Computational Study of Factors Controlling the Boat and Chair Transition States of Ireland-Claisen Rearrangements

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Computational Details

All gas phase B3LYP optimized stationary points were verified as minima or first-order saddle points by calculation of the full Hessian in Gaussian03.[15] Solvation free energy corrections were performed using UAO radii using B3LYP/6-31G(d) or 6-31+G(d) and a CPCM dielectric continuum solvent model for benzene. MO6-2X energies were computed on DFT geometries and also use B3LYP thermal and free energy corrections.

CARTESIAN COORDINATES (Å) AND ABSOLUTE ENERGIES (au)

Z*-2

B3LYP/6-31+G(d)

0 1

C 3.6394319876 0.881876848 0.0630206283

H 4.4281104166 1.4872178201 -0.3925343699

O 3.7470702265 -0.3996521749 -0.6111518411

C 2.6286764213 -1.1665119705 -0.6356506214

H 2.8584827866 -2.1736807976 -0.9716788062

C 1.3853439134 -0.7702056413 -0.3208633277

H 0.5814482301 -1.4962182094 -0.3775124529

C 1.0827172766 0.6469607855 0.0799513804

H 0.1944538402 1.0123095132 -0.4515355711

C 2.2916244599 1.5318186726 -0.2961691031

H 2.2617837619 1.6210160425 -1.3963781937

C 3.9265077478 0.7136410671 1.5524886815

H 3.2069843607 0.0436648583 2.0293465369

H 3.8727336911 1.6870493514 2.0495663813

H 4.9348491896 0.3064305879 1.6823635365

O 2.2894421356 2.8218600638 0.2805716434

C 1.2573509613 3.6801747713 -0.1798853448

H 1.2632538753 3.7546481577 -1.27866311

H 1.4602705088 4.6658993237 0.2459625359

H 0.2662361392 3.3440398062 0.1533246291

O 0.8248935679 0.791306528 1.4922274353

C -0.4342248026 0.5726076378 1.9721762503

C -1.4926495897 0.0723044661 1.3096048633

H -1.3485783138 -0.2897654193 0.297390235

O -0.5115098328 0.8818414254 3.2936204984

C 0.1277648271 2.090549817 3.7270387109

H -0.2900183564 2.9576691019 3.1993207329

H 1.2081154611 2.0501919867 3.5686760155

H -0.0939503739 2.1682766533 4.7931167226

C -2.8655794682 -0.0872456673 1.9055750312

H -3.6339667972 0.3501190436 1.253334092

H -2.9335703641 0.3957482968 2.8840816844

H -3.1274998876 -1.1469457457 2.0392635168

Version=AM64L-G03RevE.01 State=1-A\\HF=-730.8467926

Sum of electronic and zero-point Energies= -730.565099

Sum of electronic and thermal Energies= -730.548214

Sum of electronic and thermal Enthalpies= -730.547270

Sum of electronic and thermal Free Energies= -730.610360

Z*[b]-2 (H_{rel} = 3.1 kcal/mol)

B3LYP/6-31+G(d)

0 1

C 2.6108826444 3.0768119271 0.543357429

H 3.2952920208 2.9607663355 1.3994115924

O 1.7554465731 4.2035642778 0.8596360385

C 0.804421215 3.9719142089 1.8066287659

H 0.3619951286 4.9001588149 2.1558770524

C 0.4362212359 2.7630826554 2.250364923

H -0.3254391146 2.6856051799 3.0198410133

C 1.0460324416 1.4937038437 1.7232862092

H 1.7515513138 1.0799536993 2.4572795883

C 1.835349423 1.7511657055 0.4087178685

H 2.5894594263 0.9631683141 0.3063815263

C 3.4010909951 3.4537886126 -0.6988470387

H 3.9278174719 4.3995697307 -0.5359968456

H 2.7407975255 3.5584383764 -1.5639832451

H 4.1401330442 2.6764942725 -0.9232298889

O 1.0850481308 1.6309645824 -0.7908512664

C -0.1271673232 2.3714407557 -0.9531798663

H -0.8796462089 2.0728504546 -0.21693192

H -0.4836166989 2.1184343606 -1.955490634

H 0.0423545321 3.4523481831 -0.894743531

O -0.0087884373 0.5153398602 1.5485197816

C 0.267510693 -0.7555911336 1.9945603207

C -0.4099456222 -1.296068273 3.014831977

H -1.122087762 -0.6479312497 3.5195033879

O 1.2746480878 -1.4115737787 1.3399244219

C 1.0222570934 -1.6949536351 -0.0510885763

H 0.1515967901 -2.3565422098 -0.1444280348

H 1.9143156681 -2.2085030314 -0.4160080172

H 0.8584364356 -0.7740354119 -0.6174981467

C -0.2647460636 -2.7092803478 3.5013658886

H 0.0659251535 -2.7348049364 4.5490101063

H 0.464967549 -3.2636468966 2.904657767

H -1.2241133619 -3.2436332471 3.4601213535

Version=AM64L-G03RevE.01 State=1-A\\HF=-730.8419012

Sum of electronic and zero-point Energies= -730.560218

Sum of electronic and thermal Energies= -730.543544

Sum of electronic and thermal Enthalpies= -730.542600

Sum of electronic and thermal Free Energies= -730.604621

Z*-2 Conformation-1 (H_{rel} = 0.1 kcal/mol)

B3LYP/6-31+G(d)

0 1

C 3.3266152933 2.5090493861 0.3589212951

H 3.0271265739 3.4478866785 0.8510072477

O 2.9177094126 2.6131578106 -1.022478496

C 1.5893811578 2.4514716068 -1.2632333182

H 1.3472991707 2.6986259409 -2.2923469139

C 0.6818300007 2.0403348778 -0.3676306792

H -0.3586133908 1.9593202735 -0.6615457434

C 1.0856470133 1.6447302852 1.0284863098

H 0.8818992116 2.4444635827 1.7556176252

C 2.6021093688 1.354668894 1.0734334624

H 2.9344370791 1.3368717744 2.1223622523

C 4.8404916999 2.3790096018 0.3630743543

H 5.2890430624 3.210736294 -0.1896358609

H 5.1419098633 1.43883387 -0.1065303935

H 5.2207973769 2.4024309817 1.3911393399

O 2.9462676982 0.1389611408 0.4353078202

C 3.1259583756 -0.9757709157 1.2992979886

H 2.2029783819 -1.2299687796 1.8321163996

H 3.926302701 -0.7823981047 2.0306476997

H 3.4240838243 -1.8120483684 0.6613862168

O 0.3995917913 0.4658995358 1.4781002308

C -0.9075883756 0.5578542423 1.8730788837

C -1.6551526189 1.6678373137 1.991488975

H -1.1987092189 2.629134959 1.7793113016

O -1.3883999541 -0.6681846014 2.2162795461

C -1.2396417372 -1.7101977449 1.2407041958

H -1.7337315597 -2.5846896636 1.6683320227

H -0.185903605 -1.9313504864 1.0500658046

H -1.7322346451 -1.4287888483 0.301024297

C -3.0926758303 1.6761037893 2.4363623924

H -3.4789373653 0.6601215064 2.552946056

H -3.7288073213 2.2055228567 1.7135744379

H -3.2110834346 2.1913703113 3.4003352501

Version=AM64L-G03RevE.01 State=1-A\\HF=-730.8463561

Sum of electronic and zero-point Energies= -730.564917

Sum of electronic and thermal Energies= -730.548021

Sum of electronic and thermal Enthalpies= -730.547077

Sum of electronic and thermal Free Energies= -730.610038

Z*-2 Conformation-2 (H_{rel} = 1.1 kcal/mol)

B3LYP/6-31+G(d)

0 1

C 0.9170514884 -1.1975119877 -0.6933277266

H 1.2867466357 -2.1849829448 -0.9837224457

O 0.7542094021 -0.4991815893 -1.9565472114

C 0.8156678853 0.855032722 -1.9118473654

H 0.4959129965 1.2870275154 -2.8560079536

C 1.2366128458 1.5972576623 -0.8757088867

H 1.2381085848 2.6779529098 -0.9728612933

C 1.7448905507 0.9755168395 0.3929914397

H 2.6743840467 1.4745689455 0.6950745018

C 2.0269943387 -0.517502194 0.1297746223

H 2.9430250311 -0.5420435238 -0.4865727053

C -0.434918773 -1.3473626086 -0.0020839196

H -0.8899867564 -0.3760797476 0.2027419149

H-0.3075774212 -1.8716085618 0.9496588986

H -1.106326585 -1.9291030354 -0.6428004951

O 2.2176123466 -1.3127289535 1.2832753128

C 3.4112600567 -1.0549422146 2.0014289969

H 4.2941050666 -1.1229580685 1.3461546532

H 3.4800710614 -1.8224567558 2.7763213193

H 3.3953505022 -0.0673112025 2.481913885

O 0.8137482361 1.0783845597 1.5106703052

C 0.3716654175 2.3397456562 1.8145976555

C -0.9319489864 2.6351014353 1.8730582295

H -1.6194087389 1.8504341725 1.56850753

O 1.3513654982 3.2745314596 2.050070672

C 2.1719788634 3.027898518 3.1994371217

H 2.6915215636 2.0663273202 3.1231306085

H 1.5633694602 3.037287235 4.1126443963

H 2.9015082367 3.8399189629 3.2316602622

C -1.5055034277 3.9481088241 2.3228747188

H -2.181548402 3.8154180252 3.1791577641

H -2.0974948098 4.4146503179 1.5232005584

H -0.7184442145 4.650610307 2.6111356357

Version=AM64L-G03RevE.01 State=1-A\\HF=-730.8447024

Sum of electronic and zero-point Energies= -730.563292

Sum of electronic and thermal Energies= -730.546406

Sum of electronic and thermal Enthalpies= -730.545462

Sum of electronic and thermal Free Energies= -730.608750

Z*-2 Conformation-3 (H_{rel} = 4.7 kcal/mol)

B3LYP/6-31+G(d)

0 1

C 0.0361011822 3.2562427707 2.1788805213

H -0.2777889991 4.3000448627 2.0815441448

O 0.863991814 3.2694601389 3.3757087088

C 1.7858609597 2.2780540959 3.4862332651

H 2.2040657263 2.2520582467 4.4886139134

C 2.1727307978 1.4432401471 2.5091845816

H 2.9143270478 0.683818341 2.7370978552

C 1.6070968167 1.535035005 1.1188918389

H 2.3929999705 1.4639532912 0.3609063293

C 0.9152590128 2.8946381564 0.9605405178

H 1.7307718855 3.637042801 0.9264237032

C -1.1943166686 2.3809717414 2.3979702491

H -0.9178571601 1.3508001073 2.6323836352

H -1.8041892637 2.3644053775 1.4889450998

H -1.7917533174 2.7892755963 3.220290931

O 0.192954636 2.9307682181 -0.2557674875

C 0.0273693104 4.2247418577 -0.8133702625

H 0.9990092631 4.7204322061 -0.9647862915

H -0.6085393455 4.8720158364 -0.1916236149

H -0.457218524 4.0839055101 -1.7826599429

O 0.6504484303 0.477688549 0.8535442221

C 1.1272657519 -0.738870966 0.4649270463

C 0.5844357447 -1.8685645814 0.944014464

H -0.1215598805 -1.7463373116 1.7606101688

O 2.0746257386 -0.6691433876 -0.5288294453

C 3.3454095172 -1.2704801314 -0.2602214866

H 3.9623488358 -1.0688816509 -1.1390971872

H 3.2641276243 -2.3516917453 -0.1125610941

H 3.8109510309 -0.8207983223 0.6263736834

C 0.7948591938 -3.2522005621 0.3921967433

H 1.4577437159 -3.8650487819 1.0213469813

H 1.2143022841 -3.2291916181 -0.6190952149

H -0.1628311317 -3.7853827978 0.3353824236

Version=AM64L-G03RevE.01 State=1-A\\HF=-730.8388497

Sum of electronic and zero-point Energies= -730.557536

Sum of electronic and thermal Energies= -730.540533

Sum of electronic and thermal Enthalpies= -730.539588

Sum of electronic and thermal Free Energies= -730.603619

Z*-2 without Methoxy groups:

B3LYP/6-31+G(d)

0 1

C 3.6612356913 0.7416927191 0.9113844678

H 3.7264432124 -0.053502285 1.6712439456

O 3.7420468648 1.9965902448 1.6319723342

C 2.6076109219 2.3744640094 2.2838375295

H 2.8007685286 3.2140120132 2.9451666539

C 1.4021655831 1.8036604705 2.1449402189

H 0.5671967405 2.1803401642 2.7279582218

C 1.1597287204 0.6970304122 1.1521901206

H 1.0337231115 -0.2721859652 1.6630948144

C 2.3295422358 0.6256148957 0.1692861408

H 2.2977744387 -0.3101471477 -0.4001119488

C 4.8761935979 0.6814633324 -0.00071572

H 4.8251921295 1.4650839295 -0.7650164414

H 4.926335108 -0.2922534281 -0.5011586929

H 5.7954686464 0.8218791267 0.5773732008

O -0.0338139734 0.9303098952 0.3795135295

C -1.2161134829 0.6455066974 1.0092739272

C -2.3683530503 1.236109669 0.6770280326

H -2.3482306062.014914362 -0.0842153516

C -3.6966945521 0.8673001366 1.2766436026

H -4.1801352466 1.7359124987 1.7444059636

H -3.5907854654 0.0902012585 2.0432210646

H -4.392693512 0.4896091666 0.5146088559

H 2.2350992576 1.4534658486 -0.5442130483

H -1.1587048995 -0.1370720243 1.7702885784

Version=AM64L-G03RevD.01 State=1-A\\HF=-501.8036328

Sum of electronic and zero-point Energies= -501.587740

Sum of electronic and thermal Energies= -501.576123

Sum of electronic and thermal Enthalpies= -501.575179

Sum of electronic and thermal Free Energies= -501.625781

E*-2

B3LYP/6-31+G(d)

0 1

C 3.2993107756 0.0044335524 2.2746855084

H 4.2777345878 -0.4129095621 2.0204177818

O 2.8805407478 -0.7640673642 3.433406314

C 1.543839923 -0.8242238757 3.6668605496

H 1.3425077461 -1.2291193021 4.6546312659

C 0.5731582647 -0.4645128205 2.8131619519

H -0.4631428935 -0.541920736 3.1231823428

C 0.8776009174 0.0353251757 1.4312505945

H 0.2234029485 -0.4578950325 0.7045396663

C 2.3500494653 -0.2917359834 1.1003295665

H 2.3800182547 -1.3829736452 0.9312952402

C 3.4580304794 1.4755578156 2.6493952813

H 3.7935994582 2.0433096357 1.776314716

H 4.208511255 1.5679039948 3.4418554501

H 2.5169988473 1.9089052606 2.9966043865

O 2.8761352267 0.3714335349 -0.031607415

C 2.2942940127 -0.0041871499 -1.2702357747

H 2.898369483 0.4633492773 -2.0517545873

H 1.259096241 0.3514195539 -1.3609089181

H 2.3164535263 -1.0972868479 -1.4039755909

O 0.6649532247 1.4706972088 1.307215125

C -0.4864098131 1.9015977862 0.7347000896

C -0.5141080404 2.951973585 -0.1049532332

O -1.5607116314 1.1737562251 1.1708547581

C -2.8364655277 1.467195676 0.6146890213

H -3.1629492565 2.4772382828 0.8927410308

H -3.5232329498 0.7318625985 1.0379832851

H -2.8183286317 1.37672134 -0.478954293

H -1.4785048926 3.3252536538 -0.4335578437

C 0.7117230716 3.6925096697 -0.5673821557

H 0.7764688706 4.6922494457 -0.113483051

H 0.6964209401 3.8391236658 -1.65604301

H 1.6246353692 3.1500153814 -0.307258053

Version=AM64L-G03RevD.01 State=1-A\\HF=-730.8482844

Sum of electronic and zero-point Energies= -730.566172

Sum of electronic and thermal Energies= -730.549589

Sum of electronic and thermal Enthalpies= -730.548645

Sum of electronic and thermal Free Energies= -730.610810

E*[b]-2 (H_{rel} = 0.5 kcal/mol)

B3LYP/6-31+G(d)

0 1

C -1.5239805044 1.9364591614 1.735063025

H -2.032161993 1.2750811746 1.0158194119

O -1.5128422656 3.2582338101 1.1529117216

C -0.5987638563 3.4677178804 0.1658924003

H -0.756143652 4.4302953759 -0.3108461597

C 0.3745339899 2.6174795489 -0.1866341337

H 1.0422078284 2.8671906228 -1.0020532594

C 0.5679879221 1.3149070407 0.5408211103

H 0.1063214285 0.4793101704 -0.003942033

C -0.0932428895 1.403366212 1.9335288782

H -0.1533440871 0.3955019396 2.3745101375

C -2.3312028044 2.0245935035 3.0193622674

H -1.8222780278 2.6651053113 3.7444188087

H -2.4608400512 1.0265828238 3.4546528137

H -3.3217055382 2.4417785027 2.8105158068

O 0.570963318 2.2822563463 2.8211288227

C 1.5931855067 1.7214187736 3.6340922684

H 1.8303891406 2.4780065759 4.387240655

H 2.4910223088 1.4857108146 3.054507849

H 1.2368209263 0.8118177365 4.1431172067

O 1.9692598684 0.9791232242 0.7207599806

C 2.5470587824 0.178173071 -0.2126553

C 3.3264785752 -0.8662659534 0.1181022322

O 2.2679890447 0.6171706364 -1.4765016971

C 2.7445389997 -0.1510357947 -2.574599694

H 2.3867327991 -1.1867775792 -2.5137021286

H 3.8412758889 -0.1438083267 -2.6120928509

H 2.3450176162 0.3288835149 -3.469752319

H 3.8492675766 -1.387754415 -0.6769591432

C 3.5750745492 -1.3387861391 1.5242181738

H 3.4235079271 -2.4235374753 1.6077294014

H 2.9063352155 -0.8475121358 2.2358672206

H 4.607536457 -1.1366859524 1.8444785267

Version=AM64L-G03 RevD.01 State=1-A\\HF=-730.8469413

Sum of electronic and zero-point Energies= -730.565447

Sum of electronic and thermal Energies= -730.548721

Sum of electronic and thermal Enthalpies= -730.547777

Sum of electronic and thermal Free Energies= -730.610364

E*-2 Conformation-1 (H_{rel} = 2.1 kcal/mol)

B3LYP/6-31+G(d)

0 1

C -1.4038063968 0.793210661 0.1612326563

H -2.2000265711 1.3001954901 -0.3914898926

O -2.1054106238 0.1142403578 1.2397201889

C -1.4067929965 -0.1180548622 2.3802098724

H -1.9658877666 -0.7699848671 3.0455313826

C -0.2031806052 0.387858999 2.6932292581

H 0.2507721613 0.1161745356 3.6409084215

C 0.5271926134 1.3111057115 1.7606450189

H 0.9931423069 2.1344405747 2.3129631403

C -0.4927919793 1.8805758795 0.7576398686

H -1.1459985255 2.5481409214 1.3444866938

C -0.7300230973 -0.2284727736 -0.7498607208

H 0.0057318285 -0.8281257976 -0.2097193312

H -0.2155489339 0.2891302758 -1.5656248409

H -1.4913953299 -0.8906787245 -1.1759312475

O 0.0731909038 2.6092542908 -0.3173270387

C 0.4044143715 3.9541470092 -0.0006845227

H 0.7699292353 4.4112255639 -0.923641567

H 1.1894541382 4.0152924228 0.7652047315

H -0.4814901818 4.5070211628 0.3475196849

O 1.5941724329 0.6030419799 1.0559546353

C 2.8535081369 0.7553831215 1.572149968

C 3.5464841979 -0.2382304698 2.1420275228

O 3.3846896155 2.0179234852 1.445850778

C 3.6722215615 2.4007041531 0.0902903464

H 2.7805352377 2.3194481609 -0.5388546589

H 4.4721919373 1.7671567547 -0.314608232

H 4.0118762811 3.4380851238 0.1317643981

H 4.5721815766 -0.0085202891 2.4209476291

C 3.0302420623 -1.6216422564 2.4136831088

H 3.0984738405 -1.8676429127 3.4826598438

H 3.6238081302 -2.3759063093 1.8784145125

H 1.9871404382 -1.7264973728 2.1037083918

Version=AM64L-G03RevD.01 State=1-A\\HF=-730.8447551

Sum of electronic and zero-point Energies= -730.562865

Sum of electronic and thermal Energies= -730.546238

Sum of electronic and thermal Enthalpies= -730.545293

Sum of electronic and thermal Free Energies= -730.607771

E*-2 Conformation-2 (H_{rel} = 2.3 kcal/mol)

