033347\C,3.845

7582794,-1.4965772797,-0.3324477074\H,2.1324144835,-2.3527433971,-1.28

68853793\C,4.3584649572,-0.4866910103,0.4790628995\H,5.4143042934,-0.4

671222611,0.7478124807\C,-0.6865121345,0.5693262371,-0.2459841143\C,-0

.277372506,1.7690316875,-0.8307119917\C,-1.9307943902,0.5265685725,0.3

866658284\C,-1.1015542433,2.8935431278,-0.7899512045\H,-0.1302348551,-

0.6590824506,4.2366076289\C,-2.7417445625,1.656415949,0.4326894931\H,-

2.2818174355,-0.4105361444,0.8194212781\C,-2.3400484177,2.8525861021,-

0.1568891795\H,-2.9756843724,3.7368773921,-0.1183970345\O,-0.344507975

9,-1.6915686517,0.5040558592\Si,-0.045202086,-1.9564830973,2.155092298

3\C,-1.355711694,-3.2163696432,2.5816501576\H,-2.3590046433,-2.8104398
55,2.3803686641\H,-1.2291510138,-4.1255420901,1.9753602916\H,-1.307801
8746,-3.5022914201,3.6426646237\C,1.6821642801,-2.6418374921,2.4090226
264\H,1.7658963809,-3.0592745384,3.4245482895\H,1.9098802918,-3.445609
97,1.6926376976\H,1.4801909667,1.2505599599,0.9933698422\C,-0.25855891
42,-0.3949991807,3.1745938541\H,-1.2575709807,0.0492912775,3.058644516
7\H,0.4968742701,0.3695424148,2.9411916951\H,0.6926047629,1.8416042101
,-1.3290095669\C,-4.0909354205,1.5363674631,1.0926017544\F,-4.62456583
9,2.730615427,1.3484597637\F,-4.9523150393,0.8706451555,0.3215701162\F
,-4.0033235603,0.8724823346,2.2476177\C,-0.6260014272,4.1440070038,-1.
4807268103\F,-0.5783527707,3.9673173657,-2.8070254104\F,-1.423067331,5
.182220915,-1.2438599894\F,0.6064741408,4.4741724891,-1.0930294587\C,4
.7282939245,-2.6243667855,-0.8016709183\F,4.5224953948,-2.8963196628,-
2.0911139253\F,6.0195147605,-2.3447582348,-0.6417186001\F,4.4709247136
,-3.7445619499,-0.1216864086\C,3.9620696012,1.5795712303,1.8695306587\
F,3.6347347404,2.7869490569,1.4101219945\F,3.39366013,1.4530498597,3.0
725882042\F,5.2811325932,1.548636319,2.0404670468\C,-6.8828260257,-3.4
471966897,0.6626374551\H,-7.305087702,-2.8990134358,1.5198695781\H,-7.
7372816149,-3.8356263937,0.0857628531\H,-6.3171798696,-4.3053146681,1.
0520742793\H,-0.7357596848,1.338006487,-3.4449015921\H,-0.9256309175,0
.1096156879,-4.694238318\\Version=ES64L-G09RevD.01\State=1-A\HF=-2737.
4135523\RMSD=6.985e-09\RMSF=7.825e-07\Dipole=0.4485646,-0.4463643,-0.1
423265\Quadrupole=-7.2574006,-1.8669253,9.1243259,-2.3305591,-0.509739
8,-3.8593921\PG=C01 [X(C29H29F12N1O1Si1)]\\@

_ap_ conformation 0; ΔG298(MP2/CBS) = -2736.0627413

1\1\GINC-LOGIN\FOpt\RM062X\def2SVP\C29H29F12N1O1Si1\JHIOE\19-Jun-2015\

0\\#p m062x/def2svp empiricaldispersion=gd3 int=ultrafine opt freq scf

=tight\\title\\0,1\C,0.1889641885,0.5463187342,2.3127028263\C,1.442583

0715,0.8051085614,3.1587126876\C,2.1864117969,-0.5379636087,3.19670511

17\C,1.0851507723,-1.5947528388,3.0460666895\H,-0.664135873,1.13144615

47,2.6947316007\H,2.0422153053,1.6297404866,2.7530209619\H,1.124814790

6,1.0931214442,4.1707227074\H,2.8992360052,-0.6106950375,2.3633949604\

H,2.7562887469,-0.6691097362,4.1250202997\H,1.4028879229,-2.4205941029

,2.3876490273\H,0.7866829772,-2.0456686795,4.0097354444\N,-0.040417209

2,-0.8685337487,2.4795281799\C,-1.1899630827,-1.5018186516,2.083072324

2\H,-2.0241421555,-0.8315856807,1.8533536748\C,-1.3666237665,-2.835662

7348,1.9385948759\H,-0.5505871217,-3.5319219886,2.1519378579\C,-2.6228

665373,-3.3879771144,1.4554907506\H,-3.4141204125,-2.6625615086,1.2247

026133\C,-2.8657483153,-4.6896611369,1.2424443434\H,-2.0710981806,-5.4

103428535,1.4682502571\C,0.352599578,1.0088899234,0.8058151271\C,1.510

2776653,0.231319744,0.1901171949\C,1.4449223663,-1.1541345733,-0.00985

91416\C,2.7235686755,0.8738993358,-0.0579952004\C,2.5597848048,-1.8582

069286,-0.4578415264\H,3.0477731841,3.9423739851,-0.6477334126\C,3.832

970352,0.1601148123,-0.5086025837\H,2.8160835511,1.9421960009,0.132852

7635\C,3.7665606712,-1.2134632278,-0.7163699419\H,4.6334229031,-1.7701

364786,-1.0711354072\C,-0.9936098748,0.8192929831,0.086812613\C,-1.236

416457,-0.0634474821,-0.9676952027\C,-2.0564912985,1.6065569967,0.5439

846447\C,-2.5159638922,-0.186413716,-1.5076599937\H,0.5239942893,3.705

775694,-2.748608384\C,-3.3253651889,1.4970454628,-0.0181625663\H,-1.88

81523244,2.3237401299,1.3503381061\C,-3.5742888794,0.5880961174,-1.042

184227\H,-4.5704461658,0.4911775158,-1.4740853007\O,0.6423543745,2.378

2058793,0.8817081921\Si,0.5802419709,3.6146673042,-0.288807713\C,-0.789525925,4.796380562,0.1902632322\H,-1.7902642766,4.3787869793,0.0114884465\H,-0.7105009196,5.0639279834,1.254949073\H,-0.7057293758,5.7243181738,-0.3957924355\C,2.2270812888,4.5030487035,-0.1767734258\H,2.1615008324,5.4782131139,-0.6825801154\H,2.4927415804,4.6874803483,0.8750614479\H,0.5270150981,-1.7083160729,0.1995165617\C,0.3107441624,2.917755387,-2.0093880812\H,-0.7249069439,2.5813859786,-2.1619485736\H,0.9850701706,2.0731164106,-2.2195718017\H,-0.4391669151,-0.667200343,-1.3978713523\C,-4.4180143371,2.4012570917,0.4901020525\F,-5.6177303145,2.0261078069,0.0540729849\F,-4.4512792985,2.4186704076,1.8228059828\F,-4.2233473646,3.6632046378,0.0905222843\C,-2.7704593368,-1.2257015976,-2.5704188143\F,-3.1087030052,-2.394739849,-2.0260059952\F,-3.7666969074,-0.8620504747,-3.3788798944\F,-1.6889801663,-1.4333550358,-3.3208146145\C,5.1224687838,0.909899408,-0.7161962318\F,5.6764742322,1.2507716298,0.4491310341\F,6.0151833186,0.1886083927,-1.3902510876\F,4.9181091483,2.0439158705,-1.3938343845\C,2.418234539,-3.3467153022,-0.6451530483\F,2.1236280265,-3.9514052885,0.5124704436\F,1.4313623698,-3.6343598956,-1.4928058004\F,3.5348116618,-3.8997976998,-1.1130161492\C,-4.1470356771,-5.2377614092,0.6968994439\H,-3.9781125578,-5.7817885392,-0.2459030141\H,-4.611053014,-5.9518051847,1.3956799617\H,-4.8687501058,-4.4330406315,0.4990266366\\Version=ES64L-G09RevD.01\State=1-A\HF=-2737.4149493\RMSD=6.977e-09\RMSF=3.023e-06\Dipole=0.3971821,1.0182538,0.4884831\Quadrupole=-6.3629255,2.4769974,3.8859282,-0.4716406,3.6500927,-2.2909598\PG=C01 [X(C29H29F12N1O1Si1)]\\@

_ap_ conformation 1; ΔG298(MP2/CBS) = -2736.0618520

1\1\GINC-WORKER\FOpt\RM062X\def2SVP\C29H29F12N1O1Si1\JHIOE\23-Jul-2015

\0\\#p freq def2svp m062x opt empiricaldispersion=gd3 int=ultrafine\\t

itle\\0,1\C,-0.1598325969,-0.6269850967,2.3388465539\C,-1.4144017133,-

0.9385809028,3.1771353119\C,-1.5438866902,0.2452625405,4.1426778944\C,

-0.9776679103,1.4179542088,3.3417527458\H,0.701820198,-1.2250880719,2.

6861129436\H,-2.2968999627,-0.990575386,2.5239191641\H,-1.3307126588,-

1.9069885674,3.6834207121\H,-1.7468471556,1.8925324516,2.7026777102\H,

-0.5407821694,2.2065490859,3.9732527881\N,0.0746028477,0.7824427542,2.

5687920092\C,1.1661946995,1.4562131128,2.0823446029\H,2.020442528,0.81

98283997,1.8282037807\C,1.2576991862,2.7891822175,1.8727008119\H,0.399

9571204,3.4387349729,2.0765543173\C,2.4533222274,3.3907767825,1.302571

3221\H,3.2866613233,2.706943655,1.0943500527\C,2.5876719458,4.68388087

27,0.9734459722\H,1.7500045761,5.3617006473,1.1754688052\C,-0.34687180

77,-1.0292215821,0.8214702714\C,-1.5136642126,-0.2415038443,0.22741976

34\C,-1.4801596179,1.1538618949,0.1119809151\C,-2.6920279881,-0.896539

9859,-0.1318328153\C,-2.5851674115,1.8543839621,-0.3649671845\H,-3.013

1743439,-3.9828206436,-0.7121950809\C,-3.7883970882,-0.1880622643,-0.6

217473019\H,-2.7696572467,-1.9752772949,-0.0050966347\C,-3.7506789897,

1.1962239519,-0.7471288689\H,-4.6070732356,1.7496849932,-1.1312067242\

C,0.9838994974,-0.8080919481,0.0811076332\C,1.2005219891,0.1300608356,

-0.9318681048\C,2.0601993312,-1.6055032685,0.4822003908\C,2.4681693452

,0.2902178823,-1.4874557449\H,-0.4714445194,-3.6973610627,-2.779913605

8\C,3.3182279336,-1.4585474621,-0.097837228\H,1.9142680035,-2.35701015

71,1.2610479524\C,3.540574788,-0.4997458305,-1.0806083134\H,4.52810180

68,-0.3742251417,-1.5254616499\O,-0.635193479,-2.4011271988,0.86303901

28\Si,-0.5548179802,-3.6226645575,-0.3217363267\C,0.8242240567,-4.7991

449026,0.1461907391\H,1.8222698612,-4.38420567,-0.0522442597\H,0.76135
27347,-5.0589694901,1.2138920174\H,0.7308374626,-5.7314594615,-0.43140
98681\C,-2.1928768568,-4.5293522627,-0.2241633087\H,-2.1094507553,-5.5
081208875,-0.7200772117\H,-2.4709362851,-4.7055757245,0.8257285854\H,-
0.5886782557,1.7186052661,0.3910872282\C,-0.287920291,-2.9070276988,-2
.0350891323\H,0.7390520424,-2.5404175037,-2.1762370688\H,-0.9846738969
,-2.0815314208,-2.2478481841\H,0.3926556691,0.7540964975,-1.3095976575
\C,4.4273825912,-2.3757559604,0.3470428096\F,5.6166603034,-1.965431335
4,-0.08602595\F,4.4807195416,-2.4619041743,1.6764654435\F,4.2401179843
,-3.6175152553,-0.1148210175\C,2.7081286556,1.3777825348,-2.5046288841
\F,3.2050189226,2.4736379812,-1.9282532073\F,3.5870266833,0.9891116208
,-3.4302508166\F,1.5846414311,1.7270072675,-3.1279704153\C,-5.03101063
04,-0.9628620513,-0.9731396496\F,-5.6541247964,-1.4046545293,0.1211277
093\F,-5.8999590247,-0.2259348812,-1.6612024309\F,-4.73523015,-2.03922
64525,-1.7095841354\C,-2.4801774241,3.3557374061,-0.4286836716\F,-2.36
62821648,3.8791772715,0.798174223\F,-1.4019554154,3.7377361785,-1.1124
018149\F,-3.5471063044,3.9079956957,-1.002034767\C,3.7979619214,5.2715
745648,0.3184899893\H,3.5469111758,5.7018178754,-0.6640560311\H,4.2286
637198,6.0865977697,0.921307973\H,4.5740259454,4.5090148941,0.16503798
07\H,-0.9198950508,0.0820736384,5.0332296821\H,-2.5765369704,0.4112462
454,4.475062248\\Version=ES64L-G09RevD.01\State=1-A\HF=-2737.4120208\R
MSD=9.455e-09\RMSF=7.378e-06\Dipole=-0.2997064,-0.9843126,0.5971669\Qu
adrupole=-6.9542798,2.0392006,4.9150792,-0.0777253,-3.7235967,1.546787
6\PG=C01 [X(C29H29F12N1O1Si1)]\\@

***sc-endo* conformation 0; ΔG298(MP2/CBS) = -2736.0520577**

1\1\GINC-LOGIN\FOpt\RM062X\def2SVP\C29H29F12N1O1Si1\JHIOE\29-Jun-2015\

0\\#p m062x/def2svp empiricaldispersion=gd3 int=ultrafine opt freq scf

=tight\\title\\0,1\C,-0.3037674647,-0.5308584101,2.4030711308\C,-1.545

2384396,-0.512598728,3.3071224999\C,-2.217758685,0.8395485374,3.010693

7414\C,-1.0731416174,1.7417784618,2.5037930046\H,0.4975687532,-1.15892

28687,2.8253642442\H,-2.2137713983,-1.3716749028,3.1984274531\H,-1.176

61053,-0.5263335879,4.3425882684\H,-2.9867230808,0.7287887985,2.237539

742\H,-2.6949083926,1.2540191668,3.9077986257\H,-1.3085511062,2.172256

479,1.5133628262\H,-0.8470831936,2.5797910345,3.1834717841\N,0.0788484

654,0.8620853858,2.4512882464\C,1.3511805896,1.3255108611,2.2325473274

\H,2.1400658158,0.5887251615,2.4186735386\C,1.6963521023,2.5587836386,

1.8033959624\H,0.9239508192,3.2920496794,1.5548031733\C,3.0813207339,2

.899035412,1.5153073965\H,3.8334374209,2.1525827909,1.8053410983\C,3.4

878009007,4.0026171597,0.8681076789\H,2.7305680097,4.7348851288,0.5645

110506\C,-0.5374565048,-1.0287647161,0.9085002251\C,0.7485397497,-0.65

45595617,0.165578964\C,1.9846934904,-1.2124887535,0.5120364879\C,0.751

3841537,0.4432269531,-0.6922049741\C,3.1700987804,-0.6958427457,-0.003

2464613\H,-1.6040870465,1.4379520611,-2.4101072935\C,1.9416070099,0.95

85992825,-1.2006662278\H,-0.1791789291,0.9670338895,-0.9002233618\C,3.

1657195639,0.3954781633,-0.8689441806\H,4.097935235,0.8180289845,-1.24

37749747\C,-0.8760144463,-2.5290833457,0.8577291482\C,-0.0221110364,-3

.5324503227,0.3932439386\C,-2.1713785385,-2.9089489653,1.2343784523\C,

-0.4377388251,-4.8649351873,0.35207821\H,-2.315793797,-1.6718264194,-3

.1410650095\C,-2.5794849396,-4.2369896367,1.1904853373\H,-2.8886174758

,-2.1449922999,1.5323427882\C,-1.713106521,-5.2376808042,0.7572486128\

H,-2.0310834264,-6.279450174,0.7220916208\O,-1.6285310282,-0.299631079

2,0.4127051191\Si,-2.5419771382,-0.4440439223,-1.0198492518\C,-4.30359
0709,-0.851372446,-0.5288890694\H,-4.4290897668,-1.9008351704,-0.22833
41759\H,-4.635561124,-0.2087698464,0.3010805924\H,-4.9770488312,-0.668
7383761,-1.3800824279\C,-2.5229984184,1.2448519003,-1.8378212694\H,-3.
3692509958,1.3281851674,-2.5362577869\H,-2.6319985556,2.0391365236,-1.
0834717125\H,2.049928998,-2.0222402246,1.2413030293\C,-1.8300530889,-1
.7543049977,-2.1561382296\H,-2.0056051091,-2.7714780448,-1.7763716795\
H,-0.7476814466,-1.6208025661,-2.3060600192\H,0.9694344467,-3.30055607
52,0.0086697755\C,-3.9982926446,-4.5649128237,1.5763813859\F,-4.156223
031,-5.8607631333,1.8324857386\F,-4.3757329166,-3.8809798541,2.6575359
571\F,-4.8525592986,-4.2449674716,0.5972734916\C,0.5457543934,-5.90460
57097,-0.1227437115\F,1.4634845143,-6.1618483387,0.8105857784\F,-0.056
5271711,-7.0542851252,-0.420723292\F,1.1987482937,-5.489561019,-1.2089
457851\C,1.8608143145,2.1966682624,-2.0542442647\F,1.163358312,3.15660
62948,-1.4438222434\F,3.0631918123,2.6857598043,-2.3461189506\F,1.2339
712855,1.9458601973,-3.2101858663\C,4.4765273452,-1.2463025068,0.50228
73718\F,4.8131741803,-0.6720127928,1.664495566\F,4.4035372591,-2.55910
0062,0.7254768678\F,5.4738805891,-1.0277169261,-0.3504203412\C,4.90752
09318,4.2995668029,0.4980619397\H,5.0223384812,4.3764843337,-0.5953187
088\H,5.2453915153,5.2591125369,0.9202367724\H,5.5842056127,3.51162268
81,0.8582031254\\Version=ES64L-G09RevD.01\State=1-A\HF=-2737.4065048\R
MSD=5.453e-09\RMSF=2.274e-06\Dipole=-1.2249525,0.0353888,0.0610567\Qua
drupole=0.2705378,-5.6814551,5.4109173,-4.8822133,0.8212037,-0.5953863
\PG=C01 [X(C29H29F12N1O1Si1)]\\@

Dienamines Z-1C

sc-exo conformation 0; ΔG298(MP2/CBS) = -2736.0619620

1\1\GINC-WORKER\FOpt\RM062X\def2SVP\C29H29F12N1O1Si1\JHIOE\14-Jun-2015

\0\\#p m062x/def2svp empiricaldispersion=gd3 int=ultrafine opt freq sc

f=tight\\title\\0,1\C,-0.1598009445,-1.2964179647,-1.8419144276\C,0.20

15531302,-0.4076137759,-3.0430431939\C,-1.1104498819,0.272149585,-3.49

49457612\C,-2.2402338773,-0.437758424,-2.727547093\H,0.3401267428,-2.2

76763244,-1.8849893292\H,0.9925497608,0.3157425711,-2.8012877469\H,0.5

968506834,-1.0452405997,-3.8448275793\H,-1.1076205405,1.3471790215,-3.

2758262419\H,-1.2447175761,0.168503445,-4.5787543504\H,-2.7718762628,0

.259774916,-2.0507549317\H,-3.0015944735,-0.8793087847,-3.3911091744\N

,-1.5829892519,-1.4978937668,-1.9905722614\C,-2.2935578839,-2.39770651

37,-1.2372341361\H,-1.6818596779,-3.1819720886,-0.7821974746\C,-3.6289

880845,-2.3665062757,-1.0203533593\H,-4.2228370453,-1.5452471416,-1.42

64137334\C,-4.2904894528,-3.3773143923,-0.2082938696\H,-3.6453630974,-

4.1891990009,0.1464280331\C,-5.5832886119,-3.4063255281,0.1594546722\H

,-5.9074633448,-4.2382475613,0.7919048443\C,0.218916093,-0.7174399146,

-0.4295811534\C,1.7048089199,-0.358971923,-0.327092922\C,2.6599521062,

-1.2009723303,-0.9075752766\C,2.1551603772,0.6811683751,0.4880226272\C

,4.0173796132,-1.0086261217,-0.670944277\H,2.8911213597,-1.6427874624,

2.0449871199\C,3.5175158627,0.8632572347,0.7259158754\H,1.4432260204,1

.3562732185,0.9662634733\C,4.4640378093,0.0234952613,0.1511220774\H,5.

