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A. Calculated Structures and Energies.

Chapter 2 – Corner Cutting in Organocatalysis

o-chlorobenzaldehyde

B3LYP/6-31G*

OCBB3G*

E(RB+HF-LYP) = -805.165191571

Zero-point correction=	0.100612 (Hartree/Particle)
Thermal correction to Energy=	0.108104
Thermal correction to Enthalpy=	0.109048
Thermal correction to Gibbs Free Energy=	0.067881
Sum of electronic and zero-point Energies=	-805.064580
Sum of electronic and thermal Energies=	-805.057088
Sum of electronic and thermal Enthalpies=	-805.056144
Sum of electronic and thermal Free Energies=	-805.097310

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.836	27.746	86.642

C,0,0.0635074983,0.,-0.0605631261
C,0,0.0137883836,0.,1.3444347379
C,0,1.1745729015,0.,2.1060260578
C,0,2.4186212913,0.,1.4661471061
C,0,2.4976791903,0.,0.0744899992
C,0,1.3238575971,0.,-0.6787899779
H,0,-0.9698894553,0.,1.8037974637
H,0,1.1180247557,0.,3.1904497802
H,0,3.334371027,0.,2.0508166594
H,0,3.4578373538,0.,-0.4303036957
Cl,0,1.4802528699,0.,-2.4348987436
C,0,-1.2232855305,0.,-0.8077016823
O,0,-2.3100744754,0.,-0.2603890258
H,0,-1.1445154075,0.,-1.9097735533

B3LYP/6-31+G**

OCBB3+G**

E(RB+HF-LYP) = -805.187708093

Zero-point correction=	0.100174 (Hartree/Particle)
Thermal correction to Energy=	0.107722
Thermal correction to Enthalpy=	0.108666
Thermal correction to Gibbs Free Energy=	0.067332
Sum of electronic and zero-point Energies=	-805.087534

Sum of electronic and thermal Energies=	-805.079986
Sum of electronic and thermal Enthalpies=	-805.079042
Sum of electronic and thermal Free Energies=	-805.120376

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.596	27.866	86.994

C,0,0.0603668497,0.,-0.0574078273
C,0,0.0124120185,0.,1.348903725
C,0,1.1762556373,0.,2.1088773404
C,0,2.4202416181,0.,1.466442032
C,0,2.497111434,0.,0.0730470317
C,0,1.321273259,0.,-0.6786357232
H,0,-0.9684096756,0.,1.8141133613
H,0,1.1208091819,0.,3.1927843008
H,0,3.3368228923,0.,2.0488162355
H,0,3.4570062967,0.,-0.4313336221
Cl,0,1.4766071987,0.,-2.4339169978
C,0,-1.2214187105,0.,-0.8125425363
O,0,-2.3146010758,0.,-0.2725636833
H,0,-1.1397289243,0.,-1.9128426366

B3LYP/6-31G* Onsager solvent model for DMSO

OCBOnsgrB3G

E(RB+HF-LYP) = -805.167053971

Zero-point correction=	0.100626 (Hartree/Particle)
Thermal correction to Energy=	0.108121
Thermal correction to Enthalpy=	0.109065
Thermal correction to Gibbs Free Energy=	0.067892
Sum of electronic and zero-point Energies=	-805.066428
Sum of electronic and thermal Energies=	-805.058933
Sum of electronic and thermal Enthalpies=	-805.057989
Sum of electronic and thermal Free Energies=	-805.099162

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.847	27.741	86.656

C,0,0.0600286697,0.,-0.0574833549
C,0,0.0127722902,0.,1.3476513702
C,0,1.1752963922,0.,2.1069918651
C,0,2.4179609537,0.,1.4651870461
C,0,2.4956086404,0.,0.0721777119
C,0,1.3212941666,0.,-0.6775120745

H,0,-0.96887508,0.,1.8114636199
H,0,1.1214049739,0.,3.1913430672
H,0,3.3346889349,0.,2.0477065601
H,0,3.4564595465,0.,-0.4308537516
Cl,0,1.4751854539,0.,-2.4352500345
C,0,-1.2198118878,0.,-0.806517927
O,0,-2.3155510594,0.,-0.2726489242
H,0,-1.1317159948,0.,-1.9085171736

B3LYP/6-31+G Onsager solvent model for DMSO**
OCBOnsgrB3+G

E(RB+HF-LYP) = -805.189919078

Zero-point correction=	0.100160 (Hartree/Particle)
Thermal correction to Energy=	0.107714
Thermal correction to Enthalpy=	0.108659
Thermal correction to Gibbs Free Energy=	0.067314
Sum of electronic and zero-point Energies=	-805.089760
Sum of electronic and thermal Energies=	-805.082205
Sum of electronic and thermal Enthalpies=	-805.081261
Sum of electronic and thermal Free Energies=	-805.122605

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.592	27.875	87.017

C,0,0.0564157415,0.,-0.0539908561
C,0,0.0114167789,0.,1.3532999268
C,0,1.1769501525,0.,2.1102732814
C,0,2.4198366713,0.,1.4652707768
C,0,2.4948448564,0.,0.0712382161
C,0,1.3181960034,0.,-0.6771581961
H,0,-0.967387363,0.,1.8225593566
H,0,1.1258091709,0.,3.194227221
H,0,3.3374308395,0.,2.0455731211
H,0,3.4549113626,0.,-0.4326060133
Cl,0,1.4710172995,0.,-2.434330493
C,0,-1.2177292208,0.,-0.8115487789
O,0,-2.3218064273,0.,-0.2876931991
H,0,-1.1251598657,0.,-1.9113763632

B3LYP/6-31+G PCM solvent model for DMSO**
OCBPCM3+Gradii
E(RB+HF-LYP) = -805.200891262

Zero-point correction= 0.099818 (Hartree/Particle)
 Thermal correction to Energy= 0.107426
 Thermal correction to Enthalpy= 0.108370
 Thermal correction to Gibbs Free Energy= 0.066867
 Sum of electronic and zero-point Energies= -805.101073
 Sum of electronic and thermal Energies= -805.093465
 Sum of electronic and thermal Enthalpies= -805.092521
 Sum of electronic and thermal Free Energies= -805.134025

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	67.411	28.001	87.352

C,0,0.0535027811,0.,-0.0535662058
 C,0,0.0098071979,0.,1.3548607071
 C,0,1.1763823977,0.,2.1111805979
 C,0,2.41919902,0.,1.464573971
 C,0,2.493925226,0.,0.0695117845
 C,0,1.316534477,0.,-0.6769818111
 H,0,-0.9630026871,0.,1.8351949296
 H,0,1.1241880241,0.,3.1948781829
 H,0,3.3371621204,0.,2.0440045867
 H,0,3.454798117,0.,-0.4329085069
 Cl,0,1.4699659092,0.,-2.4352823191
 C,0,-1.2104406962,0.,-0.8166857229
 O,0,-2.3228434334,0.,-0.2923791184
 H,0,-1.1244314537,0.,-1.9126630753

p-nitrobenzaldehyde

B3LYP/6-31G*

PNBB3G*

E(RB+HF-LYP) = -550.071353862

Zero-point correction= 0.112672 (Hartree/Particle)
 Thermal correction to Energy= 0.121485
 Thermal correction to Enthalpy= 0.122429
 Thermal correction to Gibbs Free Energy= 0.077800
 Sum of electronic and zero-point Energies= -549.958682
 Sum of electronic and thermal Energies= -549.949869
 Sum of electronic and thermal Enthalpies= -549.948925
 Sum of electronic and thermal Free Energies= -549.993554

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	76.233	32.434	93.930

C,0,0.0054576062,0.,-0.0901276138
 C,0,-0.0350394686,0.,1.3101617849
 C,0,1.1573460707,0.,2.0502453891
 C,0,2.383479571,0.,1.3974003611
 C,0,2.3941095293,0.,0.0012407094
 C,0,1.2263151274,0.,-0.7587527141
 C,0,-1.345244042,0.,2.0126049572
 O,0,-1.4710352266,0.,3.2199559887
 H,0,1.0986165816,0.,3.1338627816
 H,0,3.3216549928,0.,1.9382841579
 N,0,3.6935595307,0.,-0.6991460351
 H,0,1.2910796227,0.,-1.8396145143
 H,0,-2.233388601,0.,1.3439657673
 O,0,3.6766228093,0.,-1.9289335149
 O,0,4.7108843205,0.,-0.0086294928
 H,0,-0.9223824238,0.,-0.6570110122

B3LYP/6-31+G**

PNBB3+G

E(RB+HF-LYP) = -550.103291252

Zero-point correction=	0.112028	(Hartree/Particle)
Thermal correction to Energy=	0.120909	
Thermal correction to Enthalpy=	0.121853	
Thermal correction to Gibbs Free Energy=	0.077007	
Sum of electronic and zero-point Energies=	-549.991264	
Sum of electronic and thermal Energies=	-549.982382	
Sum of electronic and thermal Enthalpies=	-549.981438	
Sum of electronic and thermal Free Energies=	-550.026284	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.871	32.633	94.386

C,0,0.0047077512,0.,-0.0865199076
 C,0,-0.034307542,0.,1.3150346879
 C,0,1.1602830197,0.,2.0542941802
 C,0,2.3862622426,0.,1.3984104934
 C,0,2.3951653804,0.,0.0006876257
 C,0,1.2257606189,0.,-0.758307121
 C,0,-1.3500583099,0.,2.0091651891
 O,0,-1.486456932,0.,3.2175057077
 H,0,1.1067110387,0.,3.1379496745
 H,0,3.3238790668,0.,1.9403062657
 N,0,3.6963769152,0.,-0.7023249169
 H,0,1.2854687928,0.,-1.8394642254

H,0,-2.2349759526,0.,1.3388871724
 O,0,3.6795029972,0.,-1.9332858238
 O,0,4.7163276338,0.,-0.0136096022
 H,0,-0.9226077208,0.,-0.6532233997

B3LYP/6-31G* Onsager solvent model for DMSO

PNBOnsB3G

E(RB+HF-LYP) = -550.072590041

Zero-point correction=	0.112616	(Hartree/Particle)
Thermal correction to Energy=	0.121440	
Thermal correction to Enthalpy=	0.122384	
Thermal correction to Gibbs Free Energy=	0.077715	
Sum of electronic and zero-point Energies=	-549.959974	
Sum of electronic and thermal Energies=	-549.951150	
Sum of electronic and thermal Enthalpies=	-549.950206	
Sum of electronic and thermal Free Energies=	-549.994875	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	76.205	32.466	94.015

C,0,0.0037143097,0.,-0.0956424031
 C,0,-0.0378933397,0.,1.3043121196
 C,0,1.1538048537,0.,2.0452921066
 C,0,2.3801942574,0.,1.395173791
 C,0,2.3938184602,0.,-0.0016026627
 C,0,1.2264228213,0.,-0.762893897
 C,0,-1.3463649681,0.,2.0169195954
 O,0,-1.4504192125,0.,3.2260272041
 H,0,1.0905840878,0.,3.1286772374
 H,0,3.3171642984,0.,1.9378377752
 N,0,3.6947685237,0.,-0.6953123601
 H,0,1.2894469775,0.,-1.8438814999
 H,0,-2.2420009618,0.,1.3612479105
 O,0,3.6892291893,0.,-1.9250466425
 O,0,4.7123551152,0.,-0.0012673995
 H,0,-0.9227854119,0.,-0.664334875

B3LYP/6-31+G Onsager solvent model for DMSO**

PNBB3+GOnsgr

E(RB+HF-LYP) = -550.104793624

Zero-point correction=	0.111955	(Hartree/Particle)
Thermal correction to Energy=	0.120848	

Thermal correction to Enthalpy= 0.121793
 Thermal correction to Gibbs Free Energy= 0.076906
 Sum of electronic and zero-point Energies= -549.992839
 Sum of electronic and thermal Energies= -549.983945
 Sum of electronic and thermal Enthalpies= -549.983001
 Sum of electronic and thermal Free Energies= -550.027888

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.834	32.667	94.472

C,0,0.0029633912,0.,-0.0933167444
 C,0,-0.0376311525,0.,1.3077411884
 C,0,1.1559839712,0.,2.048322976
 C,0,2.3826246468,0.,1.3959546865
 C,0,2.3950805709,0.,-0.0024339674
 C,0,1.2261555458,0.,-0.7632421623
 C,0,-1.3511091484,0.,2.0142120174
 O,0,-1.4614641476,0.,3.224538829
 H,0,1.0973450563,0.,3.1317480976
 H,0,3.3184825478,0.,1.9404152594
 N,0,3.6972089567,0.,-0.6977498484
 H,0,1.2844594133,0.,-1.8445434704
 H,0,-2.2455969828,0.,1.3593430031
 O,0,3.6926753856,0.,-1.9287455663
 O,0,4.7178063619,0.,-0.0046929491
 H,0,-0.9229454162,0.,-0.6620453491

B3LYP/6-31+G** PCM solvent model for DMSO

pnbPCMB3+G

E(RB+HF-LYP) = -550.126515939

Zero-point correction= 0.112759 (Hartree/Particle)
 Thermal correction to Energy= 0.121521
 Thermal correction to Enthalpy= 0.122465
 Thermal correction to Gibbs Free Energy= 0.078232
 Sum of electronic and zero-point Energies= -550.013757
 Sum of electronic and thermal Energies= -550.004995
 Sum of electronic and thermal Enthalpies= -550.004051
 Sum of electronic and thermal Free Energies= -550.048283

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	76.256	32.476	93.096

C,0,0.0033577409,0.,-0.0840814606

C,0,-0.0298968604,0.,1.3186914394
 C,0,1.1657375267,0.,2.0579566097
 C,0,2.3899031258,0.,1.4010545155
 C,0,2.3932670839,0.,0.0018476688
 C,0,1.2227004136,0.,-0.7577267926
 C,0,-1.3474510017,0.,1.9947207528
 O,0,-1.4979748484,0.,3.2114326963
 H,0,1.1287491152,0.,3.1414530548
 H,0,3.3207271533,0.,1.9523000891
 N,0,3.6835604386,0.,-0.6965864439
 H,0,1.265633898,0.,-1.8386404534
 H,0,-2.2235761501,0.,1.3245486473
 O,0,3.6836265405,0.,-1.9309212921
 O,0,4.7167964186,0.,-0.0213255753
 H,0,-0.9231215943,0.,-0.6492174556

Acetone

B3LYP/6-31G*

acetoneB3G*

E(RB+HF-LYP) = -193.155694048

Zero-point correction=	0.084087 (Hartree/Particle)
Thermal correction to Energy=	0.089495
Thermal correction to Enthalpy=	0.090439
Thermal correction to Gibbs Free Energy=	0.056267
Sum of electronic and zero-point Energies=	-193.071607
Sum of electronic and thermal Energies=	-193.066199
Sum of electronic and thermal Enthalpies=	-193.065255
Sum of electronic and thermal Free Energies=	-193.099427

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	56.159	16.766	71.922

C,0,-0.0366307514,0.,-0.0089558092
 C,0,1.3810551347,0.,-0.5585622358
 C,0,2.5065914926,0.,0.4637236357
 O,0,1.6031756529,0.,-1.7536678169
 H,0,-0.7528977947,0.,-0.8328099768
 H,0,-0.2041318996,0.8806309885,0.6242729261
 H,0,-0.2041318996,-0.8806309885,0.6242729261
 H,0,3.4710414746,0.,-0.0477550043
 H,0,2.4353844447,-0.8806309885,1.114849447
 H,0,2.4353844447,0.8806309885,1.114849447

B3LYP/6-31+G**

acetoneB3+G**

E(RB+HF-LYP) = -193.174509200

Zero-point correction=	0.083548 (Hartree/Particle)
Thermal correction to Energy=	0.088933
Thermal correction to Enthalpy=	0.089878
Thermal correction to Gibbs Free Energy=	0.055333
Sum of electronic and zero-point Energies=	-193.090962
Sum of electronic and thermal Energies=	-193.085576
Sum of electronic and thermal Enthalpies=	-193.084632
Sum of electronic and thermal Free Energies=	-193.119177

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	55.807	16.841	72.706

C,0,-0.036418309,-0.0142552768,-0.0086389789
C,0,1.3804234426,-0.000491796,-0.5540295357
C,0,2.5063226723,0.0144923118,0.4644028373
O,0,1.6033828062,-0.0014246441,-1.7524525427
H,0,-0.7531299642,0.0754257821,-0.8264039588
H,0,-0.184208508,0.8009016395,0.7092480706
H,0,-0.2171945056,-0.9513358055,0.5323663455
H,0,3.4691564833,-0.0762373302,-0.0407472402
H,0,2.3858008167,-0.7995233276,1.1886529078
H,0,2.4807053645,0.9524484469,1.0327954604

B3LYP/6-31G* Onsager solvent model for DMSO

acetoneOnsgrB3G*

E(RB+HF-LYP) = -193.157937889

Zero-point correction=	0.084106 (Hartree/Particle)
Thermal correction to Energy=	0.089494
Thermal correction to Enthalpy=	0.090438
Thermal correction to Gibbs Free Energy=	0.055716
Sum of electronic and zero-point Energies=	-193.073832
Sum of electronic and thermal Energies=	-193.068444
Sum of electronic and thermal Enthalpies=	-193.067500
Sum of electronic and thermal Free Energies=	-193.102222

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	56.158	16.751	73.079

C,0,-0.0342206106,0.001758477,-0.0092413531

C,0,1.3813871068,-0.0003528597,-0.5592053554
 C,0,2.5044826978,-0.0015194813,0.4630777915
 O,0,1.6042505405,-0.0014076849,-1.7571020579
 H,0,-0.7540878877,-0.00855489,-0.830212451
 H,0,-0.2022100212,0.8880907928,0.6153228145
 H,0,-0.1988640173,-0.8701383512,0.6359923823
 H,0,3.471446159,0.0075608519,-0.0440787931
 H,0,2.4361733247,-0.8868474794,1.1076035081
 H,0,2.4264845715,0.87141144,1.1230376742

B3LYP/6-31+G Onsager solvent model for DMSO**

acetoneOnsgrB3+G**

E(RB+HF-LYP) = -193.177479728

Zero-point correction=	0.083530 (Hartree/Particle)
Thermal correction to Energy=	0.088927
Thermal correction to Enthalpy=	0.089871
Thermal correction to Gibbs Free Energy=	0.055152
Sum of electronic and zero-point Energies=	-193.093950
Sum of electronic and thermal Energies=	-193.088553
Sum of electronic and thermal Enthalpies=	-193.087609
Sum of electronic and thermal Free Energies=	-193.122328

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	55.802	16.826	73.071

C,0,-0.0328711212,-0.0095439225,-0.0104529992
 C,0,1.3807883079,0.0261132342,-0.5563331967
 O,0,1.6033573718,0.0732738325,-1.7577970349
 C,0,2.5049839933,0.0003552243,0.4600861705
 H,0,-0.7531543035,-0.0583611508,-0.8286521697
 H,0,-0.2239995606,0.8866439324,0.5921890451
 H,0,-0.1680319169,-0.8680218051,0.6573849786
 H,0,3.4695386932,0.1009708557,-0.0400398305
 H,0,2.4804336732,-0.9415231079,1.0214841134
 H,0,2.3801608627,0.8037169073,1.1951319234

B3LYP/6-31+G PCM solvent model for DMSO**

acetoneB3BBPCM

E(RB+HF-LYP) = -193.188187160

Zero-point correction=	0.082768 (Hartree/Particle)
Thermal correction to Energy=	0.087392
Thermal correction to Enthalpy=	0.088336
Thermal correction to Gibbs Free Energy=	0.055650

Sum of electronic and zero-point Energies= -193.105419
 Sum of electronic and thermal Energies= -193.100795
 Sum of electronic and thermal Enthalpies= -193.099851
 Sum of electronic and thermal Free Energies= -193.132537

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	54.839	14.904	68.793

C,0,-0.0290522916,0.002642355,-0.009919448
 C,0,1.379066335,0.0252886423,-0.5473917205
 O,0,1.6035035833,0.0719275171,-1.7583919584
 C,0,2.5012821078,-0.0114445468,0.4584233273
 H,0,-0.7528434401,-0.1249439194,-0.8167306362
 H,0,-0.225269492,0.948633644,0.5099070208
 H,0,-0.1424871017,-0.7958011317,0.7310499393
 H,0,3.4637382654,0.1683200896,-0.0237324023
 H,0,2.5132307358,-0.997087648,0.9400614423
 H,0,2.3300372989,0.7260888845,1.2497254311

Proline (zwitter-ion)

B3LYP/6-31G* Onsager solvent model for DMSO
 zwitterionOnsB3G
 E(RB+HF-LYP) = -401.150698198

Zero-point correction= 0.145913 (Hartree/Particle)
 Thermal correction to Energy= 0.153096
 Thermal correction to Enthalpy= 0.154040
 Thermal correction to Gibbs Free Energy= 0.113598
 Sum of electronic and zero-point Energies= -401.004785
 Sum of electronic and thermal Energies= -400.997602
 Sum of electronic and thermal Enthalpies= -400.996658
 Sum of electronic and thermal Free Energies= -401.037101

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	96.069	26.410	85.118

N,0,0.0010971983,-0.0693800561,-0.0268009178
 C,0,-0.0420670318,-0.0202426518,1.4969430656
 C,0,1.4481993689,0.2124891433,1.9509793529
 O,0,1.643228143,0.2984812294,3.1707229174
 O,0,2.2625271378,0.2656649625,0.975626308
 C,0,-0.6533726791,-1.3735197584,1.9126485613
 C,0,-1.4256695634,-1.855990695,0.6712490107

C,0,-0.5372770956,-1.4056755323,-0.4902544962
 H,0,-0.671415866,0.8198001072,1.7985881875
 H,0,0.1460499209,-2.0785270818,2.1681736672
 H,0,-1.2910852977,-1.2675575142,2.7930022601
 H,0,-1.5928297557,-2.9364097429,0.6552668972
 H,0,-2.406583197,-1.3716800965,0.6057414107
 H,0,0.3234223539,-2.0658526569,-0.6247581189
 H,0,-1.049229398,-1.2881010217,-1.4465173156
 H,0,-0.5040538952,0.7060840086,-0.4581643253
 H,0,1.0632226567,0.0632903566,-0.1447914646

B3LYP/6-31+G Onsager solvent model for DMSO**
zwitterionOnsB3+G

E(RB+HF-LYP) = -401.194110171

Zero-point correction=	0.145600 (Hartree/Particle)
Thermal correction to Energy=	0.152808
Thermal correction to Enthalpy=	0.153752
Thermal correction to Gibbs Free Energy=	0.113551
Sum of electronic and zero-point Energies=	-401.048510
Sum of electronic and thermal Energies=	-401.041302
Sum of electronic and thermal Enthalpies=	-401.040358
Sum of electronic and thermal Free Energies=	-401.080559

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.888	26.660	84.610

N,0,0.0315789017,-0.0932801097,-0.0322960357
 C,0,-0.0302202641,-0.0311897438,1.4927998185
 C,0,1.4304860949,0.2548407705,1.9858684193
 O,0,1.5763756173,0.4277900349,3.2114424881
 O,0,2.2936341471,0.2636120502,1.0543297572
 C,0,-0.6214404053,-1.3958945541,1.9002242294
 C,0,-1.4357472781,-1.8479098962,0.6751400286
 C,0,-0.5664306465,-1.407895827,-0.5043659621
 H,0,-0.6915985152,0.7902689041,1.7771494097
 H,0,0.1880324023,-2.105316437,2.1074923238
 H,0,-1.2250160045,-1.3076393926,2.8053501962
 H,0,-1.626125532,-2.9236843338,0.652888453
 H,0,-2.4079132223,-1.3439011508,0.6406957199
 H,0,0.2641715874,-2.0954285362,-0.679268078
 H,0,-1.1031318623,-1.2530392795,-1.4411964537
 H,0,-0.4385927457,0.7011603978,-0.4666966982
 H,0,1.0761007254,0.0003801032,-0.1719026159

B3LYP/6-31+G PCM solvent model for DMSO**

zwitterionPCMB3+G

E(RB+HF-LYP) = -401.230118347

Zero-point correction=	0.146181 (Hartree/Particle)
Thermal correction to Energy=	0.153436
Thermal correction to Enthalpy=	0.154381
Thermal correction to Gibbs Free Energy=	0.113935
Sum of electronic and zero-point Energies=	-401.083938
Sum of electronic and thermal Energies=	-401.076682
Sum of electronic and thermal Enthalpies=	-401.075738
Sum of electronic and thermal Free Energies=	-401.116184

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	96.283	26.633	85.126

N,0,0.0350413296,-0.098016474,-0.0509547315
 C,0,-0.0086911641,-0.036412424,1.4679079682
 C,0,1.4047163832,0.2538562591,2.014578549
 O,0,1.4838746395,0.4589016873,3.2538954784
 O,0,2.3565754468,0.2411707697,1.1801600183
 C,0,-0.5890599483,-1.4028912971,1.8920429171
 C,0,-1.4339678402,-1.836379418,0.6844885445
 C,0,-0.5786915812,-1.4076455002,-0.5069405105
 H,0,-0.6796619798,0.7776485842,1.7448192716
 H,0,0.2200534005,-2.1210087897,2.0661243649
 H,0,-1.167116426,-1.313975968,2.8131515799
 H,0,-1.6327111746,-2.9105130178,0.6683948645
 H,0,-2.3948377442,-1.3101947938,0.6753466577
 H,0,0.2420747162,-2.1046009398,-0.683743833
 H,0,-1.121698083,-1.2433994478,-1.4361466414
 H,0,-0.4505830743,0.7005180708,-0.4622070915
 H,0,1.0288460999,-0.014184301,-0.3132644064

Proline (neutral)**B3LYP/6-31G***

ProlineB3G

E(RB+HF-LYP) = -401.148202726

Zero-point correction=	0.145511 (Hartree/Particle)
Thermal correction to Energy=	0.153024
Thermal correction to Enthalpy=	0.153968
Thermal correction to Gibbs Free Energy=	0.112570

Sum of electronic and zero-point Energies= -401.002692
 Sum of electronic and thermal Energies= -400.995179
 Sum of electronic and thermal Enthalpies= -400.994234
 Sum of electronic and thermal Free Energies= -401.035633

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	96.024	27.466	87.131

N,0,-0.130479708,0.1149941399,0.1027061796
 C,0,-0.0620726146,-0.0610954741,1.5777978958
 C,0,1.4197196356,-0.0638186915,1.942229461
 O,0,1.8509075145,1.1675624534,2.304163156
 O,0,2.1585315042,-1.0229853239,1.8845126445
 C,0,-0.7553033184,-1.4135251396,1.9255328177
 C,0,-1.3490625389,-1.8956348026,0.5853075575
 C,0,-0.4295084681,-1.2201818765,-0.4454817316
 H,0,-0.5305076997,0.7958799558,2.068441836
 H,0,-0.0082122088,-2.1242612015,2.2895022611
 H,0,-1.5132925526,-1.2901017508,2.704841572
 H,0,-1.3685043246,-2.9874108662,0.501694556
 H,0,-2.3782038324,-1.5333321999,0.4626933757
 H,0,0.5104555613,-1.777569248,-0.5376707278
 H,0,-0.8644226372,-1.1263230282,-1.4454899128
 H,0,-0.9047954845,0.7414745044,-0.1063575222
 H,0,2.8124951722,1.0845125492,2.4505695813

B3LYP/6-31+G**

ProlineB3+G

E(RB+HF-LYP) = -401.185797297

Zero-point correction= 0.144561 (Hartree/Particle)
 Thermal correction to Energy= 0.152177
 Thermal correction to Enthalpy= 0.153121
 Thermal correction to Gibbs Free Energy= 0.111406
 Sum of electronic and zero-point Energies= -401.041236
 Sum of electronic and thermal Energies= -401.033620
 Sum of electronic and thermal Enthalpies= -401.032676
 Sum of electronic and thermal Free Energies= -401.074391

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	95.493	27.880	87.796

N,0,-0.0321458605,0.026849397,0.0810079238

C,0,-0.0283638892,-0.1073763145,1.5619581196
 C,0,1.4243455933,-0.0242540361,2.0257896378
 O,0,1.7886989082,1.2537170096,2.2952575663
 O,0,2.197266156,-0.9541264974,2.1231276267
 C,0,-0.6886381286,-1.4721463445,1.8955478927
 C,0,-1.4093985812,-1.8693668651,0.5936318178
 C,0,-0.4940389446,-1.2582849461,-0.4787882628
 H,0,-0.5670349944,0.7325090329,2.011126591
 H,0,0.0910851404,-2.2007849767,2.135945313
 H,0,-1.3601082197,-1.3981826136,2.7557524442
 H,0,-1.5313099606,-2.952871956,0.4943690484
 H,0,-2.4056961173,-1.4114341232,0.5437497893
 H,0,0.3733051695,-1.907116448,-0.653285416
 H,0,-0.9833036748,-1.0913581878,-1.4431408779
 H,0,-0.6527809598,0.7805452322,-0.1928060535
 H,0,2.7358623634,1.2418666373,2.5157498396

B3LYP/6-31G* Onsager solvent model for DMSO

ProlineOnsB3G

E(RB+HF-LYP) = -401.148973536

Zero-point correction=	0.145371	(Hartree/Particle)
Thermal correction to Energy=	0.152950	
Thermal correction to Enthalpy=	0.153894	
Thermal correction to Gibbs Free Energy=	0.111981	
Sum of electronic and zero-point Energies=	-401.003602	
Sum of electronic and thermal Energies=	-400.996024	
Sum of electronic and thermal Enthalpies=	-400.995079	
Sum of electronic and thermal Free Energies=	-401.036993	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.978	27.546	88.214

N,0,-0.1026313622,0.0923735212,0.093658386
 C,0,-0.0529950297,-0.0725320619,1.5715106741
 C,0,1.4223492227,-0.0515481117,1.9586587131
 O,0,1.8290335699,1.1895089489,2.3175532038
 O,0,2.1805614885,-0.9975870696,1.9213945875
 C,0,-0.7365719593,-1.4283112878,1.9179543159
 C,0,-1.3677840041,-1.8866792002,0.5879394594
 C,0,-0.4450236081,-1.2331242414,-0.4531754394
 H,0,-0.5401307157,0.7805570005,2.0506148859
 H,0,0.0220648767,-2.1447099319,2.2463522312
 H,0,-1.4701098889,-1.3183411393,2.7219301624
 H,0,-1.4214847253,-2.9770560275,0.5003379656

H,0,-2.3869638591,-1.492951763,0.4847158007
H,0,0.4778728524,-1.8168588315,-0.5613879405
H,0,-0.891637642,-1.1244192288,-1.4464651933
H,0,-0.8472260581,0.7488065581,-0.1289985267
H,0,2.7884208421,1.1210568658,2.4823997143

B3LYP/6-31+G** Onsager solvent model for DMSO

ProlineB3+GOnsgr

E(RB+HF-LYP) = -401.186942205

Zero-point correction=	0.144448 (Hartree/Particle)
Thermal correction to Energy=	0.152108
Thermal correction to Enthalpy=	0.153053
Thermal correction to Gibbs Free Energy=	0.111130
Sum of electronic and zero-point Energies=	-401.042494
Sum of electronic and thermal Energies=	-401.034834
Sum of electronic and thermal Enthalpies=	-401.033890
Sum of electronic and thermal Free Energies=	-401.075813

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.449	27.960	88.234

N,0,0.0025198677,-0.0031022687,0.0719994048
C,0,-0.0173142573,-0.1212420783,1.5545984175
C,0,1.4245797957,-0.010895072,2.0430689745
O,0,1.7622068277,1.2757885895,2.3072569018
O,0,2.2162061525,-0.9238088495,2.1643325275
C,0,-0.6675162744,-1.4881278938,1.8869117196
C,0,-1.4251909992,-1.8594450562,0.5995095813
C,0,-0.5144460233,-1.2691535202,-0.4872068131
H,0,-0.577297004,0.7128287319,1.9888599887
H,0,0.1184050684,-2.2215850944,2.0918892477
H,0,-1.3130422625,-1.427060363,2.7675429133
H,0,-1.5793075537,-2.9385161187,0.4976288127
H,0,-2.4089893111,-1.3748009703,0.5731134066
H,0,0.3266952994,-1.9453887938,-0.6874158156
H,0,-1.0208228766,-1.0783805871,-1.4380324883
H,0,-0.5728091078,0.7798302984,-0.2176749558
H,0,2.7038666584,1.2812430463,2.5486111769

B3LYP/6-31+G** PCM solvent model for DMSO

prolinePCMradiiB3+G

E(RB+HF-LYP) = -401.207927454

Zero-point correction=	0.144002 (Hartree/Particle)
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Thermal correction to Energy=	0.151547
Thermal correction to Enthalpy=	0.152491
Thermal correction to Gibbs Free Energy=	0.111246
Sum of electronic and zero-point Energies=	-401.063925
Sum of electronic and thermal Energies=	-401.056381
Sum of electronic and thermal Enthalpies=	-401.055436
Sum of electronic and thermal Free Energies=	-401.096682

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.097	27.826	86.808

N,0,-0.00182021,0.0062790382,0.0550927909
 C,0,-0.0101216144,-0.1144066818,1.5469706233
 C,0,1.4344399422,-0.0056570713,2.0192964432
 O,0,1.7595218639,1.2490400644,2.3748985563
 O,0,2.2444473843,-0.921071273,2.043641852
 C,0,-0.6715190952,-1.473693963,1.8889517246
 C,0,-1.4237006125,-1.8526606404,0.6002557653
 C,0,-0.504269078,-1.2824186622,-0.4869105314
 H,0,-0.5642201017,0.7235885262,1.9761085959
 H,0,0.1003716434,-2.2184577733,2.1056821084
 H,0,-1.3201309876,-1.3937366004,2.7651847879
 H,0,-1.5824649592,-2.9317175581,0.5081779276
 H,0,-2.4022710209,-1.3583089509,0.5622440777
 H,0,0.343189567,-1.957079257,-0.6602079531
 H,0,-0.9976274842,-1.1089262157,-1.4469798668
 H,0,-0.6513280124,0.7452565713,-0.2009769199
 H,0,2.7052477753,1.2821544469,2.6135630179

Water

B3LYP/6-31G*

waterB3G

E(RB+HF-LYP) = -76.4089532984

Zero-point correction=	0.021167 (Hartree/Particle)
Thermal correction to Energy=	0.024002
Thermal correction to Enthalpy=	0.024946
Thermal correction to Gibbs Free Energy=	0.003500
Sum of electronic and zero-point Energies=	-76.387786
Sum of electronic and thermal Energies=	-76.384952
Sum of electronic and thermal Enthalpies=	-76.384007
Sum of electronic and thermal Free Energies=	-76.405453

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
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Total	15.061	5.997	45.136
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O,0,-0.0271960061,0.,-0.0192306237
H,0,0.0216667013,0.,0.9482044605
H,0,0.9011983635,0.,-0.2956399235

B3LYP/6-31+G**

waterB3+G

E(RB+HF-LYP) = -76.4384293843

Zero-point correction=	0.021265 (Hartree/Particle)
Thermal correction to Energy=	0.024100
Thermal correction to Enthalpy=	0.025044
Thermal correction to Gibbs Free Energy=	0.003606
Sum of electronic and zero-point Energies=	-76.417165
Sum of electronic and thermal Energies=	-76.414329
Sum of electronic and thermal Enthalpies=	-76.413385
Sum of electronic and thermal Free Energies=	-76.434823

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	15.123	6.009	45.121

O,0,-0.0242864205,0.,-0.017173234
H,0,0.0193714773,0.,0.9483643136
H,0,0.9005840018,0.,-0.2978571664

B3LYP/6-31G* Onsager solvent model for DMSO

waterOnsB3G

E(RB+HF-LYP) = -76.4128807605

Zero-point correction=	0.021153 (Hartree/Particle)
Thermal correction to Energy=	0.023988
Thermal correction to Enthalpy=	0.024932
Thermal correction to Gibbs Free Energy=	0.003479
Sum of electronic and zero-point Energies=	-76.391727
Sum of electronic and thermal Energies=	-76.388893
Sum of electronic and thermal Enthalpies=	-76.387949
Sum of electronic and thermal Free Energies=	-76.409401

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	15.053	5.995	45.151

O,0,-0.0317455425,0.,-0.022447635
 H,0,0.0269492786,0.,0.9455592859
 H,0,0.9004653226,0.,-0.2897777377

B3LYP/6-31+G Onsager solvent model for DMSO**
 waterOnsB3+G

E(RB+HF-LYP) = -76.4384293843

Zero-point correction=	0.021265	(Hartree/Particle)
Thermal correction to Energy=	0.024100	
Thermal correction to Enthalpy=	0.025044	
Thermal correction to Gibbs Free Energy=	0.003606	
Sum of electronic and zero-point Energies=	-76.417165	
Sum of electronic and thermal Energies=	-76.414329	
Sum of electronic and thermal Enthalpies=	-76.413385	
Sum of electronic and thermal Free Energies=	-76.434823	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	15.123	6.009	45.121

O,0,-0.0242864205,0.,-0.017173234
 H,0,0.0193714773,0.,0.9483643136
 H,0,0.9005840018,0.,-0.2978571664

B3LYP/6-31+G PCM solvent model for DMSO**
 waterPCMB3+G
 E(RB+HF-LYP) = -76.4500985151

Zero-point correction=	0.020977	(Hartree/Particle)
Thermal correction to Energy=	0.023813	
Thermal correction to Enthalpy=	0.024757	
Thermal correction to Gibbs Free Energy=	0.003314	
Sum of electronic and zero-point Energies=	-76.429121	
Sum of electronic and thermal Energies=	-76.426285	
Sum of electronic and thermal Enthalpies=	-76.425341	
Sum of electronic and thermal Free Energies=	-76.446785	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	14.943	6.019	45.132

O,0,-0.0237101423,0.,-0.0167656116
 H,0,0.017175859,0.,0.9508582778
 H,0,0.9022033098,0.,-0.3007584561

o*-chlorobenzaldehyde transition structures – Houk-List model*B3LYP/6-31G***

ts3aOCB

E(RB+HF-LYP) = -1323.02553860

Zero-point correction=	0.307965 (Hartree/Particle)
Thermal correction to Energy=	0.326154
Thermal correction to Enthalpy=	0.327098
Thermal correction to Gibbs Free Energy=	0.261135
Sum of electronic and zero-point Energies=	-1322.717573
Sum of electronic and thermal Energies=	-1322.699385
Sum of electronic and thermal Enthalpies=	-1322.698440
Sum of electronic and thermal Free Energies=	-1322.764404

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	204.665	70.123	138.831

C,0,2.402423363,-0.4299793473,-0.3850708974
C,0,1.2007334073,0.4767714576,-0.092855243
C,0,0.3873814395,-0.3037593787,0.9653775174
N,0,0.7571329654,-1.7181650417,0.7184739313
C,0,1.7890493087,-1.8312131672,-0.3489222339
C,0,0.2181194468,-2.7530102569,1.3452118976
C,0,-0.6572899819,-2.5168740385,2.5446762819
C,0,-1.1258549203,0.0204938309,0.8378782016
O,0,-1.8734828259,-0.7351102576,0.0692440465
C,0,0.225547657,-4.0404687398,0.729014525
O,0,-1.5223884847,1.0063382222,1.430949732
C,0,-1.1931048978,-3.8237122468,-0.4406758255
O,0,-1.0294548439,-2.7296774945,-1.1372662373
C,0,-1.1449998523,-5.1225594369,-1.2252522464
H,0,3.164659357,-0.3264249896,0.3964369794
H,0,-0.2712370997,-1.7196869431,3.1860933639
H,0,-0.7416235208,-3.4348930404,3.1296974264
H,0,2.8743713313,-0.2166083721,-1.348243314
H,0,0.595842055,0.6008060638,-0.9981261936
H,0,1.4695385144,1.4704950872,0.2707007146
H,0,-1.6663707283,-2.2245370813,2.2270215283
H,0,1.0388072917,-4.2586885456,0.0429471743
H,0,-2.0284571792,-3.8316636747,0.2793268892
H,0,-0.0068208744,-4.8732403625,1.3876535988
H,0,0.6871656671,-0.0123988091,1.9763827513
H,0,-1.4412429757,-1.57919125,-0.4532484647
H,0,2.503213015,-2.6139985521,-0.0790991066

H,0,1.2994587214,-2.0959462507,-1.2872445513
 C,0,-1.6034238553,-6.3539513678,-0.7389105033
 C,0,-1.5598677568,-7.5156315808,-1.5094327796
 C,0,-1.0442274446,-7.4599125206,-2.8034176355
 C,0,-0.5868984155,-6.2447074534,-3.317197922
 C,0,-0.6434867093,-5.0953314302,-2.5340042152
 Cl,0,-2.2834119083,-6.4893960514,0.8916891258
 H,0,-1.9315454541,-8.4471885119,-1.0957707592
 H,0,-1.0103301222,-8.3631429539,-3.4061601651
 H,0,-0.1972490973,-6.1920383396,-4.3300742841
 H,0,-0.3260285923,-4.131845175,-2.9189421072

B3LYP/6-31+G**

ts3aOCBG**

E(RB+HF-LYP) = -1323.09116405

Zero-point correction=	0.306251 (Hartree/Particle)
Thermal correction to Energy=	0.324617
Thermal correction to Enthalpy=	0.325561
Thermal correction to Gibbs Free Energy=	0.259035
Sum of electronic and zero-point Energies=	-1322.784913
Sum of electronic and thermal Energies=	-1322.766547
Sum of electronic and thermal Enthalpies=	-1322.765603
Sum of electronic and thermal Free Energies=	-1322.832129

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	203.700	70.610	140.015
C,0,2.4198017745,-0.4174025785,-0.3523227166			
C,0,1.2341549555,0.5065870157,-0.0439352944			
C,0,0.3760873803,-0.3004905393,0.9605841516			
N,0,0.7432203683,-1.7099508593,0.6898460756			
C,0,1.776613562,-1.8056996145,-0.3744903017			
C,0,0.2245681808,-2.7568441806,1.3261995233			
C,0,-0.6369614484,-2.5220429193,2.5373714612			
C,0,-1.1273256196,0.0421392297,0.7901986535			
O,0,-1.8613450844,-0.6882282054,-0.0130765073			
C,0,0.2629921457,-4.0450894083,0.7358709218			
O,0,-1.5364976789,1.0253703789,1.3870494217			
C,0,-1.2576110532,-3.8398456153,-0.4593487327			
O,0,-1.1092802063,-2.741464571,-1.1370543991			
C,0,-1.1769646343,-5.1350192803,-1.2314001588			
H,0,3.1726291539,-0.3602531306,0.4424904116			
H,0,-0.1970746051,-1.7812862014,3.2107498476			
H,0,-0.7740075065,-3.4567530095,3.0825069815			
H,0,2.9093335112,-0.1784787432,-1.300143932			

H,0,0.6562469973,0.6943934595,-0.9549876453
H,0,1.5218425137,1.4726235671,0.3741599265
H,0,-1.6279966626,-2.1519321737,2.2469989068
H,0,1.0388635929,-4.2561272253,0.0081016665
H,0,-2.0485526039,-3.8588747609,0.303603591
H,0,0.0316844904,-4.8793233579,1.3906686337
H,0,0.6398984863,-0.0390760187,1.9896015544
H,0,-1.4673333037,-1.5778987519,-0.4937972448
H,0,2.4726719314,-2.6126152519,-0.1325198977
H,0,1.2949997213,-2.0220507366,-1.3309255821
C,0,-1.6183694447,-6.3693301924,-0.731757311
C,0,-1.5528214257,-7.5384761526,-1.4911968699
C,0,-1.0336817278,-7.4879441405,-2.7854418346
C,0,-0.5932831863,-6.269913263,-3.3117270865
C,0,-0.6703259121,-5.1123987825,-2.5403550245
Cl,0,-2.2996585346,-6.4968078828,0.8964584635
H,0,-1.9105781954,-8.4717029379,-1.0699986556
H,0,-0.9840421666,-8.3963087679,-3.3782860811
H,0,-0.2023326398,-6.221681817,-4.323635719
H,0,-0.3649191256,-4.1498505807,-2.937198197

B3LYP/6-31G* Onsager solvent model for DMSO

OCBOnsgrB3G5.44

E(RB+HF-LYP) = -1323.02973810

Zero-point correction=	0.307671	(Hartree/Particle)
Thermal correction to Energy=	0.325943	
Thermal correction to Enthalpy=	0.326887	
Thermal correction to Gibbs Free Energy=	0.260660	
Sum of electronic and zero-point Energies=	-1322.722067	
Sum of electronic and thermal Energies=	-1322.703795	
Sum of electronic and thermal Enthalpies=	-1322.702851	
Sum of electronic and thermal Free Energies=	-1322.769078	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	204.532	70.286	139.387
C,0,2.4010563428,-0.4233025235,-0.3832010298			
C,0,1.203408154,0.4850404962,-0.0790877461			
C,0,0.3818681026,-0.3099647106,0.9637236439			
N,0,0.7480003943,-1.719432728,0.696872915			
C,0,1.7809893378,-1.821834041,-0.3701886056			
C,0,0.2240726981,-2.7638993665,1.3274845013			
C,0,-0.6310858763,-2.5346300746,2.5441472736			
C,0,-1.1273550985,0.0254838145,0.8364869365			
O,0,-1.8846462011,-0.7238920863,0.0706481033			