B3LYP/6-31+G(d)

0 1

C 2.2908277715 -1.0147192199 1.8625281572

H 2.983313264 -0.5543857773 2.5853715445

O 3.0891086267 -1.472419561 0.7490167513

C 3.5108754507 -0.5166574831 -0.1237155032

H 4.2188282579 -0.9256331924 -0.8376292941

C 3.1119486894 0.7609691021 -0.1232180805

H 3.5065128498 1.453178998 -0.8594243087

C 2.0930876792 1.2578726267 0.8610227484

H 2.5746344378 1.7537188936 1.7142502821

C 1.2818559909 0.0665561899 1.4247223977

H 0.722945101 0.399359914 2.3106973165

C 1.6574181151 -2.2535553407 2.4750639773

H 1.1028028606 -1.9915860956 3.3836142185

H 2.4348427695 -2.9768604953 2.7419213606

H 0.9764094605 -2.7270451775 1.7619903647

O 0.393564028 -0.4411217253 0.4434075547

C -0.9548470895 -0.5916803135 0.8633645511

H -1.5126861034 -0.9389959954 -0.0100907153

H -1.3762302785 0.363895368 1.2041452066

H -1.0536235276 -1.3364542363 1.66662932

O 1.2825208892 2.2370719646 0.1806783909

C 0.3867648634 2.9551781968 0.927106321

C -0.85537055 3.2160470894 0.5006186167

O 0.8491375822 3.4289437195 2.1323987325

C 1.8401719255 4.4627682565 2.0298789624

H 2.7220305312 4.1214572644 1.4750369588

H 2.1234996748 4.7153486224 3.0538214614

H 1.4159404218 5.3437169704 1.5318727724

H -1.4428655134 3.8892386779 1.1200726408

C -1.4679187024 2.6789116473 -0.7610407971

H -1.6411642907 3.4829918769 -1.4904351839

H -2.4457371201 2.2190156323 -0.5624095268

H -0.8215980652 1.9318736026 -1.2292671989

Version=AM64 L-G03RevD.01 State=1-A\\HF=-730.8436308

Sum of electronic and zero-point Energies= -730.562439

Sum of electronic and thermal Energies= -730.545626

Sum of electronic and thermal Enthalpies= -730.544682

Sum of electronic and thermal Free Energies= -730.607364

E*-2 Conformation-3 (H_{rel} = 3.2 kcal/mol)

B3LYP/6-31+G(d)

0 1

C 1.142748568 2.7296983627 3.2242661787

H 0.9278822213 2.0048963354 4.0261662526

O -0.1432234811 3.2318546368 2.7772054987

C -0.885053193 2.3730419887 2.0233455907

H -1.906201139 2.726937485 1.9157127898

C -0.4263770428 1.2447963702 1.4667262441

H -1.1047514621 0.6176613207 0.8955881145

C 1.0074463276 0.8110466296 1.6225451429

H 1.0814691194 0.0052951996 2.3606414962

C 1.9064473863 1.9692905383 2.1194790403

H 2.7886646686 1.5260846415 2.5954846004

C 1.9080680655 3.9127111155 3.7930357961

H 2.8454565259 3.5697291241 4.245204191

H 1.3107225388 4.410896413 4.5634213494

H 2.1513641272 4.6340430256 3.0083521579

O 2.4750639666 2.8019543566 1.1239032908

C 1.6413926346 3.4413152785 0.1590234975

H 2.3252741169 4.013697122 -0.4736405399

H 0.9222115871 4.1264269149 0.6231116349

H 1.108638232 2.7118224744 -0.4587678251

O 1.557859078 0.312170982 0.3804174986

C 1.207355836 -0.9454454679 -0.0021445905

C 0.8387020374 -1.2352305855 -1.2619202098

O 1.3572160791 -1.8331550759 1.0273813602

C 0.9921549294 -3.1888448685 0.8033553713

H -0.0528372312 -3.2650574738 0.4768673549

H 1.1203038861 -3.6949259123 1.7619572638

H 1.645161412 -3.6524277026 0.0530219463

H 0.6909553244 -2.2769966354 -1.5275782619

C 0.6739612793 -0.2190839836 -2.3587194529

H -0.3150983013 -0.3000011051 -2.8304364344

H 1.4188530218 -0.3638453412 -3.1541665002

H 0.7881688812 0.7996438366 -1.979839847

Version=AM64L-G03RevD.01 State=1-A\\HF=-730.8430482

Sum of electronic and zero-point Energies= -730.561050

Sum of electronic and thermal Energies= -730.544407

Sum of electronic and thermal Enthalpies= -730.543463

Sum of electronic and thermal Free Energies= -730.605960

E*-2 Conformation-4 (H_{rel} = 3.8 kcal/mol)

B3LYP/6-31+G(d)

0 1

C -0.453641479 -0.0104740057 -0.8960862564

H 0.150012059 -0.8782933032 -1.2077794807

O -0.203514909 1.028170048 -1.8766095169

C 1.0149895292 1.6302895238 -1.796419587

H 1.2225288652 2.2199301602 -2.6844943819

C 1.856653359 1.5338534828 -0.7590823499

H 2.8144949576 2.0426367295 -0.8006510668

C 1.527298613 0.7341422367 0.4708243456

H 2.0914585482 -0.2086443603 0.4734370289

C 0.0153514883 0.3737133804 0.521084814

H -0.096492866 -0.525481899 1.135937184

C -1.9309515992 -0.3562614877 -0.982162407

H -2.1539396744 -1.212303711 -0.335519272

H -2.1951371607 -0.6187254021 -2.0116231919

H -2.548806748 0.4862759881 -0.660152636

O -0.8180713474 1.3154734712 1.1804472897

C -0.808234343 2.6863653892 0.7752696779

H -1.5465318791 3.1778949873 1.4147602757

H -1.1049875043 2.8058197433 -0.2727571649

H 0.1720206701 3.144652013 0.9384767273

O 1.9503396146 1.4896332773 1.6327495113

C 2.570924399 0.7782467907 2.6296420324

C 3.8033372945 1.0714327466 3.0622340329

O 1.8482201053 -0.2583043629 3.1619116093

C 0.7238621571 0.1375207173 3.9723263961

H 0.0146357281 0.7398738732 3.3969381721

H 1.0772699338 0.6987223937 4.846801114

H 0.2495226101 -0.7905311903 4.2991031129

H 4.1580023482 0.5009563564 3.9171946048

C 4.7143801236 2.110119212 2.4746236547

H 5.665768553 1.6655311032 2.1507395538

H 4.9628029903 2.8830848681 3.2150906776

H 4.2544355629 2.6046812304 1.6147454962

Version=AM64L-G03RevD. 01 State=1-A\\HF=-730.8417382

Sum of electronic and zero-point Energies= -730.560101

Sum of electronic and thermal Energies= -730.543415

Sum of electronic and thermal Enthalpies= -730.542470

Sum of electronic and thermal Free Energies= -730.604426

E*-2 Conformation-5 (H_{rel} = 4.8 kcal/mol)

0 1

C 1.6749194958 3.2862286305 2.2264657433

H 0.8848510647 4.0198122954 2.4548075622

O 2.3991527776 3.7872601878 1.0850294143

C 1.7703416778 3.6733554776 -0.121855399

H 2.2917455876 4.2408037262 -0.8863306601

C 0.6662073938 2.9548900721 -0.3551723992

H 0.2358601724 2.9339843113 -1.3492650064

C -0.0029113741 2.1790861252 0.7482654219

H -0.8375808324 2.7638294893 1.1544297164

C 0.9856368613 1.9425381405 1.9107923666

H 0.4191250516 1.6219133694 2.7967587943

C 2.6675627565 3.2258186399 3.3764698489

H 2.164460125 2.9294773147 4.3043520687

H 3.1203897991 4.210821787 3.5293910975

H 3.4652501984 2.5106734642 3.1554133424

O 1.9458412662 0.9550851229 1.5631943017

C 2.0970919268 -0.1010655432 2.5005500432

H 2.4318870096 0.2673366235 3.4809386794

H 2.8614601552 -0.7684009444 2.0941513866

H 1.1620002686 -0.6640412569 2.6217601449

O -0.703583252 0.9839837248 0.3346172059

C -0.0828823809 -0.0874454245 -0.2354557559

C -0.3972428038 -1.3450435976 0.1241421117

O 0.7464705507 0.2836343236 -1.245735835

C 1.6143504626 -0.6972786241 -1.7953734795

H 1.0527860764 -1.4522292772 -2.3615197026

H 2.1960105529 -1.1867856047 -1.0048437798

H 2.2827669789 -0.1596916603 -2.4707104453

H 0.0210083415 -2.1600697616 -0.4580167198

C -1.3427276684 -1.7097659168 1.2362210076

H -2.2451925682 -2.2053782551 0.8497031999

H -1.6685675427 -0.8252415794 1.7908693067

H -0.8804881288 -2.4100953799 1.9469564184

Version=AM64L-G03RevD.01 State=1-A\\HF=-730.8402325

Sum of electronic and zero-point Energies= -730.558580

Sum of electronic and thermal Energies= -730.542028

Sum of electronic and thermal Enthalpies= -730.541084

Sum of electronic and thermal Free Energies= -730.602393

E*-2 without Methoxy groups:

B3LYP/6-31+G(d)

0 1

C 2.2169358885 -1.0889629097 1.763169401

H 1.4669720389 -1.8898324003 1.6630411761

O 2.0746708948 -0.5683670588 3.1085318893

C 1.0095420261 0.255502223 3.3107094829

H 0.86321203 0.4490863 4.3692868307

C 0.2301106006 0.7721566044 2.3495839601

H -0.604294874 1.4081124778 2.6294167183

C 0.5190793207 0.5461828614 0.8886937323

H -0.2096732152 -0.1515384525 0.4439139152

C 1.9384783185 -0.000385196 0.7263615193

H 2.0850581137 -0.3989895013 -0.2837981059

C 3.6147037708 -1.6795188402 1.6675694757

H 3.7487999513 -2.181256621 0.7024942208

H 3.7751318121 -2.4127832054 2.4647573859

H 4.3734640672 -0.8945096071 1.7619180049

O 0.4457177539 1.7740815279 0.1386282151

C -0.8145006546 2.2162955031 -0.1637845559

C -1.0836687648 3.4893022807 -0.478728044

H -2.1110511305 3.7076323567 -0.763418741

C -0.0921942271 4.6180670457 -0.4940645308

H -0.4446008506 5.4608029115 0.1160534614

H 0.057016483 5.004275115 -1.5123866256

H 0.8802055139 4.2981357921 -0.1092078107

H 2.6470614686 0.8254821054 0.8649628195

H -1.5851763355 1.4440286877 -0.1737037946

Version=AM64L-G03RevD.01 State=1-A\\HF=-501.8044446

Sum of electronic and zero-point Energies= -501.588339

Sum of electronic and thermal Energies= -501.576723

Sum of electronic and thermal Enthalpies= -501.575779

Sum of electronic and thermal Free Energies= -501.626713

Z*-A (alternative substrate)

B3LYP/6-31+G(d)

0 1

H 4.0327156649 0.1159101439 0.6180977202

C 3.1965929427 0.4474215462 -0.0185196095

O 3.6306215151 1.6083554297 -0.7467036368

C 3.6259283618 2.7851794115 -0.0577698952

H 4.1216284854 3.5675078877 -0.6234729978

C 3.084664181 2.9720047851 1.1510635077

H 3.1395336074 3.94704529 1.6232423295

C 1.9832174206 0.7491583507 0.8811282324

H 1.7349364421 -0.1648441313 1.4387187452

C 2.3713109574 1.8663323145 1.8766528637

H 3.023198113 1.4317788263 2.6488513061

C 2.9149644474 -0.6521864306 -1.0429598099

H 2.8071902535 -1.6062108019 -0.5029932841

H 3.7741880689 -0.7388618313 -1.7164156861

O 1.767528204 -0.4085816314 -1.8426447919

Si 0.3722253513 0.288100419 -1.2293594244

O 0.8631334109 1.1651306685 0.1157352004

C -0.8447281176 -1.0514586437 -0.7230752273

H -1.117091683 -1.6769551102 -1.5825852315

H -1.7668531689 -0.6162271256 -0.3179166829

H -0.423883297 -1.7098058419 0.0471238688

C -0.3353939024 1.4659876411 -2.4912713945

H 0.3996119824 2.2355046296 -2.7514014761

H -1.233221485 1.9652106798 -2.1067584026

H -0.6134697433 0.9342189648 -3.4095573404

O 1.2365289838 2.4507777036 2.5216460293

C 0.5234558041 1.7372917577 3.4439105345

C 0.8823072989 0.5978860066 4.0612132995

H 1.8691666793 0.1909304939 3.8657387307

C 0.0259516909 -0.1223993476 5.0679056345

H 0.4435213137 -0.0501424726 6.0828124038

H -0.0514042449 -1.192694867 4.8315100203

H -0.9849259748 0.2934335027 5.0975096376

O -0.6379204998 2.3694162908 3.7517505104

C -1.3153043129 3.0701853343 2.6973509691

H -0.7651841244 3.9674418386 2.4017454261

H -2.2849398258 3.3464321142 3.1163751884

H -1.4508008006 2.4227262041 1.8243227332

Version=AM64L-G03RevE.01 State=1-A\\HF=-1134.9933578

Sum of electronic and zero-point Energies= -1134.680509

Sum of electronic and thermal Energies= -1134.659960

Sum of electronic and thermal Enthalpies= -1134.659016

Sum of electronic and thermal Free Energies= -1134.730819

Z*[b]-A (H_{rel} = 0.4 kcal/mol)

B3LYP/6-31+G(d)

0 1

H -0.2389248942 -2.3068765466 1.4589759749

C -0.3776973381 -1.2219201696 1.5094912314

O -1.8076690537 -1.0387304517 1.5678769425

C -2.3246780205 0.0966088047 1.0254496343

H -3.387489457 0.1654604566 1.2372636153

C -1.6562050655 1.0082645183 0.3056506015

H -2.1911743821 1.8738923663 -0.0707059873

C 0.2280084825 -0.6025740664 0.2306178414

H -0.1846900792 -1.156318345 -0.6230530429

C -0.191733343 0.860544188 0.0177092464

H 0.0289270226 1.1409148084 -1.0175598539

C 0.2548528554 -0.7256658075 2.8190499013

H -0.2310297655 -1.2335306979 3.6584514257

H 0.1152190655 0.3545468839 2.9330076668

O 1.6405214736 -1.0604574004 2.856918215

Si 2.6491518379 -0.8692866939 1.5335778229

O 1.6357034419 -0.7750689489 0.1920894362

C 3.6994828163 -2.410993505 1.3639283299

H 4.3394231585 -2.5464896337 2.2448952043

H 4.3511613262 -2.3491061801 0.4833012715

H 3.0733019133 -3.3045081826 1.2601391836

C 3.7248029048 0.656047792 1.7003093611

H 4.3980924169 0.5528081237 2.5610392661

H 3.1174955839 1.5547764703 1.8434902241

H 4.3475345705 0.798220701 0.8077367277

O 0.6254373931 1.7012943303 0.8866786053

C 0.5661746477 3.05263746 0.6479318635

C 0.2369803729 3.9207778545 1.6119729154

H -0.0890790519 3.4926239997 2.5562925649

C 0.280579319 5.4165028133 1.4838806883

H 0.9285225658 5.8622169704 2.2512979907

H -0.7180157207 5.8543705792 1.620746704

H 0.6493148796 5.7230270555 0.5010129174

O 0.8616608398 3.4426038537 -0.6315938809

C 2.1674846947 3.0773827025 -1.107701465

H 2.9411389056 3.5648543495 -0.5012884661

H 2.2219546856 3.4383290258 -2.1366769739

H 2.314459998 1.9928225217 -1.0832047036

Version=AM64L-G03 RevE.01 State=1-A\\HF=-1134.9931848

Sum of electronic and zero-point Energies= -1134.679807

Sum of electronic and thermal Energies= -1134.659413

Sum of electronic and thermal Enthalpies= -1134.658469

Sum of electronic and thermal Free Energies= -1134.729288

Z*-A Conformation-1 (H_{rel} = 0.7 kcal/mol)

B3LYP/6-31+G(d)

0 1

H 0.4814308603 0.9225851797 4.0421555367

C -0.097017793 0.6465712663 3.146515987

O -0.4250194486 -0.7512255061 3.2441240758

C 0.562543419 -1.6291840749 2.9019114372

H 0.2758661487 -2.6472139398 3.1452034782

C 1.7287728665 -1.2977122097 2.3363339602

H 2.4571837952 -2.0671314411 2.104243814

C 0.7510861667 0.9467801674 1.8951184334

H 0.9979796712 2.0185696268 1.8876184588

C 2.0555146762 0.1273196611 1.9946491161

H 2.6757810112 0.5897534726 2.7785028498

C -1.4133034593 1.420852698 3.174015586

H -1.1824370061 2.4875060066 3.3202606165

H -2.0080955183 1.0813401384 4.0288794014

O -2.20289672 1.2491597403 2.0067849027

Si -1.5557471128 1.0411728341 0.4762137087

O 0.0475322042 0.6030135893 0.7112295057

C -1.6656202926 2.6566864575 -0.4770670152

H -1.1093807449 3.4597888138 0.0219146371

H -2.7101594068 2.981202668 -0.56665003

H -1.2603452402 2.5493975282 -1.4910339877

C -2.4382995321 -0.354926319 -0.3950239672

H -3.5016838596 -0.1222054608 -0.531362606

H -2.3625440089 -1.2789549264 0.1885407705

H -2.0045922448 -0.5396045954 -1.3856104509

O 2.8432903148 0.1286981961 0.7880403201

C 3.566888467 1.2710677273 0.5304633754

C 4.8213392726 1.4336279788 0.9705046135

H 5.2194267409 0.6421586061 1.6013833772

C 5.7020273281 2.6128539277 0.6717356248

H 5.959488599 3.1613230786 1.5888773861

H 5.2123906077 3.3110110265 -0.012598056

H 6.6502143556 2.2915426417 0.2192284052

O 2.9150725117 2.2273963314 -0.1990013101

C 2.3567479442 1.7748936611 -1.4447015372

H 1.8740722225 2.6485558332 -1.8873895951

H 1.6244102092 0.9826567824 -1.2743493082

H 3.1560829953 1.4186728342 -2.1076615145

Version=AM64L-G03RevE.01 State=1-A\\HF=-1134.9919775

Sum of electronic and zero-point Energies= -1134.679324

Sum of electronic and thermal Energies= -1134.658875

Sum of electronic and thermal Enthalpies= -1134.657931

Sum of electronic and thermal Free Energies= -1134.729827

Z*-A Conformation-2 (H_{rel} = 1.3 kcal/mol)

B3LYP/6-31+G(d)