5273466441,0.1658566499,0.3420548484\C,-0.7144260974,0.4571012636,-0.1

443198001\C,-0.5028911489,1.7226829771,-0.6933059968\C,-1.8917961476,0

.2294077299,0.5719403153\C,-1.453485159,2.7313052893,-0.5344348878\H,0

.7158624233,0.2830932146,2.929413642\C,-2.8298091842,1.2439181215,0.73

40389618\H,-2.0909053772,-0.7624764216,0.9782843303\C,-2.6248575191,2.5062491242,0.1816549458\H,-3.3601861388,3.3000794289,0.3107852621\O,-0.0372944323,-1.7711900519,0.4618022646\Si,0.4231036667,-2.0625230451,2.0711208238\C,-0.6755039559,-3.5014763101,2.527226234\H,-1.7356997747,-3.2252565958,2.4199240644\H,-0.5078277373,-3.8207895952,3.5663342086\H,-0.4799643763,-4.3608582264,1.8688804337\C,2.2392061344,-2.5221733122,2.1621571954\H,2.5112644292,-3.2561867695,1.3886418845\H,2.4561425083,-2.9691083404,3.1448549927\H,2.3525626985,-2.0370786086,-1.53744136\C,0.0910185703,-0.586178108,3.1817119879\H,-0.9643496797,-0.2782178829,3.1663379334\H,0.3418269033,-0.8721220838,4.2158340272\H,0.4082764783,1.9378871126,-1.2572269528\C,-4.1028416393,0.9257245925,1.4744253427\F,-4.7395934087,2.0311928006,1.8601917176\F,-4.9460915693,0.225409293,0.7126204525\F,-3.8573816797,0.1941498819,2.5632454542\C,-1.1847138014,4.0632657008,-1.1830563916\F,-1.1443888964,3.9446018757,-2.5160293924\F,-2.1194784602,4.962500076,-0.8886064945\F,-0.0051761285,4.5578198088,-0.8062227088\C,3.9268437186,1.9589156572,1.6756798147\F,3.4961625776,1.6946803799,2.9130751953\F,5.2482206287,2.1039695976,1.7303556072\F,3.3982254976,3.1300340648,1.3220946897\C,4.9910481104,-1.9920170013,-1.267575024\F,4.746091066,-2.1897322241,-2.5636991472\F,6.2508528227,-1.5812069089,-1.1458980859\F,4.8936203076,-3.1811603292,-0.6675948462\C,-6.6377573845,-2.4036117377,-0.1983416273\H,-7.5025896807,-2.8942889942,-0.6714144395\H,-7.0144185314,-1.8922935994,0.7018312864\H,-6.2681637492,-1.6314463081,-0.8841851908\\Version=ES64L-G09RevD.01\State=1-A\HF=-2737.4133104\RMSD=8.746e-09\RMSF=1.556e-06\Dipole=0.536801,-0.28833,-0.2287167\Quadrupole=-6.5667534,-2.6817451,9.2484986,-4.2824765,1.3455307,-4.0489024\PG=C01 [X(C29H29F12N1O1Si1)]\\@

sc-exo conformation 1; ΔG298(MP2/CBS) = -2736.0617136

1\1\GINC-LOGIN\FOpt\RM062X\def2SVP\C29H29F12N1O1Si1\JHIOE\27-Jul-2015\

0\\#p m062x/def2svp empiricaldispersion=gd3 int=ultrafine opt freq scf

=tight\\title\\0,1\C,-0.3659886243,-1.2061947937,-1.7987159643\C,0.028

6200525,-0.340080471,-3.0053289094\C,-1.2100531688,0.5206169008,-3.309

6335335\C,-2.3984351061,-0.2969488027,-2.7875680473\H,0.0515999633,-2.

2247246537,-1.8556515351\H,0.9238023883,0.2694512378,-2.8157710938\H,0

.2555109217,-0.9989697946,-3.8557841612\H,-1.1505920268,1.4850594153,-

2.7875215255\H,-1.3014961856,0.7388396512,-4.3808507728\H,-3.126326003

2,0.3389156839,-2.2548761651\H,-2.9516149452,-0.815520764,-3.591374437

6\N,-1.804765961,-1.2804995283,-1.9001546732\C,-2.56688835,-2.19879731

18,-1.2282641465\H,-1.9944510755,-2.9973163291,-0.7487128948\C,-3.9156

557779,-2.1653294057,-1.1106595006\H,-4.4762518641,-1.3409014041,-1.55

58814954\C,-4.6460958446,-3.1996132014,-0.3917150717\H,-4.0505828704,-

4.0592609929,-0.0644032411\C,-5.9562765818,-3.1956354342,-0.0904525706

\H,-6.3542572127,-4.0615082593,0.4465937903\C,0.0964042823,-0.65857448

29,-0.4011167066\C,1.6227607918,-0.6535164974,-0.2545192747\C,2.190711

03,-0.0114821456,0.8489187599\C,2.4750499379,-1.3395697034,-1.12462711

15\C,3.5635494126,-0.054075806,1.078369741\H,1.8805118388,-1.730137911

2,2.9731372402\C,3.8489790031,-1.3768087704,-0.891361599\H,2.089405000

4,-1.8468102928,-2.0083991624\C,4.4092632759,-0.7356657812,0.209836571

3\H,5.4855859821,-0.7567066856,0.3814126845\C,-0.5154899341,0.72700776

58,-0.212113173\C,0.1663854953,1.9105778854,-0.4994457631\C,-1.8659417

333,0.7993181796,0.1412561998\C,-0.4967012206,3.1369440824,-0.44481888

46\H,-0.8582399944,-0.3237123347,4.1726241793\C,-2.5163518957,2.027913

5168,0.1959476512\H,-2.4183884927,-0.1196996808,0.3558512181\C,-1.8424

209737,3.2109049613,-0.0975059183\H,-2.3548771341,4.1716473571,-0.0521

731807\O,-0.4433568614,-1.5647455562,0.5186812671\Si,-0.5186944951,-1.7496404511,2.2008150189\C,-1.9272024017,-2.9585735308,2.4021241154\H,-2.8460751469,-2.5614611313,1.9426341176\H,-1.6896427776,-3.9154042149,1.9129021229\H,-2.1308392101,-3.160892936,3.4642394857\C,1.0885347726,-2.4788589311,2.8343323776\H,0.9126614949,-2.9616625799,3.8082250776\H,1.4586066669,-3.247614187,2.1389032464\H,1.5542673954,0.5448023664,1.5415660106\C,-0.9127044254,-0.1401268664,3.087687441\H,-1.9284678611,0.2119895756,2.85631673\H,-0.2139011852,0.6782051449,2.8584635892\H,1.2214939529,1.8919641957,-0.7803806923\C,-3.9778433762,2.0323917674,0.560136823\F,-4.4656511824,3.2666298247,0.6586359724\F,-4.7046062322,1.3835822042,-0.3576607876\F,-4.1874981456,1.4157798305,1.7249669388\C,0.2535670091,4.3776894081,-0.8510590217\F,0.3522720157,4.458739823,-2.1816619218\F,-0.3510064539,5.4859498617,-0.4282600268\F,1.4962353273,4.3764455608,-0.3683773046\C,4.7358103921,-2.1639643923,-1.8227145889\F,4.2419515525,-2.1889334507,-3.0615569153\F,5.9626051696,-1.6481040683,-1.8806021725\F,4.8567078333,-3.4302404869,-1.4213767535\C,4.1043361396,0.6371593837,2.3031374135\F,3.6685480809,1.8943548489,2.3800084988\F,3.7008611027,0.0186533988,3.4185155253\F,5.4341424629,0.6607966541,2.3159105157\C,-6.935554558,-2.1090818573,-0.4222322664\H,-7.5923856385,-2.3990686269,-1.258881872\H,-7.591321882,-1.9019167303,0.4364048993\H,-6.4373528847,-1.1687747303,-0.6926875055\\Version=ES64L-G09RevD.01\State=1-A\HF=-2737.4132512\RMSD=9.709e-09\RMSF=1.827e-06\Dipole=0.1757287,-0.2622871,-0.226949\Quadrupole=-7.8182235,-1.6888129,9.5070364,-3.0727222,0.2963493,-3.6599303\PG=C01 [X(C29H29F12N1O1Si1)]\\@

ap **conformation 0; ΔG298(MP2/CBS) = -2736.0622160**

1\1\GINC-WORKER\FOpt\RM062X\def2SVP\C29H29F12N1O1Si1\JHIOE\18-Jun-2015

\0\\#p m062x/def2svp empiricaldispersion=gd3 int=ultrafine opt freq sc

f=tight\\title\\0,1\C,-0.53748425,-1.0323210615,-1.8153704667\C,-0.147

9887853,-0.0724343735,-2.9472408737\C,-1.3628102392,0.849510995,-3.128

2763355\C,-2.561793768,0.0034127795,-2.6826944332\H,-0.1111947189,-2.0

336583047,-1.9923220631\H,0.7824989201,0.4635419394,-2.7219270849\H,0.

0214090329,-0.6622627364,-3.8590993735\H,-1.2716758146,1.7418955022,-2

.4934243854\H,-1.4684393056,1.1962100074,-4.1638065825\H,-3.2792920085

,0.5984532879,-2.0936973127\H,-3.1218003385,-0.431951551,-3.5298434104

\N,-1.9782285375,-1.0667914499,-1.888005444\C,-2.7525635148,-1.9728568

803,-1.2105084275\H,-2.2103458841,-2.8429924958,-0.8261714743\C,-4.081

2496023,-1.8623405322,-0.9755083043\H,-4.6219139035,-0.9884962482,-1.3

450960208\C,-4.8127381869,-2.8692545572,-0.2206080954\H,-4.2446980825,

-3.7665257578,0.0489946386\C,-6.0913748642,-2.7916197793,0.1854424066\

H,-6.4942502909,-3.6394416744,0.7470216993\C,0.033662351,-0.5895213896

,-0.4055056592\C,-0.5450257414,0.7789440033,-0.0645559355\C,-1.9112079

022,0.9557343102,0.1910409405\C,0.2624434277,1.9141948437,-0.137223569

5\C,-2.438356751,2.2311757108,0.3756185105\H,3.3880288499,1.9111705097

,0.2586951049\C,-0.2746859521,3.1867751913,0.0519189874\H,1.3199152822

,1.8086232886,-0.3763475428\C,-1.6299501466,3.3632646357,0.3113697605\

H,-2.0475124734,4.358503012,0.4615075014\C,-0.2876986537,-1.6828257801

,0.6269842321\C,-1.0902677238,-1.5208686625,1.7565793417\C,0.304312443

6,-2.9341157324,0.4144716087\C,-1.327060556,-2.5922011464,2.6185522537

\H,2.9531816351,0.0280928083,2.9226672818\C,0.0816876732,-3.9914195997

,1.2907459174\H,0.9615684422,-3.0815720264,-0.4451403398\C,-0.74933531

78,-3.8371947073,2.3981321947\H,-0.935097903,-4.6680728578,3.078491782

8\O,1.4223850081,-0.5257005063,-0.5845788455\Si,2.7107896745,-0.494550
5216,0.5290134174\C,3.6579289988,-2.1001287182,0.3627515728\H,3.116340
6086,-2.9556639186,0.790321241\H,3.8660785658,-2.3152794151,-0.6963373
333\H,4.6234904748,-2.0219325,0.8853850624\C,3.8056146793,0.9290132669
,-0.0074477534\H,4.7907782551,0.8476323821,0.4762058711\H,3.9626130429
,0.9033662947,-1.0963059554\H,-2.5893034258,0.0999616309,0.2324443557\
C,2.0979657659,-0.2423698454,2.2836664109\H,1.6406439559,-1.1526735642
,2.6973725164\H,1.3633008465,0.5752774816,2.3473893101\H,-1.5367453308
,-0.5582387076,2.0019072392\C,0.7891901412,-5.2980715664,1.0416186663\
F,0.2490882017,-6.2958400055,1.7365792589\F,0.7567434157,-5.6299195742
,-0.2491370268\F,2.0786432602,-5.2206997295,1.3905239168\C,-2.27058167
89,-2.3884712956,3.7770486987\F,-3.539969514,-2.4495120521,3.378801357
8\F,-2.0998934557,-3.3163555202,4.7187887543\F,-2.0902556011,-1.193767
8527,4.3422146158\C,0.6427515458,4.3728423866,-0.0878940512\F,0.942917
2631,4.6034340238,-1.367775333\F,0.0990525406,5.483998735,0.4034401731
\F,1.7990650682,4.1668839171,0.5501345806\C,-3.9170114994,2.3428524083
,0.6449099642\F,-4.631719101,1.8424095862,-0.3724230391\F,-4.263218969
8,1.6549971524,1.7318460887\F,-4.299165744,3.6054272282,0.8191518751\C
,-7.0285459773,-1.6443725169,-0.0457017141\H,-7.8019644143,-1.90043605
4,-0.7881065445\H,-7.5568844736,-1.3847035357,0.8837710454\H,-6.509317
2185,-0.7419233644,-0.3937383045\\Version=ES64L-G09RevD.01\State=1-A\H
F=-2737.4141791\RMSD=6.038e-09\RMSF=2.419e-06\Dipole=1.0432658,0.15852
4,-0.6636848\Quadrupole=2.3950311,-7.199436,4.8044049,-2.0638169,2.311
9985,-0.8317058\PG=C01 [X(C29H29F12N1O1Si1)]\\@

_ap_ conformation 1; ΔG298(MP2/CBS) = -2736.0596931

1\1\GINC-LOGIN\FOpt\RM062X\def2SVP\C29H29F12N1O1Si1\JHIOE\23-Jul-2015\

0\\#p freq def2svp m062x opt empiricaldispersion=gd3 int=ultrafine\\ti

tle\\0,1\C,0.0401254471,-0.5874182351,2.3508150174\C,-1.115111587,-1.1

636371789,3.1924707446\C,-1.533360197,-0.0180750743,4.1210679026\C,-1.

2463472062,1.2318185678,3.2893740604\H,1.0141178204,-0.9623188769,2.71

25680929\H,-1.951349755,-1.442955345,2.5361123054\H,-0.8106770829,-2.0

701163094,3.7279726608\H,-2.0946062331,1.4898371116,2.6266822236\H,-1.

0211154315,2.1201760555,3.8987159652\N,-0.0581307092,0.8423967748,2.55

0114498\C,0.8502985784,1.7444507312,2.0556709311\H,1.8409737619,1.3289

96837,1.8395722708\C,0.600803789,3.0498485696,1.8014131198\H,-0.407894

9421,3.4370680237,1.9701256564\C,1.6155378998,3.941840788,1.2595401656

\H,2.6263494723,3.5252432706,1.1905754937\C,1.4218758646,5.1943904081,

0.8130381656\H,2.2925636855,5.728436518,0.4213634051\C,-0.0445827049,-

1.0521932686,0.8425223247\C,-1.3413310462,-0.5302467369,0.2250202618\C

,-1.57897081,0.8398436969,0.0599836873\C,-2.3696842739,-1.4133451524,-

0.1046867665\C,-2.7992359868,1.297562543,-0.4289686966\H,-2.0479973704

,-4.5173563225,-0.6161801135\C,-3.5836829634,-0.9469288815,-0.60876618

15\H,-2.234805927,-2.4822006338,0.0556553286\C,-3.8164512511,0.4135251

478,-0.7784268848\H,-4.7653800334,0.7767593343,-1.1721585371\C,1.22019

163,-0.5857102554,0.1009141821\C,1.2475051031,0.3198064019,-0.96196291

45\C,2.4342190781,-1.1292644852,0.535095522\C,2.4587415605,0.694556293

8,-1.5415125748\H,0.3855964123,-3.7724478771,-2.6967829048\C,3.6376390

337,-0.7683372619,-0.0648449192\H,2.4397570773,-1.8556990866,1.3504702

66\C,3.6656092198,0.1575501187,-1.103595354\H,4.6081394883,0.449495497

8,-1.5671963111\O,-0.0495572301,-2.4529597171,0.9145312974\Si,0.285467

7195,-3.6592454809,-0.2404781432\C,1.8737775228,-4.5159320062,0.257411

995\H,2.7653162697,-3.906222386,0.0544838796\H,1.8572633683,-4.7620031

417,1.3300701259\H,1.9812527561,-5.4583340919,-0.3010372069\C,-1.13396

13918,-4.8778761821,-0.1218528371\H,-0.8536657117,-5.827756985,-0.6015

426316\H,-1.3706527849,-5.0889259278,0.931751657\H,-0.8138231947,1.576

4639688,0.310385156\C,0.4102665671,-2.9449057476,-1.9704200972\H,1.346

3250291,-2.3884573724,-2.1228471213\H,-0.4336446696,-2.2759700584,-2.1

997737973\H,0.3314966312,0.745576273,-1.3680212013\C,4.9072353617,-1.4

275147665,0.4076389244\F,5.9902215444,-0.7765775765,-0.0095685508\F,4.

9538430032,-1.4944294353,1.7383041653\F,4.9960332984,-2.6826535183,-0.

047593933\C,2.4663780014,1.745111967,-2.6235767194\F,2.6050263063,2.96

58034934,-2.1075577197\F,3.4763222017,1.5580491291,-3.4748004285\F,1.3

331889893,1.7341369082,-3.3245230429\C,-4.6535881594,-1.9591843011,-0.

9228252861\F,-5.1805864212,-2.4697385381,0.1919898238\F,-5.6478481621,

-1.4303032664,-1.6322416274\F,-4.1556911079,-2.9861632704,-1.619598013

5\C,-2.9869353057,2.788809118,-0.5321915347\F,-3.0093203721,3.35290114

29,0.6835805173\F,-1.9854398028,3.3605198547,-1.2002769532\F,-4.125475

1305,3.1097244978,-1.1418611242\C,0.1209155773,5.9377268634,0.77708712

9\H,0.1250243223,6.7854141608,1.4811348366\H,-0.051625846,6.3601771653

,-0.2244976268\H,-0.7384586706,5.2989552989,1.016692213\H,-0.901975348

5,-0.0050541602,5.0211774565\H,-2.5811125713,-0.0902276197,4.439549325

9\\Version=ES64L-G09RevD.01\State=1-A\HF=-2737.4114455\RMSD=5.816e-09\

RMSF=4.379e-06\Dipole=-0.1580075,-1.0347131,0.6514286\Quadrupole=-6.36

07069,1.4910542,4.8696527,-2.6542415,-3.5099857,0.8320466\PG=C01 [X(C2

9H29F12N1O1Si1)]\\@

***sc-endo* conformation 0; ΔG298(MP2/CBS) = -2736.0518343**

1\1\GINC-WORKER\FOpt\RM062X\def2SVP\C29H29F12N1O1Si1\JHIOE\29-Jun-2015

\0\\#p m062x/def2svp empiricaldispersion=gd3 int=ultrafine opt freq sc

f=tight\\title\\0,1\C,-0.4260192049,-0.5311959972,2.4254543991\C,-1.71

8834233,-0.4054376978,3.2476211494\C,-2.2438884304,1.0094301674,2.9349

382942\C,-1.0091631465,1.7919150551,2.4391331336\H,0.2985237026,-1.220

040727,2.8898961216\H,-2.4599955753,-1.1889855109,3.0681043034\H,-1.42

98503924,-0.4741672788,4.3055850341\H,-3.0144942524,0.9757328558,2.156

751636\H,-2.681849854,1.4744606971,3.8272508473\H,-1.1623280301,2.1780

505477,1.4140308388\H,-0.7498502161,2.65010321,3.0795500188\N,0.068523

9103,0.824587244,2.5010581846\C,1.3904219474,1.1778196609,2.4060985076

\H,2.093172488,0.3921288344,2.7052132441\C,1.8705354896,2.3684834194,1

.9830052486\H,1.1726712628,3.1272627177,1.621580425\C,3.302105315,2.61

76842664,1.8964288689\H,3.9408814169,1.8199894004,2.2927664669\C,3.908

0474752,3.6840736934,1.3441152297\H,5.0022343048,3.6892994544,1.332353

4953\C,-0.6332201453,-1.0169422855,0.9213139649\C,0.6363543847,-0.5833

058972,0.1854013863\C,1.8909692911,-1.1030718601,0.5201725941\C,0.5992

664715,0.5258816686,-0.6567913979\C,3.0577979543,-0.5451350646,0.00468

75823\H,-1.8418308956,1.4706192049,-2.3203900847\C,1.771410306,1.08710

90265,-1.1585050065\H,-0.3520479984,1.0099989745,-0.8693507712\C,3.015

8755596,0.5573906074,-0.8429906046\H,3.9323321302,1.0134193248,-1.2155

774449\C,-0.9083647932,-2.530634462,0.8504257925\C,-0.0185871077,-3.48

39419628,0.347372613\C,-2.1763463938,-2.9796319282,1.2433623397\C,-0.3

719124722,-4.8330888565,0.2847511926\H,-2.4063723216,-1.6751821835,-3.

1355630046\C,-2.5241191048,-4.3241584052,1.1739118712\H,-2.9257813751,

-2.2598574994,1.5681498947\C,-1.6210190809,-5.273814457,0.7034308977\H

,-1.8915269218,-6.3281124435,0.6490384736\O,-1.7513527139,-0.326229147

2,0.432461077\Si,-2.6755860794,-0.4995512872,-0.9887017276\C,-4.405701
1601,-1.0096982711,-0.4818694108\H,-4.4728302251,-2.0726765066,-0.2114
757278\H,-4.7509395254,-0.4099269585,0.3745068958\H,-5.1048780356,-0.8
351750717,-1.3137569557\C,-2.7545542386,1.2052018752,-1.7675291412\H,-
3.5949720982,1.253679471,-2.4761951889\H,-2.9240447775,1.970289358,-0.
9942000809\H,1.9829105046,-1.9203119775,1.2390900745\C,-1.9077097755,-
1.7489132844,-2.1564570016\H,-2.0261612892,-2.7803975541,-1.7934270285
\H,-0.8351985267,-1.5561631028,-2.312709067\H,0.9531683027,-3.19851073
25,-0.0514072236\C,-3.9218818175,-4.7271798833,1.5661937602\F,-4.01152
61736,-6.0318048458,1.811014418\F,-4.3284033843,-4.0733114938,2.654804
0188\F,-4.7967057335,-4.4435600809,0.5937884571\C,0.6497733956,-5.8151
983545,-0.2305342305\F,1.592827607,-6.0528344665,0.6824158359\F,0.0949
773552,-6.9835851917,-0.5476649851\F,1.2655166758,-5.3449689603,-1.315
8704201\C,1.6476983371,2.3436023914,-1.9775409459\F,1.1114281768,3.334
0067028,-1.2580197967\F,2.8237542394,2.7670316815,-2.4333699447\F,0.84
39736996,2.1596281654,-3.0311903298\C,4.3728623989,-1.0998019152,0.482
1382606\F,4.5806629081,-0.7862074844,1.7680945152\F,4.3963759071,-2.43
18995709,0.4049261457\F,5.4012716624,-0.6292859753,-0.2160937992\C,3.2
377676009,4.8743022858,0.7268061674\H,3.6253344648,5.8099823222,1.1582
974068\H,3.4339426876,4.9181610993,-0.3567865889\H,2.1494919557,4.8622
347002,0.8639600161\\Version=ES64L-G09RevD.01\State=1-A\HF=-2737.40621
41\RMSD=8.494e-09\RMSF=3.228e-06\Dipole=-1.3121296,0.061524,0.0344004\
Quadrupole=-0.2369142,-5.2068731,5.4437873,-5.0101659,0.6398226,-0.682
9905\PG=C01 [X(C29H29F12N1O1Si1)]\\@

Predienamines 1c

conformation 0; ΔG298(MP2/CBS) = -2736.4932382

1\1\GINC-WORKER\FOpt\RM062X\def2SVP\C29H30F12N1O1Si1(1+)\JHIOE\29-Jun-

2015\0\\#p m062x/def2svp empiricaldispersion=gd3 int=ultrafine opt fre

q scf=tight\\title\\1,1\C,-0.1471786924,-1.0794807868,-1.9346743674\C,

0.2387867614,-0.1467170792,-3.0867378991\C,-1.0368288381,0.6174011,-3.

