

Supporting Information

for

Synthesis and evaluation of new guanidine-thiourea organocatalyst for the nitro-Michael reaction: Theoretical studies on mechanism and enantioselectivity

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Detailed information about the DFT calculations

Calculations of the enantiomeric excess ee

For calculation of ee the theory of the activated complex was used. Based on this theory, the kinetic constant k is a function of the free activation energy (Equation 1) [1].

$$k = \frac{k_B \cdot T}{h} e^{-\frac{\Delta G^\ddagger}{RT}} \quad (1)$$

The enantiomeric excess ee is defined as the ratio of the difference of the product concentrations to their sum. If it is assumed that the transition states are totally converted into the products, the product concentrations can be replaced by the transition state (TS) concentrations in the expression for ee. The TS concentrations are the product of the reactant concentrations and the kinetic constants. This results in the following expression (Equation 2):

$$ee = \frac{[TS_R] - [TS_S]}{[TS_R] + [TS_S]} = \frac{k_R[C_R] - k_S[C_S]}{k_R[C_R] + k_S[C_S]} \quad (2)$$

Since the starting point is the same for the R and S pathways, the reactant concentration is the same ($[C_R]=[C_S]$) and Equation 2 can be simplified to Equation 3.

$$ee = \frac{k_R - k_S}{k_R + k_S} = \frac{1 - k_S/k_R}{1 + k_S/k_R} \quad (3)$$

$$\frac{k_S}{k_R} = e^{-\frac{\Delta G_S^\ddagger - \Delta G_R^\ddagger}{RT}} = e^{-\frac{\Delta G_{RS}}{RT}} \quad (4)$$

$$ee = \frac{1 - e^{-\frac{\Delta G_{RS}}{RT}}}{1 + e^{-\frac{\Delta G_{RS}}{RT}}} \quad (5)$$

Thus, ee can be expressed simply as a function of the free-energy difference between the two TS.

Table S1: Computed absolute energies (Hartree) and zero-point vibrational energies (ZPVE, kcal·mol⁻¹) at different levels of theory.

	B3PW91/6-31G(d)		MP2/6-311++G(d,p)// B3PW91/6-31G(d)
	<i>E</i> , Hartree	<i>ZPE</i> , kcal·mol ⁻¹	<i>E</i>
7a	-1296.36288	257.4	-1293.82784
7b	-1296.35890	256.7	-1293.81598
7c	-1296.35385	257.1	-1293.81306
7d	-1296.34879	257.0	-1293.80697
14	-574.67641	120.2	-573.511336
11	-513.95497	86.3	-512.868865
Complex1	-1871.05130	378.6	-1867.36309
TS1 abst	-1871.04057	376.3	-1867.34815
Complex2	-1871.05200	379.1	-1867.36063
Complex2a	-1871.02988	378.0	-1867.32660
CatN1	-1810.33177	344.3	-1806.72577
CatN2	-1810.31678	343.8	-1806.69915
CatN3	-1810.31548	343.9	-1806.68976
CatN4	-1810.31588	344.2	-1806.69807
CatN5	-1810.31522	344.2	-1806.70782
Init1	-2385.01243	466.1	-2380.25480
TS1	-2385.01044	466.4	-2380.25619
Fin1	-2385.02907	467.5	-2380.28565
Init2	-2385.01606	466.2	-2380.25641
TS2	-2385.00825	466.6	-2380.25465
Fin2	-2385.02826	468.3	-2380.28306
Init3	-2385.01807	465.9	-2380.25365
TS3	-2385.01461	466.7	-2380.25991
Fin3	-2385.02947	467.9	-2380.28666
Init5	-2385.01579	466.4	-2380.25323
TS5	-2385.01391	466.6	-2380.25725
Fin5	-2385.03207	467.5	-2380.28914
Init6	-2385.01739	466.0	-2380.25536

TS6	-2385.01400	466.6	-2380.25929
Fin6	-2385.02935	467.9	-2380.28825
Init7	-2385.02332	466.5	-2380.26253
TS7	-2385.00833	466.9	-2380.26401
Fin7	-2385.02404	468.1	-2380.28770
Init8	-2385.02833	466.4	-2380.26937
TS8	-2385.01900	467.0	-2380.27124
Fin8	-2385.04179	468.1	-2380.30268
Init9	-2385.02758	466.0	-2380.26793
TS9	-2385.01711	466.4	-2380.26405
Fin9	-2385.04204	468.0	-2380.30140
Init10	-2385.03004	466.4	-2380.26876
TS10	-2385.01786	466.9	-2380.27004
Fin10	-2385.04011	468.2	-2380.29130
Init11	-2385.02891	466.5	-2380.26811
TS11	-2385.01568	466.4	-2380.26712
FIN11	-2385.03455	467.8	-2380.29556
Init12	-2,385.0275	466.2	-2380.26903
TS12	-2385.01904	466.8	-2380.27386
Fin12	-2385.04204	468.0	-2380.30144
	B3PW91/6–31G(d)		MP2/6–31G(d)// B3PW91/6–31G(d)
	E, Hartree	ZPE, kcal mol ⁻¹	E, Hartree
3-TABDa	-1529.74038	338.9	-1526.59967
3-TABDb	-1529.72748	338.5	-1526.58731
Init13	-2618.39687	548.7	-2611.69081
TS13	-2618.37707	548.7	-2611.67899
Fin13	-2618.40341	550.4	-2611.71183
Init14	-2618.38723	548.5	-2611.67932
TS14	-2618.38103	548.6	-2611.68187
Fin14	-2618.40422	549.9	-2611.70584
Init15	-2618.38441	548.6	-2611.67939
TS15	-2618.38408	548.9	-2611.68330
Fin15	-2618.40307	550.2	-2611.71068
Init16	-2618.39143	548.2	-2611.68258
TS16	-2618.37362	548.8	-2611.67205
Fin16	-2618.40280	550.2	-2611.70900

References

[1] Benson, S.W. *Thermochemical Kinetics*, 2nd ed.; John Wiley & Sons: New York, 1976; p 94.

Gaussian Archive Entries:

Catalyst 7

7a

1\1\FAU-CCC-ALTIX2\SP\RMP2-FC\6-31G(d)\C16H25N5S1\SHUBINA\17-Mar-2008\0\#P MP2/6-31G(D) SCF=TIGHT NAME=SHUBINA\catalyst01\0,1\S,0,0.18473,1.913306,-2.300628\N,0,-0.913453,-0.36176,-1.36578\N,0,1.327745,-0.449093,-1.678304\N,0,-0.100623,-1.753507,1.014044\N,0,0.799901,-0.162644,2.527567\N,0,-1.182663,0.270481,1.406763\C,0,-2.130887,0.283486,-0.90416\C,0,-2.339352,-0.06018,0.58703\C,0,-3.598139,0.629011,1.122061\C,0,-4.829798,0.258729,0.29031\C,0,-4.621071,0.560971,-1.195667\C,0,-3.356555,-0.115299,-1.730677\C,0,0.199961,0.316213,-1.750759\C,0,2.689975,0.041854,-1.861274\C,0,3.479431,-0.924268,-2.743255\C,0,3.329198,0.319501,-0.505288\C,0,3.279988,1.612814,0.030268\C,0,3.922523,-0.694824,0.25659\C,0,3.810757,1.885317,1.290144\C,0,4.45096,-0.426658,1.520277\C,0,4.39753,0.866787,2.041542\C,0,-0.136873,-0.598716,1.606054\H,0,-3.739751,0.353921,2.174015\H,0,-2.461291,-1.146863,0.679126\H,0,-1.974756,1.365276,-1.009029\H,0,-5.037616,-0.813849,0.41708\H,0,-5.709372,0.792759,0.670852\H,0,-5.495375,0.238838,-1.774645\H,0,-4.53709,1.648261,-1.338052\H,0,-3.47446,-1.208695,-1.699425\H,0,-3.177316,0.155927,-2.77021\H,0,-3.452547,1.72017,1.094242\H,0,-0.721421,-1.2297,-0.855576\H,0,1.241952,-1.27846,-1.097122\H,0,2.580944,0.994746,-2.387267\H,0,4.509206,-0.574518,-2.872099\H,0,3.516945,-1.935938,-2.321825\H,0,3.005641,-0.993024,-3.727016\H,0,2.809962,2.403683,-0.548971\H,0,3.987491,-1.706034,-0.138874\H,0,3.773254,2.898845,1.682696\H,0,4.91825,-1.225908,2.090983\H,0,4.82005,1.079724,3.020425\H,0,-0.962128,1.256196,1.465671\H,0,0.702581,0.782911,2.871766\H,0,1.760445,-0.401168,2.313959\H,0,0.622747,-2.336127,1.433423\Version=IA64L-G03RevC.02\State=1-A\HF=-1290.2316019\MP2=-1293.2365847\RMSD=9.679e-09\PG=C01 [X(C16H25N5S1)]\@

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7d

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11

1\1\FAU-CCC-CCDO112\Freq\RB3PW91\6-31G(d)\C8H7N1O2\SHUBINA\13-Mar-2008
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93,-0.4127059835,-0.0967717142\H,-1.4443326091,2.2236041101,0.41294494
96\H,-3.8908295608,1.8623542253,0.333069333\H,0.7769730799,1.470186162
4,0.2827373426\C,1.4845521001,-0.434711449,-0.0692128655\N,2.86027698,
0.0035644666,0.0200856992\H,1.4129173737,-1.4952617849,-0.2674932762\O
,3.1022039288,1.1865811315,0.2430215591\O,3.7089144924,-0.8711249063,-
0.1391875178\Version=AM64L-G03RevD.02\State=1-A\HF=-513.954973\RMSE=1
.806e-09\RMSE=6.033e-05\ZeroPoint=0.1375321\Thermal=0.146658\ZPE=86.30
27094\Dipole=-2.2805758,-0.2199882,-0.0531002\DipoleDeriv=1.131409,0.0
2642637,-0.6952789,-0.0771496,0.0447473,-0.0765608,-0.2903388\Polar=18
0.4451701,-6.3709142,99.3184357,-0.4435557,12.2998334,35.6417995\PG=C0
1 [X(C8H7N1O2)]\NImag=0\O,0.73089363,-0.10312621,0.72751110,-0.01632792
897,-0.05066345,0.06943599,0.04006592\O,0.00002345,-0.00007176,0.00003
13769,0.00009362,0.00002221\@

Complex1

1\1\GINC-LX64161\Freq\RB3PW91\6-31G(d)\C23H37N5O4S1\SCHENKER\27-Jan-2
008\O\#P Geom=AllCheck Guess=Read SCRF=Check GenChk RB3PW91/6-31G(d)
Freq\deprotDFT-init.com\O,1\S,-1.2771312627,-3.3542422293,0.78910574
22\N,-1.8861225442,-0.7333522049,0.8596602629\N,0.1988082757,-1.273110
3305,1.6032398814\N,-1.2381523943,1.1377529307,-2.6570776761\N,0.04596
55237,-0.7722786199,-2.4908783576\N,-2.2127923545,-0.9352759605,-1.977
7967324\C,-3.2040322229,-0.9361161559,0.2895281721\C,-3.2889422399,-0.
4054850688,-1.1570763397\C,-4.676368751,-0.6891108958,-1.7443534074\C,
-5.7845808028,-0.0874573749,-0.8768065784\C,-5.6891443156,-0.575066972
4,0.5704141479\C,-4.3005050397,-0.3151756398,1.1621247363\C,-0.9743409
706,-1.7177488624,1.0923287459\C,1.3095501815,-2.1264434592,1.99921382
89\C,2.0752692437,-1.4298167811,3.1295810234\C,2.2421563075,-2.4921306
833,0.8541988257\C,2.5870414226,-1.5597428001,-0.1277910748\C,2.822233
0087,-3.7623711859,0.8081872368\C,3.4928943997,-1.8890829482,-1.135877
5597\C,3.7318286772,-4.0937953313,-0.1942167558\C,4.0709398925,-3.1573
535965,-1.1697376611\C,-1.1578930524,-0.1227349663,-2.3638710752\H,-4.
7180497162,-0.2947296979,-2.7665458823\H,-3.1494878969,0.6841513036,-1
.1194858398\H,-3.343734093,-2.0235581072,0.2688217785\H,-5.7045900668,
1.0100891759,-0.8958461481\H,-6.7676883712,-0.3327679859,-1.2970926954
\H,-6.4558999998,-0.092406044,1.1891818066\H,-5.8945079072,-1.65451324
68,0.6044569303\H,-4.1329975403,0.7708594333,1.24399877\H,-4.225805623
9,-0.7259798402,2.1757749471\H,-4.8122405665,-1.7772897888,-1.82394387
43\H,-1.5658991557,0.2239261179,0.9635576349\H,0.3573607911,-0.2701907
635,1.617586972\H,0.8660430502,-3.0508314002,2.3821373554\H,2.90391750
42,-2.0599524228,3.4661110923\H,2.5014230577,-0.4784689372,2.787984430
3\H,1.4150755323,-1.2329944123,3.9815303703\H,2.1330214585,-0.57224186
21,-0.1229541931\H,2.546811566,-4.5037130365,1.5556807655\H,3.73732629
81,-1.1479522144,-1.8919404509\H,4.1661908557,-5.0903182951,-0.2200342
157\H,4.7742448823,-3.4177932279,-1.9567919535\H,-1.9580242264,-1.8935
162148,-1.7584266241\H,0.2540052411,-1.5036820409,-1.8220239523\H,0.82
53340607,-0.144226494,-2.6536622989\O,2.4614656334,1.3435656486,-1.870
2950203\C,2.1935657687,2.3707288518,-1.2837941424\C,0.8046730058,2.949
3947425,-1.1280411461\O,0.2929362983,1.7205226624,0.8981722626\C,0.259

6072232,2.7620794344,0.2635328473\O,-0.3235797263,3.8746647455,0.71748
85164\C,-0.9302748195,3.8002435453,2.0239686789\C,-1.4299104932,5.1844
687912,2.3718664471\O,3.1048585319,3.1674668579,-0.7022397421\C,4.4896
743428,2.7664454825,-0.7906987193\C,4.8938992102,1.9235386115,0.402595
9745\H,5.9683368513,1.7128151496,0.3580928333\H,4.687121769,2.45063022
32,1.3396250738\H,4.3620764905,0.9679987254,0.4073631087\H,4.640355038
2,2.229830896,-1.7306322705\H,5.041818516,3.7093803976,-0.819576913\H,
-0.1835733135,3.4374420855,2.7372521241\H,-1.7447256317,3.0681222995,1
.9919953208\H,-1.9024443341,5.1696661533,3.3596034953\H,-0.6046114384,
5.9026493844,2.3956820614\H,-2.1681584185,5.5301643976,1.6417523253\H,
0.819035554,4.013999524,-1.3720711378\H,-2.2107792902,1.4338613764,-2.
7175407967\H,0.1200841919,2.4064149046,-1.8146852074\Version=IA64L-G0
3RevD.01\State=1-A\HF=-1871.0513047\RMSD=3.603e-09\RMSF=8.258e-06\Zero
Point=0.6033383\Thermal=0.6395027\Dipole=0.2355631,2.435849,1.4779559\
2,0.1417466,0.2100218,0.1840004,0.2072439\Polar=337.3905057,-22.689679
7,316.9533931,-16.6448138,-1.7466225,251.8571024\PG=C01 [X(C23H37N5O4S
1)]\NImag=0\0.06550803,0.03931577,0.29857759,0.02368001,0.04524595,0.
42,0.00131590,0.00179152,-0.00000169,0.08900402,0.07177990,0.15412984\
\0.00000076,0.00000073,0.00000374,0.00000072,0.00000008,0.00000134,0.0
001207,0.00000129\@@

TS H-abs

1\1\FAU-RRZE-ALTIX-BATCH\Freq\RB3PW91\6-31G(d)\C23H37N5O4S1\SCHENKER\2
0-Jan-2008\0\#P B3PW91/6-31G(D) FREQ=NORAMAN NAME=SCHENKER GUESS=READ
GEOM=CHECK\deprotts\0,1\S.2.0181544314,2.9941592529,-0.4818915701\N
.2.0917869436,0.5171997734,0.5752940677\N,0.3560893288,1.8239353075,1.
2646300154\N,0.391322588,-2.0265228297,-1.7496023725\N,-0.3604960197,0
.1458638602,-1.944887077\N,1.9185583846,-0.2697016126,-2.1492226903\C,
3.3012159118,0.175596799,-0.1446167432\C,3.0270440338,-0.7697188026,-1
.3358494173\C,4.3080043711,-0.9863925196,-2.1429806307\C,5.416985385,-
1.5565203337,-1.2527579991\C,5.6667731082,-0.6780312113,-0.023542204\C
.4.3789551104,-0.4204401319,0.7660222395\C,1.4626591224,1.7255451821,0
.4992889515\C,-0.439640261,3.0351875879,1.4316884877\C,-1.0572934667,3
.0151432852,2.833664951\C,-1.5077616961,3.2220634856,0.3651491542\C,-2
.3467403312,2.1683326717,-0.0103509486\C,-1.703181237,4.4801253212,-0.
211145909\C,-3.3591266776,2.3707357824,-0.9474449611\C,-2.7211340703,4
.6867170556,-1.1403183864\C,-3.5528794049,3.6312445575,-1.5112660946\C
.0.6485736295,-0.7453476421,-1.920348817\H,4.0979213028,-1.6552789026,
-2.9859903933\H,2.7116707522,-1.7393606474,-0.9296084685\H,3.669673594
9,1.1273868674,-0.5459600543\H,5.1310023203,-2.5670907563,-0.924394296
7\H,6.3412427686,-1.6701385253,-1.8319888557\H,6.4189413902,-1.1408349
267,0.6269726992\H,6.0837631006,0.2864645259,-0.3460737582\H,4.0161994
862,-1.3640622127,1.2035426696\H,4.5656984085,0.2669463627,1.598979008
2\H,4.6280299479,-0.0268530367,-2.5737097735\H,1.5936679116,-0.2226303
859,1.0620367988\H,-0.023488057,0.9612938864,1.6482525124\H,0.26192287
31,3.8717282888,1.3593916038\H,-1.637602366,3.9279196663,2.9986065188\
H,-1.7389977467,2.1642532251,2.9521120489\H,-0.2778371055,2.9503608354
.3.6009485621\H,-2.204288125,1.173545735,0.4048593216\H,-1.0435266028,
5.3013763399,0.0612729294\H,-3.988045511,1.5325188552,-1.2342184471\H,
-2.8557111605,5.6705204583,-1.5836088251\H,-4.3426864013,3.7888888723,
-2.2418159164\H,1.9547033202,0.7396602859,-2.2791493001\H,-0.163457776
.1.1090383565,-1.7000698515\H,-1.2811257646,-0.1922413955,-1.660067610
4\O,-2.774135899,-0.9982718209,-0.698798255\C,-2.6011916838,-2.1855601
062,-0.4397330678\C,-1.3944934416,-2.7977311699,0.1219496587\O,-0.5277
210351,-0.9732108772,1.4507901557\C,-0.7318187481,-2.1707072092,1.2620
115489\O,-0.2402872697,-3.1084952082,2.1087297049\C,0.503916344,-2.630
5332113,3.2355202988\C,0.8150474147,-3.823541973,4.1139732672\O,-3.521
629136,-3.1258038578,-0.7508715316\C,-4.7010620337,-2.674808747,-1.437
8232012\C,-5.7663223969,-2.2080114893,-0.4632118865\H,-6.681278063,-1.
9436491736,-1.0058661754\H,-6.0090288469,-2.9980708796,0.2549335003\H,
-5.4238336863,-1.3258444342,0.0847182452\H,-4.4266992233,-1.8769984439
,-2.1335767849\H,-5.0362023013,-3.5478490505,-2.0048216418\H,-0.085960
6561,-1.8756391085,3.7658786914\H,1.423247129,-2.1425883572,2.88641082
01\H,1.3910075365,-3.5045960899,4.9893416719\H,-0.1069585389,-4.299392
1227,4.4622104216\H,1.4009752193,-4.569799321,3.5680645572\H,-1.487776
5606,-3.8750865562,0.2390756267\H,1.1813704871,-2.6342172448,-1.933387
4491\H,-0.4968197078,-2.4754795013,-0.8825894259\Version=IA64L-G03Rev

C.02\State=1-A\HF=-1871.0405724\RMSD=4.386e-09\RMSF=5.971e-06\ZPE=376.2563738\Dipole=0.673967,-1.4683188,0.6845032\DipoleDeriv=-0.5582568,-0.01426\Polar=349.4573498,-7.4619519,321.2561429,21.4128421,-20.1888357,260.4898297\PG=C01 [X(C23H37N5O4S1)]\NImag=1\0.07490186,0.04982676,0.00736676,-0.00534093,0.00296118,0.04122123,0.02898499,0.01513604\0.00000880,0.00000531,0.00000395\@\