C,0,0.2382483931,-4.0455098007,0.7164093449
 O,0,-1.52202154,1.0164991457,1.4264957269
 C,0,-1.2345366652,-3.8139940766,-0.4602886845
 O,0,-1.0755630389,-2.7187312063,-1.1464250488
 C,0,-1.1749567445,-5.1123718731,-1.2345496014
 H,0,3.1617740843,-0.3366646177,0.4012146913
 H,0,-0.1971954478,-1.7827720815,3.2103209532
 H,0,-0.7487010348,-3.4688780775,3.0964441637
 H,0,2.8771252879,-0.196779733,-1.341083799
 H,0,0.6022876334,0.6287943618,-0.9842817231
 H,0,1.477413703,1.4704524288,0.3030602357
 H,0,-1.6288190178,-2.1830952983,2.2528004213
 H,0,1.0279195326,-4.2588951078,0.0030472549
 H,0,-2.0449678257,-3.8237295896,0.2858969161
 H,0,0.0073614102,-4.8846152208,1.3666714028
 H,0,0.6795803232,-0.0329459519,1.9796515736
 H,0,-1.4593578,-1.5758047592,-0.4528912562
 H,0,2.4920766404,-2.6105941399,-0.1116488495
 H,0,1.2952524949,-2.070195122,-1.3154728201
 C,0,-1.6477181647,-6.3377715891,-0.7461373564
 C,0,-1.5778343829,-7.5099441924,-1.497802806
 C,0,-1.0221258547,-7.4706721838,-2.7759086318
 C,0,-0.553187292,-6.2613216992,-3.2934882356
 C,0,-0.6352451685,-5.1013391332,-2.528755147
 Cl,0,-2.3727257144,-6.4509435489,0.8681169134
 H,0,-1.9522144295,-8.4386335418,-1.0803438298
 H,0,-0.9588235996,-8.3836223414,-3.3609468332
 H,0,-0.1259940704,-6.2240811832,-4.291543765
 H,0,-0.2987145656,-4.1454586476,-2.9165862024

B3LYP/6-31+G** Onsager solvent model for DMSO

OCBOnsgrB3+G5.34

E(RB+HF-LYP) = -1323.09657429

Zero-point correction=	0.305336 (Hartree/Particle)
Thermal correction to Energy=	0.323806
Thermal correction to Enthalpy=	0.324750
Thermal correction to Gibbs Free Energy=	0.258023
Sum of electronic and zero-point Energies=	-1322.791239
Sum of electronic and thermal Energies=	-1322.772768
Sum of electronic and thermal Enthalpies=	-1322.771824
Sum of electronic and thermal Free Energies=	-1322.838552

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	203.191	71.004	140.441

C,0,2.4142479358,-0.410323522,-0.3536851353
 C,0,1.2324749086,0.5133513322,-0.0291913038
 C,0,0.3662216728,-0.3093282136,0.9577617644
 N,0,0.7327995185,-1.7118734174,0.6657848963
 C,0,1.7655918826,-1.7953121982,-0.3994804283
 C,0,0.2320845101,-2.7706691014,1.3057305202
 C,0,-0.5950114105,-2.5451671667,2.5438196509
 C,0,-1.1349636154,0.0414475899,0.784382361
 O,0,-1.8749152833,-0.6918361553,-0.004582908
 C,0,0.2792566323,-4.0517016167,0.7203767357
 O,0,-1.5394382236,1.0375942322,1.3727039116
 C,0,-1.3155291398,-3.8270050356,-0.4814366848
 O,0,-1.1700940107,-2.7228495706,-1.1452093266
 C,0,-1.2199790411,-5.1165882935,-1.2444167357
 H,0,3.1667940234,-0.3713918378,0.4418737527
 H,0,-0.0825627742,-1.8815173438,3.2470499149
 H,0,-0.7873903914,-3.4971137543,3.0398733896
 H,0,2.9065032305,-0.1572336718,-1.2961587387
 H,0,0.6577555728,0.7229039883,-0.9379313442
 H,0,1.5255499359,1.4690276751,0.4090031556
 H,0,-1.5599483299,-2.0844375306,2.301539679
 H,0,1.0222274312,-4.2564674413,-0.041377988
 H,0,-2.0723126692,-3.8458317759,0.312184935
 H,0,0.04891058,-4.8941890255,1.3638840431
 H,0,0.6258123675,-0.0630106336,1.9919553275
 H,0,-1.4897885974,-1.6107095605,-0.5040128044
 H,0,2.4600974254,-2.6069609704,-0.1713545009
 H,0,1.2873766177,-1.9943554003,-1.3619567018
 C,0,-1.675845056,-6.3457521054,-0.7429378158
 C,0,-1.5721622592,-7.5261673706,-1.4789672223
 C,0,-1.0011150834,-7.4922361389,-2.7520063382
 C,0,-0.5496683774,-6.2796541225,-3.2819500017
 C,0,-0.6630935701,-5.1104112112,-2.5338035332
 Cl,0,-2.4122101985,-6.4500280372,0.8640113362
 H,0,-1.9298357597,-8.4576839514,-1.0542266648
 H,0,-0.9098393836,-8.4114776472,-3.3221604297
 H,0,-0.1093281962,-6.2485558835,-4.2737218612
 H,0,-0.3340278746,-4.156535113,-2.9325059063

B3LYP/6-31+G PCM solvent model for DMSO**
 chlorobenzaldehyde TSB3BBPCM
 $E(RB+HF-LYP) = -1323.12522421$

Zero-point correction=	0.304064 (Hartree/Particle)
Thermal correction to Energy=	0.322653
Thermal correction to Enthalpy=	0.323597

Thermal correction to Gibbs Free Energy=	0.256747
Sum of electronic and zero-point Energies=	-1322.821160
Sum of electronic and thermal Energies=	-1322.802571
Sum of electronic and thermal Enthalpies=	-1322.801627
Sum of electronic and thermal Free Energies=	-1322.868477

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	202.468	71.488	140.699

C,0-2.192784	0.313937	0.440402
C,0-0.831524	-0.266570	0.607296
O,0 0.047880	0.381794	1.282953
C,0-0.237365	-0.128441	-1.499362
C,0 1.069096	-0.550780	-1.254136
C,0 1.410998	-2.016928	-1.309882
N,0 2.002496	0.310924	-0.809827
C,0 3.292986	-0.095234	-0.229382
C,0 4.046503	1.244899	-0.003861
C,0 3.401186	2.199313	-1.016220
C,0 1.929471	1.782419	-0.999771
C,0 3.203067	-0.866335	1.095721
O,0 4.179818	-1.527831	1.456077
O,0 2.132507	-0.766053	1.845954
H,0 3.825253	2.043192	-2.013967
H,0 2.330796	-2.182171	-1.879594
H,0 0.603596	-2.569589	-1.790891
H,0 3.533859	3.249331	-0.745152
H,0 3.874606	1.605386	1.016287
H,0 5.121163	1.118080	-0.142156
H,0 1.559906	-2.445313	-0.311727
H,0-0.465920	0.924952	-1.602379
H,0-0.782911	-1.358060	0.600502
H,0-0.907162	-0.815210	-2.003945
H,0 3.845029	-0.729776	-0.929191
H,0 1.243383	-0.232085	1.503429
H,0 1.408206	2.004344	-1.932909
H,0 1.384949	2.245322	-0.171673
C,0-3.302394	-0.444742	0.028000
C,0-4.573818	0.115517	-0.095235
C,0-4.757792	1.469496	0.195930
C,0-3.672508	2.249164	0.612176
C,0-2.410079	1.672648	0.732988
Cl,0-3.129160	-2.163552	-0.354531
H,0-5.407227	-0.501255	-0.413588
H,0-5.746400	1.907182	0.099079

H,0-3.811636 3.300408 0.843968
H,0-1.563151 2.265723 1.061869

***o*-chlorobenzaldehyde transition structures – Seebach-Eschenmoser model**

B3LYP/6-31+G**

seebachTSfirstmodelB3+G

E(RB+HF-LYP) = -1322.54237280

Zero-point correction=	0.293492 (Hartree/Particle)
Thermal correction to Energy=	0.312379
Thermal correction to Enthalpy=	0.313323
Thermal correction to Gibbs Free Energy=	0.243771
Sum of electronic and zero-point Energies=	-1322.248880
Sum of electronic and thermal Energies=	-1322.229994
Sum of electronic and thermal Enthalpies=	-1322.229050
Sum of electronic and thermal Free Energies=	-1322.298602

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	196.021	70.936	146.384
N,0,2.7727370383,-0.4653223538,-0.7972269094			
C,0,1.9286017998,-0.156410226,0.3769984354			
C,0,1.7661852706,-1.5016435341,1.110258734			
C,0,2.9310872493,-2.3570039666,0.5825375619			
C,0,3.0242514612,-1.9194903842,-0.8852364235			
C,0,1.9316341267,-2.6724999897,-1.7646034001			
O,0,0.9322173955,-2.0002886231,-2.1136867654			
C,0,3.0605892872,0.4070186103,-1.7579752431			
C,0,3.9308383129,0.1230680063,-2.8458284783			
O,0,2.216068267,-3.8793129055,-1.9530579292			
C,0,2.617132846,1.835003826,-1.6472452467			
C,0,5.6819378298,1.0100504604,-2.4444412094			
O,0,5.5228889809,2.2509240247,-2.1970825013			
C,0,6.2567271715,0.131855326,-1.3394563543			
H,0,1.7797414316,-1.3725550804,2.1979248216			
H,0,4.1323879186,-0.915096889,-3.0881221966			
H,0,3.7466728544,0.7407153083,-3.7205389008			
H,0,0.8146845528,-1.9603379018,0.827907418			
H,0,2.7498272321,-3.4312910668,0.6533760234			
H,0,3.860534896,-2.1187928008,1.1161482524			
H,0,3.5354146089,2.4490075379,-1.6929972511			
H,0,2.0116425722,2.0974857171,-2.5212597393			
H,0,4.0112613916,-2.1091670032,-1.3048042089			
H,0,2.4328392788,0.5877390674,1.0055400812			
H,0,0.9657399031,0.2492915255,0.0524403537			

H,0,2.0469603739,2.0634395628,-0.7471254561
H,0,6.0663386485,0.7136632666,-3.4354407601
C,0,6.88817816,-1.1032604378,-1.5389935923
C,0,7.4330578494,-1.8432105671,-0.4873959219
C,0,7.3548081525,-1.3468855999,0.8149863068
C,0,6.7428330217,-0.1106860579,1.0467001172
C,0,6.2127291919,0.6120068962,-0.0204611023
Cl,0,7.0374574254,-1.793304912,-3.1662267278
H,0,7.9075698746,-2.7970262743,-0.6935922019
H,0,7.7733444773,-1.9226497476,1.63605058
H,0,6.6854964989,0.2893831641,2.0559804539
H,0,5.7621226489,1.5903220219,0.1197843804

B3LYP/6-31G* Onsager solvent model for DMSO

seebachTSOnsB3Gfirstmodel

E(RB+HF-LYP) = -1322.47160994

Zero-point correction=	0.295633 (Hartree/Particle)
Thermal correction to Energy=	0.314204
Thermal correction to Enthalpy=	0.315149
Thermal correction to Gibbs Free Energy=	0.246215
Sum of electronic and zero-point Energies=	-1322.175977
Sum of electronic and thermal Energies=	-1322.157406
Sum of electronic and thermal Enthalpies=	-1322.156461
Sum of electronic and thermal Free Energies=	-1322.225395

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	197.166	70.071	145.084
N,0,2.8488232148,-0.639430928,-0.7884740666			
C,0,2.1806948498,-0.4018866283,0.5086666049			
C,0,1.7735650625,-1.801008994,1.0019264861			
C,0,2.7324202022,-2.7435869625,0.2579651058			
C,0,2.8431078151,-2.0807510669,-1.1181120164			
C,0,1.5982442564,-2.4711106259,-2.0495506975			
O,0,0.8283757004,-1.5395923122,-2.3734482673			
C,0,3.1629691252,0.3216967425,-1.6424106501			
C,0,3.9287384369,0.0940676733,-2.8355263521			
O,0,1.5645386441,-3.6959171488,-2.3098285042			
C,0,2.8909175765,1.7603414912,-1.3221932403			
C,0,5.6147756023,0.841991636,-2.6119694777			
O,0,5.5360027732,2.122644955,-2.6164677151			
C,0,6.2305390441,0.1963319469,-1.354505184			
H,0,1.8345764571,-1.8791867489,2.0921509361			
H,0,4.0140007712,-0.9386733175,-3.162082547			
H,0,3.6426325026,0.7575326972,-3.6498525083			

H,0,0.742998552,-2.0112129172,0.6978963334
H,0,2.3520251362,-3.7613128496,0.1508729621
H,0,3.707426349,-2.7782147362,0.7616688454
H,0,3.7963254156,2.324786464,-1.6163673792
H,0,2.0646556687,2.1199433176,-1.9495866987
H,0,3.7662789494,-2.3593478246,-1.6264842763
H,0,2.88618238,0.0792989387,1.1965400877
H,0,1.3181294254,0.2583118774,0.3778916562
H,0,2.6363312177,1.9467936814,-0.2772755211
H,0,6.0310528546,0.3451668417,-3.5175328783
C,0,6.7200451597,-1.1075943789,-1.2452745603
C,0,7.2963036427,-1.6055801374,-0.0756629207
C,0,7.400168095,-0.7753049749,1.0398594792
C,0,6.9407297442,0.5416545311,0.9623244533
C,0,6.3775188912,1.0109657699,-0.2215145851
Cl,0,6.6532834305,-2.2226091429,-2.6390581302
H,0,7.6646314341,-2.6262389915,-0.0477696322
H,0,7.8515412066,-1.1534805444,1.9531147147
H,0,7.0391626825,1.203525985,1.8190556778
H,0,6.0548277306,2.0417246815,-0.3351505338

B3LYP/6-31+G Onsager solvent model for DMSO**

seebachTSOnsB3+Gfirstmodel

E(RB+HF-LYP) = -1322.55194078

Zero-point correction=	0.294021	(Hartree/Particle)
Thermal correction to Energy=	0.312750	
Thermal correction to Enthalpy=	0.313694	
Thermal correction to Gibbs Free Energy=	0.244821	
Sum of electronic and zero-point Energies=	-1322.257920	
Sum of electronic and thermal Energies=	-1322.239190	
Sum of electronic and thermal Enthalpies=	-1322.238246	
Sum of electronic and thermal Free Energies=	-1322.307120	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	196.254	70.577	144.957

N,0,2.8078500369,-0.6650317398,-0.7958566476
C,0,2.1605449855,-0.4374120381,0.5170297037
C,0,1.7248343064,-1.8353737168,0.9867207203
C,0,2.6450471686,-2.7881742167,0.2062659577
C,0,2.7718741085,-2.1002761741,-1.1609403071
C,0,1.5437974154,-2.4519320969,-2.1074466923
O,0,0.6755161337,-1.560445741,-2.2763212538
C,0,3.1817796651,0.3069884845,-1.6146726696

C,0,3.9202031135,0.0781878545,-2.821982182
 O,0,1.5914757321,-3.6259869982,-2.554955462
 C,0,2.9470501707,1.7430285337,-1.2461032539
 C,0,5.6524783991,0.7907483465,-2.6416888484
 O,0,5.5995780448,2.0740539484,-2.7209806404
 C,0,6.2630026369,0.2073518766,-1.3571256708
 H,0,1.8122303104,-1.9409832315,2.0722534222
 H,0,3.9770007911,-0.9504947781,-3.1657485337
 H,0,3.6551575518,0.7690909966,-3.6187497805
 H,0,0.6826527122,-2.0110793483,0.7039768547
 H,0,2.2406944049,-3.7964839872,0.0975822473
 H,0,3.6266759305,-2.856416394,0.6915135404
 H,0,3.8094314685,2.325094037,-1.6062466236
 H,0,2.0569608404,2.1049123993,-1.7770819749
 H,0,3.6934163775,-2.3862831477,-1.6663756136
 H,0,2.8868624318,0.0110118662,1.204747557
 H,0,1.3135089407,0.2452503231,0.4066769986
 H,0,2.7968110647,1.9040965634,-0.1775237972
 H,0,6.0317745789,0.2335791425,-3.5223349629
 C,0,6.7260947598,-1.1027122768,-1.1921150432
 C,0,7.3167501688,-1.5527265414,-0.0088621012
 C,0,7.4601399516,-0.6700879057,1.062790581
 C,0,7.0234141828,0.6515716484,0.929141904
 C,0,6.4448471653,1.074432142,-0.2666804957
 Cl,0,6.6061068233,-2.2813752358,-2.5234185895
 H,0,7.6649719351,-2.577867845,0.0638083488
 H,0,7.9235528192,-1.0113787985,1.9838072443
 H,0,7.1514624244,1.3526366904,1.7491803112
 H,0,6.1389904491,2.1052253584,-0.4184492477

***o*-chlorobenzaldehyde transition structures – Seebach-Eschenmoser model with pyrrolidinium stabilizing alkoxide**

B3LYP/6-31G*

seebachTSsinglestableB3G

E(RB+HF-LYP) = -1535.60070285

Zero-point correction=	0.442658 (Hartree/Particle)
Thermal correction to Energy=	0.467860
Thermal correction to Enthalpy=	0.468804
Thermal correction to Gibbs Free Energy=	0.384338
Sum of electronic and zero-point Energies=	-1535.158045
Sum of electronic and thermal Energies=	-1535.132843
Sum of electronic and thermal Enthalpies=	-1535.131898
Sum of electronic and thermal Free Energies=	-1535.216365

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	293.587	93.726	177.775

C,0,2.8733867558,-2.4394896461,-0.7606551073
C,0,2.3467397972,-1.4362027316,0.0696679481
C,0,3.2614897208,-0.5829906761,0.7052773661
C,0,4.6368189505,-0.7031837767,0.5134668659
C,0,5.1287294468,-1.6982268974,-0.331081274
C,0,4.242219239,-2.5697619513,-0.9686811548
C,0,0.8656453612,-1.3829020877,0.2719461382
O,0,0.1675692882,-2.3852119178,-0.0656650364
Cl,0,2.7009187976,0.6899899888,1.7979245855
C,0,0.2966002837,0.1011354651,-1.2402554246
C,0,0.6810531632,1.4407888105,-1.1011343447
C,0,1.9189978252,1.9499132222,-1.7981951183
N,0,-0.0003529357,2.3080303667,-0.3396881701
C,0,0.3079263608,3.7431189042,-0.2305805884
C,0,-0.9540403978,4.3314654775,0.4074336614
C,0,-1.4399569625,3.1931062166,1.3149673706
C,0,-1.176003131,1.9266647999,0.4781224374
C,0,-2.4233426772,1.5287844305,-0.4029217339
O,0,-2.8329732667,2.3845474595,-1.199863979
O,0,-2.8669201655,0.3593447694,-0.1719178831
N,0,-2.4496775466,-2.771408821,0.178341576
C,0,-3.27799134,-2.4276809399,-1.0493878198
C,0,-4.6806328657,-2.0625856818,-0.5105910518
C,0,-4.6350498655,-2.3683627814,1.0030063081
C,0,-3.1645292295,-2.1595363255,1.3573737792
H,0,0.5324946029,-0.7258051493,1.0816432952
H,0,-0.7489548547,5.264081838,0.9425039051
H,0,-0.7350187475,-0.147370597,-1.0295136464
H,0,0.7659298234,-0.4529422287,-2.0455585927
H,0,-1.7043163503,4.5067544197,-0.3668524333
H,0,-2.4967305814,3.2878652207,1.577392318
H,0,-0.8564132458,3.1650434639,2.2447956648
H,0,2.4702735289,1.1177454431,-2.23993834
H,0,1.6511245333,2.6446904315,-2.6043666548
H,0,-0.8986891116,1.0723939867,1.1014926294
H,0,1.1915014833,3.891593403,0.4088279417
H,0,0.5246511218,4.1704077592,-1.2141451642
H,0,2.5862958889,2.4834683536,-1.1121849096
H,0,-1.4197282896,-2.4646651418,0.0991594114
H,0,-2.4215172224,-3.786943281,0.2934370515
H,0,-3.254777155,-3.287209807,-1.7228892857

H,0,-2.8120063753,-1.5594438697,-1.5110281178
H,0,-2.8234535333,-2.6429261295,2.2761431547
H,0,-2.9079565285,-1.0971020584,1.3304282192
H,0,-5.2833943867,-1.7042766097,1.5805402194
H,0,-4.9421081238,-3.4021271443,1.2135503221
H,0,-5.4751102927,-2.6138283759,-1.0214150372
H,0,-4.8181167602,-0.9905180333,-0.6631827787
H,0,5.309939021,-0.0251143944,1.0276494003
H,0,6.2005434917,-1.7920915557,-0.4814708797
H,0,4.6200618618,-3.3528817006,-1.6202086549
H,0,2.1642595958,-3.1155179201,-1.2274543885

B3LYP/6-31+G**

seebachTSsinglestableB3+G
E(RB+HF-LYP) = -1535.68720910

Zero-point correction=	0.439677 (Hartree/Particle)
Thermal correction to Energy=	0.465211
Thermal correction to Enthalpy=	0.466155
Thermal correction to Gibbs Free Energy=	0.380591
Sum of electronic and zero-point Energies=	-1535.247532
Sum of electronic and thermal Energies=	-1535.221999
Sum of electronic and thermal Enthalpies=	-1535.221054
Sum of electronic and thermal Free Energies=	-1535.306618

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	291.924	94.530	180.084

C,0,2.9553557733,-2.4386649184,-0.6216588745
C,0,2.4371384838,-1.3946285196,0.1651516323
C,0,3.3577369174,-0.5070091174,0.746861648
C,0,4.7318642111,-0.6363415794,0.5462607227
C,0,5.2161373492,-1.6731967925,-0.253608835
C,0,4.3234362667,-2.5777172691,-0.8379144256
C,0,0.9643558224,-1.3224719009,0.3897291039
O,0,0.2416092168,-2.3266680267,0.1119131725
Cl,0,2.8055887961,0.8187828752,1.7756998291
C,0,0.3736551615,0.1234424099,-1.2350726365
C,0,0.6905374205,1.4827804467,-1.1240710095
C,0,1.9089599939,2.0350229727,-1.8217657571
N,0,-0.0454624024,2.3356356975,-0.3966699616
C,0,0.1808580632,3.7900635055,-0.331017954
C,0,-1.1095552917,4.3285417056,0.2968458419
C,0,-1.5569605598,3.1806968568,1.2147719415

C,0,-1.2107692145,1.9130693999,0.407216135
 C,0,-2.4260942984,1.4215804539,-0.4640876734
 O,0,-2.7444749499,2.1272322866,-1.4380223611
 O,0,-2.9555433145,0.3459606263,-0.0422262705
 N,0,-2.3415250514,-2.8333558871,0.294977855
 C,0,-3.171455547,-2.5211950799,-0.9367201126
 C,0,-4.6181997041,-2.3307535229,-0.4216134261
 C,0,-4.5560398875,-2.5824065016,1.1043519455
 C,0,-3.1048413465,-2.2688331351,1.4655125033
 H,0,0.638730505,-0.6073339548,1.1488358158
 H,0,-0.9442666955,5.2699192154,0.8294070181
 H,0,-0.6427876506,-0.1833311281,-1.0333630839
 H,0,0.8997624766,-0.4374656923,-1.9983267638
 H,0,-1.8584876144,4.4816327391,-0.4839874756
 H,0,-2.620947087,3.2233501599,1.4599442375
 H,0,-0.99008716,3.1968345708,2.1544578205
 H,0,2.5113165233,1.2206368708,-2.2265446058
 H,0,1.6100029176,2.6813337686,-2.6557985867
 H,0,-0.9051210283,1.0899432959,1.0580209405
 H,0,1.0570633248,4.0064941809,0.2983412787
 H,0,0.3661369426,4.1987305423,-1.3282935812
 H,0,2.5340422779,2.6304034282,-1.1482386629
 H,0,-1.3279480481,-2.4777094748,0.2355978135
 H,0,-2.2654964591,-3.8460795531,0.4036452069
 H,0,-3.0445240382,-3.3372277969,-1.6509859512
 H,0,-2.790035877,-1.5867659967,-1.3457358608
 H,0,-2.7417786222,-2.7266847358,2.3885860259
 H,0,-2.9215631859,-1.1911925555,1.450146632
 H,0,-5.2502078388,-1.9455861921,1.6577515195
 H,0,-4.7964598837,-3.6265586084,1.3452299319
 H,0,-5.3215052241,-3.0056026881,-0.9170387108
 H,0,-4.9137083715,-1.2988361611,-0.6192120837
 H,0,5.4101660115,0.0668990353,1.0173171225
 H,0,6.2858944003,-1.7736899366,-0.4104700767
 H,0,4.695383641,-3.3912216905,-1.4535875174
 H,0,2.2445626892,-3.1379646882,-1.0497210327

B3LYP/6-31+G Onsager solvent model for DMSO**

seebachTSsinglestableOnsB3+G

E(RB+HF-LYP) = -1535.69146392

Zero-point correction=	0.439052 (Hartree/Particle)
Thermal correction to Energy=	0.464606
Thermal correction to Enthalpy=	0.465551
Thermal correction to Gibbs Free Energy=	0.380190
Sum of electronic and zero-point Energies=	-1535.252411

Sum of electronic and thermal Energies=	-1535.226858
Sum of electronic and thermal Enthalpies=	-1535.225913
Sum of electronic and thermal Free Energies=	-1535.311274

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	291.545	94.324	179.657

C,0,2.8373808399,-2.4424615822,-0.8071257237
C,0,2.3269269403,-1.4066361243,-0.0053744948
C,0,3.2553406405,-0.582098993,0.6496129406
C,0,4.6310855911,-0.7660317318,0.5136157501
C,0,5.1081664219,-1.7954120647,-0.2998106531
C,0,4.2074091377,-2.6357780925,-0.9617570673
C,0,0.8464151418,-1.2879030669,0.1671245492
O,0,0.1157434554,-2.28935986,-0.1394529088
Cl,0,2.711045411,0.7262078792,1.7127219398
C,0,0.3021737894,0.144410977,-1.3430245931
C,0,0.6891467423,1.4777672427,-1.1299333986
C,0,1.970730037,1.9980387597,-1.7303974202
N,0,-0.0279857962,2.3162771954,-0.3717640622
C,0,0.3191440474,3.7269155843,-0.132795231
C,0,-0.9377924864,4.3055790962,0.5271188957
C,0,-1.5226123472,3.1022523092,1.2829639264
C,0,-1.2651078451,1.9150590978,0.3330055096
C,0,-2.4861680268,1.6600143403,-0.631230192
O,0,-2.7037850535,2.5307361474,-1.49898676
O,0,-3.1239038798,0.5954095216,-0.3765427659
N,0,-2.3972521013,-2.7472626986,0.234350746
C,0,-3.2507998503,-2.4752272824,-0.9839117898
C,0,-4.6822033436,-2.2357890703,-0.4429115062
C,0,-4.5675065635,-2.3418167083,1.098612606
C,0,-3.0915871227,-2.0512679553,1.3717718019
H,0,0.5343678755,-0.6229774118,0.9776354358
H,0,-0.7030304343,5.1530948606,1.1789847507
H,0,-0.742805365,-0.1036404171,-1.2121774266
H,0,0.8089053016,-0.3790996242,-2.1455419154
H,0,-1.6419317299,4.623877118,-0.2458033432
H,0,-2.5868844226,3.2157917297,1.5040000353
H,0,-0.9916726807,2.9494174384,2.2310471796
H,0,2.5346192423,1.1792796504,-2.1784976712
H,0,1.7509379928,2.7307096024,-2.516717918
H,0,-1.0674972853,0.9942150781,0.8856664269
H,0,1.191347877,3.7887646398,0.5343088823
H,0,0.5711374222,4.2279707024,-1.0722792742
H,0,2.6044405434,2.4875107299,-0.9841151005

H,0,-1.3482376037,-2.445540429,0.1028721692
H,0,-2.3753318578,-3.7519038079,0.4201377196
H,0,-3.1559297403,-3.3179005346,-1.6712203908
H,0,-2.8623526933,-1.5664148779,-1.443230436
H,0,-2.7067948812,-2.4276651471,2.3220622292
H,0,-2.8839510837,-0.9846153772,1.2497909912
H,0,-5.2160692138,-1.6292330527,1.6136992239
H,0,-4.8311625767,-3.3477742885,1.4488242763
H,0,-5.3976276506,-2.9581745842,-0.8456558135
H,0,-4.9926421661,-1.2291708115,-0.7293086438
H,0,5.3157496555,-0.1189548309,1.0510317834
H,0,6.1785665213,-1.9465362674,-0.3996757565
H,0,4.5741947672,-3.448555977,-1.5808693892
H,0,2.1210584067,-3.1014710314,-1.2865841231

o-chlorobenzaldehyde transition structures – Seebach-Eschenmoser model with pyrrolidinium stabilizing alkoxide and carboxylate

B3LYP/6-31G*

SeebachTSB3Gdoublestable
E(RB+HF-LYP) = -1535.61756383

Zero-point correction=	0.441087 (Hartree/Particle)
Thermal correction to Energy=	0.466064
Thermal correction to Enthalpy=	0.467008
Thermal correction to Gibbs Free Energy=	0.382829
Sum of electronic and zero-point Energies=	-1535.176476
Sum of electronic and thermal Energies=	-1535.151500
Sum of electronic and thermal Enthalpies=	-1535.150556
Sum of electronic and thermal Free Energies=	-1535.234735

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	292.460	93.022	177.170
C,0,-4.38135543,-0.9297414818,-0.9105932392			
N,0,-2.9291272512,-1.0033629648,-1.1740751177			
C,0,-2.1606442791,-0.1584335427,-0.2319242693			
C,0,-3.2319086048,0.8164621251,0.291785757			
C,0,-4.497296726,-0.0533718862,0.3447650921			
C,0,-2.3665501764,-1.8254760256,-2.0529427309			
C,0,-3.2911141132,-2.6421376738,-2.9191875413			
C,0,-1.5798216191,-1.0127233663,0.9482544631			
O,0,-0.4788930999,-0.5664449604,1.4378348849			
C,0,-0.9599720592,-1.9240937081,-2.2370913757			
O,0,-2.2433816565,-1.9759539809,1.3353267813			
C,0,-0.2251950246,-0.3605161691,-3.3144804458			

C,0,0.8052571909,-1.1005359207,-4.1481865847
 O,0,0.1799376448,0.5383313376,-2.5011315828
 N,0,1.2591263785,0.5975755395,-0.0210108966
 C,0,1.4204715364,2.0500866742,0.3384717069
 C,0,2.8403058239,2.1733812992,0.9206932996
 C,0,3.1534035394,0.751104013,1.4164722262
 C,0,2.5181123393,-0.1287559042,0.3370910366
 H,0,-1.1465840239,-0.1546197325,-3.8778486519
 H,0,-5.423825137,0.5283659353,0.351048825
 H,0,-0.3418245607,-1.7318302542,-1.3661733101
 H,0,-0.6610902995,-2.8145671859,-2.7819573194
 H,0,-4.4657383908,-0.6890348878,1.2318537603
 H,0,-2.9554698543,1.231317839,1.2649582754
 H,0,-3.3603956972,1.6494582658,-0.4111699919
 H,0,-2.7302138059,-3.1506141372,-3.7029383656
 H,0,-3.8016975299,-3.3991386699,-2.3101768133
 H,0,-1.3818328786,0.3544405052,-0.7940720969
 H,0,-4.8863543445,-0.4740279152,-1.7727252722
 H,0,-4.7938742284,-1.9311614013,-0.7594906893
 H,0,-4.0655574388,-2.0262171753,-3.3910911574
 H,0,0.9864130573,0.4842798132,-1.0312059501
 H,0,0.4289930474,0.146403942,0.5847653125
 H,0,0.6527643054,2.2904752476,1.0797070177
 H,0,1.2534826808,2.6620193524,-0.550246603
 H,0,2.2553852447,-1.1335251452,0.6748569692
 H,0,3.1582177647,-0.201256581,-0.5486131433
 H,0,4.2239770401,0.5598174911,1.5332162108
 H,0,2.6658256011,0.5630862125,2.3799786876
 H,0,2.8943217164,2.9258404353,1.7125692216
 H,0,3.5489130085,2.464860623,0.1363463158
 C,0,0.511637234,-1.8429971587,-5.3000915554
 C,0,1.5009258365,-2.4802670732,-6.0476842516
 C,0,2.8333755906,-2.379796235,-5.6494619558
 C,0,3.1617673345,-1.6325932285,-4.5169820813
 C,0,2.156989349,-1.0012993981,-3.789891686
 Cl,0,-1.1561030252,-1.9975612227,-5.8752806303
 H,0,1.22418923,-3.0422066025,-6.933651199
 H,0,3.606497646,-2.8756443138,-6.2296235113
 H,0,4.1993191697,-1.5359101275,-4.2086129246
 H,0,2.3944569449,-0.3853306209,-2.9289328999

B3LYP/6-31+G**

SeebachTSB3+Gdoublestable

E(RB+HF-LYP) = -1535.70375441

Zero-point correction= 0.438826 (Hartree/Particle)

Thermal correction to Energy= 0.464039
 Thermal correction to Enthalpy= 0.464983
 Thermal correction to Gibbs Free Energy= 0.378335
 Sum of electronic and zero-point Energies= -1535.264929
 Sum of electronic and thermal Energies= -1535.239716
 Sum of electronic and thermal Enthalpies= -1535.238772
 Sum of electronic and thermal Free Energies= -1535.325420

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	291.189	93.628	182.366

C,0,-1.8523069993,-3.6377764543,-0.3322908459
 N,0,-1.2153608003,-2.3426511838,-0.0049581687
 C,0,-2.1342965817,-1.2051513496,-0.235179386
 C,0,-3.19960366,-1.8156352242,-1.1669450638
 C,0,-3.3003886615,-3.272346012,-0.6862368021
 C,0,0.0010520774,-2.2162577772,0.516297536
 C,0,0.8066111993,-3.476737384,0.6982358835
 C,0,-2.7864907205,-0.6979837089,1.0968030838
 O,0,-3.0883508442,0.5511862404,1.0930457105
 C,0,0.5745933414,-0.9588663306,0.8549248699
 O,0,-2.9991701182,-1.523750199,1.9899522405
 C,0,1.241577351,0.0494501157,-0.7881110966
 C,0,2.5940471811,0.4925995875,-0.2698255129
 O,0,0.3773814222,0.9510694847,-1.0796540952
 N,0,-1.7258920132,2.3398690497,-0.133115694
 C,0,-2.4656419173,2.8936523836,-1.3233393791
 C,0,-2.5788093114,4.4052213645,-1.0671724191
 C,0,-2.5405467399,4.5101879166,0.4669864748
 C,0,-1.5036210206,3.4506789678,0.8515802186
 H,0,1.3084679543,-0.8207758373,-1.453408182
 H,0,-3.7146086363,-3.9447867915,-1.4426756741
 H,0,-0.1072989734,-0.1731666758,1.1597273346
 H,0,1.4421446114,-1.0446619051,1.5013829881
 H,0,-3.9211383607,-3.3245439637,0.2110276356
 H,0,-4.1486971135,-1.2780222482,-1.1018000487
 H,0,-2.8536312193,-1.772796922,-2.2071155934
 H,0,1.83159901,-3.2373812463,0.9774230709
 H,0,0.3635195851,-4.0869251893,1.4947914011
 H,0,-1.5760133891,-0.4074395947,-0.7235284569
 H,0,-1.3298301914,-4.0955891257,-1.182164055
 H,0,-1.7895273089,-4.3186935885,0.5206688214
 H,0,0.828317281,-4.0874242436,-0.210642562
 H,0,-0.8264471905,1.8866372661,-0.4298207522
 H,0,-2.3240627554,1.5379966001,0.3468080423

H,0,-3.4484525559,2.4149168939,-1.3542365864
H,0,-1.9215684346,2.6400557396,-2.2349552457
H,0,-1.6201495724,3.0567375207,1.8630612205
H,0,-0.4844619587,3.8312518347,0.7297374178
H,0,-2.2654860348,5.5059619489,0.8252398075
H,0,-3.5160906886,4.2533021024,0.8951887589
H,0,-3.4872759511,4.8270450705,-1.5055718606
H,0,-1.7216704908,4.9311286136,-1.5036051207
C,0,3.7539476656,-0.2931284241,-0.3283633318
C,0,4.9881019185,0.1666179126,0.1334745281
C,0,5.0837480063,1.4490665373,0.6752867934
C,0,3.9474410998,2.2609370886,0.738909221
C,0,2.7278445173,1.7834580614,0.2647470605
Cl,0,3.7062768431,-1.9268620765,-1.0106241117
H,0,5.8600485122,-0.4747084225,0.0624482401
H,0,6.0424271283,1.8092953666,1.0361710763
H,0,4.0157314896,3.2641128378,1.1495005358
H,0,1.8407650186,2.4077963729,0.2790100731

B3LYP/6-31G* Onsager solvent model for DMSO

SeebachTSOnsB3Gdoublestable5.95

E(RB+HF-LYP) = -1535.61884523

Zero-point correction=	0.441596 (Hartree/Particle)
Thermal correction to Energy=	0.466529
Thermal correction to Enthalpy=	0.467473
Thermal correction to Gibbs Free Energy=	0.383805
Sum of electronic and zero-point Energies=	-1535.177250
Sum of electronic and thermal Energies=	-1535.152316
Sum of electronic and thermal Enthalpies=	-1535.151372
Sum of electronic and thermal Free Energies=	-1535.235041

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	292.751	92.989	176.095
C,0,-1.9351912246,-3.6529007677,-0.3623733352			
N,0,-1.2625429152,-2.3748276054,-0.0526335075			
C,0,-2.171355704,-1.2201381764,-0.2434481902			
C,0,-3.2655611674,-1.8051786735,-1.1554247344			
C,0,-3.3870021124,-3.2563139269,-0.6660351344			
C,0,-0.0381914174,-2.2759346068,0.4511849116			
C,0,0.7471471224,-3.5541510583,0.6005207353			
C,0,-2.7898638988,-0.7540810194,1.1219532501			
O,0,-3.0579069913,0.4969968791,1.1844230315			
C,0,0.5674421737,-1.0338790198,0.7942687469			
O,0,-3.0142102934,-1.6242907387,1.9689250294			

C,0,1.2187068329,-0.0528633393,-0.8330420686
 C,0,2.5078148597,0.5408307237,-0.2895432492
 O,0,0.2962893969,0.7481881406,-1.2184516125
 N,0,-1.6297186253,2.2355036256,-0.0812652867
 C,0,-2.3311169207,2.8557343655,-1.2603761894
 C,0,-2.2628016747,4.3690721,-1.0166688132
 C,0,-2.2610270096,4.4753882757,0.5175195514
 C,0,-1.3681575261,3.3036958298,0.9427415788
 H,0,1.4072049632,-0.9378127381,-1.4585022365
 H,0,-3.8465750403,-3.9252056155,-1.4000425705
 H,0,-0.1009776461,-0.2469003273,1.1291356202
 H,0,1.4381108162,-1.1484042858,1.4333578462
 H,0,-3.9672690511,-3.2808230864,0.2585463752
 H,0,-4.199333171,-1.2436432442,-1.0702404291
 H,0,-2.9420272838,-1.7729614194,-2.2035556759
 H,0,1.7808529325,-3.3380482292,0.868504859
 H,0,0.3044157508,-4.1751907246,1.3899241004
 H,0,-1.610050678,-0.4290645884,-0.7370850362
 H,0,-1.4512177595,-4.1193835332,-1.2308405439
 H,0,-1.8591496866,-4.3407283614,0.4846844571
 H,0,0.7452640092,-4.1471448244,-0.3215792711
 H,0,-0.7500905847,1.7499090195,-0.4039505907
 H,0,-2.2601285972,1.4535702201,0.3796843217
 H,0,-3.3632676931,2.492480926,-1.2587032669
 H,0,-1.839929662,2.5254836936,-2.1774821302
 H,0,-1.5990248589,2.8987403761,1.9302541714
 H,0,-0.3084665396,3.5742780978,0.907198047
 H,0,-1.8850474066,5.4347052649,0.8842391872
 H,0,-3.2749552006,4.3369105393,0.9108056665
 H,0,-3.0967367349,4.8994405306,-1.4850161056
 H,0,-1.332801912,4.7790753391,-1.428050169
 C,0,3.7089287102,-0.1660613036,-0.142627176
 C,0,4.8763135803,0.4356160598,0.3246818049
 C,0,4.8637303727,1.789612445,0.6572243484
 C,0,3.6885063298,2.5273786387,0.5061439817
 C,0,2.5371649498,1.9046673155,0.0330308603
 Cl,0,3.8053789977,-1.8833874713,-0.5688111339
 H,0,5.783605301,-0.152506367,0.4149844731
 H,0,5.7725152242,2.2629644856,1.0177026044
 H,0,3.6752931623,3.5875159063,0.7438782915
 H,0,1.6263646471,2.4702372543,-0.1326793943

B3LYP/6-31+G Onsager solvent model for DMSO**

SeebachTSOnsB3+Gdoublestable5.64

E(RB+HF-LYP) = -1535.70543387

Zero-point correction= 0.439215 (Hartree/Particle)
 Thermal correction to Energy= 0.464341
 Thermal correction to Enthalpy= 0.465285
 Thermal correction to Gibbs Free Energy= 0.381056
 Sum of electronic and zero-point Energies= -1535.266219
 Sum of electronic and thermal Energies= -1535.241093
 Sum of electronic and thermal Enthalpies= -1535.240149
 Sum of electronic and thermal Free Energies= -1535.324378

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	291.378	93.599	177.275

C,0,-1.9149134954,-3.6176821375,-0.4027214601
 N,0,-1.243589584,-2.3577148326,-0.0161378664
 C,0,-2.1443811754,-1.1898080138,-0.1560419472
 C,0,-3.2540578439,-1.7283808431,-1.0807952687
 C,0,-3.3678330173,-3.2071300439,-0.677187021
 C,0,-0.0039792061,-2.2848206448,0.4573501402
 C,0,0.7832193235,-3.5684055872,0.5210151207
 C,0,-2.7402537811,-0.7268345922,1.2174200945
 O,0,-3.0059154532,0.5261533035,1.2748911136
 C,0,0.6142585045,-1.0601894587,0.8430179687
 O,0,-2.9469870196,-1.5883612032,2.0822897886
 C,0,1.2478630141,-0.0151829593,-0.7484329288
 C,0,2.5690941708,0.5064346919,-0.2152900184
 O,0,0.3360242806,0.8378373908,-1.0539537126
 N,0,-1.6829775806,2.3011237287,-0.0806426009
 C,0,-2.4382541782,2.7890354843,-1.2926344237
 C,0,-2.49657709,4.3172334979,-1.1467573498
 C,0,-2.444694087,4.5292307826,0.3754128391
 C,0,-1.4346456033,3.4710180398,0.8293725895
 H,0,1.385062937,-0.8649200622,-1.4303252334
 H,0,-3.824980252,-3.8287554105,-1.4523763613
 H,0,-0.0391073538,-0.2811989702,1.2208915088
 H,0,1.4981458246,-1.2077005563,1.4559506507
 H,0,-3.9532934757,-3.2959420433,0.240990384
 H,0,-4.1890663933,-1.1776669409,-0.9520811306
 H,0,-2.9446299107,-1.6350692484,-2.1289186535
 H,0,1.8145642161,-3.3685146418,0.8068863376
 H,0,0.3385584031,-4.2433240121,1.2624663416
 H,0,-1.5806779014,-0.3872591174,-0.6273571817
 H,0,-1.4332179025,-4.0266721499,-1.3002909378
 H,0,-1.8326800238,-4.3554085859,0.4003565797
 H,0,0.7872065463,-4.0936470736,-0.4407259997
 H,0,-0.7900304761,1.8242638365,-0.3738875618