5035263239\C,-2.2109286743,-0.0748036345,-2.7972104623\H,0.2753864234,

-2.086267235,-2.0397198747\H,1.0544671117,0.5268005641,-2.7948522106\H

,0.6164417702,-0.7490682848,-3.922908408\H,-0.992168622,1.6735375072,-

3.2142102572\H,-1.1679727148,0.5884783031,-4.5912268934\H,-2.725441761

,0.5884094284,-2.083623693\H,-2.9554108546,-0.4825700753,-3.4933767148

\N,-1.614703812,-1.1962067771,-2.043557541\C,-2.3041374827,-2.09478697

36,-1.413162374\H,-1.728764064,-2.8683549145,-0.8960862869\C,-3.730794

8591,-2.0780815678,-1.2900922809\H,-4.313408763,-1.2867691746,-1.76568

76888\C,-4.3347965159,-2.9803183048,-0.4830128887\H,-3.7149497407,-3.7

535025215,-0.0089249565\C,-5.7839110836,-3.0000508344,-0.1600944654\H,

-6.3076184594,-2.2201542714,-0.7305707318\C,0.2141085786,-0.6136893817

,-0.475326827\C,1.7135420289,-0.3355644667,-0.3496277094\C,2.192119169

,0.6164731546,0.5512429478\C,2.6367130168,-1.1626436825,-0.9974438285\

C,3.5585774605,0.7256599602,0.808028836\H,2.8441588529,-1.9234792543,1

.8449299151\C,3.9982138976,-1.042769044,-0.7400450656\H,2.3137938548,-

1.9318471523,-1.7011946321\C,4.4759387163,-0.0989160522,0.1670421628\H

,5.543447568,-0.0107734926,0.3711955311\C,-0.6688294206,0.5878841428,-

0.1296113718\C,-0.4080098538,1.8706893539,-0.617667184\C,-1.8567427736

,0.3720517933,0.5702650418\C,-1.3346586849,2.8965608191,-0.434469131\H

,0.3224133383,-1.1671398399,4.1363589943\C,-2.7763070743,1.4016616022,

0.7492470063\H,-2.0770681374,-0.620541702,0.9651370269\C,-2.5299055731 ,2.6765682024,0.2467524604\H,-3.2496433867,3.4839273008,0.3850669175\O ,-0.131919266,-1.7098986565,0.3231849009\Si,0.3608811544,-2.1708381672 ,1.9095322289\C,-0.8445191591,-3.5596458282,2.2412891654\H,-1.88184595 7,-3.1898266884,2.2339229439\H,-0.7464601801,-4.3578570661,1.489882289 4\H,-0.663034265,-4.0093468241,3.2285453435\C,2.1322669437,-2.76090872 83,1.8983635891\H,2.3346660023,-3.3063551981,2.833248933\H,2.338187792 6,-3.4436264326,1.0605568398\H,1.5041255228,1.2782334401,1.080652218\C ,0.1287794215,-0.7693294707,3.1271405747\H,-0.8923547742,-0.3613226507 ,3.1257863367\H,0.8412983486,0.0533973968,2.9720581261\H,0.5220516277, 2.0868604443,-1.1498924741\C,-4.0651425896,1.0632875447,1.4548427739\F ,-4.8137901973,2.1314868406,1.6757025377\F,-4.7857394258,0.2026387733, 0.7141381912\F,-3.8305592292,0.4593780011,2.6184262905\C,-1.0276527104 ,4.2404282241,-1.0514688385\F,-1.0569520812,4.1450779916,-2.3876244523 \F,-1.9058686377,5.164222573,-0.6898727182\F,0.1890465785,4.6543410631 ,-0.715563517\C,4.9386348279,-2.0194517864,-1.4048588877\F,4.62044685, -2.1844354283,-2.6892922346\F,6.1993734481,-1.616382303,-1.3336479374\ F,4.8533904583,-3.2162951807,-0.8220749388\C,3.9996688761,1.734895906, 1.8412314984\F,3.5364892243,2.9478118922,1.5473922111\F,3.5129354878,1 .407222176,3.0411429137\F,5.3201815067,1.8008967727,1.9355036032\C,-6. 4141751823,-4.3789395383,-0.3821228046\H,-7.4710225415,-4.3609054199,- 0.0892715536\H,-6.3573161915,-4.6745391811,-1.4381642902\H,-5.90992361 74,-5.1483196576,0.2193374004\H,-5.8742366721,-2.7268745119,0.90685657 52\\Version=ES64L-G09RevD.01\State=1-A\HF=-2737.8043757\RMSD=6.307e-09 \RMSF=1.541e-06\Dipole=-3.5849766,-2.999928,-1.8062978\Quadrupole=13.4 915959,-6.6643486,-6.8272473,17.8150173,8.9006378,-1.7511274\PG=C01 [X (C29H30F12N1O1Si1)]\\@

conformation 1; ΔG298(MP2/CBS) = -2736.4920183

1\1\GINC-LOGIN\FOpt\RM062X\def2SVP\C29H30F12N1O1Si1(1+)\JHIOE\30-Jun-2

015\0\\#p m062x/def2svp empiricaldispersion=gd3 int=ultrafine opt freq

 scf=tight\\title\\1,1\C,0.1506881988,-1.0700915511,1.90664349\C,-0.21

75087666,-0.1460218192,3.0709436445\C,1.0665726644,0.610551739,3.47667

85689\C,2.2293679978,-0.080506991,2.7497530018\H,-0.2757168431,-2.0757

91819,2.0065123833\H,-1.0347504729,0.5323347935,2.7947789491\H,-0.5860

069659,-0.7538741746,3.9071747367\H,1.0211771274,1.6689952598,3.195997

859\H,1.211803239,0.572777552,4.5623125767\H,2.7375692498,0.586181879,

2.0350899814\H,2.9814832543,-0.4968835526,3.4325415001\N,1.6183111585,

-1.1944274638,1.9968316307\C,2.2928720893,-2.0928581832,1.3502157682\H

,1.7054790721,-2.8658358768,0.84628846\C,3.7151522527,-2.072876635,1.1

847544588\H,4.3097542516,-1.2743893839,1.6327992587\C,4.2924197534,-2.

978835093,0.3620456849\H,3.6560287,-3.7526943451,-0.0880457766\C,5.720

2086803,-2.9761880845,-0.0439179294\H,6.1639909809,-3.9392134532,0.261

0637781\C,-0.2222985014,-0.5880551671,0.4548010116\C,-1.7238663828,-0.

316883613,0.3400795226\C,-2.2107864309,0.6410193391,-0.5501506387\C,-2

.6404403627,-1.155377068,0.98267446\C,-3.5785120177,0.7453193997,-0.80

18811167\H,-2.8522725517,-1.9072116671,-1.8606158336\C,-4.0032591468,-

1.0413965401,0.7292513566\H,-2.311488772,-1.9295182351,1.6781218159\C,

-4.4890842102,-0.0916203683,-0.167370185\H,-5.5575400197,-0.0088706481

,-0.3687379495\C,0.6533265608,0.6220465346,0.1195603343\C,0.3861000602

,1.8987075679,0.618525908\C,1.8455370182,0.4170314502,-0.5777156958\C,

1.3100139936,2.9301030282,0.4489845903\H,-0.3470226076,-1.0878539003,-

4.1636643329\C,2.7650113967,1.4492599427,-0.7355774006\H,2.0709840371,

-0.5700740632,-0.982852244\C,2.5111763021,2.7195983107,-0.2234933506\H

,3.2305942122,3.5298866915,-0.3465039265\O,0.12578987,-1.6718136715,-0

.3588871123\Si,-0.3672274517,-2.1177440591,-1.9488877396\C,0.860118700

7,-3.4815315293,-2.3054711642\H,1.8905998894,-3.092135716,-2.300775553

5\H,0.7820575328,-4.2905016942,-1.5631562926\H,0.6799646493,-3.9228165

253,-3.2967691011\C,-2.1294570582,-2.7339976901,-1.9316478797\H,-2.333

9936623,-3.2715528823,-2.8705279409\H,-2.3171634578,-3.4286263752,-1.0

993413324\H,-1.5276968284,1.3103901769,-1.0763329131\C,-0.1614124128,-

0.6980598155,-3.1498172697\H,0.8529574376,-0.2734541478,-3.1426124768\

H,-0.8880417987,0.1104496505,-2.9861451017\H,-0.5458453877,2.105851266

,1.1512067489\C,4.0792087081,1.1162202024,-1.3940717816\F,4.7638844545

,2.1956027118,-1.7315902492\F,4.8442361992,0.3915560969,-0.5570655983\

F,3.8988368012,0.3667557256,-2.4827923073\C,0.9924831931,4.2682472013,

1.0733741495\F,0.9708994116,4.1529561862,2.4079253681\F,1.8925098595,5

.187943278,0.7578381673\F,-0.2064718917,4.6992202194,0.6982307158\C,-4

.9361325523,-2.0311626403,1.3854477984\F,-4.6164956575,-2.2054929562,2

.6682430928\F,-6.1998560316,-1.6368124437,1.3179054465\F,-4.8417307708

,-3.2218409211,0.7915040884\C,-4.0286528543,1.7721528496,-1.8136911491

\F,-3.6354345683,2.9927498071,-1.4570697279\F,-3.482379967,1.514933294

1,-3.0052814413\F,-5.3464007335,1.7808745718,-1.9563882239\C,5.8565665

989,-2.8205816372,-1.5657493986\H,6.9151721187,-2.8509519589,-1.851739

1731\H,5.3396234205,-3.632407451,-2.0968449285\H,5.4379180672,-1.86181

40828,-1.8989813331\H,6.2618084829,-2.1778026721,0.4820080736\\Version

=ES64L-G09RevD.01\State=1-A\HF=-2737.8060068\RMSD=5.532e-09\RMSF=2.229

e-06\Dipole=3.5178198,-2.9491238,1.643431\Quadrupole=12.5305175,-6.912

1884,-5.6183291,-15.982839,6.7434424,2.3938438\PG=C01 [X(C29H30F12N1O1

Si1)]\\@

conformation 2; ΔG298(MP2/CBS) = -2736.4945273

1\1\GINC-WORKER\FOpt\RM062X\def2SVP\C29H30F12N1O1Si1(1+)\JHIOE\29-Jun-

2015\0\\#p m062x/def2svp empiricaldispersion=gd3 int=ultrafine opt fre

q scf=tight\\title\\1,1\C,0.1346215662,-1.1695009659,1.8292254222\C,-0

.1293931587,-0.2629263009,3.0342065616\C,1.2148632666,0.4001134312,3.4

045424905\C,2.3055398471,-0.3791193051,2.6543192486\H,-0.3642310565,-2

.1429099959,1.9097232138\H,-0.9144496787,0.4720491133,2.8151801027\H,-

0.497767775,-0.8757017574,3.8671147579\H,1.238444411,1.4572959178,3.11

77938676\H,1.3836904297,0.3583985473,4.4866154739\H,2.8762008,0.252903

5086,1.9562105498\H,3.0137284964,-0.8844996728,3.3242662592\N,1.589317

4547,-1.4110025718,1.8771430419\C,2.1708270467,-2.3621515668,1.2159693

483\H,1.507867865,-3.0689420247,0.7089381046\C,3.5887029666,-2.5002315

738,1.069070617\H,4.2582672,-1.7581397393,1.5063504882\C,4.0729073416,

-3.521158683,0.322936216\H,3.3548763188,-4.231157412,-0.1061749286\C,5

.5053092533,-3.7660935016,0.0164406152\H,5.5891956658,-3.8306924523,-1

.0833132029\C,-0.2374897019,-0.6125266528,0.4067340549\C,-1.7260603759

,-0.2630544328,0.3304348122\C,-2.6739506966,-1.0653306438,0.9728912472

\C,-2.1788679366,0.7377423534,-0.5310456216\C,-4.0337362203,-0.8746016

482,0.7484788703\H,-2.9653847829,-1.668830523,-1.9272214179\C,-3.54311

82782,0.918629506,-0.7541270944\H,-1.4719041474,1.3823728136,-1.056443

7989\C,-4.4853275362,0.1176767828,-0.1186687778\H,-5.5514127056,0.2606

464356,-0.2974914998\C,0.68715909,0.5677511022,0.100081118\C,0.4710361

133,1.8423083549,0.6301420942\C,1.8628372907,0.3356180139,-0.615111326

9\C,1.4260027281,2.8451948831,0.4686394992\H,-0.8693744338,0.242108628

5,-3.0115039011\C,2.8129075005,1.3417809057,-0.7672421062\H,2.04916674

99,-0.6508228917,-1.0425652442\C,2.6091480308,2.6086041451,-0.22726743

6\H,3.3534568683,3.3966209862,-0.3462923862\O,0.0420631333,-1.68057644

92,-0.4531938891\Si,-0.5000178165,-2.0471431192,-2.0471020703\C,0.6191068866,-3.4875669314,-2.4537745521\H,1.6771233427,-3.1832280948,-2.4258799302\H,0.4131442607,-3.8721446673,-3.4634929303\H,0.469117477,-4.3174572457,-1.7463806318\C,-2.3009419856,-2.5401991679,-2.0270258692\H,-2.5285224418,-3.2434291507,-1.2119969293\H,-2.5488731519,-3.0368081277,-2.9779775363\H,-2.3752612189,-1.8702622508,1.6465014731\C,-0.2043392513,-0.6108504808,-3.2086567962\H,0.8377371249,-0.2597398552,-3.1983291782\H,-0.4263510451,-0.9533647067,-4.232115663\H,-0.4465179725,2.0702855139,1.1787215625\C,4.1012356515,0.9792382154,-1.4594504153\F,4.8580129757,2.0356059099,-1.7058161212\F,4.8114127634,0.1377921817,-0.6851860323\F,3.8723583758,0.3413204484,-2.6051810002\C,1.1702792252,4.1765443182,1.1340925655\F,1.2562165885,4.0437996453,2.4641413045\F,2.0487356602,5.094757267,0.7588570462\F,-0.0523134624,4.6202598499,0.8628657267\C,-3.9569636294,1.9757279216,-1.7499786826\F,-3.5129594119,1.657137765,-2.9689459271\F,-5.2744537044,2.1073489693,-1.8123019647\F,-3.4291470887,3.1566679197,-1.4360372747\C,-5.0032778357,-1.8268879292,1.406793175\F,-4.6852156674,-2.0166127885,2.6877703875\F,-6.2504359454,-1.3824571744,1.3457563073\F,-4.9589935859,-3.0196034002,0.8106675669\C,6.4900624695,-2.7551387889,0.5822897589\H,7.5142401769,-3.0200901849,0.293384296\H,6.283531479,-1.7457240669,0.2000449745\H,6.4517007221,-2.7301177922,1.6807976171\H,5.7369674147,-4.790848676,0.3593131901\\Version=ES64L-G09RevD.01\State=1-A\HF=-2737.8068925\RMSD=9.764e-09\RMSF=2.566e-06\Dipole=3.4671046,-3.4517569,1.5947592\Quadrupole=11.2424579,-3.3240735,-7.9183844,-19.8757937,8.5693222,0.8031106\PG=C01 [X(C29H30F12N1O1Si1)]\\@

TS predienamine → dienamine

conformation 0 (*trans*); ΔG298(MP2/CBS) = -3102.1127163

1\1\GINC-WORKER\FTS\RM062X\def2SVP\C35H43F12N2O2Si1(1+)\JHIOE\10-Oct-2

015\0\\#p opt=(ts,calcfc,noeigen) def2svp m062x empiricaldispersion=gd

3 int=ultrafine\\title\\1,1\C,-0.2301803182,-0.7852656989,1.4782948874

\C,-0.8424721616,-0.4534209988,2.845035974\C,-0.1138044248,0.802907775

4,3.370924762\C,1.1075380497,1.0050743962,2.4600383262\H,-0.0473165667

,-1.8605969909,1.3486031926\H,-1.9290182968,-0.3124860129,2.7772233807

\H,-0.68083832,-1.3021424186,3.5225005911\H,-0.7601147573,1.6878759076

,3.3450353099\H,0.1940964283,0.6643392571,4.413961888\H,1.0698522083,1

.9651036483,1.9173253451\H,2.0629954307,0.9642527941,3.0034843775\N,1.

0652801153,-0.1024455068,1.5027861178\C,2.020673312,-0.3190001805,0.61

2374041\H,1.8689625841,-1.190518574,-0.0309075402\C,3.1348893968,0.488

7821066,0.4136604202\H,3.2738030056,1.4060097784,0.9883209106\C,4.0293

178472,0.1667571477,-0.6056471143\H,3.8089425327,-0.7444327697,-1.1796

63871\C,5.2234048008,0.8457283779,-0.9126977656\H,6.0114167486,0.15490

70728,-0.1095772806\C,-1.0480278879,-0.3444543831,0.211719616\C,-2.461

6924796,-0.9314139199,0.2236327311\C,-3.5250120395,-0.263441374,-0.384

8030457\C,-2.6724176194,-2.2377555524,0.678006415\C,-4.7598782617,-0.8

915847478,-0.5475654432\H,-2.9565525745,-2.4082204797,-2.2674925481\C,

-3.9078545296,-2.8551495727,0.5162401397\H,-1.8698908332,-2.8070016422

,1.1493465036\C,-4.9668577699,-2.1908786569,-0.1001517585\H,-5.9330123

466,-2.6791043787,-0.2305128754\C,-1.0175745604,1.1830259876,0.1408280

778\C,-1.8404176058,1.9808623927,0.9386198898\C,-0.0372215755,1.805152

4281,-0.6341623709\C,-1.6634210767,3.3638177604,0.9744893812\H,-1.6588

893769,0.042613295,-4.3844763165\C,0.1321360378,3.1857612621,-0.593407

513\H,0.6193371675,1.2004204115,-1.2603252356\C,-0.6764893038,3.983403

8101,0.2125750542\H,-0.545224827,5.0652306094,0.2439792583\O,-0.331781

1035,-0.8924883283,-0.8619986063\Si,-0.7699903825,-1.2201544751,-2.486

1338084\C,0.903422114,-1.6176456903,-3.219635062\H,1.577232803,-0.7500

80321,-3.1420893039\H,1.3663503389,-2.4698007104,-2.6992614836\H,0.817

6413177,-1.8800416534,-4.2842804381\C,-1.9339170062,-2.6810838916,-2.5

691113774\H,-1.9823459907,-3.0491056139,-3.6057149507\H,-1.5981261722,

-3.5127115696,-1.9316708916\H,-3.4010519556,0.7549141885,-0.7577772497

\C,-1.5276627714,0.2774802499,-3.315995667\H,-0.8892793318,1.170337339

7,-3.2496659202\H,-2.5242009817,0.5233118424,-2.9220027665\H,-2.630367

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25\F,1.1782047529,5.0971129208,-1.4837829471\F,2.4440231976,3.48337404

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094,1.7144670455\C,-4.0509948106,-4.2961246347,0.9404659364\F,-3.42159

98248,-4.520083686,2.0951912597\F,-5.3230675064,-4.6445246426,1.084769

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4742110857,0.117169931,-2.5299717222\F,-6.9858192944,-0.8068123948,-1.

3036112954\C,5.8619916635,0.6874141433,-2.2811888211\H,6.9398965078,0.

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5.4177446815,1.376761654,-3.0143032033\H,5.2995107636,1.8503938085,-0.

4732836679\C,6.785352212,-2.0057375734,0.0934751687\C,8.3635757203,-0.

1974778222,0.4320084584\C,8.9183973393,-1.183397011,-0.5954673398\C,8.

2008622532,-2.4840607795,-0.2315407649\H,6.1858697935,-1.9321619346,-0

.8334523002\H,8.4024196701,0.8503087601,0.1018753916\H,8.6387863697,-0

.8709487624,-1.6128984752\H,10.011675197,-1.2580983806,-0.5551893894\H

,8.2182880687,-3.233952268,-1.0321865509\H,8.6591351435,-2.9315681678,

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5.8370884931,-3.8634362375,0.6398625637\H,6.5945822746,-2.9939726959,2

.0046604363\O,4.8030751044,-2.1983288425,1.3367186428\C,3.9844081721,-

2.857056998,2.2666068971\H,3.085156689,-2.2434831371,2.4102144889\H,3.

6846635872,-3.8560985892,1.9047725871\H,4.4922537662,-2.9764115984,3.2

396967545\H,8.9110114976,-0.2756038913,1.3831394695\\Version=ES64L-G09

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3859436,-15.4298705,8.2788433,0.3213254\PG=C01 [X(C35H43F12N2O2Si1)]\\

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conformation 1 (*trans*) ; ΔG298(MP2/CBS) = -3102.1112390

1\1\GINC-LOGIN\FTS\RM062X\def2SVP\C35H43F12N2O2Si1(1+)\JHIOE\10-Oct-20

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3.3671106318\C,-0.8414124748,1.1592886055,-2.5221357622\H,0.3512594937

,-1.7823355451,-1.6838866881\H,2.258213009,-0.0027517233,-2.7762431626

\H,1.1118074067,-0.9436477927,-3.7214347395\H,1.0447785133,2.003606356

9,-3.1988712249\H,0.2021659524,1.0765196499,-4.4369057926\H,-0.8754914

078,2.048942405,-1.8694803678\H,-1.7588444206,1.1518781014,-3.12811190

98\N,-0.8154298392,-0.0488864508,-1.6927657236\C,-1.7976504557,-0.3665

204809,-0.8693658636\H,-1.6447715342,-1.2838318475,-0.2934784852\C,-2.