Complex2

1\1\GINC-ALTIX2\Freq\RB3PW91\6-31G(d)\C23H37N5O4S1\SCHENKER\24-Jan-2008\0\#P Geom=AllCheck Guess=Read SCRF=Check GenChk RB3PW91/6-31G(d) Freq\deprotDFT-end.com\0,1S,1.5659446325,3.1877743012,-0.0810902746\N,2.0465689414,0.6206328663,0.6006252826\N,0.1871711779,1.546044814,1.5313150721\N,0.5946047197,-1.6626868418,-2.0080920582\N,-0.4695977837,0.3654499976,-1.8069188233\N,1.8321620569,0.305139267,-2.1955706826\C,3.2532101943,0.5826598243,-0.1939208768\C,3.0525695971,-0.1693335849,-1.5282418105\C,4.2971350027,-0.0439598491,-2.4055234801\C,5.5223060069,-0.5965769336,-1.6679323244\C,5.7137309815,0.0678213834,-0.3012734797\C,4.4477390034,-0.0112000594,0.5588028898\C,1.2522241989,1.7236737934,0.7272033808\C,-0.755401561,2.5887919563,1.9190927015\C,-1.2779335551,2.2638134457,3.3225236609\C,-1.9021746701,2.7800611132,0.9386504256\C,-2.5912644595,1.6857230862,0.4064288484\C,-2.3226137882,4.07076422,0.6059519124\C,-3.6759809297,1.881456872,-0.4476900356\C,-3.414736633,4.2681651865,-0.2368163698\C,-4.0947269335,3.1725700916,-0.7669862491\C,0.6488878673,-0.3246771236,-1.9699087011\H,4.1371580151,-0.5736095796,-3.352357019\H,2.9033727768,-1.2305388779,-1.2942003696\H,3.4745327614,1.6306622618,-0.430175301\H,5.3998029246,-1.6814081696,-1.5308560486\H,6.4188671674,-0.4629525734,-2.2847588737\H,6.5558260464,-0.3946420805,0.2275619622\H,5.978941161,1.1245377791,-0.4462864752\H,4.2388997455,-1.0595351572,0.8231825977\H,4.5838696484,0.5335244031,1.4996428545\H,4.4552495026,1.0143320647,-2.6567735482\H,1.6398360712,-0.2564681713,0.9296732131\H,-0.0511633069,0.5814809109,1.7642281031\H,-0.1818571278,3.5199493412,1.9559942416\H,-1.965423138,3.0469502666,3.6559022589\H,-1.829098264,1.3158109525,3.3274680276\H,-0.4510238069,2.1933551047,4.0378208304\H,-2.2745291028,0.6697528071,0.630943487\H,-1.7820002699,4.9280625608,1.0019185874\H,-4.1815557919,1.0146330806,-0.8638529369\H,-3.7261112934,5.2791430771,-0.4887189128\H,-4.9421352969,3.3248346736,-1.4310454144\H,1.7477884209,1.3214606744,-2.1646490144\H,-0.409355064,1.3236642299,-1.4788515633\H,-1.3142948763,-0.1727622435,-1.5362348599\O,-2.4890136607,-1.3164343949,-0.982385092\C,-2.3446137593,-2.5126050668,-0.663164931\C,-1.3315363343,-3.1220279327,0.1240552866\O,-0.1638906133,-1.2296157699,1.0455793155\C,-0.4468088774,-2.4450378992,0.9955899638\O,0.1713632544,-3.3217655024,1.8506771615\C,1.0717393418,-2.7668696645,2.8022517896\C,1.4505687802,-3.8689719356,3.7707010725\O,-3.2328871708,-3.4477329408,-1.1178435066\C,-4.2891544547,-2.9902039366,-1.9645165972\C,-5.5144148756,-2.5934560041,-1.1594518832\H,-6.3368971894,-2.3174249614,-1.830112666\H,-5.8487186936,-3.423230322,-0.5279210887\H,-5.2891086037,-1.7364651378,-0.5180132686\H,-3.9344931242,-2.1527403017,-2.5720867897\H,-4.5106435149,-3.8391392021,-2.6196578145\H,0.5970811685,-1.9261394456,3.3210792584\H,1.9635603808,-2.3732035516,2.2928256192\H,2.1545416823,-3.4890948543,4.5194104938\H,0.5639940799,-4.2469896886,4.2893409995\H,1.9215776445,-4.7060654234,3.2455005177\H,-1.4173786442,-4.192392539,0.2659551858\H,1.4115193434,-2.1797323533,-2.2893589572\H,-0.1175671285,-2.1772363327,-1.478208904\Version=IA64L-G03Rev D.01\State=1-A\HF=-1871.0520031\RMSD=6.696e-09\RMSF=1.531e-05\ZeroPoint=0.6041341\Thermal=0.6395171\Dipole=1.7716808,-0.6874995,-0.4639503\D 2417424,-0.1156651,0.4537434\Polar=358.9821013,-7.1488475,318.8306412,31.7559474,-3.5435083,259.2432901\PG=C01 [X(C23H37N5O4S1)]\NImag=0\0.08,-0.14319039,-0.08380734,0.11651819\0.00000560,-0.00000100,0.000006000743\@\

Complex2a

1\1\FAU-CCC-SNODE127\Freq\RB3PW91\6-31G(d)\C23H37N5O4S1\BCO166\26-Oct-2007\0\#P GEOM=ALLCHECK GUESS=READ SCRF=CHECK GENCHK RB3PW91/6-31G(D) FREQ\SSR-MH30-malon-c3\0,1S,-2.6789905077,1.8053198523,1.3808158937\N,-3.5405673627,0.669772145,-0.8934740131\N,-2.3201836221,2.5826532008,-1.1608241852\N,-0.9391593588,-1.1294846461,1.0369407083\N,0.464324

2018,-1.8488768344,-0.636560814\N,-1.7819926323,-1.5948341312,-1.11299
56838\C,-3.9297884846,-0.5624126373,-0.235438977\C,-3.2125093489,-1.78
615625,-0.8512455564\C,-3.5383725167,-3.0501968705,-0.0447257141\C,-5.
0516776901,-3.2886568632,-0.0036890135\C,-5.8067084447,-2.0661770883,0
.5234970728\C,-5.4446711985,-0.7973845025,-0.2540866147\C,-2.837658645
1,1.679306733,-0.2993643121\C,-1.2932462624,3.5897606238,-0.8406831392
\C,-1.7979902393,4.9815808977,-1.2073271294\C,0.0132207901,3.162193101
, -1.4971930667\C,0.7450265105,2.1138052617,-0.9203666919\C,0.478575592
7,3.7295526411,-2.687173174\C,1.903008255,1.6300105289,-1.52309631\C,1
.6454466236,3.2553274201,-3.2893499303\C,2.3538763196,2.2033624217,-2.
7137318477\C,-0.7493432376,-1.5191030917,-0.228970999\H,-3.026801058,-
3.9080728571,-0.4977326478\H,-3.6361972123,-1.9209604615,-1.8579877634
\H,-3.6324494767,-0.4424325746,0.8107673318\H,-5.4057063705,-3.5256504
359,-1.0181079094\H,-5.270533995,-4.1679930432,0.6134012934\H,-6.88845
84917,-2.2383179673,0.4749489229\H,-5.5629227657,-1.9160243479,1.58452
54863\H,-5.7934972367,-0.8803115262,-1.2952292683\H,-5.937027704,0.079
8036104,0.1793765707\H,-3.1392959324,-2.9415121285,0.9714539331\H,-3.5
441618275,0.6473497479,-1.9062171897\H,-2.3734232207,2.3605485617,-2.1
48964304\H,-1.1752617089,3.5334343457,0.2452210499\H,-1.0329862824,5.7
341618816,-0.9907403721\H,-2.0612166243,5.060354428,-2.2685981856\H,-2
.6922005289,5.2146307427,-0.6217422582\H,0.4111258581,1.6698632086,0.0
148667721\H,-0.0584665663,4.5541359148,-3.1494049079\H,2.4404625835,0.
8020646444,-1.0673331067\H,1.998534004,3.7127780364,-4.2106843555\H,3.
260179519,1.8321072709,-3.1855503367\H,-1.4918847995,-1.8360229731,-2.
0488594068\H,1.3257869791,-1.5721463517,-0.1159688094\H,-0.0512546142,
-0.9862683675,1.5510660058\O,3.1426028548,-1.7247386132,-0.66879947\C,
4.0366919311,-1.6956553334,0.1979896667\C,3.9567000952,-1.2838067596,1
.54639283\O,1.6490482886,-0.6713382914,1.5716931958\C,2.7742179225,-0.
8074064964,2.1194385566\O,2.9225646231,-0.4493959729,3.4344122989\C,1.
774150465,0.0718489874,4.089473859\C,2.2047477692,0.5148148538,5.47393
52823\O,5.3064355059,-2.1036424395,-0.1370849621\C,5.4828292007,-2.543
2198731,-1.4771773611\C,6.9295725402,-2.9707771917,-1.6281583561\H,7.1
198510686,-3.1397407208,-2.6497287564\H,7.605433095,-2.1356143136,-1.4
165338883\H,7.1680118572,-3.7840712736,-0.9347829429\H,4.7971092991,-3
.3724466632,-1.6932740292\H,5.2316944415,-1.733320687,-2.1742079456\H,
4.8494810299,-1.3239285145,2.1561577616\H,0.9932865185,-0.6989834394,4
.1518763319\H,1.3593308821,0.9084043172,3.5143067914\H,1.3496586594,0.
9195415695,6.0271707646\H,2.6170488115,-0.3268436104,6.0400947962\H,2.
974338769,1.2908114911,5.4090817346\H,-1.6459016743,-0.4170500949,1.21
9902691\H,0.6234163912,-2.2827437349,-1.5326891828\Version=AM64L-G03R
evC.02\State=-1\AHF=-1871.0298757\RMSD=4.002e-09\RMSF=1.900e-05\ZPE=37
8.0134707\Dipole=-4.2392139,-0.5010171,-3.1142609\DipoleDeriv=-0.44678
-0.0463698,0.1719287\Polar=352.9756016,-12.1967427,280.0327206,-35.267
031,-1.0847571,307.0678505\PG=C01 [X(C23H37N5O4S1)]\NImag=0\0.0368743
0.00063087,-0.05606856,0.18225559,0.38594361\0.00000037,0.00000935,0.
.0.0000369\@\

CatN1

1\1\FAU-CCC-SNODE130\Freq\RB3PW91\6-31G(d)\C24H32N6O2S1\SCHENKER\28-Oc
t-2007\0\#P GEOM=ALLCHECK GUESS=READ SCRF=CHECK GENCHK RB3PW91/6-31G(
D) FREQ\SSH-MH30-nitrostyrene\HF/3-21G\0,1\S,-1.3056385877,3.172063
0228,1.959841427\N,-0.9782475107,2.258928232,-0.5570505029\N,0.9437488
636,2.6489933943,0.5917405444\N,-1.1467899255,-1.608013235,0.241394630
1\N,-1.1023500521,-0.6522126856,2.4311563707\N,-2.4906689022,0.2084939
32,0.8092071493\C,-2.3957874582,2.057087714,-0.8077871065\C,-2.8108954
315,0.5883262834,-0.552130676\C,-4.3001696304,0.3920802328,-0.86168279
86\C,-4.6423502932,0.819158957,-2.2895001136\C,-4.2247379273,2.2688381
985,-2.5465848554\C,-2.7414619921,2.4856986984,-2.2380665043\C,-0.4138
741904,2.6590735031,0.6042460864\C,1.795186422,2.8977209058,1.75016749
83\C,3.114509495,3.5104289282,1.2780268295\C,2.0082852036,1.6426932464
,2.5883596133\C,1.6175945835,1.6201494598,3.9302681596\C,2.5992424212,
0.496974247,2.042528538\C,1.8141071693,0.4825773085,4.7137415241\C,2.7
946814553,-0.6423339588,2.8209869566\C,2.4028267792,-0.6535651013,4.16
10681959\C,-1.5269711339,-0.7216677197,1.1085703456\H,-4.5551044373,-0
.659979019,-0.6909073022\H,-2.2223024109,-0.0664532198,-1.2060088311\H
, -2.9301091549,2.700672317,-0.0984725969\H,-4.1230188462,0.1600438441,
-3.0010308546\H,-5.7163143505,0.693165498,-2.4757737925\H,-4.432223451

8,2.5516512626,-3.5862494298\H,-4.8270631212,2.937885815,-1.9149444138
\H,-2.1329347577,1.902096173,-2.9455152819\H,-2.464284821,3.5379625947
,-2.3735701302\H,-4.8934553555,0.9801810483,-0.1458537512\H,-0.3569666
425,1.8438891454,-1.2483382209\H,1.4093501146,2.2836168784,-0.23399627
77\H,1.2601184276,3.6269137856,2.3650049208\H,3.7571465593,3.723884443
5,2.1376328812\H,3.6611726811,2.8300923692,0.614430087\H,2.9288796731,
4.4446058368,0.7377120363\H,1.1422919567,2.4989127844,4.3591018974\H,2.
.9054473792,0.4893710395,0.9986832077\H,1.5013418228,0.4835133607,5.75
49855116\H,3.260866295,-1.5220697779,2.3830290304\H,2.5588707037,-1.54
09162958,4.7696481155\H,-2.5804005833,0.9643359778,1.4810153284\H,-1.0
966186741,0.2828511866,2.8287307533\H,-0.2208606917,-1.1170760878,2.60
56646042\H,-0.446584101,-2.213730549,0.6688132699\H,-0.1226390891,-5.7
226244351,-1.7223828456\H,-0.1149439554,-4.3317911527,-1.7081186504\H,
1.030798208,-3.6228163238,-2.1133377081\H,1.0043515178,-6.4221319234,-
2.1519094877\H,2.1447355462,-5.72802801,-2.5664744416\H,2.1608200953,-
4.3404411349,-2.5467637644\H,-0.9811736237,-3.7722554699,-1.3610612363
\H,-1.0097830149,-6.2611442108,-1.4006936691\H,0.9960673309,-7.5088626
281,-2.1697998467\H,3.0188608316,-6.2742666401,-2.9103845579\H,3.04475
45378,-3.8085851015,-2.8890068661\H,0.9758405864,-2.171868989,-2.06790
61406\H,2.02272666,-1.3276571516,-2.1253146143\H,-0.0041057397,-1.7290
799475,-1.891542834\H,1.7852845096,0.07685438,-2.0050328523\H,2.722771
8081,0.7787142087,-1.6128209033\H,0.6689689221,0.5226664441,-2.2822045
895\H,3.0763379,-1.5718788183,-2.138492257\H,Version=AM64L-G03RevC.02\St
ate=1-A\HF=-1810.3317668\RMSE=2.396e-09\RMSEF=2.917e-05\ZPE=344.320256
\Dipole=1.4229983,-2.1614795,-1.0830238\H,DipoleDeriv=-0.6196797,0.10208
-0.0433314,-0.0926641,0.17123\H,Polar=302.0139914,-20.3099069,397.922223
1,5.4359407,24.0921952,277.2352454\H,PG=C01 [X(C24H32N6O2S1)]\NImag=0\O
4,0.00016947,-0.00019124,0.00351517,-0.00441128,0.00339774,0.02097062\
\O.00002108,0.00000276,0.00001682,0.00000247,0.00007340,-0.00007905,0.
00000037\H@

CatN2

1\1\FAU-CCC-SNODE126\Freq\RB3PW91\6-31G(d)\C24H32N6O2S1\SCHENKER\25-Oc
t-2007\O\#P GEOM=ALLCHECK GUESS=READ SCRF=CHECK GENCHK RB3PW91/6-31G(
D) FREQ\ssr-mh30-nist-c4\0,1\H,S,-3.2453959396,2.6241428143,0.91735805
92\H,-2.601251671,0.4391738669,-0.5040671187\H,-0.970573573,2.01877283
73,-0.3693663923\H,-3.237397501,-1.8684032257,2.4438699757\H,-0.991890
9355,-2.6214705526,2.0636797557\H,-2.4563412776,-2.3390227345,0.302603
2198\H,-3.8333925183,-0.2742756477,-0.1912781399\H,-3.6076115656,-1.78
77051933,-0.4050602513\H,-4.8940333356,-2.5713960539,-0.1097000543\H,
6.0690772072,-2.0711893839,-0.9513511229\H,-6.2837205513,-0.5693160998
,-0.758996278\H,-5.002375608,0.2081260082,-1.0613592475\H,-2.239199752
5,1.6508680099,-0.0233424223\H,-0.3809441968,3.3257765897,-0.124336027
7\H,-0.6297796143,4.2746066789,-1.296481425\H,1.0775347459,3.141062822
9,0.2704557746\H,1.3787503388,2.318140154,1.366743389\H,2.1329653332,3
.7671823121,-0.3980514323\H,2.6922212288,2.1367947926,1.7867248336\H,3
.4538424536,3.5861361423,0.0195236018\H,3.7385404714,2.7739212665,1.11
42537851\H,-2.2913651362,-2.2596739334,1.6686444662\H,-4.7004415329,-3
.6341469676,-0.3010872393\H,-3.3707632381,-1.9343832415,-1.4712683628\
H,-4.0616284772,-0.1022456116,0.8656251675\H,-5.8750712761,-2.27490325
83,-2.016061515\H,-6.9774620739,-2.628794845,-0.6889457417\H,-7.099936
9413,-0.2112114733,-1.3994589406\H,-6.5892463569,-0.3736314777,0.27849
38343\H,-4.7315538281,0.0814476722,-2.121199111\H,-5.1421612381,1.2800
362698,-0.8880691132\H,-5.1163214279,-2.4691288781,0.9575840562\H,-1.8
985279194,-0.0791253242,-1.0197216997\H,-0.4302291415,1.3807537786,-0.
9420055547\H,-0.924003544,3.7217557925,0.7440359862\H,-0.2458151948,5.
2790804298,-1.0852424495\H,-0.1662185099,3.9112090692,-2.2217612196\H,
-1.708753245,4.3512691782,-1.4580639961\H,0.5648071426,1.823919961,1.8
920433294\H,1.9307448334,4.411261745,-1.2488114416\H,2.9013257247,1.50
62182108,2.6476072573\H,4.2581598842,4.0918327577,-0.509931473\H,4.764
2718484,2.6465344818,1.4524006503\H,-1.5951309106,-2.3719148559,-0.227
6283299\H,-0.568078459,-3.3405796799,1.4881690703\H,-0.9344760672,-2.8
63684173,3.0444352851\H,-2.9480631508,-1.9124068608,3.4201857015\H,6.8
014123416,-2.8309915344,-0.022259185\H,5.4308560912,-2.9631641992,-0.2
115862624\H,4.6186898967,-1.8320420746,-0.408967441\H,7.3811631359,-1.
5631399196,-0.0195417895\H,6.5849497028,-0.4293458116,-0.2034366199\H,
5.2167784158,-0.5573999178,-0.3963624528\H,4.9761347652,-3.9510253794,

-0.2136398418\H,7.4161659612,-3.7144010646,0.1250843586\H,8.4519765414
,-1.45523883,0.1309275748\H,7.0363081381,0.5587959489,-0.191687256\H,4
.6088931688,0.3349281132,-0.5142111089\C,3.1969352289,-2.0395034167,-0
.6154254376\C,2.2871159388,-1.1120973527,-0.962023232\H,2.8258408498,-
3.055028344,-0.4917498957\N,0.9160668212,-1.4844563492,-1.1377493657\O
,0.1625393421,-0.6088853485,-1.5784252361\O,0.5435302595,-2.62507693,-
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G03RevC.02\State=1-A\HF=-1810.3167779\RMSD=2.407e-09\RMSF=6.072e-06\ZP
E=343.757065\Dipole=5.0107801,-2.0961556,-0.8835587\DipoleDeriv=-0.804
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28772,299.9002463,23.6352612,-20.6672333,216.3537474\PG=C01 [X(C24H32N
6O2S1)]\NImag=0\0.15087115,-0.08253632,0.13595883,-0.09911185,0.09748
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.00000184,0.00000120,0.00000039\@

CatN3

1\1\FAU-CCC-SNODE133\Freq\RB3PW91/6-31G(d)\C24H32N6O2S1\SCHENKER\27-Oc
t-2007\0\#P GEOM=ALLCHECK GUESS=READ SCRF=CHECK GENCHK RB3PW91/6-31G(
D) FREQ\ssr-mh30-nitrostyrene//B3PW91/6-31G(d)\0,1\S,-2.0095072348,4
.6139456083,0.9572048725\N,-1.9299877411,1.9378817905,0.6484223157\N,-
0.4941928555,3.1141425834,-0.665586523\N,-0.7827663369,0.989436181,4.0
360673568\N,0.6533349108,-0.7585392418,3.2475856863\N,-1.3356483143,-0
.3010365977,2.1752629264\C,-2.8147536006,1.6729324163,1.7807398936\C,-
2.7204193916,0.1659692886,2.0963307333\C,-3.5974899698,-0.1878810087,3
.304426046\C,-5.0550845137,0.2127700424,3.0605513006\C,-5.1697624771,1
.6896674925,2.6773671888\C,-4.2753221713,2.0287025843,1.4832818851\C,-
1.4671214034,3.1668656813,0.2945138573\C,0.0690240509,4.2749482352,-1.
3464386304\C,-0.8073952861,4.7090522294,-2.5208630246\C,1.5234466967,3
.982342873,-1.6883303216\C,2.3967332005,3.6032559238,-0.6585146801\C,2
.0336774355,4.0894137045,-2.9843371768\C,3.7379769778,3.3420312077,-0.
9174373233\C,3.3795572722,3.8266058524,-3.2478273763\C,4.2360568742,3.
4521654247,-2.2170877697\C,-0.4852277588,0.0446372098,3.2191751262\H,-
3.5223991461,-1.2667965364,3.4944832369\H,-3.1267896213,-0.3608922451,
1.218422707\H,-2.4628508258,2.2411172549,2.6498236683\H,-5.4733440932,
-0.4028201794,2.2490234976\H,-5.6560316491,-0.0019127891,3.9537325023\
H,-6.2122038555,1.9448357486,2.4479700175\H,-4.8764482754,2.3130846318
,3.5338162693\H,-4.6030891037,1.4694002352,0.5938068793\H,-4.339928260
9,3.0931835278,1.2412476164\H,-3.1958928774,0.3256429349,4.1843164451\
H,-1.2795419636,1.1677466518,0.5032488615\H,-0.3673582072,2.2293408313
,-1.1423136387\H,0.041369087,5.0780722405,-0.5992295348\H,-0.423642665
4,5.6245291622,-2.9846737088\H,-0.8716233965,3.9306144795,-3.291134085
6\H,-1.8144268468,4.9145335281,-2.1471594809\H,2.0094075927,3.51554450
26,0.3539065807\H,1.382329254,4.3842632076,-3.8017990633\H,4.399248602
,3.0563254883,-0.102713667\H,3.7552878989,3.917202717,-4.2642919503\H,
5.2847417723,3.2503446175,-2.4211867199\H,-1.2099940973,-1.2545061727,
1.8517870322\H,0.9454712812,-1.1459786983,2.3555117882\H,1.4230352381,
-0.3679819543,3.7731634085\H,-0.0178797949,1.155208186,4.6897658557\C,
4.181697203,-6.5662046113,-3.183904982\C,3.708823271,-5.5664943628,-2.
3413386934\C,2.3645725987,-5.5468713204,-1.9302094272\C,3.3166919593,-
7.563683607,-3.6302170964\C,1.9772305972,-7.5576841734,-3.2308702133\C
,1.5035967017,-6.5612395832,-2.3898215075\H,4.3824116438,-4.7874314105
,-1.9922447393\H,5.2233233606,-6.5669930322,-3.4921829965\H,3.68249431
75,-8.3465974839,-4.2890059907\H,1.302761268,-8.3349630333,-3.57898489
31\H,0.4601546196,-6.5700830658,-2.0880909801\C,1.934370417,-4.4754309
525,-1.0479405264\C,0.7037630783,-4.2885938539,-0.5431491418\H,2.68664
5114,-3.7427764047,-0.7620528274\N,0.4346274056,-3.1736611866,0.321080
6743\O,-0.720651509,-3.0838982605,0.7402227333\O,1.3378076788,-2.38222
78044,0.5948492053\H,-0.1757900202,-4.8966030117,-0.7012314532\Versio
n=AM64L-G03RevC.02\State=1-A\HF=-1810.3154797\RMSD=5.616e-09\RMSF=1.17
9e-05\ZPE=343.9419253\Dipole=2.6474444,-4.9809638,-2.6875203\DipoleDer
17534,0.0466431,-0.0793858,0.0258003,-0.0683351,0.1088343\Polar=373.17
01181,-42.1266924,318.69212,-81.4157688,59.0931909,308.7435514\PG=C01
[X(C24H32N6O2S1)]\NImag=0\0.07127811,-0.07196346,0.25343420,-0.055930
0.00039459,0.03180134,0.04408853,0.04255104\0.00000066,-0.00000029,0.
00001710,0.00001393,-0.00000101,-0.00000161,-0.00000112\@