0 1

H 3.6028672252 0.307966912 -1.2681779894

C 3.0718159221 0.9802867996 -0.5862753408

O 4.0076361725 2.047016017 -0.3225617079

C 3.9628783625 2.6451715836 0.8982959785

H 4.6532485869 3.4828175281 0.9322575465

C 3.2057340183 2.2723526119 1.9399495353

H 3.2642136015 2.8410888984 2.8618507164

C 2.7256334787 0.1890232182 0.6934816516

H 3.6518102255 -0.2899237348 1.0385101606

C 2.2787552715 1.0944525761 1.8542691732

H 2.2978788394 0.50720168 2.7804109437

C 1.8521404884 1.5428223913 -1.3330079494

H 2.200122853 2.0713200002 -2.2266531555

H 1.3017428173 2.2486011325 -0.7008707634

O 1.0000266229 0.4843548538 -1.7615085651

Si 0.6348857368 -0.833994602 -0.7922666269

O 1.8012906931 -0.848642671 0.4200835529

C 0.8344834542 -2.3892468156 -1.8177084892

H 0.127550256 5 -2.3972347825 -2.6569003427

H 0.6472056739 -3.286027994 -1.2138321287

H 1.8479265652 -2.4627825929 -2.2287298194

C -1.0957481478 -0.7160792038 -0.0871526274

H -1.8376190445 -0.7150184888 -0.8961880545

H -1.2234399302 0.1966127285 0.5023886779

H -1.3130639643 -1.5746121858 0.5613729394

O 0.8856620362 1.4801236873 1.6410951106

C 0.192937306 1.8646356489 2.7642283533

C -0.5725832526 1.009365332 3.4544160639

H -0.5584753916 -0.0257023409 3.1232020568

C -1.4175136183 1.3630591671 4.6443542729

H -1.0694004277 0.8416032373 5.5471239992

H -2.4624495375 1.061724503 4.4885346207

H -1.3942881644 2.4373569708 4.8461558481

O 0.354499458 3.1694457862 3.146074511

C 0.1709875404 4.154353783 2.1207040666

H 0.9406574876 4.0689848886 1.3477795233

H 0.2536102118 5.121726279 2.620317287

H -0.8236194264 4.0557971976 1.6669769709

Version=AM64L-G03RevE.01 State=1-A\\HF=-1134.9914709

Sum of electronic and zero-point Energies= -1134.678396

Sum of electronic and thermal Energies= -1134.657873

Sum of electronic and thermal Enthalpies= -1134.656929

Sum of electronic and thermal Free Energies= -1134.728326

Z*-A Conformation-3 (H_{rel} = 3.1 kcal/mol)

B3LYP/6-31+G(d)

0 1

H 2.6898395201 2.745163735 -0.7838067926

C 2.8958286868 2.356028414 0.225900739

O 3.7204412753 1.1841390944 0.0885283795

C 3.0791609627 0.0220836244 -0.227386074

H 3.7945385431 -0.7683124185 -0.4316533495

C 1.751519248 -0.1412366052 -0.2719481958

H 1.341859964 -1.1134489739 -0.5271696687

C 1.5570230126 2.0324958115 0.9188053132

H 0.9491853039 2.9500062989 0.9556045741

C 0.8152564413 0.9868267615 0.075738216

H 0.4422044878 1.4922751925 -0.8243495931

C 3.7159752398 3.4037573858 0.9787257486

H 3.1958387307 4.3712018867 0.894088627

H 4.6940715942 3.5024123055 0.4955479937

O 3.9425045187 3.087857836 2.3438601521

Si 2.7933064012 2.3260546175 3.2998261304

O 1.7741288475 1.5387046355 2.2285123205

C 1.8392030864 3.6018747532 4.2966019415

H 2.5061980296 4.1484512815 4.9753040913

H 1.0604290783 3.1214241233 4.9020479891

H 1.3481756657 4.3388953778 3.6489361548

C 3.6322134363 1.0557814335 4.3791478412

H 4.3453658562 1.5309574448 5.0640027991

H 4.1787518736 0.3331753931 3.7632965934

H 2.8990286807 0.5066425293 4.9825157889

O -0.3251530766 0.5373751142 0.8269259942

C -1.3198776483 -0.0994436367 0.1408896249

C -1.8963523964 -1.1993303475 0.6466337073

H -1.4180274253 -1.621089441 1.5262270115

C -3.1730447649 -1.829266692 0.1614545396

H -3.8068703051 -2.1018862375 1.0148569902

H -2.9987508411 -2.7543902878 -0.4078654505

H -3.7514810972 -1.1467638412 -0.470011187

O -1.7327483443 0.576116111 -0.9836362452

C -1.6487736606 -0.1230553211 -2.2315263951

H -1.9711594493 0.5892855073 -2.9945462285

H -2.3037774476 -0.9995335347 -2.2522043411

H -0.6170290278 -0.4372313308 -2.43287274

Version=AM64 -G03RevE.01 State=1-A\\HF=-1134.9881215

Sum of electronic and zero-point Energies= -1134.675583

Sum of electronic and thermal Energies= -1134.655027

Sum of electronic and thermal Enthalpies= -1134.654083

Sum of electronic and thermal Free Energies= -1134.726109

Z*-A Conformation-4 (H_{rel} = 3.5 kcal/mol)

B3LYP/6-31+G(d)

0 1

H 3.7377999097 -0.0111094474 2.9171810872

C 2.9325320148 0.2502858057 2.2146638937

O 3.3714411111 -1.4565065447 1.555752161

C 2.9848909396 -1.6518683836 0.2679278158

H 3.3019979262 -2.6317074737 -0.076630243

C 2.3264078427 -0.7775868565 -0.5060335788

H 2.0874912129 -1.0603584959 -1.5251873873

C 2.7941443811 0.92897461 1.2260300232

H 3.7972483651 1.1413013856 0.8326315623

C 1.9322859002 0.5806719946 -0.0019457559

H 2.1071051808 1.338342314 -0.7755770516

C 1.6664602282 -0.543517081 3.033614903

H 1.8656590593 -1.39047274 3.698194287

H 0.8272039298 -0.7995793789 2.377858903

O 1.3433242696 0.5792729744 3.8503459456

Si 1.4209162054 2.1557864439 3.2910135175

O 2.3494351896 2.1029585256 1.8855260508

C 2.3359245256 3.1873056418 4.5599732131

H 1.7904326653 3.2090297741 5.5118098977

H 2.4517570716 4.2232156879 4.2171639353

H 3.3353505257 2.7806633917 4.7531690032

C -0.2854706179 2.855747789 2.9680766415

H -0.8722561118 2.8471290804 3.8957878873

H -0.8247760715 2.2736830085 2.2148153817

H -0.2296058476 3.8964468402 2.6237178378

O 0.5328335582 0.6708701967 0.391368886

C -0.4141850228 0.7706956721 -0.6039447496

C -0.8654114163 -0.2793933947 -1.3041843628

H -0.4563102962 -1.2505110761 -1.0410617712

C -1.9238878858 -0.219976074 -2.3684354085

H -2.8349835634 -0.7467557408 -2.0506039836

H -1.5839190937 -0.7063365706 -3.2929584907

H -2.199076951 0.812093717 -2.6014554106

O -0.9865556199 2.0064863156 -0.7218599536

C -0.106365212 3.131162724 -0.8274776776

H 0.5768761894 3.1847022491 0.024426488

H -0.7505608227 4.0124432936 -0.8404202954

H 0.4648463308 3.0849814337 -1.7652732017

Version=AM64L-G03RevE.01 State=1-A\\HF=-1134.9883199

Sum of electronic and zero-point Energies= -1134.674858

Sum of electronic and thermal Energies= -1134.654573

Sum of electronic and thermal Enthalpies= -1134.653628

Sum of electronic and thermal Free Energies= -1134.723906

E*-A

B3LYP/6-31+G(d)

0 1

H 0.5353585923 1.9540955333 3.98676415

C 0.9409972858 1.0460427472 3.5133065641

O 2.3760826418 1.1531705532 3.5068868068

C 2.9206512941 1.9317420474 2.5261721753

H 3.9848185137 2.0685586394 2.6904609797

C 2.2504626321 2.4551380702 1.4931888691

H 2.7770442335 3.0685416978 0.7692546186

C 0.3753720762 0.9322582649 2.0845017903

H 0.7235123209 0.8906456738 2.1417302575

C 0.780272358 2.190513699 1.3051454428

H 0.1776755073 3.0277734671 1.6779391419

C 0.5756508133 -0.1492300505 4.3924984461

H -0.5067339233 -0.1079711924 4.59224028

H 1.1006477465 -0.0590257298 5.3497062749

O 0.9179415628 -1.4074722759 3.8319715615

Si 0.872113106 -1.7248245175 2.1859272714

O 0.8730575528 -0.2259487578 1.4376111107

C -0.6981945294 -2.6665886291 1.7645393455

H -0.7304717145 -3.6302664092 2.288517403

H -0.7590598972 -2.8654412111 0.6871996045

H -1.5952983265 -2.1029124013 2.0496137388

C 2.4135329933 -2.6504969946 1.6832785079

H 2.4729716853 -3.6212090037 2.1908737931

H 3.3078773574 -2.0733078383 1.942458837

H 2.4256240305 -2.8340020126 0.60187833

O 0.4245918361 1.9731485876 -0.0746867015

C 0.5569633418 3.0180888096 -0.933713347

C 1.1023460866 2.8683543391 -2.1527910171

O 0.0136615733 4.1597966727 -0.4108457266

C 0.1069621679 5.3545510183 -1.175621167

H 1.1530761366 5.5896114611 -1.4100599185

H -0.320472581 6.1427270833 -0.5530345623

H -0.4666071442 5.2700139145 -2.1074991536

H 1.0743179055 3.7085491631 -2.8392353758

C 1.7036016393 1.5829730564 -2.6533949961

H 1.1210523104 1.1663156238 -3.4877199743

H 1.7410425621 0.8299437434 -1.862084788

H 2.7245828946 1.7421431577 -3.0269785728

Version=IA32L-G03 RevD.01 State=1-A\\HF=-1134.9948109

Sum of electronic and zero-point Energies= -1134.681899

Sum of electronic and thermal Energies= -1134.661467

Sum of electronic and thermal Enthalpies= -1134.660522

Sum of electronic and thermal Free Energies= -1134.732624

E*[b]-A (H_{rel} = 0.5 kcal/mol)

B3LYP/6-31+G(d)

0 1

H 1.1919790394 0.157354346 4.4191520468

C 1.5480472063 0.6703099186 3.5197433295

O 2.4783418906 1.6620357103 4.0069072747

C 2.5858926847 2.8298700267 3.3182754108

H 3.3827107682 3.4394300602 3.7340339047

C 1.8229825887 3.2183488272 2.2864664822

H 2.0181128546 4.1810757199 1.8247512271

C 0.330256492 1.3186300365 2.8267403314

H -0.2087494589 1.8933994513 3.5917218995

C 0.7269931433 2.3438315547 1.753082542

H -0.1581624043 2.9235270133 1.4825106127

C 2.302955154 -0.3543055453 2.6574600191

H 3.1230346887 -0.7740955599 3.2492953811

H 2.7238527498 0.1258995703 1.7679853762

O 1.4436804443 -1.4295124895 2.2880396937

Si -0.1367074445 -1.190255994 1.780220102

O -0.5667786704 0.3355002826 2.3435891445

C -1.2245676626 -2.4499644298 2.6404077835

H -0.946006145 -3.4709386218 2.3505867198

H -2.279414848 -2.3030690646 2.3763134526

H -1.1333232035 -2.370272112 3.7297064609

C -0.3073621202 -1.3251728587 -0.0805325958

H -0.0800814856 -2.3467090216 -0.4119876924

H 0.3659772138 -0.6351241665 -0.5973759567

H -1.3344102475 -1.0938251276 -0.3909331237

O 1.1595129262 1.6182735313 0.5620800534

C 1.1383689772 2.2739236786 -0.6294557748

C 2.1613071772 2.2136719572 -1.4996477397

O -0.0567704513 2.909122124 -0.8186571698

C -0.2224318381 3.6903376609 -1.9951472819

H 0.5606323098 4.4554594101 -2.0719215663

H -1.2005678884 4.1657198487 -1.9021364244

H -0.2055170953 3.0579765192 -2.8918509479

H 2.025199036 2.6539232775 -2.4821950369

C 3.4768450548 1.5352968441 -1.2311305778

H 3.5970245976 0.6256515491 -1.8371221766

H 3.5738277159 1.2508979419 -0.1802032169

H 4.3173162503 2.196778131 -1.4807719667

Version=IA32L-G03RevD.01 State=1-A\\HF=-1134.9948352

Sum of electronic and zero-point Energies= -1134.681030

Sum of electronic and thermal Energies= -1134.660776

Sum of electronic and thermal Enthalpies= -1134.659832

Sum of electronic and thermal Free Energies= -1134.730513

E*-A Conformation-1 (H_{rel} = 1.6 kcal/mol)

B3LYP/6-31+G(d)

0 1

H 3.7916626126 2.4518577694 -0.2314496957

C 3.2457488798 1.551421195 0.0688448738

O 3.9963988031 0.4609649728 -0.5036861195

C 3.3153693911 -0.6674531983 -0.8429517259

H 4.0068509065 -1.450825051 -1.1383956858

C 1.9838182287 -0.8184920839 -0.8488071747

H 1.5655980742 -1.7757936963 -1.1427032698

C 1.8207273356 1.6369926023 -0.5197582969

H 1.9271737856 1.869308657 -1.5877199766

C 1.0631242902 0.3003577982 -0.4606043317

H 0.2105639413 0.3524771765 -1.1443581324

C 3.2966835937 1.4586195368 1.6015467212

H 4.3442242895 1.4148615053 1.9166761679

H 2.7877684467 0.5544221351 1.9528933764

O 2.7181578395 2.6220832781 2.1879202118

Si 1.2949866476 3.3014978917 1.622441014

O 1.0865007635 2.7017324839 0.0631723045

C 1.5286306388 5.1564316471 1.5086257675

H 2.3762224656 5.4082961702 0.8609804019

H 1.7201060742 5.587337841 2.4993815212

H 0.63350493 5.6420008554 1.0999603552

C -0.1539567686 2.8776660075 2.7325347513

H 0.0019517785 3.3018093129 3.7328301049

H -0.2740067585 1.7947184268 2.8324207306

H -1.0901203218 3.2936123405 2.3386557727

O 0.5333637068 0.124681128 0.887097676

C -0.4713937009 -0.8000736177 1.0283262893

C -0.4441085044 -1.7718098166 1.9485794673

O -1.5301952712 -0.6650104107 0.1664381574

C -2.2706123589 0.5604320864 0.2854064523

H -3.0646731942 0.5040235295 -0.4619868162

H -1.6378309205 1.4329217881 0.0919963707

H -2.7088784703 0.6394231124 1.2883631387

H -1.3487257324 -2.3684443414 2.0354880767

C 0.7104957306 -2.0994079589 2.8505104795

H 1.5845179737 -1.4822899487 2.6263749999

H 1.0021771839 -3.1536992516 2.748456167

H 0.4481736903 -1.9446518726 3.9064998757

Version=IA32L-G03RevD.01 State=1-A\\HF=-1134.9928309

Sum of electronic and zero-point Energies= -1134.679353

Sum of electronic and thermal Energies= -1134.659007

Sum of electronic and thermal Enthalpies= -1134.658063

Sum of electronic and thermal Free Energies= -1134.728548

E*-A Conformation-2 (H_{rel} = 4.5 kcal/mol)

B3LYP/6-31+G(d)

0 1

H 0.8712100193 -2.1051249822 2.1876844718

C 0.8423993993 -1.432742694 1.3241363305

O 1.1957561331 -2.2659577835 0.1993732498

C 1.8457746503 -1.6816864535 -0.8407727851

H 1.9591375271 -2.3862336257 -1.6594750782

C 2.3163763239 -0.4268145906 -0.8789698497

H 2.825690009 -0.0872835293 -1.7754451263

C 1.8798230039 -0.312708333 1.5565628632

H 2.8295362707 -0.7992987822 1.8165423544

C 2.1676697204 0.5079737857 0.2855205281

H 3.0854126913 1.081023167 0.4357821992

C -0.6031271225 -0.937103041 1.1586887698

H -1.256296732 -1.8043101399 1.0164131496

H -0.6929492854 -0.2841530909 0.2836078783

O -1.0340028883 -0.2611776081 2.3363706338

Si -0.0600103176 0.8201178496 3.1677803823

O 1.5151508854 0.4983272474 2.6591317482

C -0.1675480818 0.4250785109 4.9959770462

H 0.1239632671 -0.6125741444 5.1950128857

H -1.1910109285 0.5657091416 5.3657649916

H 0.491449632 1.0803924057 5.5793542575

C -0.5551724568 2.5950655375 2.839391262

H -1.5770577918 2.7712013975 3.1997973884

H -0.5216882489 2.8356097687 1.7727495848

H 0.1071147911 3.2930853812 3.3670672643

O 1.0789428463 1.4533547965 0.0776075505

C 1.351722335 2.6820389538 -0.4728111914

C 2.2300362527 3.5917514717 -0.0221002737

O 0.5066259215 3.0003204664 -1.4975417082

C 0.3755558772 2.0515235217 -2.5606354463

H 1.3211858751 1.9610517256 -3.1125692021

H -0.3955078319 2.4515552807 -3.2218395057

H 0.0730870634 1.0697567963 -2.1850507881

H 2.316086263 4.4868264393 -0.6324275847

C 3.0261030966 3.5401350151 1.2535965355

H 4.1001187434 3.388048081 1.0691838144

H 2.6822156273 2.7524210804 1.9292170933

H 2.9362274601 4.4958009772 1.7873243063

Version=IA32L-G03RevD.01 State=1-A\\HF=-1134.9883813

Sum of electronic and zero-point Energies= -1134.674738

Sum of electronic and thermal Energies= -1134.654539

Sum of electronic and thermal Enthalpies= -1134.653595

Sum of electronic and thermal Free Energies= -1134.723413

Z*-6

B3LYP/6-31+G(d)

0 1

H 1.2569018113 -2.1335556966 0.3174143696

C 1.0734628175 -1.5658135424 1.2348621941

O 0.7607638365 -2.5754761962 2.2192585154

C -0.2970195948 -2.3974320379 3.0515561513

H -0.4270857582 -3.2711193626 3.6833625815

C -1.0915734195 -1.3207898953 3.1061387842

H -1.9072995832 -1.2998796268 3.8204925635

C -0.0942533023 -0.5838706777 0.9637106021

H -0.8504709392 -1.1269501144 0.3798211253

C -0.8233894706 -0.1303525685 2.2377374267

H -1.7565848242 0.3620279078 1.9444764766

C 2.3967728832 -0.8797728084 1.6044738575

H 3.1352824156 -1.6499294869 1.8484953561

H 2.2719576966 -0.220727339 2.470077995

O 2.8873318863 -0.1541071933 0.4746087242

Si 1.873992783 0.886546936 -0.3708709947

O 0.3266103536 0.5315148566 0.191919296

C 2.0002607672 0.4040877265 -2.2281086713

C 2.2496761631 2.7136593519 0.0840900627

O 0.0097630974 0.8597071267 2.9145265019

C -0.5049870007 1.3864781944 4.073115276

C 0.1780476806 1.3562844442 5.2232913521

H 1.109463857 0.796192175 5.217759349

C -0.2423631685 2.0257449793 6.5001625198

H 0.5260333773 2.7278840571 6.8524398338

H -0.3888517036 1.2893323983 7.3026203065

H -1.1793876878 2.5753492207 6.3741126379

O -1.7572793494 1.9351843054 3.9694851161

C -1.8771902835 3.0364581829 3.0559904435

H -1.253455006 3.8756557752 3.3886902884

H -2.9293901901 3.3277493772 3.0724369424

H -1.586268253 2.748252576 2.0404465971

C 3.4858883811 3.2567873067 -0.6678396901

H 4.3800299152 2.6469882306 -0.4880600607

H 3.7107941916 4.2751534649 -0.3172923946

H 3.3277566468 3.3163177749 -1.7504714756

C 2.5428154887 2.7844673457 1.6017613878

H 3.4344724566 2.2047686802 1.8681747212

H 1.7046350027 2.414361925 2.199142319

H 2.7294969424 3.8296537269 1.891760738

C 1.0315871833 3.6142162399 -0.2255856475

H 1.2439166734 4.6468353847 0.0899535478

H 0.1374682405 3.2775052442 0.3095833328

H 0.791513703 3.6438309608 -1.2947021066

C 3.4773406841 0.3203987391 -2.6790308628

H 4.0449109322 -0.3928541288 -2.0704163174

H 3.9884364442 1.2873704182 -2.6267165608

H 3.5282612011 -0.0179655381 -3.7249662467

C 1.3605898144 -0.9898785904 -2.4265198752

H 1.8912814567 -1.7672890482 -1.8643553164

H 1.4069499446 -1.2713008449 -3.4889916416

H 0.3052224879 -1.004927968 -2.1293189513

C 1.2423455973 1.410182489 -3.1234292128

H 1.6821496895 2.4130401119 -3.0885445984

H 0.1851676691 1.4951167313 -2.841934001

H 1.2764973617 1.0778882996 -4.1717946675

Version=AM64L-G03RevD.01 State=1-A\\HF=-1370.8558866

Sum of electronic and zero-point Energies= -1370.371489

Sum of electronic and thermal Energies= -1370.343208

Sum of electronic and thermal Enthalpies= -1370.342264

Sum of electronic and thermal Free Energies= -1370.429269

Z*[b]-6 (H_{rel} = 5.2 kcal/mol)