924759077,0.4194185417,-0.6246247183\H,-3.0591352308,1.3749970587,-1.1

350565556\C,-3.7710774585,0.0835183837,0.4295701948\H,-3.562009275,-0.8647289689,0.9470417259\C,-4.8806992552,0.8299644271,0.883534453\H,-5.8319048372,0.3192451517,0.1684121055\C,1.2276765139,-0.392534503,-0.304542435\C,2.6720843656,-0.8973028645,-0.3164323764\C,3.6671921005,-0.2581534508,0.4232409052\C,2.9764262002,-2.1228917927,-0.919368572\C,4.9282460089,-0.8373507685,0.5678595486\H,3.1197712239,-2.7077027577,1.9574078857\C,4.2370333045,-2.6910366628,-0.7742595328\H,2.2279529928,-2.6680014068,-1.4967804056\C,5.2284512383,-2.0565430119,-0.0272578517\H,6.214301798,-2.5072430999,0.090016499\C,1.0950820584,1.107094587,-0.0307474548\C,1.8936538263,2.0577704317,-0.6658876187\C,0.024080022,1.5514731664,0.749639594\C,1.6052874183,3.4188180198,-0.5407104397\H,1.6206924503,-0.6011806334,4.3168426969\C,-0.268686677,2.905291315,0.8535021921\H,-0.6109917704,0.8257375365,1.254796515\C,0.5213298754,3.8591782675,0.2112228102\H,0.2990740754,4.923635309,0.2960067885\O,0.4939718681,-1.1215772532,0.6429343584\Si,0.8784651896,-1.6418487086,2.231002791\C,-0.8053205833,-2.18814736,2.8330231513\H,-1.5016395266,-1.3354041646,2.8663377721\H,-1.2270794136,-2.9625482767,2.1746257183\H,-0.745392076,-2.6071470321,3.8482115902\C,2.099365369,-3.0557952578,2.178434807\H,2.1246090932,-3.5513282462,3.1613450586\H,1.8238349245,-3.8111564422,1.4273848438\H,3.4676103033,0.695309599,0.9157798001\C,1.5351000827,-0.2371550726,3.2803773986\H,0.8642022627,0.634009571,3.2911477765\H,2.5393444886,0.0908860158,2.9767272496\H,2.748852753,1.7514427239,-1.2741979126\C,-1.5258955159,3.3188540909,1.5748783099\F,-1.4122651728,4.5165842109,2.1309506062\F,-2.5583277011,3.3722881806,0.718366877\F,-1.8596822908,2.4424122624,2.5244422145\C,2.4755505892,4.3937418788,-1.29528094\F,2.3363486878,4.2091105825,-2.6147304717\F,2.1593233251,5.6534986062,-1.0262003569\F,3.7608926623,4.2108786134,-1.0097171047\C,4.481621

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0041234,-0.5995549693\C,5.9396316688,-0.1116742201,1.4214927205\F,6.17
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27376\F,7.0930133014,-0.7640390613,1.4854059828\C,-5.3961989444,0.6000
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075018,-0.4757090327,2.5125019568\H,-4.7342552292,1.0555313889,3.04611
83425\H,-4.8812105498,1.8755970703,0.5449229298\C,-7.2450772891,0.3303
645608,-1.7842109568\C,-6.4825031409,-1.698390415,-0.7055674258\C,-6.2
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-1.8455872643,-0.1334890005\H,-5.2290102357,-1.4553386839,-2.457120191
8\H,-6.3587417778,-2.8199806875,-2.5902975795\H,-7.0364333593,-0.48694
37096,-3.8152068019\H,-8.2751167781,-1.2754690765,-2.820990511\N,-6.94
65733312,-0.3137523321,-0.4863206465\H,-7.7206519234,-0.3082924226,0.1
807012744\H,-8.1791421909,0.9024005251,-1.7285934188\C,-7.510131359,-2
.6910219071,-0.1813167538\H,-7.0787175939,-3.709586737,-0.1902677708\H
,-8.4051653486,-2.7024917258,-0.8368561392\O,-7.8503850154,-2.28979331
88,1.1130980403\C,-8.8007986712,-3.1191258394,1.7355558998\H,-8.420539
4747,-4.1491652448,1.8428921522\H,-9.0016813298,-2.7075084877,2.730929
0885\H,-9.7424743776,-3.1493701481,1.1603548279\\Version=ES64L-G09RevD
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0152,15.4521664,8.1141643,-5.2589691\PG=C01 [X(C35H43F12N2O2Si1)]\\@

conformation 2 (*cis*); ΔG298(MP2/CBS) = -3102.1138460

1\1\GINC-LOGIN\FTS\RM062X\def2SVP\C35H43F12N2O2Si1(1+)\JHIOE\10-Oct-20

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-3.0120433767\C,-1.5453485847,0.6626451504,-1.935360312\H,0.0996263037

,-2.0498177823,-1.0998308943\H,1.5438044281,-0.2900139478,-2.763225012

1\H,0.2924472345,-1.3907148672,-3.3282996723\H,0.0969182449,1.59141807

77,-3.0236394591\H,-0.8801797216,0.5090728849,-4.0109437504\H,-1.56714

85104,1.6145156197,-1.3785941159\H,-2.5549937054,0.4856684464,-2.33571

81809\N,-1.2153114779,-0.4362056535,-1.0248669118\C,-2.0129286674,-0.8

209570839,-0.0438137214\H,-1.6672131672,-1.6898954873,0.5235217154\C,-

3.1962411295,-0.1825451804,0.3198811917\H,-3.5050947742,0.7370486331,-

0.1774024272\C,-3.9629239174,-0.6966352407,1.365392848\H,-3.603164543,

-1.6236847777,1.8310164277\C,-5.1742716194,-0.1596293522,1.8483563396\

C,1.0830498201,-0.4392147329,-0.0845706238\C,2.5284366068,-0.896002600

3,-0.3009057747\C,3.5995377498,-0.1379388528,0.1760680995\C,2.79530901

39,-2.1718857704,-0.8070016117\C,4.8964826719,-0.6490406569,0.16055537

05\H,3.5120696007,-2.2782598162,2.0975451076\C,4.0935194261,-2.6725687

105,-0.8242595832\H,1.993132926,-2.8110696274,-1.1789776248\C,5.160011

446,-1.9194952501,-0.3388712879\H,6.1749000065,-2.3175755756,-0.346786

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,4.9095451349,0.0058092009\O,0.5764601928,-1.0437200855,1.0740786954\S

i,1.2605217502,-1.3263504847,2.6200719567\C,-0.2460667178,-1.901937383,3.5646739435\H,-1.0229315755,-1.121691942,3.5721264012\H,-0.6671704761,-2.8125482082,3.1122276298\H,0.0065032892,-2.1331853003,4.6098742238\C,2.5720289901,-2.6561969686,2.5270674596\H,2.7947896401,-3.0165432423,3.5434189173\H,2.2424039875,-3.5191292331,1.9290589265\H,3.4347416245,0.8604250534,0.5853069335\C,1.9591322491,0.2459666043,3.3580722313\H,1.2235018834,1.062787237,3.3898252376\H,2.859311978,0.5987806914,2.8345411912\H,2.3248899263,1.566876522,-1.5841554552\C,-1.3756295968,3.4709869928,1.8069006041\F,-1.3569032299,4.7893832209,1.9443362227\F,-2.5811328704,3.1328083054,1.3200120461\F,-1.2807403211,2.9194989858,3.0158717031\C,1.977188414,4.1808943286,-1.8965875441\F,1.5614463129,3.8603156798,-3.1289631431\F,1.7216739237,5.4684909197,-1.7051050335\F,3.2946537463,4.0037640257,-1.8715514745\C,4.3031226402,-4.0853649039,-1.3111511013\F,3.6490446792,-4.2977534062,-2.4540524148\F,5.5866245121,-4.3562292495,-1.5088512948\F,3.8298650663,-4.9612521498,-0.4220470092\C,5.9918366097,0.1994797313,0.7586087978\F,6.0158022112,1.4094114868,0.2033079577\F,5.7801745231,0.3716118366,2.066588652\F,7.1877318683,-0.3542637581,0.6059058603\C,-5.5564899412,1.2659171785,1.4880818617\H,-6.5274800846,1.5295259099,1.9285555305\H,-4.812989818,1.9919187863,1.8496666065\H,-5.638956799,1.3797067824,0.3959421768\C,-6.3713657657,-1.9874125515,-0.8429974706\C,-8.0412451115,-2.1733857638,0.9047921693\C,-7.5804287533,-3.5662511158,0.4780455328\C,-7.0921884865,-3.3323650261,-0.9523307302\H,-5.3286828973,-2.1408664754,-0.509433449\H,-8.0246411617,-2.0204915812,1.9931964012\H,-6.7453404408,-3.8996787408,1.1127897601\H,-8.3793629574,-4.3135128625,0.5538742842\H,-6.4406027956,-4.1302374472,-1.3300705385\H,-7.952212519,-3.2423514983,-1.6356656707\N,-7.0746188207,-1.2649935109,0.2461755483\H,-7.4931979118,-0.396021984,-0.08804

60454\H,-6.0563386253,-0.8225517676,1.1227928645\H,-5.4357559439,-0.49

0852751,2.8611947112\H,-9.061307643,-1.9702832366,0.5464803877\C,-6.34

07233983,-1.1597947447,-2.109871603\H,-5.7675816992,-1.6929022563,-2.8

917292228\H,-7.3737379421,-1.0241968347,-2.4917570283\O,-5.7645864805,

0.0809442817,-1.8074623002\C,-5.7736185281,0.9814099919,-2.8875072536\

H,-5.3189695721,1.9189249779,-2.5449135006\H,-5.194781929,0.5891232347

,-3.7419128992\H,-6.8023673215,1.188148173,-3.2298411371\\Version=ES64

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283,-25.4757875,18.8961361,10.1664838,-4.4315016\PG=C01 [X(C35H43F12N2

O2Si1)]\\@

TS dienamine → product-iminium 1A

sc-exo: *R* **enantiomer unshielded side; ΔG298(MP2/CBS) = -1788.3691414**

1\1\GINC-LOGIN\FTS\RM062X\def2SVP\C40H48N3O1(1+)\JHIOE\29-Sep-2015\0\\

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4\C,0.8244648086,0.6175644166,2.2635147228\H,2.0986197905,1.2177049155

,-0.6568368433\H,3.7499780815,2.0780739177,1.4476391713\H,2.2227309908

,2.866498162,1.008093623\H,2.7260592478,0.8746170417,3.2656351844\H,1.

7194769893,2.3290683979,3.2979635981\H,0.7236209467,-0.286647863,2.884

3930919\H,-0.1330109531,1.163888811,2.3012271\N,1.0962728789,0.2431797

998,0.8780825226\C,0.2676479261,-0.5197402659,0.1712896392\H,0.5782562

152,-0.7057308596,-0.8587647475\C,-0.9203635432,-1.0579236898,0.634156

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S54

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0.0714853716\H,-10.0615440477,-1.5683945347,-1.4311700528\H,-9.5752796
874,-2.5861621915,-0.0457015632\C,-9.816889386,0.4516386541,1.08769021
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477,-2.9227928195,-1.7400426215\H,4.3437101471,-1.9291173398,-1.974243
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ap: *R* enantiomer unshielded side; ΔG298(MP2/CBS) = -1788.3703343

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***sc-exo: S* enantiomer unshielded side; ΔG298(MP2/CBS) = -1788.3684345**

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\C,-1.5751394521,-1.1953056425,-2.0736385944\H,-1.0585262318,-0.797160

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.5723271526,-1.162579999,-0.4547376964\C,-8.2234435112,-1.4142764482,2
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,3.0398700675\H,8.1834869269,0.0537009539,-0.9114709555\H,5.9036807366
,3.5391227165,0.1686405175\C,3.9746589345,-1.3480142349,-2.5266346891\
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2,-2.8319588752\H,4.4055096614,-2.2859733052,-2.1388696439\\Version=ES
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_ap_: _S_ enantiomer unshielded side; ΔG298(MP2/CBS) = -1788.3705130

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82645,0.6984577607\C,0.8100530475,-0.6318734796,-0.0613976952\H,1.1736
755202,-0.7874134625,-1.0801172529\C,-0.3791594391,-1.2337346025,0.309

0149457\H,-0.8031202465,-1.0760180133,1.3029946275\C,-1.124716235,-1.9300139561,-0.6625491505\H,-0.6307976046,-2.1219834575,-1.6249384804\C,3.9909678689,-0.1238775841,0.0026022946\C,4.3372444069,-0.7982535507,1.3311701147\C,5.4200722879,-0.3300937623,2.0837448371\C,3.5035825953,-1.7730582061,1.9017180848\C,5.669770512,-0.8227908399,3.364779884\C,3.7493671782,-2.2616968569,3.1835257697\H,2.6414189838,-2.1522360078,1.3503140388\C,4.8338704457,-1.7877966237,3.9216992448\H,5.0266194037,-2.1715200668,4.9242572994\C,3.6847637142,-1.0766972541,-1.1639760991\C,3.7492434034,-2.4688591837,-1.0912227032\C,3.3666196902,-0.4920731661,-2.401838821\C,3.4328865064,-3.2574340436,-2.2021811475\C,3.0536646663,-1.2724833193,-3.5093589193\H,3.3902833313,0.5955215982,-2.5011280101\C,3.0681249277,-2.6662753529,-3.4071170229\H,2.8225555652,-3.2840830343,-4.2718289174\O,5.0013544709,0.7805423313,-0.3949812206\H,6.0634174497,0.4469381165,1.671022853\H,4.0570367881,-2.9581297044,-0.1685026508\C,-3.1948492018,-3.1101046897,-1.5254583832\H,-2.6885025086,-3.1427141536,-2.5010475464\H,-3.2593938258,-4.1415460592,-1.1453457748\H,-4.2300931271,-2.7637270629,-1.6701829149\C,-2.4622103903,-2.2372590229,-0.5557377166\H,-2.9280825059,-2.0945537775,0.4235322035\C,-3.1713917361,-0.1137808745,-1.2881001386\H,-3.214952555,-0.5251392387,-2.3015372189\C,-2.115438479,0.8452618734,-1.1050580795\C,-1.084428239,0.9103207214,-2.0748085042\C,-2.03768044,1.7815058225,-0.0503235229\C,-0.0658279857,1.8382839827,-2.0208740833\H,-1.1044830592,0.2050595705,-2.9102809874\C,-1.0186505956,2.7130445384,0.0287600757\H,-2.8293737493,1.8307296,0.6952703545\C,0.0026585941,2.7768976345,-0.9551018876\H,0.6798386716,1.8476593014,-2.8140649044\H,-1.0398581079,3.4334137606,0.8437624641\C,-4.4364725959,-0.1611594313,-0.5865850982\C,-4.5931108457,0.0300611697,0.8049343806\C,-5.603726034,-0.4671589838,-1.3186188393\C,-5.8285092

664,-0.0300165388,1.4147753277\H,-3.7143107253,0.1732632032,1.43559088
84\C,-6.8533546182,-0.5124151715,-0.7313847663\H,-5.5235060183,-0.6440
214979,-2.3938611088\C,-7.0096712685,-0.2812830754,0.660269895\H,-5.88
64352953,0.1023509099,2.4930002683\N,0.9866448131,3.7188953067,-0.8989
799866\C,1.9042443502,3.872657866,-2.012677326\H,2.6055918433,4.682947
1623,-1.7899693638\H,2.4961434741,2.9587183381,-2.1758881081\H,1.37671
32659,4.1147973653,-2.9504190648\C,0.9203414564,4.7638481879,0.1056207
881\H,1.8081795082,5.3990352047,0.0217974532\H,0.0235716468,5.39513553
,-0.014445514\H,0.9074822613,4.3388496699,1.1208340254\H,-7.7179375754
,-0.7287744583,-1.3547722283\N,-8.2309550908,-0.3151127763,1.252892250
5\C,-9.4106016964,-0.6044056116,0.4617725367\H,-10.2924102988,-0.58173
69485,1.1095179353\H,-9.5525645131,0.1413078223,-0.3366761574\H,-9.351
877923,-1.6016382731,-0.0032500271\C,-8.3557540946,-0.078300596,2.6771
943616\H,-9.4136469965,-0.1124224872,2.955452406\H,-7.8221870771,-0.84
2118071,3.266061918\H,-7.9612406159,0.9116190971,2.9561701958\H,3.0883
219337,-3.0193915961,3.6070800424\H,6.5209481373,-0.4429522634,3.93143
43039\H,3.4838353254,-4.3438573753,-2.1192712944\H,2.812853621,-0.7956
085249,-4.4608378527\C,6.1733334115,0.2172738372,-0.9482441489\H,6.014
8527245,-0.1045068573,-1.98920235\H,6.9409530678,1.0005275978,-0.92715
6299\H,6.5259511831,-0.6487754172,-0.3651997312\\Version=ES64L-G09RevD
.01\State=1-A\HF=-1790.2890825\RMSD=4.712e-09\RMSF=1.775e-06\Dipole=-2
.350165,0.7790122,0.1551287\Quadrupole=49.9491307,-26.31287,-23.636260
7,10.4399,-8.7691493,2.2909451\PG=C01 [X(C40H48N3O1)]\\@

TS dienamine → product-iminium 1B

***sc-exo*: *R* enantiomer unshielded side; ΔG298(MP2/CBS) = -2157.1477893**

1\1\GINC-WORKER\FTS\RM062X\def2SVP\C42H54N3O1Si1(1+)\JHIOE\13-Sep-2015

\0\\#p opt=(ts,calcfc,noeigen) m062x/def2svp int=ultrafine empiricaldi

spersion=gd3\\title\\1,1\C,2.3471395679,0.9023660166,0.3604625834\C,2.

6974183084,2.0238884656,1.3450560062\C,2.0240542205,1.6387393007,2.674

0739595\C,0.8440242722,0.739643398,2.28656749\H,2.1263729728,1.2808162

574,-0.6482741029\H,3.7829138628,2.1539682286,1.4455412097\H,2.2869022

567,2.9692794099,0.9633353826\H,2.7200357729,1.0831263235,3.3128904566

\H,1.695732521,2.5209967567,3.2389387679\H,0.7819542481,-0.1600230935,

2.9197679192\H,-0.1291339219,1.2562381384,2.3350536081\N,1.1021851628,

0.3545670089,0.9020705141\C,0.2887295759,-0.4456681392,0.2199518391\H,

0.5963335155,-0.6476059601,-0.8076332028\C,-0.8830579332,-1.005852874,

0.6979418189\H,-1.2099373805,-0.8180841242,1.7214009384\C,-1.698055389

4,-1.750377779,-0.181932669\H,-1.264094834,-1.9976509879,-1.1584169386

\C,3.4354093744,-0.2062492723,0.1709559518\C,4.7173970364,0.3631718476

,-0.4529702409\C,4.7070339809,1.5044241077,-1.2631556371\C,5.916061839

4,-0.3545399388,-0.34034463\C,5.8538479906,1.9119076768,-1.9446827869\

H,5.172072173,-0.933769425,-3.0285250316\C,7.0625131666,0.0465614742,-

1.0229553437\H,5.9535006959,-1.2432249725,0.290958885\C,7.0349113023,1

.1819766938,-1.8317968448\H,7.930562354,1.4985858783,-2.367565979\C,3.

6807698153,-0.8976621657,1.5154197624\C,4.6273230079,-0.4232689045,2.4

32671969\C,2.8730646029,-1.9793808081,1.8844267242\C,4.7571871435,-1.0

110958536,3.6901334595\H,5.5428162259,-3.1507996752,-0.9219503313\C,3.

0000393235,-2.5663346295,3.1434633697\H,2.1378148138,-2.3610714532,1.1

737887638\C,3.9403671088,-2.0822241361,4.0516716896\H,4.0443954695,-2.

5442414352,5.0342404617\O,2.8352115442,-1.1023474821,-0.7317597939\Si,3.3950718206,-2.2474497377,-1.8496577098\C,1.7781254868,-3.0375154158,-2.3748186241\H,1.2494690745,-3.4545683978,-1.5035473255\H,1.9428802419,-3.8528939922,-3.094510095\H,1.1227678171,-2.2942043651,-2.855569798\C,4.2180262102,-1.4066129385,-3.305075806\H,3.5607337177,-0.6309197086,-3.7263486556\H,4.4202608322,-2.1444373901,-4.097002434\H,3.7996532427,2.0967380434,-1.3817181621\C,4.5171260869,-3.5202475216,-1.0559341949\H,4.1319055537,-3.8393232492,-0.076174803\H,4.5691931997,-4.4080657129,-1.7053102839\H,5.2774189893,0.4115156773,2.163500429\C,-3.7391602326,-1.8603302261,1.3170718605\H,-3.4947938308,-0.8833181946,1.7625905213\H,-4.8280106248,-1.9070206721,1.1782898982\H,-3.4643943487,-2.6356604381,2.0509848418\C,-3.0200527731,-2.0701343444,0.0210823052\H,-3.4946424571,-2.7275632137,-0.7114470498\C,-3.7231778999,-0.1146000458,-1.2530868224\H,-3.4999549866,-0.6840247172,-2.1594967482\C,-2.7483822777,0.8967220474,-0.9433137244\C,-1.7282899641,1.1606633823,-1.8855926809\C,-2.6704904196,1.6023627554,0.2786139401\C,-0.7594960306,2.1232526845,-1.680117739\H,-1.7236902689,0.6057824405,-2.8272008186\C,-1.7034238464,2.565069124,0.5066008621\H,-3.3738900955,1.3819979681,1.0814642728\C,-0.7256852302,2.8717399019,-0.4739322577\H,-0.0253416702,2.304425324,-2.4629599593\H,-1.7062062406,3.087910565,1.461074505\C,-5.1005035412,-0.1690675697,-0.8512632074\C,-5.7450465803,0.7841973411,-0.0289224704\C,-5.9019347533,-1.235195214,-1.3302186737\C,-7.071343294,0.6601163367,0.3294153628\H,-5.2104306883,1.6761478566,0.2931407846\C,-7.2232402933,-1.383158995,-0.9785465937\H,-5.4509712931,-1.9764991553,-1.9947898412\C,-7.8545735753,-0.4409385118,-0.1152494749\H,-7.520190084,1.4382576415,0.9426646791\N,0.2069218004,3.8457957526,-0.2667736856\C,1.1236915929,4.205651425,-1.3286874971\H,1.7717974572,5.0187864624,-0.98550

83128\H,1.7675038036,3.3564303164,-1.6123448299\H,0.5919208585,4.54510

30162,-2.2328734407\C,0.1641359769,4.633948897,0.947986172\H,0.9840454

662,5.3598063533,0.9362080631\H,-0.785468136,5.1856597216,1.0471022497

\H,0.2870664038,3.9994566286,1.8414179276\H,-7.7832910865,-2.226494685

2,-1.3762568973\N,-9.1520611434,-0.5784617069,0.2481005186\C,-9.935040

7867,-1.6921749797,-0.2536759501\H,-10.948917219,-1.6299778011,0.15314

87473\H,-10.0042628248,-1.6744383902,-1.3528371579\H,-9.5016826272,-2.