CatN4

1\1\FAU-CCC-SNODE131\Freq\RB3PW91\6-31G(d)\C24H32N6O2S1\SCHENKER\28-Oc
t-2007\0\#P GEOM=ALLCHECK GUESS=READ SCRF=CHECK GENCHK RB3PW91/6-31G(D)
D) FREQ\ssr-mh30-nist-c6\0,1\S,-0.8306210198,-2.648177093,-1.0204152
516\N,1.0278555,-2.6239112111,0.9277176517\N,1.6113102294,-1.542539647
5,-0.9862460821\N,-0.9880289023,-0.7102148064,3.3674695792\N,0.8930393
344,0.6723638041,3.9144978416\N,1.1796233356,-1.578505504,3.4909168653
\C,0.1329239942,-3.211464985,1.9226029876\C,0.7551499223,-2.970700654,
3.3122306847\C,-0.1555695428,-3.5296217409,4.4132763327\C,-0.415487350
2,-5.0235713481,4.20122836\C,-0.9737025687,-5.2981137688,2.8030355372\
C,-0.0663200477,-4.7169317458,1.7169418443\C,0.6531764254,-2.264241165
,-0.3290916335\C,1.5193843682,-1.1045120517,-2.3719200366\C,2.03550586
25,-2.1817701508,-3.3273800853\C,2.1804891959,0.2610032738,-2.51419406
94\C,1.9959589381,1.2273133726,-1.5142673688\C,2.9434369718,0.60953520
54,-3.6334567077\C,2.5528216297,2.4987188497,-1.630766101\C,3.49920933
28,1.8841482402,-3.7550627647\C,3.3072241975,2.8345267982,-2.756074044
9\C,0.2623409138,-0.5240876747,3.5727543973\H,0.317489037,-3.358959042
,5.3899835603\H,1.6982002447,-3.5407943866,3.333312391\H,-0.8353942856
,-2.7002601544,1.8734247476\H,0.5255651989,-5.580789052,4.3290603926\H
,-1.1033474223,-5.3954762421,4.9712819177\H,-1.0994251595,-6.376964962
8,2.6468835116\H,-1.9734127278,-4.850226532,2.7145910583\H,0.915946979
4,-5.2127823762,1.7405781818\H,-0.492544871,-4.8838879267,0.723278796\
H,-1.0934075771,-2.9649801327,4.4042960676\H,1.7275674467,-2.026051539
5,1.361866968\H,2.5418770677,-1.5381597617,-0.5857527165\H,0.442254474
3,-0.9917952328,-2.5542730377\H,1.8424152819,-1.916610227,-4.372380441
\H,3.1128543083,-2.3478814561,-3.2060522789\H,1.506604945,-3.115854172
7,-3.1187689905\H,1.4159384799,0.9745376735,-0.6306966316\H,3.11384508
68,-0.1152549277,-4.4237366738\H,2.401431395,3.2224040026,-0.833355645
6\H,4.0907783293,2.1285779301,-4.6341285882\H,3.7471326674,3.824483219
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CatN5

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Fin1

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TS5

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Fin5

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44N6O6S1)]\@

Init2

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\H,6.8051258945,-1.4855651071,3.2649950575\H,8.2659126158,-3.056577653
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\C,2.5920447353,-2.6349858012,-0.6181518203\H,2.5982895638,-1.69381636
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TS2

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Fin2

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Init3

1\1\GINC-A02\Freq\RB3PW91\6-31G(d)\C31H44N6O6S1\TS\29-Nov-2007\0\#P B 3PW91/6-31G(d) geom=check guess=read Freq=NoRaman Name=TS\TS3 Init\0,1\S,4.8943226117,1.0949006936,-0.9695338973\N,2.2542204782,1.422847077,-1.3835908386\N,3.08997092,-0.6095894825,-1.9872117167\N,3.3275950499,1.3186156334,1.9724648102\N,1.6481806222,0.0032691376,2.8950164402\N,1.1000514,1.5021275681,1.2413052617\C,2.2273984231,2.6998871129,-0.6977273002\C,1.1614901513,2.7106941025,0.4162978407\C,1.2584019951,4.0044504546,1.2337012588\C,1.0706376634,5.2195089582,0.3187495932\C,2.0441096095,5.2054886828,-0.8627388224\C,1.9784994758,3.8856625661,-1.6382640224\C,3.3362989562,0.612568121,-1.4643801197\C,4.0328805902,-1.7214529421,-1.9432548164\C,3.6554210557,-2.7332333797,-3.0276553768\C,4.0981470756,-2.3706495546,-0.5651367601\C,2.9329472188,-2.7228995274,0.1250092395\C,5.3351709513,-2.6484929639,0.0226764676\C,3.0055622569,-3.3405262026,1.3729421597\C,5.4119058737,-3.2691182196,1.268732252\C,4.2460771486,-3.6169546592,1.9494558587\C,2.0272810461,0.9403926447,2.0000986765\H,0.4827751455,3.9837854301,2.0064469008\H,0.1772550172,2.7066750093,-0.0631577061\H,3.2271300603,2.8405718503,-0.2754121122\H,0.0386273209,5.2185963616,-0.0604618192\H,1.1887647982,6.1439058779,0.8975751565\H,1.8365673253,6.0463511064,-1.5360252727\H,3.0695828364,5.3491679915,-0.4927047978\H,0.9949261427,3.7741267395,-2.1174708106\H,2.7312390019,3.864106379,-2.4342289358\H,2.2319187072,4.0529150467,1.7401402193\H,1.3451367636,1.0244012927,-1.6215678185\H,2.1172274042,-0.8568133927,-2.1713858622\H,5.0190845643,-1.3048266131,-2.1679001102\H,4.368595761,-3.5630732408,-3.0290380591\H,2.6572140408,-3.1506977421,-2.8533389303\H,3.6666772839,-2.2589971375,-4.0148714157\H,1.9585065077,-2.5082734088,-0.3079918319\H,6.2470681957,-2.3606491337,-0.4955333565\H,2.0887928426,-3.6147487485,1.8900021931\H,6.384031414,-3.4742359734,1.7106782411\H,4.3033772211,-4.1047034282,2.9197701679\H,0.1368174125,1.1424452903,1.3497810914\H,0.6873776529,-0.3504708066,2.7753125932\H,2.3345530824,-0.7072968879,3.1097623951\H,3.9423790246,0.7796078401,2.5673329525\O,-1.6218029429,1.9884939625,1.2165465675\C,-2.7128475633,1.4075617362,1.2873536902\C,-2.9941719265,0.0571671015,1.5992028848\O,-0.7518323244,-0.7453790629,1.8541535028\C,-1.9929938761,-0.880042896,1.9118435342\O,-2.5204145255,-2.0865114163,2.297220529\C,-1.5902120222,-3.10

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,-1.0062244957\C,-4.4500222746,-1.158910335,-1.5592558567\C,-7.1409072
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41,-0.1125449,-0.5330503,-0.0543839,-0.0467328,-0.1191563,-0.5013694,-
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TS3

1\1\GINC-A05\Freq\RB3PW91\6-31G(d)\C31H44N6O6S1\SHUBINA\08-Nov-2007\O\
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07890647\N,1.0720164427,1.3617602737,1.3071071421\C,2.3213494806,2.729
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544936,3.8462859615,1.5765102174\C,1.1795227527,5.1565597359,0.7891296
086\C,2.1946233178,5.2394703482,-0.3543899851\C,2.1321967555,4.0084042
913,-1.2643997459\C,3.4655478073,0.7379816257,-1.3644085524\C,4.182041
1331,-1.5624853417,-1.9318051067\C,3.8547390067,-2.5223455165,-3.07702
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4231373,-0.0278261987\C,5.3731971925,-2.4125465494,0.1415826469\C,3.01
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9795439\C,4.2075558106,-3.5679438473,1.9157036201\C,1.9705452555,0.629
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0.8792523451,-2.0481215409\H,-7.2837045186,0.0297813629,-2.5428956208\
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808293\H,-2.7276018811,0.5540821026,-1.5753508587\N,-0.4730872243,-0.6
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Fin3

1\1\GINC-A08\Freq\RB3PW91\6-31G(d)\C31H44N6O6S1\TS\21-Nov-2007\0\#P B
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22421449\C,-1.9607110278,5.2231128621,0.4993651255\C,-1.816984578,3.98
7009719,1.3938691816\C,-3.1888119008,0.6874278835,1.5810130952\C,-3.79
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,-1.0790626278\C,-4.1552611414,-3.6137115167,-1.7289495932\C,-2.242350
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,-1.2486592032,1.1768693922\H,2.8163414665,0.6326063816,1.0982159687\N
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InIt6

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,1.3480658688\N,-2.0084472068,2.6537682257,-0.7892468813\N,2.056044965
9,3.4097790703,0.2831731231\N,2.6726649151,1.2380868906,-0.2646570334\
N,1.3489394112,1.5699137762,1.5747424275\C,-0.3640554531,3.2552085524,
2.4034491109\C,0.732604592,2.2167157261,2.7315967048\C,1.7390712104,2.
8144928591,3.7241347686\C,1.022422513,3.2415320656,5.0097667691\C,-0.1
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5715759\C,-1.3907761923,3.4013942772,0.1510951835\C,-2.1240784883,3.03
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0600086,3.2363175557\H,0.0909177505,4.1793160671,2.0319275989\H,0.6395
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N6O6S1)]\@

TS6

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81\Thermal=0.7888435\Dipole=1.3456053,-0.6203456,1.0395684\DipoleDeriv

Fin6

1\1\GINC-A06\FOpt\RB3PW91\6-31G(d)\C31H44N6O6S1\SHUBINA\22-Nov-2007\0\ \#P B3PW91/6-31G(d) OPT Freq=NoRaman Name=SHUBINA\Fint for TS6\0,1\S ,0.2451570301,4.651510714,1.8819207318\N,-0.3451434244,2.1106461497,2.560995613\N,-1.2606065682,2.8104062546,0.6081756998\N,2.7673655575,2.5827569756,1.0669743359\N,2.6425723266,0.7516717416,-0.3539918812\N,1.8650592159,0.5372319058,1.7953643631\C,0.7445003509,2.0369121792,3.5052488823\C,1.6172597417,0.794945358,3.2167850054\C,2.8847625943,0.8281987688,4.0761401011\C,2.5028248833,0.856218233,5.5616231872\C,1.5380708481,2.0011543285,5.8891908709\C,0.3086236786,1.9988516638,4.9738465745\C,-0.4884839509,3.1210707796,1.670988907\C,-1.5076635009,3.7044674446,-0.5126797436\C,-2.8309224058,3.3075171484,-1.1730648515\C,-0.3628528752,3.7169467965,-1.5210817605\C,0.1471382983,2.525423712,-2.0514852682\C,0.1822158165,4.9288276076,-1.9534384088\C,1.1789051555,2.5512598687,-2.9918968321\C,1.2108626016,4.9583985909,-2.8952013529\C,1.7148228348,3.7687220136,-3.4174962526\C,2.3909558272,1.3036423589,0.8457141555\H,3.5024709383,-0.0505091676,3.8543190382\H,1.0220259256,-0.0772079898,3.5124531739\H,1.3353070979,2.9518950912,3.3823436177\H,2.0299950046,-0.1015646966,5.824071565\H,3.408487388,0.9336115968,6.1758631616\H,1.2274139315,1.9407510422,6.939499441\H,2.0628928054,2.9605868784,5.775273449\H,-0.3066820697,1.1058229229,5.1543853538\H,-0.3232889993,2.8715422466,5.1708765284\H,3.4810814461,1.7136414858,3.8188413664\H,-0.7875121861,1.2000758902,2.3312336331\H,-1.3563827525,1.8000802514,0.4239143996\H,-1.5979423208,4.7123257993,-0.0966992723\H,-3.0513501213,3.9720190635,-2.0145658247\H,-2.7860699644,2.2811987704,-1.5559216856\H,-3.6501789969,3.3688446852,-0.4491577382\H,-0.2478615024,1.5690621692,-1.7162077832\H,-0.1916897866,5.8589165576,-1.5317516455\H,1.5565541298,1.6132719226,-3.3948176397\H,1.6235362668,5.9127644803,-3.2135308454\H,2.5163736265,3.7883182833,-4.1522308528\H,1.4479362646,-0.3152065257,1.4344989854\H,2.2960857587,-0.1919511658,-0.5373242423\H,2.5780396061,1.3655099078,-1.1564417863\H,3.144902766,3.05765841,0.2570350655\O,1.6353798512,-1.9879903669,0.280204227\C,0.9429120377,-2.8612993705,-0.2073039695\C,0.0625984413,-2.7621411433,-1.4334901182\O,1.5328932603,-1.0626857532,-2.4220615523\C,0.5980129976,-1.832802996,-2.5024054826\O,-0.1304423798,-1.9960181152,-3.6171773846\C,0.2299950854,-1.1837206919,-4.7518248923\C,-0.5950211247,-1.6561810264,-5.9283236057\O,0.8565209025,-4.0881749881,0.3209196291\C,1.5381978446,-4.2910264076,1.5771495853\C,1.2846945346,-5.7174931292,2.0097938725\H,0.2152702932,-5.8998839917,2.1540058229\H,1.6620661216,-6.4272131219,1.2668899012\H,1.7953090566,-5.9103651038,2.9591890206\H,2.603647486,-4.0860776353,1.4326091671\H,1.1490851831,-3.5665581929,2.2996416354\H,0.0057620271,-3.7583214582,-1.8810284341\H,1.3045547862,-1.2887509424,-4.9324033216\H,0.0307025955,-0.1346914272,-4.508667404\H,-0.3580734319,-1.0538335074,-6.8117466521\H,-0.3832998583,-2.7049438063,-6.1586771206\H,-1.6649488169,-1.5582009782,-5.7210297989\H,2.1305264235,3.196103716,1.5910863758\C,-4.5085204198,-3.9941222307,-2.5530841363\C,-3.5512484958,-3.0494307866,-2.1878271662\C,-2.4403000035,-3.4111621044,-1.4198276364\C,-4.3695191048,-5.3216537503,-2.1534115884\C,-3.2672421656,-5.6945440956,-1.3854680527\C,-2.3118204126,-4.7476691102,-1.0222279715\H,-3.6674258841,-2.0145214081,-2.5020185734\H,-5.3629593042,-3.6913383795,-3.1535273339\H,-5.1138023896,-6.0607715916,-2.4387729808\H,-3.1498771087,-6.727655315,-1.0669727334\H,-1.4540820696,-5.049743187,-0.4258633437\C,-1.4343530441,-2.3531654178,-1.008223589\C,-1.5573527897,-2.0285170464,0.4439141421\H,-1.6577074924,-1.4339574157,-1.5573231383\N,-1.2249432076,-0.8229908756,0.8750717035\O,-1.3007423875,-0.5211649374,2.1194676664\O,-0.7871867335,0.0651181982,0.0423365478\H,-1.9292285951,-2.7204986115,1.185693197\Version=IA64L-G03RevD.01\State=1-A\HF=-2385.0293488\RMSD=5.772e-09\RMSF=9.400e-06\Thermal=0.\Dipole=1.4939299,-2.0671573,-1.2485828\PG=C01 [X(C31H44N6O6S1)]\@

Init7

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O6S1)]\@

TS7

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Fin7

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Init8

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3.1080058529\H,-3.2363605486,-4.8731897313,-2.4928506584\H,-4.59474315
33,-4.5658847949,-1.395457533\H,-4.2734680777,-2.0842457928,-1.7000921
158\H,-2.9171286941,-2.386290498,-2.7862838642\H,-1.0483711825,-3.1161
575893,1.0274920304\H,0.4775480681,-0.0981405318,3.6498438927\H,1.9091
290772,-0.2825656892,2.6301106411\H,2.3809969914,-1.0180230623,4.98213
99022\H,1.0776516144,-2.2192777024,4.8726049297\H,2.5286124171,-2.3860
858998,3.8631610316\H,0.773761294,0.2580974849,-2.3984429926\C,1.90220
90244,-7.4414259125,-0.3395184968\C,2.0888435616,-6.1145976726,-0.7010
366383\C,1.7823584865,-5.0808442472,0.2026331435\C,1.4053954811,-7.761
2461396,0.9270654792\C,1.1002506437,-6.7471388973,1.8334496128\C,1.291
6963243,-5.4168146303,1.4767780048\H,2.48672991,-5.8783520612,-1.68419
46933\H,2.145841605,-8.2324396201,-1.0435786335\H,1.25974729,-8.801831
9744,1.204974272\H,0.7126127082,-6.9926560287,2.8182644709\H,1.0462267
245,-4.6183494457,2.1725105537\C,1.9480727352,-3.6712772337,-0.1086135
248\C,2.1938200414,-3.1404656154,-1.3197162497\H,1.826268546,-2.973391
3283,0.7171024301\N,2.2707510759,-1.7199508514,-1.4626572273\O,2.16635
16254,-1.2757366703,-2.6157751417\O,2.4172663238,-1.008719363,-0.47163
19176\H,2.2415600088,-3.6526127085,-2.2705151375\\Version=IA64L-G03Rev
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TS8

1\1\GINC-A02\FTS\RB3PW91\6-31G(d)\C31H44N6O6S1\TS\29-Nov-2007\0\#P B3
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0.7933336414\N,2.6596682209,1.5416887926,1.0900080037\N,0.6358215362,-
0.7889904169,-2.0401952586\N,2.3334817585,0.7197232961,-2.5233744167\N
.2.8788431414,-1.4464746114,-1.9560361647\C,3.3641345273,-1.9844731934
.0.4054872267\C,2.7721054899,-2.4877128057,-0.9304735146\C,3.457421561
5,-3.7819955922,-1.3663176988\C,3.2811271424,-4.8541166894,-0.28693172
18\C,3.798556316,-4.3750021897,1.0724385811\C,3.154643079,-3.048170136
1,1.4882952902\C,3.3787082545,0.5028831393,0.61250411\C,2.9980662485,2
.9487014802,0.9284610328\C,2.4638152131,3.7245202376,2.1360078489\C,2.
4796226879,3.5367653657,-0.377760449\C,1.1693231439,3.29682466,-0.8099
541277\C,3.3021967463,4.3593060903,-1.1523973015\C,0.6967533761,3.8674
545947,-1.9918244901\C,2.8302568852,4.9357022777,-2.3318379214\C,1.525
4512955,4.6914841081,-2.7558839326\C,1.9281908425,-0.5064117825,-2.137
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093969565,-0.7783791026\H,4.4371865482,-1.8074562882,0.2687355056\H,2.
2132427612,-5.0979440961,-0.2059206639\H,3.7967114383,-5.7744967052,-0
.5872037923\H,3.6058046663,-5.1353031887,1.8391113977\H,4.8901967026,-
4.2482625012,1.0249087146\H,2.0767458183,-3.1929201119,1.6454893226\H,
3.5833431675,-2.6892116279,2.4316737937\H,4.5279103787,-3.5943861741,-
1.5418357722\H,1.8243462716,-0.7057245689,1.1102136251\H,1.7084795256,
1.3269708427,1.3907636985\H,4.0903773779,3.0034823873,0.9187650316\H,2
.7280198571,4.7829472971,2.0502332613\H,1.3706546618,3.660092751,2.195
0879606\H,2.8891662413,3.3296374574,3.0647971279\H,0.5187905916,2.6324
725422,-0.2459905024\H,4.3274067153,4.5388557853,-0.8357038878\H,-0.32
06211178,3.6580351489,-2.3125183378\H,3.4876422557,5.567363735,-2.9241
808025\H,1.1571174615,5.1359551228,-3.6771141675\H,3.8223041794,-1.086
3690624,-2.0742678133\H,3.2156160853,1.0486970726,-2.1308027732\H,1.62
93554655,1.4379276763,-2.6380154908\H,-0.0425369769,-0.0597647891,-1.7
935433262\O,-1.5162606475,0.9740921237,-1.2957597333\C,-2.3693390013,1
.0674440337,-0.411023606\C,-2.3437662252,0.5061599055,0.9206853105\O,0
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0651635\O,-1.3228995066,0.0004221761,2.920464259\C,-0.1792581861,-0.36