B3LYP/6-31+G(d)

0 1

H -0.2409583638 3.3298154668 -2.0242633367

C -0.0177463477 2.4005338783 -1.4762324251

O -1.2317899263 1.6317819247 -1.4056803811

C -2.1510854839 2.053565321 -0.4876901269

H -3.1095459441 1.5704069181 -0.6511510652

C -1.9263017761 2.9413159821 0.4894502299

H -2.7387204406 3.2364515445 1.1412879553

C 0.5046441532 2.7684581389 -0.0757377597

H 1.3926663668 3.4049920634 -0.1940282266

C -0.5774511487 3.5899981282 0.653550023

H -0.5920873544 4.5781649892 0.175144612

C 0.9889296505 1.6024756075 -2.3026367082

H 1.8018695083 2.2833142578 -2.5984723066

H 0.4949015029 1.2496534949 -3.2148801214

O 1.529213872 0.470246864 -1.6387794212

Si 1.7746454364 0.3643960072 0.0189497729

O 0.8402374104 1.6070171566 0.67156525

C 3.6464086176 0.6762870499 0.3507147761

C 1.0286025874 -1.2844028663 0.6430508322

O -0.171638811 3.9392160574 1.9916750547

C -0.3446292738 3.1417388354 3.0921625737

C 0.6832580716 2.9131168 3.9215450357

H 1.6646950855 3.1976109105 3.5536119547

C 0.5845044861 2.3686695936 5.3201316788

H 1.2714537234 2.9091624404 5.9837077644

H 0.8577315604 1.3045339126 5.384862732

H -0.4242608802 2.4826602161 5.7314055168

O -1.6562654784 2.8342959364 3.3520742324

C -1.9926296538 1.4501142559 3.5057618104

H -3.063606248 1.4278023884 3.7219068593

H -1.4470930447 0.9867911279 4.3330940878

H -1.7909199387 0.9034936948 2.5785029597

C 1.8760220759 -2.4991576552 0.2025397506

H 2.002510827 -2.5419514004 -0.8862703698

H 1.3764413751 -3.4293552793 0.5115295658

H 2.8713368361 -2.5004708865 0.6610960896

C -0.388256338 -1.43444548 34 0.0399225505

H -0.3672868266 -1.4633452232 -1.0544630414

H -1.0478974628 -0.613165764 0.3380728588

H -0.8384351473 -2.3735887967 0.3954099062

C 0.9042226396 -1.2822458951 2.1847576578

H 0.3750833131 -2.189573907 2.5129711073

H 0.3396280051 -0.4160915192 2.5457885194

H 1.8787142317 -1.2774535118 2.6841149968

C 4.5095185711 -0.1557474522 -0.6273693881

H 4.2691373252 0.0671387294 -1.6729840537

H 4.3867385301 -1.2344151459 -0.4811736313

H 5.5742213547 0.074398267 -0.4709479977

C 3.9548803096 2.1732976894 0.1066989349

H 3.7129967543 2.4867159856 -0.9169536361

H 5.0299419191 2.3581945862 0.250966804

H 3.4158124584 2.8240146611 0.8046507974

C 4.0535966916 0.3363155124 1.8015254383

H 3.959991806 -0.7336848312 2.0178206605

H 3.4548373008 0.8841983438 2.5395118349

H 5.107211532 0.6077408804 1.9661808123

Version=AM64L-G03RevD.01 State=1-A\\HF=-1370.8477591

Sum of electronic and zero-point Energies= -1370.363247

Sum of electronic and thermal Energies= -1370.335309

Sum of electronic and thermal Enthalpies= -1370.334365

Sum of electronic and thermal Free Energies= -1370.420033

Z*-6 Conformation-1 (H_{rel} = 1.0 kcal/mol)

B3LYP/6-31+G(d)

0 1

H 3.3177356209 1.2431105608 3.1856135559

C 2.3561538322 0.7218736826 3.152679816

O 2.3455105484 -0.0808414364 4.3534410447

C 1.9687707062 -1.3844457551 4.2853884556

H 2.0935422694 -1.8607389605 5.2534930937

C 1.5071437081 -2.0217758956 3.2014844406

H 1.2305156252 -3.0672714068 3.2794331551

C 2.3089458093 -0.1141303725 1.8496678775

H 3.2940994693 -0.5856084291 1.7266245649

C 1.3165009036 -1.2878913534 1.9074330875

H 1.5026079053 -1.9390600257 1.0447753152

C 1.2644704805 1.7983620687 3.2416022754

H 1.3238537271 2.2796672908 4.2229833949

H 0.2670484194 1.3609768302 3.1213694898

O 1.5056245072 2.8012475617 2.2529457056

Si 1.8100492844 2.3636005347 0.6575163771

O 2.076029327 0.7016884912 0.7131750879

C 3.4350757369 3.248664753 0.1362914869

C 0.2611848717 2.6650601561 -0.4352262419

O -0.0399238434 -0.7704650994 1.7503748079

C -0.9945027033 -1.6972198084 1.4043025597

C -1.3735927003 -1.8826245399 0.1332362568

H -0.8333352028 -1.3138776668 -0.619018024

C -2.4609255536 -2.8119044557 -0.3237019669

H -2.0585269367 -3.6105025699 -0.9627778525

H -3.2108477002 -2.2763651142 -0.9219255156

H -2.96664657 -3.281719328 0.5241702414

O -1.5200540518 -2.4301215304 2.4345824925

C -1.9994721272 -1.6826917674 3.5599612733

H -2.7647141802 -0.96177343 3.2442596174

H -1.1823054627 -1.1589400147 4.064432164

H -2.4423345522 -2.4164742023 4.2365838212

C 0.1232667544 4.1463268399 -0.8542119078

H 0.0889322305 4.820091185 0.011079085

H -0.8154808135 4.2841937669 -1.4112010439

H 0.9376143907 4.4760274345 -1.5089294041

C -0.9930668511 2.2815484975 0.3859387521

H -1.104050869 2.9168196505 1.2726925372

H -0.966298692 1.2380045908 0.7123450369

H -1.8926140479 2.4168716813 -0.2333838559

C 0.3109257091 1.7822923762 -1.704057232

H -0.6101815436 1.9222894267 -2.28951815

H 0.3902508158 0.7196094875 -1.4521941353

H 1.1532911026 2.0352681201 -2.3584033794

C 3.3692507107 4.7623271911 0.4477168435

H 3.1681379214 4.9475938979 1.5091770588

H 2.5994749806 5.2788935728 -0.1348812896

H 4.3330222316 5.2340647285 0.2032560605

C 4.6114695286 2.6477233628 0.9404479396

H 4.499208779 2.8173723598 2.0177418121

H 5.5529441229 3.1273636645 0.6344043509

H 4.7211962671 1.5705099285 0.7675956624

C 3.7290136004 3.0423010612 -1.3670626758

H 2.9676022132 3.5010806765 -2.0073182479

H 3.7957004925 1.9792261304 -1.6306283365

H 4.6927097981 3.5053916012 -1.626777338

Version=AM64L-G03RevD.01State=1-A\\HF=-1370.8542693

Sum of electronic and zero-point Energies= -1370.369953

Sum of electronic and thermal Energies= -1370.341671

Sum of electronic and thermal Enthalpies= -1370.340727

Sum of electronic and thermal Free Energies= -1370.427582

Z*-6 Conformation-2 (H_{rel} = 2.8 kcal/mol)

B3LYP/6-31+G(d)

0 1

H 3.6489041205 2.389440924 -0.3981914592

C 3.028084437 1.5144497519 -0.6135954306

O 3.4672400912 1.0826798237 -1.921925038

C 2.5474513737 0.7226665462 -2.8525301201

H 3.0404372684 0.461338582 -3.7843406921

C 1.2181728536 0.6932818562 -2.6862657598

H 0.5935196038 0.3820451359 -3.5172020576

C 1.5454188904 1.9590730518 -0.5839202563

H 1.482221463 2.9215962383 -1.1108950263

C 0.6069169788 1.0182977784 -1.3563629951

H -0.363005709 1.513207406 -1.4573156849

C 3.3849509202 0.4453506652 0.4301469714

H 4.4305179573 0.1530865322 0.2894364237

H 2.7521161998 -0.4417448575 0.320241136

O 3.2646925401 1.0021232016 1.7404650572

Si 1.8836524699 1.8517987399 2.1879870784

O 1.0833768792 2.1637547381 0.7401355134

C 2.4811449563 3.5224235236 2.9259578502

C 0.7362679756 0.7696066932 3.2838743091

O 0.4056811547 -0.1877244735 -0.567858477

C -0.6829612667 -0.959252623 -0.8568310601

C -0.5671592668 -2.291595531 -0.9617721868

H 0.4486595847 -2.6760540775 -0.9790701551

C -1.6978904708 -3.2852443655 -0.969428663

H -1.415835078 -4.1769348008 -0.3963837191

H -1.9565610128 -3.6304367329 -1.9815366061

H -2.6050671673 -2.878308328 -0.5099560452

O -1.8521853447 -0.2409713665 -0.8756247364

C -2.6942363962 -0.3734085594 -2.0262849888

H -3.4534229967 0.4063602357 -1.9304743655

H -3.1825561291 -1.3516703007 -2.0666258046

H -2.1197203556 -0.2196427904 -2.9481357025

C 1.1479951703 0.8004663018 4.7734228459

H 2.1843602512 0.4732620805 4.9238779956

H 0.5048759313 0.1144979667 5.3446303894

H 1.0372631425 1.7939122057 5.2215106891

C 0.828655611 -0.6973160071 2.7997147988

H 1.8417714947 -1.0993680719 2.9187762191

H 0.5387158724 -0.8040272729 1.7510741404

H 0.1503209915 -1.3231107056 3.3992738621

C -0.730580214 1.2427783834 3.1529019531

H -1.3824829318 0.5952064579 3.758426962

H -1.0794361326 1.1942454468 2.1164422326

H -0.8720675094 2.2703492457 3.5094492844

C 3.5291916733 3.2983803577 4.0409671844

H 4.3820515495 2.7110157978 3.6812555223

H 3.1113611274 2.7855130305 4.9131291006

H 3.9153708546 4.2685449637 4.3885738623

C 3.1512871901 4.3452389418 1.8007118584

H 4.03851115 3.8413692089 1.399343923

H 3.4825038606 5.3164547509 2.1975528288

H 2.462068662 4.547434895 0.9722315638

C 1.2986516823 4.3474594933 3.4832280022

H 0.8079266625 3.8553958143 4.3303105069

H 0.536242223 4.540127616 2.7179967526

H 1.6596151632 5.3235764819 3.840480213

Version=AM64L-G03RevD.01 State=1-A\\HF=-1370.8515896

Sum of electronic and zero-point Energies= -1370.367060

Sum of electronic and thermal Energies= -1370.338720

Sum of electronic and thermal Enthalpies= -1370.337776

Sum of electronic and thermal Free Energies= -1370.426192

Z*-6 Conformation-3 (H_{rel} = 3.7 kcal/mol)

B3LYP/6-31+G(d)

0 1

H 2.8790284045 -1.4939749566 1.302329606

C 2.1294211042 -1.205853371 0.5593367929

O 2.2964583508 -2.171199474 -0.5021068666

C 2.352900996 -1.7474026055 -1.7890329592

H 2.5679106495 -2.5820356105 -2.4500456031

C 2.1768463141 -0.4911421852 -2.2190201655

H 2.2504204275 -0.2836610676 -3.2802008735

C 2.4239673022 0.2528579156 0.125638677

H 3.5127449452 0.3482959193 0.0110975961

C 1.8451741356 0.60932902 -1.2559123885

H 2.2941131241 1.5561077013 -1.5794372725

C 0.7570518575 -1.39504971 1.2206328799

H 0.6020402807 -2.4617561295 1.4109940746

H -0.0486775708 -1.0281273624 0.5757936574

O 0.7502286373 -0.7253180457 2.4833821265

Si 1.2854588429 0.8637732887 2.603505123

O 2.0084964972 1.1850929624 1.1136689388

C 2.6193795934 0.900173687 3.9900797325

C -0.2060475662 2.0537660993 2.8007887127

O 0.4125132212 0.825898661 -1.0996335396

C -0.3052887435 1.2919214783 -2.179303809

C -0.7760293344 0.4976715389 -3.1507504663

H -0.5593543892 -0.5621003801 -3.0566544494

C -1.608919542 0.9510118099 -4.3156646161

H -2.6256737458 0.5363173761 -4.2608593836

H -1.1793614878 0.6072740346 -5.2667778429

H -1.694059528 2.0405145434 -4.3486791634

O -0.6627067952 2.6110156288 -2.1060440649

C 0.3600716894 3.5568623665 -1.787647471

H 0.8352934586 3.3223412042 -0.8308316761

H -0.1390545022 4.5254608706 -1.7201080027

H 1.1169896496 3.5928191977 -2.5839935797

C -0.7767504172 2.0150347325 4.2369893272

H -1.0618683599 1.0002741266 4.5413070648

H -1.6824795329 2.6373270245 4.2885316307

H -0.0730694509 2.4078496241 4.9795448336

C -1.3206465897 1.5964975425 1.8292904755

H -1.6727757766 0.5856647169 2.0664353012

H -0.9902213919 1.6066413943 0.7868316999

H -2.182666304 2.2750504384 1.9144309122

C 0.1867206236 3.5080254515 2.4537547674

H -0.7019347472 4.1544553685 2.5084537759

H 0.5921456988 3.5874454037 1.4397559479

H 0.9309729667 3.9190894987 3.1450608509

C 2.1101352189 0.1824807304 5.2626430146

H 1.815799121 -0.8519059774 5.0521106252

H 1.2519882924 0.6891611174 5.7162288308

H 2.9092035369 0.1562862797 6.0189081591

C 3.882363071 0.1553648457 3.4980400166

H 3.6809767824 -0.9027018982 3.293343013

H 4.6587400096 0.1895181645 4.276627289

H 4.3050185903 0.6098771804 2.5940167168

C 3.0282119016 2.3476397026 4.3456233605

H 2.2011074883 2.9180892436 4.7821221457

H 3.3948259929 2.8998178365 3.471009268

H 3.8398669994 2.335133047 5.0883972498

Version=AM64L-G03RevD.01 State=1-A\\ HF=-1370.8500946

Sum of electronic and zero-point Energies= -1370.365542

Sum of electronic and thermal Energies= -1370.337374

Sum of electronic and thermal Enthalpies= -1370.336430

Sum of electronic and thermal Free Energies= -1370.422864

E*-6

B3LYP/6-31+G(d)

0 1

H 0.1627522583 -0.9015313777 3.9050982019

C 0.0965996326 -0.7629271295 2.8138064481

O 0.4154667592 -2.0230082563 2.1963548634

C 1.7406523823 -2.3288133117 2.0996137333

H 1.8787283042 -3.3548453996 1.7734707815

C 2.7508747708 -1.4902430858 2.3593857965

H 3.7743214958 -1.8359697302 2.2598321123

C 1.0719225674 0.3538413427 2.4016757913

H 0.8142608491 1.2575286504 2.9668833379

C 2.5081482733 -0.0685455447 2.7787738615

H 2.6235228237 0.0467882647 3.8649196976

C -1.3578925346 -0.4379939065 2.4716036764

H -1.6954654768 0.3580352875 3.153093429

H -1.9702081084 -1.3271179503 2.6597604303

O -1.5755930416 -0.0416185717 1.125984459

Si -0.4528624219 0.7889476411 0.1893882889

O 1.002919978 0.6142007434 1.0094973838

C -0.9806277681 2.640142662 0.1573825932

C -0.2503776203 -0.1005782674 -1.4948784029

O 3.497050323 0.7622657552 2.1365020697

C 3.9948274638 1.8259208763 2.8172103173

C 5.2923819676 2.1700323946 2.7459298366

O 3.0104525448 2.4882670981 3.5013924391

C 3.391649579 3.5858288883 4.3229856624

H 4.1405245765 3.2784929242 5.0637915476

H 2.4804267766 3.912907159 4.8272328493

H 3.7916156037 4.408627216 3.7173243892

C -1.4261122015 0.1921901827 -2.4532732377

H -2.3940072072 -0.0883420771 -2.0192334066

H -1.3017809017 -0.3894695858 -3.3787885964

H -1.4764258542 1.2483134266 -2.7408977365

C -0.1947416886 -1.6253858018 -1.2426527744

H -1.1114278393 -1.9975288012 -0.7728409204

H 0.646641273 -1.8996047509 -0.5986355123

H -0.0672816862 -2.149420067 -2.2018858098

C 1.0765804309 0.3295506242 -2.1653680204

H 1.9387538601 0.128756919 -1.5203527259

H 1.0909598937 1.3940624617 -2.4244700221

H 1.2163872958 -0.2348581882 -3.0996309894

C -2.4789561451 2.7727406658 -0.202736664

H -3.1143533678 2.2096698592 0.490707899

H -2.6993049187 2.4213004925 -1.2164235936

H -2.7824408264 3.8295136506 -0.1514440235

C -0.773649791 3.2356133289 1.571079442

H -1.360810917 2.7072903093 2.3331733321

H -1.1060103746 4.2848168624 1.5825553263

H 0.2797915184 3.2221092063 1.8726735527

C -0.1379325815 3.4692905014 -0.8364576072

H -0.3021368195 3.1640884216 -1.8758469053

H 0.9363308788 3.3943239564 -0.6275949702

H -0.4141146918 4.5322740549 -0.7644331592

H 5.6066664996 3.0944706462 3.2186531738

C 6.3368426887 1.3862822966 1.9988828932

H 6.7286924946 1.9532020784 1.1422756269

H 5.9301076625 0.4469387089 1.6149231136

H 7.194661358 1.1511762461 2.644026721

Version=AM64L-G03RevD.01 State=1-A\\HF=-1370.8607194

Sum of electronic and zero-point Energies= -1370.376041

Sum of electronic and thermal Energies= -1370.348059

Sum of electronic and thermal Enthalpies= -1370.347115

Sum of electronic and thermal Free Energies= -1370.433609

E*[b]-6 (H_{rel} = 2.0 kcal/mol)

B3LYP/6-31+G(d)