6575792527,0.0515549364\C,-9.7696138989,0.4000830087,1.1228545694\H,-1

0.8016089924,0.0988386414,1.3268002409\H,-9.2363615697,0.4699830285,2.

0837669755\H,-9.787832612,1.4008543482,0.6623215288\H,5.5045763103,-0.

6322250274,4.3886340719\H,2.3634336645,-3.4104698821,3.412769056\H,7.9

820753036,-0.5313607992,-0.9205937904\H,5.8209595181,2.8046646892,-2.5

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527e-09\RMSF=6.220e-07\Dipole=-3.366396,1.1633955,0.3105417\Quadrupole

=72.8003054,-30.9634493,-41.8368561,13.6726738,-5.8117164,3.7290919\PG

=C01 [X(C42H54N3O1Si1)]\\@

ap: R enantiomer unshielded side; ΔG298(MP2/CBS) = -2157.1462519

1\1\GINC-WORKER\FTS\RM062X\def2SVP\C42H54N3O1Si1(1+)\JHIOE\14-Sep-2015

\0\\#p def2svp m062x opt=(ts,calcfc,noeigen) empiricaldispersion=gd3 i

nt=ultrafine\\title\\1,1\C,2.2519782293,0.7198524501,0.5579615667\C,2.

678775618,1.6813886432,1.6740739437\C,2.1369608463,1.0692686818,2.9721

568309\C,0.8734663347,0.3222260854,2.5412294819\H,1.9550141085,1.27647

41816,-0.3414594547\H,3.7664112841,1.8189694926,1.6791359603\H,2.21778

1947,2.6604892649,1.4856200181\H,2.8631602734,0.3642465875,3.398285547

1\H,1.9204114216,1.827742138,3.7351768213\H,0.736848233,-0.6289154828,

3.0793848685\H,-0.0450884065,0.9207349934,2.6710058273\N,1.0691332853,

0.0597170182,1.1152999878\C,0.2194544479,-0.6716923151,0.4038414525\H,0.4766679318,-0.8001220582,-0.6504361155\C,-0.9540605669,-1.2419331406,0.8681127536\H,-1.2763801773,-1.0908779622,1.8988885663\C,-1.7912421196,-1.9034110782,-0.0523738347\H,-1.3568440469,-2.1262216964,-1.0346568336\C,3.4058143575,-0.2487997633,0.1050664427\C,3.8776901737,-1.041031978,1.325375305\C,5.086917962,-0.7114099951,1.9439984585\C,3.0630796877,-2.0103850067,1.9340429346\C,5.4775345743,-1.3288192533,3.133595788\H,7.4946130766,0.8601941907,0.3804396345\C,3.4509004463,-2.6254668851,3.1221823931\H,2.1100140442,-2.2927757796,1.4837389563\C,4.6601377909,-2.2852462902,3.7297914598\H,4.9630620015,-2.7668740842,4.6602618919\C,2.9259138344,-1.1114628833,-1.0755544536\C,2.9415483072,-2.50798941,-1.0972036818\C,2.4832154168,-0.4367074727,-2.2247820936\C,2.4851731722,-3.2099561187,-2.2162024507\H,6.1713429124,-1.9156729985,-0.6175784125\C,2.0284933316,-1.1318469521,-3.3413727125\H,2.516560551,0.6546723889,-2.2518481662\C,2.0168801561,-2.5285935582,-3.3360165955\H,1.6641102035,-3.0797364609,-4.2086633431\O,4.3917345503,0.6420449918,-0.3451077344\Si,5.7419003469,0.4299210962,-1.3616774453\C,5.3668943246,1.2415547185,-3.0088863862\H,4.6599515154,0.6501355852,-3.6075353888\H,6.2930384969,1.3516765776,-3.5933355891\H,4.9451406534,2.2473148148,-2.8587578142\C,7.1260645268,1.3699441341,-0.5214497202\H,6.7890072088,2.3770630501,-0.2338950088\H,7.9783685881,1.4835763071,-1.2081421898\H,5.7195686993,0.0571982562,1.502163932\C,6.1707155461,-1.3797839095,-1.5791551228\H,5.4701018597,-1.8860774217,-2.2585577262\H,7.1811779832,-1.4594138718,-2.0096338248\H,3.3317975173,-3.0670905606,-0.2483129902\C,-3.8656355825,-1.9580944811,1.4055171672\H,-3.5620724327,-1.0279134307,1.9100408008\H,-4.9520120255,-1.9201320258,1.2464986381\H,-3.6597766533,-2.792599266,2.0954758193\C,-3.1383101625,-2.1461570623,0.1105720055\H,

-3.6288592464,-2.7606813201,-0.648105531\C,-3.6785791745,-0.1850509443,-1.1034477431\H,-3.4682899876,-0.7331689814,-2.0261108536\C,-2.6692511734,0.7897593852,-0.7650758716\C,-1.6336496776,1.0406856929,-1.6922577553\C,-2.5790861001,1.4646791457,0.4719311452\C,-0.6376447373,1.9705056964,-1.459011133\H,-1.6333734861,0.5027230173,-2.6439087665\C,-1.5852926474,2.3935773375,0.7283645063\H,-3.2958108853,1.2481660545,1.2643017536\C,-0.594130145,2.6964546268,-0.2398344206\H,0.109598757,2.1446774967,-2.2314675629\H,-1.5810953139,2.8957902092,1.6937729668\C,-5.074021129,-0.1567568788,-0.7487686145\C,-5.6819472511,0.8198745272,0.0720506662\C,-5.9255280802,-1.1583211164,-1.2754215492\C,-7.0259228517,0.7771938263,0.3832614248\H,-5.1008762653,1.6664940098,0.4336316968\C,-7.2658872198,-1.2248666731,-0.9718934334\H,-5.5023914139,-1.9151894735,-1.9409376875\C,-7.8639106777,-0.2597679657,-0.1110170625\H,-7.4431201664,1.570961453,0.9988658516\N,0.36090534,3.6444262003,-0.0080779961\C,1.2784871258,4.0214534419,-1.0658757749\H,1.9250434515,4.8294166248,-0.7085624503\H,1.9295891813,3.1814799653,-1.3595586987\H,0.7457335448,4.3754468248,-1.964052876\C,0.288314211,4.4493496583,1.1951796882\H,1.1266293782,5.1536728894,1.20831628\H,-0.6517436959,5.0239183657,1.2499014906\H,0.3612477083,3.8251650136,2.1005100872\H,-7.8657559758,-2.021348577,-1.4065112409\N,-9.1802426939,-0.3177556298,0.2056514547\C,-10.0163402428,-1.3669855606,-0.3460216754\H,-11.0378593847,-1.2449906935,0.0268331784\H,-10.0453039232,-1.3242829429,-1.4463717961\H,-9.6592470807,-2.3650031244,-0.0466624662\C,-9.7617202114,0.6828436093,1.0797271462\H,-10.8175660566,0.4467148648,1.2436429753\H,-9.2581151182,0.6996128772,2.0589343379\H,-9.6989124249,1.6913079686,0.6401856202\H,2.8038371148,-3.3782530319,3.575072243\H,6.4255488812,-1.0530574681,3.5975023712\H,2.5092168748,-4.3004967014,-2.2102567588\H,1.6944972652,-0.5840136

946,-4.2242923309\\Version=ES64L-G09RevD.01\State=1-A\HF=-2159.4949215

\RMSD=7.909e-09\RMSF=9.055e-07\Dipole=-3.7489672,0.6376286,0.3567635\Q

uadrupole=67.4445202,-30.9673512,-36.477169,9.640168,-2.3712629,5.8713

915\PG=C01 [X(C42H54N3O1Si1)]\\@

sc-exo: *S* enantiomer unshielded side; ΔG298(MP2/CBS) = -2157.1468505

1\1\GINC-WORKER\FTS\RM062X\def2SVP\C42H54N3O1Si1(1+)\JHIOE\24-Sep-2015

\0\\#p def2svp freq m062x opt=(ts,calcfc,noeigen) empiricaldispersion=

gd3 int=ultrafine\\title\\1,1\C,2.1839220101,0.8004787908,0.5121104961

\C,2.3320243429,1.6951472964,1.7488938209\C,1.2961675695,1.2038710733,

2.7832081684\C,0.3963079486,0.1950550182,2.0525538639\H,2.1732051909,1

.3787607348,-0.4227352891\H,3.357155398,1.6710425327,2.1382573566\H,2.

1284334841,2.7336357799,1.4569804282\H,1.7852749868,0.7248278936,3.639

4064819\H,0.7038839413,2.0409837712,3.1771062098\H,0.4882846414,-0.820

5431214,2.4738526711\H,-0.6669713989,0.4806803204,2.0662379948\N,0.862

0810165,0.1999505715,0.6711482796\C,0.2140264168,-0.4094660346,-0.3157

891858\H,0.6849646792,-0.320273108,-1.297554456\C,-0.981499936,-1.0957

276276,-0.1972710977\H,-1.4528880485,-1.2291476104,0.778997196\C,-1.66

68961824,-1.5098327622,-1.3565196903\H,-1.1336756028,-1.4154351321,-2.

3122719674\C,3.2813754593,-0.3004462472,0.3189309609\C,4.6821996734,0.

3205216758,0.2440617201\C,4.8761962584,1.5695644192,-0.3605705937\C,5.

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02198574,0.2308151122\C,2.5996845215,-3.1312261839,3.5376009391\H,2.39
9482523,-3.8304162845,4.350470674\O,2.9530907581,-0.8730101974,-0.9241
76497\Si,3.8429930597,-1.7864676492,-2.0486616202\C,2.4927552345,-2.30
61387258,-3.2376358993\H,1.7092200622,-2.8725990199,-2.7110060646\H,2.
8895327203,-2.9439279281,-4.041184641\H,2.0274262014,-1.4253108939,-3.
7060191187\C,5.1169687033,-0.7228297892,-2.9128917712\H,4.6607593241,0
.2027835062,-3.2949540036\H,5.5350406038,-1.2728073385,-3.7703992233\H
,4.0231989567,2.1616415506,-0.6945275089\C,4.643084906,-3.2849390684,-
1.2600996293\H,3.9020792388,-3.949159359,-0.7932306875\H,5.1693896705,
-3.8580947512,-2.0395891837\H,4.2624321669,-0.2295675443,2.915710336\C
,-3.6826346027,-2.4183338094,-2.5997654423\H,-3.1444070939,-2.16445249
26,-3.5244528741\H,-3.74794561,-3.5160268532,-2.5390034964\H,-4.717356
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687896029\C,-2.614944888,1.8871423641,0.2236536102\C,-0.6456602971,2.4
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1,-0.3331036904,-1.6596371722\N,-8.7523468147,-0.6696204899,0.96731214
65\C,-9.9393149665,-0.7762512642,0.1421515095\H,-10.8065204234,-0.9652
281367,0.7824120467\H,-10.1239699522,0.1534586641,-0.4193432699\H,-9.8
581103268,-1.6051784183,-0.5792906939\C,-8.8525480562,-0.83810815,2.40
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4892953354,-4.2603355825,2.070334986\H,3.7900103887,-1.804085236,4.755
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\Quadrupole=61.0158933,-29.7334765,-31.2824168,15.0441112,-5.6383762,-
0.5889876\PG=C01 [X(C42H54N3O1Si1)]\\@

ap: *S* enantiomer unshielded side; ΔG298(MP2/CBS) = -2157.1455540

1\1\GINC-LOGIN\FTS\RM062X\def2SVP\C42H54N3O1Si1(1+)\JHIOE\28-Sep-2015\
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d3 int=ultrafine\\title\\1,1\C,2.0833820543,0.3992581861,0.7873817351\
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.0810471616\C,0.4086125751,-0.7134738714,2.1831304047\H,1.9325183093,1
.2854399378,0.1560043447\H,3.3501486018,0.9042273326,2.4907269408\H,1.

8194056979,1.7965316908,2.3951695304\H,2.2281498074,-1.0970516602,3.29
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504664,-0.374245774,0.8273636405\C,0.1214786413,-0.6831319624,-0.24553
89495\H,0.5369930868,-0.3546109928,-1.2014029882\C,-1.0978616847,-1.33
69548327,-0.2501929468\H,-1.5727234892,-1.6474579528,0.6829526166\C,-1
.8043858172,-1.4563648526,-1.4628609006\H,-1.2618784091,-1.1961171759,
-2.3820626526\C,3.3182420984,-0.3585586117,0.1767945644\C,3.6036348429
,-1.5914143051,1.0356734304\C,4.6875046572,-1.5873724695,1.9181086587\
C,2.7247541186,-2.6869231385,1.0683888213\C,4.8948006707,-2.6435019833
,2.8071162853\H,5.7712917503,-1.0002651457,-2.2936223033\C,2.929454343
,-3.740295346,1.956717541\H,1.863938363,-2.7239833139,0.3985995643\C,4
.0152350868,-3.7223981648,2.8330950921\H,4.1747936965,-4.5474061249,3.
5283541556\C,3.0556610343,-0.6573836517,-1.3100597302\C,3.0965094506,-
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210408967,-0.7165176531\H,7.4093943912,-0.7928945465,-1.6262786642\H,5
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3,-1.5566102719,-2.8603250815\C,-3.1534126189,-1.7100252466,-1.5649510

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84136429,-0.4448627155,-0.037111805\H,-10.971809731,-0.6919864175,0.52

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-1.1127534789,-0.9121130703\C,-9.0799664107,-1.0510979027,2.1883681345

\H,-10.1474436704,-1.1723312967,2.3969659687\H,-8.5847591747,-2.020013

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TS dienamine → product-iminium 1C

***sc-exo: R* enantiomer unshielded side; ΔG298(MP2/CBS) = -3504.067938**

1\1\GINC-LOGIN\FTS\RM062X\def2SVP\C46H50F12N3O1Si1(1+)\JHIOE\28-Aug-20
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,1.100292518,-0.4745345759,-2.1971131783\C,0.5289072162,0.8336321592,-
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,-1.4550591426,-0.3366837534\H,2.1810292394,-0.565468813,-2.3704661498
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2,-2.7135658455\H,0.2366756857,0.7317897856,-3.8192682026\H,-0.7501084
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55,-0.9913294215,0.260412059\C,2.9236420173,-2.2717865532,-0.280540653
9\C,4.2308284894,-0.6624984358,0.9138757466\C,3.9559449319,-3.19973292

04,-0.1516609806\H,3.7780387426,-0.9687493437,3.6037472501\C,5.2596964

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6,-2.0135862519\F,4.8138059782,-5.3291610665,-0.67671076\F,2.745661257

9,-5.2062246037,-0.0859986433\C,-5.3150122475,2.0938302132,0.444549287

6\H,-5.0142212485,1.7308143346,-0.5504286293\H,-6.4079825577,2.016016534,0.5160490867\H,-5.0499997268,3.1618441331,0.5042690117\C,-4.6461931624,1.3190531025,1.5383359303\H,-5.1696888747,1.258116653,2.4953902857\C,-5.2050667889,-0.8905282644,1.0762847701\H,-5.0838178712,-1.1128308923,2.1400016843\C,-4.145948535,-1.4405909797,0.2546501252\C,-3.1936073635,-2.2784074965,0.8713094646\C,-3.9370875505,-1.1574868723,-1.1118616487\C,-2.1592330711,-2.8716736721,0.1702699245\H,-3.2950292505,-2.5002338065,1.9367567225\C,-2.9085484869,-1.7452976085,-1.8323970909\H,-4.5866475508,-0.4517164919,-1.6298945131\C,-1.992387428,-2.6343328128,-1.2177617006\H,-1.4921559841,-3.5482862604,0.7002494249\H,-2.8190370033,-1.511080794,-2.8916092209\C,-6.5723522876,-0.6512962531,0.6911129195\C,-7.0868138924,-0.7996508406,-0.6166657545\C,-7.4946651153,-0.2598513538,1.6923345577\C,-8.4087705965,-0.5387561258,-0.9143512019\H,-6.4512048835,-1.1801485851,-1.4141078928\C,-8.8146504644,0.0126196055,1.4171262808\H,-7.1453821994,-0.1611364255,2.7235077929\C,-9.3182562475,-0.1040414321,0.0889672528\H,-8.7533411769,-0.6950086718,-1.9340746477\N,-0.9869048322,-3.2359919105,-1.9327736993\C,-0.1741824216,-4.2592869174,-1.3003698437\H,0.6471399402,-4.5358604702,-1.971744543\H,0.2747525604,-3.888959675,-0.3673422128\H,-0.7512174588,-5.1691256135,-1.0568117846\C,-1.0592310525,-3.2316581185,-3.3827657082\H,-0.1975549417,-3.7755359249,-3.784968177\H,-1.9823020733,-3.7103144956,-3.7528785814\H,-1.0224688184,-2.2076103024,-3.7843364241\H,-9.4721478732,0.3099933314,2.2309723384\N,-10.6128895226,0.1694461563,-0.1998439846\C,-11.5238256653,0.5772038568,0.853358901\H,-12.5139871287,0.7540987924,0.4225603098\H,-11.6201229075,-0.2003988311,1.6275275354\H,-11.1887630795,1.5086835245,1.3361245374\C,-11.0981732028,0.0347570396,-1.5602243841\H,-12.1519028746,0.3274620237,-1.5962288119\H,-10.5379350158,0.6843256537,-2.2

507874721\H,-11.0173228347,-1.0041727953,-1.917982627\\Version=ES64L-G

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,-34.4751567,-6.496273,3.9717244,5.5016262\PG=C01 [X(C46H50F12N3O1Si1)

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sc-exo: R **enantiomer shielded side; ΔG298(MP2/CBS) = -3504.0551837**

1\1\GINC-WORKER\FTS\RM062X\def2SVP\C46H50F12N3O1Si1(1+)\JHIOE\29-Aug-2

015\0\\#p opt=(calcfc,noeigen,ts) m062x/def2svp int=ultrafine empirica

ldispersion=gd3\\title\\1,1\C,1.1669364258,-0.0975180083,-2.2754422852

\C,1.5475723079,1.1012557152,-3.162563298\C,0.3191452698,2.0251681756,

-3.1603972547\C,-0.8719524422,1.0870050575,-2.958747072\H,1.5585308491

,-1.0467310341,-2.6738395029\H,2.4503002213,1.616786498,-2.809412779\H

,1.7527245874,0.7403793529,-4.180638949\H,0.378141554,2.7518234659,-2.

3393676433\H,0.2357733646,2.5945753721,-4.0935631525\H,-1.63555294,1.5

048439295,-2.2837107662\H,-1.3677306372,0.8212175617,-3.9073641435\N,-

0.2933773681,-0.1232171129,-2.3751102315\C,-1.0328758377,-1.1862842155

,-2.0690206783\H,-0.4725982767,-2.0533808258,-1.7187770404\C,-2.408821

9856,-1.2986748447,-2.175285582\H,-3.0265801036,-0.4720117845,-2.53352

4126\C,-2.9997669359,-2.5365378338,-1.8529697233\H,-2.3215550255,-3.31

035707,-1.4713705022\C,1.6500170415,-0.020947838,-0.7863048215\C,3.173

0917727,-0.1194533795,-0.6767641601\C,4.0257650329,-0.3669604855,-1.75

16520216\C,3.722594197,-0.0372331694,0.6066985084\C,5.3918087989,-0.55

40585869,-1.5386638565\H,3.8822200055,-2.8993818233,-0.6405879817\C,5.

0869837972,-0.2153753324,0.8099278959\H,3.0699663144,0.1673673003,1.45

98494542\C,5.9372818115,-0.4813958286,-0.2617327899\H,7.0063766131,-0.