12184899,3.7038823482\C,-0.6717411852,-0.7127988893,5.0913802893\O,-3.5452999901,1.7005450201,-0.6426781029\C,-3.7446423937,2.2175259107,-1.9630348069\C,-5.1422154884,2.7969692135,-2.0158710546\H,-5.3430010952,3.2022969784,-3.0136563286\H,-5.8877494019,2.0270934872,-1.7951685501\H,-5.257142744,3.6047023254,-1.2860490022\H,-2.9843043089,2.9795188553,-2.1709353874\H,-3.6070614213,1.4124321272,-2.69323235\H,-3.1859106999,0.7688863749,1.5497413622\H,0.5250029694,0.478653517,3.7303092363\H,0.3185658827,-1.2113950245,3.2260084801\H,0.1746521803,-0.9914636095,5.7282264912\H,-1.1852240153,0.1370460232,5.552489682\H,-1.3657999638,-1.5581710938,5.0533739214\H,0.3347579944,-1.7469564731,-1.8319813853\C,-6.4485559037,-1.1426210557,-0.9326377566\C,-5.0713426061,-1.3031729259,-0.8164239973\C,-4.4595442769,-1.3592084177,0.4448208108\C,-7.2434899077,-1.0288773862,0.2080335148\C,-6.6486095986,-1.0762579719,1.4681009101\C,-5.2717895522,-1.2377811444,1.5827039207\H,-4.469281574,-1.3896523311,-1.7163491436\H,-6.9044565472,-1.11086009,-1.9191273631\H,-8.3194469233,-0.9064064453,0.1147485505\H,-7.2585537244,-0.9915006564,2.363823777\H,-4.8110411508,-1.2769087661,2.5674357945\C,-3.0113170568,-1.5812913796,0.626801408\C,-2.2514476434,-2.2201783029,-0.3504654991\H,-2.6973683212,-1.7677961275,1.6497205773\N,-1.0205915423,-2.749763723,-0.0535682437\O,-0.3607359624,-3.2602927739,-1.0121630202\O,-0.5672162044,-2.7377755208,1.1090120505\H,-2.5182863326,-2.3113177552,-1.3923590714\Version=IA64L-G03RevD.01\State=1-A\HF=-2385.0190008\RMSD=8.012e-09\RMSF=2.464e-06\Thermal=0.\Dipole=-1.0091578,0.9480822,-0.1225105\PG=C01 [X(C31H44N6O6S1)]\@

Fin8

1\1\GINC-A06\FOpt\RB3PW91\6-31G(d)\C31H44N6O6S1\TS\20-Dec-2007\0\#P B 3PW91/6-31G(d) Opt Freq=NoRaman Name=TS\Fin TS8\0,1\S,-0.0944834667,4.758309844,0.6559886373\N,1.2312774342,2.3989775952,0.6099469696\N,-0.8966639957,2.3078428002,1.41098624\N,0.0762624246,1.3884504688,-2.5091803357\N,-0.9851026788,3.4614440136,-2.3887331424\N,1.2889117394,3.3501663307,-2.0903568309\C,2.4363422578,2.9929739773,0.0624089887\C,2.4869861065,2.7850215749,-1.4689804006\C,3.7486675403,3.4098978456,-2.0652050837\C,4.9989138926,2.8170802657,-1.4102741725\C,4.9624518749,2.9823909184,0.1109227676\C,3.6859862123,2.3881891364,0.7120229269\C,0.0945363227,3.0706714441,0.895913886\C,-2.2913877344,2.7166386664,1.5198002912\C,-2.9367737809,2.028542019,2.724441059\C,-3.0502471674,2.4346173459,0.2281821908\C,-2.9546167206,1.1856084752,-0.400432185\C,-3.8449353948,3.4226743494,-0.3595571932\C,-3.6271989594,0.9388997685,-1.5973400726\C,-4.5237557686,3.1780516389,-1.5557222867\C,-4.4123725388,1.9370852115,-2.1824924201\C,0.1346323341,2.6964465093,-2.2984614297\H,3.7582612209,3.2420494982,-3.1485160934\H,2.4976529787,1.7055491405,-1.659072294\H,2.3893296737,4.0670664495,0.2768960579\H,5.0600335902,1.7489900134,-1.6601400351\H,5.8968264821,3.2914162385,-1.8251656149\H,5.8419931999,2.5093339688,0.5648141218\H,5.0189616295,4.0522349305,0.3613238774\H,3.6630620865,1.2999679192,0.5675621277\H,3.6461668896,2.5729978424,1.7924591885\H,3.729653501,4.5000057766,-1.9089706448\H,1.216423792,1.3663692591,0.5493075414\H,-0.7149411669,1.3134801105,1.5535136244\H,-2.2819843755,3.7980048475,1.6821757549\H,-3.9824422495,2.3390850447,2.8167313613\H,-2.9112707361,0.9390579823,2.6201905168\H,-2.4083042643,2.3025591515,3.6436696216\H,-2.3399104694,0.4018267789,0.0354380761\H,-3.9194381821,4.3993429301,0.1140010109\H,-3.5375265151,-0.0394865442,-2.0639596253\H,-5.1316968298,3.9616686248,-2.0014304175\H,-4.9370040532,1.7459473353,-3.1154123739\H,1.1569524183,4.339761613,-1.9063741342\H,-1.029759365,4.2064132494,-1.6912540264\H,-1.8634308305,2.9653347587,-2.4855440946\H,-0.8379507213,0.9592103679,-2.455351639\O,-1.570849434,-2.0343047329,-0.9279678892\C,-1.476167203,-2.6661936874,0.1023150496\C,-0.2369007392,-2.7796423546,0.971493194\O,-0.8887987869,-0.5980815149,1.8295666022\C,-0.1181140035,-1.5438714117,1.848799704\O,0.8342180729,-1.7116699252,2.7650186938\C,1.0948015992,-0.5934153349,3.6334482377\C,2.1770426998,-1.0131367711,4.602742124\O,-2.4847829883,-3.3728756587,0.6381705008\C,-3.7366864504,-3.3296503187,-0.0712709299\C,-4.707273287,-4.2280212631,0.6631243291\H,-5.6768621905,-4.222423127,0.153831786\H,-4.3394339103,-5.2584279172,0.6932330194\H,-4.8570797574,-3.8844485426,1.691436819\H,-4.0842865821,-2.2916357777,-0.1063860522\H,-3.568918975,-3.6600408332,-1.1017242309\H,-0.4002778502,-3.6083066438,1.6700664248\H,0.1664439384,-0.3192903674,4.1450475686\H,1.410551722,0.25

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Init9

1\1\FAU-CCC-CCDH153\SP\RB3PW91\6-31G(d)\C31H44N6O6S1\SHUBINA\28-Jul-20
08\0\#P B3PW91/6-31G(d) SCF=Tight Name=SHUBINA\Init TS 9 R\0,1\S,0,
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7,0.786433,-1.97522\N,0,-3.248193,1.519079,-1.419021\C,0,-3.08969,2.17
3889,0.940103\C,0,-2.839887,2.60169,-0.525273\C,0,-3.590505,3.900761,-
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,0.62198,-1.957312\H,0,-3.42425,4.19102,-1.867227\H,0,-1.771164,2.7813
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,0,8.973561,-0.202535,0.624418\H,0,7.202247,-0.645102,2.310099\H,0,4.8
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TS9

1\1\FAU-CCC-CCDH153\SP\RB3PW91\6-31G(d)\C31H44N6O6S1\SHUBINA\28-Jul-20

08\0\#P B3PW91\6-31G(d) SCF=Tight Name=SHUBINA\TS9 R\0,1\S,0,-4.704
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,-2.019157\N,0,-2.214953,2.026045,-1.864858\C,0,-2.109074,2.867495,0.4
38332\C,0,-1.478399,2.92581,-0.973251\C,0,-1.488292,4.350851,-1.52772\
C,0,-0.78986,5.317848,-0.568916\C,0,-1.413822,5.263978,0.827655\C,0,-1
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5,-1.707063,1.479377\C,0,-3.156406,-2.663737,2.514904\C,0,-4.194747,-2
.446104,0.222744\C,0,-5.550528,-2.519586,-0.106624\C,0,-3.264526,-3.09
6752,-0.597122\C,0,-5.975077,-3.229531,-1.229823\C,0,-3.687219,-3.8003
21,-1.72539\C,0,-5.04444,-3.871906,-2.04388\C,0,-1.937889,0.714168,-2.
013503\H,0,-1.010305,4.358587,-2.514195\H,0,-0.444409,2.572017,-0.9036
13\H,0,-3.167381,3.143817,0.357165\H,0,0.275737,5.056237,-0.503586\H,0
,-0.838216,6.336894,-0.971708\H,0,-0.876581,5.935144,1.508873\H,0,-2.4
48765,5.632974,0.778086\H,0,-0.372196,3.50401,1.542391\H,0,-1.907788,3
.804056,2.36349\H,0,-2.530883,4.671782,-1.675786\H,0,-1.140378,1.17325
6,1.183213\H,0,-1.802213,-0.908401,1.228532\H,0,-4.635849,-1.219945,1.
905031\H,0,-3.865112,-3.468587,2.732301\H,0,-2.230252,-3.118373,2.1462
41\H,0,-2.934072,-2.131022,3.446026\H,0,-6.278083,-2.001859,0.513869\H
,0,-2.201265,-3.034942,-0.377766\H,0,-7.034249,-3.272549,-1.471975\H,0
,-2.951167,-4.302012,-2.349585\H,0,-5.372908,-4.424202,-2.920966\H,0,-
3.210139,2.223403,-1.90047\H,0,0.12929,0.813747,-1.832204\H,0,-0.56313
3,-0.764052,-1.893915\H,0,-2.786007,-1.101723,-2.320085\H,0,-3.836615,
0.098728,-1.744896\O,0,1.913765,1.21303,-1.590951\C,0,2.903841,1.07518
,-0.86828\C,0,2.956485,0.711361,0.520973\O,0,0.698526,1.278815,1.07757
1\C,0,1.834076,0.919013,1.390833\O,0,2.16186,0.642698,2.684194\C,0,1.1
05283,0.750676,3.643353\C,0,1.696255,0.466634,5.008242\O,0,4.155421,1.
209895,-1.383854\C,0,4.230177,1.525918,-2.777424\C,0,5.696377,1.639924
,-3.138057\H,0,5.804783,1.874466,-4.202707\H,0,6.179534,2.433373,-2.55
8952\H,0,6.221065,0.701311,-2.933671\H,0,3.728019,0.743121,-3.357815\H
,0,3.691858,2.461773,-2.966592\H,0,3.934712,0.70723,0.983622\H,0,0.316
124,0.03316,3.390514\H,0,0.669842,1.755012,3.59524\H,0,0.918168,0.5401
13,5.77576\H,0,2.122926,-0.540825,5.048286\H,0,2.486509,1.185143,5.248
473\C,0,6.306362,-2.378071,-1.015789\C,0,4.941369,-2.122996,-0.942068\
C,0,4.323986,-1.879811,0.295129\C,0,7.084475,-2.392048,0.142065\C,0,6.
486348,-2.145363,1.377496\C,0,5.121675,-1.890331,1.451401\H,0,4.353602
,-2.110959,-1.855047\H,0,6.766077,-2.568803,-1.982206\H,0,8.150811,-2.
59328,0.081042\H,0,7.083957,-2.15347,2.285336\H,0,4.656723,-1.691371,2
.41425\C,0,2.880969,-1.652416,0.440645\C,0,1.961378,-2.050468,-0.51330
9\H,0,2.512741,-1.580095,1.458661\N,0,0.614874,-2.104114,-0.237593\O,0
,-0.155611,-2.400139,-1.19813\O,0,0.169389,-1.881285,0.909392\H,0,2.18
8912,-2.292685,-1.540469\Version=AM64L-G03RevD.02\State=1-A\HF=-2385.
0171108\RMSD=4.259e-09\Thermal=0.\Dipole=1.2645905,0.452724,-0.3944132
\PG=C01 [X(C31H44N6O6S1)]\@

Fin9

1\1\FAU-CCC-CCDH154\SP\RB3PW91\6-31G(d)\C31H44N6O6S1\SHUBINA\28-Jul-20
08\0\#P B3PW91\6-31G(d) SCF=Tight Name=SHUBINA\Fin TS9 R\0,1\S,0,-4
.4365,1.26469,0.34854\N,0,-1.76017,1.5415,0.51121\N,0,-2.5722,-0.46985
,1.21331\N,0,-2.93345,-0.42881,-2.27356\N,0,-0.64957,-0.0949,-2.3257\N
,0,-2.12831,1.73552,-2.313\C,0,-1.78821,2.83627,-0.1358\C,0,-1.31333,2
.72583,-1.60373\C,0,-1.3835,4.08146,-2.30831\C,0,-0.58331,5.13935,-1.5
4445\C,0,-1.04123,5.24352,-0.08796\C,0,-0.97288,3.88853,0.62166\C,0,-2
.84687,0.75078,0.72061\C,0,-3.58363,-1.41382,1.68661\C,0,-2.96782,-2.2
4495,2.81659\C,0,-4.16554,-2.30651,0.59737\C,0,-5.54862,-2.35218,0.402
15\C,0,-3.345,-3.13268,-0.18117\C,0,-6.10899,-3.20681,-0.54721\C,0,-3.
90545,-3.9816,-1.13628\C,0,-5.28824,-4.0252,-1.32038\C,0,-1.87461,0.40
644,-2.26664\H,0,-1.02091,3.97695,-3.33775\H,0,-0.27361,2.37937,-1.608
13\H,0,-2.84099,3.14429,-0.14738\H,0,0.48416,4.87513,-1.57218\H,0,-0.6
7712,6.10926,-2.04793\H,0,-0.4277,5.97673,0.44988\H,0,-2.07399,5.62024
,-0.05898\H,0,0.06905,3.55647,0.70544\H,0,-1.36325,3.96588,1.64295\H,0
,-2.43615,4.39559,-2.37337\H,0,-0.8495,1.21499,0.83388\H,0,-1.59717,-0
.81516,1.16273\H,0,-4.40304,-0.81004,2.08844\H,0,-3.69474,-2.97497,3.1
8578\H,0,-2.08296,-2.78768,2.46713\H,0,-2.6681,-1.59719,3.64808\H,0,-6
.19083,-1.70042,0.99008\H,0,-2.26264,-3.08961,-0.07182\H,0,-7.18736,-3
.22579,-0.68649\H,0,-3.25521,-4.61803,-1.73261\H,0,-5.72178,-4.69121,-
2.06268\H,0,-3.12217,1.9423,-2.26642\H,0,0.15918,0.51347,-2.28076\H,0,

-0.51267,-1.04624,-1.89633\H,0,-2.73414,-1.41701,-2.16462\H,0,-3.74709
,-0.12085,-1.7379\O,0,2.07697,0.89348,-1.37883\C,0,2.91161,0.92577,-0.
49585\C,0,2.92042,0.08513,0.76519\O,0,1.03703,1.45213,1.48529\C,0,1.84
09,0.56912,1.72133\O,0,1.99517,-0.0013,2.91578\C,0,0.99384,0.31439,3.9
0269\C,0,1.33611,-0.455,5.15858\O,0,3.97934,1.73478,-0.52978\C,0,4.096
75,2.58933,-1.68345\C,0,5.38958,3.36228,-1.54783\H,0,5.51638,4.02648,-
2.40931\H,0,5.38787,3.97286,-0.63955\H,0,6.2469,2.68342,-1.5064\H,0,4.
08016,1.96761,-2.58455\H,0,3.22364,3.24972,-1.71991\H,0,3.8691,0.27327
,1.27959\H,0,0.01835,0.02755,3.49986\H,0,0.9922,1.39681,4.06778\H,0,0.
59468,-0.24184,5.93594\H,0,1.33314,-1.53219,4.96616\H,0,2.32303,-0.171
36,5.53826\C,0,5.90753,-2.16352,-1.71943\C,0,4.64745,-1.74457,-1.29742
\C,0,4.22922,-1.94817,0.0238\C,0,6.77353,-2.79299,-0.82661\C,0,6.36878
, -3.00101,0.49039\C,0,5.10761,-2.58086,0.90897\H,0,3.97787,-1.26147,-2
.00561\H,0,6.21172,-2.00102,-2.75066\H,0,7.75529,-3.12276,-1.15674\H,0
,7.03329,-3.49626,1.19409\H,0,4.7968,-2.75123,1.93772\C,0,2.87098,-1.4
7312,0.51083\C,0,1.78531,-1.94637,-0.39393\H,0,2.69874,-1.88566,1.5134
1\N,0,0.52054,-1.88505,-0.04852\O,0,-0.39372,-2.31145,-0.8683\O,0,0.16
111,-1.38915,1.08685\H,0,1.98334,-2.40745,-1.35017\Version=AM64L-G03R
evD.02\State=1-AHF=-2385.0420358\RMSD=8.889e-09\Thermal=0.\Dipole=2.1
224925,1.5761175,-0.4381603\PG=C01 [X(C31H44N6O6S1)]\@

Init10

1\1\FAU-CCC-CCDH155\SP\RB3PW91\6-31G(d)\C31H44N6O6S1\SHUBINA\28-Jul-20
08\0\#P B3PW91\6-31G(d) SCF=Tight Name=SHUBINA\Init TS10 S\0,1\S,0,
-4.68922,1.67535,0.10279\N,0,-2.05948,2.11013,0.58356\N,0,-2.96102,0.3
2418,1.65864\N,0,-2.96347,-0.38985,-2.27095\N,0,-0.74269,0.1132,-1.798
37\N,0,-2.29846,1.81395,-2.22612\C,0,-2.02466,3.27978,-0.26613\C,0,-1.
52856,2.93323,-1.68965\C,0,-1.63098,4.15978,-2.59789\C,0,-0.80093,5.31
105,-2.02053\C,0,-1.20368,5.6361,-0.57936\C,0,-1.15828,4.39687,0.32144
\C,0,-3.16241,1.35798,0.81234\C,0,-3.93009,-0.72612,1.92966\C,0,-3.698
15,-1.27386,3.33998\C,0,-3.89281,-1.83718,0.88771\C,0,-5.08385,-2.3374
,0.35463\C,0,-2.67981,-2.38863,0.45569\C,0,-5.07012,-3.36689,-0.58691\
C,0,-2.65946,-3.41601,-0.48993\C,0,-3.85826,-3.90785,-1.01305\C,0,-1.9
8048,0.5194,-2.05379\H,0,-1.28845,3.89915,-3.60631\H,0,-0.47903,2.6362
2,-1.63278\H,0,-3.06073,3.63058,-0.34552\H,0,0.26152,5.03061,-2.04554\
H,0,-0.9058,6.19987,-2.65475\H,0,-0.5493,6.41701,-0.17288\H,0,-2.22309
,6.04871,-0.57222\H,0,-0.12561,4.03622,0.41954\H,0,-1.51776,4.63852,1.
32841\H,0,-2.68445,4.46607,-2.68539\H,0,-1.16221,1.72852,0.91047\H,0,-
1.99742,0.17489,1.96864\H,0,-4.9167,-0.25543,1.88706\H,0,-4.44069,-2.0
4389,3.57109\H,0,-2.70639,-1.73194,3.4298\H,0,-3.78085,-0.47148,4.0807
3\H,0,-6.03091,-1.90396,0.66883\H,0,-1.73871,-1.99744,0.83696\H,0,-6.0
0736,-3.73764,-0.99497\H,0,-1.70727,-3.81964,-0.8245\H,0,-3.84335,-4.7
0652,-1.75047\H,0,-3.30205,1.98169,-2.21301\H,0,-0.03327,0.74296,-1.38
468\H,0,-0.58426,-0.86856,-1.59599\H,0,-2.78542,-1.33187,-1.93812\H,0,
-3.8969,-0.07274,-2.02269\O,0,1.14565,1.75442,-0.58069\C,0,2.14505,1.4
001,0.08182\C,0,2.21256,0.65484,1.26949\O,0,-0.12422,0.34657,1.73037\C
,0,1.08729,0.19846,1.98953\O,0,1.46254,-0.49003,3.11176\C,0,0.42109,-0
.97533,3.95047\C,0,1.07145,-1.59163,5.17293\O,0,3.39832,1.76036,-0.367
66\C,0,3.44155,2.53267,-1.56516\C,0,4.89813,2.8049,-1.88277\H,0,4.9789
4,3.41166,-2.79152\H,0,5.38028,3.34696,-1.06264\H,0,5.44548,1.8705,-2.
04573\H,0,2.94957,1.98801,-2.38018\H,0,2.88678,3.46759,-1.42096\H,0,3.
18568,0.48417,1.71222\H,0,-0.17676,-1.71885,3.40682\H,0,-0.24983,-0.15
329,4.22794\H,0,0.30642,-1.98813,5.84965\H,0,1.73826,-2.41139,4.88671\
H,0,1.66067,-0.84553,5.71565\C,0,7.02348,-3.44215,-0.51295\C,0,5.64695
, -3.53642,-0.65925\C,0,4.83226,-2.40021,-0.49552\C,0,7.61363,-2.21382,
-0.20228\C,0,6.81864,-1.08134,-0.03546\C,0,5.43721,-1.17144,-0.17554\H
,0,5.19944,-4.50081,-0.88349\H,0,7.64151,-4.32758,-0.63498\H,0,8.69214
, -2.14474,-0.08598\H,0,7.27317,-0.12521,0.2089\H,0,4.81696,-0.28618,-0
.05666\C,0,3.3856,-2.43149,-0.6434\C,0,2.66675,-3.44729,-1.15277\H,0,2
.83935,-1.54734,-0.31167\N,0,1.24014,-3.35803,-1.25656\O,0,0.66235,-4.
33064,-1.73955\O,0,0.66637,-2.3356,-0.86711\H,0,3.03725,-4.38705,-1.53
84\Version=AM64L-G03RevD.02\State=1-AHF=-2385.0300439\RMSD=1.742e-09
\Thermal=0.\Dipole=1.6317228,-0.6308108,-0.8722403\PG=C01 [X(C31H44N6O
6S1)]\@