H,0,-2.2633116349,1.5375909399,0.4484889158
H,0,-3.436218487,2.3427074469,-1.2629578456
H,0,-1.9249850674,2.4494283581,-2.1937208432
H,0,-1.5569914318,3.1472220008,1.8647780123
H,0,-0.4070818118,3.8171112504,0.6818819703
H,0,-2.139210086,5.5394891652,0.6606271833
H,0,-3.4247092192,4.3313824335,0.8247521502
H,0,-3.392390998,4.7379537668,-1.6109770608
H,0,-1.6253204855,4.7797666925,-1.6241427503
C,0,3.762206168,-0.2304202763,-0.2148166722
C,0,4.9687016603,0.3047776667,0.2377935319
C,0,5.0017872888,1.616549953,0.7127474215
C,0,3.8311580861,2.3798752327,0.7208132649
C,0,2.6401819118,1.825980283,0.2564318796
Cl,0,3.7956261747,-1.8969972522,-0.8145572568
H,0,5.8691948008,-0.2990446656,0.2059604117
H,0,5.9402630023,2.0388209047,1.0588355784
H,0,3.8521025053,3.4069225444,1.0730652699
H,0,1.7304962073,2.4153129281,0.2203330393

***o*-chlorobenzaldehyde transition structures – Seebach-Eschenmoser model with protonated proline stabilizing alkoxide**

B3LYP/6-31+G Onsager solvent model for DMSO (carboxylic acid towards carboxylate)**
seebachsinglestablewithPROLINEOnsB3+G
E(RB+HF-LYP) = -1724.29474818

Zero-point correction=	0.453755 (Hartree/Particle)
Thermal correction to Energy=	0.481222
Thermal correction to Enthalpy=	0.482166
Thermal correction to Gibbs Free Energy=	0.392889
Sum of electronic and zero-point Energies=	-1723.840993
Sum of electronic and thermal Energies=	-1723.813526
Sum of electronic and thermal Enthalpies=	-1723.812582
Sum of electronic and thermal Free Energies=	-1723.901859

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	301.972	102.649	187.900

C,0,-0.4950740039,2.4152913531,-0.708512199
N,0,-1.3509161388,2.3071217867,0.4982907815
C,0,-2.1712543674,3.5286939566,0.669218781
C,0,-1.3383630136,4.6049755037,-0.0244391426
C,0,-0.7464904883,3.8591024546,-1.2289423697
C,0,-1.5295735896,1.1867590581,1.2075830951

C,0,-2.7151388082,1.1288837653,2.1335712873
 C,0,0.9929816787,2.103168591,-0.5479879808
 O,0,1.5520884403,2.4497933495,0.5964614148
 C,0,-0.6516563442,0.0690361705,1.1238114142
 C,0,-0.7475485801,-1.2841196945,-0.2818200119
 C,0,-2.0605973466,-1.9849554849,-0.048076124
 C,0,-2.0734062718,-3.191924183,0.6691017959
 C,0,-3.2577165632,-3.8915193877,0.8935173968
 C,0,-4.4660309598,-3.3994797436,0.3906571907
 C,0,-4.4831184008,-2.2076682678,-0.3360054513
 C,0,-3.2879140136,-1.5192004495,-0.542447598
 Cl,0,-3.3705135806,-0.0144289641,-1.4756513429
 O,0,0.3380829807,-1.9714004673,-0.106540818
 O,0,1.5810203513,1.5570421326,-1.4753282356
 O,0,3.7644447236,1.1239749128,0.6989644578
 C,0,4.3106885904,0.0392952014,1.085198725
 O,0,5.3020694897,-0.1129353071,1.8154327582
 C,0,3.6323139822,-1.2803665321,0.5710640651
 N,0,2.6997194496,-0.9889808098,-0.5815674455
 C,0,3.2437467555,-1.6334636344,-1.8252116161
 C,0,4.6982478875,-1.9722038429,-1.4815823403
 C,0,4.6257957836,-2.3139593556,0.016185548
 H,0,-0.782646977,-0.6001779086,-1.1385750262
 H,0,-1.9435039699,5.46620707,-0.3170740392
 H,0,0.3800946477,0.3190261407,0.9192906982
 H,0,-0.7549604544,-0.6148589755,1.9605722028
 H,0,-0.5435500951,4.9506674541,0.6445876576
 H,0,0.166965948,4.317738656,-1.6141432298
 H,0,-1.4689878052,3.8219757185,-2.0494125971
 H,0,-2.8869508732,0.0991852839,2.4486325517
 H,0,-2.5273762196,1.7276478267,3.0337538702
 H,0,-0.8492991505,1.684694368,-1.4382399681
 H,0,-3.1452461695,3.3992044118,0.1788924143
 H,0,-2.3399493369,3.7270328121,1.7289283041
 H,0,-3.6266421561,1.5085313618,1.6636717584
 H,0,2.6708604251,0.0382231106,-0.6935445629
 H,0,1.6768981733,-1.3506187734,-0.3939481648
 H,0,3.0367497221,-1.682390051,1.3954310961
 H,0,2.653740625,-2.5349742095,-2.0134477424
 H,0,3.1189425498,-0.9511760058,-2.6681172186
 H,0,5.3408368164,-1.0980139178,-1.6397186532
 H,0,5.0811952417,-2.792031349,-2.0974008201
 H,0,4.2399591243,-3.3317933395,0.1522466325
 H,0,5.5798451076,-2.2266225137,0.5392163115
 H,0,-5.4094704155,-1.8180490546,-0.7438550768
 H,0,-5.3940142111,-3.9386869097,0.5528536558

H,0,-3.2411665636,-4.8231964513,1.4510092499
H,0,-1.1200774416,-3.5674717284,1.0268977104
H,0,2.4777928154,2.0240158619,0.6587889502

B3LYP/6-31+G Onsager solvent model for DMSO (carboxylic acid away from carboxylate)**

seebachsinglestablewithPROLINEAWAYOnsB3+G
E(RB+HF-LYP) = -1724.27034732

Zero-point correction=	0.453318 (Hartree/Particle)
Thermal correction to Energy=	0.481581
Thermal correction to Enthalpy=	0.482525
Thermal correction to Gibbs Free Energy=	0.389735
Sum of electronic and zero-point Energies=	-1723.817029
Sum of electronic and thermal Energies=	-1723.788766
Sum of electronic and thermal Enthalpies=	-1723.787822
Sum of electronic and thermal Free Energies=	-1723.880612

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	302.197	104.314	195.292

C,0,-3.298622811,-1.0906098864,0.3598835105
N,0,-2.5578944607,-2.0872767859,-0.4959034464
C,0,-3.0771525736,-1.9473944036,-1.9170650125
C,0,-4.2038326089,-0.8989953405,-1.8447071839
C,0,-4.6422626377,-0.9052638504,-0.3718339261
O,0,0.0012509328,-2.0601460077,-0.5852168599
C,0,0.8830355207,-1.2910222656,-0.0752054801
C,0,2.3127514273,-1.716838278,-0.1164625212
C,0,2.6928637436,-2.7476661562,-0.9939396288
C,0,4.0003897698,-3.2237704986,-1.0339375715
C,0,4.9650371989,-2.6815398446,-0.1787596289
C,0,4.614783563,-1.66475995,0.7115666747
C,0,3.3023953109,-1.1941920029,0.7317873158
Cl,0,2.9131230727,0.0812342476,1.8978440965
C,0,0.8451584976,0.3934326782,-1.4565629758
C,0,1.5069859673,1.5587812869,-1.0436505171
N,0,0.9225148409,2.4730399564,-0.2566046423
C,0,1.5690723056,3.7129183975,0.202584724
C,0,0.4182342194,4.5179155061,0.8174820219
C,0,-0.527028405,3.4287043988,1.3486362265
C,0,-0.4487609667,2.3232653873,0.276981589
C,0,-1.5675985308,2.4835420036,-0.8206754224
O,0,-2.4280203014,1.551724216,-0.8206583001
C,0,2.9399626464,1.7974002808,-1.4477409463

O,0,-1.5060729714,3.5027084658,-1.5377353142
 H,0,0.6174173956,-0.6545088579,0.7732124479
 H,0,0.7695309212,5.2029128335,1.5959720813
 H,0,-0.2371061934,0.3887172348,-1.4453287597
 H,0,1.3109422711,-0.1648669012,-2.2601726663
 H,0,-0.0905268844,5.0846171359,0.0336344263
 H,0,-1.5514414351,3.7841351214,1.4842058947
 H,0,-0.1687254591,3.0446513285,2.3118497673
 H,0,3.3398326501,0.9159487502,-1.949892048
 H,0,3.0043060507,2.6438189,-2.142409568
 H,0,-0.5416396497,1.3288989454,0.7193350324
 H,0,2.3415576343,3.476890792,0.9492413356
 H,0,2.0485502139,4.2327237806,-0.6324414531
 H,0,3.5759588995,2.0225975544,-0.5856704504
 H,0,-1.4573150734,-1.9656548625,-0.4632943625
 H,0,-2.7359485503,-3.0292174299,-0.1423213081
 H,0,-3.4256233038,-2.928995795,-2.2454801328
 H,0,-2.2438798825,-1.6406083366,-2.5500845637
 C,0,-3.4430508453,-1.5278206622,1.7993032263
 H,0,-2.7593724559,-0.1336904559,0.3030126654
 H,0,-5.1156419694,0.0293371542,-0.0674448683
 H,0,-5.3236699508,-1.737435381,-0.1512031491
 H,0,-5.0213155251,-1.1442810132,-2.5280401814
 H,0,-3.8081802932,0.0910242591,-2.0869175128
 H,0,5.3461773475,-1.2477065443,1.395191183
 H,0,5.9840441093,-3.0556291424,-0.1903094261
 H,0,4.2653779012,-4.0256348861,-1.7158295117
 H,0,1.9227716282,-3.1745501401,-1.6278332489
 O,0,-3.1409113599,-2.8386212282,1.98385792
 O,0,-3.8246833049,-0.8015499386,2.6875808014
 H,0,-3.2725506361,-3.05900277,2.9225046478

***o*-chlorobenzaldehyde transition structures – Seebach-Eschenmoser model with protonated proline stabilizing alkoxide and carboxylate**

B3LYP/6-31+G Onsager solvent model for DMSO**

seebachdoublestablewithPROLINEOnsB3+G

E(RB+HF-LYP) = -1724.28357288

Zero-point correction=	0.453065 (Hartree/Particle)
Thermal correction to Energy=	0.481038
Thermal correction to Enthalpy=	0.481983
Thermal correction to Gibbs Free Energy=	0.390964
Sum of electronic and zero-point Energies=	-1723.830507
Sum of electronic and thermal Energies=	-1723.802534
Sum of electronic and thermal Enthalpies=	-1723.801590

Sum of electronic and thermal Free Energies= -1723.892609

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	301.856	103.752	191.565

C,0,2.5404994833,-2.7969692105,-0.9737416935
C,0,2.4225173399,-1.6765146625,-0.1346209321
C,0,3.5950889212,-1.1963398925,0.4675526811
C,0,4.8380879048,-1.7896049624,0.2427471378
C,0,4.9265967567,-2.8920230395,-0.6082102323
C,0,3.7730027758,-3.3977301501,-1.2165184651
C,0,1.05932997,-1.1014506612,0.123241917
O,0,0.0372527354,-1.8540914015,-0.0694208039
Cl,0,3.5434387055,0.1796463462,1.5815045208
C,0,0.8917102265,0.3569579561,-1.3382740599
C,0,1.487309829,1.596535158,-1.013773044
C,0,2.859880101,1.9360088814,-1.5333114375
N,0,0.8843447427,2.4815726105,-0.2167055682
C,0,1.4476277156,3.7958888627,0.1540638747
C,0,0.2826925959,4.5172075105,0.8416965058
C,0,-0.5331031694,3.3687764524,1.4560468895
C,0,-0.4408686183,2.2509738726,0.3963949202
C,0,-1.624691562,2.3390614017,-0.6281309254
O,0,-1.5861801727,3.2431100607,-1.4729818097
O,0,-2.553064428,1.4763523919,-0.4393212764
N,0,-2.378361228,-0.9673044485,0.4852810281
C,0,-2.6540099942,-1.193000309,1.9360773653
C,0,-2.9588077696,-2.6903755533,1.998086318
C,0,-3.78677921,-2.9428072724,0.7195519008
C,0,-3.3014760718,-1.8607440433,-0.2963836027
H,0,1.0416450257,-0.3920487595,0.9591561594
H,0,0.6329920204,5.2377794209,1.5859907254
H,0,-0.1895426027,0.3142755653,-1.3298131474
H,0,1.3479692897,-0.1760871242,-2.1654923546
H,0,-0.320249258,5.0383646999,0.0941201059
H,0,-1.5700690841,3.6441461479,1.6628977911
H,0,-0.0766138547,3.0326035032,2.3947132582
H,0,3.327351565,1.0491858268,-1.9628589499
H,0,2.779437549,2.6938167031,-2.3229415604
H,0,-0.4408333797,1.2627004624,0.8602864917
H,0,2.2953281699,3.6530628717,0.837593646
H,0,1.8057468822,4.3231723655,-0.7342826187
H,0,3.5160362947,2.3314106659,-0.7534248421
H,0,-1.3675573635,-1.2977280859,0.2751371725
H,0,-2.4433843063,0.0782218022,0.1797067074

H,0,-3.512178367,-0.5820999472,2.2282611542
H,0,-1.7810505675,-0.8924715248,2.5194099688
C,0,-4.4598619544,-1.0880415787,-0.9089192395
H,0,-2.7353322154,-2.2932415042,-1.1215138047
H,0,-3.6412480022,-3.947245237,0.3168442069
H,0,-4.8536686954,-2.8163196291,0.924499349
H,0,-3.4973799252,-2.9699201837,2.9070189615
H,0,-2.0235008787,-3.2583118354,1.9680887293
H,0,5.7186123001,-1.3982126281,0.7405045522
H,0,5.8914767108,-3.3594220673,-0.7791232776
H,0,3.8353068137,-4.2662775063,-1.8651858413
H,0,1.6277912864,-3.1897182946,-1.4104443901
O,0,-5.0597366791,-0.2823764215,-0.0058675098
O,0,-4.8377036759,-1.2139259086,-2.0527534868
H,0,-5.698528677,0.2746963033,-0.4806521647

p-nitrobenzaldehyde transition structures – Houk-List model

B3LYP/6-31G*

ts3aPNBB3G*

E(RB+HF-LYP) = -1067.93254846

Zero-point correction=	0.320021 (Hartree/Particle)
Thermal correction to Energy=	0.339586
Thermal correction to Enthalpy=	0.340530
Thermal correction to Gibbs Free Energy=	0.270495
Sum of electronic and zero-point Energies=	-1067.612528
Sum of electronic and thermal Energies=	-1067.592963
Sum of electronic and thermal Enthalpies=	-1067.592018
Sum of electronic and thermal Free Energies=	-1067.662054

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	213.093	74.789	147.401

C,0,2.4017853779,-0.4617458838,-0.3886470696
C,0,1.2115895507,0.4596692251,-0.0943818024
C,0,0.3998969809,-0.3045929366,0.976192132
N,0,0.7454439547,-1.7266088336,0.7290313415
C,0,1.7750532172,-1.8565740286,-0.3418452782
C,0,0.191607823,-2.7481186083,1.3581281613
C,0,-0.6768255245,-2.4990198839,2.559517844
C,0,-1.1113869726,0.0357864997,0.8689631104
O,0,-1.8756206315,-0.7085837293,0.103828868

C,0,0.1738960054,-4.0379581456,0.7335685288
 O,0,-1.4928997629,1.0186221786,1.4750042357
 C,0,-1.2010624249,-3.805825659,-0.4446951876
 O,0,-1.0410408003,-2.7011534235,-1.1263011499
 C,0,-1.1455063885,-5.0979064721,-1.2400077098
 H,0,3.1703786084,-0.3614475293,0.3868619049
 H,0,-0.2818988988,-1.7019802901,3.1953880925
 H,0,-0.7649391052,-3.4126181191,3.1512688099
 H,0,2.8692249379,-0.2592199678,-1.3561682732
 H,0,0.6002214184,0.5832137139,-0.9952396912
 H,0,1.4935596606,1.4528401502,0.2603736462
 H,0,-1.6843122218,-2.1982570413,2.2445414453
 H,0,1.0053850784,-4.2768115976,0.0757601128
 H,0,-2.0569020962,-3.8333055239,0.2586020211
 H,0,-0.0742030144,-4.8649109998,1.3963511371
 H,0,0.717320631,-0.0166331053,1.9826732242
 H,0,-1.4530652001,-1.5447998441,-0.428788436
 H,0,2.4816343262,-2.6446931993,-0.0677537493
 H,0,1.2776317578,-2.1227179282,-1.2752515635
 C,0,-1.5880794896,-6.3083303129,-0.68756509
 C,0,-1.5376235258,-7.4883582253,-1.421662958
 C,0,-1.0385125166,-7.4422035449,-2.723419557
 C,0,-0.6052039716,-6.2507702608,-3.3043767917
 C,0,-0.6645625899,-5.0798951532,-2.5551655581
 H,0,-1.9852616731,-6.3269965204,0.3249194848
 H,0,-1.8774243267,-8.4319762452,-1.0130005981
 N,0,-0.9755388975,-8.6841123168,-3.5060502373
 H,0,-0.2400682995,-6.2576677361,-4.3241878624
 H,0,-0.3631616218,-4.1287082926,-2.9799925416
 O,0,-0.5305205033,-8.6178156401,-4.6522979986
 O,0,-1.3680078713,-9.7208717694,-2.9690435896

B3LYP/6-31+G**

ts3aPNBB3+G**

E(RB+HF-LYP) = -1068.00757742

Zero-point correction=	0.318400 (Hartree/Particle)
Thermal correction to Energy=	0.338144
Thermal correction to Enthalpy=	0.339088
Thermal correction to Gibbs Free Energy=	0.268506
Sum of electronic and zero-point Energies=	-1067.689178
Sum of electronic and thermal Energies=	-1067.669433
Sum of electronic and thermal Enthalpies=	-1067.668489
Sum of electronic and thermal Free Energies=	-1067.739072

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	212.189	75.325	148.553

C,0,-0.6660494993,-5.0898073413,-2.5843137593
C,0,-1.1706438424,-5.109852475,-1.2763640937
C,0,-1.6144456442,-6.3233644316,-0.7288035883
C,0,-1.5414609776,-7.5054192547,-1.4600441948
C,0,-1.0188937889,-7.4575985988,-2.7538571569
C,0,-0.5843074276,-6.2627642129,-3.3303445622
C,0,-1.2643581358,-3.8270964701,-0.4845755878
O,0,-1.130357916,-2.7128160187,-1.13460683
H,0,-2.0292640272,-6.3438111223,0.2758957241
C,0,0.2283191383,-4.0526096816,0.7143262142
C,0,0.2088477767,-2.7662708084,1.3187693229
C,0,-0.6439721831,-2.5316567929,2.535975764
N,0,0.7320428005,-1.7236655631,0.6841734539
C,0,0.3871622518,-0.3104950891,0.9714759333
C,0,1.2360696936,0.4927801952,-0.0429022174
C,0,2.4125592965,-0.4382672175,-0.3645902394
C,0,1.7594510187,-1.8217789615,-0.3885941145
C,0,-1.1149729995,0.0488370602,0.8359147828
O,0,-1.506806596,1.0224684984,1.4566981453
O,0,-1.8727409414,-0.6620617636,0.0331707485
H,0,3.1722564823,-0.3898404174,0.4240470368
H,0,-0.2016470049,-1.7891354984,3.2054531822
H,0,-0.7738494478,-3.4651604065,3.0852446361
H,0,2.8957258823,-0.1991195305,-1.3154190509
H,0,0.6481660756,0.6839613922,-0.9468140565
H,0,1.5337586599,1.4566082438,0.3730725875
H,0,-1.6375838682,-2.1634088072,2.251967514
H,0,1.0173577132,-4.2733538481,0.0031049349
H,0,-2.0688894533,-3.8798959322,0.2702005084
H,0,-0.010119618,-4.8873695343,1.3677183868
H,0,0.6753711968,-0.0611491343,1.9968679112
H,0,-1.4888155384,-1.5320874113,-0.4607632701
H,0,2.4510880396,-2.634741768,-0.1545310805
H,0,1.2686552914,-2.0299206819,-1.3418208369
H,0,-1.8823837862,-8.4493856719,-1.0532031308
N,0,-0.9322478918,-8.701925975,-3.533981612
H,0,-0.2016641783,-6.2656828556,-4.3436406442
H,0,-0.3638269236,-4.1390345437,-3.0095602704
O,0,-0.4670538414,-8.6356314694,-4.6736635366
O,0,-1.3267197861,-9.742642101,-3.0030379538

B3LYP/6-31G* Onsager solvent model for DMSO
PNBOnsB3G5.55

E(RB+HF-LYP) = -1067.93735896

Zero-point correction=	0.320863 (Hartree/Particle)
Thermal correction to Energy=	0.340559
Thermal correction to Enthalpy=	0.341503
Thermal correction to Gibbs Free Energy=	0.271053
Sum of electronic and zero-point Energies=	-1067.616496
Sum of electronic and thermal Energies=	-1067.596800
Sum of electronic and thermal Enthalpies=	-1067.595856
Sum of electronic and thermal Free Energies=	-1067.666306

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	213.704	75.052	148.276

C,0,2.1074466678,0.7847202166,-0.6828821035
C,0,1.5687375492,-0.4225235722,-0.2176174639
C,0,2.4299623909,-1.4084828255,0.286011988
C,0,3.8046181001,-1.2049245268,0.3214945486
C,0,4.313067806,0.0042704778,-0.1564463603
C,0,3.4794938679,1.0076784896,-0.6532544897
C,0,0.0794160855,-0.6676427325,-0.3391393422
O,0,-0.5928264102,0.1445865893,-1.0818454269
H,0,0.20199150361,-2.3517127807,0.6397758675
C,0,-0.4693437323,-0.4795223152,1.489391848
C,0,-1.8684358336,-0.6464777702,1.299627078
C,0,-2.4642826121,-2.0276471126,1.3496702753
N,0,-2.6054863887,0.3579792975,0.842558112
C,0,-3.9275020503,0.1958215351,0.1904944862
C,0,-4.3380583731,1.6416666261,-0.1758871164
C,0,-3.5826115514,2.5103653841,0.8373800883
C,0,-2.235764435,1.795397338,0.9683714999
C,0,-3.946125979,-0.7096450743,-1.065102671
O,0,-5.0031285861,-1.2124883203,-1.3818271831
O,0,-2.8354682516,-0.8531910426,-1.7716460163
H,0,-4.1030630205,2.5206259304,1.8015450269
H,0,-3.4666906515,-2.0191904012,1.7888710181
H,0,-1.8308136172,-2.6877004361,1.9451595825
H,0,-3.4652687964,3.5458089257,0.506617585
H,0,-4.0028901561,1.8708517005,-1.1938967671
H,0,-5.4223534586,1.7623438194,-0.1433017947
H,0,-2.5512299782,-2.4535487955,0.3422452598
H,0,-0.0979302366,0.5181068032,1.7028913305

H,0,-0.1240045559,-1.7520660806,-0.4423996978
H,0,0.0229647988,-1.253562383,2.0732359522
H,0,-4.6395005579,-0.2388427973,0.8979957504
H,0,-1.9771735079,-0.3773241196,-1.4387752168
H,0,-1.749317682,1.95897666,1.9335359711
H,0,-1.542875246,2.0577144774,0.1668944464
H,0,4.4845301187,-1.959207299,0.6977872372
N,0,5.7639691609,0.2117001745,-0.1645985874
H,0,3.9148217118,1.930095149,-1.0179237952
H,0,1.4279232098,1.5237001866,-1.0934765374
O,0,6.1931804161,1.279861417,-0.6065997701
O,0,6.4805687487,-0.6975828125,0.260830388

B3LYP/6-31+G Onsager solvent model for DMSO**
PNBOnsB3+G5.38

$$E(RB+HF-LYP) = -1068.01308607$$

Zero-point correction=	0.318825 (Hartree/Particle)
Thermal correction to Energy=	0.338733
Thermal correction to Enthalpy=	0.339677
Thermal correction to Gibbs Free Energy=	0.268533
Sum of electronic and zero-point Energies=	-1067.694261
Sum of electronic and thermal Energies=	-1067.674353
Sum of electronic and thermal Enthalpies=	-1067.673409
Sum of electronic and thermal Free Energies=	-1067.744553

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	212.558	75.704	149.737

C,0,2.1459983746,0.7771005136,-0.6817183023
C,0,1.594959985,-0.4317146751,-0.2294846306
C,0,2.4461277116,-1.4272693923,0.2768232209
C,0,3.8231175152,-1.2350327071,0.3211307459
C,0,4.3450293143,-0.027453951,-0.1511515589
C,0,3.5207926832,0.9882364943,-0.6433959576
C,0,0.117734617,-0.6843626585,-0.3799199942
O,0,-0.5612679735,0.1054119618,-1.1263779698
H,0,2.0273005422,-2.3680404958,0.6249623198
C,0,-0.478102574,-0.4224978769,1.5384607117
C,0,-1.8579684062,-0.6108540845,1.3004580833
C,0,-2.4450135344,-1.9957626754,1.3754408787
N,0,-2.6069390524,0.3760635657,0.808629674
C,0,-3.9296492885,0.1792786938,0.1693710407

C,0,-4.4178215177,1.6180432043,-0.1346693161
 C,0,-3.6532742582,2.4906594137,0.8695175674
 C,0,-2.2780791721,1.8215572352,0.9318515243
 C,0,-3.9301899408,-0.6765174784,-1.1190197821
 O,0,-4.9743314447,-1.2020326656,-1.452771172
 O,0,-2.8247188768,-0.7602654023,-1.843473273
 H,0,-4.1338402074,2.460319013,1.8532975509
 H,0,-3.4175385859,-1.9881012649,1.8767931375
 H,0,-1.7776917976,-2.6558420759,1.9306840726
 H,0,-3.5874383654,3.5362330947,0.5584744718
 H,0,-4.1471251765,1.8939106763,-1.1597100449
 H,0,-5.5027338865,1.6890306938,-0.044947903
 H,0,-2.5973691871,-2.4232781659,0.3772615752
 H,0,-0.0988151985,0.5817207717,1.6910661046
 H,0,-0.1079857322,-1.764721213,-0.4141386161
 H,0,0.0197010043,-1.1841875598,2.1307195571
 H,0,-4.6103134787,-0.3149806374,0.8683030382
 H,0,-1.9492326685,-0.3413979559,-1.4848089501
 H,0,-1.7537483853,1.9954786619,1.8741430239
 H,0,-1.6338260775,2.123391914,0.1020349325
 H,0,4.4918452555,-1.9982789313,0.6991572006
 N,0,5.7988362126,0.1636055751,-0.1619326388
 H,0,3.9622981383,1.9108745644,-0.9995873603
 H,0,1.4784766906,1.5278152512,-1.0906522094
 O,0,6.2421355447,1.2292711175,-0.6014356724
 O,0,6.5091311972,-0.756422549,0.25637992

B3LYP/6-31+G** PCM solvent model for DMSO

nitrobenzaldehydeTSB3BBPCM

E(RB+HF-LYP) = -1068.05264838

Zero-point correction=	0.316468 (Hartree/Particle)
Thermal correction to Energy=	0.336315
Thermal correction to Enthalpy=	0.337259
Thermal correction to Gibbs Free Energy=	0.267065
Sum of electronic and zero-point Energies=	-1067.736181
Sum of electronic and thermal Energies=	-1067.716333
Sum of electronic and thermal Enthalpies=	-1067.715389
Sum of electronic and thermal Free Energies=	-1067.785584

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	211.041	76.061	147.738

C,0,1.552154 -0.537943 -0.363927

C,0,0.108496 -0.883016 -0.495725
 O,0,-0.642927 -0.202355 -1.278377
 C,0,-0.415838 -0.341738 1.558043
 C,0,-1.784490 -0.528883 1.351803
 C,0,-2.409321 -1.873666 1.614936
 N,0,-2.530055 0.425997 0.769009
 C,0,-3.891024 0.207978 0.249275
 C,0,-4.368783 1.624470 -0.173796
 C,0,-3.522302 2.565466 0.692260
 C,0,-2.162847 1.866393 0.740586
 C,0,-3.994262 -0.750731 -0.945204
 O,0,-5.092031 -1.242072 -1.210977
 O,0,-2.943729 -0.987464 -1.697778
 H,0,-3.942682 2.640141 1.700856
 H,0,-3.317064 -1.767716 2.217630
 H,0,-1.708736 -2.511709 2.154477
 H,0,-3.451603 3.571286 0.271986
 H,0,-4.153728 1.792265 -1.234847
 H,0,-5.443628 1.735320 -0.023792
 H,0,-2.686097 -2.391275 0.689340
 H,0, 0.015624 0.651228 1.531280
 H,0,-0.119001 -1.942842 -0.327010
 H,0, 0.109606 -1.072199 2.162654
 H,0,-4.538329 -0.194604 1.034035
 H,0,-1.980543 -0.600531 -1.429770
 H,0,-1.582528 2.112765 1.631500
 H,0,-1.561514 2.084790 -0.146431
 C,0,2.438334 -1.472328 0.200222
 C,0,3.792423 -1.183341 0.318639
 C,0,4.253095 0.056849 -0.138092
 C,0,3.394879 1.001232 -0.713295
 C,0,2.043818 0.695011 -0.825814
 H,0, 2.064878 -2.429898 0.550165
 H,0, 4.478045 -1.899199 0.753040
 N,0, 5.667603 0.373359 -0.014120
 H,0, 3.781024 1.949332 -1.064829
 H,0, 1.361805 1.408886 -1.273852
 O,0, 6.067209 1.476768 -0.408944
 O,0, 6.424683 -0.470633 0.483561

Chapter 3 – Base Catalyzed Isomerization of Flourinated Imines
Deprotonation TS B3LYP/6-31G* Onsager solvent model for benzene

Dimethylamine TS 1

Eme2nhdeprotA
E(RB+HF-LYP) = -1068.21174549

Zero-point correction=	0.328422 (Hartree/Particle)
Thermal correction to Energy=	0.349373
Thermal correction to Enthalpy=	0.350317
Thermal correction to Gibbs Free Energy=	0.276428
Sum of electronic and zero-point Energies=	-1067.883324
Sum of electronic and thermal Energies=	-1067.862372
Sum of electronic and thermal Enthalpies=	-1067.861428
Sum of electronic and thermal Free Energies=	-1067.935318

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	219.235	78.519	155.513

C,0,-4.1582763928,0.9104692082,-3.1967868311
C,0,-3.601256708,-0.0120838841,-2.2812091048
C,0,-4.3966392441,-0.3912752362,-1.1780455881
C,0,-5.6767955,0.1274676616,-0.9949485781
C,0,-6.2090141472,1.0481411778,-1.9028550538
C,0,-5.4389154837,1.4294046538,-3.0052115386
C,0,-2.207463766,-0.4804255389,-2.3857797554
N,0,-1.5498603402,-0.2525361412,-3.5558531879
C,0,-0.4708115097,-0.8005087055,-4.0309261085
C,0,-0.0153245414,-0.2151215148,-5.3470964486
F,0,1.3379533116,-0.0963676655,-5.4151969077
C,0,0.33833602,-1.9078062415,-3.4690140036
C,0,0.9417679999,-2.8652839462,-4.3112748933
C,0,1.701149123,-3.907309237,-3.7875895633
C,0,1.8856835109,-4.0278792893,-2.4076003063
C,0,1.3045362358,-3.0855740474,-1.559319481
C,0,0.5418289697,-2.0409815065,-2.0817233609
F,0,-0.3693934695,-0.97229742,-6.4303756344
F,0,-0.5228476124,1.0194704698,-5.5712160669
N,0,-1.5177443507,2.0634286261,-1.5295425148
C,0,-0.3177877081,2.5628122131,-2.2455911364
H,0,-2.3658802844,2.4492041191,-1.9559359685
C,0,-1.5328205624,2.310244235,-0.0695787797

H,0,-3.576040976,1.1815158501,-4.0735008132
H,0,-5.8440476073,2.1309988729,-3.7316471119
H,0,-7.2067114819,1.4529585678,-1.7578843424
H,0,-6.2653253346,-0.1912499052,-0.1374466815
H,0,-3.9986869377,-1.1096297103,-0.463137735
H,0,-1.9622246706,-1.3492192242,-1.7650046617
H,0,-1.6662048878,0.9248610143,-1.75516894
H,0,0.8031722039,-2.7915247661,-5.3844751343
H,0,0.21498317265,-4.6330296571,-4.4618205472
H,0,0.2477043891,-4.8436261692,-2.0002051808
H,0,0.14494031663,-3.1574915616,-0.4840831889
H,0,0.01235312814,-1.3034516672,-1.4058299141
H,0,-1.4518858036,3.3802422153,0.1425298018
H,0,-2.4664492787,1.9176897466,0.3379345643
H,0,-0.6888433646,1.7842250177,0.3827628794
H,0,-0.2285311125,3.6476094462,-2.1324778735
H,0,0.5649685796,2.0778477578,-1.8227754568
H,0,-0.4088569433,2.2896431816,-3.2976988525

Dimethylamine TS 2

Eme2nhdeprotB

E(RB+HF-LYP) = -1068.21069165

Zero-point correction=	0.331388 (Hartree/Particle)
Thermal correction to Energy=	0.352113
Thermal correction to Enthalpy=	0.353057
Thermal correction to Gibbs Free Energy=	0.279687
Sum of electronic and zero-point Energies=	-1067.879304
Sum of electronic and thermal Energies=	-1067.858578
Sum of electronic and thermal Enthalpies=	-1067.857634
Sum of electronic and thermal Free Energies=	-1067.931004

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	220.954	78.184	154.420

C,0,-4.419241875,0.7771113879,-3.1808390034
C,0,-3.7779541985,-0.0748684419,-2.2491324056
C,0,-4.46855359,-0.3539840138,-1.047309058
C,0,-5.7182377225,0.2012423165,-0.7820285323
C,0,-6.3279091993,1.0572115135,-1.7044300257
C,0,-5.6669319117,1.3322724226,-2.9067826315
C,0,-2.4339327359,-0.611802063,-2.4664233008
N,0,-1.7788719198,-0.3241027193,-3.5976023004

C,0,-0.6330533856,-0.7674533881,-4.0724840027
 C,0,-0.2442811547,-0.1533416449,-5.3870859402
 F,0,1.0842282954,0.149289354,-5.4498240846
 C,0,0.2728754429,-1.7865969559,-3.5071173042
 C,0,1.0528775511,-2.6202368088,-4.3414857384
 C,0,1.9179417253,-3.5715273828,-3.8109211791
 C,0,2.0412209432,-3.7332928603,-2.4279394066
 C,0,1.2871948094,-2.9172406347,-1.5850898288
 C,0,0.4197477382,-1.9618142291,-2.113793387
 F,0,-0.4747745973,-0.9583475252,-6.4731164886
 F,0,-0.9079251963,1.0040598962,-5.6489451291
 N,0,-1.2755298459,1.9982090685,-1.8091250078
 H,0,-0.2648415328,1.8385812515,-1.7757273825
 C,0,-1.5859713972,2.94612443,-2.9236991477
 C,0,-1.7719597244,2.4261060028,-0.4705762161
 H,0,-3.9223635044,0.9685160035,-4.1275976472
 H,0,-6.1372832335,1.9775424754,-3.6462187738
 H,0,-7.3016732125,1.4914062448,-1.4958554464
 H,0,-6.2213015501,-0.03628902,0.1528121177
 H,0,-4.0091813453,-1.0200007951,-0.3183564927
 H,0,-2.1217208946,-1.4158026047,-1.7934332293
 H,0,-1.703062325,1.0339538458,-2.0520195483
 H,0,0.9667227786,-2.5235352415,-5.4178821777
 H,0,0.24982754487,-4.1977713063,-4.4848985019
 H,0,0.27139074446,-4.4808758304,-2.0160676761
 H,0,1.3768136861,-3.0178584281,-0.5058139572
 H,0,-0.1308042442,-1.3244775314,-1.4310223468
 H,0,-1.0859345724,3.9000353595,-2.7397543899
 H,0,-1.2504944512,2.4907963303,-3.8552762735
 H,0,-2.6679692209,3.0771004006,-2.9546992169
 H,0,-1.3405956609,3.3945782029,-0.208636621
 H,0,-2.8594901473,2.4906305692,-0.5181023311
 H,0,-1.4855485146,1.6733483496,0.2657640132

Dimethylamine TS 3

Eme2nhdeprotC
 E(RB+HF-LYP) = -1068.21101450

Zero-point correction=	0.328679 (Hartree/Particle)
Thermal correction to Energy=	0.349513
Thermal correction to Enthalpy=	0.350458
Thermal correction to Gibbs Free Energy=	0.277270
Sum of electronic and zero-point Energies=	-1067.882336
Sum of electronic and thermal Energies=	-1067.861501

Sum of electronic and thermal Enthalpies= -1067.860557
 Sum of electronic and thermal Free Energies= -1067.933745

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	219.323	78.501	154.037

C,0,-4.4496417819,0.7339878039,-3.2628244567
 C,0,-3.7654194936,0.0219641901,-2.2546965031
 C,0,-4.4493791425,-0.2101143087,-1.0435754644
 C,0,-5.7468224199,0.2560613577,-0.842349235
 C,0,-6.4060903938,0.9722111825,-1.8451328794
 C,0,-5.7459513182,1.2023567556,-3.0559747806
 C,0,-2.3674485967,-0.4299784035,-2.4053455816
 N,0,-1.7681934557,-0.2698048974,-3.6107242029
 C,0,-0.6690499718,-0.7708570586,-4.1013325734
 C,0,-0.2760260159,-0.1681101394,-5.4306536915
 F,0,1.0316521668,0.2297140981,-5.4309937803
 C,0,0.2492991694,-1.7821271253,-3.5262903953
 C,0,1.0200914138,-2.623296894,-4.3606691378
 C,0,1.8861927344,-3.5736044984,-3.8300068637
 C,0,2.0198972116,-3.7243189656,-2.4471193711
 C,0,1.2758374296,-2.9002618172,-1.6046518961
 C,0,0.4058688422,-1.9460305707,-2.1334365228
 F,0,-0.3976471923,-1.0210697329,-6.4916322714
 F,0,-1.0033136758,0.9257474941,-5.7499712592
 N,0,-1.1298323761,1.9873626848,-1.7280172369
 C,0,0.3494938738,1.834960215,-1.7163568356
 C,0,-1.6263725961,2.9051963532,-2.7919258038
 H,0,-1.451697855,2.3150637019,-0.81439947
 H,0,-3.9474584107,0.893146059,-4.2125295501
 H,0,-6.2514457408,1.7434313131,-3.8533696175
 H,0,-7.417666283,1.3369505266,-1.6887419492
 H,0,-6.2473378137,0.0574082841,0.1027857887
 H,0,-3.9505132999,-0.7702041083,-0.2538432447
 H,0,-2.0822258679,-1.2484084057,-1.7348900894
 H,0,-1.6301898996,0.9459575928,-1.8985407463
 H,0,0.9299366089,-2.5346382335,-5.4365468659
 H,0,2.459855716,-4.2056081964,-4.5037947186
 H,0,2.6945307007,-4.4699467564,-2.0351583532
 H,0,1.3726968928,-2.9935686583,-0.5255843536
 H,0,-0.1375453251,-1.3067033923,-1.4497674746
 H,0,-1.1527709399,3.886242231,-2.6921935385
 H,0,-1.3897028929,2.4562038466,-3.7571625997
 H,0,-2.709496251,2.9893714352,-2.697127357
 H,0,0.8274405046,2.7917910271,-1.48786432

H,0,0.6260501143,1.091601348,-0.9663945181
H,0,0.6645346306,1.4831866619,-2.6996552795

1-2 motion SM side TS B3LYP/6-31G* Onsager solvent model for benzene

Dimethylamine TS 1

Eme2nh1-2TSA

E(RB+HF-LYP) = -1068.21499337

Zero-point correction=	0.332154 (Hartree/Particle)
Thermal correction to Energy=	0.353055
Thermal correction to Enthalpy=	0.354000
Thermal correction to Gibbs Free Energy=	0.280495
Sum of electronic and zero-point Energies=	-1067.882839
Sum of electronic and thermal Energies=	-1067.861938
Sum of electronic and thermal Enthalpies=	-1067.860994
Sum of electronic and thermal Free Energies=	-1067.934498

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	221.546	78.520	154.703

C,0,-4.3950009554,0.6537586392,-2.9768900874
C,0,-3.6673178813,-0.088179114,-2.0130270424
C,0,-4.3236318218,-0.3815325245,-0.7959758141
C,0,-5.6197341563,0.0603126528,-0.5453148572
C,0,-6.3143159224,0.8121903939,-1.4980893261
C,0,-5.6898939624,1.0974184512,-2.7176645583
C,0,-2.293952647,-0.5296348122,-2.2350559127
N,0,-1.6369196933,-0.1215800637,-3.3066856239
C,0,-0.4219653208,-0.4003216452,-3.7744348967
C,0,-0.0896579927,0.3222549114,-5.037178393
F,0,1.1843124865,0.81658466,-5.0453565823
C,0,0.5831810121,-1.3339420294,-3.2408290884
C,0,1.4901235783,-2.0091550365,-4.091883843
C,0,2.4504670604,-2.878962126,-3.5860299908
C,0,2.5445056412,-3.1198166021,-2.2122795647
C,0,1.6638079364,-2.4615582421,-1.3534503135
C,0,0.7035711683,-1.5841647441,-1.8550511679
F,0,-0.190889095,-0.4057331628,-6.1893970022
F,0,-0.9006272538,1.4225792776,-5.2544559157
N,0,-1.5079054339,2.5655039027,-2.6453281156
C,0,-0.0920137913,2.8616224258,-2.2717897028
H,0,-1.5372589539,2.3409054978,-3.651169221

C,0,-2.492602982,3.6271281263,-2.2885000649
 H,0,-3.9314239623,0.8369167728,-3.9428511866
 H,0,-6.2279474207,1.6531391297,-3.4834078722
 H,0,-7.3255170889,1.156651651,-1.3006838551
 H,0,-6.0925271381,-0.1805792493,0.4042501603
 H,0,-3.7958055229,-0.9617395502,-0.041167556
 H,0,-1.9018993182,-1.2715269103,-1.5353486827
 H,0,-1.7902503686,1.6483912016,-2.2381728481
 H,0,1.4289007691,-1.8553072915,-5.1637357807
 H,0,3.1277669026,-3.3809185852,-4.273666543
 H,0,3.291288902,-3.8051432791,-1.8200088769
 H,0,1.7284714614,-2.6220129632,-0.2794506907
 H,0,0.0623400456,-1.0579816811,-1.157354602
 H,0,-2.2419297868,4.5439307921,-2.825598738
 H,0,-3.4878564891,3.2727896467,-2.5600885513
 H,0,-2.4447442995,3.8007780611,-1.2122000978
 H,0,0.2029009424,3.8104219015,-2.7239052774
 H,0,-0.0195023892,2.9265863609,-1.1851197823
 H,0,0.5319807411,2.0509281565,-2.6507201348

Dimethylamine TS 2

Eme2nh1-2TSB

E(RB+HF-LYP) = -1068.21052118

Zero-point correction=	0.332002 (Hartree/Particle)
Thermal correction to Energy=	0.352766
Thermal correction to Enthalpy=	0.353710
Thermal correction to Gibbs Free Energy=	0.279982
Sum of electronic and zero-point Energies=	-1067.878519
Sum of electronic and thermal Energies=	-1067.857756
Sum of electronic and thermal Enthalpies=	-1067.856811
Sum of electronic and thermal Free Energies=	-1067.930540

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	221.364	78.270	155.174

C,0,-4.5612764057,0.6489549538,-3.3370277618
 C,0,-3.7831133622,0.1546627736,-2.2602731355
 C,0,-4.4053799895,0.0902575161,-0.9913794286
 C,0,-5.71771423,0.5162398104,-0.8035727201
 C,0,-6.4628615913,1.0248028163,-1.8725436821
 C,0,-5.8716914877,1.078250518,-3.1401906047
 C,0,-2.3844734215,-0.2336011128,-2.4125138249
 N,0,-1.7707175188,-0.0727400593,-3.5835438362