6246417788,-0.1030210348\C,1.1423727562,1.2947564295,-0.1976334344\C,1

.9251945177,2.4515085368,-0.1659848932\C,-0.1964791011,1.3774827332,0.1880880082\C,1.3643868392,3.6710116233,0.2090817249\H,2.9715377935,-2.1349328809,2.2934777819\C,-0.7490700126,2.6046791877,0.5506598314\H,-0.8033428382,0.4704056401,0.1719519366\C,0.0213593809,3.7642752306,0.5634064345\H,-0.4141934589,4.7231304731,0.8450495948\O,1.0497582787,-1.0812021473,-0.0839540011\Si,1.5495894158,-2.6774879749,0.2824983523\C,0.0097837798,-3.7318211834,0.0835737814\H,-0.8886819937,-3.1905797152,0.4205111423\H,0.1082702144,-4.6349009887,0.7056362362\H,-0.1358985899,-4.0690458477,-0.954538806\C,2.8868613912,-3.3019525469,-0.8767496306\H,2.6773834132,-3.1001315003,-1.9386101148\H,2.9355882911,-4.3965878731,-0.7597825684\H,3.6529177826,-0.4369124717,-2.7740483555\C,2.1289073329,-2.7968891144,2.0526494475\H,1.2980866785,-2.5967457042,2.7444659665\H,2.4631326651,-3.8319892197,2.2290883248\H,2.9803851238,2.4195211574,-0.4449106409\C,-2.2152881134,2.6523616949,0.8848661107\F,-2.6403183993,3.8803736855,1.1467218474\F,-2.9491212563,2.180195848,-0.1391468783\F,-2.5101725173,1.8827318949,1.9377143401\C,2.2170359827,4.9140499235,0.1336773895\F,1.7149502067,5.8982163124,0.8720878376\F,3.4588266003,4.6722087072,0.5455211006\F,2.2933877163,5.3497483027,-1.1256725634\C,5.6225868914,-0.0922298698,2.2155329107\F,4.9692079057,-0.9151567429,3.0443125981\F,6.9142227449,-0.3871373536,2.2817100596\F,5.4527176617,1.1426094185,2.6829098852\C,6.2559956032,-0.924772167,-2.7186985239\F,5.9074427712,-0.2321978323,-3.8035796715\F,7.5421510359,-0.7029892884,-2.4772901647\F,6.1121476397,-2.2177598876,-3.0141367203\C,-4.7985315394,-4.2882941661,-1.8415642495\H,-4.1704700836,-4.8759181522,-1.1544791469\H,-5.8449686068,-4.3784154978,-1.5154992831\H,-4.7329862175,-4.7557449471,-2.8362707145\C,-4.3428859003,-2.8561789696,-1.8926019643\H,-5.0097082375,-2.1360552364,-2.3718837992\C,-4.8441909426,-2.168771659

1,0.1822796372\H,-5.4051573519,-3.1061503529,0.2022933879\C,-5.6649051647,-1.0120408844,-0.1072549785\C,-6.874002994,-1.2104847693,-0.8199107237\C,-5.3973762012,0.3095812648,0.3141211976\C,-7.7268387075,-0.1797999926,-1.1381860334\H,-7.1400268495,-2.2226148841,-1.1368153937\C,-6.2389674723,1.3601081197,0.0054199794\H,-4.5372761556,0.5275120313,0.9415341753\C,-7.4264134244,1.157243272,-0.7461077983\H,-8.639981972,-0.4011136544,-1.6862971533\H,-5.9811942676,2.3519995355,0.3704041\C,-3.6874001956,-2.186435099,1.0607040237\C,-2.7668729123,-1.1248361543,1.191829261\C,-3.4781988264,-3.3103767182,1.8882074906\C,-1.7801583123,-1.1326580648,2.159720178\H,-2.8321629823,-0.2719813783,0.5178778259\C,-2.4878976967,-3.3425350503,2.8536563524\H,-4.1490430296,-4.1683417233,1.7976795856\C,-1.6320348564,-2.2272947948,3.0477005929\H,-1.1212503404,-0.271831936,2.2444029516\N,-8.2509953915,2.185921248,-1.0615173236\C,-9.479464973,1.9379591137,-1.7916642455\H,-10.0019425001,2.8867639868,-1.9476635728\H,-9.2781630379,1.4918032952,-2.7783467423\H,-10.1510879008,1.2636982626,-1.2368009989\C,-7.9236018457,3.5328084452,-0.6358029658\H,-8.6871473641,4.2229808983,-1.0075925331\H,-7.8906800891,3.6142721437,0.4626151181\H,-6.9481657578,3.8522272889,-1.0349868005\H,-2.4013925851,-4.2219368016,3.4884240369\N,-0.7045365935,-2.1935334737,4.0477314632\C,-0.5655629079,-3.3258587918,4.9408845293\H,0.2627415498,-3.1393067678,5.6322513072\H,-1.4799877649,-3.5016304941,5.5327015061\H,-0.3358449457,-4.2446512121,4.3790496614\C,-0.014793817,-0.9520186185,4.3402033325\H,0.6274934538,-1.0950579471,5.2152619511\H,0.6248506885,-0.6353416668,3.4992456371\H,-0.7247545234,-0.1365860137,4.5559920012\\Version=ES64L-G09RevD.01\State=1-A\HF=-3506.2517512\RMSD=4.385e-09\RMSF=7.715e-07\Dipole=-4.9519914,-1.3792386,-0.7958947\Quadrupole=38.2852094,-16.9056376,-21.3795717,-11.7269075,15.9336802,-12.7446373\PG=C01 [

X(C46H50F12N3O1Si1)]\\@

ap: **R** enantiomer unshielded side; ΔG298(MP2/CBS) = -3504.0686885

1\1\GINC-WORKER\FTS\RM062X\def2SVP\C46H50F12N3O1Si1(1+)\JHIOE\03-Sep-2

015\0\\#p opt=(calcfc,ts,noeigen) def2svp m062x empiricaldispersion=gd

3 int=ultrafine\\title\\1,1\C,1.1207825422,-0.5304315431,1.4540624584\

C,1.5263986809,-1.6839253209,2.3825886151\C,1.2665151546,-2.9691240854

,1.586276582\C,0.0951672156,-2.6145479955,0.6698402655\H,0.6270400832,

0.2557883015,2.0397463377\H,2.5635444824,-1.5775388757,2.7221288148\H,

0.882117026,-1.6456552181,3.2706393131\H,2.1455028271,-3.2470953664,0.

9894319645\H,1.0301532594,-3.8206484947,2.2361651138\H,0.1783492166,-3

.0691002672,-0.3297773417\H,-0.8812958034,-2.9018856909,1.0974283636\N

,0.1447168237,-1.1544850096,0.5557664253\C,-0.7165954291,-0.4848135765

,-0.2040640648\H,-0.6089120543,0.6001016593,-0.2025899011\C,-1.7522510

06,-1.01967543,-0.9483600587\H,-1.9547034205,-2.0910456951,-0.94380135

12\C,-2.6274412678,-0.1237560876,-1.5928408874\H,-2.2928977235,0.91828

71818,-1.6705591444\C,2.3488322549,0.1411794444,0.7433716788\C,3.07596

37705,-0.94144697,-0.0478535196\C,4.2333828274,-1.5212625036,0.4661623

241\C,2.5244018247,-1.470400659,-1.2205381047\C,4.8289510958,-2.604981

6552,-0.1785330211\H,5.5279889134,0.4816623624,3.6229216378\C,3.107757

3057,-2.5730282373,-1.8379568865\H,1.6267205123,-1.0305402328,-1.66243

44125\C,4.2697395582,-3.1510325396,-1.328649447\H,4.7309201049,-4.0062

753501,-1.8226225716\C,1.9311455491,1.3333574322,-0.1309338923\C,2.585

8021105,1.6406257446,-1.3221677082\C,0.9676445124,2.2338619384,0.33994

56148\C,2.2872864117,2.8148562341,-2.0189652012\H,6.1026943641,0.57965

3166,0.5125855031\C,0.6303026172,3.3654397075,-0.3894951877\H,0.449256

8328,2.0545805078,1.2823889893\C,1.2983168433,3.6814452528,-1.57372821

54\H,1.0548495204,4.5853006975,-2.1333869651\O,3.1288025782,0.61373980

41,1.8032810048\Si,4.3623894198,1.8002283492,1.87121118\C,3.6207977653

,3.5173573964,1.7543155768\H,3.3381994585,3.7779689807,0.723163232\H,4

.3669765156,4.2542645713,2.0899158057\H,2.73311844,3.6235820019,2.3963

87685\C,5.0952161803,1.4908903597,3.5577174116\H,4.3263773061,1.583258

8845,4.3386669653\H,5.8934870236,2.2149971415,3.7771199095\H,4.6646902

473,-1.1379550831,1.3918216639\C,5.6383979713,1.575960893,0.5165732548

\H,5.2382324472,1.782947914,-0.4865877419\H,6.4404827346,2.3106086609,

0.6942527308\H,3.3524249621,0.9733709845,-1.7206816493\C,-0.5317898546

,4.2059881783,0.067106951\F,-0.3980042951,5.4788076713,-0.2712968572\F

,-1.6732201228,3.761325945,-0.4882626258\F,-0.7023339298,4.1376481996,

1.3907495298\C,3.0897115166,3.1189754366,-3.2610264109\F,3.0380372426,

2.1033072908,-4.1203940631\F,2.6494060246,4.2093557642,-3.8782654047\F

,4.3730702568,3.3091198226,-2.9507365903\C,2.4152003443,-3.1554690773,

-3.0438629427\F,2.084360839,-2.2061363869,-3.916724453\F,3.1664786122,

-4.0538013347,-3.6667557375\F,1.2752769105,-3.7616618844,-2.6803978625

\C,6.0896264883,-3.1722518739,0.4243884276\F,5.8708922555,-3.585586311

5,1.6741071147\F,6.5564393792,-4.2003724004,-0.2736972287\F,7.04505990

51,-2.2424470712,0.4832844865\C,-4.5197459793,-1.76820341,-1.974163794

6\H,-4.2439452414,-2.3328927558,-1.0707312395\H,-5.6159945147,-1.72712

47502,-2.0290353648\H,-4.1629128,-2.3381299246,-2.8470295584\C,-3.9308

754785,-0.3911353509,-1.9670497936\H,-4.4308379987,0.3610558096,-2.581

6777207\C,-4.7387307262,0.6013380174,-0.0818793013\H,-4.5903655447,1.5

821978817,-0.5428132483\C,-3.8076423952,0.3341743723,1.0009228616\C,-2

.9632638891,1.3763989558,1.4342238309\C,-3.6261925249,-0.9212971343,1.

6164402354\C,-2.0600289978,1.2142052525,2.472307376\H,-3.0413745768,2.

3588772046,0.9624452551\C,-2.725066514,-1.1050698222,2.6531407082\H,-4

.192905181,-1.7858011532,1.2688938289\C,-1.9256170851,-0.0357953413,3.1287940343\H,-1.4851089326,2.0795799214,2.7993364577\H,-2.6465677719,-2.0924330673,3.1043316813\C,-6.0946388028,0.1162427948,-0.1828971922\C,-6.6846706682,-0.8225986292,0.6919888169\C,-6.9195917421,0.6258913393,-1.2142879542\C,-7.9863728802,-1.2524210591,0.5298661883\H,-6.1297358334,-1.1896318536,1.5536896164\C,-8.2170975982,0.2064858002,-1.3989421174\H,-6.5122526183,1.3773347039,-1.8958746392\C,-8.7955286902,-0.7666918935,-0.5336836803\H,-8.3951297409,-1.9577603526,1.2499035378\N,-1.059713178,-0.2039773257,4.1759723733\C,-0.3308829712,0.9376164686,4.6930326604\H,0.3148937913,0.6092356702,5.5140896971\H,0.318543706,1.3828058739,3.9211865235\H,-1.0030422605,1.7267740413,5.0710985228\C,-1.1390088243,-1.412609643,4.9737087763\H,-0.4079971438,-1.3552903207,5.787024583\H,-2.1416332137,-1.5503147822,5.4127900748\H,-0.9036580081,-2.3079416059,4.3764101462\H,-8.799438761,0.63722269,-2.2103837154\N,-10.0690145369,-1.1954680624,-0.7071988499\C,-10.8802657985,-0.6534038478,-1.7808916356\H,-11.8677062076,-1.1243116298,-1.757181777\H,-11.0163521743,0.434555334,-1.6749610873\H,-10.4292560172,-0.852853187,-2.7657093856\C,-10.6326784945,-2.1813123301,0.195049188\H,-11.6518829916,-2.4193029029,-0.1242581046\H,-10.0448432788,-3.1125493232,0.1879290964\H,-10.6752980699,-1.8058133262,1.2300496074\\Version=ES64L-G09RevD.01\State=1-A\HF=-3506.2554498\RMSD=7.088e-09\RMSF=6.385e-07\Dipole=-6.0359397,-0.8208861,2.0426016\Quadrupole=76.879712,-42.7440338,-34.1356782,23.6614095,18.0842017,-4.9719478\PG=C01 [X(C46H50F12N3O1Si1)]\\@

***sc-exo: S* enantiomer unshielded side; ΔG298(MP2/CBS) = -3504.066979**

1\1\GINC-LOGIN\FTS\RM062X\def2SVP\C46H50F12N3O1Si1(1+)\JHIOE\01-Sep-20

15\0\\#p opt=(ts,calcfc,noeigen) m062x/def2svp empiricaldispersion=gd3

int=ultrafine\\title\\1,1\C,0.591160833,-0.4722364967,-0.5462447397\C

,0.7214534045,-0.3897378528,-2.0723819129\C,-0.0375705402,0.8813482646

,-2.4825701095\C,-1.1318368357,1.0296983939,-1.4245762967\H,0.45047604

35,-1.504793698,-0.1979077483\H,1.7676070206,-0.3812746331,-2.40696831

03\H,0.2435108007,-1.2800999263,-2.5041414124\H,0.6277073873,1.7547664

953,-2.470167611\H,-0.4550476062,0.8044524927,-3.4936934773\H,-1.30327

20563,2.0768397385,-1.1298018506\H,-2.0968438402,0.6007047737,-1.74868

3919\N,-0.6451637504,0.2595051425,-0.2813592414\C,-1.3505482086,0.1311

93191,0.8377550495\H,-0.9114489439,-0.5262072602,1.5910427914\C,-2.578

0254236,0.7240089053,1.0783769282\H,-3.0374249393,1.381088728,0.336896

215\C,-3.3250816099,0.3243808944,2.1995422073\H,-2.8062906566,-0.27536

4769,2.9593083499\C,1.7948232496,0.0922906611,0.2720885926\C,3.0369277

898,-0.7832002212,0.0681935083\C,2.9835089414,-2.0496844029,-0.5192932

573\C,4.2676506715,-0.3369304359,0.5565975647\C,4.126636659,-2.8431332

869,-0.6030887938\H,4.2419812471,-0.839362546,3.2465106862\C,5.4050299

032,-1.1355041526,0.4721216114\H,4.350458381,0.6578376307,1.0020979299

\C,5.3489601623,-2.3991119667,-0.108772988\H,6.2435249539,-3.017765999

1,-0.184504693\C,2.0203439539,1.5443232191,-0.1440023389\C,2.931871767

9,1.918157186,-1.1345829486\C,1.1729836829,2.517645042,0.3885984044\C,

2.971287989,3.2341862339,-1.5929723124\H,3.6435785365,2.1834492041,2.4

707391671\C,1.2203537441,3.8286354296,-0.0761475247\H,0.4577351438,2.2

439525247,1.1671666014\C,2.1168385401,4.2034361761,-1.0727004665\H,2.1

529565687,5.2312540367,-1.4347341394\O,1.3709482545,0.0149440071,1.603

1938161\Si,2.0301962348,0.3577509761,3.1374809778\C,0.490675042,0.3147

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3,-2.0556659\PG=C01 [X(C46H50F12N3O1Si1)]\\@

sc-exo: S enantiomer shielded side; ΔG298(MP2/CBS) = -3504.059340

1\1\GINC-WORKER\FTS\RM062X\def2SVP\C46H50F12N3O1Si1(1+)\JHIOE\31-Aug-2
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961279969\C,0.3205253288,-2.4302787634,2.7917097367\H,2.3127298039,0.1508335116,2.8736041712\H,3.6180937698,-2.2334761516,2.1665643066\H,3.0600579106,-1.8606931968,3.8003334456\H,1.7589526686,-3.6919162882,1.7550201683\H,1.8153388826,-3.8586421743,3.5083403219\H,-0.3969482204,-2.7955151061,2.0371366951\H,-0.1520208394,-2.546879966,3.780957638\N,0.6049228176,-1.0166539042,2.5652490234\C,-0.3724307263,-0.0996685997,2.5343112552\H,-0.0395826243,0.9286711839,2.3805741707\C,-1.7183604427,-0.3613466544,2.6526611827\H,-2.0710879704,-1.3795173259,2.822716441\C,-2.658908137,0.6982765082,2.539605946\H,-2.2470328876,1.6951144013,2.3419316378\C,2.2235053569,-0.329843969,0.7903006007\C,3.6909880793,-0.060898,0.4560112019\C,4.6488490712,0.223464982,1.4296311727\C,4.055682801,0.0519304139,-0.889542128\C,5.932757221,0.6249465762,1.0623030577\H,4.2103399139,2.7558477816,-0.0242761082\C,5.3378817965,0.4566877841,-1.2476865605\H,3.3273037308,-0.1709964281,-1.6733030772\C,6.2922889794,0.7475277999,-0.275637269\H,7.2975996281,1.0620043936,-0.5567792827\C,1.6267358103,-1.4271182985,-0.0904736127\C,2.3655965909,-2.5438851699,-0.4870314905\C,0.2670322096,-1.3770582029,-0.4018349867\C,1.7457681375,-3.6006580573,-1.1514970756\H,2.4457443776,2.0663092351,-2.2881656922\C,-0.3441108721,-2.4445772903,-1.055965837\H,-0.3156721724,-0.5025443474,-0.1054294381\C,0.383799687,-3.5684224405,-1.4375013107\H,-0.0966369611,-4.4020787456,-1.9499394704\O,1.4780954921,0.8458895573,0.6230671993\Si,1.7180107978,2.4339851193,0.0663167225\C,0.3493613709,3.3538433345,0.9535209105\H,-0.6118948363,2.8287047448,0.8564059526\H,0.2111236597,4.3707145268,0.5540331264\H,0.5970092968,3.4469587399,2.0228366757\C,3.370996668,3.1625101712,0.5580796719\H,3.5893789298,3.0198071693,1.6273435209\H,3.3339212729,4.2478784114,0.3716376099\H,4.4171257061,0.1482301355,2.4931233917\C,1.5302447178,2.4311370328,-1.7993433747\H,

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86,-3.4793931669,-1.0408863762\H,-9.1437778743,-3.4464978268,0.7416814

171\C,-10.5262715816,-0.7029523405,-0.3209967392\H,-11.4280971022,-1.3

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ap: S enantiomer unshielded side; ΔG298(MP2/CBS) = -3504.067664

1\1\GINC-WORKER\FTS\RM062X\def2SVP\C46H50F12N3O1Si1(1+)\JHIOE\05-Sep-2

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N,-0.1590442482,-0.7793325456,0.6180872459\C,-0.8754181947,-0.0648476125,-0.2443926052\H,-0.5841600359,0.9799210142,-0.3582292459\C,-1.9716198384,-0.5031006204,-0.9652566304\H,-2.3464822401,-1.5236353258,-0.8661442843\C,-2.7010634829,0.442405021,-1.7079218635\H,-2.240276614,1.4302960283,-1.8460090572\C,2.2600716952,0.0443413715,0.734198002\C,2.7600900953,-1.2688887094,0.1425233949\C,3.7610775798,-1.9889076507,0.7903807079\C,2.1342026766,-1.8413292281,-0.970689584\C,4.1307165723,-3.2538597656,0.3343791463\H,5.4458372656,0.8127142879,-0.5689060206\C,2.4869307147,-3.1183960269,-1.3971004063\H,1.3562395167,-1.2978563412,-1.5129617094\C,3.4929388186,-3.8385212017,-0.7543393201\H,3.7761133785,-4.8327617272,-1.0999527115\C,2.1111712443,1.1494535529,-0.3221824077\C,2.8315273817,1.144292346,-1.5166035297\C,1.3517816234,2.2840454603,-0.0246499917\C,2.7912040822,2.2429037534,-2.3785211053\H,3.9998831744,3.3407595639,0.191933321\C,1.2702089289,3.3496134907,-0.910631549\H,0.7924785413,2.34994201,0.9085928515\C,2.0007687024,3.3516777128,-2.0974093434\H,1.9588334786,4.1975442064,-2.7840559489\O,3.104007415,0.5038528104,1.7501693848\Si,4.5509793517,1.418407558,1.7010745877\C,5.1632020352,1.2577120775,3.4548527295\H,4.4120440537,1.6332505494,4.1649798546\H,6.0890271156,1.8331629734,3.601118905\H,5.3750007492,0.2079739536,3.7061318821\C,5.7828278542,0.7188648753,0.4738210774\H,6.0424577721,-0.3317197643,0.666520321\H,6.71023931,1.3077804011,0.5605943985\H,4.243462683,-1.5681651002,1.6735975988\C,4.1857989461,3.2055702759,1.2682025354\H,3.3185943505,3.5961639767,1.8223411599\H,5.0583130749,3.8226724394,1.5335916377\H,3.4486667308,0.2855429199,-1.7880392685\C,0.3191997974,4.4635027075,-0.5675240197\F,0.5365415125,5.5586430013,-1.2759493058\F,-0.9505057163,4.0776150646,-0.791639779\F,0.3891644176,4.7784441081,0.7310369804\C,3.6554557544,2.1974422484,-3.6157639671\F,3.4172621755,

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01408868,-0.247433919\C,-10.845302023,-1.4036164664,-0.6438498932\H,-1
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02,-3.4330489964,0.115292272\H,-10.5981601347,-3.8298221406,0.07270108
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.1281674\PG=C01 [X(C46H50F12N3O1Si1)]\\@

product-iminium 1C

_S_ enantiomer; ΔG298(MP2/CBS) = -3504.1060819

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29,-0.7512569876,2.2773615966\C,-0.6884610688,0.4766640393,2.862101113
3\C,0.4714822575,0.7739042914,1.9057395969\H,-0.8425442774,-1.80303339
93,0.4274882604\H,-2.4964035577,-0.7149239401,2.4349402339\H,-1.041871
9579,-1.6708730679,2.7486870107\H,-1.3609824998,1.3392243155,2.9300056
988\H,-0.3222044818,0.2773234625,3.8762105232\H,0.5377710058,1.8362694
863,1.6263136386\H,1.4497151826,0.4510461426,2.2967845009\N,0.19726194
53,-0.0251764141,0.6999514635\C,0.9920781193,-0.0772697085,-0.32703120
11\H,0.6946764293,-0.7555597037,-1.1304297288\C,2.2138810237,0.6500462
641,-0.4482175467\H,2.5244373024,1.3416609674,0.33677646\C,3.073878716
,0.2959928717,-1.433598002\H,2.7244967327,-0.4065551526,-2.2027456135\