TS10

1\1\FAU-CCC-CCDH155\SP\RB3PW91\6-31G(d)\C31H44N6O6S1\SHUBINA\28-Jul-20
08\0\#P B3PW91\6-31G(d) SCF=Tight Name=SHUBINA\TS10 S\0,1\S,0,-4.76
9333,1.034621,0.670417\N,0,-2.126551,1.322384,1.106951\N,0,-2.920405,-
0.811715,1.293602\N,0,-3.076326,0.017031,-2.131892\N,0,-0.794072,0.341
305,-1.865277\N,0,-2.283688,2.128612,-1.646771\C,0,-2.143336,2.727109,
0.744184\C,0,-1.550532,2.93855,-0.669891\C,0,-1.589312,4.415266,-1.064
465\C,0,-0.857877,5.276341,-0.031769\C,0,-1.423668,5.063907,1.374101\C
,0,-1.39738,3.585462,1.770803\C,0,-3.193285,0.48617,1.049485\C,0,-3.91
4884,-1.884662,1.311408\C,0,-3.51626,-2.917684,2.368039\C,0,-4.110624,
-2.518016,-0.059733\C,0,-5.380844,-2.5499,-0.641588\C,0,-3.033976,-3.0
85756,-0.755147\C,0,-5.579681,-3.135914,-1.892568\C,0,-3.231076,-3.666
3,-2.008434\C,0,-4.504954,-3.6947,-2.580919\C,0,-2.027433,0.817349,-1.
848723\H,0,-1.146422,4.534556,-2.060009\H,0,-0.509726,2.600154,-0.6644
94\H,0,-3.198379,3.024304,0.726116\H,0,0.210379,5.017081,-0.038905\H,0
, -0.9256,6.333444,-0.316195\H,0,-0.858293,5.655728,2.104402\H,0,-2.459
647,5.431171,1.409454\H,0,-0.35863,3.236434,1.840741\H,0,-1.857845,3.4
38431,2.754896\H,0,-2.637681,4.743341,-1.138573\H,0,-1.194664,0.933148
,1.254811\H,0,-1.945151,-1.120503,1.343875\H,0,-4.858503,-1.415502,1.6
02481\H,0,-4.260879,-3.719247,2.403414\H,0,-2.543357,-3.364882,2.14029
8\H,0,-3.460236,-2.448433,3.356246\H,0,-6.218634,-2.098115,-0.115669\H
,0,-2.033532,-3.050863,-0.33013\H,0,-6.574589,-3.147564,-2.331064\H,0,
-2.38535,-4.103104,-2.534547\H,0,-4.656374,-4.149458,-3.556806\H,0,-3.
271085,2.355061,-1.708304\H,0,0.028278,0.942521,-1.74628\H,0,-0.620161
, -0.635983,-1.609328\H,0,-2.884696,-0.966071,-2.288334\H,0,-3.92914,0.
191908,-1.596852\O,0,1.756153,1.556951,-1.816824\C,0,2.795463,1.220002
, -1.250611\C,0,2.973568,0.688778,0.086138\O,0,0.740178,1.022282,0.8802
99\C,0,1.940971,0.851119,1.081063\O,0,2.434311,0.67756,2.330872\C,0,1.
471842,0.660906,3.395819\C,0,2.223438,0.421555,4.687794\O,0,3.987971,1
.294465,-1.894475\C,0,3.943847,1.783593,-3.24181\C,0,5.365806,1.818643
, -3.759816\H,0,5.378816,2.188075,-4.790952\H,0,5.987689,2.480116,-3.14
834\H,0,5.813454,0.819779,-3.746019\H,0,3.305074,1.127667,-3.844268\H,
0,3.484302,2.778046,-3.248348\H,0,3.989679,0.722178,0.458336\H,0,0.735
224,-0.126588,3.200308\H,0,0.939886,1.618549,3.416353\H,0,1.523349,0.4
16986,5.5301\H,0,2.741634,-0.542691,4.670034\H,0,2.965834,1.207331,4.8
60007\C,0,6.181104,-2.279561,1.616594\C,0,4.835135,-1.977125,1.443333\
C,0,4.298359,-1.813644,0.156478\C,0,7.018706,-2.427956,0.51018\C,0,6.4
99572,-2.262906,-0.772474\C,0,5.15394,-1.952859,-0.946075\H,0,4.199955
, -1.846448,2.314215\H,0,6.57991,-2.400387,2.620649\H,0,8.069647,-2.668
192,0.648772\H,0,7.14361,-2.3753,-1.640935\H,0,4.753251,-1.819513,-1.9
47559\C,0,2.87144,-1.524231,-0.080632\C,0,1.879123,-1.986574,0.791253\
H,0,2.569099,-1.489184,-1.122805\N,0,0.574333,-2.067677,0.393156\O,0,-
0.310083,-2.252422,1.275542\O,0,0.274262,-2.006766,-0.830891\H,0,2.020
289,-2.169809,1.845848\Version=AM64L-G03RevD.02\State=1-A\HF=-2385.01
78577\RMSD=5.485e-09\Thermal=0.\Dipole=1.2474084,0.8086933,-0.4041417\
PG=C01 [X(C31H44N6O6S1)]\@

Fin10

1\1\FAU-CCC-CCDH156\SP\RB3PW91\6-31G(d)\C31H44N6O6S1\SHUBINA\28-Jul-20
08\0\#P B3PW91\6-31G(d) SCF=Tight Name=SHUBINA\Fin10 S\0,1\S,0,4.56
495,-2.04026,0.49841\N,0,1.98822,-1.53078,1.14926\N,0,3.39646,0.22219,
1.38971\N,0,3.09654,-0.43772,-2.04413\N,0,0.80218,-0.19385,-1.89753\N,
0,1.79713,-2.29991,-1.61635\C,0,1.5348,-2.85358,0.78372\C,0,0.87797,-2
.86505,-0.62027\C,0,0.4472,-4.27943,-1.00857\C,0,-0.51132,-4.85812,0.0
3607\C,0,0.10387,-4.82867,1.43736\C,0,0.55799,-3.41762,1.82072\C,0,3.2
6182,-1.07146,1.04889\C,0,4.6297,0.99117,1.34081\C,0,4.65928,1.96029,2
.52654\C,0,4.79791,1.72645,0.01729\C,0,6.01508,1.66719,-0.66666\C,0,3.
75325,2.48769,-0.52614\C,0,6.19538,2.35288,-1.86858\C,0,3.9321,3.16996
, -1.73021\C,0,5.15365,3.10674,-2.40465\C,0,1.88419,-0.96568,-1.82201\H
,0,-0.02019,-4.2552,-2.00004\H,0,-0.01271,-2.2282,-0.59101\H,0,2.42919
, -3.48787,0.74576\H,0,-1.43925,-4.27052,0.03689\H,0,-0.78381,-5.88426,
-0.2399\H,0,-0.61838,-5.19983,2.17469\H,0,0.96688,-5.50938,1.47434\H,0
, -0.31817,-2.75705,1.89234\H,0,1.04552,-3.4172,2.80244\H,0,1.33875,-4.
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5684,-2.13863\H,0,5.2897,3.64045,-3.34207\H,0,2.70418,-2.75985,-1.6281

3\H,0,-0.11957,-0.6205,-1.93111\H,0,0.80397,0.72654,-1.4077\H,0,3.1530
8,0.55899,-2.21743\H,0,3.88464,-0.84388,-1.53181\O,0,-2.06871,-0.66681
,-2.1653\C,0,-3.14892,-0.48207,-1.64294\C,0,-3.40356,0.25944,-0.33944\
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,-0.37316,1.83134\C,0,-4.17326,-1.29126,2.94562\C,0,-4.96623,-0.61914,
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,0,-5.59384,-2.10593,-3.77516\H,0,-5.55674,-2.7001,-4.69429\H,0,-6.076
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,-4.12819\H,0,-3.56073,-2.5838,-3.16232\H,0,-4.40334,0.69849,-0.40355\
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3.70814\C,0,-4.66248,4.16594,1.26101\C,0,-4.13662,2.90045,1.00357\C,0,
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2,-0.04959\C,0,-2.38413,3.89885,-0.30916\H,0,-4.61531,2.0266,1.43778\H
,0,-5.55178,4.26202,1.87972\H,0,-4.46528,6.28818,0.93223\H,0,-2.41938,
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.0798\C,0,-1.35578,1.02889,0.97621\H,0,-1.7776,1.5024,-1.00384\N,0,-0.
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993,-0.9220885\PG=C01 [X(C31H44N6O6S1)]\@

INIT11

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23811871\C,2.6090128766,2.5013577101,0.5214725222\C,3.1840715142,3.869
1173266,0.8921740566\C,2.6836001758,4.9428385452,-0.0781761831\C,2.993
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387703176,-3.5055679875,-0.317017735\C,1.8479628556,-3.4564643843,0.41
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434,0.5994639085\H,4.0750031801,2.0966659596,-1.0046730403\H,1.5985007
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.688512876\H,1.3492642775,3.2085802341,-1.8560386991\H,2.7313056726,2.
9200264376,-2.9206444278\H,4.2829315482,3.8186839354,0.8610081571\H,1.
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37,-4.0815655802,2.1786074558\H,4.8294866987,-5.540253695,1.7507564657
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,1.3345316314\H,3.8439120412,-0.9432562784,1.3841638977\H,2.4611745406
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,-4.6741386136,-3.3406191262,3.1451224012\H,-2.1553088792,-3.347084560
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22652\C,-6.0153868295,2.6869942105,0.0534757924\H,-5.0144499422,-0.297
7734088,1.3549723977\H,-7.4172081777,-0.800597047,1.0069263708\H,-8.92
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720922\O,-0.9684610961,3.8876474319,-0.032751267\O,-1.1284132206,2.348
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33e-06\Thermal=0.\Dipole=-1.7277952,1.0054263,0.3095872\PG=C01 [X(C31H
44N6O6S1)]\@

TS11

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0.00000085,-0.00000176,-0.00000109\@

FIN 11

1\1\GINC-A06\FOpt\RB3PW91\6-31G(d)\C31H44N6O6S1\SHUBINA\05-Aug-2008\O\
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3\C,3.9056194771,-3.5385160081,-0.7202961634\C,1.5990523676,-4.0064297
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Init 12

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TS12

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Fin 12

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3-TABDa

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Catalyst1\O,1\C,0,4.38453,-0.10633,0.05509\C,0,2.89478,-0.05048,-0.30
81\C,0,2.21958,-1.41577,-0.06976\C,0,2.95213,-2.52798,-0.8328\C,0,4.43
979,-2.57105,-0.48169\C,0,5.09974,-1.21296,-0.72581\N,0,0.82973,-1.309
19,-0.47988\C,0,-0.21195,-1.89839,0.14602\S,0,-0.04004,-3.00649,1.4120
1\N,0,-1.42782,-1.50602,-0.33021\C,0,-2.71528,-2.07181,0.05621\C,0,-3.
73801,-0.94696,0.13203\C,0,-3.09438,-3.2467,-0.84405\C,0,-3.54778,0.06
901,1.07991\C,0,-4.44964,1.12164,1.19257\C,0,-5.56365,1.18223,0.35275\
C,0,-5.76335,0.18089,-0.59242\C,0,-4.8568,-0.87606,-0.701\N,0,2.20357,
1.05996,0.35461\C,0,1.27429,1.7997,-0.36336\N,0,0.81752,2.96544,0.2354
9\C,0,0.90598,3.21144,1.66654\C,0,2.11835,2.53458,2.27788\C,0,2.15604,
1.09024,1.80973\C,0,-0.26253,3.67357,-0.43506\C,0,-0.02056,3.66855,-1.
93471\C,0,0.09386,2.21998,-2.39686\N,0,0.93333,1.39573,-1.55007\H,0,4.
51603,-0.30467,1.12813\H,0,4.83631,0.87229,-0.14771\H,0,2.82131,0.1741
,-1.37739\H,0,2.23317,-1.66095,1.00117\H,0,2.83087,-2.34926,-1.91127\H

,0.2.46289,-3.48168,-0.60619\H,0,4.94177,-3.35173,-1.06672\H,0,4.55887
,-2.84974,0.57562\H,0,5.06934,-0.97992,-1.80025\H,0,6.15929,-1.24123,-
0.44173\H,0,0.65189,-0.51495,-1.10864\H,0,-1.43749,-0.88909,-1.13313\H
,0,-3.17952,-2.94591,-1.89527\H,0,-4.04607,-3.69158,-0.53271\H,0,-2.31
68,-4.01215,-0.7682\H,0,-2.68047,0.02087,1.73486\H,0,-4.28966,1.89357,
1.94179\H,0,-6.27152,2.00275,0.44009\H,0,-6.62859,0.21627,-1.25003\H,0
,-5.03493,-1.65108,-1.44109\H,0,-0.00999,2.85386,2.16975\H,0,0.94832,4
.29762,1.82097\H,0,2.05806,2.5891,3.37061\H,0,3.0364,3.04171,1.95968\H
,0,1.28681,0.53422,2.19687\H,0,3.04753,0.59132,2.19505\H,0,-1.24077,3.
21966,-0.19921\H,0,-0.27823,4.69771,-0.04301\H,0,0.91056,4.20874,-2.14
582\H,0,-0.83331,4.18625,-2.45722\H,0,0.48762,2.18018,-3.42186\H,0,-0.
91452,1.77688,-2.44836\H,0,-2.55642,-2.46363,1.06806\Version=AM64L-G0
3RevD.02\State=1-A\HF=-1529.7549559\RMSD=4.106e-09\Thermal=0.\Dipole=-
0.0648415,3.0706615,-0.7545704\PG=C01 [X(C22H33N5S1)]\@

3TABD-b

1\1\FAU-CCC-CCDH159\SP\RB3PW91\6-31G(d)\C22H33N5S1\SHUBINA\10-Aug-2008
\0\#P B3PW91/6-31G(d) SCF=Tight Name=SHUBINA SCRF=(PCM,Solvent=THF)\
Catalyst2\0,1\C,0,4.11614,-0.7813,-0.39996\C,0,2.65994,-0.64929,-0.86
658\C,0,1.75119,-1.61578,-0.07974\C,0,2.23488,-3.04942,-0.33156\C,0,3.
68741,-3.21818,0.11971\C,0,4.61286,-2.21925,-0.57886\N,0,0.37725,-1.40
068,-0.52356\C,0,-0.7267,-1.75957,0.18889\S,0,-0.68622,-2.7018,1.58105
\N,0,-1.88588,-1.26877,-0.33922\C,0,-3.22802,-1.57769,0.14371\C,0,-4.1
0821,-0.34995,-0.04775\C,0,-3.75663,-2.86919,-0.47865\C,0,-3.69158,0.8
716,0.50087\C,0,-4.46681,2.01846,0.36757\C,0,-5.6798,1.96825,-0.32166\
C,0,-6.10456,0.76233,-0.87073\C,0,-5.32407,-0.38751,-0.73494\N,0,2.140
44,0.72832,-0.95344\C,0,2.02116,1.49533,0.21984\N,0,1.53747,2.79806,0.
05062\C,0,1.73299,3.53377,-1.18565\C,0,1.56452,2.62323,-2.38473\C,0,2.
46093,1.41261,-2.20311\C,0,1.51463,3.63895,1.23911\C,0,1.07325,2.82717
,2.4443\C,0,2.00748,1.63025,2.58969\N,0,2.25794,0.93107,1.34755\H,0,4.
17373,-0.48035,0.65057\H,0,4.74638,-0.08842,-0.97359\H,0,2.62317,-0.99
807,-1.9107\H,0,1.81977,-1.38888,0.98833\H,0,2.14142,-3.27769,-1.40411
\H,0,1.58057,-3.7411,0.20702\H,0,4.02176,-4.24556,-0.0718\H,0,3.7444,-
3.06901,1.20721\H,0,4.6592,-2.45982,-1.65216\H,0,5.6375,-2.31031,-0.19
616\H,0,0.28677,-0.54387,-1.0648\H,0,-1.83975,-0.87056,-1.2694\H,0,-3.
85774,-2.78453,-1.56749\H,0,-4.73229,-3.13939,-0.06005\H,0,-3.05603,-3
.67848,-0.25489\H,0,-2.74637,0.91255,1.03726\H,0,-4.1273,2.95391,0.805
98\H,0,-6.28823,2.86305,-0.42656\H,0,-7.04755,0.71023,-1.40961\H,0,-5.
6756,-1.31854,-1.1697\H,0,2.73352,4.0048,-1.21256\H,0,0.99952,4.34986,
-1.21172\H,0,1.82642,3.15812,-3.30447\H,0,0.51958,2.3001,-2.46336\H,0,
3.52002,1.72392,-2.24126\H,0,2.31047,0.70146,-3.02256\H,0,2.5072,4.087
73,1.42376\H,0,0.81982,4.46587,1.04502\H,0,0.04429,2.48174,2.28603\H,0
,1.07951,3.45033,3.34628\H,0,1.59341,0.91051,3.30754\H,0,2.97026,1.958
38,3.01338\H,0,-3.10476,-1.75405,1.21957\Version=AM64L-G03RevD.02\Sta
te=1-A\HF=-1529.7446412\RMSD=8.195e-09\Thermal=0.\Dipole=0.2504432,2.9
391154,-2.6529998\PG=C01 [X(C22H33N5S1)]\@

Init13

1\1\FAU-CCC-CCDH158\SP\RB3PW91\6-31G(d)\C37H52N6O6S1\SHUBINA\11-Aug-20
08\0\#P B3PW91/6-31G(d) SCF=Tight Name=SHUBINA SCRF=(PCM,Solvent=THF)
\Aza INIT 1R\0,1\C,0,-1.52159,4.68467,-2.32805\C,0,-1.41721,3.31906,
-1.63554\C,0,-1.69766,3.4669,-0.11687\C,0,-0.7172,4.47895,0.4967\C,0,-
0.74763,5.82703,-0.22485\C,0,-0.50437,5.65742,-1.72487\N,0,-1.60805,2.
20228,0.58152\C,0,-2.64781,1.54307,1.15118\S,0,-4.27393,2.02768,0.9835
5\N,0,-2.27926,0.46171,1.87568\C,0,-3.19469,-0.46677,2.52069\C,0,-3.43
234,-1.72415,1.69481\C,0,-2.67811,-0.80722,3.92164\C,0,-4.73466,-2.141
99,1.40608\C,0,-4.96541,-3.31921,0.69353\C,0,-3.89282,-4.09277,0.25269
\C,0,-2.58702,-3.68075,0.52488\C,0,-2.36341,-2.50612,1.24161\N,0,-2.27
803,2.29511,-2.26601\C,0,-1.91895,0.98457,-2.24834\N,0,-2.81025,0.0232
2,-2.59796\C,0,-4.23461,0.32594,-2.68696\C,0,-4.40974,1.66881,-3.35991
\C,0,-3.65544,2.71088,-2.56063\C,0,-2.48131,-1.40306,-2.51728\C,0,-0.9
9975,-1.6514,-2.72687\C,0,-0.2273,-0.74768,-1.79006\N,0,-0.65953,0.632
65,-1.96972\H,0,-2.52278,5.11569,-2.19663\H,0,-1.35497,4.56283,-3.4062
3\H,0,-0.37838,3.0128,-1.76046\H,0,-2.72626,3.82083,0.01809\H,0,0.2938
4,4.05451,0.44518\H,0,-0.96648,4.60183,1.55716\H,0,0.00313,6.49843,0.2
1001\H,0,-1.7248,6.30759,-0.06898\H,0,0.51247,5.27672,-1.89234\H,0,-0.