C,0,-0.5542762102,-0.4092246156,-3.9850553721
 C,0,-0.2738756737,-0.0718218225,-5.4181346657
 F,0,0.9621649134,0.4788942185,-5.5995731258
 C,0,0.5128487098,-1.0884078679,-3.2283636388
 C,0,1.4614378583,-1.9194587988,-3.8701413758
 C,0,2.4830269683,-2.5397125839,-3.1584459733
 C,0,2.6033421145,-2.3627235425,-1.7772070731
 C,0,1.6842741687,-1.541966659,-1.1234619126
 C,0,0.6602742264,-0.9167642466,-1.8334671996
 F,0,-0.3042424659,-1.1492259067,-6.2679909784
 F,0,-1.1613337921,0.8182436811,-5.9431482388
 N,0,-1.7822883337,2.7284456713,-2.7097752182
 H,0,-0.7613531557,2.798779846,-2.6696261776
 C,0,-2.2565024084,3.2580105765,-4.0263746613
 C,0,-2.3908081826,3.3893672761,-1.5174568304
 H,0,-4.1174085829,0.6576511341,-4.3284773504
 H,0,-6.4465537193,1.4437174842,-3.9889830266
 H,0,-7.4858143023,1.3588580813,-1.7241266924
 H,0,-6.1637562758,0.4532130014,0.1865849341
 H,0,-3.8394168965,-0.3009579737,-0.1474555149
 H,0,-1.9412651645,-0.7852670478,-1.5796387223
 H,0,-1.9827775045,1.6858966989,-2.666281384
 H,0,1.3856036353,-2.0852420028,-4.938612066
 H,0,3.1900992379,-3.1743069732,-3.688409103
 H,0,3.3988953873,-2.8535148873,-1.2228105834
 H,0,1.7663023151,-1.3781237524,-0.0512226654
 H,0,-0.0159952359,-0.2595867625,-1.2988385835
 H,0,-1.9637622606,4.3063182445,-4.1177123493
 H,0,-1.8123145238,2.646872646,-4.8109163973
 H,0,-3.3414555772,3.1556797862,-4.0513155965
 H,0,-2.1738188182,4.4590166472,-1.5428054353
 H,0,-3.4662329867,3.211927224,-1.5469123948
 H,0,-1.9722414579,2.9376030101,-0.6169776337

Dimethylamine TS 3

Eme2nh1-2TSC

E(RB+HF-LYP) = -1068.21205391

Zero-point correction=	0.332377 (Hartree/Particle)
Thermal correction to Energy=	0.352939
Thermal correction to Enthalpy=	0.353883
Thermal correction to Gibbs Free Energy=	0.281869
Sum of electronic and zero-point Energies=	-1067.879677
Sum of electronic and thermal Energies=	-1067.859115

Sum of electronic and thermal Enthalpies= -1067.858171
 Sum of electronic and thermal Free Energies= -1067.930185

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	221.472	78.199	151.566

C,0,0.2854133559,-2.1067555191,-2.0951453799
 C,0,0.2416158679,-1.8250686186,-3.4810998177
 C,0,1.1712069308,-2.5185577032,-4.2945994109
 C,0,2.0717763861,-3.4311740203,-3.7562342424
 C,0,2.0894941066,-3.6993179963,-2.3844341373
 C,0,1.1902270668,-3.0237291105,-1.5607053504
 C,0,-0.6880055958,-0.8290114199,-4.0422626723
 C,0,-0.2603393131,-0.1140704966,-5.2886844721
 F,0,-1.0717972172,0.9216359285,-5.6233646965
 N,0,-1.8370288278,-0.3859305938,-3.5531232566
 C,0,-2.5311397683,-0.709134566,-2.466922035
 C,0,-3.8410734703,-0.1019669492,-2.230837585
 C,0,-4.4477627846,0.7842312975,-3.1533513528
 C,0,-5.6716091134,1.3861704132,-2.8725412491
 C,0,-6.3415391759,1.1239488779,-1.6720760287
 C,0,-5.766155127,0.2352101284,-0.7592144797
 C,0,-4.5397984514,-0.366086904,-1.0316660006
 F,0,1.0005083875,0.433335478,-5.1673968715
 F,0,-0.1881916337,-0.895796223,-6.4086854316
 N,0,-1.1587185718,1.980774163,-1.9667988721
 C,0,-1.6232133224,2.9468422176,-3.0120327001
 C,0,0.3239522784,1.7781196252,-1.9389402238
 H,0,-1.4810669229,2.292520307,-1.0463901826
 H,0,-3.9450063242,0.9622022447,-4.0997039408
 H,0,-6.11769041,2.0562603998,-3.6049157053
 H,0,-7.2969656188,1.5946374033,-1.4576575463
 H,0,-6.2767896766,0.0102648355,0.1745729234
 H,0,-4.1049880835,-1.0552635637,-0.3093943338
 H,0,-2.2655274819,-1.541921361,-1.8108566897
 H,0,-1.6351316845,1.0467561251,-2.1402008405
 H,0,1.1800504179,-2.3417762771,-5.3631040518
 H,0,2.765876608,-3.9436941459,-4.4187449961
 H,0,2.7901756725,-4.4182579805,-1.9684568342
 H,0,1.1914807371,-3.205146155,-0.4880922598
 H,0,-0.3763212374,-1.5820894769,-1.4176215427
 H,0,-1.1317230121,3.9092932359,-2.8538475088
 H,0,-1.3677794062,2.5266147704,-3.9838268127
 H,0,-2.7062354133,3.0405466176,-2.9277400158
 H,0,0.8075303529,2.7130115639,-1.6480172992

H,0,0.5543124085,0.9878766004,-1.2228406435
H,0,0.6454770676,1.4675168477,-2.9327494541

1-2 motion product side TS B3LYP/6-31G* Onsager solvent model for benzene

Dimethylamine TS 1

Eme2nhpdtside1-2tsA
E(RB+HF-LYP) = -1068.21354491

Zero-point correction=	0.331441 (Hartree/Particle)
Thermal correction to Energy=	0.352294
Thermal correction to Enthalpy=	0.353239
Thermal correction to Gibbs Free Energy=	0.279866
Sum of electronic and zero-point Energies=	-1067.882104
Sum of electronic and thermal Energies=	-1067.861251
Sum of electronic and thermal Enthalpies=	-1067.860306
Sum of electronic and thermal Free Energies=	-1067.933679

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	221.068	78.465	154.426

C,0,-2.3212884763,1.2258964417,-1.4115514048
C,0,-1.6412969336,0.7881817554,-0.2528387234
C,0,-1.6631666193,1.6342365344,0.8752270877
C,0,-2.3168821901,2.8640730549,0.844430067
C,0,-2.9716410819,3.2883307814,-0.3144993523
C,0,-2.9718252379,2.4553044472,-1.4391732564
C,0,-0.9171749919,-0.4799679083,-0.1948010114
N,0,-0.7615467836,-1.2185405493,-1.2581151247
C,0,-0.0636320343,-2.3867632431,-1.3968077356
C,0,-0.4423614036,-3.1344040924,-2.625132032
F,0,0.5718953057,-3.9091477634,-3.1078169339
C,0,0.6108162379,-3.1361836893,-0.3138118371
C,0,0.5113698382,-4.5399603279,-0.1879829808
C,0,1.1918940428,-5.2304215221,0.8125638773
C,0,1.9845010108,-4.5505881651,1.7392135698
C,0,2.0942318074,-3.1620610397,1.6384653425
C,0,1.425636842,-2.4717490115,0.6303914031
F,0,-1.5078664806,-3.9923284354,-2.5021364807
F,0,-0.7977958881,-2.2985445361,-3.6606317276
N,0,1.028784634,-0.1849627103,-3.0314895335
C,0,1.3662292902,-0.291466824,-4.4771473452
H,0,0.00428878,-0.1293521473,-2.8687998336
C,0,1.7122184115,0.9228029229,-2.3061341459

H,0,-2.3561740282,0.5662673979,-2.274668024
H,0,-3.4933554232,2.7659635231,-2.3419336777
H,0,-3.4790478358,4.2487514681,-0.3406177386
H,0,-2.3120323054,3.4972414182,1.7286460089
H,0,-1.1529924587,1.3158409765,1.7824687086
H,0,-0.5320324106,-0.7737179676,0.7863527046
H,0,1.184636424,-1.1024139683,-2.5341111114
H,0,-0.1130435216,-5.0942093919,-0.8795503157
H,0,1.0908836738,-6.3119278792,0.8737987481
H,0,2.5086270408,-5.0911962038,2.5228981053
H,0,2.7155392085,-2.6115303529,2.3413734273
H,0,1.5570985643,-1.3959565569,0.5575106639
H,0,1.5080162452,1.8650652441,-2.8184584113
H,0,1.3154926141,0.9566231674,-1.2912731966
H,0,2.786587023,0.7308199769,-2.2934764862
H,0,1.0687196343,0.6291162603,-4.9832778783
H,0,2.443344231,-0.438069835,-4.5788933248
H,0,0.8276922452,-1.1442342497,-4.8870590908

Dimethylamine TS 2

Eme2nhpdtside1-2tsB
E(RB+HF-LYP) = -1068.21057373

Zero-point correction=	0.331672 (Hartree/Particle)
Thermal correction to Energy=	0.352642
Thermal correction to Enthalpy=	0.353586
Thermal correction to Gibbs Free Energy=	0.279350
Sum of electronic and zero-point Energies=	-1067.878902
Sum of electronic and thermal Energies=	-1067.857932
Sum of electronic and thermal Enthalpies=	-1067.856988
Sum of electronic and thermal Free Energies=	-1067.931224

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	221.286	78.594	156.243

C,0,-1.7671162538,1.7721564565,0.6608683312
C,0,-2.0109778713,0.6642487549,-0.1883534022
C,0,-3.3546853218,0.4697715355,-0.5943198022
C,0,-4.3739254552,1.3200727234,-0.1770177194
C,0,-4.1069207394,2.4091061408,0.6566379211
C,0,-2.792142009,2.6225894413,1.0719314245
C,0,-0.9370837813,-0.2713183126,-0.5612108775
C,0,-1.3268044317,-1.6578483249,-0.9472059359
F,0,-0.2663944117,-2.5001441305,-1.0718181274

N,0,0.3980021951,-0.0450142549,-0.6561854504
 C,0,1.0963701243,1.0483726491,-0.5114212939
 C,0,2.5532654382,1.0175607967,-0.6128123296
 C,0,3.2649452483,-0.1612624732,-0.9310310032
 C,0,4.6547179898,-0.164695294,-0.9910756091
 C,0,5.3840701573,1.0035458624,-0.7392682177
 C,0,4.6950448325,2.1797996717,-0.4338971915
 C,0,3.3029921327,2.1871032418,-0.3717882136
 F,0,-2.1400641645,-2.2588374225,0.014560541
 F,0,-2.0388778107,-1.7886077751,-2.1050363412
 N,0,0.1574833755,-1.6102299358,1.855792366
 C,0,0.1556827717,-0.6804627542,3.0222242623
 H,0,-0.6546350952,-2.234406488,1.8967271932
 C,0,1.4092884955,-2.4045522519,1.680282657
 H,0,2.6957613743,-1.0598976544,-1.1505157815
 H,0,5.1782452558,-1.084459623,-1.2441318886
 H,0,6.4697950627,0.9961813119,-0.7845492097
 H,0,5.2459303829,3.0974165257,-0.2395186272
 H,0,2.7778694471,3.109585683,-0.129903593
 H,0,0.648646642,2.0332583196,-0.352185802
 H,0,-0.0149506038,-1.0503450183,0.9728531667
 H,0,-3.5999802805,-0.3560609186,-1.2510602092
 H,0,-5.390494318,1.1319382178,-0.5156122982
 H,0,-4.9046743816,3.0749254821,0.9742552733
 H,0,-2.5569270696,3.4578318476,1.7282299392
 H,0,-0.7642712357,1.9586129381,1.0263650006
 H,0,0.2582086675,-1.2512996867,3.9473444505
 H,0,0.994290109,0.0073927664,2.9061504699
 H,0,-0.7815698794,-0.1219744596,3.0143724091
 H,0,1.6037313533,-2.9834309945,2.5854720773
 H,0,1.2684734496,-3.0579698485,0.8202054829
 H,0,2.2267953506,-1.7110044514,1.4780948775

Dimethylamine TS 3

Eme2nhpdtside1-2tsC
 E(RB+HF-LYP) = -1068.21347742

Zero-point correction=	0.331924 (Hartree/Particle)
Thermal correction to Energy=	0.352910
Thermal correction to Enthalpy=	0.353854
Thermal correction to Gibbs Free Energy=	0.279729
Sum of electronic and zero-point Energies=	-1067.881553
Sum of electronic and thermal Energies=	-1067.860567
Sum of electronic and thermal Enthalpies=	-1067.859623
Sum of electronic and thermal Free Energies=	-1067.933748

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	221.454	78.654	156.009

C,0,3.2171273261,1.9313666197,0.1586011384
C,0,2.474662759,0.797379257,-0.2372371824
C,0,3.1758208561,-0.424812737,-0.3764101141
C,0,4.5397522732,-0.502386201,-0.1125526927
C,0,5.2569904595,0.6298162084,0.2923010902
C,0,4.5831975942,1.8474616411,0.4194346789
C,0,1.0375427508,0.9013154203,-0.4656109934
N,0,0.3173974215,-0.1794473555,-0.6518441641
C,0,-1.0180484577,-0.3404460652,-0.7381952996
C,0,-1.4339417964,-1.7671658772,-0.7671370515
F,0,-2.562140546,-2.0081499957,-1.4704615186
C,0,-2.0565936014,0.7030891606,-0.7490575788
C,0,-1.8291520169,1.9629813526,-1.3464088514
C,0,-2.8020201802,2.9611286627,-1.3300800576
C,0,-4.0400604553,2.7407411243,-0.7241543627
C,0,-4.2928845936,1.4957207397,-0.1411328084
C,0,-3.3221170244,0.4982722206,-0.1480457304
F,0,-0.4851111278,-2.6100099479,-1.2131353012
F,0,-1.7441572354,-2.2734057474,0.5349918466
N,0,0.0982089839,-0.6519703492,2.1470805035
C,0,0.9191499315,-1.8841520593,2.3441680355
H,0,0.7079245469,0.1726849583,2.1556916308
C,0,-1.045397289,-0.4952996111,3.0894349174
H,0,2.6243226066,-1.2953447313,-0.720715433
H,0,0.50547574328,-1.4532880047,-0.2336037951
H,0,0.6322001159,0.5644969208,0.4972432485
H,0,0.5125863556,2.7387551615,0.7264869755
H,0,0.27055427498,2.8869258077,0.2623375861
H,0,0.6094432409,1.9081114175,-0.4238943601
H,0,-0.2679169758,-0.6695726718,1.1653837828
H,0,-3.5424419812,-0.4578564775,0.3167046014
H,0,-5.253269778,1.3015013588,0.3312120156
H,0,-4.7953986816,3.5217946136,-0.7082161084
H,0,-2.591779252,3.9167725032,-1.8054053553
H,0,-0.8921744631,2.1444562283,-1.8612713579
H,0,0.1284641689,-1.9156361189,3.372205706
H,0,0.2813933111,-2.74190951,2.1292738473
H,0,0.17504092981,-1.8462132429,1.6390456584
H,0,-0.6718789538,-0.4415703684,4.1135332192
H,0,-1.587031867,0.4150861606,2.8278261784
H,0,-1.7001156692,-1.3572514653,2.9613854563

Chapter 4 – Dynamic Effects in the Roush Allylboration of Aldehydes
Exploratory calculations B3LYP/6-31G*

TS for reaction of 38 and formaldehyde

hchoTSG*

E(RB+HF-LYP) = -485.813681946

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	114.255	36.287	94.162
Zero-point correction=		0.172617	(Hartree/Particle)
Thermal correction to Energy=		0.182077	
Thermal correction to Enthalpy=		0.183021	
Thermal correction to Gibbs Free Energy=		0.138282	
Sum of electronic and zero-point Energies=		-485.641065	
Sum of electronic and thermal Energies=		-485.631605	
Sum of electronic and thermal Enthalpies=		-485.630661	
Sum of electronic and thermal Free Energies=		-485.675400	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	114.255	36.287	94.162

C,0,-0.4820279424,2.722126265,-0.1046951043
 B,0,-0.1161768708,1.1036314714,-0.3552145136
 O,0,-1.0715011878,0.3786288202,-1.1389840787
 C,0,-1.3021423594,-0.8663855678,-0.4838693256
 C,0,-0.1719894982,-0.9737376714,0.5613800231
 O,0,0.213884784,0.3738287858,0.8068718434
 C,0,-0.7200375762,3.3369708159,-1.4086168814
 C,0,0.2416823616,3.9077499273,-2.185712462
 O,0,1.2346747756,1.3002505549,-1.2682869442
 C,0,1.0577429183,1.6697104744,-2.4556571963
 H,0,1.9071518513,2.0809028908,-3.0059103298
 H,0,-0.4951318552,-1.4429989205,1.49773498
 H,0,-2.2930287381,-0.8523867072,-0.0060993484
 H,0,0.6801940403,-1.5481055648,0.1652288999
 H,0,0.3375540469,3.1876043528,0.4504476473
 H,0,-1.3826824887,2.6981755501,0.5173890796
 H,0,-1.6971461395,3.1588748455,-1.8593019995
 H,0,0.0180109038,4.2789104214,-3.1826903122
 H,0,1.2027632375,4.1938529698,-1.7650309836
 H,0,0.1742924946,1.3466949426,-3.0090748655
 H,0,-1.2866187576,-1.6880376562,-1.2108721281

TS for reaction of 38 and acetaldehyde

allTSG*

E(RB+HF-LYP) = -525.138013744

Zero-point correction=	0.201122 (Hartree/Particle)
Thermal correction to Energy=	0.211896
Thermal correction to Enthalpy=	0.212840
Thermal correction to Gibbs Free Energy=	0.165153
Sum of electronic and zero-point Energies=	-524.936892
Sum of electronic and thermal Energies=	-524.926118
Sum of electronic and thermal Enthalpies=	-524.925174
Sum of electronic and thermal Free Energies=	-524.972861

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	132.967	41.361	100.366

C,0,-0.5131368045,2.7228150571,-0.0797766231
C,0,-0.1193416769,1.3622442952,-0.3586856322
C,0,-0.8789757224,0.4760187788,-1.0783660366
B,0,-0.0734137012,3.6088558288,-1.4865411818
O,0,-0.4242342461,4.9814026623,-1.3965713534
C,0,0.6028694551,5.706826364,-2.0593757363
H,0,0.7361566457,6.6842638125,-1.5807530371
O,0,-0.9441996888,2.8829137329,-2.5570849998
C,0,-0.5844503996,1.720964255,-2.9476523176
C,0,-1.4982037166,0.9742049173,-3.8766982312
O,0,1.3216553404,3.4858371128,-1.8248400671
C,0,1.8466756689,4.8028737146,-1.945910007
H,0,2.4419275383,5.0521498043,-1.0537233204
H,0,0.3344270542,5.8749810977,-3.1148928349
H,0,-1.5857635029,2.864152446,0.0750445508
H,0,0.0629543948,3.1996173621,0.7167526373
H,0,0.9291405575,1.1121538333,-0.1936580864
H,0,-0.4988045442,-0.5118002348,-1.3259557869
H,0,-1.9559009725,0.6067222316,-1.1473670514
H,0,0.4858800035,1.5093756342,-2.9908247403
H,0,-1.2699159501,-0.094104551,-3.8993539027
H,0,-2.5450328954,1.1300273664,-3.6049249538
H,0,-1.3499729264,1.3725917442,-4.8907162751
H,0,2.5038880891,4.8711877346,-2.822172013

TS for reaction of 38 and acetaldehyde (mPW1K/6-31G*)

allTSMPW1KB3G

E(RmPW+HF-PW91) = -524.981188775

Zero-point correction= 0.207684 (Hartree/Particle)
 Thermal correction to Energy= 0.218141
 Thermal correction to Enthalpy= 0.219086
 Thermal correction to Gibbs Free Energy= 0.172042
 Sum of electronic and zero-point Energies= -524.773504
 Sum of electronic and thermal Energies= -524.763047
 Sum of electronic and thermal Enthalpies= -524.762103
 Sum of electronic and thermal Free Energies= -524.809147

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	136.886	39.992	99.012

C,0,-0.511611233,2.7179105655,-0.0848376723
 C,0,-0.1250013789,1.3630999079,-0.3887265462
 C,0,-0.8936842637,0.4913216017,-1.0879802057
 B,0,-0.0779169922,3.604958875,-1.4427644349
 O,0,-0.404415821,4.9731001086,-1.3589872164
 C,0,0.5835890007,5.6584034773,-2.0782158817
 H,0,0.7322974519,6.6507767896,-1.6542005345
 O,0,-0.9472456807,2.9065573522,-2.5301949194
 C,0,-0.5684274239,1.7745398981,-2.9260666082
 C,0,-1.453383442,1.0146557544,-3.8516343812
 O,0,1.3012228859,3.4722063967,-1.8037147418
 C,0,1.8176168576,4.7672639645,-1.9656359894
 H,0,2.4219466543,5.0377003033,-1.0952142101
 H,0,0.2835376423,5.7765693868,-3.1245411561
 H,0,-1.5774534421,2.8474715998,0.0832639647
 H,0,0.0623268594,3.160987922,0.7246908049
 H,0,0.9166347512,1.1067329316,-0.2334729143
 H,0,-0.5244931721,-0.4898621452,-1.3509347687
 H,0,-1.9613368637,0.6440103662,-1.1650361667
 H,0,0.4981369645,1.5726936735,-2.9420080609
 H,0,-1.2079387345,-0.0425288283,-3.8724728993
 H,0,-2.4979649515,1.1558438088,-3.5918747256
 H,0,-1.2987755219,1.4164103881,-4.8555577168
 H,0,2.4565658537,4.8154509019,-2.8479290194

TS for reaction of 38 and pivalaldehyde

tbutTSG*

E(RB+HF-LYP) = -643.077891996

Zero-point correction= 0.285854 (Hartree/Particle)
 Thermal correction to Energy= 0.300752
 Thermal correction to Enthalpy= 0.301696

Thermal correction to Gibbs Free Energy=	0.244761
Sum of electronic and zero-point Energies=	-642.792038
Sum of electronic and thermal Energies=	-642.777140
Sum of electronic and thermal Enthalpies=	-642.776196
Sum of electronic and thermal Free Energies=	-642.833131

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	188.724	57.570	119.830

C,0,-0.4481973463,2.7633586441,-0.0176827791
 B,0,-0.072693516,3.5952374621,-1.483896754
 O,0,1.3130898579,3.4741634017,-1.8630991372
 C,0,1.8287453757,4.7915198061,-2.0099534376
 C,0,0.5781141428,5.6855325242,-2.119205704
 O,0,-0.4312084703,4.9697688537,-1.420431382
 C,0,-0.0476156576,1.4042958587,-0.2716105177
 C,0,-0.8202612227,0.4855367547,-0.9395570091
 O,0,-0.9700745392,2.834773016,-2.4839925396
 C,0,-0.6345452287,1.6574545824,-2.8648280913
 C,0,-1.5442155741,0.9499155033,-3.8631327532
 H,0,0.7149307048,6.6745404278,-1.6657896148
 H,0,2.433815988,5.0588388172,-1.1294038563
 H,0,0.2891302005,5.8278981742,-3.1732820187
 H,0,-1.5158698484,2.9029209511,0.1678129136
 H,0,0.154912609,3.2796276967,0.7323358317
 H,0,1.0098151782,1.1731293759,-0.1386710159
 H,0,-0.4295909149,-0.5044595918,-1.1548365866
 H,0,-1.9017940684,0.5874663389,-0.9475303801
 H,0,0.4345216137,1.4405548379,-2.9378464435
 C,0,-1.2112192469,-0.5474438112,-3.9716013123
 C,0,-3.0323501783,1.1690265612,-3.5490190229
 C,0,-1.2024446076,1.6345921595,-5.2190325597
 H,0,0.24738396857,4.8506693412,-2.8958476307
 H,0,-1.7915046905,1.1741188522,-6.0203489161
 H,0,-1.4324870415,2.7035146507,-5.1855426692
 H,0,-0.1420031744,1.5191218961,-5.4722204566
 H,0,-3.6481299785,0.7740854648,-4.3647880849
 H,0,-3.3297285783,0.6529174587,-2.6299252724
 H,0,-3.2559596052,2.2324452755,-3.4294816702
 H,0,-1.7174950643,-0.9796589658,-4.8418180504
 H,0,-0.13416833,-0.711303476,-4.1000924638
 H,0,-1.5384174743,-1.1028898417,-3.0878996157

TS for reaction of 38 and benzaldehyde

PhCHOTShpG*

E(RB+HF-LYP) = -716.879396314

Zero-point correction=	0.254330 (Hartree/Particle)
Thermal correction to Energy=	0.268164
Thermal correction to Enthalpy=	0.269108
Thermal correction to Gibbs Free Energy=	0.213144
Sum of electronic and zero-point Energies=	-716.625066
Sum of electronic and thermal Energies=	-716.611232
Sum of electronic and thermal Enthalpies=	-716.610288
Sum of electronic and thermal Free Energies=	-716.666253

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	168.276	54.513	117.788

C,0,-0.4509319704,2.6818783365,0.0049541696
 B,0,-0.0080783036,1.0419698201,-0.4428167024
 O,0,-1.0340136182,0.3926194633,-1.2168414287
 C,0,-1.4188468179,-0.7793794893,-0.5087559647
 C,0,-0.2682391757,-1.0231977839,0.487211928
 O,0,0.287477626,0.2664760467,0.7100657148
 C,0,-0.6996048536,3.312007901,-1.2570987443
 C,0,0.2976272343,3.8037631432,-2.0724600161
 O,0,1.2357466978,1.3034862692,-1.2847071672
 C,0,1.0995798355,1.7876725596,-2.4739348581
 C,0,2.3103318874,2.1589190939,-3.2297332395
 H,0,-0.6056069094,-1.4527645477,1.4379648944
 H,0,-2.3710146897,-0.6061059833,0.0169244933
 H,0,0.4892722391,-1.6959700256,0.0544203346
 H,0,0.388664778,3.0834608663,0.5760304428
 H,0,-1.3326126253,2.5327507901,0.6306076646
 H,0,-1.6842001753,3.1569752829,-1.6991197608
 H,0,0.0642537737,4.2041408118,-3.0552406436
 H,0,1.2411071706,4.1283606982,-1.6430488823
 H,0,0.2258063939,1.47409586,-3.0473731164
 H,0,-1.5625991316,-1.6135646128,-1.2068671839
 C,0,2.2238929204,2.3628996289,-4.615204465
 C,0,3.3612683525,2.6900226894,-5.350100601
 C,0,4.5949545129,2.8163215059,-4.706762723
 C,0,4.6877112434,2.6092151763,-3.3269165211
 C,0,3.5536749094,2.2807733656,-2.5892269007
 H,0,1.2626704859,2.2604692134,-5.1138861328
 H,0,3.2871046529,2.8430497248,-6.4231323404
 H,0,5.4826759969,3.0708972183,-5.279285216
 H,0,5.64843002,2.6995456826,-2.8274929603
 H,0,3.6145805399,2.1040442945,-1.5202110737

TS for reaction of 38 and 44a

PNBTShpG*

E(RB+HF-LYP) = -921.378685827

Zero-point correction=	0.256811 (Hartree/Particle)
Thermal correction to Energy=	0.273217
Thermal correction to Enthalpy=	0.274162
Thermal correction to Gibbs Free Energy=	0.211581
Sum of electronic and zero-point Energies=	-921.121874
Sum of electronic and thermal Energies=	-921.105468
Sum of electronic and thermal Enthalpies=	-921.104524
Sum of electronic and thermal Free Energies=	-921.167105

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	171.446	63.167	131.711

C,0,3.5579551436,2.2453868078,-2.5797905045
C,0,2.3124003855,2.1368494653,-3.2216152741
C,0,2.2206938459,2.3641099636,-4.604719194
C,0,3.3487230771,2.7057082171,-5.3409785397
C,0,4.5697652426,2.8149598493,-4.6765841762
C,0,4.6922061663,2.5872693433,-3.305409478
C,0,1.1072629672,1.7445117115,-2.468632363
O,0,1.2411016781,1.2819504472,-1.2797911324
B,0,-0.0238100069,1.0381165691,-0.4268257578
O,0,0.2681420416,0.2638498474,0.7221894695
C,0,-0.28841947,-1.0272058581,0.4988351224
C,0,-1.4252465883,-0.7877328568,-0.5150182479
O,0,-1.0409749115,0.3944656841,-1.210659695
C,0,-0.4332713213,2.6798488363,-0.0054100614
C,0,-0.6845861587,3.318501879,-1.2673965013
C,0,0.3024209178,3.8375260291,-2.0719213608
H,0,-0.6404362421,-1.4482624957,1.4475763473
H,0,-2.3878843191,-0.6256547799,-0.0066337405
H,0,0.4747934827,-1.7039159289,0.0835923079
H,0,0.4071489228,3.0842033197,0.5629090604
H,0,-1.3158658721,2.5481781794,0.6236920898
H,0,-1.6700901285,3.1667733121,-1.7083229006
H,0,0.0692265039,4.2413162812,-3.0533302434
H,0,1.2537809304,4.1421933113,-1.6451819184
H,0,0.2226197929,1.4525552949,-3.0361738675
H,0,-1.5483213888,-1.6179585801,-1.2211545549
H,0,1.2600020624,2.2704640708,-5.1041616717
H,0,3.3025203037,2.8846491414,-6.4079010579

N,0,5.76933361,3.1777213594,-5.449108861
 H,0,5.6635585816,2.6762342877,-2.8348975564
 H,0,3.6225052453,2.0486747586,-1.5150930215
 O,0,6.8346817559,3.264969688,-4.839951169
 O,0,5.6321107501,3.3727938448,-6.6564365483

TS for reaction of 38 and 44a (MP2/6-31G*)

pnitrobenzaldehyde-MP2-TS

E(RHF) = -915.916550392

Zero-point correction=	0.259217 (Hartree/Particle)
Thermal correction to Energy=	0.275778
Thermal correction to Enthalpy=	0.276722
Thermal correction to Gibbs Free Energy=	0.213490
Sum of electronic and zero-point Energies=	-918.362749
Sum of electronic and thermal Energies=	-918.346187
Sum of electronic and thermal Enthalpies=	-918.345243
Sum of electronic and thermal Free Energies=	-918.408475

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	173.053	63.628	133.084

C,0,3.5296831191,2.2588870825,-2.536793283
 C,0,2.2883600054,2.1121214644,-3.1768161894
 C,0,2.1889462039,2.3006877368,-4.5636334655
 C,0,3.3097390842,2.6465921857,-5.3118782805
 C,0,4.5260498003,2.7938266527,-4.6466555499
 C,0,4.6587044126,2.6050714326,-3.2703563009
 C,0,1.0953720462,1.7221945652,-2.4108859683
 O,0,1.2504741397,1.286880005,-1.2162500938
 B,0,-0.0717553641,1.0965186475,-0.3732548882
 O,0,0.1882211074,0.291531821,0.7675969246
 C,0,-0.2392781075,-1.020353047,0.3893441076
 C,0,-1.4062810765,-0.7648621098,-0.5638802318
 O,0,-1.071907475,0.4725454657,-1.2044905074
 C,0,-0.4059650148,2.7160778756,-0.0049560929
 C,0,-0.649753515,3.3244655527,-1.2887032645
 C,0,0.3517854273,3.8215571298,-2.0827471892
 H,0,-0.5197966551,-1.5838476214,1.2843934298
 H,0,-2.3491488796,-0.6499255175,-0.0131973818
 H,0,0.5750197751,-1.5520344731,-0.1233899049
 H,0,0.4379753291,3.133518848,0.547662226
 H,0,-1.2918214523,2.6369607378,0.6291240568
 H,0,-1.6285907411,3.1588822335,-1.7399721477
 H,0,0.1459034082,4.1987933417,-3.0806252628

H,0,1.3047973723,4.1085488725,-1.6473245727
H,0,0.2004097613,1.4135409036,-2.9583119444
H,0,-1.5320096848,-1.5518746383,-1.3150901914
H,0,1.2275108098,2.1768028011,-5.0591354702
H,0,3.2586879346,2.7961389577,-6.3846933179
N,0,5.7157598206,3.1601263588,-5.4273545511
H,0,5.6292744005,2.7236370023,-2.8012069165
H,0,3.5949755931,2.0916745448,-1.4650008177
O,0,6.7895409066,3.2863133702,-4.8144052387
O,0,5.5731665085,3.3220508179,-6.6514197216

TS for reaction of 38 and *p*-aminobenzaldehyde

PNH2BTSG*

E(RB+HF-LYP) = -772.235576541

Zero-point correction=	0.271087 (Hartree/Particle)
Thermal correction to Energy=	0.286334
Thermal correction to Enthalpy=	0.287278
Thermal correction to Gibbs Free Energy=	0.228457
Sum of electronic and zero-point Energies=	-771.964489
Sum of electronic and thermal Energies=	-771.949242
Sum of electronic and thermal Enthalpies=	-771.948298
Sum of electronic and thermal Free Energies=	-772.007120

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.677	60.402	123.800

C,0,3.5645936651,2.2745413891,-2.575342111
C,0,2.3200432296,2.1565854124,-3.2174004444
C,0,2.2634712775,2.3583022508,-4.6056237007
C,0,3.4040054552,2.6667943324,-5.3331726699
C,0,4.6498794745,2.7870269267,-4.6878897319
C,0,4.7087669531,2.5836567302,-3.2942555219
C,0,1.1026954931,1.8093703866,-2.4731439689
O,0,1.2315999333,1.3133440711,-1.2777593011
B,0,-0.0010573597,1.0354171835,-0.4565184493
O,0,0.2877890687,0.2765067386,0.7122988789
C,0,-0.2858542758,-1.0089633992,0.5190255907
C,0,-1.4285663582,-0.7737364059,-0.4879275618
O,0,-1.0204917515,0.3688692814,-1.2271005534
C,0,-0.4903579637,2.6791382537,-0.0009182536
C,0,-0.7208303563,3.2954496835,-1.2678091014
C,0,0.294869282,3.7676686513,-2.0786805617
H,0,-0.6340018309,-1.4107177743,1.4783798543
H,0,-2.3793894178,-0.5705466452,0.0305453589

H,0,0.4631154203,-1.7039797793,0.1063586596
H,0,0.3396602032,3.0815505212,0.5829128021
H,0,-1.3785305876,2.5103451458,0.6094544571
H,0,-1.6978041581,3.1335039737,-1.724265808
H,0,0.0719907856,4.1679117142,-3.0641021798
H,0,1.2231502393,4.1135207956,-1.6328828215
H,0,0.2424894328,1.4766048849,-3.0564915013
H,0,-1.585033638,-1.6252334776,-1.1622900798
H,0,1.3109123221,2.263910648,-5.1225975641
H,0,3.3406123558,2.8164521701,-6.4084522271
N,0,5.786234457,3.1476986462,-5.3996739836
H,0,5.6648985154,2.6687395971,-2.7827525961
H,0,3.621022616,2.1039148837,-1.504968216
H,0,6.6721701543,2.9046042614,-4.9759738978
H,0,5.7678283639,2.9598379483,-6.3935607953

TS for reaction of 38 and 44b

panisaldehydeTShp

E(RB+HF-LYP) = -831.403758153

Zero-point correction=	0.287244 (Hartree/Particle)
Thermal correction to Energy=	0.303645
Thermal correction to Enthalpy=	0.304589
Thermal correction to Gibbs Free Energy=	0.242741
Sum of electronic and zero-point Energies=	-831.116515
Sum of electronic and thermal Energies=	-831.100113
Sum of electronic and thermal Enthalpies=	-831.099169
Sum of electronic and thermal Free Energies=	-831.161017

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	190.540	63.578	130.170

C,0,3.4810573973,2.2535144579,-2.5090612249
C,0,2.2632981155,2.130290683,-3.1738699123
C,0,2.1718973063,2.3343609048,-4.5568866869
C,0,3.3395524969,2.6639430452,-5.268772175
C,0,4.5566154844,2.7899934107,-4.6195960116
C,0,4.6366414172,2.5873493697,-3.23125129
C,0,0.8943969605,2.1868966265,-5.270476996
O,0,-0.0917675697,1.6062440564,-4.6601296665
B,0,-1.4434875473,1.5397653931,-5.3385738719
C,0,-1.9888729025,3.2134976334,-5.1705796733
C,0,-0.9858390657,3.946951875,-5.8765123777
C,0,0.2465575203,4.2613118701,-5.3377740892
O,0,5.8740251874,2.7333832168,-2.6867931396

O,0,-2.3392594179,0.6638074962,-4.6667141144
 C,0,-2.5205236857,-0.4654518059,-5.5106876002
 C,0,-2.2112703679,0.0570334396,-6.9278565457
 O,0,-1.3241460404,1.147791963,-6.719415516
 H,0,-3.5433048923,-0.8475913851,-5.4076658567
 H,0,-3.1265377236,0.404674381,-7.4329859423
 H,0,-1.8229373945,-1.2701399319,-5.2280772157
 H,0,-2.0494457168,3.4023645309,-4.0969529137
 H,0,-2.9740171797,3.1966121914,-5.6390454064
 H,0,-1.0973097566,4.0184949891,-6.9588594399
 H,0,1.001371409,4.7606521529,-5.9392070889
 H,0,0.3537712659,4.3734540882,-4.2626594645
 H,0,0.9393650317,2.0806037094,-6.3555573105
 H,0,-1.7378425202,-0.6991093434,-7.5667847961
 H,0,3.2875608909,2.8187733083,-6.3441292406
 H,0,5.463958834,3.0397833092,-5.1600417568
 H,0,3.5226564298,2.0834048805,-1.4394128598
 H,0,1.3685527363,1.8598293842,-2.6223278285
 C,0,6.0272770768,2.5388393365,-1.287351226
 H,0,7.0856443852,2.7029957641,-1.0787151836
 H,0,5.4278098407,3.2574476054,-0.7139393597
 H,0,5.7521709948,1.5185903938,-0.9909602189

TS for reaction of 38 and 44b (MP2/6-31G*)

anisaldehyde-mp2-freq-B3G

E(RHF) = -826.336719782

Zero-point correction=	0.290432	(Hartree/Particle)
Thermal correction to Energy=	0.306886	
Thermal correction to Enthalpy=	0.307831	
Thermal correction to Gibbs Free Energy=	0.245958	
Sum of electronic and zero-point Energies=	-828.512042	
Sum of electronic and thermal Energies=	-828.495588	
Sum of electronic and thermal Enthalpies=	-828.494644	
Sum of electronic and thermal Free Energies=	-828.556517	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	192.574	63.875	130.222

1	6	0	-2.961689	-0.697574	-0.744112
2	6	0	-1.576657	-0.546658	-0.696338
3	6	0	-0.971584	0.158581	0.349553
4	6	0	-1.773690	0.715427	1.359062
5	6	0	-3.152511	0.570542	1.318794
6	6	0	-3.754978	-0.134370	0.265442

7	6	0	0.487523	0.305292	0.414961
8	8	0	1.214069	-0.441462	-0.344466
9	5	0	2.734457	-0.128833	-0.363539
10	6	0	2.748544	1.285390	-1.317123
11	6	0	1.986280	2.215745	-0.530910
12	6	0	0.612258	2.257867	-0.553562
13	8	0	-5.117496	-0.214179	0.325708
14	8	0	3.461451	-1.201578	-0.957555
15	6	0	3.973215	-1.946702	0.149130
16	6	0	4.221644	-0.886138	1.220876
17	8	0	3.205730	0.093324	0.986385
18	1	0	4.878554	-2.480352	-0.157330
19	1	0	5.213006	-0.428507	1.099435
20	1	0	3.229281	-2.680092	0.492866
21	1	0	2.321629	1.042557	-2.291884
22	1	0	3.812799	1.516057	-1.392274
23	1	0	2.500384	2.707699	0.295594
24	1	0	0.059878	2.915501	0.111630
25	1	0	0.070678	1.892801	-1.421386
26	1	0	0.927531	0.646289	1.356477
27	1	0	4.138258	-1.274744	2.241878
28	1	0	-1.311495	1.260058	2.181311
29	1	0	-3.791538	0.988522	2.091727
30	1	0	-3.403908	-1.254565	-1.563146
31	1	0	-0.950217	-0.989254	-1.466828
32	6	0	-5.772127	-0.929218	-0.721388
33	1	0	-6.834236	-0.873765	-0.486737
34	1	0	-5.585741	-0.465117	-1.695540
35	1	0	-5.454546	-1.976877	-0.744978

TS for reaction of 39 and acetaldehyde

ZcroteqTShpG*

E(RB+HF-LYP) = -564.452353059

Zero-point correction=	0.229809 (Hartree/Particle)
Thermal correction to Energy=	0.241962
Thermal correction to Enthalpy=	0.242906
Thermal correction to Gibbs Free Energy=	0.192083
Sum of electronic and zero-point Energies=	-564.222544
Sum of electronic and thermal Energies=	-564.210391
Sum of electronic and thermal Enthalpies=	-564.209447
Sum of electronic and thermal Free Energies=	-564.260270

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	151.834	46.451	106.966

C,0,-0.4352535495,2.7294491753,-0.1057853954
 B,0,-0.053186278,3.6142868634,-1.5515700951
 O,0,1.3468933439,3.5276079427,-1.8863875903
 C,0,1.8496790784,4.8562457632,-1.946143082
 C,0,0.5924358232,5.7397102705,-2.0661043435
 O,0,-0.4356374507,4.9785531685,-1.4462065258
 C,0,-0.1391036186,1.360308842,-0.4302552949
 C,0,-0.9952155378,0.4968570688,-1.0854679806
 O,0,-0.8995790316,2.8706406257,-2.603776772
 C,0,-0.5278810545,1.6838218841,-2.9329091478
 C,0,-1.3672028784,0.947131162,-3.9371102228
 H,0,0.6962029247,6.7071561695,-1.5603645539
 H,0,2.4131139962,5.088083787,-1.0284231276
 H,0,0.3452617758,5.9289977408,-3.1231804092
 H,0,-1.4758624871,2.9422373551,0.1452687532
 H,0,0.2429872871,3.1687822434,0.6285160641
 H,0,0.9090969494,1.0653028791,-0.3730434948
 H,0,-0.6016962661,-0.4863608767,-1.3422769376
 C,0,-2.5015520347,0.6136624782,-1.0281982569
 H,0,0.5432748753,1.4738023388,-2.9246066102
 H,0,-1.1445284924,-0.1229641126,-3.9465993583
 H,0,-2.4326956693,1.1078255785,-3.7590149936
 H,0,-1.1293912161,1.3504391921,-4.9316036864
 H,0,2.5311384504,4.9661926399,-2.7993496543
 H,0,-2.9814706541,-0.0722504943,-1.7331232503
 H,0,-2.8688559094,0.3571980746,-0.0258110876
 H,0,-2.8417753762,1.6292452403,-1.2539109463

TS for reaction of 39 and pivalaldehyde

ZbutTShpG*

E(RB+HF-LYP) = -682.387714847

Zero-point correction=	0.314947 (Hartree/Particle)
Thermal correction to Energy=	0.331107
Thermal correction to Enthalpy=	0.332051
Thermal correction to Gibbs Free Energy=	0.272483
Sum of electronic and zero-point Energies=	-682.072768
Sum of electronic and thermal Energies=	-682.056608
Sum of electronic and thermal Enthalpies=	-682.055664
Sum of electronic and thermal Free Energies=	-682.115232

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	207.773	62.481	125.371

C,0,-0.2390429473,2.7035925106,-0.0126440498
 C,0,0.0172459189,1.3441051583,-0.3793054664
 C,0,-0.9315224004,0.4815285879,-0.9047064554
 B,0,-0.0968352171,3.5773420197,-1.5283780861
 O,0,-1.0360889498,2.8090056388,-2.4508209338
 C,0,-0.6874055054,1.6178737955,-2.8137068111
 C,0,-1.5080382848,0.9441554286,-3.9151417683
 C,0,-0.9047161119,1.5441026131,-5.2196037781
 O,0,1.2550765831,3.5365210899,-2.0315641777
 C,0,1.7124588463,4.8793549077,-2.117315467
 C,0,0.4258422941,5.726730793,-2.0868031508
 O,0,-0.5056264384,4.9304588476,-1.3670435419
 C,0,-1.2944586281,-0.5785106311,-3.937072607
 C,0,-3.0028181637,1.2987963084,-3.8624037945
 H,0,0.5578976171,6.6924626309,-1.5842391539
 H,0,2.3630437212,5.1140961735,-1.259626285
 H,0,0.0582379409,5.9179764599,-3.1080489584
 H,0,-1.2335150459,2.9141083813,0.3837083468
 H,0,0.5409905086,3.1681066468,0.5927179398
 H,0,1.0638629352,1.0566297006,-0.4846817892
 H,0,-0.5841599635,-0.508799819,-1.1919993701
 C,0,-2.4009848242,0.6031350599,-0.5602588297
 H,0,0.3849835479,1.4195591976,-2.8782066054
 H,0,2.2966270244,5.0227818826,-3.0352560115
 H,0,-1.4161169372,1.1138583777,-6.0884352409
 H,0,-1.0305218385,2.630791207,-5.2449027283
 H,0,0.1644342512,1.3207148558,-5.3116924484
 H,0,-3.4947725404,0.9492772015,-4.7772517331
 H,0,-3.5066696378,0.829000353,-3.0149379021
 H,0,-3.1456116241,2.3801242717,-3.7865327801
 H,0,-1.7049432259,-0.9996191917,-4.8616920085
 H,0,-0.2284948211,-0.8351582805,-3.9017081591
 H,0,-1.7929787411,-1.0727949282,-3.0978856379
 H,0,-2.9952922528,-0.1616535787,-1.0681433631
 H,0,-2.552263906,0.4690494505,0.5192162958
 H,0,-2.8065581835,1.5836198797,-0.8271114896