0 1

H 3.2437740493 -1.2943672233 1.286032103

C 2.5645208173 -0.9735362407 0.4901549269

O 2.9647238415 -1.7566731085 -0.6572671516

C 3.1018063755 -1.1557582851 -1.8674033343

H 3.4624900251 -1.8711053422 -2.6007213551

C 2.8459952775 0.1287736703 -2.1501454852

H 2.9950870871 0.4864063008 -3.1635712622

C 2.7520960407 0.5495172952 0.2857778392

H 3.8315647678 0.7537044718 0.3190433466

C 2.2991957256 1.0433087531 -1.0962947944

H 2.6438645015 2.0720096026 -1.2238314627

C 1.1468877359 -1.3812521273 0.9204449607

H 1.0995830664 -2.4733139563 0.9804308858

H 0.4005195145 -1.0349913393 0.1979801965

O 0.8735771911 -0.865450069 2.2247222136

Si 1.1811456889 0.7476196835 2.5893037733

O 2.141503147 1.2977053801 1.3218973351

C 2.2280222172 0.7588921844 4.2007007389

C -0.4384416156 1.7813620741 2.5874541735

O 0.8395425123 1.0581397161 -1.1284660327

C 0.2425261159 1.8216936283 -2.0825900045

C -0.7177857172 1.3431061832 -2.8917200306

O 0.7055789581 3.1077117985 -2.0340013913

C 0.2147830104 4.0326487545 -2.9958552118

H 0.4011512904 3.6748059402 -4.0166722978

H 0.7600160223 4.9620815605 -2.821747907

H -0.8602421356 4.2067677092 -2.8601555597

C -1.1836579206 1.7176951639 3.9398600368

H -1.4316398435 0.6886098237 4.2281674754

H -2.1318166765 2.2702163307 3.860976714

H -0.6137193503 2.1719670193 4.7578200116

C -1.3822117745 1.2150815413 1.4998022888

H -1.6782721103 0.1824258925 1.7191289295

H -0.9239234635 1.2369846108 0.5073529945

H -2.2992237807 1.8222706244 1.4584798877

C -0.1266530863 3.259113249 2.2504020155

H -1.0635074217 3.8360231866 2.2211698223

H 0.3587800036 3.3573502366 1.2741328065

H 0.5215540791 3.7313089064 2.9987212158

C 1.5374684109 -0.0493891988 5.3237337544

H 1.3352877039 -1.0809929746 5.0125692372

H 0.5903898272 0.3978107317 5.642087947

H 2.1910202075 -0.0904108478 6.2082511404

C 3.5931318383 0.0941871164 3.9063547257

H 3.4800359063 -0.9548216799 3.6083212465

H 4.2159662704 0.1084248251 4.8131548453

H 4.1469706094 0.6213981076 3.1204399958

C 2.4922823983 2.2025608216 4.6854034788

H 1.5712888404 2.723348063 4.9700719185

H 2.9968284316 2.8051497556 3.9197546456

H 3.1432052395 2.1865958285 5.5724413476

H -1.237787774 2.0396676942 -3.54180239

C -1.1641854196 -0.0930609063 -2.9304051256

H -0.5008299907 -0.7327174448 -2.3425573434

H -1.1753568224 -0.4732706416 -3.9608411788

H -2.183909843 -0.2113328497 -2.5364916551

Version=AM64L-G03RevD.01 State=1-A\\HF=-1370.8579896

Sum of electronic and zero-point Energies= -1370.372836

Sum of electronic and thermal Energies= -1370.344855

Sum of electronic and thermal Enthalpies= -1370.343911

Sum of electronic and thermal Free Energies= -1370.430315

E*-6 Conformation-1 (H_{rel} = 3.3 kcal/mol)

B3LYP/6-31+G(d)

0 1

H 1.2295835218 -2.0127280131 0.3084803492

C 1.0568047756 -1.4777568184 1.2474601121

O 0.8000728933 -2.5232918032 2.2108661614

C -0.2656554828 -2.4244586184 3.0469289883

H -0.3607110919 -3.3292873435 3.6399486853

C -1.0996028408 -1.3814492502 3.1480894438

H -1.9171814666 -1.4214280829 3.8595554572

C -0.1422470835 -0.5187018586 1.0361098747

H -0.8914549492 -1.057543193 0.4394998441

C -0.8681516324 -0.1436454223 2.3363631902

H -1.8142827437 0.3401276693 2.0754136412

C 2.3720614692 -0.7677436849 1.5980933894

H 3.1355260547 -1.5238333778 1.8064788364

H 2.2549283657 -0.1300271926 2.480711562

O 2.8129163895 -0.0073221397 0.4710606707

Si 1.7499634081 1.0324189312 -0.3133687719

O 0.2343424792 0.6430985056 0.3102698799

C 1.8145155731 0.5920920328 -2.1837743573

C 2.1112081631 2.8532199546 0.1699681721

O -0.0552814078 0.8285300984 3.0616627995

C -0.6322117018 1.3735375578 4.1807380194

C -0.0330723793 1.3919038491 5.3771033067

O -1.88217402 1.9130000994 4.0019128201

C -1.9494972848 3.0239897405 3.0958489677

H -1.3364798287 3.8544769063 3.4685492316

H -2.999155768 3.323535323 3.0644937061

H -1.6129409331 2.7447033113 2.0917012473

C 3.3345691121 3.4202419441 -0.5851144675

H 4.2335202101 2.809954717 -0.4333639297

H 3.5600501729 4.4309156226 -0.2135368237

H 3.1596653734 3.5052513424 -1.6636216139

C 2.4202672982 2.8929236637 1.6859797492

H 3.3225376977 2.3193195273 1.9287837167

H 1.594173546 2.4974319219 2.2847608088

H 2.596139198 3.9333922964 1.9985426159

C 0.8844782848 3.7522751871 -0.107883195

H 1.0901122434 4.7767593217 0.237053119

H -0.0062140486 3.3948782795 0.4194451946

H 0.6406157064 3.8115642121 -1.1746748592

C 3.2765892973 0.5286913503 -2.6851434623

H 3.8703832187 -0.1889528604 -2.1076728279

H 3.7805848548 1.4994576881 -2.6338462438

H 3.2949455957 0.2080002104 -3.7377175495

C 1.1778179903 -0.8018477776 -2.3929665325

H 1.7296460057 -1.5874910497 -1.8635714255

H 1.195361959 -1.0602433887 -3.4621466196

H 0.1314760111 -0.8322016287 -2.0661790843

C 1.0222254933 1.613317262 -3.0303226086

H 1.4676068731 2.6138837347 -2.9995684243

H -0.0216506538 1.6977715191 -2.7028451589

H 1.0103292628 1.2971471409 -4.0841590469

H -0.54315073 1.9531258002 6.1560395411

C 1.25954531 0.7109640531 5.7225305938

H 2.0488606958 1.4405210525 5.9526890051

H 1.6117577878 0.0798844539 4.9022516274

H 1.1429337551 0.0786472236 6.6130926742

Version=AM64L-G03RevD.01 State=1-A\\HF=-1370.8554837

Sum of electronic and zero-point Energies= -1370.370788

Sum of electronic and thermal Energies= -1370.342620

Sum of electronic and thermal Enthalpies= -1370.341676

Sum of electronic and thermal Free Energies= -1370.428101

E*-6 Conformation-2 (H_{rel} = 6.5 kcal/mol)

B3LYP/6-31+G(d)

0 1

H -0.154875324 0.1973848489 -1.7380330778

C 0.8648699704 0.4342019643 -1.4205209399

O 1.6821344855 0.073243149 -2.5569665009

C 2.8192586364 -0.6416197483 -2.366115722

H 3.2728281998 -0.886439858 -3.3222661023

C 3.3338951965 -1.0137994108 -1.1866445767

H 4.2523551757 -1.591388637 -1.1693583206

C 1.1735107815 -0.3948106962 -0.1487812263

H 0.7669289202 -1.403267278 -0.3091651224

C 2.677216309 -0.6084788191 0.0986206879

H 2.7889059668 -1.387048547 0.8554661485

C 0.9180793223 1.9533800598 -1.2051354834

H 0.7692937786 2.4508549028 -2.1688141404

H 1.8844256127 2.2631886522 -0.792089233

O -0.155116661 2.3423887513 -0.3469647067

Si -0.4246586955 1.5279693402 1.1001379522

O 0.5417548637 0.1499461592 0.9991355384

C -2.2753092872 1.0066216465 1.1073326392

C 0.1965384954 2.5716878397 2.5848334337

O 3.2425526089 0.6260109052 0.6228723276

C 4.4370464313 0.5746995402 1.2978049346

C 4.7339590742 -0.1855945146 2.3638825708

O 5.3211092884 1.5282891579 0.8806385478

C 5.6158693854 1.5978219326 -0.5179222644

H 6.1511547707 0.695925811 -0.8428803197

H 6.2610089843 2.4701007236 -0.6401930159

H 4.707089852 1.7193731152 -1.1139888328

C -0.8090253101 3.6807307017 2.9700594282

H -1.0412556412 4.3408945428 2.1251461127

H -0.3758695107 4.3075067781 3.7635595116

H -1.7522604601 3.2785050651 3.3565485043

C 1.5255850357 3.2514579616 2.1774032596

H 1.3844998186 3.9430882318 1.3384948667

H 2.2912435757 2.5235307773 1.8946972833

H 1.9154890655 3.8340648157 3.025276502

C 0.457571754 1.6754313035 3.8174202258

H 0.8530505791 2.2867489058 4.642332113

H 1.1942180147 0.8951784772 3.6008151093

H -0.4531635531 1.1867565031 4.182920022

C -3.1901557463 2.2101034891 0.7792176227

H -2.9271333568 2.6663569375 -0.1819612414

H -3.1470869018 2.9912169439 1.5450638238

H -4.2362814736 1.8747737671 0.715290019

C -2.4981937221 -0.069976452 0.0195454631

H -2.2847958321 0.3136044214 -0.9851427469

H -3.5508011041 -0.3897442188 0.0252553883

H -1.8845938254 -0.9630783821 0.1883613218

C -2.6843776861 0.4027157783 2.4698104122

H -2.6256352371 1.1335762637 3.2838642165

H -2.0597891815 -0.457165808 2.7430616656

H -3.7257786168 0.0502704805 2.4256178229

H 5.7561675911 -0.0944354128 2.7207666998

C 3.7976262561 -1.0609887488 3.1524484559

H 3.9353927125 -2.1317048725 2.9381297315

H 2.7469615973 -0.8133068294 2.9738343377

H 3.9845650168 -0.9327524117 4.2262788738

Version=AM64L-G03RevD.01 State=1-A\\HF=-1370.8505779

Sum of electronic and zero-point Energies= -1370.365653

Sum of electronic and thermal Energies= -1370.337542

Sum of electronic and thermal Enthalpies= -1370.336598

Sum of electronic and thermal Free Energies= -1370.423155

TS

2-Z*-boat-TS:

B3LYP/6-31+G(d)

0 1

C 0.7109983495 1.7665398951 0.1327773837

C 2.0938705017 1.2932442302 -0.3559570731

C 3.2251307373 1.4960449631 0.6353711971

H -0.3445941403 2.0832882109 3.2255963586

O 2.1119380241 -0.1095860902 -0.7397821142

O 0.6054210871 1.5537237778 1.5222521531

C -0.3951648672 1.1673104504 -0.7544854878

H 0.6907867711 2.8583221682 -0.052092664

O -1.3479576685 -0.0579373667 0.4603530363

C 0.0026317833 0.2947769624 -1.7827436908

H -1.2845924208 1.7721041665 -0.8904602005

C 1.1209698078 -0.4832570958 -1.5664808856

H -0.7072193984 -0.0275942751 -2.5379047549

H 1.371674109 -1.360452616 -2.1539723186

C -1.2655360633 -1.2952412293 0.1139168358

C -0.1396912193 -2.0738430225 0.2580553581

O -2.3262499698 -1.8596714352 -0.5752777923

C -0.0466443005 -3.5273207295 -0.1055479202

H 0.6623226403 -1.628906625 0.8360439575

C -3.5485071613 -1.1265300068 -0.5839731757

H -3.4469134509 -0.1716967957 -1.1116529303

H -3.9003577111 -0.9295732719 0.4354402767

H -4.2660667962 -1.761729213 -1.1086666047

H -0.7469234625 -3.7895289601 -0.9045664962

H -0.2766246768 -4.1765985686 0.7541255004

H 0.9691436113 -3.7880231439 -0.430672278

H -1.4386876968 1.8269795545 1.8402348836

H -0.4286129113 3.3148905573 1.9332197032

H 2.2963411636 1.8457569513 -1.2844236293

C -0.471359751 2.2345688388 2.1506258742

H 3.049324535 0.9234580424 1.5486636396

H 3.3004554064 2.5551551719 0.9048155281

H 4.1726951385 1.1813265047 0.1861683302

Version=AM64L-G03RevD.01 State=1-A\\HF=-730.8124617

Sum of electronic and zero-point Energies= -730.533426

Sum of electronic and thermal Energies= -730.516899

Sum of electronic and thermal Enthalpies= -730.515955

Sum of electronic and thermal Free Energies= -730.577708

2-Z*-boat-TS without methoxy groups:

B3LYP/6-31+G(d)

0 1

C 0.7175683381 1.7729815816 0.0420701693

C 2.119390066 1.3281578475 -0.3807985866

C 3.1816652162 1.513333515 0.6883029285

O 2.1447696662 -0.0865564368 -0.7548754579

C -0.3253444083 1.2546142536 -0.9112898978

H 0.7036328721 2.8712926063 0.0666274947

O -1.3147298556 -0.0495877367 0.5699437326

C 0.0257580217 0.2647558586 -1.8163590208

H -1.2504120955 1.806077841 -1.0279350697

C 1.1479775642 -0.5072547076 -1.5462141815

H -0.6916772056 -0.1162551949 -2.5359896268

H 1.3961954167 -1.4181938343 -2.0803459746

C -1.245175744 -1.2789275453 0.2172319432

C -0.0949250189 -2.0523825598 0.2414013005

C -0.0752259567 -3.5049839734 -0.1438723721

H 0.7742614303 -1.6564968704 0.7609243655

H -1.0148305611 -3.8036721807 -0.6249030439

H 0.071046397 -4.1541499238 0.7326412654

H 0.7439080096 -3.7393285553 -0.8393010745

H 2.4019482161 1.8678030319 -1.2962853202

H 2.9255162822 0.9507208917 1.592501813

H 3.2619737994 2.5741243981 0.9520625644

H 4.1580409643 1.172259994 0.3289613592

H -2.1457918536 -1.7387671074 -0.235517973

H 0.4754604392 1.4234348072 1.0530186632

Version=AM64L-G03RevD.01 State=1-A\\HF=-501.7574369

Sum of electronic and zero-point Energies= -501.544453

Sum of electronic and thermal Energies= -501.533097

Sum of electronic and thermal Enthalpies= -501.532152

Sum of electronic and thermal Free Energies= -501.581191

2-Z*-chair-TS:

B3LYP/6-31+G(d)

0 1

C -1.3461585393 -1.1902416471 -0.3959925732

C -0.7934080218 -0.8078810261 -1.793994728

C -1.5243487726 0.3297295842 -2.4838582289

H -3.4261291648 -1.4300991354 1.1551070949

O 0.6217400359 -0.4578731343 -1.8012391207

O -2.139097118 -0.1456752251 0.1329858893

C -0.246150596 -1.731091989 0.5083514589

H -2.0201826184 -2.0519756751 -0.5725065371

O 0.314075857 -0.220959606 1.6536067522

C 0.9683827038 -2.0902279356 -0.0996158692

H -0.5765965581 -2.2862230543 1.3789921737

C 1.4319540287 -1.2684009556 -1.1043487365

H 1.6755698462 -2.7353815332 0.4103502385

H 2.4421577564 -1.2969830035 -1.4996317271

C 1.1340639891 0.6011884985 1.0876238472

C 2.460502699 0.3189395059 0.8389534627

O 0.6614263196 1.7992624439 0.589170226

C 3.445443231 1.2700951811 0.2233390592

H 2.8391430059 -0.5958689093 1.2810181443

C -0.4251038573 2.3989106564 1.2975920704

H -0.5373613486 3.3986570621 0.8700960818

H -0.1917796292 2.4817564861 2.3670748177

H -1.3451959697 1.8291087893 1.1625001126

H 4.1689252244 0.7375019392 -0.4090778928

H 4.0325725911 1.7972424991 0.9919978418

H 2.9447386335 2.0275220396 -0.3855910741

H -3.5591044796 0.3164627824 1.4990399964

H -2.185155737 -0.6097436134 2.1663531811

H -0.850499534 -1.7184662008 -2.4052544016

C -2.8566133176 -0.4986721821 1.3068774923

H -2.586740953 0.0877403019 -2.5876523264

H -1.0981498931 0.4867670217 -3.479864177

H -1.4359198138 1.2518800346 -1.9054025483

Version=AM64L-G03RevD.01 State=1-A\\HF=-730.8099353

Sum of electronic and zero-point Energies= -730.530673

Sum of electronic and thermal Energies= -730.514228

Sum of electronic and thermal Enthalpies= -730.513283

Sum of electronic and thermal Free Energies= -730.574281

2-Z*-chair-TS without methoxy groups:

B3LYP/6-31+G(d)

0 1

C -1.2186365138 -0.9964146057 -0.3634281683

C -0.7092275149 -0.8157218452 -1.7963040594

C -1.3997754436 0.2950119449 -2.5682383713

O 0.7187822384 -0.5188083847 -1.819855898

C -0.2863991251 -1.8696231445 0.4403953678

H -2.2165183706 -1.4529608889 -0.4107823441

O 0.4116395462 -0.450401855 1.8752546448

C 0.9637651006 -2.1650488466 -0.0882262775

H -0.6947363844 -2.4599183854 1.2515895069

C 1.4910884693 -1.2928559332 -1.0338021243

H 1.6425695668 -2.8335644474 0.430299157

H 2.5193823649 -1.3300435207 -1.3775872136

C 1.0988785061 0.4265351767 1.2403915444

C 2.4087914505 0.2553277087 0.8219441758

C 3.1948880121 1.3269116214 0.1208062962

H 2.9569371522 -0.5933548232 1.2270360324

H 3.757247538 0.9327349343 -0.7372119961

H 3.9348426227 1.787998569 0.792196581

H 2.5392224424 2.1233512623 -0.250844789

H -0.8151150405 -1.7721918039 -2.3287883119

H -2.4725840428 0.084228242 -2.6463259849

H -0.9895780678 0.3758650197 -3.5801055113

H -1.2717244133 1.2584690562 -2.0629730197

H -1.3434568987 -0.025359148 0.1310413826

H 0.5797168053 1.3398340973 0.8885193805

Version=AM64L-G03RevD.01 State=1-A\\HF=-501.7591013

Sum of electronic and zero-point Energies= -501.545763

Sum of electronic and thermal Energies= -501.534564

Sum of electronic and thermal Enthalpies= -501.533620

Sum of electronic and thermal Free Energies= -501.582265

2-E*-boat-TS:

B3LYP/6-31+G(d)

0 1

C 1.3468733794 1.000929214 -0.2372736704

C 2.3153794081 -0.1906767403 -0.0869567305

C 3.2080371763 -0.1394691318 1.138691084

H 0.1941724945 3.0086816399 2.092692367

O 1.6435911584 -1.4834379323 -0.0731303486

O 0.9558386302 1.4618946162 1.037768389

C 0.2288059663 0.6536267584 -1.2284078377

H 1.9415629846 1.8008368137 -0.720728348

O -1.4367268943 0.5478756601 -0.0752772357

C 0.2364110572 -0.6292370343 -1.799345317

H -0.2014452746 1.4792293553 -1.7830767233

C 0.7526945019 -1.6694912653 -1.055771654

H -0.4224592932 -0.8700441728 -2.6264885609

H 0.5791112474 -2.7173343225 -1.276749684

C -1.9335459587 -0.6359742229 -0.1043468755

C -1.5730919486 -1.6870452456 0.7082702608

O -2.8355967319 -0.9507656331 -1.1149932188

C -0.7153410373 -1.5412970738 1.9258829898

H -2.0987676734 -2.6271386761 0.55463926

C -3.484803393 0.1476105906 -1.7480770008

H -2.7810237311 0.7729632693 -2.3093888108

H -4.0065267187 0.7770892092 -1.0167159325

H -4.2085424465 -0.2960504812 -2.4361032852

H -0.2680795333 -0.5460122766 1.9774003637

H 0.0910425566 -2.2869043313 1.9511257956

H -1.3140789644 -1.693334907 2.8375385232

H -0.6799107277 2.6717520742 0.5743175678

H 0.9276565632 3.4838668076 0.5342321775

H 2.9246139789 -0.2042944298 -1.0016294143

C 0.3077210139 2.727070288 1.0428535907

H 3.8972241871 -0.9901038534 1.1308354785

H 2.6143553732 -0.1628236437 2.0548241708

H 3.7938486496 0.7860090774 1.1343886292

Version=AM64L-G03RevD.01 State=1-A\\HF=-730.8108672

Sum of electronic and zero-point Energies= -730.531690

Sum of electronic and thermal Energies= -730.515350

Sum of electronic and thermal Enthalpies= -730.514406

Sum of electronic and thermal Free Energies= -730.574726

2-E*-boat-TS without methoxy groups:

B3LYP/6-31+G(d)

0 1

C 1.337032584 0.9355563524 -0.2779865565

C 2.3316836223 -0.2166849385 -0.1212756393

C 3.1533004944 -0.1673873061 1.1542618504

O 1.6557523029 -1.5175859868 -0.138700952

C 0.3633972235 0.6572156928 -1.3892859277

H 1.9078936263 1.8510355831 -0.4841827726

O -1.4817509819 0.6167456635 -0.034323603

C 0.2340332351 -0.6382415192 -1.8554255049

H -0.087406078 1.4864692936 -1.9205120854

C 0.7136364052 -1.6828806185 -1.070651628

H -0.4576274625 -0.8803667153 -2.6557398988

H 0.4870196874 -2.7272769167 -1.2534253255

C -1.932705341 -0.5773340881 -0.0627530453

C -1.4937916956 -1.6354906814 0.7242931439

C -0.6404128507 -1.4877725701 1.9468390185

H -1.992488861 -2.5932671133 0.5716090061

H -0.4522518571 -0.42991628 2.1575544271

H 0.3327305465 -1.9895046291 1.8476639928

H -1.1397761434 -1.9298734743 2.8206128215

H 2.9922379132 -0.2358746796 -0.9999550218

H 3.8314042278 -1.0250158972 1.2126455735

H 2.5053067908 -0.1726471356 2.0368900143

H 3.754552584 0.7489110234 1.1719607734

H 0.7757107452 1.1093339058 0.6485908005

H -2.6874807174 -0.8281469647 -0.8327034613

Version=AM64L-G03RevD.01 State=1-A\\HF=-501.7552902

Sum of electronic and zero-point Energies= -501.542161

Sum of electronic and thermal Energies= -501.530830

Sum of electronic and thermal Enthalpies= -501.529886

Sum of electronic and thermal Free Energies= -501.578719

2-E*-chair-TS:

B3LYP/6-31+G(d)

0 1

C -0.5779053123 0.9026490519 -1.3720069656

C 0.7242687855 1.7157608845 -1.155080288

C 0.5426402276 3.0346301702 -0.4267839016

H -3.1509496954 0.9355847969 -1.8017019741

O 1.7729197599 0.9900770903 -0.4474051766

O -1.5868494455 1.3218076862 -0.4760732393

C -0.2948464138 -0.5921746201 -1.4272402427

H -0.9188691736 1.1659600533 -2.3935110614

O -0.7585532103 -1.2996734472 0.4182104055

C 1.0417670866 -0.9985704419 -1.5360841957

H -1.0715438158 -1.2144565532 -1.8565456193

C 1.9854273345 -0.2695322569 -0.8411388757

H 1.2940771944 -2.0035091679 -1.852738349

H 2.9994390897 -0.6077088363 -0.6546150734

C 0.1973045692 -1.1168383646 1.2597438596

C 1.3357841254 -1.8882368093 1.3580013177

O 0.1817345783 0.0045143253 2.0761844958

C 1.5186117075 -3.2233118598 0.7003081895

H 2.0532389237 -1.5977103124 2.1220517041

C -1.0896809326 0.35501213 2.6232823613

H -1.4968572891 -0.4760915878 3.2161055601

H -1.7966630609 0.6340731429 1.8405284221

H -0.9049357145 1.2101118267 3.2784999902

H 2.4556082126 -3.2873801107 0.1263188805

H 0.6843677761 -3.4540280848 0.0324010369

H 1.570171061 -4.0192051849 1.4585061002

H -3.5766989918 1.315272262 -0.1102146414

H -2.9076591723 -0.2921968014 -0.5088447056

H 1.145510221 1.8898148306 -2.1543419105

C -2.8702651396 0.7770781741 -0.7474626361

H -0.1727483702 3.6662031753 -0.9630560762

H 1.503110247 3.556858213 -0.371188572

H 0.1650448377 2.8662166264 0.5838911809

Version=AM64L-G03RevD.01 State=1-A\\HF=-730.807843

Sum of electronic and zero-point Energies= -730.528367

Sum of electronic and thermal Energies= -730.512189

Sum of electronic and thermal Enthalpies= -730.511244

Sum of electronic and thermal Free Energies= -730.571164

2-E*-chair-TS without methoxy groups:

B3LYP/6-31+G(d)

0 1

C -0.5456352864 0.8872530865 -1.2177780617

C 0.7594135481 1.6864303942 -1.1557869435

C 0.6354461075 3.0297777721 -0.4582938838

O 1.8076202224 0.9480209533 -0.4580577643

C -0.2865533511 -0.5510167692 -1.5936757249

H -1.197789543 1.3591366416 -1.9653591535

O -0.8627996744 -1.5011437197 0.2520795511

C 1.024238276 -1.0108268968 -1.6015903573

H -1.0674220041 -1.1051160033 -2.1004373083

C 1.9528292249 -0.341217126 -0.812273104

H 1.2595052898 -2.0152501597 -1.933790995

H 2.9474540252 -0.7196580529 -0.6030211816

C 0.0299799838 -1.1683392618 1.1108651926

C 1.2541526757 -1.7951029886 1.2821878764

C 1.5959944014 -3.1616932293 0.7608841651

H 1.9148075583 -1.3714066445 2.0393187984

H 2.5710581685 -3.1865059367 0.2521863584

H 0.8291370685 -3.518728531 0.0680029706

H 1.6629944272 -3.8823105037 1.5894510718

H 1.1351973231 1.8218390482 -2.1803798775

H -0.0900182332 3.6593222566 -0.9863149803

H 1.5988479328 3.5496505414 -0.445514381

H 0.2958704257 2.9009779574 0.5751311424

H -0.1228056433 -0.2323553407 1.6792244783

H -1.0835229233 0.9322625126 -0.2630578884

Version=AM64L-G03RevD.01 State=1-A\\HF=-501.7578549

Sum of electronic and zero-point Energies= -501.544166

Sum of electronic and thermal Energies= -501.533094

Sum of electronic and thermal Enthalpies= -501.532150

Sum of electronic and thermal Free Energies= -501.580352

A-Z*-boat-TS: (alternative substrate)

B3LYP/6-31+G(d)

0 1

C 0.6591260047 2.1079144178 -0.322561291

C 2.0410953236 1.3940831671 -0.4252279925

C 2.5575506197 0.7680119621 0.8810812303

O 2.7276476471 1.7859812134 1.8655796529

O 2.09222773 0.3603093814 -1.4545591875

O 0.4268249207 2.7150456614 0.9336046573

C -0.4883875154 1.229732534 -0.7468520676

H 0.6715523709 2.9308542144 -1.055866267

O -0.4658068717 -0.1821826217 0.8146768896

C -0.2857799339 0.3848686377 -1.8342037195

H -1.475713422 1.604746913 -0.5017801012

C 0.9835396193 -0.1167480907 -2.0321139152

H -1.1104411617 -0.0936802193 -2.35127488

H 1.2230627311 -0.8569520064 -2.7875198991

C -0.5878663986 -1.3633040715 0.335467062

C 0.4426880523 -2.1270539383 -0.1859577525

O -1.8567624681 -1.8951948756 0.1882970772

C 0.2778021806 -3.5254786318 -0.710278275

H 1.4477183222 -1.7670374059 -0.0058979359

C -2.912919393 -1.2355737688 0.8857710967

H -3.0805278545 -0.2219640449 0.5072755167

H -2.7020467903 -1.1796386798 1.959686894

H -3.8021585291 -1.8457952868 0.7120133724

H -0.6805600458 -3.6552469816 -1.2235324013

H 0.3114667919 -4.2745291964 0.097074214

H 1.0842040408 -3.7780911041 -1.4099034682

H 3.5379683235 0.3212789978 0.6870175467

C 1.8652467384 4.3273715752 2.8798895096

H 2.783847905 2.1289224021 -0.7503828372

Si 1.3442409962 2.6152644345 2.334169788

H 1.8714490301 -0.0070073508 1.231790587

C 0.3698417613 1.7069664146 3.6483063977

H 0.9907932639 4.9454404163 3.1181617194

H 2.4381422043 4.8353701408 2.0957530885

H 2.4928379598 4.2758836142 3.7784666798

H -0.5162479616 2.2840297943 3.9425764245

H 0.9758627632 1.5396223983 4.547625884

H 0.0264810451 0.7397799838 3.2656267022

Version=AM64L-G03RevD.01 State=1-A\\HF=-1134.9588102

Sum of electronic and zero-point Energies= -1134.648469

Sum of electronic and thermal Energies= -1134.628037

Sum of electronic and thermal Enthalpies= -1134.627093

Sum of electronic and thermal Free Energies= -1134.697409

A-Z*-chair-TS:

B3LYP/6-31+G(d)

0 1

C -1.0267942506 -0.9413970427 -0.3880805045

C -0.3217098504 -0.5323121696 -1.7261305968

C -0.9101268232 0.7421292053 -2.3424010428

O 1.1028728199 -0.3028098121 -1.6386011386

C -0.0481614321 -1.4165370261 0.6605770762

O 0.4850138632 0.1355511271 1.7932720511

C 1.2143162243 -1.8250442117 0.207974415

H -0.4958071538 -1.8901907075 1.5266537352

C 1.8044512814 -1.080352903 -0.7929081241

H 1.853436696 -2.4390253711 0.8331692161

H 2.8426886643 -1.1800532464 -1.0905052344

C 1.303239054 0.9341086195 1.2090148789

C 2.6412550338 0.6600198816 0.9967027143

O 0.8122530058 2.0948264865 0.6318222221

C 3.6139103085 1.5959781612 0.3381322868

H 3.0343450975 -0.1987766861 1.5288964159

C -0.2695527226 2.7101608973 1.3386772577

H -0.5516200093 3.5846524954 0.7468154078

H 0.0637145988 3.0370284448 2.3328350784

H -1.1137013654 2.0265074958 1.4422435504

H 4.4132508488 1.0405180089 -0.169948661

H 4.1056778791 2.2530873331 1.072603488

H 3.1186931378 2.2390313944 -0.3949597972

H -1.6093774191 -1.8464751026 -0.6319943427

H -0.4439537596 -1.3672602947 -2.4279609866

H -0.5258360581 0.8738312822 -3.3575830619

H -0.5990340761 1.6042831837 -1.7394040086

O -2.3332349507 0.633462181 -2.4225881954

Si -3.1455334629 0.5586687373 -0.9508396173

C -4.5473064129 -0.670009904 -1.1459860521

H -4.1785713182 -1.6727611624 -1.3923328535

H -5.2185376128 -0.3588984868 -1.9564627797

H -5.1413148302 -0.74192536 -0.2266622157

O -1.939000074 0.0360456019 0.101419769

C -3.7416777432 2.2249586791 -0.3458048761

H -4.1015228422 2.1610492475 0.6886130181

H -4.5703019905 2.5849144775 -0.9681573901

H -2.9439033552 2.9745405457 -0.3793851017

Version=AM64L-G03RevD.01 State=1-A\\HF=-1134.9541662

Sum of electronic and zero-point Energies= -1134.643422

Sum of electronic and thermal Energies= -1134.623355

Sum of electronic and thermal Enthalpies= -1134.622411

Sum of electronic and thermal Free Energies= -1134.691783

A-E*-boat-TS:

B3LYP/6-31+G(d)

0 1

C 1.3222997211 1.0699505667 -0.2304937644

C 2.2813766402 -0.1432583931 -0.031239954

C 2.9548442046 -0.1609973159 1.3504703351

H 2.2506047833 -0.584940286 2.0782750412

O 1.669791634 -1.4470675152 -0.1831468145

O 0.9171550313 1.6868488274 0.9823682665

C 0.1639703741 0.7242459365 -1.1407761782

H 1.913629041 1.8027920985 -0.8075984082

O -1.3979894665 0.3836134145 0.1591399053

C 0.2073572079 -0.4990789166 -1.8215312103

H -0.3643679005 1.5696425787 -1.5651205728

C 0.7841458679 -1.5791077497 -1.1839229891

H -0.4669208196 -0.6995726257 -2.6469163271

H 0.6749620566 -2.6063197499 -1.5130364769

C -1.8704126586 -0.7843978273 -0.0507164859

C -1.4482909638 -1.9493518015 0.5600893453

O -2.8053110687 -0.9602856693 -1.0632840301

C -0.5936927391 -1.9586936267 1.7886173528

H -1.9547480751 -2.8690537758 0.2753087742

C -3.4721086422 0.2143326863 -1.5194464785

H -2.7893512037 0.9011756067 -2.0325439781

H -3.9472379987 0.749355314 -0.6890148515

H -4.233537975 -0.135145603 -2.2208416966

H -0.2002412612 -0.9593269926 1.9913683371

H 0.2473906828 -2.6600169268 1.7073446572

H -1.1829495746 -2.2704312668 2.6650826107

O 3.3712468786 1.1495289995 1.7286101123

C 2.7830617989 3.9428368032 1.5404676821

H 3.0414024345 -0.0827734588 -0.8210319181

Si 2.1246599611 2.2521239219 2.0045318416

H 3.8405178465 -0.80229026 1.3270528498

C 1.4396100477 2.1866974189 3.743108548

H 2.023024667 4.7179628293 1.696853749

H 3.097363965 3.9806801955 0.4908072981

H 3.6553730767 4.1980180351 2.1553676563

H 0.5416788483 2.8114944184 3.8260029596

H 2.1740494818 2.5496920332 4.4723925523

H 1.1566440966 1.1651180764 4.0214022601

Version=AM64L-G03RevD.01 State=1-A\\HF=-1134.9518246

Sum of electronic and zero-point Energies= -1134.641399

Sum of electronic and thermal Energies= -1134.621265

Sum of electronic and thermal Enthalpies= -1134.620321

Sum of electronic and thermal Free Energies= -1134.689929

A-E*-chair-TS:

B3LYP/6-31+G(d)

0 1

C 0.1457621291 1.4711392004 -1.1241974004

C 1.4742129316 2.26332203 -1.0961619568

C 1.3581126677 3.7586117061 -0.8008816252

O 2.4460652986 1.6771061261 -0.1984168213

O -0.7630040194 1.7955465319 -0.0853325556

C 0.4622830712 -0.0238171858 -1.2121025286

H -0.3239574737 1.7283294391 -2.0914576302

O -0.0718680293 -1.0013952658 0.472845934

C 1.8198019923 -0.3869458296 -1.210444922

H -0.2657100134 -0.6385486544 -1.7264787888

C 2.6920560079 0.3805401051 -0.4674921995

H 2.1146892445 -1.3937290052 -1.4771960987

H 3.6869963697 0.0678465319 -0.1699846408

C 0.7005841931 -0.7574156777 1.4700816027

C 1.947842891 -1.3114277152 1.6806626607

O 0.3076148012 0.1884308294 2.4057083723

C 2.4697601925 -2.5403978253 0.9953601419

H 2.4753552156 -0.9756227847 2.5709347467

C -1.0803816623 0.1217861352 2.7379706882

H -1.3374378968 -0.8801532938 3.1092419212

H -1.7068482596 0.3607722844 1.8753662546

H -1.2348930729 0.8512365739 3.535656847

H 3.4435362694 -2.3844361145 0.505115937

H 1.7615405642 -2.911036805 0.2495025958

H 2.6275930616 -3.3414478654 1.7326054384

H 1.9069566565 2.1647746593 -2.103245981

H 0.9985213162 4.2508314974 -1.7189307397

H 2.3588798125 4.1472647359 -0.5856769398

O 0.5173270922 4.0933734699 0.290632823

Si -1.0059485714 3.3973590179 0.3614184839

C -2.1694952444 4.221053288 -0.8695550147

H -2.3064417606 5.2827745817 -0.6286592866

H -3.1567249381 3.7421891137 -0.8482576599

H -1.7998201553 4.1616316848 -1.9011575359

C -1.6137785501 3.5338645523 2.1153964338

H -0.873798408 3.1251438485 2.8099901451

H -2.5620914172 3.0045440054 2.2619503462

H -1.7747293063 4.589383074 2.368004953

Version=AM64L-G03RevD.01 State=1-A\\HF=-1134.9447832

Sum of electronic and zero-point Energies= -1134.633675

Sum of electronic and thermal Energies= -1134.614050

Sum of electronic and thermal Enthalpies= -1134.613106

Sum of electronic and thermal Free Energies= -1134.681187

6-Z*-boat-TS:

B3LYP/6-31+G(d)

0 1

C 0.7007106831 1.988822775 -0.0418736692

C 2.0770013293 1.2539022369 -0.0708913482

C 2.4380700082 0.5523421772 1.2466270532

O 2.5842457123 1.5276815241 2.2788275397

O 2.226337124 0.2797236359 -1.1441572565

O 0.296141146 2.3670755736 1.2628705979

C -0.3895123968 1.2258362768 -0.7456906382

H 0.8182101293 2.9172987736 -0.6244289354

O -0.6423591943 -0.3459199033 0.595438726

C -0.0470878277 0.5185135816 -1.8961313883

H -1.390031525 1.6213814368 -0.6093470572

C 1.2081521258 -0.0504381902 -1.9479777182

H -0.7980600889 0.1636673929 -2.5937695767

H 1.5327438766 -0.7150409773 -2.7407810786

C -0.7105487996 -1.461407101 -0.0298400284

C 0.3782937384 -2.1981084307 -0.4622156399

O -1.9486603155 -1.924081284 -0.4379892996

C 0.2827805626 -3.526415947 -1.157467832

H 1.3436511221 -1.890769441 -0.0801137806

C -3.0908857843 -1.3044135912 0.1521698545

H -3.0569993162 -1.3736004338 1.2452755384

H -3.9520417116 -1.8575470106 -0.2296428807

H -3.1741268389 -0.2499931672 -0.1310223201

H -0.6040066159 -3.5854716637 -1.79637702

H 0.218770399 -4.3612248918 -0.4412088639

H 1.1706356767 -3.7097286727 -1.7757671439

H 3.4035167584 0.05141813 1.1229078604

C 1.9850579787 4.2892943845 2.7859012722

H 2.8602157484 1.990334012 -0.2751636275

Si 1.2656090765 2.5160414059 2.6289580204

H 1.6775425315 -0.1898273431 1.5033318948

C 0.2188487194 1.8416583934 4.0844473568

C 0.1309557694 0.3025405919 3.9469297786

H 1.1171997848 -0.1684858839 4.0397005139

H -0.3089681241 -0.001770717 2.9916575872

H -0.5013231109 -0.1000642994 4.7527925533

C 0.8479920042 2.172799344 5.4558340243

H 1.8715714063 1.7879041345 5.545481336

H 0.2538090162 1.7064746425 6.2556309805

H 0.8716060232 3.2496236027 5.6576188885

C -1.2149594392 2.4198594027 4.0265898721

H -1.2345207092 3.5099596 4.1423436896

H -1.8169101069 1.9952865987 4.8441809953

H -1.7106400649 2.1701007348 3.0825533614

C 3.176571569 4.3062721356 3.7727067957

H 3.9571514591 3.5964136075 3.4763788577

H 2.874768701 4.0661387872 4.7977342811

H 3.6274033004 5.3100665296 3.7936085218

C 0.9179770951 5.3064707072 3.2487302882

H 1.3486964893 6.3188215686 3.2654682524

H 0.5513368618 5.09519683 4.2594474221

H 0.0520763759 5.3310770956 2.5750931965

C 2.5059697052 4.7345257912 1.3984891777

H 3.2909840118 4.0678724337 1.0221055155

H 2.9433168657 5.7413763027 1.4718352997

H 1.7037210856 4.7835367979 0.6521901996

Version=AM64L-G03RevD.01 State=1-A\\HF=-1370.8250927

Sum of electronic and zero-point Energies= -1370.343336

Sum of electronic and thermal Energies= -1370.315222

Sum of electronic and thermal Enthalpies= -1370.314278

Sum of electronic and thermal Free Energies= -1370.400271

6-Z*-chair-TS:

B3LYP/6-31+G(d)

0 1

C -1.3775564801 0.3730027613 -0.4364688548

C -1.6199933609 0.7195393576 1.0659297507

C -0.7184031172 -0.0655131786 2.0228939981

O -1.4438435035 2.1132658775 1.4095810462

C -1.5564615403 1.5806449524 -1.3294289594

O 0.189177145 2.4961934335 -1.7166181707

C -2.2460811985 2.668339196 -0.7726281884

H -1.6443668805 1.3648374686 -2.3877716909

C -1.9629809403 2.9995960744 0.536806065

H -2.6823823252 3.4289733307 -1.4109749444

H -2.2755221782 3.9226073982 1.0130900171

C 0.6520742316 3.1889431663 -0.7403485711

C 0.1160514833 4.3867218143 -0.3048734865

O 1.7026758585 2.6713870455 0.004118141

C 0.6664597358 5.2148998152 0.8204323391

H -0.6188829467 4.8405747702 -0.9595676533

C 2.7137663764 2.0419658339 -0.7881417645

H 3.4900078895 1.7202068685 -0.0908673857

H 3.1395742897 2.7598607974 -1.5022524556

H 2.3120442576 1.1855892857 -1.333762208

H 1.2265251295 4.6024709479 1.5319510731

H -0.1372713407 5.7311267148 1.3629497186

H 1.3460468528 5.9987202645 0.4502810815

H -2.2353706711 -0.254365489 -0.7152403941

H -2.6732047565 0.494064811 1.2792842026

H -1.1094278958 0.003318862 3.042265108

H 0.2811437001 0.3820957061 2.0092483945

O -0.6868982712 -1.4470087716 1.6612329264

Si -0.0004925758 -1.8370457725 0.1679840338

C -1.0529923744 -3.301821535 -0.5092418975

O -0.1937434907 -0.3846006725 -0.6857670244

C 1.8900857549 -2.1354755275 0.2993105595

C 2.496466565 -1.0671263544 1.2402105707

H 2.284224904 -0.0480455052 0.9069294101

H 3.5899332657 -1.1850668595 1.2728309441

H 2.1267078067 -1.1771043055 2.2665024025

C 2.222346507 -3.5213900512 0.8989962909

H 1.7622806536 -3.6673302054 1.8841582231

H 3.3107344511 -3.6098127697 1.0322314834

H 1.9105689895 -4.3481979557 0.2520207823

C 2.554970433 -2.0156649622 -1.0926048856

H 2.3472016833 -1.0500584585 -1.5640412439

H 2.2227105942 -2.8012726834 -1.7801455906

H 3.6462402671 -2.1122019436 -0.9911130283

C -1.2172106419 -4.3726676845 0.5981059137

H -1.7068093024 -3.9605406615 1.4872719762

H -0.2621124632 -4.8060478199 0.9113718704

H -1.8411125629 -5.1970447093 0.2216771279

C -0.4086019111 -3.9481805599 -1.7566947516

H -0.2655107967 -3.2252433786 -2.569701603

H -1.0624926227 -4.7456380673 -2.1396818815

H 0.5620643096 -4.4060450008 -1.5391463708

C -2.4689101347 -2.8235959477 -0.9081589199

H -2.4453004572 -2.1265041455 -1.7542761869

H -2.9969232201 -2.3478147027 -0.0732836462

H -3.072223174 -3.6885208743 -1.2218636927

Version=IA32L-G03RevD.01 State=1-A\\HF=-1370.8139985

Sum of electronic and zero-point Energies= -1370.331076

Sum of electronic and thermal Energies= -1370.303529

Sum of electronic and thermal Enthalpies= -1370.302585

Sum of electronic and thermal Free Energies= -1370.386616

6-E*-boat-TS:

B3LYP/6-31+G(d)

0 1

C -0.5215887162 -0.2640979093 -1.3384338858

C -0.8258220284 1.2357699003 -1.012958187

C -1.5351390686 1.4323079451 0.3324716663

H -0.9082509746 1.0465527309 1.1395694762

O 0.3352398824 2.1220784388 -1.0223366545

O -1.2825285576 -1.1809106185 -0.5712238512

C 0.9404855416 -0.5910311157 -1.2671918122

H -0.7931926613 -0.4219934077 -2.3953472258

O 1.2422606027 -0.4817628775 0.8971374474

C 1.8552231647 0.3795682933 -1.6622916703

H 1.183364619 -1.645959339 -1.3225717201

C 1.542145215 1.6957991992 -1.3957518534

H 2.8838454037 0.133219543 -1.8984646593

H 2.2342504872 2.5198781138 -1.5286535311

C 2.4015127975 0.0338082073 1.0251243569

C 2.717928835 1.3548410762 1.2883078787

O 3.5104613516 -0.7588811896 0.7322304946

C 1.773904241 2.3856521325 1.8269808693

H 3.7807178824 1.5825154981 1.3430818646

C 3.359020019 -2.1593044395 0.956737716

H 2.5403412202 -2.5856434655 0.3691312082

H 3.1727542232 -2.3664371479 2.0187015511

H 4.3074294243 -2.6115331195 0.6570540208

H 0.7359730592 2.0597225283 1.7647785067

H 1.864677101 3.3479721345 1.3042519919

H 1.9902439733 2.5873822434 2.8878517707

O -2.8033533789 0.7779873766 0.3024853522

C -4.2220338395 -1.2757341829 -1.1129150294

H -1.4730102558 1.6406698222 -1.7977675707

Si -2.7936729888 -0.8979241063 0.1126423229

H -1.7105032902 2.5005746828 0.4923512763

C -2.7720538961 -1.8295763903 1.7854467552

C -1.8034086509 -1.0946514721 2.7440757125

H -0.7886581286 -1.0300109417 2.3370987777

H -1.7471835235 -1.6445726962 3.6956506573

H -2.1530314326 -0.0809863629 2.9754650277

C -4.1699609841 -1.8714635038 2.4417972309

H -4.0981431649 -2.3459432186 3.4316303049

H -4.890566868 -2.4540145428 1.8566242568

H -4.5868104803 -0.8676401663 2.5920783406

C -2.2529980798 -3.2740941029 1.5894911356

H -1.2447721979 -3.2833061622 1.1619905724

H -2.9037612913 -3.871385755 0.9405644443

H -2.2082190445 -3.7838015044 2.5636058896

C -5.5281307152 -0.5917809942 -0.6434786541

H -5.4005124142 0.4907677439 -0.5314343232

H -5.8869901519 -0.9888665308 0.312251349

H -6.3229136984 -0.760888547 -1.3854929951

C -4.4659140227 -2.7925938868 -1.2734428687

H -3.5643899171 -3.3228015387 -1.6053801856

H -5.2458243431 -2.9667854928 -2.0296712801

H -4.8083055834 -3.2600007226 -0.343515291

C -3.8451589999 -0.6966637556 -2.496985632

H -2.9541990279 -1.1804979582 -2.9151112772

H -3.667325138 0.384692644 -2.454830512

H -4.6684515298 -0.8632210898 -3.2074095554

Version=AM64L-G03RevD.01 State=1-A\\HF=-1370.8173818

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Sum of electronic and thermal Energies= -1370.307626

Sum of electronic and thermal Enthalpies= -1370.306682

Sum of electronic and thermal Free Energies= -1370.392714

6-E*-chair-TS:

B3LYP/6-31+G(d)

0 1

C -0.4768381621 -1.3540404918 0.8396323813

C -0.7337671089 -2.2298722848 -0.395976057

C -2.1943036753 -2.3457611829 -0.8110111762

O 0.0323281898 -1.7430952755 -1.5316558469

O -1.0143054213 -0.0440266546 0.6667900698

C 1.0281945106 -1.3480667087 1.0970310469

H -0.9691290095 -1.8425341857 1.6938011274

O 2.0082505064 0.5951685172 1.5891324225

C 1.8572929991 -1.5533950855 -0.0066928447

H 1.3847996778 -1.4886912357 2.1067544205

C 1.332021381 -1.546310452 -1.2798164824

H 2.9320260345 -1.550991922 0.1075972824

H 1.9233899617 -1.4586577309 -2.1853787686

C 2.0158760485 1.4392182672 0.6372685296

C 2.9054486168 1.4738836293 -0.4288027398

O 1.0569010897 2.4437295419 0.6189279704

C 4.1929468895 0.7085696426 -0.4913159088

H 2.763092533 2.2752459797 -1.1500077008

C 0.4830760411 2.741453543 1.8911747247

H 1.2640829005 2.9654240246 2.628642906

H -0.1277660955 1.9127532559 2.2562691282

H -0.1358027623 3.6287501047 1.7373850086

H 4.2697552736 0.0506744389 -1.37115769

H 4.3390521586 0.1026666035 0.4079378405

H 5.0429472832 1.4043850688 -0.5637196377

H -0.3599246353 -3.2428939596 -0.1831273257

H -2.6955908172 -2.9853160922 -0.0678110825

H -2.2452566429 -2.8567760162 -1.7799236743

O -2.8742461391 -1.114130393 -0.9306951764

Si -2.5389566381 0.2526823442 -0.0058288959

C -3.8226417394 0.3642221249 1.4254212218

C -2.4697273551 1.6990825854 -1.2594006368

C -3.6609381722 1.5726411524 -2.2423254828

H -3.660848424 0.6076992305 -2.759979969

H -3.5848309669 2.3627478925 -3.0039371542

H -4.6320364044 1.6915541003 -1.74866607

C -1.1566762343 1.584179959 -2.0698054554

H -0.2764071226 1.7164423961 -1.4348124179

H -1.1384112413 2.3683808932 -2.8416916849

H -1.0762980547 0.617236758 -2.5792677672

C -2.5188848883 3.0898129427 -0.5916141224

H -1.6826466521 3.2428188899 0.0971769963

H -3.4539331135 3.2581643382 -0.0445063037

H -2.4501665402 3.8702280041 -1.3637977928

C -5.2176532988 0.7768523152 0.9044368096

H -5.5858138568 0.0956224687 0.1274548319

H -5.2222979861 1.7921818771 0.4934053786

H -5.9447466583 0.7578245824 1.7301999676

C -3.3648040712 1.3680768792 2.507817345

H -2.3967583506 1.0880643943 2.938628386

H -4.0979902543 1.3930553662 3.3281427672

H -3.275231609 2.3890376731 2.1210639234

C -3.9514358742 -1.030596767 2.0824720125

H -3.0021572807 -1.3760537408 2.510031368

H -4.307851111 -1.7875215322 1.3739884557

H -4.676407728 -0.9888000739 2.9091415426

Version=AM64L-G03RevD.01 State=1-A\\HF=-1370.8055224

Sum of electronic and zero-point Energies= -1370.324088

Sum of electronic and thermal Energies= -1370.296158

Sum of electronic and thermal Enthalpies= -1370.295214

Sum of electronic and thermal Free Energies= -1370.380519

Products

8-chair product

B3LYP/6-31+G(d)

0 1

C 0.6696779716 2.1360881468 -0.3885744756

C 1.055789679 2.9433667276 0.8689680095

C -0.0243312994 2.9892147088 1.9513829813

O 2.2729850208 2.4639656424 1.4351509179

O 0.0642853107 0.8643061089 -0.1174989444

C 1.8887938517 1.9198853524 -1.2480882139

H -0.0582543121 2.7413567213 -0.9542431149

O 6.0433664516 3.2402985187 -0.3257277992

C 3.1239773354 2.1978766714 -0.8195869802

H 1.7176362356 1.5308838471 -2.2499347353

C 3.3926562832 2.7048093494 0.5769230846

H 3.9829084478 2.0956193967 -1.4775344881

C 5.9127959802 2.65526952170.7330426203

C 4.6167492119 2.0768339503 1.2783375485

O 6.9427237526 2.4246027095 1.5767360642

C 4.6488158693 0.535504843 1.2255240184

C 8.2354109083 2.8894225086 1.1425863245

H 8.9243773831 2.609017932 1.9396969206

H 8.2233085652 3.9738514701 1.0051904987

H 8.5159234388 2.4089565386 0.2014627011

H 3.708065906 0.1365717833 1.6107321189

H 5.4696943333 0.1501453543 1.8376769623

H 4.7802092589 0.1709961944 0.2007847488

H 1.2114475789 3.9879939403 0.5416833217

H -0.8290512199 3.6514694099 1.5995473366

H 0.4102729259 3.434919664 2.8525232462

O -0.5679481534 1.7280800959 2.3221341368

Si -0.9248494776 0.5335845948 1.1979559466

C -0.3750500427 -1.1242140469 1.9800698718

C -2.7572031471 0.6774332 0.6225768318

C -0.931292362 -1.2510444739 3.418188815

H -2.025075899 -1.3063394485 3.4442503167

H -0.6214460885 -0.4079208172 4.0455188486

H -0.5479924872 -2.1725530032 3.8815072472

C 1.1684277175 -1.1188751568 2.0562153205

H 1.5407156353 -0.2643299891 2.6317882507

H 1.6213994594 -1.0770690152 1.0602198402

H 1.5178301726 -2.037924196 2.5507599951

C -0.8229830355 -2.3442125327 1.1458425511

H -1.913738366 -2.4479310802 1.1112467843

H -0.4242011452 -3.2672070555 1.5927980593

H -0.4540404043 -2.2954673118 0.1137149486

C -3.747978185 0.1312402924 1.6742760094

H -4.7819552812 0.3080676744 1.3411364623

H -3.6299629483 0.6224667184 2.648104866

H -3.6389717136 -0.9487040785 1.8249455642

C -2.9652506109 -0.0761919815 -0.7118861147

H -3.9996583808 0.0623023444 -1.0614789328

H -2.7975995724 -1.1543441309 -0.6130376971

H -2.2950125552 0.2936915469 -1.4960913778

C -3.0854381366 2.1719246222 0.3900821864

H -4.1167620124 2.2737946195 0.0199474533

H -2.4298111561 2.6313644674 -0.3605769254

H -3.0107847827 2.7552817959 1.3150810908

H 4.5500141752 2.375806399 2.3318774568

H 3.5623839154 3.7960629353 0.5280715217

Version=AM64L-G03RevE.01 State=1-A HF=-1370.9122919

Sum of electronic and zero-point Energies= -1370.426969

Sum of electronic and thermal Energies= -1370.399043

Sum of electronic and thermal Enthalpies= -1370.398099

Sum of electronic and thermal Free Energies= -1370.484424

7-chair product

B3LYP/6-31+G(d)

\0 1\

C 0.6696779716 2.1360881468 -0.3885744756

C 1.055789679 2.9433667276 0.8689680095

C -0.0243312994 2.9892147088 1.9513829813

O 2.2729850208 2.4639656424 1.4351509179

O 0.0642853107 0.8643061089 -0.1174989444

C 1.8887938517 1.9198853524 -1.2480882139

H -0.0582543121 2.7413567213 -0.9542431149

O 6.0433664516 3.2402985187 -0.3257277992

C 3.1239773354 2.1978766714 -0.8195869802

H 1.7176362356 1.5308838471 -2.2499347353

C 3.3926562832 2.7048093494 0.5769230846

H 3.9829084478 2.0956193967 -1.4775344881

C 5.9127959802 2.6552695217 0.7330426203

C 4.6167492119 2.0768339503 1.2783375485

O 6.9427237526 2.4246027095 1.5767360642

C 4.6488158693 0.535504843 1.2255240184

C 8.2354109083 2.8894225086 1.1425863245

H 8.9243773831 2.609017932 1.9396969206

H 8.2233085652 3.9738514701 1.0051904987

H 8.5159234388 2.4089565386 0.2014627011

H 3.708065906 0.1365717833 1.6107321189

H 5.4696943333 0.1501453543 1.8376769623

H 4.7802092589 0.1709961944 0.2007847488

H 1.2114475789 3.9879939403 0.5416833217

H -0.8290512199 3.6514694099 1.5995473366

H 0.4102729259 3.434919664 2.8525232462

O -0.5679481534 1.7280800959 2.3221341368

Si -0.9248494776 0.5335845948 1.1979559466

C -0.3750500427 -1.1242140469 1.9800698718

C -2.7572031471 0.6774332 0.6225768318

C -0.931292362 -1.2510444739 3.418188815

H -2.025075899 -1.3063394485 3.4442503167

H -0.6214460885 -0.4079208172 4.0455188486

H -0.5479924872 -2.1725530032 3.8815072472

C 1.1684277175 -1.1188751568 2.0562153205

H 1.5407156353 -0.2643299891 2.6317882507

H 1.6213994594 -1.0770690152 1.0602198402

H 1.5178301726 -2.037924196 2.5507599951

C -0.8229830355 -2.3442125327 1.1458425511

H -1.913738366 -2.4479310802 1.1112467843

H -0.4242011452 -3.2672070555 1.5927980593

H -0.4540404043 -2.2954673118 0.1137149486

C -3.747978185 0.1312402924 1.6742760094

H -4.7819552812 0.3080676744 1.3411364623

H -3.6299629483 0.6224667184 2.648104866

H -3.6389717136 -0.9487040785 1.8249455642

C -2.9652506109 -0.0761919815 -0.7118861147

H -3.9996583808 0.0623023444 -1.0614789328

H -2.7975995724 -11543441309 -0.6130376971

H -2.2950125552 0.2936915469 -1.4960913778

C -3.0854381366 2.1719246222 0.3900821864

H -4.1167620124 2.2737946195 0.0199474533

H -2.4298111561 2.6313644674 -0.3605769254

H -3.0107847827 2.7552817959 1.3150810908

H 4.5500141752 2.375806399 2.3318774568

H 3.5623839154 3.7960629353 0.5280715217

Version=AM64L-G03RevE.01 Stat =1-A HF=-1370.9122919

Sum of electronic and zero-point Energies= -1370.422518

Sum of electronic and thermal Energies= -1370.394387

Sum of electronic and thermal Enthalpies= -1370.393443

Sum of electronic and thermal Free Energies= -1370.481215

COMPLETE REFERENCE 15

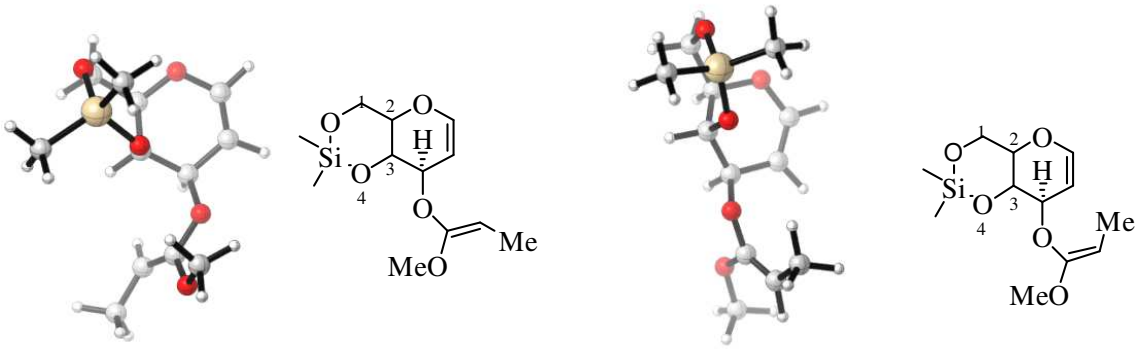
(12) Frisch M. J.; Trucks G. W.; Schlegel H. B.; Scuseria G. E.; Robb M. A.; Cheeseman J. R.; J. A. Montgomery J.; Vreven T.; Kudin K. N.; Burant J. C.; Millam J. M.; Iyengar S. S.; J. Tomasi; Barone V.; Mennucci B.; Cossi M.; Scalmani G.; Rega N.; Petersson G. A.; Nakatsuji H.; Hada M.; Ehara M.; Toyota K.; Fukuda R.; Hasegawa J.; Ishida M.; Nakajima T.; Honda Y.; Kitao O.; Nakai H.; Klene M.; Li X.; Knox J. E.; Hratchian H. P.; Cross J. B.; Adamo C.; Jaramillo J.; Gomperts R.; Stratmann R. E.; Yazyev O.; Austin A.