57204,6.6245,-2.23857\H,0,-0.66868,1.81586,0.73263\H,0,-1.27922,0.2559
1,1.91614\H,0,-1.70474,-1.30974,3.87645\H,0,-3.37571,-1.48242,4.42772\
H,0,-2.57201,0.1037,4.52028\H,0,-5.57441,-1.53604,1.7394\H,0,-5.98607,
-3.62914,0.48064\H,0,-4.0713,-5.01092,-0.30208\H,0,-1.73568,-4.25813,0
.17429\H,0,-1.33983,-2.19673,1.4383\H,0,-4.68473,0.32548,-1.68422\H,0,
-4.69934,-0.47364,-3.27241\H,0,-5.46841,1.94493,-3.39885\H,0,-4.03444,
1.61826,-4.38936\H,0,-4.17331,2.9036,-1.6118\H,0,-3.60844,3.6403,-3.13
218\H,0,-2.80301,-1.79935,-1.5453\H,0,-3.07004,-1.90863,-3.29123\H,0,-
0.72397,-1.44308,-3.76777\H,0,-0.77072,-2.69961,-2.51262\H,0,0.84626,-
0.77332,-1.99367\H,0,-0.3668,-1.04889,-0.7465\H,0,-4.14502,0.06658,2.6
1244\H,0,0.00534,1.30777,-1.56742\C,0,2.7544,0.76915,0.49888\C,0,1.779
81,0.25142,1.36889\C,0,2.48928,1.68275,-0.53617\O,0,0.5484,0.4463,1.38
926\O,0,2.34453,-0.58884,2.31245\O,0,1.39262,2.15079,-0.91822\O,0,3.63
79,2.0809,-1.16977\C,0,1.47457,-1.09482,3.32291\C,0,2.33349,-1.72131,4
.40351\C,0,3.48628,3.00503,-2.2415\C,0,4.86096,3.2387,-2.83564\H,0,3.7
8889,0.50589,0.67651\H,0,0.79318,-1.83496,2.88535\H,0,0.86662,-0.27733
,3.72541\H,0,3.01048,-0.97957,4.83977\H,0,2.93634,-2.54372,4.00401\H,0
,1.69955,-2.12186,5.20239\H,0,3.05185,3.94103,-1.86792\H,0,2.79099,2.6
0227,-2.98829\H,0,5.28598,2.30219,-3.21144\H,0,5.54501,3.64562,-2.0838
6\H,0,4.79918,3.94925,-3.66757\C,0,7.72712,-3.16759,1.19574\C,0,6.8614
4,-2.21051,1.7214\C,0,5.49542,-2.29663,1.4722\C,0,4.97514,-3.34369,0.6
9103\C,0,5.86103,-4.30373,0.16764\C,0,7.22276,-4.21445,0.41868\C,0,3.5
3717,-3.37412,0.47207\C,0,2.8514,-4.28881,-0.23325\N,0,1.42319,-4.1842
4,-0.36292\O,0,0.87725,-5.01594,-1.08961\O,0,0.82376,-3.29293,0.23865\
H,0,8.79477,-3.10144,1.38848\H,0,7.24955,-1.39468,2.32495\H,0,4.81258,
-1.55545,1.88003\H,0,5.48297,-5.12221,-0.43871\H,0,7.89743,-4.96126,0.
00875\H,0,2.96269,-2.56816,0.92669\H,0,3.24241,-5.14358,-0.76761\\Vers
ion=AM64L-G03RevD.02\State=1-A\HF=-2618.4178756\RMSD=7.839e-09\Thermal
=0.\Dipole=1.2538443,-0.8539138,-2.4491173\PG=C01 [X(C37H52N6O6S1)]\@

TS13

1\1\FAU-CCC-CCDH160\SP\RB3PW91\6-31G(d)\C37H52N6O6S1\SHUBINA\11-Aug-20
08\0\#P B3PW91/6-31G(d) SCF=Tight Name=SHUBINA SCRF=(PCM,Solvent=THF)
\Aza TS1 R\0,1\C,0,-1.017792,4.300402,-1.222357\C,0,-1.185187,2.8401
64,-0.780976\C,0,-1.799051,2.724657,0.637084\C,0,-1.058566,3.616964,1.
645671\C,0,-0.891094,5.056773,1.161899\C,0,-0.199509,5.090996,-0.20060
2\N,0,-1.773427,1.342283,1.071635\C,0,-2.855338,0.570687,1.351106\O,0,
-4.455318,1.143641,1.196476\N,0,-2.557821,-0.678838,1.760701\C,0,-3.53
1692,-1.681494,2.182606\C,0,-3.920098,-2.62949,1.053537\C,0,-2.977573,
-2.417576,3.405122\C,0,-5.215746,-2.589881,0.528514\C,0,-5.606638,-3.4
68461,-0.482317\C,0,-4.702549,-4.402595,-0.9843\C,0,-3.404688,-4.44599
8,-0.472213\C,0,-3.014762,-3.566027,0.536897\N,0,-1.981978,2.058702,-1
.758086\C,0,-1.700087,0.755336,-2.024692\N,0,-2.646761,-0.050843,-2.56
1564\C,0,-4.041611,0.377637,-2.607541\C,0,-4.073348,1.810783,-3.089252\
C,0,-3.280631,2.653684,-2.111279\C,0,-2.395893,-1.460167,-2.868829\C,
0,-0.930271,-1.704641,-3.168724\C,0,-0.111423,-1.130545,-2.03134\N,0,-
0.474534,0.266161,-1.823298\H,0,-1.994754,4.791442,-1.311723\H,0,-0.54
9736,4.3246,-2.214646\H,0,-0.071793,2.416151,-0.727944\H,0,-2.852758,3
.019689,0.606763\H,0,-0.070718,3.179014,1.823932\H,0,-1.607642,3.58223
3,2.594143\H,0,-0.315286,5.628979,1.899809\H,0,-1.872875,5.54715,1.083
78\H,0,0.809195,4.663434,-0.115515\H,0,-0.078605,6.123646,-0.55042\H,0
, -0.840875,0.982593,1.273185\H,0,-1.589174,-1.012547,1.705193\H,0,-2.0
07297,-2.876689,3.188354\H,0,-3.670302,-3.203818,3.722253\H,0,-2.83939
4,-1.715153,4.233658\H,0,-5.918947,-1.856185,0.91486\H,0,-6.621076,-3.
42564,-0.872401\H,0,-5.006993,-5.096417,-1.764594\H,0,-2.693542,-5.176
095,-0.852878\H,0,-1.998168,-3.60399,0.91958\H,0,-4.506131,0.281623,-1
.616665\H,0,-4.56242,-0.289403,-3.300125\H,0,-5.099963,2.188804,-3.129
65\H,0,-3.650116,1.870972,-4.099303\H,0,-3.867638,2.782342,-1.193671\H
,0,-3.092694,3.63787,-2.547693\H,0,-2.729052,-2.082196,-2.02751\H,0,-3
.016507,-1.715075,-3.735264\H,0,-0.65213,-1.227212,-4.116192\H,0,-0.75
1667,-2.780215,-3.265597\H,0,0.95624,-1.128013,-2.257386\H,0,-0.266877
, -1.692704,-1.101971\H,0,-4.428258,-1.126184,2.471202\H,0,0.296885,0.8
36839,-1.479149\C,0,3.422365,0.799521,0.569681\C,0,2.329408,1.194112,1
.424548\C,0,3.290944,0.899146,-0.864401\O,0,1.143761,1.27986,1.101739\
O,0,2.762577,1.41627,2.687759\O,0,2.261421,0.868301,-1.541404\O,0,4.50
8927,0.996236,-1.456917\C,0,1.762225,1.608688,3.696645\C,0,2.450466,1.
506811,5.041166\C,0,4.515503,1.039595,-2.886341\C,0,5.958247,1.163816,

-3.328468\H,0,4.417726,0.978598,0.959403\H,0,0.991201,0.842319,3.57834
\H,0,1.300413,2.593766,3.560254\H,0,3.248394,2.251124,5.134936\H,0,2.8
85163,0.511336,5.174042\H,0,1.725459,1.675043,5.845018\H,0,3.909713,1.
887262,-3.226992\H,0,4.050534,0.128301,-3.279917\H,0,6.544532,0.310698
,-2.973663\H,0,6.409613,2.079402,-2.932859\H,0,6.015431,1.195863,-4.42
2223\C,0,6.956844,-2.688342,-0.895659\C,0,6.986414,-2.139486,0.385615\
C,0,5.809027,-1.70456,0.98522\C,0,4.576215,-1.81012,0.323834\C,0,4.562
894,-2.360196,-0.966847\C,0,5.739508,-2.795361,-1.568686\C,0,3.352832,
-1.375023,1.026317\C,0,2.103233,-1.899219,0.710283\N,0,1.039361,-1.784
224,1.576526\O,0,-0.098991,-2.157292,1.155448\O,0,1.185239,-1.355696,2
.734998\H,0,7.874363,-3.032829,-1.365823\H,0,7.92837,-2.053326,0.92130
9\H,0,5.836892,-1.280012,1.986361\H,0,3.625339,-2.449185,-1.508136\H,0
,5.705872,-3.224624,-2.567148\H,0,3.488663,-1.108606,2.070769\H,0,1.84
3789,-2.350876,-0.233614\Version=AM64L-G03RevD.02\State=1-A\HF=-2618.
3975699\RMSD=5.562e-09\Thermal=0.\Dipole=0.5743984,0.5179885,-4.208538
6\PG=C01 [X(C37H52N6O6S1)]\@

Fin13

1\1\FAU-CCC-CCDH160\SP\RB3PW91\6-31G(d)\C37H52N6O6S1\SHUBINA\11-Aug-20
08\0\#P B3PW91\6-31G(d) SCF=Tight Name=SHUBINA SCRF=(PCM,Solvent=THF)
\Aza Fin 1R\0,1\C,0,-0.54226,4.11248,-1.32218\C,0,-0.90398,2.70364,-
0.83605\C,0,-1.40798,2.70245,0.62987\C,0,-0.42282,3.44228,1.5477\C,0,-
0.06448,4.83597,1.03201\C,0,0.48597,4.75977,-0.3921\N,0,-1.60021,1.344
33,1.0821\C,0,-2.7797,0.79166,1.46199\S,0,-4.26921,1.62951,1.40602\N,0
, -2.65503,-0.47964,1.89012\C,0,-3.74066,-1.32144,2.36352\C,0,-4.18789,
-2.33366,1.31583\C,0,-3.31986,-2.00747,3.66739\C,0,-5.51324,-2.34411,0
.87101\C,0,-5.95138,-3.29032,-0.05629\C,0,-5.06481,-4.2434,-0.55323\C,
0,-3.73676,-4.2365,-0.12245\C,0,-3.29955,-3.28884,0.80204\N,0,-1.88472
,2.04267,-1.73191\C,0,-1.80561,0.71825,-2.02299\N,0,-2.89759,0.03895,-
2.4418\C,0,-4.22001,0.65185,-2.35665\C,0,-4.10713,2.07711,-2.85214\C,0
, -3.1202,2.80848,-1.96445\C,0,-2.86791,-1.40319,-2.69586\C,0,-1.49175,
-1.85992,-3.14241\C,0,-0.46929,-1.35939,-2.14279\N,0,-0.63007,0.08211,
-1.9788\H,0,-1.43267,4.75399,-1.33817\H,0,-0.16812,4.05399,-2.35272\H,
0,0.02472,2.12794,-0.84575\H,0,-2.38361,3.19688,0.68169\H,0,0.49651,2.
85176,1.63387\H,0,-0.87291,3.49692,2.54618\H,0,0.67383,5.29621,1.69972
\H,0,-0.95259,5.48574,1.04846\H,0,1.41354,4.17309,-0.38915\H,0,0.7356,
5.76062,-0.7665\H,0,-0.73813,0.80048,1.26084\H,0,-1.74027,-0.93458,1.7
245\H,0,-2.43204,-2.63249,3.51777\H,0,-4.12615,-2.64772,4.04112\H,0,-3
.08438,-1.2556,4.42774\H,0,-6.2068,-1.59934,1.25494\H,0,-6.98779,-3.28
36,-0.38635\H,0,-5.40491,-4.9886,-1.26872\H,0,-3.03749,-4.97812,-0.502
89\H,0,-2.25718,-3.28384,1.11332\H,0,-4.5927,0.62276,-1.32336\H,0,-4.8
9123,0.06113,-2.98675\H,0,-5.07448,2.58655,-2.79819\H,0,-3.77977,2.079
8,-3.89911\H,0,-3.5943,3.01004,-0.99627\H,0,-2.84382,3.75965,-2.42749\
H,0,-3.17768,-1.93832,-1.78898\H,0,-3.61333,-1.6071,-3.4725\H,0,-1.271
07,-1.46872,-4.14331\H,0,-1.47119,-2.95306,-3.19411\H,0,0.5517,-1.5168
6,-2.49706\H,0,-0.57343,-1.84384,-1.16221\H,0,-4.57868,-0.64805,2.5648
8\H,0,0.20423,0.55989,-1.66062\C,0,3.64225,0.10784,0.45645\C,0,3.14004
,1.19623,1.39628\C,0,3.28017,0.48806,-0.96388\O,0,2.71576,2.27273,1.02
9\O,0,3.41686,0.88613,2.66735\O,0,2.18104,0.41045,-1.47716\O,0,4.35603
,0.93717,-1.62256\C,0,2.95312,1.81662,3.66102\C,0,3.42929,1.31837,5.00
771\C,0,4.13941,1.37665,-2.97594\C,0,5.46637,1.86605,-3.51242\H,0,4.73
549,0.17169,0.52566\H,0,1.86123,1.85367,3.60464\H,0,3.34428,2.81202,3.
42664\H,0,4.52258,1.27101,5.04615\H,0,3.03069,0.32051,5.21525\H,0,3.08
665,1.99655,5.79666\H,0,3.38059,2.16608,-2.96997\H,0,3.74354,0.53846,-
3.55928\H,0,6.21181,1.06486,-3.50097\H,0,5.84561,2.69945,-2.91305\H,0,
5.34565,2.21073,-4.54502\C,0,6.18047,-4.01562,-0.95165\C,0,6.33863,-3.
60473,0.37052\C,0,5.3974,-2.76113,0.95816\C,0,4.28405,-2.31328,0.24027
\C,0,4.1358,-2.73464,-1.08658\C,0,5.07443,-3.57748,-1.67842\C,0,3.2880
9,-1.36019,0.88519\C,0,1.89394,-1.85501,0.65987\N,0,0.81674,-1.22034,1
.07401\O,0,-0.34705,-1.77157,0.95424\O,0,0.88661,-0.0367,1.57546\H,0,6
.91139,-4.67619,-1.41126\H,0,7.19352,-3.94569,0.94946\H,0,5.5247,-2.44
838,1.99283\H,0,3.26951,-2.40301,-1.65443\H,0,4.93973,-3.89582,-2.7096
\H,0,3.49741,-1.34956,1.96474\H,0,1.72023,-2.86095,0.30538\Version=AM
64L-G03RevD.02\State=1-A\HF=-2618.4246743\RMSD=4.231e-09\Thermal=0.\Di
pole=1.3946914,-0.0084721,-4.0059284\PG=C01 [X(C37H52N6O6S1)]\@

Init14

1\1\FAU-CCC-CCDH161\SP\RB3PW91\6-31G(d)\C37H52N6O6S1\SHUBINA\11-Aug-20
08\0\#P B3PW91/6-31G(d) SCF=Tight Name=SHUBINA SCRf=(PCM,Solvent=THF)
\Aza INIT S\0,1\C,0,-1.41439,2.71099,0.99516\C,0,-0.25724,3.38728,1.74534\C,0,
-0.20604,4.89579,1.50517\C,0,-0.15199,5.21827,0.01127\N,0,-1.37303,1.2
7769,1.18694\C,0,-2.36803,0.5447,1.76094\S,0,-3.9087,1.1803,2.13123\N,
0,-2.02307,-0.73329,1.9996\C,0,-2.87066,-1.71849,2.65559\C,0,-3.67772,
-2.55805,1.67371\C,0,-1.99828,-2.59435,3.55994\C,0,-5.06924,-2.62047,1
.78318\C,0,-5.81886,-3.43086,0.93007\C,0,-5.18256,-4.1907,-0.04915\C,0
, -3.79343,-4.12675,-0.17298\C,0,-3.04473,-3.31474,0.67854\N,0,-2.44141
,2.41263,-1.26876\C,0,-2.28106,1.15338,-1.75201\N,0,-3.35106,0.3782,-2
.03119\C,0,-4.68303,0.77458,-1.58072\C,0,-4.85163,2.25379,-1.85355\C,0
, -3.77528,3.00834,-1.09799\C,0,-3.21438,-1.00307,-2.49968\C,0,-1.90952
, -1.21948,-3.24374\C,0,-0.76973,-0.69042,-2.39525\N,0,-1.05755,0.6923,
-2.03484\H,0,-2.26252,5.0432,-0.31352\H,0,-1.31571,4.81842,-1.78982\H,
0,-0.39878,2.71866,-0.89727\H,0,-2.36764,3.06154,1.40781\H,0,0.6864,2.
92383,1.42953\H,0,-0.36533,3.16415,2.81251\H,0,0.66238,5.32547,2.01985
\H,0,-1.09532,5.37078,1.9448\H,0,0.78429,4.83282,-0.4173\H,0,-0.14997,
6.30315,-0.15133\H,0,-0.43183,0.86661,1.26711\H,0,-1.10861,-1.0621,1.6
627\H,0,-1.22979,-3.11536,2.97887\H,0,-2.61299,-3.34468,4.06783\H,0,-1
.49723,-1.97789,4.31363\H,0,-5.569,-2.02037,2.54007\H,0,-6.90115,-3.46
7,1.03195\H,0,-5.76312,-4.82969,-0.71066\H,0,-3.28868,-4.72084,-0.9324
4\H,0,-1.96332,-3.25449,0.56903\H,0,-4.80593,0.55129,-0.51205\H,0,-5.4
0549,0.18049,-2.14791\H,0,-5.83203,2.60175,-1.51305\H,0,-4.78186,2.440
8,-2.93218\H,0,-4.02004,3.01224,-0.02844\H,0,-3.73078,4.04083,-1.45593
\H,0,-3.28814,-1.68178,-1.64014\H,0,-4.06892,-1.20613,-3.15499\H,0,-1.
93088,-0.69693,-4.20749\H,0,-1.77787,-2.28801,-3.44096\H,0,-0.61826,-1
.2906,-1.48844\H,0,0.1654,-0.67797,-2.96048\H,0,-3.57691,-1.15447,3.27
196\H,0,-0.24001,1.26562,-1.85762\C,0,2.37387,-1.48641,0.99072\C,0,1.3
2585,-2.30976,0.53423\C,0,2.17819,-0.27671,1.68251\O,0,0.09176,-2.1312
8,0.58087\O,0,1.81772,-3.46102,-0.04256\O,0,1.13339,0.3186,1.98259\O,0
,3.3963,0.2826,2.06775\C,0,0.86171,-4.4193,-0.47103\C,0,1.62562,-5.602
35,-1.03345\C,0,3.31669,1.45561,2.874\C,0,4.68146,1.69476,3.48999\H,0,
3.38307,-1.86469,0.88901\H,0,0.19833,-3.98224,-1.22945\H,0,0.22822,-4.
72276,0.37211\H,0,2.27555,-6.04139,-0.26966\H,0,2.25262,-5.29477,-1.87
7\H,0,0.93047,-6.37484,-1.38153\H,0,2.54843,1.32093,3.64191\H,0,3.0095
1,2.31155,2.25827\H,0,5.44594,1.84546,2.71994\H,0,4.98117,0.84261,4.10
902\H,0,4.65729,2.58854,4.12384\C,0,8.40934,-0.5059,-0.75242\C,0,7.491
83,-0.56292,0.29501\C,0,6.17362,-0.16849,0.08944\C,0,5.75348,0.28336,-
1.17487\C,0,6.69161,0.33857,-2.22335\C,0,8.00583,-0.05186,-2.01161\C,0
,4.36039,0.66957,-1.32701\C,0,3.75572,1.00663,-2.48193\N,0,2.36617,1.3
3071,-2.51403\O,0,1.8445,1.43674,-3.62559\O,0,1.74431,1.47587,-1.45207
\H,0,9.43983,-0.81219,-0.59185\H,0,7.80214,-0.91537,1.27482\H,0,5.4497
3,-0.20841,0.90005\H,0,6.39429,0.69532,-3.20569\H,0,8.72208,-0.0029,-2
.82739\H,0,3.75167,0.65887,-0.42519\H,0,4.18781,1.00826,-3.47284\\Vers
ion=AM64L-G03RevD.02\State=1-A\HF=-2618.4102567\RMSD=5.750e-09\Thermal
=0\Dipole=0.9866721,1.1740434,-3.8842565\PG=C01 [X(C37H52N6O6S1)]\@

TS14

1\1\FAU-CCC-CCDH162\SP\RB3PW91\6-31G(d)\C37H52N6O6S1\SHUBINA\11-Aug-20
08\0\#P B3PW91/6-31G(d) SCF=Tight Name=SHUBINA SCRf=(PCM,Solvent=THF)
\Aza_TS1 S\0,1\C,0,-1.371704,4.591875,-0.998584\C,0,-1.43054,3.07861
2,-0.745781\C,0,-1.005687,2.740367,0.707883\C,0,0.371618,3.350498,1.01
4923\C,0,0.443744,4.845513,0.70954\C,0,0.037596,5.126765,-0.736774\N,0,
-0.950436,1.309704,0.932942\C,0,-1.805588,0.588023,1.704386\S,0,-3.23
6457,1.228239,2.373182\N,0,-1.416749,-0.690099,1.88023\C,0,-2.129527,-
1.690874,2.657626\C,0,-2.996256,-2.593368,1.788554\C,0,-1.12142,-2.497
409,3.481595\C,0,-4.36264,-2.72271,2.052075\C,0,-5.160216,-3.5798,1.29
2638\C,0,-4.59886,-4.319366,0.253587\C,0,-3.236418,-4.191091,-0.022958
\C,0,-2.441337,-3.334537,0.736865\N,0,-2.758117,2.511475,-1.077025\C,0
, -2.883958,1.22977,-1.514578\N,0,-4.097945,0.622426,-1.527209\C,0,-5.2
37629,1.207072,-0.830275\C,0,-5.229273,2.701771,-1.053163\C,0,-3.91115
,3.257129,-0.555516\C,0,-4.232208,-0.795711,-1.866084\C,0,-3.219905,-1
.203006,-2.91851\C,0,-1.841617,-0.81933,-2.425612\N,0,-1.832243,0.5830
82,-2.024385\H,0,-2.057668,5.127011,-0.329634\H,0,-1.689563,4.79958,-2
.028294\H,0,-0.693464,2.640899,-1.422104\H,0,-1.755185,3.147508,1.3971