TS for reaction of 40 and acetaldehyde

EcrotTShpG*

E(RB+HF-LYP) = -564.454743549

Zero-point correction=	0.229247 (Hartree/Particle)
Thermal correction to Energy=	0.241609
Thermal correction to Enthalpy=	0.242553
Thermal correction to Gibbs Free Energy=	0.191159
Sum of electronic and zero-point Energies=	-564.225496

Sum of electronic and thermal Energies= -564.213134
 Sum of electronic and thermal Enthalpies= -564.212190
 Sum of electronic and thermal Free Energies= -564.263584

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	151.612	46.808	108.168

C,0,-0.487515692,2.7345325277,-0.1010284696
 B,0,-0.0772826192,3.6230023909,-1.5395684299
 O,0,1.3159975551,3.5087315531,-1.8889166762
 C,0,1.8447343531,4.8270351442,-1.9607746682
 C,0,0.6037165829,5.7363927353,-2.0577875306
 O,0,-0.4303288889,4.9946474554,-1.425235202
 C,0,-0.0788864019,1.3890897427,-0.3888704691
 C,0,-0.8224754398,0.4694328801,-1.1010951867
 O,0,-0.9598963224,2.8932559987,-2.5561094282
 C,0,-0.6221242047,1.7131036978,-2.9404765736
 C,0,-1.5829606174,1.0049157865,-3.853439505
 H,0,0.7353424888,6.6995425456,-1.5503204518
 H,0,2.4312228857,5.0475676031,-1.0549188248
 H,0,0.344347112,5.9352019605,-3.1102384711
 H,0,-1.5577338607,2.8747093539,0.0656173824
 H,0,0.104226063,3.2282115684,0.6724844306
 H,0,0.9767669804,1.1568536887,-0.2358629913
 C,0,-0.3240233951,-0.9307028967,-1.3661389249
 H,0,-1.903211835,0.6088131532,-1.1272929361
 H,0,0.4444898639,1.5046287847,-3.049172668
 H,0,-1.3896688061,-0.0686452224,-3.9085768167
 H,0,-2.6157095227,1.1861781506,-3.5445124207
 H,0,-1.4567746669,1.41641184,-4.8647264075
 H,0,2.5111435735,4.9219744799,-2.8275442922
 H,0,-0.6537754169,-1.3168407183,-2.3377223056
 H,0,0.7705043514,-0.976084997,-1.339234012
 H,0,-0.7036651202,-1.6301092063,-0.609194151

TS for reaction of 40 and pivalaldehyde

EtbutTShpG*

E(RB+HF-LYP) = -682.388846756

Zero-point correction= 0.313893 (Hartree/Particle)
 Thermal correction to Energy= 0.330264
 Thermal correction to Enthalpy= 0.331208
 Thermal correction to Gibbs Free Energy= 0.270666
 Sum of electronic and zero-point Energies= -682.074954
 Sum of electronic and thermal Energies= -682.058583

Sum of electronic and thermal Enthalpies= -682.057639
 Sum of electronic and thermal Free Energies= -682.118180

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	207.244	62.829	127.421

C,0,-0.6412403154,2.8070983997,-0.0951452066
 C,0,-0.1374115126,1.4812892113,-0.2551807729
 C,0,-0.73274039,0.4633039891,-0.9822609752
 B,0,-0.0953282121,3.5911898951,-1.5705889909
 O,0,-0.9160574314,2.8083619828,-2.5709701971
 C,0,-0.622265252,1.593396291,-2.8947408406
 C,0,-1.585822735,0.9530053746,-3.9004130975
 C,0,-1.2619132492,1.6749339339,-5.2404163284
 O,0,1.3174991138,3.4445634351,-1.8013445862
 C,0,1.8742631758,4.750668571,-1.8753443439
 C,0,0.6636339077,5.6732057917,-2.1205844196
 O,0,-0.4383966669,4.9714225895,-1.5616250433
 C,0,-1.3480328515,-0.5523678296,-4.0926060347
 C,0,-3.0543855365,1.2221696512,-3.5297406314
 H,0,0.7653593526,6.6527416468,-1.6381079167
 H,0,2.3806229984,5.000022038,-0.9294121936
 H,0,0.5066540422,5.836780882,-3.1990775372
 H,0,-1.7271440534,2.9137214435,-0.0721545545
 H,0,-0.157581716,3.389972975,0.6904408377
 H,0,0.9071120345,1.3305473165,0.0237943163
 C,0,-0.0403606457,-0.8847128987,-1.0946188153
 H,0,-1.8173276902,0.4738956611,-1.0672714788
 H,0,0.4384561889,1.3424098808,-2.9894929258
 H,0,2.6177621756,4.8002778907,-2.6809117128
 H,0,-1.8955375041,1.2698880919,-6.0380261192
 H,0,-1.4448252036,2.7499433017,-5.1591491423
 H,0,-0.2158917139,1.5255746762,-5.5336040217
 H,0,-3.7106748015,0.8810736623,-4.3382689891
 H,0,-3.3450028854,0.683743482,-2.6205079909
 H,0,-3.2311865344,2.2881266774,-3.3662628013
 H,0,-1.931894723,-0.9074594466,-4.9492336348
 H,0,-0.2944345871,-0.7758560148,-4.2981394257
 H,0,-1.65841707,-1.1318815017,-3.2192828331
 H,0,-0.7514995605,-1.7111287559,-0.9892802384
 H,0,0.4744187817,-1.0245325286,-2.0523276372
 H,0,0.7156260702,-0.9984097661,-0.3095677174

TS for reaction of 41 and acetaldehyde
 dimethylTShpG**

E(RB+HF-LYP) = -375.838783206

Zero-point correction=	0.209153 (Hartree/Particle)
Thermal correction to Energy=	0.220136
Thermal correction to Enthalpy=	0.221080
Thermal correction to Gibbs Free Energy=	0.174252
Sum of electronic and zero-point Energies=	-375.629631
Sum of electronic and thermal Energies=	-375.618647
Sum of electronic and thermal Enthalpies=	-375.617703
Sum of electronic and thermal Free Energies=	-375.664531

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.137	42.119	98.558

C,0,-0.4451910799,2.8286954061,-0.1046441128
C,0,-0.1282184179,1.4274756187,-0.2800413516
C,0,-0.9246055741,0.5297172071,-0.9345916792
H,0,-0.5995196007,-0.4943185515,-1.1012399159
B,0,0.0289732467,3.6627447149,-1.5620715659
O,0,-0.8159983584,2.8663801253,-2.5940624817
C,0,-0.5266617443,1.6891044804,-2.9647974657
C,0,-1.4809136555,0.9587809231,-3.8616634517
C,0,-0.5564813762,5.1650228681,-1.5328897437
C,0,1.6182288719,3.5550625187,-1.8597230676
H,0,-1.5123252749,3.0201008277,0.0389391831
H,0,0.1372784469,3.3132938388,0.6843831032
H,0,0.8954006893,1.1192963835,-0.060446477
H,0,-1.9854990106,0.7257614787,-1.0688575596
H,0,0.5172460319,1.3721138417,-2.9573208064
H,0,-1.3377343919,-0.1229148709,-3.801547674
H,0,-2.5155501908,1.2158169712,-3.6221988665
H,0,-1.2854635879,1.2659116916,-4.8995681936
H,0,-0.2968181715,5.722180062,-2.4446151482
H,0,-1.650403923,5.1953837928,-1.4349733984
H,0,-0.1413857852,5.7346444074,-0.6902383406
H,0,1.8710957992,4.0019633184,-2.832620234
H,0,2.1774025576,4.128783013,-1.1080356518
H,0,2.0515334995,2.5439249332,-1.8507281005

TS for reaction of 41 and acetone

aceallTShpG*

E(RB+HF-LYP) = -415.152534476

Zero-point correction=	0.237359 (Hartree/Particle)
Thermal correction to Energy=	0.249652

Thermal correction to Enthalpy= 0.250596
 Thermal correction to Gibbs Free Energy= 0.201239
 Sum of electronic and zero-point Energies= -414.915175
 Sum of electronic and thermal Energies= -414.902883
 Sum of electronic and thermal Enthalpies= -414.901939
 Sum of electronic and thermal Free Energies= -414.951295

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	156.659	47.797	103.879

C,0,-0.6128617897,5.1210658432,-1.5787535248
 B,0,0.101120405,3.6721653015,-1.5382803592
 C,0,1.7208789602,3.7484423498,-1.6014741743
 C,0,-0.4660813965,2.8310371229,-0.076934961
 C,0,-0.1508604494,1.4416826504,-0.2450192029
 C,0,-0.9230088645,0.5659472751,-0.9698340952
 O,0,-0.5955576303,2.8182733948,-2.6005393188
 C,0,-0.4391159741,1.5947990514,-2.9531132974
 C,0,-1.5829599378,1.0313749027,-3.770601458
 H,0,-0.6124502091,-0.4662254111,-1.1095936181
 H,0,-1.5361406709,3.0417477659,-0.0124609813
 H,0,0.0866223174,3.3305238756,0.7227029733
 H,0,0.8574590249,1.1210168076,0.0221274371
 H,0,-1.9814995784,0.767385682,-1.1105399988
 C,0,0.925063,1.0024428875,-3.2430707274
 H,0,-1.6180841159,-0.0600522263,-3.725089447
 H,0,-2.5352837614,1.4501543098,-3.4389509594
 H,0,-1.4335460505,1.3174159472,-4.8219899617
 H,0,-0.2838636958,5.7058171658,-2.4504010288
 H,0,-1.7084102963,5.0578857043,-1.6258336166
 H,0,-0.3572032756,5.7156984569,-0.691213923
 H,0,0.20730351543,4.033011492,-2.603664929
 H,0,0.20663316496,4.5433806381,-0.9258947337
 H,0,0.2274128622,2.8449313656,-1.3111510887
 H,0,0.8693227182,-0.0876681946,-3.2994742864
 H,0,0.12496854573,1.3725567808,-4.2268416895
 H,0,0.16754163873,1.292818061,-2.5123210295

TS for reaction of 42 and acetaldehyde

subsallTShpG*

E(RB+HF-LYP) = -415.157796215

Zero-point correction= 0.237271 (Hartree/Particle)
 Thermal correction to Energy= 0.249764
 Thermal correction to Enthalpy= 0.250708

Thermal correction to Gibbs Free Energy=	0.200439
Sum of electronic and zero-point Energies=	-414.920525
Sum of electronic and thermal Energies=	-414.908032
Sum of electronic and thermal Enthalpies=	-414.907088
Sum of electronic and thermal Free Energies=	-414.957358

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.729	47.673	105.801

C,0,-0.7262700147,5.1431145842,-1.615556301
 B,0,0.0855707639,3.74841474,-1.5916421833
 O,0,1.6086502059,4.1233858924,-1.7306237538
 C,0,2.539161323,3.2784342109,-1.6270889946
 H,0,2.3788887913,2.3738481827,-1.0377215877
 C,0,-0.1697327123,2.8586023236,-0.2600195329
 C,0,-0.1562645159,2.9092978298,-3.0724678718
 C,0,0.7992663315,1.8065138724,-3.2296687106
 C,0,2.0751501238,2.0296000587,-3.6664687
 C,0,3.948267346,3.7001226678,-1.9109097367
 H,0,2.7956767842,1.217999406,-3.7419176986
 H,0,-0.0570264274,3.6534888372,-3.868607074
 H,0,-1.1948911026,2.561507057,-3.03673373
 C,0,0.3916869055,0.4308113841,-2.7604177344
 H,0,2.3376846636,2.9560369876,-4.1688437969
 H,0,4.5681442977,2.8493805567,-2.2042069142
 H,0,3.9754777191,4.472807279,-2.6827713939
 H,0,4.3745743628,4.122910744,-0.9891106717
 H,0,-0.5603522689,5.7334909823,-0.7030359584
 H,0,-0.4550786169,5.780663774,-2.4686048766
 H,0,-1.8091736176,4.9669974146,-1.679534857
 H,0,0.0257652548,3.4491884488,0.6469689913
 H,0,-1.225622671,2.5592006489,-0.2060133638
 H,0,0.412436465,1.9306298222,-0.1615967435
 H,0,1.2439510783,-0.2518559771,-2.6778052337
 H,0,-0.1258902381,0.4722020232,-1.7966008582
 H,0,-0.3169902307,-0.0040517511,-3.4782267141

TS for reaction of 42 and acetone

acesubsallTShpG**

E(RB+HF-LYP) = -454.471453452

Zero-point correction=	0.265475 (Hartree/Particle)
Thermal correction to Energy=	0.279248
Thermal correction to Enthalpy=	0.280192
Thermal correction to Gibbs Free Energy=	0.227609

Sum of electronic and zero-point Energies=	-454.205978
Sum of electronic and thermal Energies=	-454.192206
Sum of electronic and thermal Enthalpies=	-454.191262
Sum of electronic and thermal Free Energies=	-454.243844

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	175.231	53.308	110.670

C,0,-0.6055544106,5.1465764051,-1.6163324742
 B,0,0.0988189669,3.6931663592,-1.5126134756
 C,0,-0.1473981924,2.8665694374,-3.0427311178
 C,0,0.8166349292,1.7948495924,-3.2085606062
 C,0,0.4309628912,0.3948782251,-2.8004779585
 O,0,1.6164526041,3.9548893787,-1.5889373219
 C,0,2.6188437788,3.1597522379,-1.6263653133
 C,0,3.9147618274,3.8042475754,-2.073223492
 C,0,-0.4139598823,2.8518091074,-0.2221972761
 C,0,2.1138222578,2.0727683511,-3.5791634871
 C,0,2.7658727914,1.9917254563,-0.6738059058
 H,0,2.8442740452,1.2735136815,-3.6842885483
 H,0,-0.0407508988,3.6509978033,-3.7959597431
 H,0,-1.185136643,2.5214850837,-2.9994220728
 H,0,2.3408044221,2.9958482179,-4.1027883482
 H,0,4.6190219437,3.0706970874,-2.4736491729
 H,0,3.7214126669,4.5816215734,-2.8150920478
 H,0,4.3856860115,4.277770805,-1.1994028225
 H,0,-0.50295684,5.7169115192,-0.6815890224
 H,0,-0.1869524567,5.7663555669,-2.4212803774
 H,0,-1.6838970217,5.0529907311,-1.8063003954
 H,0,-0.090211356,3.3332828963,0.7121627771
 H,0,-1.5128022895,2.8681354957,-0.2016734278
 H,0,-0.1263074192,1.7952000987,-0.1470163979
 H,0,1.2988040267,-0.262677658,-2.6871171694
 H,0,-0.1465841924,0.3906065286,-1.8697562744
 H,0,-0.218338145,-0.041070487,-3.5718356328
 H,0,3.5688988438,1.3252864296,-0.9989863228
 H,0,3.0421074269,2.3962276023,0.3111526198
 H,0,1.8468133138,1.4242778985,-0.5532971924

Transition structures for reaction of 43 and 44a – Si facial attack – TS 46

B3LYP/6-31G*

pnbDIPESiTSB3G

E(RB+HF-LYP) = -1534.40468617

Zero-point correction= 0.455519 (Hartree/Particle)
 Thermal correction to Energy= 0.486190
 Thermal correction to Enthalpy= 0.487135
 Thermal correction to Gibbs Free Energy= 0.389548
 Sum of electronic and zero-point Energies= -1533.949167
 Sum of electronic and thermal Energies= -1533.918496
 Sum of electronic and thermal Enthalpies= -1533.917551
 Sum of electronic and thermal Free Energies= -1534.015139

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	305.089	114.130	205.389

C,0,-1.7794732598,0.0198836975,-4.2307863738
 C,0,-1.933366482,0.7337336309,-3.0303580136
 C,0,-1.6895242194,2.1165026454,-3.0071692649
 C,0,-1.2874811379,2.7820379651,-4.1590822768
 C,0,-1.1343840042,2.0470710805,-5.3340498921
 C,0,-1.3773085333,0.6740417419,-5.3883710803
 C,0,-2.3850061153,0.0570034271,-1.8009019792
 O,0,-2.8678285077,-1.1309956004,-1.8970343835
 B,0,-3.1656122559,-1.9036650514,-0.6216651382
 O,0,-4.0377278229,-2.9961177969,-0.9196542838
 C,0,-5.1466266014,-2.9293235943,-0.0653009277
 C,0,-5.0081504901,-3.915748097,1.1003943798
 O,0,-6.2198522081,-4.1556936138,1.6452930344
 C,0,-6.2700077665,-5.0347153605,2.810134174
 N,0,-0.7067874081,2.7442363054,-6.5577745618
 O,0,-0.4975089716,3.9547231804,-6.4812352829
 C,0,-1.5713368604,-2.3740091642,-0.1330998162
 C,0,-0.9250826605,-1.1141911596,0.1076245222
 C,0,-0.3630063603,-0.3429041038,-0.8858425513
 O,0,-3.7820688254,-1.0887005848,0.4032649344
 C,0,-5.1321976251,-1.4575804382,0.4782676419
 C,0,-6.0136646496,-0.523831736,-0.362615035
 O,0,-7.3128664879,-0.8414533689,-0.1957723308
 C,0,-8.2999543293,-0.0588749346,-0.9370044405
 O,0,-5.6038129067,0.3716060217,-1.0685164247
 O,0,-3.9652112122,-4.3856487937,1.4976291117
 O,0,-0.5827666884,2.0743106304,-7.5824782768
 H,0,-5.4913490701,-1.4046346069,1.5132599894
 H,0,-6.0727094029,-3.1532650819,-0.6038274173
 H,0,-1.1486170915,-2.9659643871,-0.9478167684
 H,0,-1.7713875172,-2.9827786581,0.7500426139
 H,0,-1.1099378726,-0.6419598488,1.0726338075
 H,0,0.0453504219,0.6394993932,-0.6647315564

H,0,-0.0136281561,-0.8065585214,-1.8039487719
H,0,-2.7196253808,0.6756566821,-0.969328918
C,0,-9.499947702,-0.9746152456,-1.1303812828
C,0,-8.6197084961,1.2142692909,-0.1608731248
H,0,-7.8498885984,0.199068284,-1.8999390947
C,0,-7.6607352825,-5.6531132844,2.8071238368
H,0,-5.5043041097,-5.8027967792,2.6678971446
C,0,-5.9609832945,-4.2280848993,4.0670827596
H,0,-1.8214745027,2.671245131,-2.0822095526
H,0,-1.0958546621,3.8477066153,-4.1660995816
H,0,-1.2531151982,0.1471894372,-6.3263215433
H,0,-1.9900454548,-1.0439503864,-4.2432384949
H,0,-9.371505911,1.8031993947,-0.6983488147
H,0,-9.0169557675,0.9721582936,0.8312629881
H,0,-7.7231631259,1.8293337597,-0.0445556428
H,0,-10.2770233903,-0.4579795618,-1.7041312407
H,0,-9.2151002748,-1.8809172073,-1.6738873299
H,0,-9.9234511845,-1.2700104966,-0.1641999244
H,0,-7.7624177771,-6.3526458024,3.6439783193
H,0,-8.4305707582,-4.8801681363,2.9085044049
H,0,-7.8411949498,-6.1996490247,1.876215838
H,0,-6.0178790734,-4.8721843038,4.9518620632
H,0,-4.952773891,-3.8075650119,4.016019958
H,0,-6.6825191358,-3.4121749659,4.1885138715

B3LYP/6-31+G**

pnbDIPESiTBSB3+G

E(RB+HF-LYP) = -1534.49624260

Zero-point correction=	0.452470 (Hartree/Particle)
Thermal correction to Energy=	0.483368
Thermal correction to Enthalpy=	0.484313
Thermal correction to Gibbs Free Energy=	0.385483
Sum of electronic and zero-point Energies=	-1534.043773
Sum of electronic and thermal Energies=	-1534.012874
Sum of electronic and thermal Enthalpies=	-1534.011930
Sum of electronic and thermal Free Energies=	-1534.110759

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	303.318	114.832	208.003

C,0,-3.7016247747,-0.613022223,1.0480395288
C,0,-3.2204224573,-0.4407026143,-0.2613802675
C,0,-4.0771152759,0.0570258568,-1.2575339623
C,0,-5.3997787656,0.3705107192,-0.9614556142

C,0,-5.8533067387,0.1807240964,0.3446339192
 C,0,-5.0216487991,-0.3035829323,1.3568476715
 C,0,-1.8155551809,-0.737298466,-0.6005122422
 O,0,-0.9754494426,-0.9015072765,0.36339552
 B,0,0.4292492485,-1.3707448405,0.0471919733
 O,0,1.2801854796,-1.1342583475,1.173807463
 C,0,2.4070835941,-0.4107701708,0.7530883934
 C,0,3.6286031185,-1.3257083737,0.5943387722
 O,0,4.7647333466,-0.6059652661,0.7003979854
 C,0,6.0389702523,-1.3030031845,0.5152391654
 N,0,-7.2531332426,0.5081046716,0.6666691223
 O,0,-7.9663212687,0.9339607716,-0.2437074584
 C,0,0.1594234776,-3.0543309271,-0.2917532122
 C,0,-0.7123131511,-3.0193553646,-1.4296070047
 C,0,-2.0780058437,-2.8356839883,-1.3399410767
 O,0,1.0084776638,-0.7080272663,-1.1029425907
 C,0,1.9905226657,0.1817177673,-0.6411093194
 C,0,1.4451662998,1.6134582556,-0.5277837914
 O,0,2.4349131664,2.4602224771,-0.1850778727
 C,0,2.1075759069,3.880827084,-0.0347753086
 O,0,0.2941620042,1.9379081833,-0.7311838962
 O,0,3.5825201246,-2.5180206193,0.3782008586
 O,0,-7.6301033081,0.3356549799,1.8269136637
 H,0,2.8358908621,0.2134809989,-1.3385635856
 H,0,2.65563344,0.3750976819,1.4718327801
 H,0,-0.2700351667,-3.4827782679,0.6157244462
 H,0,1.173271688,-3.4111496327,-0.4768637085
 H,0,-0.247636493,-2.8898255813,-2.406988601
 H,0,-2.6830400801,-2.7409211963,-2.2368932513
 H,0,-2.6065885239,-3.1169656549,-0.4339973711
 H,0,-1.4338095494,-0.3675008988,-1.5515682802
 C,0,3.0754865804,4.4283939577,1.0039900899
 C,0,2.2156175523,4.565315175,-1.3931075929
 H,0,1.077444308,3.9362034941,0.3280079963
 C,0,7.0583535613,-0.5435581103,1.3521340797
 H,0,5.9064969929,-2.3198041972,0.8954484376
 C,0,6.3781083716,-1.3465555021,-0.9709165102
 H,0,-3.7024336825,0.2055212165,-2.2661960886
 H,0,-6.0750079042,0.757919276,-1.7140712577
 H,0,-5.4130121693,-0.4261104147,2.3591328696
 H,0,-3.0282919071,-0.9763839894,1.8164705142
 H,0,1.9783347758,5.6299052966,-1.2929807966
 H,0,3.2320881402,4.4754149504,-1.791049861
 H,0,1.5139028839,4.1270547733,-2.1075750023
 H,0,2.8734853296,5.4906218071,1.1759974284
 H,0,2.9685887511,3.8995361353,1.9554720216

H,0,4.1111546406,4.3246947712,0.6640907217
H,0,8.0370830969,-1.0284802486,1.2763004305
H,0,7.1572698067,0.4895690978,1.0028199932
H,0,6.7630201944,-0.5264291675,2.4052209981
H,0,7.3343591763,-1.8593590447,-1.1201445786
H,0,5.6119725184,-1.8904078848,-1.5298464531
H,0,6.4647187062,-0.3327978424,-1.3766922879

B3LYP/6-31+G Onsager solvent model for dichloromethane**

pnbDIPESiTSOnsB3+G
E(RB+HF-LYP) = -1534.49866212

Zero-point correction=	0.452256	(Hartree/Particle)
Thermal correction to Energy=	0.483201	
Thermal correction to Enthalpy=	0.484145	
Thermal correction to Gibbs Free Energy=	0.385431	
Sum of electronic and zero-point Energies=	-1534.046406	
Sum of electronic and thermal Energies=	-1534.015462	
Sum of electronic and thermal Enthalpies=	-1534.014517	
Sum of electronic and thermal Free Energies=	-1534.113231	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	303.213	115.048	207.760

C,0,3.740922586,-0.6814402599,-1.0715608322
C,0,3.2478955267,-0.4618234892,0.2272822504
C,0,4.1118502219,0.0207655587,1.2254870806
C,0,5.4520410048,0.2644028274,0.944718829
C,0,5.9187624889,0.0212443284,-0.3491004508
C,0,5.0781771913,-0.4430367614,-1.3648628036
C,0,1.8285034941,-0.6961421105,0.547876345
O,0,1.0029388189,-0.870722242,-0.4195863459
B,0,-0.4226315666,-1.3112661722,-0.1052777254
O,0,-1.2643123937,-1.0565792021,-1.2286967669
C,0,-2.3996166647,-0.3488660912,-0.7920523617
C,0,-3.6085619702,-1.2811555751,-0.6276147716
O,0,-4.7487088934,-0.5732022215,-0.6930755127
C,0,-6.0199889173,-1.280067914,-0.4841818679
N,0,7.3356842088,0.2629720905,-0.6521691538
O,0,8.0605178595,0.6715253936,0.2588139409
C,0,-0.1685750786,-3.0018156282,0.2280818745
C,0,0.6722650217,-2.981147477,1.3897160444
C,0,2.0432218635,-2.8394477166,1.3412424816
O,0,-0.9780571076,-0.6453640633,1.0473914418
C,0,-1.9758765883,0.2395899222,0.600767381

C,0,-1.4422561809,1.674861922,0.4862163029
 O,0,-2.4547255094,2.5209048432,0.2342103261
 C,0,-2.1546007257,3.9504971972,0.096155799
 O,0,-0.2775795785,1.9958554349,0.6111376367
 O,0,-3.5368383645,-2.4778909248,-0.4387906874
 O,0,7.7274845232,0.0397989093,-1.8012579377
 H,0,-2.8131308014,0.2570872115,1.306911703
 H,0,-2.6621054122,0.4372384204,-1.5053137401
 H,0,0.2788597781,-3.4333976471,-0.6692164887
 H,0,-1.1932408397,-3.3422937987,0.3832815861
 H,0,0.1823087562,-2.8362814586,2.3522446935
 H,0,2.6245854753,-2.7481002302,2.2541698723
 H,0,2.5910685028,-3.1240521661,0.44781638
 H,0,1.4418074352,-0.3182325258,1.4936036097
 C,0,-3.2072833889,4.5108024828,-0.848844635
 C,0,-2.1648659561,4.5974608233,1.4766293103
 H,0,-1.1563067193,4.0258609568,-0.3444221507
 C,0,-7.0614303396,-0.5135649023,-1.2853788714
 H,0,-5.89007862,-2.2904341638,-0.8815137051
 C,0,-6.3179152156,-1.3419413059,1.0092996992
 H,0,3.7285977137,0.208940017,2.22410735
 H,0,6.1314564465,0.6368360156,1.7010551972
 H,0,5.4770998768,-0.6056800522,-2.3583134589
 H,0,3.0614326622,-1.0281449998,-1.8422525343
 H,0,-1.9483896773,5.6672981806,1.3867547508
 H,0,-3.1464579358,4.4855759671,1.9486426443
 H,0,-1.4060916381,4.150143266,2.1241010456
 H,0,-3.0314447841,5.5795789259,-1.0079299814
 H,0,-3.1711932399,4.0074246255,-1.8193649418
 H,0,-4.2114483583,4.3864615461,-0.4313594383
 H,0,-8.036003844,-1.0025291849,-1.189633665
 H,0,-7.1560460869,0.5142768217,-0.9204827166
 H,0,-6.7947014158,-0.4829531118,-2.3458160453
 H,0,-7.267463228,-1.8606410057,1.1770987005
 H,0,-5.5356567816,-1.8889218318,1.5425274902
 H,0,-6.400407634,-0.3339524539,1.4293328238

B3LYP/6-31+G PCM solvent model for dichloromethane**

pnDIPESiTSPCMB3+G

E(RB+HF-LYP) = -1534.52242985

Zero-point correction=	0.450482 (Hartree/Particle)
Thermal correction to Energy=	0.481454
Thermal correction to Enthalpy=	0.482398
Thermal correction to Gibbs Free Energy=	0.383607
Sum of electronic and zero-point Energies=	-1534.071948

Sum of electronic and thermal Energies= -1534.040976
 Sum of electronic and thermal Enthalpies= -1534.040032
 Sum of electronic and thermal Free Energies= -1534.138823

		E (Thermal)	CV	S	
		KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin	
Total		302.117	115.052	207.922	
1	6	0	3.740704	-0.559059	-1.033088
2	6	0	3.280572	-0.410287	0.287418
3	6	0	4.145244	0.083584	1.279502
4	6	0	5.457183	0.423288	0.965816
5	6	0	5.889790	0.261389	-0.352804
6	6	0	5.049431	-0.223498	-1.360032
7	6	0	1.886595	-0.729687	0.652254
8	8	0	1.018966	-0.865544	-0.296347
9	5	0	-0.372823	-1.377166	0.014336
10	8	0	-1.208995	-1.175592	-1.142413
11	6	0	-2.360088	-0.458753	-0.770831
12	6	0	-3.588006	-1.375608	-0.680100
13	8	0	-4.709685	-0.642033	-0.692096
14	6	0	-6.005028	-1.326097	-0.570157
15	7	0	7.270353	0.616375	-0.693151
16	8	0	8.003261	1.042944	0.204907
17	6	0	-0.074815	-3.036060	0.371766
18	6	0	0.849808	-3.009232	1.474874
19	6	0	2.208686	-2.834717	1.317555
20	8	0	-1.003721	-0.702231	1.133040
21	6	0	-2.012403	0.143186	0.637921
22	6	0	-1.542441	1.602582	0.540765
23	8	0	-2.572213	2.392687	0.209534
24	6	0	-2.343635	3.838482	0.069924
25	8	0	-0.404979	1.981665	0.746466
26	8	0	-3.546233	-2.588907	-0.597266
27	8	0	7.640160	0.472467	-1.862711
28	1	0	-2.877665	0.132792	1.311432
29	1	0	-2.579545	0.323820	-1.505243
30	1	0	0.321466	-3.479150	-0.545594
31	1	0	-1.068509	-3.419210	0.610719
32	1	0	0.435155	-2.894205	2.479422
33	1	0	2.857867	-2.743698	2.184300
34	1	0	2.687733	-3.099669	0.378455
35	1	0	1.537874	-0.395805	1.631700
36	6	0	-3.327971	4.318169	-0.986148
37	6	0	-2.534328	4.501224	1.429225
38	1	0	-1.313332	3.971835	-0.275036

39	6	0	-7.007619	-0.454341	-1.311241
40	1	0	-5.903276	-2.299110	-1.062039
41	6	0	-6.333014	-1.514036	0.906541
42	1	0	3.787557	0.207277	2.300836
43	1	0	6.131407	0.809201	1.723775
44	1	0	5.415784	-0.331884	-2.376082
45	1	0	3.067327	-0.930467	-1.801596
46	1	0	-2.373212	5.580800	1.338741
47	1	0	-3.551217	4.334444	1.800551
48	1	0	-1.821407	4.111397	2.161257
49	1	0	-3.195168	5.392436	-1.150871
50	1	0	-3.164584	3.801456	-1.936498
51	1	0	-4.360289	4.142902	-0.665569
52	1	0	-7.995970	-0.924533	-1.281632
53	1	0	-7.081932	0.535234	-0.848083
54	1	0	-6.717127	-0.329169	-2.358573
55	1	0	-7.300930	-2.016463	1.008079
56	1	0	-5.578016	-2.130129	1.403050
57	1	0	-6.392813	-0.545713	1.415009

mPW1K/6-31G*

pnbDIPESimpw1kG

E(RmPW+HF-PW91) = -1533.92592316

Zero-point correction=	0.471191 (Hartree/Particle)
Thermal correction to Energy=	0.501036
Thermal correction to Enthalpy=	0.501981
Thermal correction to Gibbs Free Energy=	0.406012
Sum of electronic and zero-point Energies=	-1533.454732
Sum of electronic and thermal Energies=	-1533.424887
Sum of electronic and thermal Enthalpies=	-1533.423943
Sum of electronic and thermal Free Energies=	-1533.519911

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	314.405	110.500	201.982

C,0,-3.5858997342,-0.4602040886,0.9814528568
C,0,-3.037264901,-0.3579587124,-0.2944593873
C,0,-3.8120004032,0.1063095785,-1.3532546687
C,0,-5.1314992008,0.4562810515,-1.1500651731
C,0,-5.6548610279,0.3356493336,0.1243434369
C,0,-4.9039057776,-0.1141670417,1.1965394779
C,0,-1.6277092876,-0.6924955017,-0.5280526916
O,0,-0.8713458946,-0.8713083747,0.4663491475

B,0,0.5269616681,-1.4212658676,0.1901454509
 O,0,1.3565703704,-1.1324868104,1.3066368534
 C,0,2.4536900031,-0.4182544232,0.8650734897
 C,0,3.6628888516,-1.3203529794,0.6956615208
 O,0,4.7673714044,-0.587271063,0.5746574471
 C,0,6.0010194836,-1.2877939132,0.3575809909
 N,0,-7.0460984644,0.7004205852,0.3464344112
 O,0,-7.678957959,1.0908676407,-0.605978851
 C,0,0.1988398124,-3.0436420187,-0.0935651516
 C,0,-0.6451248631,-3.0159276897,-1.2575601382
 C,0,-1.9913295991,-2.8272788724,-1.213133266
 O,0,1.1109223932,-0.8003317273,-0.9694704399
 C,0,2.0257380448,0.1329453323,-0.5155969203
 C,0,1.4027037233,1.5146973785,-0.4151755264
 O,0,2.2948374034,2.3970089789,0.0169686943
 C,0,1.8631711759,3.7597977675,0.1627558556
 O,0,0.2675779164,1.7769525091,-0.7017293612
 O,0,3.6303983644,-2.5165758073,0.6501632294
 O,0,-7.4799427237,0.5881087262,1.4682443787
 H,0,2.8724522331,0.2130489306,-1.1984370138
 H,0,2.7152306423,0.3806324586,1.5566163316
 H,0,-0.2741007486,-3.4566360658,0.792974339
 H,0,1.1811989776,-3.4781449744,-0.2542256168
 H,0,-0.1516795115,-2.922095755,-2.2178581624
 H,0,-2.5731096465,-2.7380522939,-2.1192185321
 H,0,-2.5426309193,-3.0369221008,-0.307564986
 H,0,-1.1793422686,-0.3991272705,-1.469362889
 C,0,2.7607309669,4.372602843,1.2093116761
 C,0,1.9412648242,4.4578256411,-1.1756267512
 H,0,0.8313550709,3.73888948,0.5061403533
 C,0,7.0929826352,-0.3790621086,0.8665060914
 H,0,5.961640602,-2.2048433852,0.9412919759
 C,0,6.140202204,-1.6252391598,-1.1094327013
 H,0,-3.3764533947,0.1983832714,-2.3374945803
 H,0,-5.7545007055,0.8199602796,-1.9498026576
 H,0,-5.3569562505,-0.1814751715,2.1714947804
 H,0,-2.9654158234,-0.8020787514,1.7949183911
 H,0,1.6327454769,5.4970520435,-1.0744233612
 H,0,2.9615680429,4.4385676471,-1.555918296
 H,0,1.2850968728,3.977447092,-1.8968295854
 H,0,2.4730414005,5.4068246258,1.3888001497
 H,0,2.6880293533,3.8280705177,2.1481436104
 H,0,3.7988570489,4.3564314634,0.8817951469
 H,0,8.0626877548,-0.8610121251,0.7564484986
 H,0,7.1076398529,0.5542638417,0.3059315561
 H,0,6.942076997,-0.1456065996,1.91810623

H,0,7.0813193467,-2.1428961212,-1.2879505042
H,0,5.3298267164,-2.2744149142,-1.4311235779
H,0,6.1298224705,-0.7174173289,-1.7114065811

mPW1K/6-31+G**

pnbDIPESimpw1k+G

E(RmPW+HF-PW91) = -1533.99888250

Zero-point correction=	0.468224	(Hartree/Particle)
Thermal correction to Energy=	0.498239	
Thermal correction to Enthalpy=	0.499183	
Thermal correction to Gibbs Free Energy=	0.402387	
Sum of electronic and zero-point Energies=	-1533.530659	
Sum of electronic and thermal Energies=	-1533.500643	
Sum of electronic and thermal Enthalpies=	-1533.499699	
Sum of electronic and thermal Free Energies=	-1533.596495	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	312.650	111.083	203.724

C,0,3.5894693498,-0.5782240847,-1.0536450738
C,0,3.0722686448,-0.4907018062,0.2367104976
C,0,3.8817767778,-0.0685050351,1.2875222004
C,0,5.2056729359,0.2541424775,1.0620326316
C,0,5.697239367,0.1486870777,-0.2269857991
C,0,4.9111638165,-0.2584868923,-1.2919361777
C,0,1.6600560503,-0.7951270111,0.4984971582
O,0,0.8725308596,-0.9158266657,-0.4840706172
B,0,-0.5324638196,-1.4234539765,-0.196631646
O,0,-1.3750620099,-1.081994658,-1.2900775487
C,0,-2.4398289163,-0.337625042,-0.8168836595
C,0,-3.6826473564,-1.1947867564,-0.6531162099
O,0,-4.7611597161,-0.424724752,-0.5394741796
C,0,-6.0243240995,-1.0741611577,-0.3200456009
N,0,7.0930809867,0.4854804357,-0.4735467528
O,0,7.757357713,0.8411627728,0.4722382521
C,0,-0.2607294493,-3.0669586845,0.0410411792
C,0,0.6134454038,-3.0969148125,1.1790459623
C,0,1.9655883668,-2.9443248092,1.1008520475
O,0,-1.0799531159,-0.809427293,0.9855270395
C,0,-1.9713969316,0.164572927,0.5704314142
C,0,-1.308641591,1.530833742,0.5016446341
O,0,-2.1687134171,2.448347451,0.0822786542
C,0,-1.7071590457,3.8077581696,-0.0165996899

O,0,-0.1690927822,1.7529400865,0.8086008793
O,0,-3.6925813318,-2.3925991724,-0.6077775729
O,0,7.5000705552,0.3868110955,-1.6076455087
H,0,-2.8027208254,0.2543529373,1.2709923845
H,0,-2.6793814725,0.4859554166,-1.4865578293
H,0,0.1715208675,-3.4663450253,-0.8715676706
H,0,-1.2569130847,-3.4608463433,0.2181001135
H,0,0.1521585855,-3.0209351923,2.1569163066
H,0,2.570516476,-2.9007096094,1.9946866643
H,0,2.4844412485,-3.1460274308,0.1747492371
H,0,1.245276906,-0.5100421083,1.4584773035
C,0,-2.5519148624,4.4619609735,-1.0812369394
C,0,-1.8229018844,4.4754834731,1.3340657207
H,0,-0.6634709414,3.773411078,-0.3218021363
C,0,-7.076801719,-0.1417150921,-0.8665617678
H,0,-6.0103226601,-2.0071701326,-0.8795810726
C,0,-6.1918800448,-1.3664367449,1.1534191844
H,0,3.4706435573,0.0139160197,2.282980739
H,0,5.8543837943,0.5854696238,1.8556913097
H,0,5.3395238431,-0.3148249913,-2.2789256196
H,0,2.9429932568,-0.8860710625,-1.8606076462
H,0,-1.4841549644,5.5076016697,1.2679702648
H,0,-2.8577821678,4.4759010981,1.6719265603
H,0,-1.2091091889,3.9649129284,2.0711735839
H,0,-2.238520536,5.4944934527,-1.2201484691
H,0,-2.4502101489,3.9426007297,-2.0309057876
H,0,-3.6022254237,4.4574080852,-0.7964296661
H,0,-8.0629544559,-0.586997675,-0.7525171234
H,0,-7.0650304332,0.8070690139,-0.3333906496
H,0,-6.9089174969,0.0547693137,-1.9225665404
H,0,-7.1501467667,-1.8512373044,1.3300962402
H,0,-5.4077662804,-2.0307657689,1.5067133726
H,0,-6.164632422,-0.4435359579,1.7305514194

mPW1K/6-31+G Onsager solvent model for dichloromethane**

pnbDIPESimpw1kOns+G

E(RmPW+HF-PW91) = -1534.00067629

Zero-point correction=	0.468082 (Hartree/Particle)
Thermal correction to Energy=	0.498108
Thermal correction to Enthalpy=	0.499053
Thermal correction to Gibbs Free Energy=	0.402573
Sum of electronic and zero-point Energies=	-1533.532594
Sum of electronic and thermal Energies=	-1533.502568
Sum of electronic and thermal Enthalpies=	-1533.501624
Sum of electronic and thermal Free Energies=	-1533.598103

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	312.568	111.205	203.058

C,0,-3.6272537364,-0.5171698429,0.992579177
C,0,-3.0754274877,-0.3593393614,-0.2769702669
C,0,-3.8575362563,0.1203042155,-1.3239815954
C,0,-5.1893485424,0.423292218,-1.1178091173
C,0,-5.7174360887,0.240485592,0.1484859833
C,0,-4.9566290935,-0.2187682292,1.211379077
C,0,-1.6574841664,-0.6584113751,-0.5140698027
O,0,-0.9053107666,-0.8502915362,0.4800429599
B,0,0.5017345068,-1.3800207199,0.2024623761
O,0,1.3277751682,-1.0915010827,1.3195405784
C,0,2.4401602708,-0.3949010755,0.8768063148
C,0,3.6337623672,-1.3183262431,0.6995983954
O,0,4.7512951794,-0.6103823594,0.6078352737
C,0,5.9819611255,-1.320207972,0.3692738699
N,0,-7.1224897525,0.5439800218,0.3726401678
O,0,-7.7684474694,0.9435952833,-0.568871569
C,0,0.1859815677,-3.0078946249,-0.0929633046
C,0,-0.6388896522,-2.9744200625,-1.2670995686
C,0,-1.9896241553,-2.7999408473,-1.2422073389
O,0,1.0783040811,-0.7477324927,-0.9507931521
C,0,2.0140620114,0.1696146315,-0.4998490314
C,0,1.4166990679,1.562755732,-0.3950145144
O,0,2.3344911391,2.43317044,-0.0062862488
C,0,1.9527582132,3.8169812849,0.1095459354
O,0,0.2740897893,1.8361372099,-0.6484694959
O,0,3.5684601533,-2.5140346876,0.6284458508
O,0,-7.5633479151,0.37393205,1.487098229
H,0,2.8560523597,0.2359984043,-1.1891047275
H,0,2.7172391825,0.3940982329,1.5729026974
H,0,-0.2947624501,-3.4239292416,0.7874353591
H,0,1.1796313769,-3.4204934501,-0.2404257836
H,0,-0.1330923903,-2.869555513,-2.2198031845
H,0,-2.5536052367,-2.7042243101,-2.1585900074
H,0,-2.5522935477,-3.0213492049,-0.3466178255
H,0,-1.2099985434,-0.3433565341,-1.4497683826
C,0,2.8782788825,4.4224534092,1.1349418771
C,0,2.0486076667,4.4761986273,-1.2466727985
H,0,0.9226908826,3.8392669925,0.4593942225
C,0,7.0799451192,-0.4619413431,0.9456196669
H,0,5.9151116836,-2.2673972765,0.9002225551
C,0,6.135229937,-1.5735501591,-1.1124082233

H,0,-3.4194029347,0.2599576948,-2.3012730373
H,0,-5.8163678543,0.795992049,-1.9105349272
H,0,-5.4104002332,-0.3316061005,2.181890438
H,0,-2.9996742898,-0.8654555782,1.7980099479
H,0,1.7705972876,5.5254640356,-1.1694560448
H,0,3.0667893911,4.420662098,-1.6271105532
H,0,1.3782682517,4.0000283641,-1.9571183255
H,0,2.6317307894,5.4716876546,1.2826509271
H,0,2.7883631567,3.911098765,2.090220817
H,0,3.9131440639,4.3575999276,0.8054394999
H,0,8.041192961,-0.9550021874,0.8186322643
H,0,7.1213162154,0.5016431123,0.4417306604
H,0,6.9208779858,-0.2894947901,2.007180967
H,0,7.0671265482,-2.101489035,-1.3042581278
H,0,5.3185130187,-2.1845622255,-1.4877330245
H,0,6.1589121616,-0.6329485847,-1.6599771089

M05/6-31G*

pnbDIPESiTSM05G

E(RM05+HF-M05) = -1533.50285647

Zero-point correction=	0.460467	(Hartree/Particle)
Thermal correction to Energy=	0.490941	
Thermal correction to Enthalpy=	0.491885	
Thermal correction to Gibbs Free Energy=	0.394290	
Sum of electronic and zero-point Energies=	-1533.042389	
Sum of electronic and thermal Energies=	-1533.011915	
Sum of electronic and thermal Enthalpies=	-1533.010971	
Sum of electronic and thermal Free Energies=	-1533.108567	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	308.070	113.265	205.407