C,-2.1138761383,-0.1886741323,-0.204060974\C,-3.4326468868,-0.9648019512,-0.1389917957\C,-3.440492676,-2.3435776216,0.0923774278\C,-4.6326882183,-0.3490795167,-0.4994412186\C,-4.6129214097,-3.080507772,-0.0429057214\H,-4.1884732864,-1.8499258584,-2.855640586\C,-5.8018093823,-1.0951939202,-0.6388107757\H,-4.6697609837,0.7244477859,-0.6928549772\C,-5.8078602872,-2.4667780569,-0.411922309\H,-6.7247591725,-3.0469072324,-0.52113957\C,-2.2657474459,1.3017922602,0.1049720218\C,-3.1127647944,1.7795975121,1.1087564321\C,-1.4303498888,2.2090209296,-0.5474964465\C,-3.1008813646,3.1282747743,1.4591713423\H,-4.1176230083,1.1910843664,-2.8861764288\C,-1.4202611832,3.5534166034,-0.1853973654\H,-0.7702143574,1.8594431877,-1.3433223839\C,-2.25352265,4.0312528521,0.8211182293\H,-2.2453292618,5.0844946536,1.1032494791\O,-1.5320064805,-0.3669396893,-1.4646318913\Si,-2.170194372,-0.3853634047,-3.0587315814\C,-0.5871458114,-0.4285007944,-4.0515498873\H,0.0388345706,0.4507754884,-3.8334592374\H,-0.7976994997,-0.4274740068,-5.1311010629\H,-0.0083423252,-1.3376638599,-3.8271072366\C,-3.1981885992,-1.9229207853,-3.3292267938\H,-2.6950102073,-2.8221537549,-2.9427199987\H,-3.3590492343,-2.0665760794,-4.4089593484\H,-2.5321615137,-2.8787582749,0.3713002274\C,-3.151739794,1.1678237917,-3.4106536779\H,-2.5920606671,2.0828342397,-3.1667558322\H,-3.3765609499,1.1948592802,-4.4887959228\H,-3.7905565653,1.1042148698,1.6363892256\C,-0.4209064766,4.4468647592,-0.8735722461\F,-0.5878120746,5.7233620312,-0.5614387783\F,0.8248400777,4.0960204706,-0.5205839538\F,-0.4959898301,4.3219536876,-2.1980029935\C,-3.9632037726,3.568310542,2.6168525313\F,-3.4241179448,3.155435464,3.770339496\F,-4.0811070545,4.8878105169,2.6737031317\F,-5.1797916712,3.0368977853,2.5403275066\C,-7.040856718,-0.3758692503,-1.1140880043\F,-6.8749176444,0.0377049734,-2.3738764737\F,-8.1122187173,-1.1564142381,-1.0755277374\F,-7.2

79561258,0.7046910527,-0.37444179\C,-4.5439304081,-4.5774096214,0.1380
549131\F,-3.7209628572,-4.8985533754,1.1393379113\F,-5.7359171582,-5.0
984942181,0.3950296272\F,-4.0680928483,-5.1615130227,-0.962183339\C,4.
9602657299,1.1996887238,-2.8357852067\H,4.7513875854,0.4674301793,-3.6
303614378\H,4.442737686,2.1366235441,-3.0819788931\H,6.0420791101,1.39
00864615,-2.8259921359\C,4.5226891402,0.6584032327,-1.476339392\H,4.69
49936604,1.4138163767,-0.6942539115\C,5.3203872688,-0.634024056,-1.080
680485\H,5.2839739627,-1.3024926829,-1.9576990351\C,4.5537637367,-1.32
42161648,0.0379031673\C,3.6662707125,-2.3629324169,-0.2514729262\C,4.5
146601882,-0.7867747713,1.3269351936\C,2.6880710998,-2.7687016102,0.65
27134014\H,3.707709352,-2.8468821791,-1.2313073076\C,3.5474112226,-1.1
765568244,2.2466223009\H,5.2415425687,-0.0218436693,1.6124938252\C,2.5
629052885,-2.1349234974,1.9074789886\H,2.0221571637,-3.583237254,0.372
6040897\H,3.5661001162,-0.7317367589,3.2404287196\C,6.7800657553,-0.36
51027704,-0.776957269\C,7.2472569875,0.7947006436,-0.1500580953\C,7.73
11283009,-1.3440959054,-1.0888633377\C,8.5913582265,0.9740406803,0.158
173906\H,6.5607885657,1.6045946843,0.1080661558\C,9.0763650416,-1.1900
777223,-0.789544256\H,7.4079160916,-2.264496303,-1.5822591366\C,9.5487
670958,-0.0188208813,-0.150755999\H,8.8960550174,1.9011643596,0.639351
6047\N,1.5166570875,-2.4369515974,2.7694900026\C,0.7559302794,-3.64496
64819,2.517247935\H,0.0121082982,-3.7775476893,3.3118032942\H,0.214579
7915,-3.5811181905,1.5591800492\H,1.389752649,-4.5487320117,2.48312835
47\C,1.6086453408,-1.9946370504,4.1472484773\H,0.692493558,-2.27984959
55,4.6789585559\H,2.4722370451,-2.4299915867,4.6815392551\H,1.69766220
97,-0.8993529886,4.2040935749\H,9.7667911668,-1.9864177581,-1.06014053
85\N,10.8754589614,0.1473247509,0.1480389713\C,11.8246803358,-0.885065
3105,-0.1995450578\H,12.8260474267,-0.5761070466,0.1182801328\H,11.590

2491465,-1.8407911346,0.2986092183\H,11.8540537674,-1.0675354274,-1.28

72291758\C,11.3199880144,1.36492432,0.7849879422\H,12.4021389918,1.314

6618349,0.9450347821\H,11.108395513,2.2537857398,0.1663006494\H,10.838

3049863,1.5126891758,1.7663894174\\Version=ES64L-G09RevD.01\State=1-A\

HF=-3506.2794184\RMSD=8.418e-09\RMSF=2.052e-06\Dipole=3.2030421,-0.795

086,0.5363514\Quadrupole=47.090038,-31.1651207,-15.9249173,5.3893528,4

.9922114,-0.066725\PG=C01 [X(C46H50F12N3O1Si1)]\\@

***R* enantiomer; ΔG298(MP2/CBS) = -3504.1036746**

1\1\GINC-WORKER\FOpt\RM062X\def2SVP\C46H50F12N3O1Si1(1+)\JHIOE\11-Aug-

2015\0\\#p freq def2svp m062x opt empiricaldispersion=gd3 int=ultrafin

e\\title\\1,1\C,1.9316721659,-0.1840307717,-2.4031210403\C,2.764610172

2,0.7759051417,-3.2592789813\C,1.9073243003,2.0446542835,-3.4268329323

\C,0.4542395131,1.5835466416,-3.2651377797\H,2.0360590066,-1.233787380

7,-2.7105845667\H,3.740493337,0.991304833,-2.8053303914\H,2.9565960164

,0.3093826953,-4.2356447933\H,2.1570993711,2.7939181104,-2.6666509198\

H,2.0684490865,2.511082837,-4.4055021805\H,-0.1283655248,2.2277178377,

-2.5913053075\H,-0.0805917104,1.5071609234,-4.2228539933\N,0.547195391

7,0.2269514437,-2.691331573\C,-0.4809125825,-0.530409288,-2.4494558451

\H,-0.2648679391,-1.5463244876,-2.1117325141\C,-1.8420517937,-0.122199

7307,-2.5433476574\H,-2.0970661524,0.9142640406,-2.7760480348\C,-2.806

784017,-1.0173846864,-2.2101513824\H,-2.5006867087,-2.0463426653,-1.97

71687946\C,2.1767829047,-0.1593857899,-0.8503062735\C,3.5568269715,-0.

721105119,-0.5014996505\C,4.3596641449,-1.4236207507,-1.3986756793\C,3

.9756595618,-0.6140260817,0.8290352381\C,5.5394236695,-2.028987634,-0.

9648163417\H,3.3486689306,-3.4187790255,0.4542233274\C,5.1523087768,-1

.2215889496,1.25357772\H,3.3718291691,-0.0513255965,1.5458736516\C,5.9

468672695,-1.9392844869,0.3612637242\H,6.8707018677,-2.4131176827,0.69
41714199\C,2.0187402348,1.2772838719,-0.3476672149\C,3.0949181169,2.16
83928804,-0.3300802713\C,0.7466486871,1.7434087998,-0.0076216715\C,2.8
895931786,3.5137464343,-0.0345935339\H,2.1788437236,-1.7498662881,2.75
30846402\C,0.553800673,3.0955492689,0.2766732811\H,-0.0952041628,1.045
839167,0.0193955896\C,1.6169383077,3.9950674855,0.2590676399\H,1.45811
44691,5.0534024166,0.4696677809\O,1.165533144,-0.9481949584,-0.3017577
272\Si,1.0536260909,-2.3996899562,0.6079498559\C,-0.660969689,-2.98482
77901,0.1501479265\H,-1.3817673172,-2.1539883039,0.2283497218\H,-0.998
8765302,-3.7723014074,0.8404296745\H,-0.6914075506,-3.4098633835,-0.86
67846145\C,2.3430064737,-3.6495400055,0.0735616623\H,2.4039851319,-3.7
513640037,-1.0211885905\H,2.0541798698,-4.6327413066,0.4779171368\H,4.
0929505141,-1.5270435344,-2.4514597337\C,1.1666066989,-2.0307296992,2.
4310565515\H,0.4549832583,-1.2409832332,2.7176981161\H,0.8917024291,-2
.9415886623,2.9870155579\H,4.1067628939,1.8263857283,-0.5587361104\C,-
0.8355243226,3.5821734161,0.6007710939\F,-0.9753973826,4.8779581063,0.
3580741668\F,-1.7469236734,2.9258753211,-0.1341827931\F,-1.1448402643,
3.3747836391,1.8823979462\C,4.0551790766,4.4650961167,-0.1547624828\F,
4.2559922861,4.7814203626,-1.4376298806\F,3.841684699,5.5920478151,0.5
121931353\F,5.1770689871,3.9120845851,0.2969025258\C,5.5302089067,-1.1
021647147,2.7107117514\F,4.6348449559,-1.7328244109,3.4779117397\F,6.7
217465366,-1.6290618159,2.957077607\F,5.5452954769,0.1718372381,3.0953
882692\C,6.3252007226,-2.8483519183,-1.9598441167\F,6.4082820512,-2.21
81539666,-3.1325167529\F,7.5547096338,-3.0995325602,-1.5316535966\F,5.
7192853559,-4.0152115378,-2.1834750706\C,-4.9701868027,-1.2760722533,-
3.3717675179\H,-4.8140902155,-2.3603951178,-3.4766241962\H,-6.04952023
07,-1.0920710279,-3.281515732\H,-4.6023122009,-0.7809260472,-4.2801804

721\C,-4.264346815,-0.7403242578,-2.1168394124\H,-4.4235378786,0.349380042,-2.0671091412\C,-4.8253746826,-1.4036376021,-0.8267959877\H,-4.7907672083,-2.4921466447,-1.0086273183\C,-6.2787649965,-1.0336774837,-0.6064531143\C,-7.3095985802,-1.9223144697,-0.9248212269\C,-6.6442384269,0.2206010517,-0.1045085898\C,-8.6478552609,-1.5858388957,-0.7599182839\H,-7.0635484677,-2.9152452709,-1.311707563\C,-7.9732062035,0.5812644473,0.0651321783\H,-5.8688581677,0.9365308754,0.1810625259\C,-9.018973443,-0.316002112,-0.2610754217\H,-9.4078348043,-2.3208923699,-1.0169823218\H,-8.2003016563,1.5670483239,0.4660871242\C,-3.9554072732,-1.129206398,0.3888788149\C,-3.2402329514,0.059720069,0.5647196463\C,-3.8761498765,-2.0739518091,1.4206804652\C,-2.4594364483,0.2901835835,1.6937816994\H,-3.2875261363,0.852319844,-0.1854871018\C,-3.1054009794,-1.8676942243,2.5567257022\H,-4.4427588984,-3.0047124101,1.3323618606\C,-2.3643318971,-0.6732254877,2.7219202419\H,-1.9563172725,1.247777559,1.7942751934\N,-10.3347179649,0.030441698,-0.0944226216\C,-11.3729104431,-0.9192621053,-0.4207288885\H,-12.350860381,-0.4664580142,-0.2261079315\H,-11.3399118924,-1.2119659079,-1.4837792801\H,-11.2958553713,-1.8377305071,0.185888323\C,-10.6739853518,1.3307332314,0.4349674444\H,-11.7636438047,1.4241005062,0.4917704898\H,-10.2660221264,1.4820407142,1.4489675044\H,-10.2969183332,2.1449600051,-0.2066923779\H,-3.0890192736,-2.6375898679,3.326122994\N,-1.5916042353,-0.4481784079,3.8354650822\C,-1.5906916335,-1.4116152802,4.9128484019\H,-0.9180746238,-1.0665464267,5.7054425428\H,-2.5951642109,-1.5502448474,5.3485294792\H,-1.2301897138,-2.3957275556,4.5701187122\C,-0.9466044443,0.8338532769,4.0022576411\H,-0.3810613286,0.8351896445,4.9402105157\H,-0.2392045221,1.0403188613,3.1791167936\H,-1.6705714601,1.6665382122,4.0302384661\\Version=ES64L-G09RevD.01\State=1-A\HF=-3506.285438\RMSD=3.745e-09\RMSF=2.620e-06\Dip

ole=-2.2178516,-0.639671,-2.2742771\Quadrupole=34.6771568,-26.2371408,

-8.440016,1.6771301,0.1026271,-4.582699\PG=C01 [X(C46H50F12N3O1Si1)]\\

@

Catalyst base model

ΔG298(MP2/CBS) = -365.6493814

1\1\GINC-LOGIN\FOpt\RM062X\def2SVP\C6H13N1O1\JHIOE\12-Oct-2015\0\\#p f

req def2svp m062x empiricaldispersion=gd3 int=ultrafine opt\\Title Car

d Required\\0,1\C,-2.097658,-1.08209,-0.05726\C,-2.605501,0.349512,0.1

88171\C,-1.356764,1.240019,-0.02898\C,-0.239772,0.246171,-0.382832\N,-

0.685673,-0.975314,0.264312\H,-0.130554,-1.776238,-0.026548\H,-2.97151

8,0.450465,1.218149\H,-1.496907,1.990119,-0.818421\H,-0.188673,0.13257

7,-1.487984\H,-1.09868,1.774992,0.89696\H,-3.433302,0.609491,-0.484362

\H,-2.275842,-1.363147,-1.116291\H,-2.59899,-1.827874,0.575825\C,1.135

643,0.642964,0.098331\H,1.42959,1.623029,-0.329847\H,1.112189,0.741679

,1.201931\O,2.03889,-0.356305,-0.287565\C,3.337766,-0.135101,0.172216\

H,3.750368,0.816073,-0.2139\H,3.969442,-0.960224,-0.17997\H,3.379188,-

0.102157,1.27691\\Version=ES64L-G09RevD.01\State=1-A\HF=-365.966861\RM

SD=4.225e-09\RMSF=7.430e-06\Dipole=0.1270029,0.2546729,-0.0696243\Quad

rupole=2.4979616,-0.2571651,-2.2407965,0.7300255,1.3328408,0.3775725\P

G=C01 [X(C6H13N1O1)]\\@

Protonated catalyst base model

ΔG298(MP2/CBS) = -366.0764578

1\1\GINC-WORKER\FOpt\RM062X\def2SVP\C6H14N1O1(1+)\JHIOE\12-Oct-2015\0\

\#p freq def2svp m062x empiricaldispersion=gd3 opt int=ultrafine\\Titl

e Card Required\\1,1\C,-1.6298687172,-1.2748682723,0.2862405007\C,-1.8

542322268,-0.011233394,1.1124483905\C,-1.5202735022,1.1209238367,0.135

6338835\C,-0.2943842154,0.6001391505,-0.6089861006\N,-0.5252413102,-0.

9031950219,-0.6822884801\H,0.3931380575,-1.3362439094,-0.4702119004\H,

-1.3070206827,2.0747947186,0.6363482787\H,-2.3516199243,1.2916410642,-

0.5631909824\H,-1.3252503867,-2.156196853,0.8609566585\H,-2.5126104704

,-1.5307203934,-0.3118480421\H,-0.7589641974,-1.1935050379,-1.63638999

64\H,-0.2007883689,0.9678619744,-1.6378806845\C,1.02149444,0.819491922

5,0.1392642585\H,1.3894704172,1.8342008385,-0.0918480928\H,0.868704212

4,0.7611715736,1.2348939431\O,1.9052492929,-0.1711431933,-0.2939259889

\C,3.2165324134,-0.0622696701,0.2317037395\H,3.7968028602,-0.903687843

9,-0.1602883374\H,3.6834708709,0.8817234827,-0.088739008\H,3.201955611

,-0.1062743592,1.3327675937\H,-1.1854399059,0.0064756713,1.9842909662\

H,-2.8828843276,0.0398186453,1.4886244406\\Version=ES64L-G09RevD.01\St

ate=1-A\HF=-366.3520236\RMSD=4.263e-09\RMSF=1.667e-06\Dipole=-0.768012

9,-0.5728418,-0.4029115\Quadrupole=5.2054272,-1.5454095,-3.6600178,2.4

855554,1.5699385,1.393443\PG=C01 [X(C6H14N1O1)]\\@

Michler's electrophile

ΔG298(MP2/CBS) = -768.0232526

1\1\GINC-LOGIN\FOpt\RM062X\def2SVP\C17H21N2(1+)\JHIOE\02-Sep-2015\0\\#

 freq def2svp m062x empiricaldispersion=gd3 opt\\Title Card Required\\

1,1\C,-3.9347664386,0.1289648803,-0.0467088732\C,-2.8100970853,0.94297

61831,-0.4037455202\C,-1.5399432072,0.4319759794,-0.3961825495\C,-1.27

86561112,-0.9267631324,-0.0473550419\C,-2.4132991886,-1.7490743176,0.2

193838932\C,-3.6888236017,-1.2513219657,0.240063681\H,-2.9602556515,1.

9738203594,-0.7159740972\H,-0.7228976729,1.0693794496,-0.732582462\H,-

2.2535194581,-2.8063257325,0.4421145691\H,-4.5146591639,-1.9192469707,

0.4727509211\C,0.0000164813,-1.5136208814,0.0001422115\H,0.0000335903,

-2.6098669706,0.0001083848\C,1.2786710539,-0.9267253432,0.0476421849\C

,1.5399234351,0.432012778,0.3965030135\C,2.413333247,-1.7489863971,-0.