02\H,0,1.122617,2.822834,0.411993\H,0,0.61169,3.146258,2.063986\H,0,1.459079,5.213906,0.902016\H,0,-0.222788,5.398467,1.387733\H,0,0.751889,4.650233,-1.422593\H,0,0.065638,6.203236,-0.945946\H,0,-0.035786,0.880215,0.784085\H,0,-0.541428,-0.982659,1.437301\H,0,-0.405546,-3.016637,2.834258\H,0,-1.639353,-3.249929,4.085037\H,0,-0.561228,-1.832225,4.146492\H,0,-4.805301,-2.139701,2.856598\H,0,-6.221173,-3.668696,1.514797\H,0,-5.216554,-4.992943,-0.335774\H,0,-2.789102,-4.767794,-0.82978\H,0,-1.383156,-3.230568,0.506142\H,0,-5.185483,0.966908,0.240698\H,0,-6.141009,0.751168,-1.248094\H,0,-6.047337,3.178055,-0.503154\H,0,-5.366882,2.919224,-2.119434\H,0,-3.884014,3.223547,0.541287\H,0,-3.814392,4.294436,-0.881949\H,0,-4.115662,-1.405604,-0.960041\H,0,-5.253954,-0.939048,-2.23386\H,0,-3.439039,-0.700194,-3.868061\H,0,-3.277687,-2.283174,-3.084534\H,0,-1.538498,-1.443534,-1.57617\H,0,-1.080243,-0.917043,-3.202726\H,0,-2.788611,-1.139447,3.33434\H,0,-0.883368,0.962173,-1.935319\O,0,2.912689,-1.256316,0.591447\O,0,1.86166,-1.985332,-0.067083\O,0,2.62034,-0.379641,1.697906\O,0,0.64118,-1.857448,0.051643\O,0,2.387936,-2.880821,-0.946071\O,0,1.569638,0.21475,1.932244\O,0,3.717176,-0.201426,2.485248\O,0,1.454747,-3.638016,-1.721554\O,0,2.249803,-4.598105,-2.581717\O,0,3.554495,0.696648,3.587563\O,0,4.860955,0.716627,4.352955\H,0,3.882025,-1.737657,0.602667\H,0,0.855177,-2.953674,-2.33197\H,0,0.772928,-4.172845,-1.050443\H,0,2.855144,-5.267556,-1.962084\H,0,2.918568,-4.055657,-3.257729\H,0,1.571759,-5.208273,-3.188503\H,0,2.72145,0.356885,4.212959\H,0,3.288755,1.692132,3.212277\H,0,5.683464,1.049381,3.711696\H,0,5.106085,-0.281188,4.730642\H,0,4.786975,1.400261,5.205866\O,0,7.744574,0.017152,-0.667312\O,0,7.02996,1.013712,-0.005736\O,0,5.643401,1.070343,-0.1172\O,0,4.94614,0.141988,-0.903334\O,0,5.677305,-0.862824,-1.557416\O,0,7.060913,-0.924025,-1.439086\O,0,3.485449,0.267733,-1.040221\O,0,2.860241,-0.034699,-2.242381\N,0,1.570629,0.365311,-2.502394\O,0,1.040044,0.029888,-3.580533\O,0,0.948298,1.077487,-1.657398\H,0,8.826817,-0.031292,-0.578383\H,0,7.552796,1.749229,0.600509\H,0,5.089483,1.849149,0.400681\H,0,5.151551,-1.616533,-2.136925\H,0,7.610002,-1.712267,-1.948097\H,0,3.005612,1.03686,-0.444718\H,0,3.288972,-0.630614,-3.033947\Version=AM64L-G03RevD.02\State=1-A\HF=-2618.4011773\RMSD=7.874e-09\Thermal=0.\Dipole=-1.153963,0.4305293,-1.4879182\PG=C01 [X(C37H52N6O6S1)]\@

Fin14

1\1\FAU-CCC-CCDH154\SP\RB3PW91\6-31G(d)\C37H52N6O6S1\SHUBINA\11-Aug-2008\0\#P B3PW91/6-31G(d) SCF=Tight Name=SHUBINA SCRF=(PCM,Solvent=THF)\Aza Fin 1S\0,1\O,0,2.25971,4.48255,-0.12184\O,0,2.00164,2.968,-0.08648\O,0,1.2716,2.47225,-1.3607\O,0,-0.00015,3.30109,-1.60205\O,0,0.26803,4.80592,-1.61947\O,0,0.95304,5.25155,-0.32761\N,0,0.9319,1.06805,-1.23826\O,0,1.35352,0.06049,-2.03894\O,0,2.50883,0.26159,-3.27224\N,0,0.76526,-1.1303,-1.77909\O,0,1.15133,-2.39721,-2.38321\O,0,2.21506,-3.1193,-1.56483\O,0,-0.09346,-3.26181,-2.59404\O,0,3.42345,-3.49793,-2.15486\O,0,4.39376,-4.18299,-1.42295\O,0,4.16781,-4.49645,-0.08439\O,0,2.96603,-4.11667,0.51669\O,0,1.99855,-3.43268,-0.2171\N,0,3.24353,2.21185,0.1623\O,0,3.32726,1.24029,1.10549\N,0,4.51814,0.60981,1.32169\O,0,5.67434,0.77247,0.44716\O,0,5.66169,2.13369,-0.21322\O,0,4.30231,2.33599,-0.84707\O,0,4.59633,-0.52509,2.24041\O,0,3.68402,-0.30778,3.43424\O,0,2.28157,-0.07943,2.91469\N,0,2.28325,0.94231,1.87577\H,0,2.94288,4.75031,-0.9389\H,0,2.747,4.77954,0.81504\H,0,1.32607,2.79782,0.75392\H,0,1.93742,2.55717,-2.22718\H,0,-0.71515,3.067,-0.80236\H,0,-0.44765,2.97168,-2.54711\H,0,-0.67492,5.34858,-1.75963\H,0,0.90703,5.06081,-2.47809\H,0,0.28191,5.0745,0.52408\H,0,1.1606,6.32862,-0.34956\H,0,0.27579,0.85658,-0.4806\H,0,0.02561,-1.16861,-1.08001\H,0,-0.57429,-3.50572,-1.64052\H,0,0.18156,-4.20084,-3.08524\H,0,-0.82063,-2.73133,-3.21676\H,0,3.60866,-3.24188,-3.1954\H,0,5.3281,-4.46936,-1.90025\H,0,4.91983,-5.03574,0.48696\H,0,2.77834,-4.36476,1.55952\H,0,1.06699,-3.1343,0.25901\H,0,5.67822,-0.02217,-0.31362\H,0,6.57185,0.64417,1.06343\H,0,6.44383,2.18184,-0.97778\H,0,5.85941,2.91824,0.52707\H,0,4.12465,1.61491,-1.65736\H,0,4.23274,3.33455,-1.27881\H,0,4.33831,-1.45694,1.71579\H,0,5.64154,-0.60491,2.55782\H,0,4.02638,0.55954,4.01118\H,0,3.71058,-1.18214,4.09265\H,0,1.87835,-1.01211,2.49486\H,0,1.58092,0.26297,3.68033\H,0,1.58429,-2.14755,-3.35622\H,0,1.30962,1.25722,1.64231\O,0,-3.36773,-0.91052,0.60794\O,0,-2.23,-1.81,1.06114\O,0,-3.70129,-1.19756,-0.84931\O,0,-1.13454,-1.87665,0.53707\O,0,-2.58322,-2.52754,2.13173\O,0,-3.00

566,-0.88258,-1.78845\O,0,-4.87023,-1.84636,-0.96079\C,0,-1.55995,-3.3
5945,2.71357\C,0,-2.15667,-4.0243,3.93401\C,0,-5.29272,-2.14181,-2.307
56\C,0,-6.63996,-2.82376,-2.22266\H,0,-4.24178,-1.12981,1.22467\H,0,-0
.70383,-2.72652,2.9673\H,0,-1.23257,-4.08931,1.96551\H,0,-3.02018,-4.6
3973,3.66274\H,0,-2.47882,-3.27708,4.6656\H,0,-1.40912,-4.67006,4.4070
2\H,0,-4.53681,-2.77701,-2.78139\H,0,-5.33828,-1.20481,-2.87166\H,0,-7
.37694,-2.17352,-1.74111\H,0,-6.57385,-3.75451,-1.65024\H,0,-6.99787,-
3.0639,-3.22956\C,0,-6.29259,3.17722,-0.0923\C,0,-5.27413,2.99827,-1.0
255\C,0,-4.19551,2.16355,-0.7342\C,0,-4.11249,1.49864,0.49413\C,0,-5.1
4395,1.68552,1.42267\C,0,-6.22372,2.51592,1.13397\C,0,-2.93291,0.58147
,0.78811\C,0,-2.31122,0.79196,2.13045\N,0,-1.04882,1.16045,2.27981\O,0
,0.51901,1.30274,3.41683\O,0,-0.30351,1.39456,1.21982\H,0,-7.13358,3.
82891,-0.31607\H,0,-5.31529,3.51027,-1.98405\H,0,-3.40746,2.01977,-1.4
6918\H,0,-5.10021,1.18592,2.38788\H,0,-7.01199,2.65096,1.87084\H,0,-2.
15898,0.76484,0.0405\H,0,-2.84252,0.64296,3.06071\\Version=AM64L-G03Re
vD.02\State=1-A\HF=-2618.4309272\RMSD=4.123e-09\Thermal=0.\Dipole=1.49
14125,-1.1423334,1.5656164\PG=C01 [X(C37H52N6O6S1)]\@

Init15

1\1\FAU-CCC-CCDH158\SP\RB3PW91\6-31G(d)\C37H52N6O6S1\SHUBINA\11-Aug-20
08\0\#P B3PW91/6-31G(d) SCF=Tight Name=SHUBINA SCRF=(PCM,Solvent=THF)
\Aza INIT 2R\O,1\C,0,-1.40786,4.6967,-0.64071\C,0,-1.42909,3.17113,-
0.48086\C,0,-1.09332,2.74565,0.97104\C,0,0.23797,3.37379,1.41355\C,0,0
.27399,4.88814,1.21177\C,0,-0.04202,5.25654,-0.23774\N,0,-1.02058,1.30
297,1.08098\C,0,-1.867,0.53155,1.8151\S,0,-3.26732,1.13738,2.58053\N,0
,-1.49582,-0.76184,1.87815\C,0,-2.20143,-1.79807,2.61623\C,0,-3.17862,
-2.57947,1.7471\C,0,-1.17754,-2.72436,3.27927\C,0,-4.51839,-2.69666,2.
12623\C,0,-5.41209,-3.45727,1.37154\C,0,-4.97461,-4.11171,0.22196\C,0,
-3.63996,-3.99247,-0.17049\C,0,-2.74834,-3.22983,0.5832\N,0,-2.70652,2
.58086,-0.94149\C,0,-2.74422,1.36466,-1.54295\N,0,-3.89519,0.65605,-1.
58449\C,0,-5.0358,1.05636,-0.76446\C,0,-5.19398,2.55687,-0.87693\C,0,-
3.91611,3.21092,-0.39024\C,0,-3.98708,-0.67135,-2.19695\C,0,-2.92437,-
0.87705,-3.25899\C,0,-1.57917,-0.48412,-2.68363\N,0,-1.66573,0.88023,-
2.17272\H,0,-2.16651,5.16355,0.00051\H,0,-1.65198,4.95758,-1.67851\H,0
,0.62616,2.79376,-1.11453\H,0,-1.89489,3.08076,1.63925\H,0,1.05364,2.
90324,0.85036\H,0,0.40416,3.11339,2.46463\H,0,1.25883,5.2767,1.49986\H
,0,-0.45773,5.37102,1.87626\H,0,0.73389,4.84965,-0.90104\H,0,-0.03759,
6.34536,-0.37199\H,0,-0.09311,0.89323,0.90774\H,0,-0.69339,-1.06301,1.
30942\H,0,-0.53905,-3.20584,2.53066\H,0,-1.68803,-3.50911,3.84711\H,0,
-0.53684,-2.15478,3.96052\H,0,-4.86429,-2.18029,3.0188\H,0,-6.45083,-3
.53766,1.68382\H,0,-5.66656,-4.71233,-0.36397\H,0,-3.2894,-4.50402,-1.
06476\H,0,-1.171245,-3.12633,0.26526\H,0,-4.87941,0.7505,0.27894\H,0,-5
.91341,0.53321,-1.1551\H,0,-6.0276,2.90787,-0.26029\H,0,-5.40591,2.828
69,-1.91832\H,0,-3.87,3.14529,0.70376\H,0,-3.90965,4.26424,-0.68324\H,
0,-3.90024,-1.43429,-1.41252\H,0,-4.98973,-0.75641,-2.63178\H,0,-3.145
37,-0.26655,-4.14294\H,0,-2.91903,-1.92723,-3.56769\H,0,-1.25908,-1.16
17,-1.88216\H,0,-0.79402,-0.4836,-3.4398\H,0,-2.77754,-1.28328,3.39053
\H,0,-0.79213,1.40131,-2.1818\C,0,2.64681,-1.61928,0.54881\C,0,1.54179
,-2.23954,-0.07932\C,0,2.57155,-0.38949,1.24448\O,0,0.33771,-1.92404,-
0.05849\O,0,1.9421,-3.35657,-0.77794\O,0,1.65786,0.44938,1.25524\O,0,3
.72395,-0.1413,1.94891\C,0,0.91832,-4.12114,-1.40148\C,0,1.58783,-5.27
302,-2.12498\C,0,3.75494,1.07252,2.692\C,0,5.04024,1.07918,3.49536\H,0
,3.57479,-2.17345,0.60076\H,0,0.35265,-3.48995,-2.09757\H,0,0.21205,-4
.48841,-0.64576\H,0,2.14835,-5.89931,-1.42331\H,0,2.28462,-4.90259,-2.
8843\H,0,0.83724,-5.89823,-2.62165\H,0,2.87406,1.13336,3.34153\H,0,3.7
0832,1.93161,2.00987\H,0,5.91102,1.01254,2.83507\H,0,5.06979,0.22868,4
.18419\H,0,5.11726,2.00177,4.08202\C,0,7.97088,-0.33659,-0.37052\C,0,7
.26753,-1.46898,-0.77992\C,0,5.94596,-1.3532,-1.19344\C,0,5.29922,-0.1
0531,-1.20332\C,0,6.02194,1.02725,-0.78814\C,0,7.34343,0.91103,-0.3768
\C,0,3.92866,-0.04405,-1.68561\C,0,3.15842,1.06522,-1.76727\N,0,1.8640
6,0.97635,-2.32741\O,0,1.49483,-0.06398,-2.87202\O,0,1.14231,1.99399,-
2.25116\H,0,9.00503,-0.42368,-0.04762\H,0,7.74936,-2.44292,-0.77517\H,
0,5.39143,-2.23531,-1.50358\H,0,5.55088,2.00593,-0.7949\H,0,7.88994,1.
79632,-0.06242\H,0,3.50498,-0.96189,-2.08057\H,0,3.38081,2.05004,-1.38
421\\Version=AM64L-G03RevD.02\State=1-A\HF=-2618.4050044\RMSD=3.042e-0
9\Thermal=0.\Dipole=-0.4722647,1.2991822,-2.968396\PG=C01 [X(C37H52N6O
6S1)]\@

TS15

1\1\FAU-CCC-CCDH162\SP\RB3PW91\6-31G(d)\C37H52N6O6S1\SHUBINA\11-Aug-20
08\0\#P B3PW91\6-31G(d) SCF=Tight Name=SHUBINA SCRF=(PCM,Solvent=THF)
\Aza_TS2 R\0,1\C,0,-1.230097,4.56121,-0.90321\C,0,-1.343768,3.056797
,-0.619384\C,0,-0.983753,2.718147,0.849214\C,0,0.38267,3.320296,1.2174
46\C,0,0.489542,4.809715,0.897961\C,0,0.173917,5.070423,-0.574103\N,0,
-0.937646,1.28182,1.053593\C,0,-1.786312,0.561623,1.832623\S,0,-3.1945
88,1.209846,2.537294\N,0,-1.405833,-0.722765,1.998239\C,0,-2.162366,-1
.732509,2.722059\C,0,-3.117876,-2.505708,1.821385\C,0,-1.186114,-2.667
592,3.440891\C,0,-4.472612,-2.598818,2.150518\C,0,-5.350651,-3.345187,
1.364296\C,0,-4.882085,-4.009033,0.232262\C,0,-3.531744,-3.914275,-0.1
10104\C,0,-2.656107,-3.16672,0.676147\N,0,-2.67457,2.526926,-0.996406\
C,0,-2.816625,1.31727,-1.597767\N,0,-4.029227,0.710794,-1.619191\C,0,-
5.10757,1.193523,-0.762572\C,0,-5.158202,2.701161,-0.878185\C,0,-3.819
716,3.25876,-0.435135\C,0,-4.268809,-0.568839,-2.287774\C,0,-3.231228,
-0.847805,-3.35905\C,0,-1.859765,-0.619329,-2.757842\N,0,-1.792588,0.7
35133,-2.226655\H,0,-1.943252,5.130112,-0.292398\H,0,-1.481821,4.74565
5,-1.955209\H,0,-0.592187,2.572981,-1.244409\H,0,-1.753832,3.115366,1.
51995\H,0,1.16167,2.777133,0.666436\H,0,0.566412,3.127481,2.28031\H,0,
1.496069,5.169229,1.146423\H,0,-0.20943,5.380184,1.527496\H,0,0.909819
,4.559565,-1.209884\H,0,0.239812,6.141405,-0.802776\H,0,-0.025076,0.85
1988,0.887337\H,0,-0.573522,-1.043896,1.498042\H,0,-0.528459,-3.175916
,2.726784\H,0,-1.735738,-3.432459,3.998804\H,0,-0.562672,-2.10038,4.14
0204\H,0,-4.842798,-2.073935,3.028252\H,0,-6.401446,-3.407035,1.637899
\H,0,-5.562066,-4.598792,-0.378144\H,0,-3.156824,-4.43364,-0.989675\H,
0,-1.607263,-3.089052,0.397127\H,0,-4.938067,0.881511,0.276795\H,0,-6.
034777,0.734683,-1.118059\H,0,-5.943898,3.118105,-0.239734\H,0,-5.3801
83,2.982035,-1.915035\H,0,-3.7527,3.211755,0.658663\H,0,-3.741321,4.30
301,-0.748806\H,0,-4.269235,-1.371828,-1.538111\H,0,-5.274162,-0.52329
1,-2.723992\H,0,-3.377279,-0.181656,-4.217791\H,0,-3.338404,-1.879424,
-3.70978\H,0,-1.653793,-1.343979,-1.959732\H,0,-1.050835,-0.705005,-3.
483718\H,0,-2.75953,-1.193684,3.463548\H,0,-0.854854,1.16483,-2.279488
\C,0,2.936595,-1.441558,0.390332\C,0,1.778042,-2.207906,-0.061012\C,0,
2.749144,-0.413776,1.397732\O,0,0.595936,-2.033721,0.21853\O,0,2.18059
4,-3.219992,-0.865175\O,0,1.777354,0.324517,1.520949\O,0,3.844916,-0.2
82889,2.182338\C,0,1.144359,-4.006838,-1.462952\C,0,1.80988,-5.027412,
-2.361585\C,0,3.798634,0.762418,3.162136\C,0,5.09753,0.712232,3.937802
\H,0,3.839863,-2.032962,0.495428\H,0,0.48016,-3.34221,-2.02466\H,0,0.5
55194,-4.487874,-0.673521\H,0,2.4846,-5.672742,-1.78966\H,0,2.388457,-
4.533189,-3.148468\H,0,1.051473,-5.6589,-2.83732\H,0,2.92783,0.610615,
3.809512\H,0,3.663915,1.725755,2.657193\H,0,5.953008,0.85267,3.269701\
H,0,5.212587,-0.251755,4.443574\H,0,5.112819,1.503355,4.69549\C,0,7.77
3243,0.164153,-0.537219\C,0,7.293821,-1.000685,-1.134641\C,0,5.930734,
-1.154553,-1.368103\C,0,5.016968,-0.150727,-1.014201\C,0,5.513174,1.01
153,-0.406244\C,0,6.876409,1.168323,-0.17365\C,0,3.58115,-0.349838,-1.
319314\C,0,2.756503,0.763041,-1.577341\N,0,1.576529,0.600929,-2.228763
\O,0,1.199326,-0.528325,-2.620787\O,0,0.859085,1.637369,-2.448967\H,0,
8.837802,0.289388,-0.356593\H,0,7.983279,-1.7898,-1.42421\H,0,5.560799
, -2.063996,-1.836817\H,0,4.829714,1.802005,-0.110162\H,0,7.240754,2.08
0821,0.292069\H,0,3.368245,-1.213966,-1.943591\H,0,2.958714,1.777578,-
1.271333\Version=AM64L-G03RevD.02\State=1-A\HF=-2618.4042425\RMSE=4.5
48e-09\Thermal=0.\Dipole=-1.1092337,0.1222557,-1.2866652\PG=C01 [X(C37
H52N6O6S1)]\@