C,0,3.6544108031,-0.5675924615,-1.0354620614
C,0,3.140475302,-0.4196759807,0.2595948088
C,0,3.9681073934,0.046907933,1.2883300443
C,0,5.2965136597,0.3566535466,1.0355198504
C,0,5.7834549137,0.1900808176,-0.2564155678
C,0,4.9817974081,-0.2662716108,-1.2987504993
C,0,1.7245826817,-0.7090208656,0.5433613276
O,0,0.9203279263,-0.8637920787,-0.4283545618
B,0,-0.5040274833,-1.3850626128,-0.1398245477
O,0,-1.3332089344,-1.0854361475,-1.2630465314
C,0,-2.4377857768,-0.3781957539,-0.8151663442
C,0,-3.6529482584,-1.2891506331,-0.6589207051

O,0,-4.7740056768,-0.5514465548,-0.6266947712
 C,0,-6.0272984797,-1.2407692524,-0.3986255242
 N,0,7.1999226632,0.5140785907,-0.5310123006
 O,0,7.8677350618,0.9362575159,0.3955057946
 C,0,-0.203692801,-3.0361348988,0.1276159352
 C,0,0.6490732835,-3.0395383556,1.2840664488
 C,0,2.0090489076,-2.8680532954,1.2367183697
 O,0,-1.086131702,-0.7654455907,1.030020918
 C,0,-2.0133066523,0.1633443721,0.582585233
 C,0,-1.4056054403,1.5630257834,0.4945837488
 O,0,-2.3479750857,2.449576996,0.1473886167
 C,0,-1.9540606425,3.8369007644,-0.0024514322
 O,0,-0.2472808628,1.8319212995,0.7115247421
 O,0,-3.6111004001,-2.4904624856,-0.5420104494
 O,0,7.6067192669,0.3361472635,-1.6645345253
 H,0,-2.8673815514,0.223310437,1.2680885509
 H,0,-2.6954123124,0.4344335863,-1.500995723
 H,0,0.24910128,-3.4404849434,-0.7782590128
 H,0,-1.2082125796,-3.4304272884,0.2851027461
 H,0,0.1598207528,-2.9335504294,2.2518842451
 H,0,2.5951494393,-2.8053116283,2.1496407743
 H,0,2.5589735535,-3.1077439636,0.3306000197
 H,0,1.321919455,-0.3889389038,1.504387933
 C,0,-2.8976902932,4.4339067511,-1.0235140944
 C,0,-2.0033510254,4.5194577875,1.3502684072
 H,0,-0.927424286,3.841329061,-0.3779230586
 C,0,-7.0988154028,-0.3995042104,-1.0573631613
 H,0,-5.9512711519,-2.2168204058,-0.8853963212
 C,0,-6.2279987666,-1.4316652986,1.0920971396
 H,0,3.565556989,0.1733814815,2.2892704225
 H,0,5.9565455787,0.7241335884,1.8111423386
 H,0,5.4048974736,-0.3730210487,-2.2898553045
 H,0,2.997454319,-0.9107879004,-1.8271212394
 H,0,-1.7318715404,5.5741645459,1.2502248178
 H,0,-3.0097376439,4.4632243134,1.7754566379
 H,0,-1.3002643497,4.0529323536,2.0435756882
 H,0,-2.6364940461,5.4788990958,-1.2116411841
 H,0,-2.8404648932,3.8908502686,-1.9700477085
 H,0,-3.931344634,4.3966918608,-0.6680011818
 H,0,-8.074645712,-0.881099238,-0.9489772747
 H,0,-7.1532902621,0.5924224101,-0.599599743
 H,0,-6.8942949317,-0.2747661806,-2.1234022831
 H,0,-7.1839861941,-1.9268613771,1.2850308367
 H,0,-5.4340252201,-2.0540078691,1.5105516326
 H,0,-6.2316931187,-0.4666781601,1.6078340836

Transition structures for reaction of 43 and 44a – *Re* facial attack

B3LYP/6-31+G PCM solvent model for dichloromethane**

pnbDIPEReTSPCMB3+G

E(RB+HF-LYP) = -1534.52188229

Zero-point correction=	0.450510 (Hartree/Particle)
Thermal correction to Energy=	0.481502
Thermal correction to Enthalpy=	0.482446
Thermal correction to Gibbs Free Energy=	0.383351
Sum of electronic and zero-point Energies=	-1534.071372
Sum of electronic and thermal Energies=	-1534.040380
Sum of electronic and thermal Enthalpies=	-1534.039436
Sum of electronic and thermal Free Energies=	-1534.138531

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	302.147	115.030	208.563

1	6	0	4.805872	-0.730535	1.470699
2	6	0	3.532726	-0.886190	0.934683
3	6	0	3.225805	-0.348111	-0.327685
4	6	0	4.207795	0.352955	-1.048628
5	6	0	5.485717	0.516232	-0.523765
6	6	0	5.765044	-0.032042	0.730524
7	6	0	1.872251	-0.472648	-0.904796
8	8	0	0.898698	-0.807129	-0.121175
9	5	0	-0.468478	-1.124771	-0.704435
10	8	0	-1.420709	-1.218741	0.373689
11	6	0	-2.437312	-0.241319	0.197049
12	1	0	-2.534873	0.356653	1.109348
13	7	0	7.108559	0.135059	1.292115
14	8	0	7.342954	-0.350557	2.403214
15	8	0	-0.939547	-0.122730	-1.631152
16	6	0	-1.984702	0.607141	-1.034640
17	1	0	-2.810871	0.724615	-1.748038
18	6	0	-0.187384	-2.633291	-1.487734
19	6	0	0.865045	-2.361355	-2.432391
20	6	0	2.199423	-2.321103	-2.085462
21	8	0	7.947050	0.753330	0.628741
22	1	0	0.578595	-1.949287	-3.403179
23	1	0	2.552096	-2.864587	-1.212644
24	1	0	2.951250	-2.039895	-2.817999
25	1	0	1.646499	0.141314	-1.779550
26	1	0	0.077732	-3.343772	-0.700376
27	1	0	-1.152817	-2.869303	-1.940845

28	6	0	-1.540221	2.013431	-0.620696
29	6	0	-3.763032	-0.976201	-0.053393
30	1	0	3.968723	0.776932	-2.023039
31	1	0	6.249971	1.058968	-1.070959
32	1	0	5.054994	-1.139260	2.445024
33	1	0	2.768862	-1.418710	1.495899
34	8	0	-2.604870	2.716621	-0.201787
35	8	0	-0.400084	2.434287	-0.667905
36	6	0	-2.407345	4.099928	0.257681
37	6	0	-3.484249	4.352424	1.302033
38	1	0	-1.411875	4.149839	0.710861
39	6	0	-2.487790	5.036314	-0.942246
40	1	0	-2.342240	6.070715	-0.612892
41	1	0	-1.713017	4.800748	-1.677046
42	1	0	-3.468594	4.963142	-1.424477
43	1	0	-3.377589	5.365984	1.702132
44	1	0	-4.483321	4.258655	0.863185
45	1	0	-3.398379	3.644602	2.131816
46	8	0	-4.403270	-1.201970	1.098596
47	8	0	-4.156224	-1.333248	-1.151025
48	6	0	-5.655789	-1.974912	1.071365
49	6	0	-6.476639	-1.480283	2.252568
50	1	0	-6.158066	-1.739853	0.127209
51	6	0	-5.321783	-3.460440	1.136232
52	1	0	-6.247200	-4.045923	1.117594
53	1	0	-4.709864	-3.763936	0.282417
54	1	0	-4.783208	-3.695531	2.060463
55	1	0	-7.438761	-2.002276	2.274136
56	1	0	-5.958286	-1.673847	3.197759
57	1	0	-6.669849	-0.406418	2.172606

Transition structures for reaction of 43 and 44b – Si facial attack – TS 47

B3LYP/6-31G*

panisaldehydeDIPESiTSB3G

E(RB+HF-LYP) = -1444.42905672

Zero-point correction=	0.486011 (Hartree/Particle)
Thermal correction to Energy=	0.516646
Thermal correction to Enthalpy=	0.517591
Thermal correction to Gibbs Free Energy=	0.420647
Sum of electronic and zero-point Energies=	-1443.943046
Sum of electronic and thermal Energies=	-1443.912410
Sum of electronic and thermal Enthalpies=	-1443.911466
Sum of electronic and thermal Free Energies=	-1444.008410

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	324.200	114.500	204.035

C,0,3.6104299693,-0.6182378815,-1.0480325201
C,0,3.1449656298,-0.474906165,0.2569731173
C,0,3.9941432444,-0.0416248322,1.2829561772
C,0,5.3337754275,0.2515995405,0.971359721
C,0,5.8098157524,0.1119022781,-0.3220366105
C,0,4.9503867385,-0.326601648,-1.3434944017
C,0,3.5072983566,0.1297567668,2.6609041859
O,0,2.2212485538,0.1457526988,2.8565421086
B,0,1.7015110116,0.1928864343,4.2580736116
O,0,2.4038060427,1.1278319825,5.1185562544
C,0,1.5539237814,2.2164084189,5.3427108377
C,0,1.8495197645,3.3698731193,4.3739684575
O,0,2.6730980901,3.3439673497,3.4870850842
O,0,5.5108270315,-0.4309737465,-2.5788417597
O,0,0.3111693211,0.5451757791,4.2553826267
C,0,0.1175975058,1.6207041705,5.1292218886
C,0,-0.4581059055,1.155019203,6.4717554325
O,0,-0.4045227312,0.0260807558,6.9062359041
C,0,1.9942975326,-1.4433111878,4.8125402923
C,0,3.4179892332,-1.5254730828,4.7194145217
C,0,4.0872793469,-1.7460992331,3.528053201
O,0,-1.0096257418,2.2038155778,7.1228510343
C,0,-1.5603123309,1.9536826688,8.4501031766
C,0,-0.4402795611,2.0105334988,9.4840403688
C,0,-2.6392362073,3.0066559442,8.6607117576
O,0,1.0615283818,4.4283810349,4.6629453474
C,0,1.2040829491,5.6189002843,3.8308143991
C,0,2.3531536958,6.4707205079,4.3604557275
C,0,-0.1453852609,6.3219175863,3.8698549359
H,0,1.6816220649,2.6065896813,6.36038894
H,0,-0.5655012307,2.3604350744,4.6993734037
H,0,1.4374513957,-2.0934938984,4.1347423629
H,0,1.5715595031,-1.4343581808,5.8172961928
H,0,3.9915856912,-1.1263208809,5.5563625719
H,0,5.1735202598,-1.7330097381,3.4972972247
H,0,3.6051885352,-2.3180877563,2.7404195989
H,0,4.1134541514,0.7391808617,3.3310690532
H,0,1.4348975481,5.2796692826,2.8168505254
H,0,-1.996432833,0.9505373923,8.4357521177
H,0,6.0033348076,0.5995822992,1.7544815639
H,0,6.8401903282,0.3408189807,-0.5744066256
H,0,2.9280032546,-0.9482717824,-1.8227197568

H,0,2.1059598342,-0.6859405571,0.4887602812
H,0,2.4609871471,7.3770314702,3.7536978006
H,0,2.1652318028,6.7708199752,5.3975549296
H,0,3.2942787847,5.9157633418,4.3160234105
H,0,-0.1188259923,7.2211723621,3.2446874498
H,0,-0.9373000524,5.6650985913,3.496388462
H,0,-0.3988050225,6.6204046208,4.8930678024
H,0,-3.1221726589,2.8610784908,9.6332329771
H,0,-2.2095312839,4.0142413357,8.6365171051
H,0,-3.4047220371,2.9397880885,7.8812844755
H,0,-0.8454695879,1.8453932519,10.4888808905
H,0,0.3053876512,1.2357197655,9.2853708511
H,0,0.0502105526,2.9904728426,9.4673617425
C,0,4.694581215,-0.8593934111,-3.65988664
H,0,5.3429410479,-0.8664644706,-4.5375962344
H,0,4.3008447907,-1.8699496473,-3.4909070611
H,0,3.8588157112,-0.1688102089,-3.8307862925

B3LYP/6-31+G**

panisaldehydeDIPESiTSB3+G
E(RB+HF-LYP) = -1444.51875273

Zero-point correction=	0.482734	(Hartree/Particle)
Thermal correction to Energy=	0.513610	
Thermal correction to Enthalpy=	0.514554	
Thermal correction to Gibbs Free Energy=	0.416856	
Sum of electronic and zero-point Energies=	-1444.036018	
Sum of electronic and thermal Energies=	-1444.005143	
Sum of electronic and thermal Enthalpies=	-1444.004199	
Sum of electronic and thermal Free Energies=	-1444.101897	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	322.295	115.282	205.623

C,0,5.2734693471,-0.1721161319,-1.2914502822
C,0,3.9567328071,-0.5163474012,-0.9848059867
C,0,3.4726710335,-0.4229925851,0.3264327525
C,0,4.3420118832,0.0301493991,1.3360114164
C,0,5.6542493615,0.3732629803,1.0459047787
C,0,6.1302832213,0.2720845283,-0.272548045
C,0,2.0801046687,-0.765068856,0.6616646514
O,0,1.2247339824,-0.8678427849,-0.3172689083
B,0,-0.1660473222,-1.3245807589,-0.033732877
O,0,-0.7758079114,-0.6956742293,1.1253975426
C,0,-1.7715659783,0.1805983369,0.6754143769

C,0,-1.2687836182,1.6310580256,0.6154579945
 O,0,-0.140093872,1.9912190747,0.8704009278
 O,0,7.4309604499,0.6323320123,-0.4601342919
 O,0,-1.0125798272,-1.0705893396,-1.1663017019
 C,0,-2.1547286192,-0.3774241289,-0.7434438248
 C,0,-3.3698273059,-1.3077245448,-0.6344007616
 O,0,-3.3215470038,-2.5071527226,-0.4628298481
 C,0,0.0619041578,-3.0403659382,0.2693900979
 C,0,0.9316682329,-3.0223986506,1.4010491582
 C,0,2.2959047845,-2.791190565,1.3050705404
 O,0,-4.5119050843,-0.592202984,-0.7286610888
 C,0,-5.7807577741,-1.304853705,-0.5830722177
 C,0,-6.1370732815,-1.4050498605,0.8965898246
 C,0,-6.7980753066,-0.5242423887,-1.4032696509
 O,0,-2.2760261677,2.4549872932,0.2558287261
 C,0,-1.9901620249,3.8865788124,0.1550499741
 C,0,-2.1794809911,4.5328097382,1.5235347565
 C,0,-2.9295530277,4.4311341074,-0.9116096575
 H,0,-2.6290993791,0.1701114932,1.3595396324
 H,0,-2.403086641,0.4274476277,-1.4413602974
 H,0,0.4887637199,-3.4380036185,-0.652930576
 H,0,-0.9574683017,-3.3844918425,0.4420149921
 H,0,0.4685896948,-2.9172909724,2.3823392732
 H,0,2.9022528535,-2.7227876359,2.2037180863
 H,0,2.8256248779,-3.0781460807,0.4015190162
 H,0,1.6972778834,-0.3966194186,1.6136148307
 H,0,-0.9476390035,3.9858318584,-0.1601279226
 H,0,-5.6366887235,-2.3066185317,-0.9976874882
 H,0,3.9791966496,0.1215772004,2.3567162031
 H,0,6.3289243351,0.7293282113,1.8173257493
 H,0,5.6159235576,-0.2469801458,-2.316494322
 H,0,3.2869448158,-0.846733951,-1.7720318565
 H,0,-1.9775719133,5.6075547469,1.4596252296
 H,0,-3.2076879998,4.3957578642,1.8754106213
 H,0,-1.4925005781,4.1010485202,2.2560652939
 H,0,-2.7522430092,5.5025859825,-1.0515304544
 H,0,-2.76714563,3.927398293,-1.8689025222
 H,0,-3.9752046882,4.2896637126,-0.6188902454
 H,0,-7.7733817996,-1.0198308456,-1.3565654467
 H,0,-6.9098820248,0.4946125737,-1.0176458266
 H,0,-6.4908349069,-0.4657809481,-2.4514989754
 H,0,-7.0901372622,-1.931562317,1.0161798462
 H,0,-5.3719699504,-1.9614467296,1.4444299015
 H,0,-6.2374626861,-0.4072847984,1.3373894203
 C,0,7.9796016936,0.5656318953,-1.772823853
 H,0,9.0138667069,0.897588019,-1.6778888507

H,0,7.9599437176,-0.459886692,-2.161388722
H,0,7.4448791777,1.2303407961,-2.4621181134

B3LYP/6-31+G Onsager solvent model for dichloromethane**
panisaldehydeDIPESiTSOnsB3+G
E(RB+HF-LYP) = -1444.51911756

Zero-point correction=	0.482585 (Hartree/Particle)
Thermal correction to Energy=	0.513485
Thermal correction to Enthalpy=	0.514429
Thermal correction to Gibbs Free Energy=	0.416495
Sum of electronic and zero-point Energies=	-1444.036532
Sum of electronic and thermal Energies=	-1444.005632
Sum of electronic and thermal Enthalpies=	-1444.004688
Sum of electronic and thermal Free Energies=	-1444.102622

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	322.217	115.329	206.120

C,0,5.2447334824,-0.1342908919,-1.2847635256
C,0,3.9346844827,-0.504821466,-0.9802462016
C,0,3.4508323903,-0.433449906,0.33245442
C,0,4.3141347534,0.0228161664,1.346034304
C,0,5.6198306768,0.3908964218,1.0584549491
C,0,6.0956488183,0.3134600794,-0.2620563906
C,0,2.0634244582,-0.7977417152,0.6668609144
O,0,1.2071485925,-0.902367712,-0.3144193687
B,0,-0.1776629108,-1.3653057787,-0.030865634
O,0,-0.7940604385,-0.7440083346,1.1288254454
C,0,-1.7751344281,0.146612857,0.6740871906
C,0,-1.2490259171,1.589613035,0.6139058099
O,0,-0.1196529509,1.9311496563,0.8898115205
O,0,7.3880091645,0.6988955938,-0.4467877548
O,0,-1.0277347345,-1.1192516461,-1.1632158214
C,0,-2.1615593478,-0.4105010505,-0.7440404318
C,0,-3.3884985343,-1.3244550807,-0.6353863196
O,0,-3.3594764998,-2.5260462226,-0.4738366419
C,0,0.0573285743,-3.0843459209,0.2736958733
C,0,0.931336511,-3.0566150175,1.4004904195
C,0,2.2930661983,-2.8055486197,1.2975885192
O,0,-4.5208317404,-0.5904578084,-0.7174712522
C,0,-5.7987731916,-1.2827092618,-0.5687907619
C,0,-6.1464539855,-1.3895641065,0.912769538
C,0,-6.8093020956,-0.4780426506,-1.3743862926
O,0,-2.2350187934,2.4271587141,0.2308634243

C,0,-1.9229025221,3.8548603255,0.1298719284
 C,0,-2.1222705063,4.5090165415,1.4928619584
 C,0,-2.8357205463,4.4109805016,-0.9534491461
 H,0,-2.6345149283,0.1508630039,1.355966018
 H,0,-2.3988467857,0.3962149299,-1.4437197352
 H,0,0.4822799573,-3.4770366549,-0.651515655
 H,0,-0.959990746,-3.4318295032,0.450999727
 H,0,0.4716408653,-2.9550371652,2.3837790731
 H,0,2.9020165108,-2.7338485296,2.1942046672
 H,0,2.8223884641,-3.0925732609,0.3937392326
 H,0,1.6760061497,-0.4291209943,1.6169298983
 H,0,-0.8741314393,3.9342934294,-0.1693845257
 H,0,-5.6750452205,-2.2834629629,-0.9927417727
 H,0,3.9507433519,0.0994524657,2.367789884
 H,0,6.2889638207,0.7517694655,1.8324088412
 H,0,5.5866940553,-0.1895929968,-2.3112032878
 H,0,3.2692647325,-0.8361902405,-1.7707929091
 H,0,-1.9001281282,5.5795766649,1.4282524534
 H,0,-3.1582811797,4.391952749,1.8288461631
 H,0,-1.4543983622,4.0684812195,2.23769093
 H,0,-2.636338858,5.4781353163,-1.0955332583
 H,0,-2.66774787,3.9000675395,-1.9059796051
 H,0,-3.8882286708,4.2906442901,-0.6760472119
 H,0,-7.7928107507,-0.957101803,-1.3243576342
 H,0,-6.90027151,0.5392280442,-0.9794262372
 H,0,-6.5087697114,-0.4153205456,-2.4243017645
 H,0,-7.108464636,-1.8992123935,1.0351726212
 H,0,-5.387396524,-1.9643263894,1.4500052213
 H,0,-6.2246872045,-0.3939239892,1.3626416734
 C,0,7.9327232896,0.6746539598,-1.7632767466
 H,0,8.9590850796,1.0287452923,-1.6644627534
 H,0,7.9352653417,-0.3422310994,-2.1742925033
 H,0,7.3793459471,1.3422044557,-2.4345804761

B3LYP/6-31+G** PCM solvent model for dichloromethane

panisaldehydeDIPESiTSPCMB3+G
 E(RB+HF-LYP) = -1444.54163546

Zero-point correction=	0.481013 (Hartree/Particle)
Thermal correction to Energy=	0.511904
Thermal correction to Enthalpy=	0.512848
Thermal correction to Gibbs Free Energy=	0.415521
Sum of electronic and zero-point Energies=	-1444.060623
Sum of electronic and thermal Energies=	-1444.029731
Sum of electronic and thermal Enthalpies=	-1444.028787
Sum of electronic and thermal Free Energies=	-1444.126115

			E (Thermal)	CV	S
			KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total			321.225	115.488	204.843
1	6	0	5.305894	-0.042258	-1.266608
2	6	0	4.001870	-0.429224	-0.956076
3	6	0	3.516798	-0.347694	0.357064
4	6	0	4.373612	0.130496	1.367342
5	6	0	5.673732	0.516224	1.073053
6	6	0	6.149207	0.430777	-0.247827
7	6	0	2.139228	-0.734504	0.704825
8	8	0	1.260646	-0.816774	-0.264638
9	5	0	-0.114785	-1.322608	0.007397
10	8	0	-0.785533	-0.685334	1.132165
11	6	0	-1.810655	0.138570	0.639601
12	6	0	-1.390202	1.615922	0.587367
13	8	0	-0.287375	2.037017	0.879506
14	8	0	7.437026	0.832297	-0.439532
15	8	0	-0.940981	-1.106427	-1.160418
16	6	0	-2.119551	-0.440389	-0.786667
17	6	0	-3.320759	-1.395593	-0.739607
18	8	0	-3.248423	-2.610349	-0.736263
19	6	0	0.146425	-3.014110	0.335327
20	6	0	1.061873	-2.992233	1.436330
21	6	0	2.416948	-2.747014	1.278572
22	8	0	-4.462447	-0.693260	-0.694532
23	6	0	-5.737351	-1.418073	-0.605735
24	6	0	-6.050916	-1.698275	0.859478
25	6	0	-6.768580	-0.534512	-1.291675
26	8	0	-2.424555	2.372523	0.192985
27	6	0	-2.240673	3.826580	0.086955
28	6	0	-2.531376	4.463403	1.440918
29	6	0	-3.180034	4.287602	-1.017543
30	1	0	-2.687402	0.087270	1.296653
31	1	0	-2.356652	0.353972	-1.502863
32	1	0	0.547162	-3.425898	-0.594205
33	1	0	-0.852991	-3.389987	0.556465
34	1	0	0.643024	-2.906355	2.442153
35	1	0	3.062141	-2.678478	2.150371
36	1	0	2.905104	-3.017656	0.345853
37	1	0	1.775113	-0.396941	1.677755
38	1	0	-1.197927	4.001376	-0.197158
39	1	0	-5.612416	-2.358822	-1.152003
40	1	0	4.011995	0.205390	2.392587
41	1	0	6.337651	0.892138	1.848564

42	1	0	5.645428	-0.111534	-2.294442
43	1	0	3.349259	-0.790195	-1.747806
44	1	0	-2.406192	5.549364	1.372171
45	1	0	-3.560455	4.254261	1.752541
46	1	0	-1.846086	4.089974	2.206977
47	1	0	-3.073145	5.367383	-1.164251
48	1	0	-2.947579	3.787287	-1.962288
49	1	0	-4.222425	4.075952	-0.757024
50	1	0	-7.744039	-1.031737	-1.281404
51	1	0	-6.865159	0.426238	-0.774964
52	1	0	-6.489714	-0.344842	-2.332463
53	1	0	-7.002450	-2.235182	0.936885
54	1	0	-5.274392	-2.317676	1.317239
55	1	0	-6.137067	-0.762561	1.422379
56	6	0	7.988754	0.775333	-1.758257
57	1	0	9.012185	1.139623	-1.664989
58	1	0	7.997883	-0.252849	-2.137783
59	1	0	7.430749	1.419809	-2.447112

mPW1K/6-31G*

panisaldehydeDIPESimpw1kG

E(RmPW+HF-PW91) = -1443.99958178

Zero-point correction=	0.502237 (Hartree/Particle)
Thermal correction to Energy=	0.532001
Thermal correction to Enthalpy=	0.532945
Thermal correction to Gibbs Free Energy=	0.438198
Sum of electronic and zero-point Energies=	-1443.497345
Sum of electronic and thermal Energies=	-1443.467581
Sum of electronic and thermal Enthalpies=	-1443.466637
Sum of electronic and thermal Free Energies=	-1443.561384

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	333.836	110.892	199.413

C,0,5.1397289826,-0.0314602691,-1.1673055108
C,0,3.8258518102,-0.3990503449,-0.9410032171
C,0,3.2836304664,-0.3581244924,0.3364926043
C,0,4.0844509049,0.0686249607,1.3954956116
C,0,5.3925238578,0.4357739084,1.1842913354
C,0,5.931173543,0.3857999349,-0.1011250129
C,0,1.8889836805,-0.7261055581,0.5773410701
O,0,1.1101537666,-0.8458405603,-0.4287548915
B,0,-0.2700992334,-1.3728371863,-0.1826036254
O,0,-0.8852021752,-0.7884095168,0.9852407231

C,0,-1.8076932364,0.138928879,0.5412659028
 C,0,-1.2100530875,1.5343460341,0.4836134444
 O,0,-0.0937108062,1.8179899416,0.8150747264
 O,0,7.2153182058,0.7617399759,-0.2113900089
 O,0,-1.0972803777,-1.0696914751,-1.3034883357
 C,0,-2.2094127894,-0.3853570618,-0.8578373271
 C,0,-3.4100446453,-1.3052888238,-0.7292960823
 O,0,-3.3711245406,-2.502304604,-0.7348012226
 C,0,0.0088668321,-3.0295783454,0.0702725955
 C,0,0.844777409,-3.0105284406,1.2290862146
 C,0,2.1898017732,-2.7724793054,1.1810094238
 O,0,-4.5233008904,-0.5874219838,-0.5830733231
 C,0,-5.7498440968,-1.3078987547,-0.4027985058
 C,0,-5.8933009496,-1.710778559,1.0473541772
 C,0,-6.848910581,-0.3886497844,-0.8768754032
 O,0,-2.10788675,2.4070361659,0.0351452305
 C,0,-1.6998296161,3.779175205,-0.066501218
 C,0,-1.841366591,4.4481364945,1.2818016698
 C,0,-2.5704053265,4.3969399798,-1.1331222575
 H,0,-2.6655409562,0.1902886814,1.2136545641
 H,0,-2.4754684046,0.4276574281,-1.531517714
 H,0,0.4793575529,-3.4185242605,-0.8278141364
 H,0,-0.9856280151,-3.4381829891,0.2157864701
 H,0,0.3503215967,-2.9306733662,2.1902030683
 H,0,2.7705923317,-2.6981405853,2.0890655003
 H,0,2.7443062896,-2.9968548826,0.2813404813
 H,0,1.44475202,-0.4186399056,1.5168138387
 H,0,-0.6556485664,3.7871888219,-0.3710679732
 H,0,-5.6996970942,-2.1986012967,-1.0253658151
 H,0,3.6703339778,0.1175587553,2.3930568183
 H,0,6.02216906,0.7720199056,1.9932935634
 H,0,5.5335955026,-0.0670351665,-2.1701049675
 H,0,3.2013467284,-0.711640643,-1.7640577631
 H,0,-1.5527261441,5.4958105321,1.2130656552
 H,0,-2.8739751811,4.3984199994,1.6245216299
 H,0,-1.2007064886,3.9665150115,2.0159911863
 H,0,-2.2992169013,5.4409197917,-1.2793513608
 H,0,-2.4504944752,3.8747219987,-2.0798038591
 H,0,-3.6196732781,4.3512038897,-0.8461218128
 H,0,-7.8144012168,-0.8843124492,-0.7930668982
 H,0,-6.8753530417,0.5190617132,-0.2760510823
 H,0,-6.6951279835,-0.1075261263,-1.91636421
 H,0,-6.8297731274,-2.2456137033,1.1980155032
 H,0,-5.0773380887,-2.364612164,1.3444031064
 H,0,-5.8951594901,-0.8301895381,1.6886147074
 C,0,7.8108030804,0.7386925936,-1.4792313468

H,0,8.8322131501,1.0738389554,-1.3376011846
H,0,7.818527221,-0.2681302994,-1.8981360533
H,0,7.3042784027,1.4135038846,-2.1700077036

mPW1K/6-31+G**

panisaldehydeDIPESimpw1k+G

E(RmPW+HF-PW91) = -1444.07187176

Zero-point correction=	0.498992	(Hartree/Particle)
Thermal correction to Energy=	0.528955	
Thermal correction to Enthalpy=	0.529899	
Thermal correction to Gibbs Free Energy=	0.434290	
Sum of electronic and zero-point Energies=	-1443.572880	
Sum of electronic and thermal Energies=	-1443.542917	
Sum of electronic and thermal Enthalpies=	-1443.541973	
Sum of electronic and thermal Free Energies=	-1443.637581	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	331.924	111.533	201.226

1	6	0	5.155434	-0.110604	-1.188461
2	6	0	3.836933	-0.465044	-0.958440
3	6	0	3.306544	-0.444955	0.324553
4	6	0	4.122911	-0.053314	1.385881
5	6	0	5.435719	0.299835	1.171929
6	6	0	5.961980	0.270602	-0.119481
7	6	0	1.908463	-0.797401	0.573474
8	8	0	1.113473	-0.868700	-0.427754
9	5	0	-0.272544	-1.370347	-0.185854
10	8	0	-0.872077	-0.796093	0.996522
11	6	0	-1.780105	0.158929	0.579720
12	6	0	-1.161388	1.547406	0.558726
13	8	0	-0.050686	1.807762	0.929808
14	8	0	7.251221	0.630945	-0.235340
15	8	0	-1.102695	-1.023882	-1.293757
16	6	0	-2.199651	-0.325580	-0.829200
17	6	0	-3.422532	-1.219135	-0.718974
18	8	0	-3.408792	-2.417803	-0.732516
19	6	0	-0.033515	-3.041177	0.025165
20	6	0	0.819659	-3.070423	1.168858
21	6	0	2.170580	-2.857319	1.105127
22	8	0	-4.521894	-0.480217	-0.582506
23	6	0	-5.770498	-1.169177	-0.415022
24	6	0	-5.950120	-1.545925	1.037843
25	6	0	-6.838872	-0.233015	-0.923618

26	8	0	-2.031863	2.441884	0.103300
27	6	0	-1.611694	3.815135	0.047626
28	6	0	-1.819042	4.459555	1.398990
29	6	0	-2.421071	4.458857	-1.050756
30	1	0	-2.631863	0.209996	1.260042
31	1	0	-2.449288	0.507109	-1.484274
32	1	0	0.412563	-3.411541	-0.892557
33	1	0	-1.037953	-3.421760	0.176289
34	1	0	0.344414	-3.013105	2.141399
35	1	0	2.763161	-2.822731	2.007593
36	1	0	2.705810	-3.067046	0.190529
37	1	0	1.483287	-0.504815	1.527219
38	1	0	-0.552825	3.820354	-0.202557
39	1	0	-5.728506	-2.069976	-1.024033
40	1	0	3.718146	-0.019049	2.387816
41	1	0	6.075539	0.609244	1.983535
42	1	0	5.539287	-0.128708	-2.195294
43	1	0	3.201421	-0.749257	-1.783584
44	1	0	-1.513420	5.503591	1.363857
45	1	0	-2.869248	4.419394	1.683145
46	1	0	-1.226117	3.958913	2.159593
47	1	0	-2.134313	5.502752	-1.159999
48	1	0	-2.254330	3.956309	-2.000329
49	1	0	-3.484031	4.417078	-0.820844
50	1	0	-7.815407	-0.706976	-0.848159
51	1	0	-6.856577	0.684617	-0.338544
52	1	0	-6.662254	0.026143	-1.964612
53	1	0	-6.897920	-2.063504	1.173873
54	1	0	-5.153609	-2.208502	1.365528
55	1	0	-5.954004	-0.655730	1.664898
56	6	0	7.839284	0.627440	-1.508913
57	1	0	8.865807	0.944587	-1.366127
58	1	0	7.829550	-0.370410	-1.947875
59	1	0	7.337781	1.325465	-2.179475

mPW1K/6-31+G Onsager solvent model for dichloromethane**
panisaldehydeDIPESiOnsmpw1k+G
E(RmPW+HF-PW91) = -1444.07244437

Zero-point correction=	0.498920 (Hartree/Particle)
Thermal correction to Energy=	0.528879
Thermal correction to Enthalpy=	0.529823
Thermal correction to Gibbs Free Energy=	0.434234
Sum of electronic and zero-point Energies=	-1443.573525
Sum of electronic and thermal Energies=	-1443.543566
Sum of electronic and thermal Enthalpies=	-1443.542621

Sum of electronic and thermal Free Energies= -1443.638211

		E (Thermal)	CV	S	
		KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin	
Total		331.876	111.536	201.185	
1	6	0	5.124009	-0.100118	-1.194783
2	6	0	3.811888	-0.477308	-0.964632
3	6	0	3.285981	-0.481364	0.320395
4	6	0	4.101129	-0.092513	1.384030
5	6	0	5.407669	0.282065	1.170318
6	6	0	5.929412	0.278955	-0.123691
7	6	0	1.892896	-0.852350	0.571524
8	8	0	1.091658	-0.912885	-0.429788
9	5	0	-0.288926	-1.415459	-0.187062
10	8	0	-0.889817	-0.852008	0.999677
11	6	0	-1.773671	0.127512	0.587735
12	6	0	-1.122829	1.502189	0.585275
13	8	0	-0.016710	1.732815	0.987628
14	8	0	7.210691	0.661002	-0.238685
15	8	0	-1.124971	-1.067844	-1.291141
16	6	0	-2.199407	-0.335601	-0.826987
17	6	0	-3.452945	-1.186160	-0.730783
18	8	0	-3.486736	-2.384271	-0.761270
19	6	0	-0.051470	-3.091655	0.015169
20	6	0	0.810681	-3.120681	1.150509
21	6	0	2.160080	-2.891776	1.075683
22	8	0	-4.525407	-0.408298	-0.585209
23	6	0	-5.797344	-1.051240	-0.425618
24	6	0	-5.991616	-1.437232	1.023243
25	6	0	-6.830268	-0.070111	-0.923202
26	8	0	-1.958994	2.418250	0.111084
27	6	0	-1.503542	3.782424	0.073169
28	6	0	-1.731152	4.426123	1.421314
29	6	0	-2.266551	4.449983	-1.043759
30	1	0	-2.626472	0.192001	1.265710
31	1	0	-2.417534	0.510217	-1.476694
32	1	0	0.387348	-3.454166	-0.909062
33	1	0	-1.054578	-3.472323	0.173721
34	1	0	0.343501	-3.070205	2.127352
35	1	0	2.759535	-2.861307	1.973704
36	1	0	2.689500	-3.099847	0.157308
37	1	0	1.469305	-0.561236	1.526450
38	1	0	-0.438665	3.761702	-0.148441
39	1	0	-5.789571	-1.946541	-1.044349
40	1	0	3.699351	-0.074591	2.387640

41	1	0	6.045564	0.592136	1.983140
42	1	0	5.504224	-0.096735	-2.203151
43	1	0	3.177308	-0.757824	-1.791785
44	1	0	-1.398240	5.461991	1.399069
45	1	0	-2.789388	4.411985	1.676878
46	1	0	-1.171517	3.908312	2.195482
47	1	0	-1.950571	5.486515	-1.140493
48	1	0	-2.086479	3.947322	-1.990863
49	1	0	-3.336079	4.434702	-0.842498
50	1	0	-7.824355	-0.506972	-0.850920
51	1	0	-6.811839	0.841775	-0.329325
52	1	0	-6.644545	0.193020	-1.961617
53	1	0	-6.958285	-1.920411	1.154266
54	1	0	-5.219794	-2.132115	1.343082
55	1	0	-5.961627	-0.554547	1.660040
56	6	0	7.791618	0.703288	-1.515581
57	1	0	8.810938	1.041049	-1.369871
58	1	0	7.802722	-0.283444	-1.978870
59	1	0	7.269746	1.406168	-2.164927

M05/6-31G*

panisaldehydeDIPESiTSM05G

E(RM05+HF-M05) = -1443.53896591

Zero-point correction=	0.490981 (Hartree/Particle)
Thermal correction to Energy=	0.521464
Thermal correction to Enthalpy=	0.522408
Thermal correction to Gibbs Free Energy=	0.425607
Sum of electronic and zero-point Energies=	-1443.047985
Sum of electronic and thermal Energies=	-1443.017502
Sum of electronic and thermal Enthalpies=	-1443.016557
Sum of electronic and thermal Free Energies=	-1443.113359

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	327.224	113.736	203.737

C,0.5.2196769997,-0.1024685703,-1.2336052475
C,0,3.9001832556,-0.4494077681,-0.9703535033
C,0,3.375026891,-0.3633539165,0.3216721387
C,0,4.2071652447,0.0861230882,1.357934914
C,0,5.5215763806,0.435324089,1.1118359066
C,0,6.0407531413,0.3424779014,-0.1888135721
C,0,1.9761485393,-0.7054966382,0.6006213887
O,0,1.1642898955,-0.8423046911,-0.382260527
B,0,-0.2390137701,-1.3666865899,-0.1200268815

O,0,-0.8620249607,-0.7645148738,1.0440917487
 C,0,-1.8043732766,0.1403673826,0.5883242709
 C,0,-1.2421361727,1.5601880315,0.5305076879
 O,0,-0.1019355733,1.8700737503,0.7809093609
 O,0,0.73319553118,0.7066282098,-0.3303511903
 O,0,-1.0636968554,-1.0771875916,-1.256581528
 C,0,-2.1873628552,-0.3952514439,-0.8251510891
 C,0,-3.3934562185,-1.3229923152,-0.7043964694
 O,0,-3.3439836888,-2.5251131181,-0.5996668806
 C,0,0.0419911928,-3.0307124787,0.1471534512
 C,0,0.8873094956,-3.0192467271,1.3043951089
 C,0,2.2423694574,-2.791981229,1.2567128757
 O,0,-4.5255083555,-0.5979611107,-0.6881142298
 C,0,-5.7725739207,-1.3031258936,-0.4872116133
 C,0,-6.0007586065,-1.500810223,0.998931633
 C,0,-6.8427270223,-0.4742808861,-1.1642308229
 O,0,-2.2088608781,2.4193058282,0.1698063177
 C,0,-1.8606405749,3.8198115519,0.0552591374
 C,0,-1.9661656195,4.4761439815,1.4180480088
 C,0,-2.7990972321,4.4046340165,-0.9779953549
 H,0,-2.6751298639,0.1686436907,1.2556646467
 H,0,-2.4457421335,0.4211745236,-1.5068690029
 H,0,0.5027406954,-3.4249132762,-0.7590511548
 H,0,-0.9636242089,-3.4236358776,0.2961424373
 H,0,0.3922795714,-2.922366324,2.2703531543
 H,0,2.8243982473,-2.7219815795,2.1716997983
 H,0,2.8012214466,-3.0377093729,0.3579811821
 H,0,1.5630001565,-0.3791548255,1.5559249246
 H,0,-0.8257907319,3.8681834549,-0.2940549667
 H,0,-5.675560933,-2.2772514595,-0.9743633659
 H,0,3.8115775681,0.1682921621,2.3670749996
 H,0,6.1721701299,0.7895896203,1.9040334973
 H,0,5.5966927394,-0.1740180812,-2.2471643444
 H,0,3.2548722047,-0.7814867133,-1.7771344401
 H,0,-1.7289413572,5.5413395673,1.3435550614
 H,0,-2.9798454149,4.3775717256,1.8177788084
 H,0,-1.2639991115,4.0208076322,2.119719137
 H,0,-2.5730487941,5.4627354199,-1.1366358369
 H,0,-2.6966319653,3.8851593973,-1.9339458699
 H,0,-3.8395999948,4.3205913843,-0.6515340594
 H,0,-7.8142066969,-0.968739489,-1.0762104452
 H,0,-6.9188608021,0.5156273111,-0.7049044832
 H,0,-6.6189622587,-0.3433516152,-2.2256762198
 H,0,-6.95404759,-2.0084552451,1.172445789
 H,0,-5.2068638392,-2.113662089,1.4313813998
 H,0,-6.0260731596,-0.5371218959,1.5165757815

C,0,7.9282009153,0.637247382,-1.6056836814
 H,0,8.9569909975,0.9723571781,-1.4742392738
 H,0,7.9283702428,-0.3880185626,-1.993287207
 H,0,7.4227477161,1.2957751913,-2.3213503053

Transition structures for reaction of 43 and 44b – Re facial attack

B3LYP/6-31+G PCM solvent model for dichloromethane**
 panisaldehydeDIPEReTSPCMB3+G
 E(RB+HF-LYP) = -1444.54117082

Zero-point correction= 0.480886 (Hartree/Particle)
 Thermal correction to Energy= 0.511891
 Thermal correction to Enthalpy= 0.512835
 Thermal correction to Gibbs Free Energy= 0.414562
 Sum of electronic and zero-point Energies= -1444.060285
 Sum of electronic and thermal Energies= -1444.029280
 Sum of electronic and thermal Enthalpies= -1444.028336
 Sum of electronic and thermal Free Energies= -1444.126609

Total	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
	321.216	115.552	206.833

1	6	0	-6.204935	0.538934	-0.946570
2	6	0	-5.454761	-0.620283	-1.204410
3	6	0	-4.210203	-0.784322	-0.595629
4	6	0	-3.692735	0.193848	0.265708
5	6	0	-4.455422	1.351815	0.512672
6	6	0	-5.696047	1.526451	-0.083917
7	6	0	-2.373303	0.050738	0.904566
8	8	0	-1.532690	-0.815532	0.389244
9	5	0	-0.225580	-1.094964	1.054455
10	6	0	-0.685556	-1.905186	2.526724
11	6	0	-1.587610	-0.984281	3.152184
12	6	0	-2.900793	-0.823591	2.739505
13	8	0	-7.428660	0.798641	-1.485190
14	6	0	-8.009815	-0.160427	-2.373910
15	8	0	0.594394	-1.955045	0.241054
16	6	0	1.630098	-1.179829	-0.312578
17	6	0	1.797433	0.020483	0.673632
18	1	0	2.585932	-0.171731	1.413997
19	8	0	0.540128	0.119249	1.319382
20	1	0	1.348024	-0.796622	-1.305993
21	1	0	-1.158062	-0.210182	3.793284
22	1	0	-3.422133	-1.656849	2.275251

23	1	0	-3.529173	-0.072907	3.211218
24	1	0	-1.949265	0.962604	1.333184
25	1	0	-1.134097	-2.847270	2.201092
26	1	0	0.258624	-2.058210	3.052973
27	6	0	2.098351	1.340849	-0.042538
28	6	0	2.912429	-1.987003	-0.471602
29	1	0	-4.067045	2.124385	1.175856
30	1	0	-6.286462	2.421776	0.098416
31	1	0	-5.820794	-1.393234	-1.871553
32	1	0	-3.629429	-1.680602	-0.801554
33	1	0	-8.972325	0.257994	-2.669319
34	1	0	-7.383854	-0.304670	-3.261867
35	1	0	-8.165835	-1.121070	-1.869931
36	8	0	3.850620	-1.220711	-1.051726
37	8	0	3.070974	-3.143625	-0.131197
38	6	0	5.178566	-1.797788	-1.307946
39	6	0	5.710555	-1.090883	-2.545586
40	6	0	6.051623	-1.609566	-0.072850
41	1	0	5.032093	-2.864151	-1.508260
42	1	0	7.044856	-2.033216	-0.256239
43	1	0	6.168560	-0.545936	0.160248
44	1	0	5.621368	-2.117107	0.795008
45	1	0	6.691329	-1.500281	-2.808728
46	1	0	5.038070	-1.233489	-3.396627
47	1	0	5.822925	-0.016889	-2.364835
48	8	0	3.078975	2.013230	0.572632
49	8	0	1.495530	1.733260	-1.026190
50	6	0	3.474534	3.326140	0.039390
51	6	0	3.947358	4.138479	1.235571
52	6	0	4.545295	3.125459	-1.026393
53	1	0	2.580723	3.777255	-0.403383
54	1	0	4.236634	5.141845	0.906403
55	1	0	3.151905	4.236854	1.980312
56	1	0	4.815219	3.668136	1.710273
57	1	0	4.848958	4.097358	-1.429852
58	1	0	5.428611	2.638634	-0.599708
59	1	0	4.168001	2.516448	-1.852170