2191729912\C,2.8100604286,0.9430585484,0.4040251002\H,0.7228663133,1.0

693784373,0.7329466913\C,3.688836965,-1.2511875653,-0.2398984384\H,2.2

535811666,-2.8062307995,-0.4419559423\C,3.9347459871,0.1290891015,0.04

69135837\H,2.9601875312,1.9739008296,0.7162605682\H,4.514693601,-1.919

0606099,-0.4726842367\N,-5.176041125,0.6373391531,-0.0111376573\N,5.17

60294891,0.6374292482,0.0112053738\C,6.3117509971,-0.2173269667,-0.305

9716892\H,7.2242659162,0.3855576983,-0.3024066826\H,6.4241242389,-1.02

11949177,0.4369879665\H,6.1986450735,-0.6689682066,-1.3026854216\C,5.4

075730049,2.0438638673,0.3087529588\H,6.4648267558,2.272978333,0.14763

2948\H,4.8106558838,2.6885560833,-0.3524116103\H,5.157315746,2.2789360

452,1.3547742723\C,-6.3118826403,-0.2173147146,0.3059037703\H,-6.19893

99351,-0.6689798716,1.3026230397\H,-7.2243336201,0.3856664411,0.302250

3992\H,-6.4242667724,-1.021159595,-0.4370796869\C,-5.4074279007,2.0437

734807,-0.3087881238\H,-5.1569677031,2.2787699907,-1.3547783146\H,-6.4

646886957,2.2729877741,-0.1478559654\H,-4.8105589341,2.6884422963,0.35

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3e-09\RMSF=5.001e-06\Dipole=0.0000078,0.4710672,-0.0001214\Quadrupole=

60.148508,-19.8706268,-40.2778811,0.0008666,-1.37499,-0.0000246\PG=C01

 [X(C17H21N2)]\\@

Chemical Exchange Saturation Transfer in Chemical Reactions: A Mechanistic Tool for NMR Detection and Characterization of Transient Intermediates

Geometry of stationary points (most stable conformations)

***exo*-oxazolidinone + DPU**

1\1\GINC-WORKER1\FOpt\RTPSSTPSS\def2SVP/W06\C23H29N3O3\JHIOE\09-May-20
17\0\\#p tpsstpss/def2svp/w06 empiricaldispersion=gd3 scrf=(cpcm,solve
nt=n,n-DiMethylFormamide,read) opt int=ultrafine\\title\\0,1\C,-1.8931
520135,1.9076239109,-0.3230357501\C,-1.6467014096,4.2107435123,0.19111
26099\C,-3.0520489729,4.0445277726,-0.3912125564\H,-2.301196548,0.9891
057102,0.1397425265\H,-1.5920048449,4.93159841,1.0233454106\H,-0.93407
18413,4.5349658706,-0.5990810733\H,-3.7895229206,3.9922810108,0.428483
1942\H,-3.3347971572,4.8733515737,-1.0597245779\C,0.0487240683,2.49952
69207,0.8140310867\N,-1.345341637,2.8430183047,0.6823200963\O,0.445130
8612,1.931027115,-0.5266256479\C,-0.6624100671,1.5012013627,-1.1384848
142\O,-0.6293939681,0.8542057589,-2.1815149904\C,0.3218568015,1.429059
5633,1.869058646\H,0.0760835776,1.8808071035,2.8487488111\C,1.75795745
58,0.8646757994,1.8811427304\H,1.9690588203,0.487420029,0.8652044228\H
,-0.3973260467,0.6029878368,1.7140006903\C,-2.9697974335,2.6864756844,
-1.1229460401\H,-3.9289733732,2.1472870025,-1.1398394907\H,-2.64039601
06,2.8154160969,-2.1676807983\C,2.8118169693,1.9349831698,2.2122953414
\H,2.8167952666,2.7553684934,1.4726239955\H,2.6302814866,2.3766923893,
3.2102575344\H,3.8231962226,1.4910763507,2.215844592\C,1.8475621164,-0
.3290137676,2.8462645833\H,1.1514285266,-1.1313587469,2.5454435761\H,2
.8672675469,-0.7534757159,2.8456995949\H,1.6047121364,-0.0236084177,3.
8815567156\C,0.3318339449,-2.0073736662,-0.5114078731\O,0.6535778664,-
2.8075351938,0.3711909234\N,-0.9809467808,-1.7581129527,-0.8977977476\
H,-1.1090521202,-1.0517052617,-1.6279187432\N,1.2308662255,-1.24094844
11,-1.2435746847\H,0.8186144361,-0.5196263554,-1.8478480539\C,2.617822
6997,-1.1196610841,-1.0473264285\C,3.2579816615,-0.0103354934,-1.64939
58292\C,3.3871803482,-2.0270815911,-0.2850215422\C,4.6326747261,0.1902

603821,-1.487043576\H,2.6610365755,0.704399133,-2.2262794995\C,4.76360
75982,-1.8076534784,-0.1284816355\H,2.8979608263,-2.8784051806,0.18792
75585\C,5.398185861,-0.7051698631,-0.7212558663\H,5.1062810863,1.05884
97882,-1.9575975523\H,5.3463991647,-2.5169422089,0.4699404098\H,6.4732
981917,-0.5450907315,-0.5898496741\C,-2.1712586723,-2.2071613063,-0.30
11788121\C,-3.38097299,-1.6547231738,-0.7883946995\C,-2.2230058882,-3.
1582834981,0.743255168\C,-4.6098717021,-2.0386509177,-0.2410184218\H,-
3.3493129561,-0.9200154059,-1.6015025671\C,-3.4641899697,-3.5296544698
,1.280839416\H,-1.295238079,-3.5898444045,1.1188465802\C,-4.6626151803
,-2.9789096843,0.8013039585\H,-5.5317781549,-1.5960810946,-0.633754295
7\H,-3.4878771239,-4.267005533,2.0911668909\H,-5.6240328451,-3.2786870
6,1.2307751164\H,0.6731146383,3.3947546426,0.949821062\\Version=ES64L-
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pole=-1.2930581,3.0343326,0.0427922\Quadrupole=5.2194012,0.5990893,-5.
8184905,-2.1630566,2.8182429,-1.81857\PG=C01 [X(C23H29N3O3)]\\@

endo-oxazolidinone + DPU

1\1\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP/W06\C23H29N3O3\ROOT\09-May-2017\
0\\#p tpsstpss/def2svp/w06 empiricaldispersion=gd3 scrf=(cpcm,solvent=
n,n-DiMethylFormamide,read) opt int=ultrafine\\title\\0,1\C,1.45388161
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2\C,3.1025692677,-3.5341685474,1.9554293038\H,1.1634017382,-3.63353683
14,-0.6426277988\H,4.4124227251,-1.8967277512,1.2387984942\H,2.8540910
054,-1.3658007814,1.9504888015\H,3.8138454697,-4.260015475,1.525351314
4\H,3.2291068245,-3.5330610132,3.0496264078\C,2.3178326125,-1.11524645
96,-0.6949415884\N,2.717348006,-2.2988987854,0.0009054616\O,0.94964755
04,-0.7592635581,-0.0902054299\C,0.4237340617,-1.8997880938,0.38230526
93\O,-0.7048502503,-1.9588062497,0.849291508\C,3.2214712848,0.09704328
08,-0.6081321064\H,2.6984051067,0.9361286706,-1.1009758779\C,4.6087905
046,-0.0993806008,-1.2637609705\H,5.1072185003,-0.9477688803,-0.756222
8482\H,3.3479902469,0.376479168,0.4523385859\C,1.6587917607,-3.8781927
847,1.5178582705\H,1.5223729256,-4.9516156368,1.3190419035\H,0.9196063
206,-3.5826837843,2.280997662\C,4.510602859,-0.4377524394,-2.761804062
5\H,3.9985058403,-1.4002242987,-2.9361258625\H,3.958573964,0.349589675

7,-3.3083260102\H,5.5186075249,-0.5146642667,-3.2057764828\C,5.4617198
075,1.1600177699,-1.0332174078\H,5.563471822,1.3833965459,0.0438457513
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-1.9544437234,-0.6425193497,0.3734197145\N,-1.0198166211,1.5729113199,
0.2679836104\H,-0.4161742038,0.7470710662,0.3230170335\C,-0.3424660024
,2.7953981047,0.4111696461\C,1.0041602625,2.734600878,0.8447890926\C,-
0.917305421,4.0600085069,0.1453839362\C,1.761610049,3.9010762239,0.992
1500044\H,1.4472975608,1.7595907533,1.0697825853\C,-0.1462783972,5.220
7056928,0.3084322246\H,-1.9544271155,4.1157038557,-0.1854311227\C,1.19
23537946,5.1576274359,0.7255506438\H,2.8032187578,3.8236467461,1.32334
80043\H,-0.6068472111,6.1926285604,0.0975977092\H,1.7827635215,6.07220
86106,0.8431655959\C,-3.9274084271,-0.5968025676,-0.2161949641\C,-3.99
48799442,-2.0060858216,-0.0804405372\C,-5.0847786371,0.1054729049,-0.6
276175331\C,-5.1848620402,-2.6909004929,-0.3486149561\H,-3.100945274,-
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,-5.0427586912,1.1899417841,-0.7288200373\C,-6.3342668551,-1.994261220
6,-0.7586519464\H,-5.2112478927,-3.7805489948,-0.2360435034\H,-7.15496
0757,-0.0384649248,-1.2114761577\H,-7.2652943402,-2.5311353283,-0.9684
021525\H,2.0600635488,-1.3648449327,-1.7377810149\\Version=ES64L-G09Re
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8,2.1717863,3.4398831,-2.1816851\PG=C01 [X(C23H29N3O3)]\\@

_Z_-iminium + DPU

1\1\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP/W06\C23H29N3O3\ROOT\09-May-2017\
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ad) empiricaldispersion=gd3 opt int=ultrafine\\title\\0,1\C,-2.3260180
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112\C,-3.7703378109,-2.0783081257,-2.7901326004\H,-2.527925009,-2.1805
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30898891,0.0429741568,-3.0189200003\H,-4.5963410882,-2.6609829028,-2.3
466737406\H,-3.7854468108,-2.2264941341,-3.8808475116\C,-3.8257959832,

0.2250585321,-0.0989363669\H,-4.604205196,0.9332970021,-0.4142158147\N
,-3.4055566927,-0.5859086659,-1.0178670774\O,-0.9167528236,0.291705856
8,-0.2908478671\C,-0.9269434316,-0.9088133549,-0.6681784381\O,0.051403
0244,-1.66813525,-0.8840572503\C,-3.4217803866,0.2390546447,1.32916940
86\H,-2.6203022658,-0.4848262498,1.5393054356\C,-4.642796221,0.0089715
307,2.269298607\H,-5.4100319976,0.7666733108,2.0164535121\H,-3.0037024
716,1.245335629,1.5224707147\C,-2.4209225505,-2.4573780524,-2.15005488
74\H,-2.3465558115,-3.5293650871,-1.9160389141\H,-1.5826433541,-2.2033
211269,-2.8187327111\C,-5.2515930252,-1.3882893655,2.0611424743\H,-5.5
893934757,-1.5384337395,1.0195759216\H,-4.5127625125,-2.1767903068,2.2
959483127\H,-6.123886477,-1.5332075808,2.7216620301\C,-4.213083703,0.2
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0728725468,0.0919634878,4.4073815209\H,-3.430924499,-0.4964400382,4.01
97380622\C,2.7728441691,0.7305387645,0.0672727597\O,3.8870096138,1.219
1648011,0.3033132743\N,2.5195740506,-0.6319167424,-0.0092830332\H,1.57
5171353,-0.9374003934,-0.3400768836\N,1.6247447786,1.478128412,-0.1533
688976\H,0.7141443018,0.9671686466,-0.2135013139\C,1.5084142239,2.8722
782803,-0.2336408352\C,0.2067923704,3.3956733468,-0.4506873213\C,2.592
4805729,3.7773469748,-0.1224511928\C,-0.000620633,4.7754278243,-0.5492
010086\H,-0.6326125966,2.6983049408,-0.5415315863\C,2.3642417715,5.157
623966,-0.2262519956\H,3.5951797852,3.3851807924,0.0477736619\C,1.0758
773753,5.6724528306,-0.4382052161\H,-1.016264065,5.1522242166,-0.71628
18877\H,3.2170977289,5.8407635031,-0.1371642023\H,0.9120636202,6.75251
23638,-0.5156198357\C,3.4073921826,-1.6863589862,0.2448630958\C,2.9067
137697,-3.0026463336,0.0666065405\C,4.7481542178,-1.5233742721,0.67213
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87509,-0.2606486811\C,5.5482280606,-2.6511543899,0.9088847973\H,5.1432
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2608\H,3.3091112639,-5.1194849346,0.1596605416\H,6.5831022027,-2.50291
45314,1.239129358\H,5.6878455771,-4.8228656538,0.9167108914\\Version=E
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06\Dipole=-8.8073483,-1.2745358,-0.8234744\Quadrupole=14.2329333,-12.0
585813,-2.174352,1.2655675,6.7214813,2.1674415\PG=C01 [X(C23H29N3O3)]\
\@

_E_-iminium + DPU

1\1\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP/W06\C23H29N3O3\ROOT\15-May-2017\
0\\#p tpsstpss/def2svp/w06 scrf=(cpcm,solvent=n,n-DiMethylFormamide,re
ad) empiricaldispersion=gd3 opt int=ultrafine\\title\\0,1\C,-1.6794133
038,-2.1765674288,-0.6773847147\C,-3.8331286825,-1.6322643894,-1.73074
70518\C,-3.236839848,-2.8695251536,-2.408290754\H,-1.6264268756,-2.984
5488408,0.072082728\H,-4.889250092,-1.7326442303,-1.4442241286\H,-3.70
45222072,-0.7217490054,-2.3424846729\H,-3.6486457165,-3.7831468646,-1.
9456219212\H,-3.4663647568,-2.8919273253,-3.4847621258\C,-3.2891007314
,-0.8019331636,0.5473393227\H,-2.5591061814,-0.8421434894,1.3635003042
\N,-2.9887583402,-1.4861957123,-0.5114303377\O,-0.6736810448,-0.080662
2213,0.0461702317\C,-0.461527757,-1.2283338214,-0.4308946805\O,0.64204
07512,-1.7424773756,-0.7493414598\C,-4.5346416951,-0.0095059257,0.7337
665337\H,-4.9948176463,0.2444110386,-0.2366728628\C,-4.3032733453,1.27
15163625,1.577548752\H,-3.8789157739,0.9519555471,2.5496020557\H,-5.25
0473756,-0.6701104226,1.2671084625\C,-1.7345324979,-2.739822096,-2.112
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6494703,-2.80855341\C,-3.292011796,2.2062753137,0.8932522284\H,-2.3255
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,-0.7689104427,-0.1815431257\N,1.5824351317,1.6023239086,-0.2247667558
\H,0.7855967994,0.9315618647,-0.1520868835\C,1.2113688029,2.9168378515
,-0.536479513\C,-0.1371014181,3.1251679783,-0.9243712948\C,2.084360415
3,4.0309203846,-0.492414958\C,-0.6006858319,4.405972944,-1.2411915699\
H,-0.8097989164,2.2629841418,-0.9717654908\C,1.6038706232,5.3070549554
,-0.8230570806\H,3.1224997149,3.8796854153,-0.1956565455\C,0.265811007
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\H,2.2948445134,6.1572190431,-0.782246694\H,-0.0962558855,6.5147406916
,-1.444637854\C,3.9042657173,-1.1067183078,0.5354071303\C,3.6568433849
,-2.5036922347,0.4954281322\C,5.1758517798,-0.6546827761,0.9653558911\
C,4.6491068102,-3.4148725347,0.8716331681\H,2.6733275157,-2.8538833692

,0.1635566313\C,6.157080949,-1.5841426456,1.3411749841\H,5.3777100041, 0.4163731822,0.9918418871\C,5.9104682597,-2.9652630721,1.2993367684\H, 4.4322382711,-4.4884775288,0.8305099015\H,7.134919179,-1.2141172054,1. 6711064966\H,6.6865388357,-3.6797618255,1.5935186905\\Version=ES64L-G0 9RevD.01\State=1-A\HF=-1283.282459\RMSD=7.265e-09\RMSF=3.081e-06\Dipol e=-8.4933168,-2.798089,-0.466351\Quadrupole=11.8350709,-5.3651327,-6.4 699382,11.0489552,2.782214,3.3642656\PG=C01 [X(C23H29N3O3)]\\@

TS Ring Opening *endo*-oxazolidinone + DPU

1\1\GINC-WORKER0\FTS\RTPSSTPSS\def2SVP/W06\C23H29N3O3\JHIOE\18-May-201 7\0\\#p tpsstpss/def2svp/w06 empiricaldispersion=gd3 scrf=(cpcm,solven t=n,n-DiMethylFormamide,read) opt=(ts,calcfc,noeigen) int=ultrafine\\t itle\\0,1\C,-1.3927084451,-2.943102568,-0.1378541067\C,-3.2766330622,- 2.1916244499,-1.4130789051\C,-2.8871087419,-3.565421572,-1.9688124287\ H,-1.1959483855,-3.5309910499,0.7763862787\H,-4.3624369913,-2.02547861 96,-1.350425941\H,-2.8230906497,-1.3725842823,-2.006384347\H,-3.577980 0829,-4.3298658573,-1.573791313\H,-2.934168427,-3.5945599871,-3.068507 6497\C,-2.5768733853,-1.1584649721,0.7506559706\N,-2.6846334664,-2.237 4451303,-0.0545288293\O,-0.8172012806,-0.6439688787,0.1974312436\C,-0. 3433005819,-1.7888581318,-0.1896928889\O,0.8194989138,-1.9884298503,-0 .5726520124\C,-3.473945366,0.0305491803,0.6136182401\H,-3.0076090301,0 .8646083608,1.165538438\C,-4.9083948065,-0.2069091242,1.1705225558\H,- 5.3553867977,-1.0437124033,0.5999681892\H,-3.5367612502,0.3251824757,- 0.4475147051\C,-1.4586899297,-3.8015315468,-1.4220629376\H,-1.26295907 54,-4.863842986,-1.213598869\H,-0.6895215645,-3.4520949171,-2.13028422 37\C,-4.8999996618,-0.5929162094,2.6594177455\H,-4.375537644,-1.548281 7223,2.8365745474\H,-4.4052242718,0.1883667651,3.2656047123\H,-5.93312 88802,-0.7071328618,3.0309958517\C,-5.7581587341,1.0497778726,0.920137 1482\H,-5.7886554774,1.3068071203,-0.1534488309\H,-6.7948580085,0.8917 281996,1.2653733966\H,-5.3444480002,1.9170596756,1.4670797204\C,2.4350 828116,1.3746212812,-0.0478010765\O,3.2596477526,2.2932383552,0.033193 2989\N,2.7555262918,0.0262317732,-0.0024836033\H,2.0016632155,-0.65558 71001,-0.2216195824\N,1.067449695,1.5717627436,-0.199918264\H,0.454744 582,0.7459296079,-0.1178644238\C,0.3810376549,2.7808348024,-0.39059554

16\C,-1.0116890771,2.6914389149,-0.6370730768\C,0.9837358033,4.0606072
353,-0.3521456169\C,-1.7817301834,3.8435118676,-0.8246791745\H,-1.4766
712084,1.7023933556,-0.6830691597\C,0.1973265428,5.2055204165,-0.55102
61288\H,2.0545369372,4.1397540716,-0.1643462856\C,-1.1838222601,5.1146
410164,-0.7839404345\H,-2.8574997481,3.7428014137,-1.0083449921\H,0.68
1089094,6.1885552045,-0.5172574351\H,-1.7845607221,6.0179968061,-0.932
6471351\C,4.0108275817,-0.554403059,0.234443222\C,4.0809253493,-1.9703
964802,0.1920981769\C,5.1890878579,0.176778164,0.5193823274\C,5.291196
311,-2.6312880392,0.4271346675\H,3.1710645694,-2.5392330527,-0.0270534
541\C,6.3928494697,-0.5042345173,0.7541596549\H,5.1461248933,1.2655747
292,0.5477018192\C,6.4605475627,-1.9053218273,0.7112107474\H,5.3182373
766,-3.7261739675,0.3881073584\H,7.2943657316,0.079615334,0.973361014\
H,7.4074102461,-2.4238691296,0.8949287943\H,-2.1959560468,-1.380192449
9,1.7539522539\\Version=ES64L-G09RevD.01\State=1-A\HF=-1283.2728014\RM
SD=4.182e-09\RMSF=8.548e-07\Dipole=-5.8084804,-2.9534151,0.0952037\Qua
drupole=1.8203083,0.8853617,-2.70567,2.2093804,2.0196214,2.00474\PG=C0
1 [X(C23H29N3O3)]\\@

TS Ring Opening *exo*-oxazolidinone + DPU

1\1\GINC-WORKER1\FTS\RTPSSTPSS\def2SVP/W06\C23H29N3O3\JHIOE\17-May-201
7\0\\#p tpsstpss/def2svp/w06 empiricaldispersion=gd3 scrf=(cpcm,solven
t=n,n-DiMethylFormamide,read) opt=(ts,calcfc,noeigen) int=ultrafine\\t
itle\\0,1\C,-1.7703659025,-2.6077078276,0.2076097901\C,-3.145608726,-2
.7976143297,-1.7540896439\C,-2.8368347734,-4.2233381545,-1.2911684756\
H,-1.9082606443,-2.5783292918,1.3008931271\H,-4.1791738769,-2.64457664
63,-2.0989049517\H,-2.4451203006,-2.4640270181,-2.5444209907\H,-3.7029
671413,-4.6267687517,-0.7387652551\H,-2.6224867203,-4.896635724,-2.135
6126102\C,-2.9109137369,-0.6777055769,-0.502345587\N,-2.9107675283,-2.
0171422581,-0.5137618688\O,-0.9089626324,-0.5645360594,-0.726936359\C,
-0.5691685239,-1.6677677859,-0.1498210563\O,0.5906769363,-2.012923608,
0.1346494929\C,-2.9705175476,0.1394709659,0.7540534309\H,-2.414588257,
-0.3396379286,1.5773671901\C,-4.4406573219,0.4022946908,1.1973586462\H
,-4.9979460625,0.7719739273,0.3137725156\H,-2.4821877939,1.1038914059,
0.5390178526\C,-1.6293129682,-4.0491015826,-0.3412838676\H,-1.62262065

82,-4.7938329318,0.4683802636\H,-0.6742897827,-4.1371080577,-0.8848647723\C,-5.1275899701,-0.8747966532,1.7077935358\H,-5.1341712557,-1.6705218575,0.9433722321\H,-4.6036649025,-1.2669291329,2.5993899596\H,-6.1730945804,-0.663844773,1.9932505105\C,-4.4536797465,1.5125178563,2.2628020172\H,-4.0040406137,2.4440164365,1.8758846651\H,-5.4879648397,1.7339595116,2.5795182594\H,-3.8827436329,1.2025611676,3.1574561742\C,2.3536189937,1.3232192903,-0.1335346808\O,3.1873567491,2.2289761383,-0.0096264562\N,2.642674329,-0.0286037775,-0.022349497\H,1.8489115417,-0.701039635,-0.0395778457\N,1.0097253753,1.5472790455,-0.4086348483\H,0.4068086883,0.7302340084,-0.6037339399\C,0.3528148921,2.7839421768,-0.5012737298\C,-0.9274696295,2.7954387823,-1.1092755285\C,0.8766314777,3.9988347334,0.001054213\C,-1.6696535202,3.9790594532,-1.1922573984\H,-1.3284556941,1.8638942112,-1.5208062058\C,0.1240990052,5.1778982211,-0.099988304\H,1.8657224232,4.0053706336,0.4596901818\C,-1.1507122595,5.1832646584,-0.6881339567\H,-2.6589715489,3.957725351,-1.6628980073\H,0.5459643106,6.1085863991,0.2965814\H,-1.7288844868,6.1106362164,-0.7565180071\C,3.8945728147,-0.6237761077,0.1990881223\C,3.9160879607,-2.0329676796,0.3596411908\C,5.1181818645,0.0858507016,0.2613852322\C,5.1225735795,-2.7077991794,0.5739153047\H,2.9715798502,-2.5849623799,0.3169016689\C,6.3176604412,-0.6088279098,0.4771300781\H,5.1111507544,1.1695421944,0.1453409732\C,6.3369793193,-2.0031721421,0.6346759127\H,5.1109073889,-3.7969441673,0.6952106386\H,7.2543787779,-0.0411499535,0.5220293205\H,7.2807090808,-2.5326685416,0.8027146422\H,-3.3285699748,-0.1994947541,-1.3996856985\\Version=ES64L-G09RevD.01\State=1-A\HF=-1283.2697754\RMSD=5.525e-09\RMSF=9.967e-07\Dipole=-6.0005938,-2.775788,-0.457033\Quadrupole=1.2382403,1.8582955,-3.0965358,3.0841969,4.5751633,4.9025814\PG=C01 [X(C23H29N3O3)]\\@