Fin15

1\1\FAU-CCC-CCDH160\SP\RB3PW91\6-31G(d)\C37H52N6O6S1\SHUBINA\11-Aug-20
08\0\#P B3PW91\6-31G(d) SCF=Tight Name=SHUBINA SCRF=(PCM,Solvent=THF)
\Aza Fin 2R\0,1\C,0,-1.1825,4.52632,-0.97359\C,0,-1.32904,3.03221,-0
.64866\C,0,-0.98063,2.72517,0.82911\C,0,0.38805,3.32325,1.19792\C,0,0.
51742,4.80176,0.84028\C,0,0.22641,5.02042,-0.64348\N,0,-0.9422,1.29076
,1.06144\C,0,-1.78757,0.58001,1.84757\S,0,-3.20248,1.23348,2.532\N,0,-
1.40277,-0.70109,2.04794\C,0,-2.19147,-1.70924,2.74107\C,0,-3.09822,-2
.48762,1.79584\C,0,-1.25464,-2.63776,3.51817\C,0,-4.47121,-2.56564,2.0
4227\C,0,-5.30656,-3.3098,1.20862\C,0,-4.7762,-3.98628,0.11182\C,0,-3.
40642,-3.90752,-0.14759\C,0,-2.57402,-3.16285,0.6863\N,0,-2.6695,2.522

19,-1.01548\C,0,-2.83445,1.3143,-1.61873\N,0,-4.07115,0.75086,-1.66724
\C,0,-5.14716,1.2581,-0.82411\C,0,-5.14784,2.76763,-0.92088\C,0,-3.799
15,3.27175,-0.44735\C,0,-4.33593,-0.51753,-2.34532\C,0,-3.28996,-0.814
8,-3.40325\C,0,-1.92554,-0.64338,-2.76738\N,0,-1.81669,0.69787,-2.2155
8\H,0,-1.89101,5.1289,-0.38994\H,0,-1.41833,4.68214,-2.03368\H,0,-0.58
051,2.51563,-1.2542\H,0,-1.75212,3.13423,1.49015\H,0,1.16722,2.75987,0
.66889\H,0,0.55698,3.1568,2.26803\H,0,1.52534,5.15444,1.0931\H,0,-0.18
284,5.39943,1.44282\H,0,0.95997,4.47427,-1.25176\H,0,0.31543,6.08209,-
0.90564\H,0,-0.05493,0.84483,0.83077\H,0,-0.55046,-1.02814,1.59248\H,0
,-0.55525,-3.14861,2.84729\H,0,-1.83494,-3.39996,4.04791\H,0,-0.67497,
-2.06514,4.25007\H,0,-4.88937,-2.03062,2.89181\H,0,-6.37273,-3.35992,1
.41742\H,0,-5.4234,-4.57341,-0.53563\H,0,-2.98415,-4.43595,-0.9998\H,0
,-1.50863,-3.09955,0.47465\H,0,-5.00773,0.92984,0.21501\H,0,-6.08298,0
.83347,-1.19971\H,0,-5.92996,3.20214,-0.28958\H,0,-5.34216,3.06879,-1.
95752\H,0,-3.74911,3.19293,0.64573\H,0,-3.68669,4.3214,-0.7297\H,0,-4.
36711,-1.32787,-1.60359\H,0,-5.33392,-0.44276,-2.79471\H,0,-3.39766,-0
.12908,-4.2524\H,0,-3.42595,-1.83614,-3.77407\H,0,-1.76803,-1.38798,-1
.97717\H,0,-1.10255,-0.75438,-3.4743\H,0,-2.82569,-1.16442,3.44621\H,0
,-0.84016,1.07964,-2.24785\C,0,3.06684,-1.25096,0.187\C,0,1.86747,-2.1
6256,-0.02469\C,0,2.84839,-0.31471,1.3465\O,0,0.83701,-2.16909,0.62435
\O,0,2.18835,-3.11458,-0.90882\O,0,1.90935,0.44369,1.48014\O,0,3.86071
,-0.38711,2.22384\C,0,1.15281,-4.05094,-1.24377\C,0,1.74325,-5.05717,-
2.20743\C,0,3.80334,0.52612,3.33642\C,0,5.09367,0.37616,4.11131\H,0,3.
8966,-1.91874,0.44246\H,0,0.32296,-3.4942,-1.68971\H,0,0.79393,-4.5282
1,-0.32554\H,0,2.58479,-5.58845,-1.75113\H,0,2.09715,-4.56353,-3.11769
\H,0,0.9833,-5.79485,-2.48714\H,0,2.9234,0.28622,3.94281\H,0,3.67075,1
.54217,2.95086\H,0,5.95475,0.60641,3.47628\H,0,5.20825,-0.64414,4.4904
1\H,0,5.0973,1.06319,4.96437\C,0,7.74232,0.47761,-0.81735\C,0,7.32675,
-0.67522,-1.48065\C,0,5.96904,-0.97216,-1.58197\C,0,5.00108,-0.12892,-
1.02562\C,0,5.43284,1.02535,-0.36104\C,0,6.78927,1.3275,-0.25841\C,0,3
.53132,-0.49238,-1.1371\C,0,2.70736,0.68079,-1.53782\N,0,1.47428,0.492
03,-1.96597\O,0,0.95088,-0.67329,-1.94653\O,0,0.7763,1.49101,-2.4174\H
,0,8.80049,0.71458,-0.73999\H,0,8.05991,-1.34286,-1.92681\H,0,5.6516,-
1.87107,-2.10691\H,0,4.7002,1.70043,0.07476\H,0,7.10203,2.23284,0.2566
4\H,0,3.42658,-1.2719,-1.90341\H,0,3.08949,1.68789,-1.60767\\Version=A
M64L-G03RevD.02\State=1-A\HF=-2618.4244936\RMSE=9.687e-09\Thermal=0\Di
pole=-0.7639447,-0.5349354,-0.7582634\PG=C01 [X(C37H52N6O6S1)]\@

Init16

1\1\FAU-CCC-CCDH153\SP\RB3PW91\6-31G(d)\C37H52N6O6S1\SHUBINA\14-Aug-20
08\0\#P B3PW91\6-31G(d) SCF=Tight Name=SHUBINA SCRF=(PCM,Solvent=THF)
\Aza Init 3R\0,1\C,0,0.644164,4.280816,-1.776562\C,0,0.933253,2.9848
36,-1.007016\C,0,0.551604,1.755751,-1.871165\C,0,-0.930648,1.837936,-2
.265755\C,0,-1.263388,3.153645,-2.971964\C,0,-0.844424,4.358492,-2.127
886\N,0,0.83579,0.506947,-1.200216\C,0,1.735826,-0.418396,-1.623634\S,
0,2.844238,-0.140547,-2.889196\N,0,1.683613,-1.58361,-0.944603\C,0,2.5
18825,-2.742671,-1.218552\C,0,3.750925,-2.796846,-0.325014\C,0,1.68188
5,-4.019689,-1.102255\C,0,5.024664,-2.923944,-0.884454\C,0,6.156064,-3
.024355,-0.074334\C,0,6.028521,-2.99656,1.312653\C,0,4.76159,-2.862943
,1.883424\C,0,3.634345,-2.761942,1.06991\N,0,2.328049,2.904126,-0.5249
99\C,0,2.625273,2.24074,0.621555\N,0,3.917621,1.957127,0.933419\C,0,4.
965992,2.050914,-0.077798\C,0,4.744331,3.300556,-0.89922\C,0,3.363392,
3.230047,-1.516231\C,0,4.256024,1.160523,2.113085\C,0,3.27826,1.419171
,3.243303\C,0,1.877575,1.176506,2.722857\N,0,1.662727,1.939365,1.50018
\H,0,1.215076,4.31532,-2.71352\H,0,0.950052,5.144621,-1.172175\H,0,0.2
75412,3.011675,-0.137885\H,0,1.168789,1.759392,-2.777109\H,0,-1.537999
,1.742782,-1.356644\H,0,-1.165365,0.981499,-2.908061\H,0,-2.337233,3.1
97582,-3.19226\H,0,-0.743816,3.192864,-3.940589\H,0,-1.438273,4.386233
,-1.204072\H,0,-1.046214,5.294011,-2.664381\H,0,0.233805,0.239411,-0.4
1394\H,0,0.971089,-1.660979,-0.216173\H,0,1.361049,-4.192379,-0.068442
\H,0,2.276786,-4.885481,-1.410886\H,0,0.788448,-3.95311,-1.730426\H,0,
5.129177,-2.93557,-1.966895\H,0,7.138687,-3.123014,-0.529776\H,0,6.908
213,-3.080922,1.946239\H,0,4.650811,-2.84833,2.965696\H,0,2.650608,-2.
652303,1.522343\H,0,4.960503,1.155599,-0.715451\H,0,5.923732,2.08971,0
.450807\H,0,5.489621,3.372499,-1.697826\H,0,4.844584,4.186497,-0.26037
3\H,0,3.343542,2.469588,-2.308578\H,0,3.111199,4.19904,-1.951518\H,0,4
.274017,0.09356,1.849851\H,0,5.272373,1.444083,2.40787\H,0,3.38068,2.4

51656,3.598587\H,0,3.495687,0.750587,4.082307\H,0,1.118083,1.504807,3.438485\H,0,1.697103,0.114357,2.521229\H,0,2.857606,-2.63135,-2.252584\H,0,0.666978,1.970433,1.237227\C,0,-2.151874,0.057264,2.127099\C,0,-2.017707,1.411443,1.779004\C,0,-1.208053,-0.950116,1.830669\O,0,-1.085959,1.999737,1.18671\O,0,-3.114133,2.146416,2.17091\O,0,-0.140206,-0.862125,1.187074\O,0,-1.586574,-2.149546,2.368695\C,0,-3.057562,3.548262,1.928223\C,0,-4.287124,4.170459,2.559247\C,0,-0.758937,-3.275927,2.098947\C,0,-1.379067,-4.469937,2.79709\H,0,-3.014822,-0.227344,2.715803\H,0,-3.027673,3.740226,0.848049\H,0,-2.136683,3.96337,2.354802\H,0,-4.311075,3.976831,3.63653\H,0,-5.202169,3.76129,2.118305\H,0,-4.286241,5.254896,2.402026\H,0,0.257416,-3.088182,2.469163\H,0,-0.698313,-3.436304,1.017066\H,0,-2.390727,-4.654917,2.421991\H,0,-1.440793,-4.301829,3.877349\H,0,-0.776126,-5.36739,2.619509\C,0,-8.036742,0.052289,0.022802\C,0,-6.87968,0.514229,0.646417\C,0,-5.648616,-0.063378,0.350711\C,0,-5.557034,-1.116611,-0.57571\C,0,-6.733754,-1.572548,-1.198545\C,0,-7.959214,-0.993006,-0.901707\C,0,-4.240947,-1.682148,-0.841694\C,0,-3.957943,-2.681543,-1.69114\N,0,-2.603873,-3.150427,-1.853481\O,0,-2.450846,-4.111037,-2.606501\O,0,-1.693223,-2.585123,-1.250565\H,0,-8.998931,0.502101,0.254147\H,0,-6.932517,1.324508,1.368377\H,0,-4.746957,0.298989,0.838915\H,0,-6.690454,-2.385706,-1.917827\H,0,-8.859885,-1.355843,-1.38991\H,0,-3.406528,-1.252004,-0.289207\H,0,-4.648926,-3.237486,-2.309878\Version=AM64L-G03RevD.02\State=1-A\HF=-2618.4145171\RMSE=7.961e-09\Thermal=0.Dipole=0.7133284,3.0008854,1.8816873\PG=C01 [X(C37H52N6O6S1)]\@

TS16

1\1\FAU-CCC-CCDH158\SP\RB3PW91\6-31G(d)\C37H52N6O6S1\SHUBINA\11-Aug-2008\0\#P B3PW91/6-31G(d) SCF=Tight Name=SHUBINA SCRF=(PCM,Solvent=THF)\Aza_TS1\0,1\C,0,1.182474,4.580707,-0.093551\C,0,1.327248,3.052331,-0.018393\C,0,1.292366,2.434242,-1.439763\C,0,0.012951,2.868689,-2.173313\C,0,-0.163371,4.386227,-2.206258\C,0,-0.119036,4.971678,-0.795346\N,0,1.361093,0.988008,-1.403938\C,0,2.365623,0.226649,-1.926461\S,0,3.92175,0.839205,-2.248424\N,0,2.007736,-1.048776,-2.156512\C,0,2.919865,-2.144007,-2.453956\C,0,3.322443,-2.883263,-1.184242\C,0,2.274572,-3.071256,-3.486336\C,0,4.672114,-3.033631,-0.85482\C,0,5.055118,-3.721675,0.297734\C,0,4.086729,-4.264262,1.140414\C,0,2.735422,-4.113825,0.821896\C,0,2.354437,-3.430052,-0.331151\N,0,2.538102,2.649248,0.73121\C,0,2.572893,1.49857,1.45435\N,0,3.758817,1.002658,1.889434\C,0,5.020185,1.495106,1.345619\C,0,4.943914,3.000252,1.240488\C,0,3.771063,3.356123,0.35214\C,0,3.843225,-0.258029,2.6286\C,0,2.609272,-0.463639,3.482153\C,0,1.399671,-0.364651,2.580235\N,0,1.441746,0.888182,1.830572\H,0,2.00955,5.019841,-0.665351\H,0,1.225519,5.001265,0.919254\H,0,0.449754,2.6994,0.528339\H,0,2.172708,2.77826,-1.994971\H,0,-0.848698,2.411907,-1.666732\H,0,0.038983,2.454509,-3.187522\H,0,-1.109802,4.640937,-2.699014\H,0,0.635362,4.837593,-2.812637\H,0,-0.975426,4.604367,-0.215354\H,0,-0.202468,6.065082,-0.827057\H,0,0.474133,0.504162,-1.259767\H,0,1.008936,-1.270345,-2.067018\H,0,1.317853,-3.461253,-3.123606\H,0,2.936577,-3.917,-3.698572\H,0,2.09202,-2.525854,-4.418469\H,0,5.429679,-2.603105,-1.506135\H,0,6.110883,-3.833696,0.534712\H,0,4.38154,-4.806446,2.036075\H,0,1.972238,-4.538534,1.470008\H,0,1.298073,-3.320874,-0.569656\H,0,5.208354,1.040308,0.363578\H,0,5.81247,1.185162,2.033729\H,0,5.859922,3.405194,0.798368\H,0,4.827986,3.437068,2.239938\H,0,4.008182,3.106109,-0.68978\H,0,3.577366,4.427613,0.428392\H,0,3.97414,-1.093878,1.927218\H,0,4.743506,-0.201788,3.250168\H,0,2.566872,0.294257,4.273895\H,0,2.646273,-1.449405,3.955843\H,0,0.463381,-0.367068,3.13907\H,0,1.354528,-1.209358,1.886921\H,0,3.816723,-1.689031,-2.884508\H,0,0.537941,1.1636,1.448056\C,0,-3.073785,-0.23561,1.221338\C,0,-2.555555,1.111721,1.28177\C,0,-2.226942,-1.375985,1.508732\O,0,-1.392293,1.511677,1.185087\O,0,-3.585724,1.992071,1.421164\O,0,-1.012354,-1.44698,1.41373\O,0,-2.983612,-2.464493,1.820484\C,0,-3.254766,3.379181,1.478801\C,0,-4.510367,4.131446,1.868511\C,0,-2.255655,-3.691271,1.96887\C,0,-3.255131,-4.782625,2.288515\H,0,-4.100891,-0.330889,1.5518\H,0,-2.885644,3.704187,0.498263\H,0,-2.446076,3.533305,2.201716\H,0,-4.866137,3.809056,2.852161\H,0,-5.310319,3.956246,1.142356\H,0,-4.307965,5.207392,1.908899\H,0,-1.517188,-3.57657,2.770869\H,0,-1.70718,-3.895407,1.04277\H,0,-3.978713,-4.904586,1.475825\H,0,-3.805959,-4.553743,3.206764\H,0,-2.735129,-5.736973,2.426657\C,0,-7.691848,-0.275963,-1.008312\C,0,-6.8758

54,0.783776,-1.398437\C,0,-5.490222,0.657757,-1.338244\C,0,-4.893409,-
0.532091,-0.900237\C,0,-5.726476,-1.588428,-0.500101\C,0,-7.109997,-1.
460594,-0.554083\C,0,-3.418974,-0.642124,-0.893453\C,0,-2.803282,-1.84
5646,-1.254646\N,0,-1.487362,-1.888001,-1.635061\O,0,-0.941891,-2.9993
83,-1.812337\O,0,-0.853275,-0.812111,-1.846941\H,0,-8.773706,-0.179767
,-1.052652\H,0,-7.318134,1.712271,-1.751229\H,0,-4.857343,1.487185,-1.
644473\H,0,-5.28375,-2.503544,-0.11754\H,0,-7.739045,-2.288903,-0.2373
11\H,0,-2.881927,0.245492,-1.213132\H,0,-3.25718,-2.821474,-1.168181\\
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Fin16

1\1\FAU-CCC-CCDH161\SP\RB3PW91\6-31G(d)\C37H52N6O6S1\SHUBINA\13-Aug-20
08\0\#P B3PW91/6-31G(d) SCF=Tight Name=SHUBINA SCRF=(PCM,Solvent=THF)
\Aza Fin 3R\0,1\C,0,-1.171522,4.434121,0.387963\C,0,-1.347371,2.9116
24,0.360269\C,0,-1.869496,2.365586,1.71526\C,0,-0.952737,2.836518,2.85
7551\C,0,-0.74739,4.35152,2.863776\C,0,-0.219587,4.841308,1.514785\N,0
,-1.915285,0.925411,1.681021\C,0,-3.0195,0.147184,1.754467\S,0,-4.6079
32,0.775155,1.846937\N,0,-2.734116,-1.171557,1.745885\C,0,-3.706446,-2
.248094,1.823058\C,0,-3.88988,-2.95152,0.483972\C,0,-3.301049,-3.22921
7,2.928171\C,0,-5.151539,-2.994253,-0.117395\C,0,-5.349855,-3.666925,-
1.323886\C,0,-4.282598,-4.308933,-1.948632\C,0,-3.016821,-4.266172,-1.
361161\C,0,-2.819691,-3.591987,-0.156779\N,0,-2.199187,2.468488,-0.766
705\C,0,-1.948986,1.30102,-1.418603\N,0,-2.932875,0.659948,-2.08589\C,
0,-4.322814,1.081321,-1.930932\C,0,-4.363445,2.59353,-1.982069\C,0,-3.
511024,3.128747,-0.848942\C,0,-2.715218,-0.621224,-2.763357\C,0,-1.272
141,-0.785549,-3.20137\C,0,-0.366178,-0.501077,-2.020104\N,0,-0.707332
,0.808121,-1.468606\H,0,-2.135757,4.928893,0.561276\H,0,-0.801013,4.77
6091,-0.587017\H,0,-0.34867,2.49074,0.224547\H,0,-2.889338,2.724203,1.
893751\H,0,0.017803,2.331856,2.758006\H,0,-1.387298,2.496912,3.804565\
H,0,-0.055576,4.629656,3.668414\H,0,-1.700488,4.854897,3.08335\H,0,0.7
75282,4.411704,1.329597\H,0,-0.098649,5.93176,1.518352\H,0,-0.989176,0
.455621,1.741178\H,0,-1.747931,-1.438004,1.585981\H,0,-2.312012,-3.659
187,2.733311\H,0,-4.021915,-4.051272,2.99529\H,0,-3.264469,-2.71207,3.
892527\H,0,-5.986637,-2.492761,0.366953\H,0,-6.340616,-3.691758,-1.772
105\H,0,-4.43473,-4.84191,-2.884363\H,0,-2.177761,-4.766589,-1.839809\
H,0,-1.823716,-3.553716,0.278424\H,0,-4.733117,0.708384,-0.982417\H,0,
-4.88785,0.638378,-2.756141\H,0,-5.387463,2.959595,-1.85673\H,0,-3.995
593,2.941838,-2.955118\H,0,-4.041103,2.974073,0.099023\H,0,-3.340769,4
.200272,-0.988845\H,0,-3.010507,-1.437143,-2.091804\H,0,-3.386996,-0.6
44488,-3.628836\H,0,-1.04457,-0.097664,-4.024824\H,0,-1.118766,-1.8070
89,-3.562692\H,0,0.681589,-0.451923,-2.322157\H,0,-0.463602,-1.261786,
-1.233511\H,0,-4.655627,-1.775519,2.091454\H,0,0.064539,1.318944,-1.05
6747\C,0,3.794149,0.231453,-0.598853\C,0,3.143633,1.517443,-1.088404\C
,0,3.720135,-0.758957,-1.754835\O,0,1.99101,1.858105,-0.91017\O,0,4.02
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.843229,-1.522692\C,0,3.52749,3.478833,-2.345756\C,0,4.67866,4.143522,
-3.066824\C,0,4.440139,-2.863166,-2.544857\C,0,5.32735,-3.996473,-2.08
1556\H,0,4.853347,0.457257,-0.432918\H,0,3.121554,4.10902,-1.547647\H,
0,2.706192,3.225473,-3.023804\H,0,5.071533,3.495643,-3.856427\H,0,5.49
2529,4.377452,-2.373498\H,0,4.338108,5.077973,-3.525334\H,0,4.785775,-
2.422634,-3.485654\H,0,3.403035,-3.182836,-2.687962\H,0,4.973022,-4.40
7612,-1.131551\H,0,6.359876,-3.658598,-1.948546\H,0,5.321818,-4.797345
,-2.828605\C,0,5.865572,-1.712347,3.808002\C,0,4.57279,-1.279736,4.108
614\C,0,3.732063,-0.826994,3.09803\C,0,4.162441,-0.791617,1.762142\C,0
,5.4543,-1.236999,1.471214\C,0,6.299229,-1.69183,2.486414\C,0,3.155791
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6903,1.089458\O,0,-0.096596,-1.91122,0.885787\O,0,0.648503,-0.063769,1
.860587\H,0,6.525284,-2.064034,4.59746\H,0,4.218428,-1.292619,5.136709
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