Roush ester**B3LYP/6-31G***

allylDIPEB3G

E(RB+HF-LYP) = -984.337966629

Zero-point correction=

0.340007 (Hartree/Particle)

Thermal correction to Energy=

0.362511

Thermal correction to Enthalpy= 0.363456
 Thermal correction to Gibbs Free Energy= 0.283586
 Sum of electronic and zero-point Energies= -983.997959
 Sum of electronic and thermal Energies= -983.975455
 Sum of electronic and thermal Enthalpies= -983.974511
 Sum of electronic and thermal Free Energies= -984.054380

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	227.479	79.947	168.099

C,0,-0.6928121108,3.4043810485,-0.4831929267
 B,0,-1.4939628235,2.0643779101,-0.6552349001
 O,0,-2.0351197813,1.3564288316,0.3970872275
 C,0,-2.8604069072,0.3329406739,-0.1330591621
 C,0,-4.3323654768,0.7343480689,-0.0150086763
 O,0,-5.1084427517,-0.3637466,-0.0518756739
 C,0,-6.5588200688,-0.1629525299,-0.0308221509
 C,0,0.4238437702,3.5896790401,-1.477362
 C,0,1.7050040305,3.7866859385,-1.1650577678
 O,0,-1.7763549611,1.4851450752,-1.8750105349
 C,0,-2.4364152836,0.252143912,-1.6432677746
 C,0,-1.4735841645,-0.9153330302,-1.8700280179
 O,0,-2.1748048699,-2.0405588645,-2.102864935
 C,0,-1.417307021,-3.2848213706,-2.2508315917
 O,0,-0.2699325373,-0.8357635471,-1.7941242043
 O,0,-4.7254760483,1.8761991297,0.0510831806
 H,0,-3.2957160363,0.1496780671,-2.3110999173
 H,0,-2.6920277702,-0.6067007697,0.3987373411
 H,0,-0.3197653846,3.483260539,0.5448354008
 H,0,-1.4308174954,4.2171027313,-0.6006145222
 H,0,0.1363928923,3.5388526776,-2.5276696467
 H,0,2.4676757377,3.9014246985,-1.9306235174
 H,0,0.20421375634,3.8360354691,-0.1312905553
 C,0,-2.3622610243,-4.3999504002,-1.8277968819
 C,0,-0.9270172888,-3.406873454,-3.68916844
 H,0,-0.5613072996,-3.2221189254,-1.5726289583
 C,0,-7.1450987062,-1.4336634737,0.5661925491
 H,0,-6.7533141441,0.6962812475,0.6172425708
 C,0,-7.0468460719,0.1349242933,-1.4440581099
 H,0,-0.3769130801,-4.3456748892,-3.8185027465
 H,0,-1.7720842276,-3.4038311727,-4.3866120138
 H,0,-0.2560793903,-2.5806642227,-3.9391186734
 H,0,-1.8487455168,-5.3657684224,-1.8838687094
 H,0,-2.7066544921,-4.2514832733,-0.7995194733
 H,0,-3.2386402636,-4.4373062568,-2.4840559979

H,0,-8.2339688196,-1.3427618807,0.6420249958
H,0,-6.914763118,-2.3014195469,-0.0616344715
H,0,-6.7435941416,-1.6148910484,1.5680322109
H,0,-8.1351250374,0.2620843433,-1.4454297859
H,0,-6.5969945241,1.0572885366,-1.8220512265
H,0,-6.7961443556,-0.6896005538,-2.1208635132

B3LYP/6-31+G**

allylDIPEB3+G

E(RB+HF-LYP) = -984.403985383

Zero-point correction=	0.337622	(Hartree/Particle)
Thermal correction to Energy=	0.360288	
Thermal correction to Enthalpy=	0.361233	
Thermal correction to Gibbs Free Energy=	0.280740	
Sum of electronic and zero-point Energies=	-984.066364	
Sum of electronic and thermal Energies=	-984.043697	
Sum of electronic and thermal Enthalpies=	-984.042753	
Sum of electronic and thermal Free Energies=	-984.123245	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	226.084	80.499	169.410

C,0,-0.6148705272,3.4266257475,-0.4580849538
B,0,-1.4329047093,2.0970114756,-0.6210707029
O,0,-2.1003667666,1.4869360281,0.4208405587
C,0,-2.8791792538,0.4179555562,-0.0929018759
C,0,-4.3647873236,0.7862127285,-0.0676672718
O,0,-5.1134586629,-0.3277757946,0.0167319583
C,0,-6.5737060023,-0.1783951352,-0.0227914688
C,0,0.4436988008,3.6617647577,-1.5025680886
C,0,1.7386391176,3.8759199957,-1.251423185
O,0,-1.617887369,1.4308523121,-1.814711975
C,0,-2.3709553164,0.250091981,-1.5746581665
C,0,-1.475001646,-0.9839504244,-1.706900554
O,0,-2.1861989645,-2.0255642598,-2.1733069477
C,0,-1.5042239085,-3.3204744344,-2.2947774683
O,0,-0.3074061707,-1.0152166351,-1.3870606533
O,0,-4.7910477479,1.916727896,-0.1522576666
H,0,-3.1910579004,0.1819571429,-2.29296997
H,0,-2.7178548091,-0.4809491476,0.5068112187
H,0,-0.1872600908,3.4702860324,0.5508074322
H,0,-1.3605233407,4.2391364465,-0.4992478542
H,0,0.1052668204,3.6419519673,-2.5383753159
H,0,2.4537739699,4.0309876466,-2.0540163617
H,0,2.1282611385,3.8968180884,-0.2357210687

C,0,-2.5834595228,-4.3794252795,-2.1259568046
 C,0,-0.7866478552,-3.38200682,-3.638325319
 H,0,-0.775288355,-3.3748721631,-1.4812983787
 C,0,-7.1344299097,-1.3582620134,0.7569963203
 H,0,-6.8097340174,0.7647014796,0.477789268
 C,0,-7.0346540969,-0.1259584744,-1.4748103685
 H,0,-0.2788990247,-4.3467789332,-3.7423813186
 H,0,-1.5004574853,-3.2779672796,-4.4623538949
 H,0,-0.0350697415,-2.5924203759,-3.7158119388
 H,0,-2.1345158671,-5.3764306659,-2.1799675913
 H,0,-3.0833210639,-4.2789490059,-1.1582027505
 H,0,-3.3366343778,-4.2980453056,-2.9165641239
 H,0,-8.2267453825,-1.293958489,0.7903630018
 H,0,-6.8596227241,-2.3059170938,0.2821864467
 H,0,-6.7583992111,-1.3620576034,1.7840812391
 H,0,-8.1242990414,-0.0236435571,-1.5137366117
 H,0,-6.5970325102,0.7309888081,-1.9935875565
 H,0,-6.7563681509,-1.0445291992,-2.0022112383

B3LYP/6-31+G Onsager solvent model for dichloromethane**

allylDIPEOnsB3+G

E(RB+HF-LYP) = -984.407145973

Zero-point correction=	0.337640 (Hartree/Particle)
Thermal correction to Energy=	0.360272
Thermal correction to Enthalpy=	0.361216
Thermal correction to Gibbs Free Energy=	0.281540
Sum of electronic and zero-point Energies=	-984.069506
Sum of electronic and thermal Energies=	-984.046874
Sum of electronic and thermal Enthalpies=	-984.045930
Sum of electronic and thermal Free Energies=	-984.125606

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	226.074	80.531	167.692

C,0,3.656954277,-1.7022186755,-0.1925462707
 B,0,2.225804552,-1.0488775778,-0.1775645979
 O,0,1.2735585783,-1.3056418022,-1.1383194969
 C,0,0.0397866755,-0.7360616258,-0.7153350643
 C,0,-0.9063294491,-1.8366417713,-0.222846581
 O,0,-2.1775233347,-1.4400655694,-0.3604417525
 C,0,-3.2457625735,-2.323660198,0.1391068989
 C,0,4.7265625671,-0.9191781194,0.5181720341
 C,0,5.8844369634,-0.5255950548,-0.0224481876
 O,0,1.7625489488,-0.2114446549,0.8119671384

C,0,0.4493784804,0.2173349031,0.4668815527
 C,0,0.4675796527,1.6799341369,0.0112977398
 O,0,-0.7412446663,2.2259117787,0.2016520996
 C,0,-0.9648308097,3.6078646917,-0.2552987261
 O,0,1.4267781058,2.2272437061,-0.4885965825
 O,0,-0.5332341113,-2.8872393707,0.2549460979
 H,0,-0.2117083571,0.116888098,1.3304349639
 H,0,-0.4258428684,-0.1985768656,-1.5439905054
 H,0,3.9500746685,-1.9208050529,-1.2262551843
 H,0,3.5318909082,-2.6825480816,0.2984518406
 H,0,4.5113993309,-0.6483943771,1.5517461424
 H,0,6.6064647197,0.0554034116,0.5445145624
 H,0,6.1393089869,-0.7550166497,-1.0553606171
 C,0,-2.4371713774,3.6933725186,-0.6261811325
 C,0,-0.5517706348,4.5668629498,0.8546361887
 H,0,-0.3308409973,3.7564160094,-1.1338660702
 C,0,-4.4619819551,-2.0367971659,-0.7273629251
 H,0,-2.8970528104,-3.3498823811,-0.0048967212
 C,0,-3.46550786,-2.0474301242,1.6213275183
 H,0,-0.7229025404,5.5992437409,0.5323733997
 H,0,-1.1428731472,4.3884754867,1.7588413112
 H,0,0.509245506,4.4558421404,1.0934929926
 H,0,-2.6664438485,4.6965247863,-0.9989689462
 H,0,-2.6885075741,2.9713003204,-1.4082152561
 H,0,-3.0716852464,3.4983124214,0.2440849434
 H,0,-5.2918861313,-2.6824389419,-0.4238298934
 H,0,-4.7818308683,-0.9954794042,-0.6204550319
 H,0,-4.2461881923,-2.2284021661,-1.7823148431
 H,0,-4.2661699731,-2.6900959248,2.0015450992
 H,0,-2.5610800002,-2.2575207641,2.1988864201
 H,0,-3.759715594,-1.0050017811,1.780990442

B3LYP/6-31+G PCM solvent model for dichloromethane**

allylDIPEpcmB3+G

E(RB+HF-LYP) = -984.419408447

Zero-point correction=	0.336478 (Hartree/Particle)
Thermal correction to Energy=	0.359114
Thermal correction to Enthalpy=	0.360059
Thermal correction to Gibbs Free Energy=	0.280591
Sum of electronic and zero-point Energies=	-984.082930
Sum of electronic and thermal Energies=	-984.060294
Sum of electronic and thermal Enthalpies=	-984.059350
Sum of electronic and thermal Free Energies=	-984.138817

E (Thermal)

CV

S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	225.348	80.654	167.254

C,0,-0.5965702016,3.4423500144,-0.4415008958
 B,0,-1.4122825091,2.1120657015,-0.6130712915
 O,0,-2.0804303562,1.4996776007,0.4280094072
 C,0,-2.8595791258,0.4237807401,-0.0851896576
 C,0,-4.3476381016,0.7821687955,-0.0404638697
 O,0,-5.0844330505,-0.3308389042,-0.0199570142
 C,0,-6.5538539487,-0.2100458149,-0.0539912862
 C,0,0.4396821062,3.7095755354,-1.5007353575
 C,0,1.7407023623,3.9167388403,-1.2684828442
 O,0,-1.5988699685,1.4474102938,-1.8073455503
 C,0,-2.3597665959,0.2649787142,-1.5701198081
 C,0,-1.4696851188,-0.9727566206,-1.713300406
 O,0,-2.1893888657,-2.0092677475,-2.1487341485
 C,0,-1.534880313,-3.3255027583,-2.267236757
 O,0,-0.2902365582,-0.9980032817,-1.4190982392
 O,0,-4.7760777668,1.9201105912,-0.0585555183
 H,0,-3.1800442796,0.2081607895,-2.2913361624
 H,0,-2.6861542664,-0.475286073,0.5158924496
 H,0,-0.1483560202,3.4681992113,0.5600465593
 H,0,-1.3476422587,4.2521175447,-0.4529212367
 H,0,0.0788607218,3.7296823886,-2.5314494632
 H,0,2.4388892206,4.1013617478,-2.0811147857
 H,0,2.1505396313,3.9034612291,-0.2596184457
 C,0,-2.6330834967,-4.3548264737,-2.0498959477
 C,0,-0.8636657624,-3.4231816732,-3.6316635641
 H,0,-0.7867705225,-3.3835903074,-1.4695695617
 C,0,-7.0860942791,-1.4364050054,0.6710137535
 H,0,-6.8108169142,0.703403902,0.4924957168
 C,0,-7.009386946,-0.1070234658,-1.5040300441
 H,0,-0.3798289333,-4.4005834429,-3.7314819513
 H,0,-1.6025731762,-3.3212064703,-4.4336336957
 H,0,-0.0990024099,-2.6511056118,-3.7522741658
 H,0,-2.2046235671,-5.361008471,-2.1000401088
 H,0,-3.1003061529,-4.2283004074,-1.0689565213
 H,0,-3.4063548582,-4.2701736614,-2.8206647719
 H,0,-8.1794931097,-1.3945794514,0.7046903922
 H,0,-6.7921347871,-2.3553749877,0.1532003439
 H,0,-6.7116595893,-1.477083942,1.6981392378
 H,0,-8.1007724456,-0.0238581607,-1.5390704028
 H,0,-6.587031174,0.7769090416,-1.9902715339
 H,0,-6.7138156129,-0.9987719493,-2.0668248533

mPW1K/6-31G*

allylDIPEmpw1kG

E(RmPW+HF-PW91) = -984.044199128

Zero-point correction=	0.351166 (Hartree/Particle)
Thermal correction to Energy=	0.373159
Thermal correction to Enthalpy=	0.374103
Thermal correction to Gibbs Free Energy=	0.295415
Sum of electronic and zero-point Energies=	-983.693033
Sum of electronic and thermal Energies=	-983.671041
Sum of electronic and thermal Enthalpies=	-983.670096
Sum of electronic and thermal Free Energies=	-983.748784

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	234.161	77.673	165.613

C,0,-0.6974364715,3.2597245565,-0.3896870787
 B,0,-1.4978554883,1.9353390326,-0.5916050349
 O,0,-1.9961761353,1.1859520675,0.4407787975
 C,0,-2.8524156151,0.2243235291,-0.0992046746
 C,0,-4.2930911141,0.674836447,0.0407189267
 O,0,-5.1094685389,-0.3599676538,-0.0983894922
 C,0,-6.5234879409,-0.0931520592,-0.0662959349
 C,0,0.2216636477,3.6044661267,-1.5151096128
 C,0,1.5227567033,3.8163122209,-1.3955792605
 O,0,-1.8327947192,1.4097909664,-1.810714607
 C,0,-2.4558937743,0.1780655912,-1.596560991
 C,0,-1.4796153469,-0.9546188011,-1.8451342189
 O,0,-2.1405427389,-2.0914354706,-2.0177595271
 C,0,-1.3584222096,-3.2877256122,-2.1872438456
 O,0,-0.289692041,-0.8359334048,-1.8334853912
 O,0,-4.6301544556,1.8107117487,0.2085727692
 H,0,-3.3156857125,0.0605791024,-2.2512079005
 H,0,-2.7232648848,-0.7339011587,0.3969216474
 H,0,-0.1598508231,3.2203769544,0.5576713411
 H,0,-1.4517007566,4.046912201,-0.2714940075
 H,0,-0.232839846,3.6669883026,-2.4966127753
 H,0,2.1381223248,4.0522297907,-2.2512764169
 H,0,2.0230632137,3.7560958059,-0.4381840303
 C,0,-2.2435438371,-4.4287175439,-1.7507612871
 C,0,-0.9079910304,-3.3939819616,-3.6258147768
 H,0,-0.4908246275,-3.2023666925,-1.5364798249
 C,0,-7.1790185687,-1.3792294589,0.3717069413
 H,0,-6.6870498528,0.692203885,0.6680606415
 C,0,-6.9776949368,0.3779604825,-1.4284768316

H,0,-0.3332143791,-4.3073052028,-3.7697724293
H,0,-1.7683623513,-3.4214804808,-4.2928737759
H,0,-0.277689145,-2.5501777001,-3.8938784229
H,0,-1.7015159052,-5.3694697852,-1.8250342707
H,0,-2.5654067253,-4.2983604942,-0.7198580133
H,0,-3.128199118,-4.4915990502,-2.3821459879
H,0,-8.2563049389,-1.2425157527,0.4429980179
H,0,-6.9804094901,-2.1743966083,-0.344867114
H,0,-6.8071344144,-1.6915007275,1.3449558576
H,0,-8.0495959485,0.5678421244,-1.4191893674
H,0,-6.4741751422,1.3011202841,-1.7043746163
H,0,-6.7717158659,-0.3806156003,-2.182426422

mPW1K/6-31+G**

allylDIPEmpw1k+G

E(RmPW+HF-PW91) = -984.096716555

Zero-point correction=	0.348854 (Hartree/Particle)
Thermal correction to Energy=	0.370963
Thermal correction to Enthalpy=	0.371907
Thermal correction to Gibbs Free Energy=	0.292762
Sum of electronic and zero-point Energies=	-983.747863
Sum of electronic and thermal Energies=	-983.725753
Sum of electronic and thermal Enthalpies=	-983.724809
Sum of electronic and thermal Free Energies=	-983.803954

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	232.783	78.099	166.575

C,0,-0.6595658545,3.2745751399,-0.3685693948
B,0,-1.4646159836,1.9561771749,-0.5784322951
O,0,-2.0044295739,1.2292135015,0.4498385758
C,0,-2.8460230692,0.2564424235,-0.093779678
C,0,-4.2937968191,0.6938215297,0.0178459622
O,0,-5.0974511263,-0.3542214008,-0.0829901212
C,0,-6.5178752083,-0.1100463099,-0.0786678899
C,0,0.2368869438,3.6526697007,-1.5005108838
C,0,1.539653612,3.8771047152,-1.3967475437
O,0,-1.7678121991,1.4091800329,-1.7964732233
C,0,-2.4209384291,0.1919517658,-1.5855645096
C,0,-1.4689653923,-0.96642536,-1.8122191955
O,0,-2.1525426055,-2.0791448374,-2.0382222395
C,0,-1.4039129331,-3.3000874785,-2.2000598404
O,0,-0.276478216,-0.8845065553,-1.7466063069
O,0,-4.6469619199,1.8318237251,0.1403515308

H,0,-3.2696397847,0.0908423326,-2.257149567
H,0,-2.7187142999,-0.6934398695,0.4187086461
H,0,-0.1059926487,3.2157980413,0.5683274351
H,0,-1.414537729,4.0550249029,-0.2184695649
H,0,-0.2316021301,3.734735601,-2.4740381666
H,0,2.1351942232,4.1397081377,-2.2582271161
H,0,2.0545816527,3.7983360022,-0.4487100129
C,0,-2.3348511402,-4.4173745963,-1.8008120828
C,0,-0.9175400569,-3.404195775,-3.6266587577
H,0,-0.5525638669,-3.2477973724,-1.5243291269
C,0,-7.157321956,-1.3771788652,0.4306780793
H,0,-6.6997377375,0.7151071224,0.6065802522
C,0,-6.9659091114,0.2717296791,-1.4701359608
H,0,-0.3606075765,-4.3294991463,-3.7602957832
H,0,-1.7590110815,-3.4084730514,-4.3172397072
H,0,-0.2598376429,-2.5751559084,-3.8723385993
H,0,-1.8187817071,-5.3721595366,-1.8748156132
H,0,-2.6777499962,-4.2916669307,-0.7767637287
H,0,-3.2042728486,-4.4463689299,-2.4546544013
H,0,-8.2366991793,-1.2517059225,0.4814251823
H,0,-6.9398725444,-2.2120667975,-0.2326554223
H,0,-6.7936931011,-1.622482017,1.4253796683
H,0,-8.0395422116,0.4488063438,-1.4771122143
H,0,-6.4737814866,1.1828579671,-1.7998632426
H,0,-6.7473162646,-0.5285291787,-2.1751361425

mPW1K/6-31+G Onsager solvent model for dichloromethane**

allylDIPEOnsmpw1k+G

E(RmPW+HF-PW91) = -984.099641025

Zero-point correction=	0.348754	(Hartree/Particle)
Thermal correction to Energy=	0.370906	
Thermal correction to Enthalpy=	0.371851	
Thermal correction to Gibbs Free Energy=	0.292275	
Sum of electronic and zero-point Energies=	-983.750887	
Sum of electronic and thermal Energies=	-983.728735	
Sum of electronic and thermal Enthalpies=	-983.727791	
Sum of electronic and thermal Free Energies=	-983.807366	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	232.747	78.163	167.481

C,0,3.5441258531,-1.6456107697,-0.2569756576
B,0,2.1254360172,-0.9918321707,-0.2278853195
O,0,1.2051829101,-1.1524156346,-1.2255915381

C,0,-0.0211026449,-0.6537853045,-0.7699287703
 C,0,-0.9142161448,-1.7957017291,-0.321309528
 O,0,-2.1763111404,-1.4104812417,-0.317966903
 C,0,-3.1713680922,-2.3414989734,0.1629295995
 C,0,4.5657774537,-0.9670982139,0.5916188325
 C,0,5.7400504679,-0.5218104694,0.1639058317
 O,0,1.6350742621,-0.2480295473,0.8081236117
 C,0,0.3690341467,0.2287118401,0.4452742186
 C,0,0.4475657783,1.6880351694,0.0377356571
 O,0,-0.7547256657,2.2327456489,0.0899544493
 C,0,-0.8989656796,3.6042385033,-0.3394399685
 O,0,1.4521192292,2.2348907825,-0.3204120426
 O,0,-0.5053031696,-2.871842429,0.0151671336
 H,0,-0.3279414736,0.1284500176,1.2730488242
 H,0,-0.5218129282,-0.0908515596,-1.5525420932
 H,0,3.8839665902,-1.7347149151,-1.2883704619
 H,0,3.3917602639,-2.6709437475,0.0993325023
 H,0,4.3006133253,-0.8225057559,1.6322247207
 H,0,6.4279283581,-0.0218398706,0.8296426009
 H,0,6.0424549107,-0.6264968917,-0.869624264
 C,0,-2.3255979787,3.7488266124,-0.8049801286
 C,0,-0.5438856371,4.5231805534,0.8055443014
 H,0,-0.205372579,3.7552890603,-1.1641517968
 C,0,-4.4616019614,-1.9613483619,-0.5174472637
 H,0,-2.8514201825,-3.3351997779,-0.1429572712
 C,0,-3.238920147,-2.2628088449,1.6697580106
 H,0,-0.6613657463,5.5595593293,0.4957639156
 H,0,-1.2008897879,4.3458440251,1.6548549505
 H,0,0.487191797,4.376458765,1.1155359439
 H,0,-2.4946493953,4.7599472556,-1.1682546111
 H,0,-2.5460022855,3.0546776034,-1.6120228954
 H,0,-3.0191680862,3.5600545623,0.0116122868
 H,0,-5.2531121666,-2.6430778348,-0.2148633312
 H,0,-4.7595159823,-0.9510340596,-0.245086184
 H,0,-4.3615111709,-2.012622608,-1.5986195995
 H,0,-3.9953064518,-2.9510969857,2.040899481
 H,0,-2.286879471,-2.5364374118,2.1173827442
 H,0,-3.509646395,-1.2579086203,1.9883730122

M05/6-31G*

allylDIPEM05G

E(RM05+HF-M05) = -983.747157125

Zero-point correction=	0.343949 (Hartree/Particle)
Thermal correction to Energy=	0.366068
Thermal correction to Enthalpy=	0.367012

Thermal correction to Gibbs Free Energy=	0.289265
Sum of electronic and zero-point Energies=	-983.403208
Sum of electronic and thermal Energies=	-983.381089
Sum of electronic and thermal Enthalpies=	-983.380145
Sum of electronic and thermal Free Energies=	-983.457892

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	229.711	79.172	163.633

C,0,-0.7012402163,3.3452864138,-0.4179541127
 B,0,-1.4996504922,2.0124399877,-0.6223241487
 O,0,-1.9981663696,1.2486366595,0.413800032
 C,0,-2.8432097049,0.2755499535,-0.1357834834
 C,0,-4.299540724,0.6994215141,0.0141677059
 O,0,-5.0937839407,-0.3710539192,-0.0932116528
 C,0,-6.5295236254,-0.1504716957,-0.0816766658
 C,0,0.3553491936,3.5948739712,-1.4498792226
 C,0,1.6482778876,3.7984671277,-1.1970165178
 O,0,-1.830169556,1.4837809248,-1.8550194566
 C,0,-2.4519036005,0.24588846,-1.6441304023
 C,0,-1.4777035171,-0.8945171996,-1.9179418935
 O,0,-2.1601270474,-2.0359622036,-2.0698726184
 C,0,-1.3976728917,-3.2606181709,-2.2413473834
 O,0,-0.2778336352,-0.7807917808,-1.9366186763
 O,0,-4.6652754751,1.8404103093,0.1540076121
 H,0,-3.3244936985,0.1387272968,-2.2941190848
 H,0,-2.6898192406,-0.689466459,0.3525177158
 H,0,-0.2810370408,3.372305115,0.592059002
 H,0,-1.4487140044,4.1531322238,-0.4544312613
 H,0,0.0161420943,3.5897320524,-2.4852540757
 H,0,2.3642469483,3.9622894972,-1.996861359
 H,0,2.039465152,3.8030711284,-0.1819096807
 C,0,-2.2568243769,-4.3716173547,-1.6786217327
 C,0,-1.0523929901,-3.4324701403,-3.7067318701
 H,0,-0.479233027,-3.1508857886,-1.6580727313
 C,0,-7.1448928518,-1.4214201403,0.460648047
 H,0,-6.7190512905,0.6881568909,0.5931854952
 C,0,-6.987537469,0.2077931262,-1.4812500868
 H,0,-0.489615111,-4.3587854289,-3.8533029851
 H,0,-1.9603082145,-3.4831452437,-4.3149301243
 H,0,-0.4358356371,-2.6028451883,-4.0585484061
 H,0,-1.7231751847,-5.3240212033,-1.7375874033
 H,0,-2.5033896775,-4.1814426753,-0.6312123309
 H,0,-3.1906892279,-4.4661467404,-2.2402702572
 H,0,-8.2313693235,-1.3152801485,0.5217586209

H,0,-6.9192216442,-2.2726988818,-0.188087659
H,0,-6.7655564413,-1.6412333404,1.4613780071
H,0,-8.0712620485,0.3531086108,-1.4966199126
H,0,-6.5187741822,1.136107788,-1.815591535
H,0,-6.739113798,-0.5909263476,-2.1864595076

p-anisaldehyde**B3LYP/6-31G***

panisaldehydeB3G

E(RB+HF-LYP) = -460.098688151

Zero-point correction=	0.143121	(Hartree/Particle)
Thermal correction to Energy=	0.151928	
Thermal correction to Enthalpy=	0.152872	
Thermal correction to Gibbs Free Energy=	0.109205	
Sum of electronic and zero-point Energies=	-459.955567	
Sum of electronic and thermal Energies=	-459.946760	
Sum of electronic and thermal Enthalpies=	-459.945816	
Sum of electronic and thermal Free Energies=	-459.989484	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.336	32.932	91.906

C,0,-0.0045316639,0.,0.1231946683
C,0,0.0602484416,0.,1.524462398
C,0,1.3072357013,0.,2.1468716703
C,0,2.4895169191,0.,1.3995633237
C,0,2.409355964,0.,-0.0061454086
C,0,1.1805070645,0.,-0.6387417483
H,0,-0.8417148657,0.,2.1250274946
H,0,1.362017515,0.,3.2338094731
C,0,3.7968937677,0.,2.0775236045
H,0,3.3327218413,0.,-0.5772949909
H,0,1.0966788095,0.,-1.7209004284
O,0,-1.1574730448,0.,-0.5932926917
C,0,-2.395418273,0.,0.1051961473
H,0,-3.1701790568,0.,-0.6630703597
H,0,-2.5027749578,-0.8954555693,0.7304821493
H,0,-2.5027749578,0.8954555693,0.7304821493
O,0,4.8766891455,0.,1.513624823
H,0,3.7393816389,0.,3.1899197379

B3LYP/6-31+G**

panisaldehydeB3+G

E(RB+HF-LYP) = -460.129560795

Zero-point correction=	0.142307	(Hartree/Particle)
Thermal correction to Energy=	0.151184	
Thermal correction to Enthalpy=	0.152129	
Thermal correction to Gibbs Free Energy=	0.108295	

Sum of electronic and zero-point Energies= -459.987254
 Sum of electronic and thermal Energies= -459.978376
 Sum of electronic and thermal Enthalpies= -459.977432
 Sum of electronic and thermal Free Energies= -460.021265

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	94.870	33.150	92.255

C,0,-0.0040275267,0.,0.1235798126
 C,0,0.0620113895,0.,1.5250835443
 C,0,1.3122548656,0.,2.1456702538
 C,0,2.4946782319,0.,1.3961793487
 C,0,2.4117190162,0.,-0.0114102216
 C,0,1.1802892562,0.,-0.6415454972
 H,0,-0.837351753,0.,2.1285546397
 H,0,1.3672507749,0.,3.2320582116
 C,0,3.797247505,0.,2.0832013925
 H,0,3.3316268155,0.,-0.5876129673
 H,0,1.0957750474,0.,-1.7233041608
 O,0,-1.1600871274,0.,-0.5902889921
 C,0,-2.4036015581,0.,0.1065237859
 H,0,-3.1735423449,0.,-0.6652376593
 H,0,-2.5097686789,-0.8966042985,0.7287318802
 H,0,-2.5097686789,0.8966042985,0.7287318802
 O,0,4.8847739956,0.,1.5282060192
 H,0,3.7369017702,0.,3.1935907297

B3LYP/6-31+G Onsager solvent model for dichloromethane**
 panisaldehydeB3+GOs
 E(RB+HF-LYP) = -460.135075105

Zero-point correction= 0.142298 (Hartree/Particle)
 Thermal correction to Energy= 0.151163
 Thermal correction to Enthalpy= 0.152107
 Thermal correction to Gibbs Free Energy= 0.108373
 Sum of electronic and zero-point Energies= -459.992777
 Sum of electronic and thermal Energies= -459.983912
 Sum of electronic and thermal Enthalpies= -459.982968
 Sum of electronic and thermal Free Energies= -460.026702

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	94.856	33.185	92.047

C,0,-0.0068051436,0.,0.1272109208

C,0,0.0669659041,0.,1.5313882302
 C,0,1.3174661474,0.,2.1453400353
 C,0,2.5030793023,0.,1.3932643264
 C,0,2.4128636999,0.,-0.0161821101
 C,0,1.1809747877,0.,-0.6407092542
 H,0,-0.8311300066,0.,2.1364189958
 H,0,1.3731628077,0.,3.2317083184
 C,0,3.7949754812,0.,2.080176643
 H,0,3.3296511917,0.,-0.5976858302
 H,0,1.0891296791,0.,-1.7218814121
 O,0,-1.1526775509,0.,-0.5805110713
 C,0,-2.4127375537,0.,0.1069020879
 H,0,-3.1709450294,0.,-0.6747405566
 H,0,-2.5205315761,-0.8981121155,0.7238331646
 H,0,-2.5205315761,0.8981121155,0.7238331646
 O,0,4.8987070122,0.,1.5423667839
 H,0,3.724763423,0.,3.1899795631

B3LYP/6-31+G PCM solvent model for dichloromethane**
 anisaldehydeB3+GPCM
 E(RB+HF-LYP) = -460.141637535

Zero-point correction=	0.141615 (Hartree/Particle)
Thermal correction to Energy=	0.150515
Thermal correction to Enthalpy=	0.151459
Thermal correction to Gibbs Free Energy=	0.107590
Sum of electronic and zero-point Energies=	-460.000023
Sum of electronic and thermal Energies=	-459.991123
Sum of electronic and thermal Enthalpies=	-459.990178
Sum of electronic and thermal Free Energies=	-460.034048

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	94.450	33.247	92.330

C,0,-0.0021528777,0.,0.122482637
 C,0,0.0641014923,0.,1.5252814132
 C,0,1.3142723066,0.,2.1437090574
 C,0,2.4987602396,0.,1.3908935366
 C,0,2.4145910066,0.,-0.0189090927
 C,0,1.1820310094,0.,-0.6464419646
 H,0,-0.8325928196,0.,2.1352090186
 H,0,1.369668566,0.,3.2324679499
 C,0,3.7865795354,0.,2.0884666163
 H,0,3.3297059112,0.,-0.6076293887
 H,0,1.0993871482,0.,-1.7313578336

O,0,-1.1575831569,0.,-0.5891638504
 C,0,-2.4069367737,0.,0.1110301313
 H,0,-3.1759152116,0.,-0.6616365816
 H,0,-2.5084198254,-0.896958106,0.7320363864
 H,0,-2.5084198254,0.896958106,0.7320363864
 O,0,4.8905719311,0.,1.5451187881
 H,0,3.718730389,0.,3.1971178978

mPW1K/6-31G*

panisaldehydempw1kG

E(RmPW+HF-PW91) = -459.954156981

Zero-point correction=	0.147893	(Hartree/Particle)
Thermal correction to Energy=	0.156497	
Thermal correction to Enthalpy=	0.157441	
Thermal correction to Gibbs Free Energy=	0.114162	
Sum of electronic and zero-point Energies=	-459.806264	
Sum of electronic and thermal Energies=	-459.797660	
Sum of electronic and thermal Enthalpies=	-459.796716	
Sum of electronic and thermal Free Energies=	-459.839995	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	98.203	31.977	91.090

C,0,-0.0016358886,0.,0.1252088095
 C,0,0.0597291846,0.,1.5148063286
 C,0,1.2980767227,0.,2.1346309642
 C,0,2.4703391512,0.,1.3944930367
 C,0,2.3948556988,0.,-0.0002553799
 C,0,1.1755659871,0.,-0.6296696085
 H,0,-0.837832669,0.,2.1115344637
 H,0,1.3496491321,0.,3.21541878
 C,0,3.7705767131,0.,2.0691338425
 H,0,3.3142918971,0.,-0.5662880455
 H,0,1.0920784874,0.,-1.7055059567
 O,0,-1.1415207966,0.,-0.5806121436
 C,0,-2.3596287324,0.,0.113228623
 H,0,-3.1359221507,0.,-0.6435486568
 H,0,-2.4634697471,-0.8900214301,0.7342933364
 H,0,-2.4634697471,0.8900214301,0.7342933364
 O,0,4.835355529,0.,1.5070212183
 H,0,3.7193422283,0.,3.1725290512

mPW1K/6-31+G**

panisaldehydempw1k+G

E(RmPW+HF-PW91) = -459.978576850

Zero-point correction=	0.147048 (Hartree/Particle)
Thermal correction to Energy=	0.155718
Thermal correction to Enthalpy=	0.156662
Thermal correction to Gibbs Free Energy=	0.113230
Sum of electronic and zero-point Energies=	-459.831528
Sum of electronic and thermal Energies=	-459.822859
Sum of electronic and thermal Enthalpies=	-459.821915
Sum of electronic and thermal Free Energies=	-459.865347

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	97.714	32.175	91.410

C,0,-0.0013645881,0.,0.1251368562
C,0,0.060891945,0.,1.515090551
C,0,1.3015356807,0.,2.1334966219
C,0,2.4738221279,0.,1.3916991155
C,0,2.3964899378,0.,-0.0041762862
C,0,1.1753332487,0.,-0.6319334411
H,0,-0.835150516,0.,2.1134855846
H,0,1.3541179444,0.,3.2140769249
C,0,3.770488221,0.,2.0730726453
H,0,3.3139403259,0.,-0.5734926611
H,0,1.0918214249,0.,-1.7076231023
O,0,-1.1431293628,0.,-0.5780228951
C,0,-2.3645392414,0.,0.1142764073
H,0,-3.1383789669,0.,-0.6443188689
H,0,-2.46802875,-0.8908634596,0.7334812589
H,0,-2.46802875,0.8908634596,0.7334812589
O,0,4.840482366,0.,1.517376738
H,0,3.7160769533,0.,3.175606293

mPW1K/6-31+G Onsager solvent model for dichloromethane**

panisaldehydempw1kOns+G

E(RmPW+HF-PW91) = -459.983570675

Zero-point correction=	0.147030 (Hartree/Particle)
Thermal correction to Energy=	0.155689
Thermal correction to Enthalpy=	0.156633
Thermal correction to Gibbs Free Energy=	0.113282
Sum of electronic and zero-point Energies=	-459.836541
Sum of electronic and thermal Energies=	-459.827882
Sum of electronic and thermal Enthalpies=	-459.826937
Sum of electronic and thermal Free Energies=	-459.870288

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	97.696	32.200	91.239

C,0,-0.0032875202,0.,0.128651897
C,0,0.0657909403,0.,1.520788803
C,0,1.3067171227,0.,2.1332949054
C,0,2.4807922746,0.,1.3887372621
C,0,2.3972189148,0.,-0.0084627463
C,0,1.1757410846,0.,-0.6312351691
H,0,-0.8290328922,0.,2.1206889794
H,0,1.3596111862,0.,3.2139031454
C,0,3.76822971,0.,2.0703423011
H,0,3.3117207978,0.,-0.5826146012
H,0,1.0852935403,0.,-1.7064137535
O,0,-1.1365457616,0.,-0.5694421156
C,0,-2.3711710732,0.,0.1142300191
H,0,-3.1354894272,0.,-0.6526393849
H,0,-2.4775214822,-0.8920255065,0.7292979523
H,0,-2.4775214822,0.8920255065,0.7292979523
O,0,4.8521062821,0.,1.529861003
H,0,3.7037287851,0.,3.1724255502

M05/6-31G*

panisaldehydeM05G

E(RM05+HF-M05) = -459.795289592

Zero-point correction=	0.143941 (Hartree/Particle)
Thermal correction to Energy=	0.152792
Thermal correction to Enthalpy=	0.153736
Thermal correction to Gibbs Free Energy=	0.109955
Sum of electronic and zero-point Energies=	-459.651349
Sum of electronic and thermal Energies=	-459.642498
Sum of electronic and thermal Enthalpies=	-459.641553
Sum of electronic and thermal Free Energies=	-459.685334

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.878	32.988	92.144

C,0,-0.0068412748,0.,0.1282590666
C,0,0.0604916645,0.,1.5275569555
C,0,1.3061943964,0.,2.1464072548
C,0,2.4852097505,0.,1.4007304467
C,0,2.4023265532,0.,-0.0013230864

C,0,1.1765139384,0.,-0.6328596253
 H,0,-0.8393260123,0.,2.1309488257
 H,0,1.3593482355,0.,3.2329030844
 C,0,3.795598741,0.,2.0703831959
 H,0,3.325547797,0.,-0.5717708926
 H,0,1.0920800786,0.,-1.714509094
 O,0,-1.1518901483,0.,-0.5811773904
 C,0,-2.3859029973,0.,0.1011886679
 H,0,-3.1551630721,0.,-0.670875184
 H,0,-2.4974484142,-0.8944570298,0.7246254979
 H,0,-2.4974484142,0.8944570298,0.7246254979
 O,0,4.8676560252,0.,1.5027824528
 H,0,3.7394331528,0.,3.1828153265

***p*-nitrobenzaldehyde**

B3LYP/6-31+G PCM solvent model for dichloromethane**

PNBpcmB3+G

E(RB+HF-LYP) = -550.118460808

Zero-point correction=	0.111176 (Hartree/Particle)
Thermal correction to Energy=	0.120097
Thermal correction to Enthalpy=	0.121041
Thermal correction to Gibbs Free Energy=	0.076009
Sum of electronic and zero-point Energies=	-550.007285
Sum of electronic and thermal Energies=	-549.998364
Sum of electronic and thermal Enthalpies=	-549.997420
Sum of electronic and thermal Free Energies=	-550.042451

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.362	32.719	94.777

C,0,0.0037281027,0.,-0.0844583634
 C,0,-0.030379981,0.,1.3179860863
 C,0,1.1649082345,0.,2.0579038129
 C,0,2.389890309,0.,1.4008778511
 C,0,2.3939338945,0.,0.0017396552
 C,0,1.2237644991,0.,-0.7580639316
 C,0,-1.348899407,0.,2.0000742423
 O,0,-1.4950593745,0.,3.213642053
 H,0,1.1231112956,0.,3.1449767583
 H,0,3.3249992057,0.,1.9526587267
 N,0,3.6889252991,0.,-0.699559897
 H,0,1.2686899289,0.,-1.8425749555
 H,0,-2.2300968679,0.,1.3253215735

O,0,3.6828492327,0.,-1.9327876501
 O,0,4.7179296926,0.,-0.0197692687
 H,0,-0.926255064,0.,-0.652460693

mPW1K/6-31G*

PNBmpw1kG

E(RmPW+HF-PW91) = -549.878481355

Zero-point correction=	0.117015 (Hartree/Particle)
Thermal correction to Energy=	0.125624
Thermal correction to Enthalpy=	0.126568
Thermal correction to Gibbs Free Energy=	0.082298
Sum of electronic and zero-point Energies=	-549.761467
Sum of electronic and thermal Energies=	-549.752857
Sum of electronic and thermal Enthalpies=	-549.751913
Sum of electronic and thermal Free Energies=	-549.796184

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.830	31.414	93.175

C,0,0.0156828262,0.,-0.0872253369
 C,0,-0.0219223269,0.,1.301222405
 C,0,1.1583027724,0.,2.0385429409
 C,0,2.3759412464,0.,1.3910608902
 C,0,2.3851790389,0.,0.0058554055
 C,0,1.2285990622,0.,-0.750427401
 C,0,-1.3237971068,0.,2.0014777143
 O,0,-1.4396425273,0.,3.1960104879
 H,0,1.0976439857,0.,3.1159756696
 H,0,3.309401372,0.,1.9286604062
 N,0,3.6692499871,0.,-0.6851364876
 H,0,1.2944071401,0.,-1.8254569822
 H,0,-2.2089798623,0.,1.3444059159
 O,0,3.6512973667,0.,-1.8927512435
 O,0,4.6669247425,0.,-0.0050911837
 H,0,-0.9062487169,0.,-0.6516162004

mPW1K/6-31+G**

PNBmpw1k+G

E(RmPW+HF-PW91) = -549.902877995

Zero-point correction=	0.116365 (Hartree/Particle)
Thermal correction to Energy=	0.125024
Thermal correction to Enthalpy=	0.125968
Thermal correction to Gibbs Free Energy=	0.081583

Sum of electronic and zero-point Energies= -549.786513
 Sum of electronic and thermal Energies= -549.777854
 Sum of electronic and thermal Enthalpies= -549.776910
 Sum of electronic and thermal Free Energies= -549.821295

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.453	31.599	93.416

C,0,0.0152231212,0.,-0.0847695813
 C,0,-0.0212281751,0.,1.30460902
 C,0,1.1603395149,0.,2.0415169614
 C,0,2.3781124968,0.,1.3917699935
 C,0,2.3859103643,0.,0.0055642318
 C,0,1.2283598784,0.,-0.7503427532
 C,0,-1.3269359025,0.,1.9991090271
 O,0,-1.4497564117,0.,3.194165462
 H,0,1.1025710905,0.,3.1191933557
 H,0,3.3119462626,0.,1.9291249802
 N,0,3.6711770987,0.,-0.6873857225
 H,0,1.2920649775,0.,-1.8257165317
 H,0,-2.2103519051,0.,1.3403218724
 O,0,3.65177732,0.,-1.8956964752
 O,0,4.6698513776,0.,-0.0075447265
 H,0,-0.9070221082,0.,-0.6484121136

mPW1K/6-31+G** Onsager solvent model for dichlormethane

PNBmpw1k+GOns

E(RmPW+HF-PW91) = -549.904196794

Zero-point correction= 0.116311 (Hartree/Particle)
 Thermal correction to Energy= 0.124982
 Thermal correction to Enthalpy= 0.125926
 Thermal correction to Gibbs Free Energy= 0.081489
 Sum of electronic and zero-point Energies= -549.787886
 Sum of electronic and thermal Energies= -549.779215
 Sum of electronic and thermal Enthalpies= -549.778270
 Sum of electronic and thermal Free Energies= -549.822708