J.; Cammi R.; Pomelli C.; Ochterski J. W.; Ayala P. Y.; Morokuma K.; Voth G. A.; Salvador P.; Dannenberg J. J.; Zakrzewski V. G.; Dapprich S.; Daniels A. D.; Strain M. C.; Farkas O.; Malick D. K.; Rabuck A. D.; Raghavachari K.; Foresman J. B.; Ortiz J. V.; Cui Q.; Baboul A. G.; Clifford S.; Cioslowski J.; Stefanov B. B.; Liu G.; Liashenko A.; Piskorz P.; Komaromi I.; Martin R. L.; Fox D. J.; Keith T.; Al-Laham M. A.; Peng C. Y.; Nanayakkara A.; Challacombe M.; Gill P. M. W.; Johnson B.; Chen W.; Wong M. W.; Gonzalez C.; Pople J. A.; Revision D.01; Gaussian Inc.: Wallingford CT 2004.

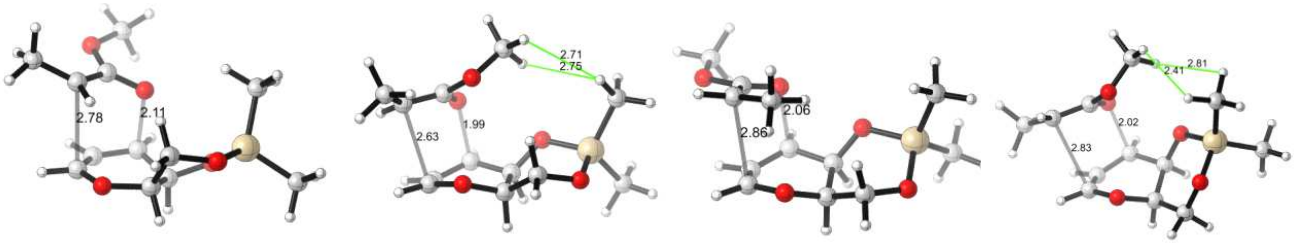
Computational Details

All gas phase B3LYP/6-31+G(d) optimized stationary points were verified as minima or first-order saddle points by calculation of the full Hessian in Gaussian03.[12] Solvation free energy corrections were performed using 6-31+G(d,p) and a CPCM dielectric continuum solvent model for benzene (ε =2.247). Conformational search was done at AM1 level of theory using S*PARTAN* (©Wavefunction, Inc). All obtained conformers within a 5 kcal/mol energy range were subsequently optimized with B3LYP/6-31+G(d) in Gaussian03.

Alternative Substrate (A)



Z*-**A** (0.9) **E***-**A** (0.0)



Z*-**A**-boat-TS (20.1) Z*-**A**-chair-TS (23.3) E*-**A**-boat-TS (25.4) E*-**A**-chair-TS (30.3)

Figure S1. Realative reactant isomer Energies (H in kcal/mol) (top) and TSs (bottom) ($\Delta H^{\ddagger}$ given in kcal/mol).

Table S1. Activation parameters for model **A** in kcal/mol.

Compound	$\Delta H^{\ddagger}$	$\Delta(\Delta H^{\ddagger})$	$\Delta G^{\ddagger}$	$\Delta(\Delta G^{\ddagger})$
E*-**A**-boat-TS	25.4	5.3	26.8	5.8
E*-**A**-chair-TS	30.3	10.2	32.3	11.3

E/Z isomerization

Uncatalyzed for substrate 6

H	0.55124600	2.63379100	-2.21727800
C	-0.06473600	2.12843600	-1.45604400
O	-0.44883100	3.11450800	-0.48314700
C	0.49726400	3.45419800	0.43404800
H	0.19291300	4.32595300	1.00438100
C	1.65586000	2.81111200	0.62589900
H	2.35346200	3.17160000	1.37435300
C	0.76357400	0.98564200	-0.84091500
H	1.08968200	0.33507800	-1.66218200
C	2.00978000	1.58849200	-0.15879000
H	2.77508800	1.78713700	-0.91627000
C	-1.34272400	1.63429200	-2.13514200
H	-1.05546100	1.09481900	-3.05071200
H	-1.94052600	2.50412700	-2.42926300
O	-2.15709600	0.80634400	-1.32107300
Si	-1.57129800	-0.25694500	-0.15785000
O	0.02018400	0.23828800	0.10392100
C	-1.58846900	-2.02231100	-0.91992100
C	-2.51420000	0.01647800	1.48467100
O	2.61696200	0.63927400	0.80288200
C	3.33451500	-0.41051600	0.44138700
C	3.94623000	-1.30011200	1.35995700
O	3.39972700	-0.50360500	-0.88518000
C	4.16881400	-1.57667300	-1.49160800
H	4.59453500	-2.17066200	-0.67466900
H	4.93416200	-1.10238100	-2.10998000
H	3.47517600	-2.14721900	-2.11331500
C	-3.92587500	-0.61109600	1.45107500
H	-4.53149000	-0.22787000	0.62032100
H	-4.45866500	-0.36895200	2.38246200
H	-3.89435100	-1.70369600	1.37411300
C	-2.66136500	1.53793800	1.72126400
H	-3.22250100	2.02673300	0.91785100
H	-1.68813600	2.03240800	1.80112000
H	-3.20037900	1.70874000	2.66505900
C	-1.71516800	-0.58373700	2.66657900
H	-0.70758900	-0.15934000	2.73309100
H	-1.61731600	-1.67279400	2.59993700
H	-2.23505900	-0.36166300	3.61035700
C	-2.96728700	-2.32829300	-1.55097800
H	-3.24072700	-1.58701500	-2.31072600
H	-3.77115900	-2.35621500	-0.80787700
H	-2.94170100	-3.31419500	-2.03905400
C	-0.52519300	-2.08462600	-2.04289800
H	-0.70929200	-1.34363700	-2.83123600
H	-0.54902000	-3.07471500	-2.52206600
H	0.48927700	-1.93463300	-1.65581100
C	-1.24895700	-3.11018700	0.12266700
H	-2.01457400	-3.18910300	0.90244900
H	-0.28521600	-2.92760000	0.61351900
H	-1.18635900	-4.09241200	-0.36937700
H	4.66958700	-0.71487500	1.94721900
C	2.94394800	-2.00742600	2.29229500

H	2.25147800	-2.64622700	1.72676600
H	2.32772800	-1.34173100	2.92454500
H	3.49971400	-2.67436100	2.96167700

Zero-point correction= 0.480858 (Hartree/Particle)
Thermal correction to Energy= 0.508605
Thermal correction to Enthalpy= 0.509549
Thermal correction to Gibbs Free Energy= 0.423906
Sum of electronic and zero-point Energies= -1370.294541
Sum of electronic and thermal Energies= -1370.266793
Sum of electronic and thermal Enthalpies= -1370.265849
Sum of electronic and thermal Free Energies= -1370.351492

E'-6-reactant TMS analogue (OTMS instead of OMe)

H	0.20651400	-1.34197400	-2.99831200
C	0.90181000	-1.16443600	-2.16180900
O	1.59134400	-2.39922100	-1.89991800
C	0.90672300	-3.32934000	-1.17460300
H	1.43048700	-4.28003200	-1.17069900
C	-0.25125200	-3.11614300	-0.53881600
H	-0.72084800	-3.92806000	0.00646700
C	0.09010400	-0.67663400	-0.94811300
H	-0.46771900	0.21877000	-1.24852100
C	-0.92263800	-1.77155700	-0.54534800
H	-1.74867300	-1.75051300	-1.26797600
C	1.94674200	-0.15072200	-2.62859100
H	1.41640800	0.69708100	-3.08907500
H	2.56982000	-0.61840100	-3.39918000
O	2.80941400	0.31982900	-1.60425400
Si	2.35108300	0.50910800	0.00238400
O	0.93084900	-0.37522000	0.15393000
C	2.00179000	2.38144100	0.28174600
C	3.64779400	-0.33180400	1.13030800
O	-1.46564200	-1.53692100	0.76543200
C	-2.66723300	-0.90520100	0.88192800
C	-3.51640600	-1.22734700	1.87319700
O	-2.84594800	0.07023800	-0.05105600
C	4.95261900	0.49002600	1.22646400
H	5.39818500	0.67415400	0.24081100
H	5.69393600	-0.06225300	1.82294600
H	4.80196100	1.45833000	1.71721100
C	3.98659500	-1.71854900	0.53451600
H	4.40378500	-1.64173100	-0.47509100
H	3.10417400	-2.36417600	0.48468200
H	4.73108100	-2.21763100	1.17307000
C	3.06729700	-0.54443000	2.54911700
H	2.13755200	-1.12346200	2.52322300
H	2.86194900	0.39938300	3.06620400
H	3.79213800	-1.09994400	3.16297000
C	3.15570800	3.23979900	-0.28729700
H	3.32484900	3.03860400	-1.35127900
H	4.10200700	3.07056900	0.23784800
H	2.91229400	4.30801600	-0.18184200
C	0.70607700	2.75595800	-0.47716800
H	0.78353600	2.55809600	-1.55397400
H	0.50786100	3.83263100	-0.36344300
H	-0.16577400	2.21752300	-0.08882800
C	1.79725700	2.72541400	1.77353400
H	2.70933700	2.57435300	2.36183100
H	0.99771400	2.12875000	2.22974500

H	1.51802200	3.78494200	1.87823900
H	-4.40988900	-0.62164700	1.98955200
C	-3.29605300	-2.33519100	2.86588800
H	-3.15620000	-1.94529800	3.88465200
H	-2.40936000	-2.92268300	2.61301600
H	-4.15872600	-3.01540800	2.90143900
Si	-4.15352700	1.10777700	-0.38196500
C	-3.56549400	2.05325400	-1.89789500
H	-2.64080800	2.60431900	-1.68862100
H	-3.37213700	1.37758900	-2.74006000
H	-4.32083900	2.78073500	-2.22210500
C	-5.70245400	0.10917200	-0.77653700
H	-6.06037000	-0.46697600	0.08362500
H	-6.51441500	0.77875000	-1.09015000
H	-5.51911200	-0.59632500	-1.59636400
C	-4.43543600	2.28366600	1.06360900
H	-5.15850600	3.06101100	0.78248500
H	-4.82514300	1.77752700	1.95381200
H	-3.50229700	2.78509100	1.34798700

Zero-point correction= 0.557129 (Hartree/Particle)
Thermal correction to Energy= 0.591853
Thermal correction to Enthalpy= 0.592797
Thermal correction to Gibbs Free Energy= 0.490157
Sum of electronic and zero-point Energies= -1739.718334
Sum of electronic and thermal Energies= -1739.683610
Sum of electronic and thermal Enthalpies= -1739.682666
Sum of electronic and thermal Free Energies= -1739.785306

Product of the rearrangement of E'-6-reactant TMS analogue (OTMS instead of OMe)

H	-0.82774100	-3.03478900	-0.57311100
C	-1.12819800	-1.97142100	-0.55225900
O	-0.05521500	-1.17580800	-1.04510000
C	1.19090400	-1.43862000	-0.39606000
H	1.58052000	-2.41094800	-0.74655600
C	1.03116900	-1.48221800	1.10483700
H	1.94537600	-1.48013200	1.69385400
C	-1.44538100	-1.61721700	0.91417100
H	-2.07110800	-2.42660500	1.32381700
C	-0.16299200	-1.54006700	1.70147500
H	-0.24817100	-1.53166400	2.78628400
C	-2.31827900	-1.83202500	-1.50270200
H	-3.03093100	-2.64103800	-1.28013600
H	-1.96110900	-1.97089800	-2.52881900
O	-2.98218400	-0.57596000	-1.44993000
Si	-3.26645300	0.24347300	-0.01406600
O	-2.15624000	-0.38244000	1.07868800
C	-5.04913900	-0.17274300	0.58314100
C	-2.82557500	2.08941100	-0.27451300
O	4.03008100	-1.65661700	-0.04487900
C	3.56045100	-0.55984000	-0.29984000
C	2.16392400	-0.33411400	-0.86060300
O	4.24721900	0.58504800	-0.15111400
C	-3.92038700	2.84715100	-1.05809900
H	-4.12242900	2.38832100	-2.03396800
H	-3.59412700	3.88131900	-1.24428900
H	-4.86622200	2.90228900	-0.50712400
C	-1.50875100	2.16143100	-1.08237700
H	-1.61416000	1.70986900	-2.07439000
H	-0.68836500	1.64853200	-0.56973900

H	-1.21734400	3.21428400	-1.21600100
C	-2.59771200	2.78432700	1.08876500
H	-1.80936000	2.28922800	1.66651100
H	-3.50255800	2.80965700	1.70644200
H	-2.28777600	3.82719500	0.92361400
C	-6.06688700	-0.00879100	-0.56929700
H	-5.80381600	-0.62853800	-1.43422500
H	-6.14492900	1.02787200	-0.91433100
H	-7.06813700	-0.31498400	-0.22995600
C	-5.07428200	-1.65119400	1.04082000
H	-4.80395800	-2.34132900	0.23189000
H	-6.08951000	-1.92309500	1.36708900
H	-4.39928600	-1.83029300	1.88582200
C	-5.48271400	0.70444200	1.77801300
H	-5.57188800	1.76189100	1.50482400
H	-4.78206200	0.63062200	2.61909600
H	-6.46910500	0.38012200	2.14309000
Si	5.88645500	0.67454900	0.41669800
C	5.97759800	-0.01426300	2.16391100
H	5.25848900	0.48434800	2.82564800
H	5.76723000	-1.08875800	2.17778400
H	6.97903400	0.14294200	2.58601100
C	7.01160800	-0.24062900	-0.77889800
H	6.90940400	0.14849100	-1.79951300
H	8.06257800	-0.12233300	-0.48348400
H	6.78126600	-1.31101000	-0.79679200
C	6.20295200	2.52697200	0.38845300
H	7.22212800	2.75634900	0.72536800
H	6.08529400	2.93538800	-0.62253000
H	5.50527800	3.05879400	1.04659800
C	2.25745300	-0.25954200	-2.40053000
H	2.62114400	-1.20770500	-2.81436200
H	1.27084900	-0.05349700	-2.82163500
H	2.94264000	0.53863100	-2.70435000
H	1.79897100	0.62907800	-0.48705000

Zero-point correction= 0.558278 (Hartree/Particle)
Thermal correction to Energy= 0.592652
Thermal correction to Enthalpy= 0.593596
Thermal correction to Gibbs Free Energy= 0.491794
Sum of electronic and zero-point Energies= -1739.771322
Sum of electronic and thermal Energies= -1739.736948
Sum of electronic and thermal Enthalpies= -1739.736003
Sum of electronic and thermal Free Energies= -1739.837806

E'-6-boat TS - TMS analogue (OTMS instead of OMe)

C	-0.54864200	1.17501800	-1.17065200
C	-0.82477400	2.33005200	-0.15138300
C	-1.32752900	1.83326300	1.20939400
H	-0.57344200	1.18989300	1.66861500
O	0.30622600	3.21767100	0.10841500
O	-1.13765400	-0.06254800	-0.80838400
C	0.90817700	1.00307000	-1.47958100
H	-1.00351000	1.48197900	-2.12688700
O	1.58472900	0.13445200	0.42216300
C	1.72135400	2.12994200	-1.49437800
H	1.16252100	0.12165100	-2.05559300
C	1.43865400	3.13314200	-0.59009000
H	2.69908900	2.12216700	-1.96204700

H	2.08281700	3.98748300	-0.41466300
C	2.73726300	0.65204800	0.60808700
C	3.04296800	1.74377900	1.40343600
O	3.78743600	0.17296600	-0.16166000
C	2.17691300	2.29098200	2.49714600
H	4.08631600	2.05331500	1.40019000
H	1.16489300	1.88854800	2.45386300
H	2.11259100	3.38765900	2.47117200
H	2.59198900	2.02757300	3.48267200
O	-2.56523100	1.14283000	1.03948400
C	-4.12642900	-0.19349300	-0.96051800
H	-1.58822400	2.99238700	-0.57239400
Si	-2.53348100	-0.26375600	0.10848600
H	-1.50812100	2.69406900	1.86043600
C	-2.21773100	-1.83659900	1.15444800
C	-1.11858300	-1.51418100	2.19639000
H	-0.18873800	-1.17964000	1.72421300
H	-0.89208200	-2.41960400	2.77951100
H	-1.44567400	-0.74473200	2.90656600
C	-3.48496100	-2.29741100	1.90846700
H	-3.23824400	-3.15192800	2.55577400
H	-4.28038400	-2.62584300	1.22987600
H	-3.89316200	-1.50876300	2.55314200
C	-1.70827300	-2.98807300	0.25547000
H	-0.78763900	-2.71067400	-0.26849800
H	-2.44671800	-3.29579500	-0.49363800
H	-1.48801400	-3.86907800	0.87667500
C	-5.35955700	0.07431000	-0.06516600
H	-5.24587800	0.99837100	0.51267600
H	-5.54984100	-0.74204900	0.64010600
H	-6.25805400	0.17900300	-0.69193700
C	-4.34622800	-1.49485800	-1.76271300
H	-3.49314400	-1.73011400	-2.41151500
H	-5.23033400	-1.38986100	-2.40919700
H	-4.52350400	-2.35884400	-1.11283800
C	-3.99608500	0.97681300	-1.96386800
H	-3.16912700	0.82356400	-2.66754900
H	-3.84886800	1.93839500	-1.45759900
H	-4.91752500	1.06046200	-2.55899400
Si	4.07691600	-1.46790400	-0.49182100
C	2.94571500	-2.13580500	-1.84753100
H	3.22765400	-3.16486900	-2.10879400
H	1.89981900	-2.14538400	-1.52167700
H	3.01680200	-1.53592400	-2.76422600
C	3.87478700	-2.47754000	1.08748100
H	4.11378100	-3.53438700	0.90924800
H	4.54072800	-2.11380100	1.87987600
H	2.84559100	-2.42382900	1.46064400
C	5.86287300	-1.48050800	-1.09182200
H	6.18596400	-2.49512500	-1.35909800
H	5.98555700	-0.84669800	-1.97905800
H	6.54251200	-1.10301400	-0.31821200

Zero-point correction= 0.555388 (Hartree/Particle)
Thermal correction to Energy= 0.589566
Thermal correction to Enthalpy= 0.590510
Thermal correction to Gibbs Free Energy= 0.490834
Sum of electronic and zero-point Energies= -1739.679581
Sum of electronic and thermal Energies= -1739.645403
Sum of electronic and thermal Enthalpies= -1739.644459
Sum of electronic and thermal Free Energies= -1739.744134

Table S1. Activation parameters (in kcal/mol) for models **2'** and **6'** at 298 K, calculated with MO6-2X//B3LYP/6-31+G(d).[19,20]

TSs	$\Delta H^{\ddagger}$	$\Delta\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$	$\Delta\Delta G^{\ddagger}$
*Z****-2'**-boat-TS	**20.2**	**0.0**	**20.5**	**0.0**
*Z****-2'-**chair-TS	26.5	6.3	27.8	7.3
*E****-2'**-boat-TS	27.8	7.6	28.9	8.4
*E****-2'**-chair-TS	28.6	8.4	29.3	8.8
*Z****-6'**-boat-TS	**24.7**	**0.0**	**25.4**	**0.0**
*Z****-6'**-chair-TS	31.1	6.4	33.0	7.6
*E****-6'-**boat-TS	32.2	7.5	32.5	7.1
*E****-6'**-chair-TS	42.2	17.5	42.9	17.5

Table S2: Electronic energies of reactants and transition states calculated with MO6-2X.

E*-2'	-730.7101
E*-2'-boat-TS	-730.6627
E*-2'-chair-TS	-730.6615
Z*-2'	-730.7080
Z*-2'-boat-TS	-730.6730
Z*-2'-chair-TS	-730.6629
E*-6'	-1370.6392
E*-6'-boat-TS	-1370.5850
E*-6'-chair-TS	-1370.5687
Z*-6'	-1370.6352
Z*-6'-boat-TS	-1370.5930
Z*-6'-chair-TS	-1370.5835