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.427	31.624	93.526

C,0,0.0137233365,0.,-0.0904408462
 C,0,-0.0240703725,0.,1.2984426169
 C,0,1.1565587662,0.,2.036511188

C,0,2.3747546043,0.,1.3897181584
 C,0,2.3852026639,0.,0.003274336
 C,0,1.2285573945,0.,-0.7542506287
 C,0,-1.327375123,0.,2.0031677733
 O,0,-1.4281423924,0.,3.199843179
 H,0,1.0945879871,0.,3.1139569078
 H,0,3.307068796,0.,1.9292552886
 N,0,3.6719002527,0.,-0.6835221409
 H,0,1.2910144933,0.,-1.8297750435
 H,0,-2.2188593649,0.,1.3573694342
 O,0,3.6632695657,0.,-1.8916896671
 O,0,4.6711201765,0.,-0.0004703523
 H,0,-0.907271784,0.,-0.6558832036

M05/6-31G*

PNBM05G

E(RM05+HF-M05) = -549.756749379

Zero-point correction=	0.113676	(Hartree/Particle)
Thermal correction to Energy=	0.122520	
Thermal correction to Enthalpy=	0.123465	
Thermal correction to Gibbs Free Energy=	0.078629	
Sum of electronic and zero-point Energies=	-549.643074	
Sum of electronic and thermal Energies=	-549.634229	
Sum of electronic and thermal Enthalpies=	-549.633285	
Sum of electronic and thermal Free Energies=	-549.678121	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	76.883	32.395	94.365

C,0,0.0074521792,0.,-0.0880836078
 C,0,-0.0329474338,0.,1.3086013493
 C,0,1.1560955014,0.,2.0474565115
 C,0,2.3798770228,0.,1.3961044967
 C,0,2.3906297044,0.,0.0037090535
 C,0,1.2260662645,0.,-0.7548066104
 C,0,-1.3411226459,0.,2.0134167558
 O,0,-1.4659677801,0.,3.2159303624
 H,0,1.0968242429,0.,3.130840309
 H,0,3.3189250263,0.,1.9357024887
 N,0,3.6951116846,0.,-0.6999390582
 H,0,1.2918286368,0.,-1.8357913154
 H,0,-2.2260444531,0.,1.3409055099
 O,0,3.6730965714,0.,-1.9166600181
 O,0,4.700714848,0.,-0.0152170759

H,0,-0.9185013694,0.,-0.656661151

Roush ester dimethyl ester derivative

B3LYP/6-31G*

allylDMEB3G

E(RB+HF-LYP) = -827.062272269

Zero-point correction=	0.226861	(Hartree/Particle)
Thermal correction to Energy=	0.244202	
Thermal correction to Enthalpy=	0.245146	
Thermal correction to Gibbs Free Energy=	0.177099	
Sum of electronic and zero-point Energies=	-826.835411	
Sum of electronic and thermal Energies=	-826.818070	
Sum of electronic and thermal Enthalpies=	-826.817126	
Sum of electronic and thermal Free Energies=	-826.885174	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	153.239	59.161	143.218

C,0,-0.7698531148,3.3651023688,-0.6738870105
 C,0,0.3045061483,3.514280985,-1.7195194712
 C,0,1.593460716,3.7445198736,-1.4681898587
 B,0,-1.558070392,2.0090696664,-0.7464877979
 O,0,-1.8639074892,1.3558080867,-1.9226508276
 C,0,-2.5071765335,0.1341191653,-1.6040204284
 C,0,-1.5408986304,-1.03554667,-1.7926634578
 O,0,-0.3370427086,-0.9558896897,-1.754068784
 O,0,-2.0652142028,1.3581286739,0.3587527427
 C,0,-2.8903982002,0.2961255707,-0.0885823711
 C,0,-4.3615701672,0.6881698877,0.0496859027
 O,0,-4.7780117635,1.8221072657,0.0447823083
 O,0,-5.1295567473,-0.416321382,0.1178956296
 C,0,-6.5495302622,-0.1799230515,0.1702612105
 O,0,-2.235436154,-2.1799201903,-1.9524814126
 C,0,-1.4393165715,-3.3749627687,-2.0647423488
 H,0,-3.3831922758,-0.0115085107,-2.2414171737
 H,0,-2.6950279371,-0.6091310745,0.4915531549
 H,0,-0.3585189906,3.5006997014,0.3334876805
 H,0,-1.5235726681,4.161687399,-0.8018584421
 H,0,-0.0226225705,3.4065125631,-2.7537770133
 H,0,2.3239208484,3.8310652679,-2.2680553866
 H,0,1.9695195589,3.8510757869,-0.4523173364
 H,0,-2.1529920735,-4.1920441675,-2.1694954815
 H,0,-0.7882968047,-3.3159228325,-2.9405109267

H,0,-0.824663238,-3.5100799408,-1.1710656094
H,0,-7.008500186,-1.1679178057,0.2027389639
H,0,-6.8054007695,0.3946269377,1.0639469755
H,0,-6.8776628206,0.3706048842,-0.7150974302

B3LYP/6-31+G**

allylDMEB3+G

E(RB+HF-LYP) = -827.114947692

Zero-point correction=	0.225457	(Hartree/Particle)
Thermal correction to Energy=	0.242847	
Thermal correction to Enthalpy=	0.243791	
Thermal correction to Gibbs Free Energy=	0.175992	
Sum of electronic and zero-point Energies=	-826.889491	
Sum of electronic and thermal Energies=	-826.872101	
Sum of electronic and thermal Enthalpies=	-826.871157	
Sum of electronic and thermal Free Energies=	-826.938956	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	152.389	59.493	142.695

C,0,-0.711854156,3.3838584756,-0.6503054992
C,0,0.3217933868,3.5863654714,-1.7264865527
C,0,1.6165540217,3.8372576647,-1.5113991919
B,0,-1.5078996538,2.0345024732,-0.7328535256
O,0,-1.7264111225,1.3205804311,-1.8929862109
C,0,-2.4466427732,0.1380589639,-1.5820551569
C,0,-1.5374065455,-1.0847958708,-1.7101827425
O,0,-0.3454648331,-1.0874453881,-1.5061220193
O,0,-2.1207156909,1.448886956,0.3567160519
C,0,-2.8974926994,0.3476123549,-0.0860946018
C,0,-4.3859148179,0.6900940064,-0.0114374058
O,0,-4.8488056984,1.799412664,-0.1497894613
O,0,-5.112382728,-0.4272922359,0.1806567682
C,0,-6.5465886426,-0.2556438322,0.1958007296
O,0,-2.2645814986,-2.1718865871,-2.0340624236
C,0,-1.5375878628,-3.4174519591,-2.1142392918
H,0,-3.2952616132,0.0304514643,-2.2617703873
H,0,-2.6945272021,-0.5263508234,0.5373528064
H,0,-0.2657567685,3.484177981,0.3463722747
H,0,-1.4730352578,4.18029535,-0.7161372406
H,0,-0.0357605299,3.5089019931,-2.7530442576
H,0,2.3132851041,3.9660447535,-2.3345009205
H,0,2.0245144197,3.9160169849,-0.5057851804
H,0,-2.2824862461,-4.1702938627,-2.3681411017

H,0,-0.7694210561,-3.3541702906,-2.8879274681
H,0,-1.0672691145,-3.6434467506,-1.1546053399
H,0,-6.9547159122,-1.2535210536,0.3498633641
H,0,-6.8357171642,0.4126010203,1.0097343672
H,0,-6.887473345,0.1617156456,-0.7543503827

B3LYP/6-31+G Onsager solvent model for dichloromethane**

DMEOns+G

E(RB+HF-LYP) = -827.117299967

Zero-point correction=	0.225465 (Hartree/Particle)
Thermal correction to Energy=	0.242834
Thermal correction to Enthalpy=	0.243778
Thermal correction to Gibbs Free Energy=	0.176546
Sum of electronic and zero-point Energies=	-826.891835
Sum of electronic and thermal Energies=	-826.874466
Sum of electronic and thermal Enthalpies=	-826.873522
Sum of electronic and thermal Free Energies=	-826.940754

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	152.381	59.522	141.501

C,0,-0.7174359549,3.3669153894,-0.6345646916
C,0,0.3027751285,3.5883569795,-1.7179982602
C,0,1.5973771516,3.8540258961,-1.5163011715
B,0,-1.5077528157,2.0111862041,-0.7259207017
O,0,-1.7514511409,1.32708803,-1.8964176531
C,0,-2.4529163211,0.1289642581,-1.5884460278
C,0,-1.5283530032,-1.0809749038,-1.7393673808
O,0,-0.3258075866,-1.0550144917,-1.6040883629
O,0,-2.0861528624,1.4022141882,0.3663885773
C,0,-2.8892174178,0.3204847488,-0.0879738807
C,0,-4.3707035573,0.6935278739,0.0036028325
O,0,-4.8029871171,1.8213582106,-0.085610234
O,0,-5.1171036519,-0.4125260309,0.1460094234
C,0,-6.5514984785,-0.2239799329,0.1670256867
O,0,-2.2549440495,-2.1815461522,-1.9946828528
C,0,-1.5258640163,-3.4273006026,-2.0843410976
H,0,-3.3074431938,0.0160255834,-2.2594060213
H,0,-2.6988155199,-0.5667355874,0.5197987555
H,0,-0.2632469578,3.4602806133,0.3590337737
H,0,-1.4872559713,4.1558051362,-0.6877940032
H,0,-0.0630874106,3.506543651,-2.7413498851
H,0,2.2847350371,3.9872803372,-2.3469029764
H,0,2.0153875092,3.9303553236,-0.5144136611

H,0,-2.2803457796,-4.1891323559,-2.2730023404
H,0,-0.8064544667,-3.380608207,-2.9044401291
H,0,-0.9997003398,-3.6241055042,-1.1478225498
H,0,-6.9708663581,-1.2222648533,0.279421828
H,0,-6.831820306,0.4131955448,1.0081424588
H,0,-6.8840765495,0.2351166536,-0.7663594545

B3LYP/6-31+G** PCM solvent model for dichloromethane

DMEPCM+G

E(RB+HF-LYP) = -827.130582461

Zero-point correction=	0.224623 (Hartree/Particle)
Thermal correction to Energy=	0.241915
Thermal correction to Enthalpy=	0.242859
Thermal correction to Gibbs Free Energy=	0.176251
Sum of electronic and zero-point Energies=	-826.905960
Sum of electronic and thermal Energies=	-826.888668
Sum of electronic and thermal Enthalpies=	-826.887724
Sum of electronic and thermal Free Energies=	-826.954331

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	151.804	59.576	140.188

C,0,-0.7020974547,3.3645311607,-0.6257528998
C,0,0.2953034569,3.602455877,-1.7288806015
C,0,1.5978971477,3.8466476931,-1.547426585
B,0,-1.5019823565,2.0179125224,-0.7185870014
O,0,-1.7636426118,1.3334262725,-1.8878142096
C,0,-2.4651020269,0.13366144,-1.5776482614
C,0,-1.5421983716,-1.0743352025,-1.7459430046
O,0,-0.3306235358,-1.035739892,-1.68140531
O,0,-2.0748640551,1.4014072176,0.3770423067
C,0,-2.8823490819,0.3178927925,-0.0711576729
C,0,-4.3626369155,0.6854389539,0.0440294922
O,0,-4.7937039899,1.8205716935,0.0690929015
O,0,-5.1134974831,-0.4215041898,0.0697392458
C,0,-6.5501121432,-0.23401807,0.0979384489
O,0,-2.2663373169,-2.1839678622,-1.9367328828
C,0,-1.5332385287,-3.4295097406,-2.0383303519
H,0,-3.326582517,0.0236747077,-2.2455237924
H,0,-2.6827729741,-0.5718253228,0.5362057346
H,0,-0.2239086457,3.4392404016,0.3591281046
H,0,-1.4669176414,4.1613367659,-0.6478588783
H,0,-0.0978130933,3.5683308996,-2.7473552895
H,0,2.2663213153,4.0086961204,-2.3893449471

H,0,2.0386919176,3.8890299958,-0.5525192781
H,0,-2.2926632578,-4.1988543274,-2.1695072799
H,0,-0.8615158297,-3.3968097211,-2.898749929
H,0,-0.9591835827,-3.6022198283,-1.1253559105
H,0,-6.9695639899,-1.2388978376,0.1046572458
H,0,-6.8367295508,0.312214098,0.9990651459
H,0,-6.8732028837,0.3157493822,-0.7887845403

Chapter 5 – Mechanism of Mukaiyama Aldol Reaction

p-tolualdehyde 49

B3LYP/6-31G*

ptol-B3G

E(RB+HF-LYP) = -384.892341620

Zero-point correction=	0.137704 (Hartree/Particle)
Thermal correction to Energy=	0.145903
Thermal correction to Enthalpy=	0.146848
Thermal correction to Gibbs Free Energy=	0.103384
Sum of electronic and zero-point Energies=	-384.754638
Sum of electronic and thermal Energies=	-384.746438
Sum of electronic and thermal Enthalpies=	-384.745494
Sum of electronic and thermal Free Energies=	-384.788957

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.556	29.856	91.476

C,0,1.2032971879,-0.0885654862,2.1632601653
C,0,-0.0090037525,-0.0002158422,1.4538670885
C,0,-1.2033480157,0.0880320179,2.1802024285
C,0,-1.1916775835,0.0881073046,3.5739420406
C,0,0.0187272022,-0.0002678165,4.2702581386
C,0,1.2215834825,-0.0889927431,3.5505153486
C,0,-0.0110310891,-0.0022425756,-0.0556923315
C,0,0.0256537806,0.0003108948,5.7478455833
O,0,1.024471729,-0.0724937145,6.4392560992
H,0,0.5800128151,0.831535254,-0.4542654155
H,0,0.4306284995,-0.9252544283,-0.4513844418
H,0,-1.0253077715,0.0830689041,-0.4570155013
H,0,-2.1486835143,0.1571780486,1.6476602979
H,0,-2.1262599032,0.157217033,4.1272090901
H,0,2.1534559099,-0.1568593577,4.1038336496
H,0,2.138347857,-0.157366148,1.6116204154
H,0,-0.9826108341,0.074627655,6.2144893444

B3LYP/6-31+G**

ptol-B3+G

E(RB+HF-LYP) = -384.919910249

Zero-point correction=	0.137012 (Hartree/Particle)
Thermal correction to Energy=	0.145233
Thermal correction to Enthalpy=	0.146177
Thermal correction to Gibbs Free Energy=	0.103009
Sum of electronic and zero-point Energies=	-384.782899
Sum of electronic and thermal Energies=	-384.774678
Sum of electronic and thermal Enthalpies=	-384.773733
Sum of electronic and thermal Free Energies=	-384.816901

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.135	30.022	90.854

C,0,1.2048443347,-0.0889127316,2.1603817002
C,0,-0.0092756663,-0.0002486744,1.4511437012
C,0,-1.2034563603,0.0881795486,2.1802617582
C,0,-1.1887972474,0.088111978,3.5755111928
C,0,0.023672291,-0.0006096099,4.272019668
C,0,1.2265277456,-0.0895477471,3.5491413769
C,0,-0.0121379361,-0.0021454887,-0.058229695
C,0,0.0203853506,0.0006976327,5.7494570755
O,0,1.0147164669,-0.0721080691,6.4516625657
H,0,0.5772846578,0.8327831595,-0.4544722392
H,0,0.4305949402,-0.9246089014,-0.451626409
H,0,-1.0263112955,0.0816441306,-0.4578753014
H,0,-2.1500745652,0.1575094674,1.6511170494
H,0,-2.1227015778,0.1573223744,4.1289775088
H,0,2.1612587346,-0.1578166339,4.097030964
H,0,2.1392440446,-0.1578471844,1.6085703916
H,0,-0.9875199174,0.0754157493,6.2125296924

B3LYP/6-31G* PCM solvent model for dichloromethane

ptol-PCM-B3G

E(RB+HF-LYP) = -384.900517222

Zero-point correction=	0.137194 (Hartree/Particle)
Thermal correction to Energy=	0.145409
Thermal correction to Enthalpy=	0.146353
Thermal correction to Gibbs Free Energy=	0.102646
Sum of electronic and zero-point Energies=	-384.763323
Sum of electronic and thermal Energies=	-384.755108
Sum of electronic and thermal Enthalpies=	-384.754164

Sum of electronic and thermal Free Energies= -384.797871

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.246	29.893	91.990

C,0,1.2062640837,-0.0885196148,2.1613686522
C,0,-0.0090898617,-0.000183483,1.454574231
C,0,-1.2040734293,0.0880997375,2.182122026
C,0,-1.1909609046,0.0883668458,3.5761197218
C,0,0.0228605525,-0.0002759119,4.2709280533
C,0,1.226424379,-0.0890787251,3.5487901242
C,0,-0.0126735048,-0.0022767598,-0.0545495787
C,0,0.0194065922,0.0006103938,5.7431298913
O,0,1.0169273899,-0.0745792861,6.447589342
H,0,0.579516184,0.8314747655,-0.4518761167
H,0,0.4317877028,-0.9247836454,-0.4486999955
H,0,-1.0275762381,0.082029866,-0.4542680394
H,0,-2.1521954204,0.1572508949,1.6511280962
H,0,-2.126433638,0.1575941208,4.1314078413
H,0,2.1652709464,-0.1574222163,4.0942628154
H,0,2.1423818481,-0.1572693063,1.6082438509
H,0,-0.9895826817,0.0767813244,6.2053300846

Titanium tetrachloride

B3LYP/6-31G*

TiCl4-B3G

E(RB+HF-LYP) = -2690.47851346

Zero-point correction=	0.005761	(Hartree/Particle)
Thermal correction to Energy=	0.012987	
Thermal correction to Enthalpy=	0.013931	
Thermal correction to Gibbs Free Energy=	-0.026050	
Sum of electronic and zero-point Energies=	-2690.472752	
Sum of electronic and thermal Energies=	-2690.465527	
Sum of electronic and thermal Enthalpies=	-2690.464583	
Sum of electronic and thermal Free Energies=	-2690.504564	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	8.149	20.846	84.147

Ti,0,-0.0000001889,0.,-0.0000001889
Cl,0,-0.0000002297,0.0000001531,2.1777295848
Cl,0,2.0531831455,0.0000002146,-0.7259100749

Cl,0,-1.0265916056,-1.7781090983,-0.7259100077
 Cl,0,-1.0265920658,1.7781087305,-0.7259102578

B3LYP/6-31+G**

TiCl4-B3+G

E(RB+HF-LYP) = -2690.49053183

Zero-point correction=	0.005704	(Hartree/Particle)
Thermal correction to Energy=	0.012961	
Thermal correction to Enthalpy=	0.013905	
Thermal correction to Gibbs Free Energy=	-0.026177	
Sum of electronic and zero-point Energies=	-2690.484828	
Sum of electronic and thermal Energies=	-2690.477571	
Sum of electronic and thermal Enthalpies=	-2690.476627	
Sum of electronic and thermal Free Energies=	-2690.516709	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	8.133	20.888	84.359

Ti,0,-0.0000001889,0.,-0.0000001889
 Cl,0,-0.0000002298,0.0000001534,2.1807045405
 Cl,0,2.0559879606,0.0000002149,-0.7269017268
 Cl,0,-1.0279940128,-1.7805381397,-0.7269016594
 Cl,0,-1.0279944736,1.7805377714,-0.7269019098

B3LYP/gen (SDD on Ti, 6-31G* on Cl) PCM solvent model for dichloromethane

TiCl4-PCM-B3G-SDD

E(RB+HF-LYP) = -1899.38448916

Zero-point correction=	0.005573	(Hartree/Particle)
Thermal correction to Energy=	0.012876	
Thermal correction to Enthalpy=	0.013820	
Thermal correction to Gibbs Free Energy=	-0.026332	
Sum of electronic and zero-point Energies=	-1899.378916	
Sum of electronic and thermal Energies=	-1899.371613	
Sum of electronic and thermal Enthalpies=	-1899.370669	
Sum of electronic and thermal Free Energies=	-1899.410821	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	8.080	21.012	84.507

Ti,0,-0.0000001889,0.,-0.0000001889
 Cl,0,-0.0000002296,0.0000001526,2.1701390779
 Cl,0,2.046026747,0.0000002139,-0.7233799061

Cl,0,-1.0230134072,-1.7719114748,-0.7233798391
 Cl,0,-1.0230138657,1.7719111083,-0.7233800883

TMS enol ether of pinacolone **48**

B3LYP/6-31G*

TMS-enol-ether-pinacolone-B3G

E(RB+HF-LYP) = -719.784995546

Zero-point correction=	0.272281 (Hartree/Particle)
Thermal correction to Energy=	0.288762
Thermal correction to Enthalpy=	0.289706
Thermal correction to Gibbs Free Energy=	0.228515
Sum of electronic and zero-point Energies=	-719.512714
Sum of electronic and thermal Energies=	-719.496234
Sum of electronic and thermal Enthalpies=	-719.495289
Sum of electronic and thermal Free Energies=	-719.556481

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	181.201	59.899	128.788

C,0,0.3699895077,-0.5124527149,-0.3445404814
 O,0,0.5910237154,-0.6370139631,1.0032847267
 C,0,1.3950751469,0.4252024629,-0.9826105756
 C,0,2.8132860385,-0.1400653655,-0.7363186608
 C,0,1.1726985969,0.5741593124,-2.49719551
 C,0,1.2776587802,1.8169628079,-0.3181223782
 C,0,-0.6254972141,-1.1340705192,-0.9909492736
 H,0,-1.3317982863,-1.7783234326,-0.4793830138
 H,0,-0.768061785,-1.0097682496,-2.055487361
 H,0,1.9246143231,1.25316426,-2.9150988194
 H,0,1.2655363551,-0.3862778182,-3.0163610924
 H,0,0.1850762374,0.9920042523,-2.7216650523
 H,0,0.026911662,2.5001790174,-0.7357851245
 H,0,0.2865817062,2.2516700099,-0.4934522192
 H,0,1.4357248275,1.7520068593,0.7618738176
 H,0,3.5676833112,0.5296736087,-1.1663618909
 H,0,3.0160212218,-0.2430849666,0.3331915564
 H,0,2.928492663,-1.1252589813,-1.2035776894
 Si,0,-0.1043910664,-1.6298985517,2.1841721807
 C,0,0.86143917,-1.2013198819,3.7397183
 C,0,-1.9293425225,-1.213180666,2.4242043322
 C,0,0.1324226576,-3.4461085481,1.7329431109
 H,0,-0.2906967222,-4.0960452337,2.5091378386
 H,0,-0.3476408948,-3.7037622886,0.7831444974

H,0,1.1977132637,-3.6882498835,1.6415847628
H,0,0.5141146357,-1.793741996,4.5950365823
H,0,1.9317669956,-1.3972371478,3.6094823021
H,0,0.745072003,-0.1425175097,3.9976997748
H,0,-2.3383796999,-1.7698272474,3.2770165687
H,0,-2.0586047066,-0.1448787973,2.6340643201
H,0,-2.5400839208,-1.4536408283,1.5477014712

B3LYP/6-31+G**

TMS-enol-ether-pinacolone-B3+G
E(RB+HF-LYP) = -719.830380998

Zero-point correction=	0.270196 (Hartree/Particle)
Thermal correction to Energy=	0.286775
Thermal correction to Enthalpy=	0.287719
Thermal correction to Gibbs Free Energy=	0.225609
Sum of electronic and zero-point Energies=	-719.560185
Sum of electronic and thermal Energies=	-719.543606
Sum of electronic and thermal Enthalpies=	-719.542662
Sum of electronic and thermal Free Energies=	-719.604772

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.954	60.361	130.722

C,0,0.3854835131,-0.5372488026,-0.3589288018
O,0,0.6116370398,-0.6849630322,0.982886957
C,0,1.3964530441,0.4267718825,-0.9827014664
C,0,2.8226838741,-0.1298564151,-0.7569657998
C,0,1.1647340845,0.6090624961,-2.4930639904
C,0,1.2687076473,1.8024810554,-0.2852669921
C,0,-0.6043340934,-1.1652681137,-1.0140842676
H,0,-1.2927707728,-1.8324776135,-0.5091042146
H,0,-0.7525777754,-1.0233211586,-2.0750964971
H,0,1.9079545717,1.3058858262,-2.8953196587
H,0,1.2671238749,-0.3362959108,-3.0363032197
H,0,0.1729687939,1.0226567682,-2.7041096035
H,0,2.0070900753,2.5015406662,-0.6942130817
H,0,0.2721856689,2.2301116669,-0.4425808576
H,0,1.4379179702,1.7138474664,0.7908735055
H,0,3.5659750643,0.5600647249,-1.1724909887
H,0,3.0299801377,-0.2573197981,0.3085672905
H,0,2.9468436298,-1.1004754316,-1.2501786458
Si,0,-0.1048764131,-1.6428702025,2.1833127852
C,0,0.8667649071,-1.1933976026,3.7282727316
C,0,-1.9235087872,-1.1925117643,2.4003303384

C,0,0.1044226885,-3.471445694,1.7740366948
 H,0,-0.2754599278,-4.0909566893,2.5956702163
 H,0,-0.4305976991,-3.7603398441,0.863945529
 H,0,1.1624983995,-3.7184045556,1.6319072651
 H,0,0.5097145122,-1.7621538052,4.5948455054
 H,0,1.9331369782,-1.4086468331,3.6000418877
 H,0,0.7648118698,-0.127604921,3.960157025
 H,0,-2.3319547692,-1.6912680995,3.2879002609
 H,0,-2.0410505507,-0.1122837712,2.5420932825
 H,0,-2.5375515563,-1.4850164943,1.5429138106

B3LYP/6-31G* PCM solvent model for dichloromethane

TMS-enol-ether-pinacolone-PCM-B3G

E(RB+HF-LYP) = -719.786273658

Zero-point correction=	0.271742 (Hartree/Particle)
Thermal correction to Energy=	0.288256
Thermal correction to Enthalpy=	0.289200
Thermal correction to Gibbs Free Energy=	0.227911
Sum of electronic and zero-point Energies=	-719.514532
Sum of electronic and thermal Energies=	-719.498018
Sum of electronic and thermal Enthalpies=	-719.497074
Sum of electronic and thermal Free Energies=	-719.558362

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	180.883	60.031	128.993

C,0,0.3695052165,-0.5125516582,-0.3448416764
 O,0,0.589583867,-0.6364773746,1.0023783776
 C,0,1.3949259517,0.4254367626,-0.9827971846
 C,0,2.8130521887,-0.1400256344,-0.7361768053
 C,0,1.173715857,0.5754785241,-2.4974818922
 C,0,1.2781000433,1.8171175624,-0.3180050825
 C,0,-0.6252789164,-1.1348410395,-0.992749936
 H,0,-1.3313886633,-1.7804226177,-0.4821026304
 H,0,-0.7664099377,-1.0103246565,-2.0578442678
 H,0,1.9262079648,1.2548281733,-2.9139561896
 H,0,1.2667665036,-0.3846771131,-3.0173138104
 H,0,0.1861232743,0.9933340895,-2.7225478882
 H,0,2.028028669,2.4997776711,-0.7354452238
 H,0,0.287291108,2.252633203,-0.4938993178
 H,0,1.4355144967,1.7515358701,0.7621452897
 H,0,3.567416692,0.5299086021,-1.1660828446
 H,0,3.0151642503,-0.2435143665,0.3334976711
 H,0,2.9282045422,-1.125206306,-1.2037920242

Si,0,-0.1055587957,-1.6306036278,2.1853203431
 C,0,0.8619897244,-1.2006090188,3.7389485611
 C,0,-1.9299302488,-1.2136449159,2.4252146564
 C,0,0.1317840996,-3.4461405037,1.7334335114
 H,0,-0.2870594291,-4.0937979469,2.5139560329
 H,0,-0.3545026589,-3.7059291987,0.7871929609
 H,0,1.197060768,-3.6873944035,1.6375319608
 H,0,0.5131318166,-1.7928263539,4.5938809955
 H,0,1.9321221188,-1.3984366343,3.6084888191
 H,0,0.7459369373,-0.1414464284,3.9963694441
 H,0,-2.336094503,-1.7711380864,3.278941514
 H,0,-2.0597922034,-0.1453158541,2.6355805276
 H,0,-2.5412047334,-1.4564307191,1.5495031087

TS 51 – Open TS, trans anti-periplanar attack

B3LYP/6-31G*

Re-ptol-anti-periplanar-open-TS-1-B3G

E(RB+HF-LYP) = -3795.15363491

Zero-point correction=	0.420138 (Hartree/Particle)
Thermal correction to Energy=	0.453868
Thermal correction to Enthalpy=	0.454812
Thermal correction to Gibbs Free Energy=	0.350138
Sum of electronic and zero-point Energies=	-3794.733497
Sum of electronic and thermal Energies=	-3794.699767
Sum of electronic and thermal Enthalpies=	-3794.698823
Sum of electronic and thermal Free Energies=	-3794.803497

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	284.806	118.553	220.305

C,0,0.6427120413,2.7620745119,0.2570981133
 C,0,0.6570522559,1.7205212362,-0.6867991163
 C,0,1.6327582634,1.7298674281,-1.6928217001
 C,0,2.5703331912,2.7596057475,-1.7574235747
 C,0,2.5629597207,3.8037157694,-0.8221783405
 C,0,1.5853501108,3.781925469,0.187123807
 C,0,-0.4004797372,0.6799209183,-0.670043637
 O,0,-1.4641061022,0.9616093758,0.0396494865
 Ti,0,-3.2929283564,0.4291264263,0.2158052362
 Cl,0,-3.7318688455,-1.6330746992,0.9778725822
 C,0,3.5497987252,4.94193022,-0.9157231082
 Cl,0,-3.1584917036,1.3238466714,2.3365354336
 Cl,0,-3.0739762894,-0.3700164382,-1.9873908466

Cl,0,-5.0335255545,1.7019445209,-0.350730815
 C,0,0.2967976815,-0.8888085578,0.3426999479
 C,0,1.3532363183,-1.5043572479,-0.3397799422
 O,0,2.5982481946,-1.115449074,-0.1780785436
 Si,0,3.6683953904,-0.6261349131,1.1060601147
 C,0,2.8438723781,0.483182886,2.374105868
 C,0,1.1796407258,-2.5837148103,-1.4068163391
 C,0,-0.2691942254,-3.0939037199,-1.5058219124
 C,0,1.6239050859,-2.013664239,-2.7784870557
 C,0,2.1059888098,-3.7690601537,-1.031549777
 C,0,5.0389264947,0.2480876947,0.178792114
 C,0,4.2323595899,-2.238023882,1.8882940496
 H,0,-0.645660015,-1.4229049246,0.3617458064
 H,0,0.5312122952,-0.3423115238,1.2493942901
 H,0,1.6101167842,-2.8177062143,-3.521817261
 H,0,0.9397503618,-1.2332863007,-3.1284907411
 H,0,2.6373045242,-1.6040627591,-2.7341024304
 H,0,1.9802881423,-4.5673535477,-1.7703358357
 H,0,3.1584559433,-3.4737740075,-1.0213249041
 H,0,1.8486671835,-4.1808082279,-0.0489777039
 H,0,-0.321237831,-3.8639782869,-2.2826517952
 H,0,-0.6040099049,-3.5512093505,-0.5684436916
 H,0,-0.9819431171,-2.3096159007,-1.7772468801
 H,0,3.6105436663,0.8271494237,3.0811496061
 H,0,2.3908626341,1.3710594983,1.9219686651
 H,0,2.0785033665,-0.0366679675,2.9606131865
 H,0,3.3916762758,-2.7909103812,2.3231651825
 H,0,4.7278614573,-2.891921871,1.1626623408
 H,0,4.9451064073,-2.035812397,2.6974037983
 H,0,5.8363946884,0.5501859163,0.8683541607
 H,0,5.4836062233,-0.4030311855,-0.5818160449
 H,0,4.6642504824,1.1483086017,-0.319641201
 H,0,-0.5859582495,0.166358897,-1.6167571372
 H,0,1.6472983434,0.9436550916,-2.4423048144
 H,0,3.3090016576,2.7611839743,-2.5554442032
 H,0,1.5549699054,4.5871088285,0.9174020759
 H,0,-0.1280965386,2.7708723043,1.0214203369
 H,0,3.0870850329,5.8227544077,-1.3798065248
 H,0,3.9033305627,5.2492519979,0.0745338864
 H,0,4.4204995552,4.6719737641,-1.5214422119

B3LYP/6-31+G**

Re-ptol-anti-periplanar-open-TS-1-B3+G
 E(RB+HF-LYP) = -3795.22788912

Zero-point correction= 0.417376 (Hartree/Particle)

Thermal correction to Energy= 0.451318
 Thermal correction to Enthalpy= 0.452263
 Thermal correction to Gibbs Free Energy= 0.346891
 Sum of electronic and zero-point Energies= -3794.810513
 Sum of electronic and thermal Energies= -3794.776571
 Sum of electronic and thermal Enthalpies= -3794.775627
 Sum of electronic and thermal Free Energies= -3794.880998

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	283.207	119.195	221.772

C,0,0.5676959085,2.6067286659,0.2155739355
 C,0,0.6782426483,1.4929312558,-0.6347329486
 C,0,1.6841393929,1.48309362,-1.6112627771
 C,0,2.5586679986,2.563459066,-1.7376497103
 C,0,2.4547359896,3.6804665136,-0.8958204078
 C,0,1.4461034649,3.6784633514,0.0840657402
 C,0,-0.3194545783,0.3917329828,-0.561825514
 O,0,-1.4132341216,0.6669071991,0.1083242161
 Ti,0,-3.2576526123,0.1374511308,0.2239130181
 Cl,0,-3.6555248304,-1.8680350669,1.1371108149
 C,0,3.3681899051,4.8711470374,-1.0599002978
 Cl,0,-3.2550804559,1.2378421352,2.2507700506
 Cl,0,-2.9163170099,-0.8027479672,-1.9111054369
 Cl,0,-5.031463501,1.2771301082,-0.5191412205
 C,0,0.4342027323,-1.0499764611,0.5432533847
 C,0,1.5102677707,-1.6882087352,-0.0953693174
 O,0,2.7444941329,-1.2681080616,0.0501477291
 Si,0,3.8062754114,-0.6411147677,1.2848613531
 C,0,2.984033542,0.6292196386,2.3884854188
 C,0,1.3651125705,-2.838297077,-1.0911878878
 C,0,-0.0698763975,-3.3924073203,-1.1529519623
 C,0,1.7897801223,-2.3397834518,-2.4980206659
 C,0,2.3266578638,-3.9714203708,-0.6474243907
 C,0,5.2036760884,0.0830609698,0.2733332249
 C,0,4.3282381481,-2.1539024521,2.2661530993
 H,0,-0.4848446063,-1.6193216693,0.6103029504
 H,0,0.6609890326,-0.4447166909,1.4135867607
 H,0,1.7899681102,-3.1876130012,-3.1900524382
 H,0,1.0868396612,-1.5984683269,-2.8898262572
 H,0,2.7939238387,-1.907469371,-2.4836087615
 H,0,2.2184209631,-4.817219423,-1.3331772376
 H,0,3.3696340505,-3.6467086634,-0.6642332457
 H,0,2.0863836326,-4.3270238781,0.3603340995
 H,0,-0.1013720784,-4.2102024617,-1.8795450712

H,0,-0.39026788,-3.7994199852,-0.1885291037
H,0,-0.8036074466,-2.6474871742,-1.4714177733
H,0,3.7536283449,1.0654999243,3.0380883079
H,0,2.5293160488,1.4453127856,1.819843614
H,0,2.2221066227,0.1925456621,3.04215731
H,0,3.4705774596,-2.6371573425,2.746777106
H,0,4.8290872918,-2.8953213536,1.6355490702
H,0,5.0268252812,-1.8609231441,3.0589664861
H,0,6.0053976322,0.4386910232,0.9309167302
H,0,5.6309032696,-0.6656322815,-0.401827376
H,0,4.8586556217,0.9306102672,-0.3271956412
H,0,-0.4629338196,-0.1781907774,-1.4836967029
H,0,1.7728871465,0.6413084366,-2.2915242778
H,0,3.3213535438,2.5457428957,-2.5120971017
H,0,1.3388847814,4.5378381037,0.7412807878
H,0,-0.2277696304,2.6289243132,0.9536133615
H,0,2.8508180547,5.6885039609,-1.5773231221
H,0,3.6971319267,5.2600476164,-0.090714131
H,0,4.2559449635,4.619338612,-1.6469987913

B3LYP/6-31+G PCM solvent model for dichloromethane**

Re-ptol-anti-periplanar-open-TS-1-PCM-B3+G

E(RB+HF-LYP) = -3795.25045761

Zero-point correction=	0.415527	(Hartree/Particle)
Thermal correction to Energy=	0.449864	
Thermal correction to Enthalpy=	0.450808	
Thermal correction to Gibbs Free Energy=	0.344791	
Sum of electronic and zero-point Energies=	-3794.834930	
Sum of electronic and thermal Energies=	-3794.800594	
Sum of electronic and thermal Enthalpies=	-3794.799650	
Sum of electronic and thermal Free Energies=	-3794.905667	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	282.294	120.091	223.131

1	6	0	0.427892	2.583019	0.332105
2	6	0	0.558348	1.496091	-0.557589
3	6	0	1.546970	1.542075	-1.558199
4	6	0	2.380161	2.653570	-1.669778
5	6	0	2.256485	3.739954	-0.788831
6	6	0	1.266099	3.683268	0.212636
7	6	0	-0.361717	0.365267	-0.505378
8	8	0	-1.464519	0.493200	0.185955
9	22	0	-3.297136	0.062468	0.206350

10	17	0	-4.082018	-1.959046	0.822166
11	6	0	3.143382	4.952490	-0.913620
12	17	0	-3.334616	0.798988	2.417353
13	17	0	-3.006915	-0.701424	-1.993802
14	17	0	-4.800379	1.598668	-0.445898
15	6	0	0.621838	-1.137097	0.754200
16	6	0	1.638565	-1.695644	-0.006590
17	8	0	2.851498	-1.175040	-0.032657
18	14	0	4.019478	-0.544755	1.095472
19	6	0	3.284259	0.756842	2.227854
20	6	0	1.458459	-2.880892	-0.955315
21	6	0	0.032398	-3.458926	-0.914568
22	6	0	1.796426	-2.431952	-2.399732
23	6	0	2.460489	-3.982809	-0.523195
24	6	0	5.329156	0.156859	-0.041066
25	6	0	4.625392	-2.023855	2.078022
26	1	0	-0.287415	-1.704665	0.893444
27	1	0	0.871039	-0.426088	1.531674
28	1	0	1.755140	-3.300445	-3.064812
29	1	0	1.075868	-1.697468	-2.775369
30	1	0	2.798721	-2.000380	-2.457779
31	1	0	2.335752	-4.854289	-1.173844
32	1	0	3.493944	-3.638378	-0.607056
33	1	0	2.280277	-4.303532	0.508582
34	1	0	-0.029241	-4.302399	-1.609296
35	1	0	-0.226687	-3.833744	0.081063
36	1	0	-0.725853	-2.731757	-1.220601
37	1	0	4.101991	1.206864	2.805455
38	1	0	2.787946	1.559906	1.675464
39	1	0	2.574576	0.334907	2.947485
40	1	0	3.811167	-2.501504	2.634621
41	1	0	5.090833	-2.776820	1.433727
42	1	0	5.375676	-1.694801	2.807500
43	1	0	6.166835	0.550082	0.547024
44	1	0	5.720565	-0.614619	-0.712778
45	1	0	4.931719	0.974284	-0.651147
46	1	0	-0.413241	-0.290276	-1.374292
47	1	0	1.650210	0.721950	-2.263294
48	1	0	3.131165	2.681231	-2.457774
49	1	0	1.151407	4.518993	0.901834
50	1	0	-0.337888	2.561370	1.102408
51	1	0	2.560766	5.826725	-1.229407
52	1	0	3.603287	5.204970	0.048336
53	1	0	3.939053	4.795152	-1.646508

TS 52 – open TS, syn-clinical attack**B3LYP/6-31G***

Re-ptol-syn-clinical-open-TS-1-B3G

E(RB+HF-LYP) = -3795.15601466

Zero-point correction=	0.419868	(Hartree/Particle)
Thermal correction to Energy=	0.453646	
Thermal correction to Enthalpy=	0.454590	
Thermal correction to Gibbs Free Energy=	0.350955	
Sum of electronic and zero-point Energies=	-3794.736147	
Sum of electronic and thermal Energies=	-3794.702369	
Sum of electronic and thermal Enthalpies=	-3794.701424	
Sum of electronic and thermal Free Energies=	-3794.805060	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	284.667	118.688	218.119

C,0,0.1562797826,-0.480580786,-0.2814623976
C,0,0.1728378258,-0.6766595199,1.109178243
H,0,1.0425459842,-0.7927432209,-0.8189514889
C,0,1.435797351,-0.9021211632,1.9303185452
O,0,-0.9216158077,-0.6673698632,1.8297199739
C,0,1.4682434349,0.0799340596,3.1255994429
C,0,1.3488194213,-2.3570157242,2.4694645198
C,0,2.7187258075,-0.7472406475,1.0942451403
H,0,2.2478865694,-2.5696938247,3.0575726425
H,0,0.4763099319,-2.4933094987,3.1150963882
H,0,1.2996262871,-3.0876671958,1.653503853
H,0,2.3493904477,-0.1348208672,3.7391213946
H,0,1.5382879999,1.1145078063,2.7844625262
H,0,0.5770969698,-0.0207047292,3.7497660515
H,0,3.5860546785,-0.8772158667,1.7494229613
H,0,2.7895037829,-1.5065952308,0.3065200541
H,0,2.7909027202,0.2456658575,0.6434807054
Si,0,-2.6401917456,-0.8212655323,1.6053319574
C,0,-3.2664058769,-0.7313063324,3.3658119554
C,0,-3.3145686495,0.5825695197,0.5601604858
C,0,-2.9215258951,-2.5071606566,0.820844853
H,0,-3.9964256786,-2.6900636147,0.699906072
H,0,-2.4615645111,-2.5903257505,-0.1701317563
H,0,-2.5181640722,-3.3103271642,1.447622314
H,0,-4.356652178,-0.8453772291,3.3976608898
H,0,-2.8283100572,-1.5186063754,3.9890157018
H,0,-3.0180261451,0.2350723717,3.8183762342

H,0,-4.4094662744,0.5927677413,0.6363694552
H,0,-2.9486179592,1.551919511,0.9157777637
H,0,-3.0645243617,0.4862934466,-0.5019092507
H,0,-0.7772795323,-0.6984475341,-0.7921512545
C,0,0.2130528139,1.4674493,-0.7229584565
O,0,1.1843104629,2.0629091738,-0.0883770138
H,0,-0.7934081761,1.6639481219,-0.3398200121
C,0,0.3195449711,1.3757604436,-2.2057944173
C,0,1.5637661301,1.4891159383,-2.843686641
C,0,1.6468074066,1.4258844495,-4.2299476205
C,0,0.4998628891,1.2552558034,-5.0214660512
C,0,-0.7393536404,1.1455949468,-4.3755792887
C,0,-0.8304279413,1.2035973077,-2.9875289751
H,0,2.4541728015,1.643365126,-2.2430479124
H,0,2.6174118972,1.5207807539,-4.7110793394
C,0,0.5996724971,1.2248959714,-6.5272619445
H,0,-1.6425453397,1.0227733684,-4.9683263751
H,0,-1.8053406423,1.1328418551,-2.5094806776
H,0,-0.2935212389,0.7843794672,-6.9812743092
H,0,0.7093893669,2.2391259106,-6.9331780368
H,0,1.4707962726,0.6495780248,-6.8596947171
Ti,0,1.3558517496,3.7899917861,0.8535687515
Cl,0,3.4283581422,3.1136904843,1.4326238723
Cl,0,1.1564770375,4.8863190141,-1.082621698
Cl,0,-0.6271555871,3.2107216985,1.8741427747
Cl,0,1.4779488776,5.653190068,2.1320091112

B3LYP/6-31+G**

Re-ptol-syn-clinical-open-TS-1-B3+G

E(RB+HF-LYP) = -3795.23189286

Zero-point correction=	0.417115 (Hartree/Particle)
Thermal correction to Energy=	0.451069
Thermal correction to Enthalpy=	0.452013
Thermal correction to Gibbs Free Energy=	0.347695
Sum of electronic and zero-point Energies=	-3794.814778
Sum of electronic and thermal Energies=	-3794.780824
Sum of electronic and thermal Enthalpies=	-3794.779880
Sum of electronic and thermal Free Energies=	-3794.884198

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	283.050	119.315	219.555

C,0,0.1739134863,-0.4760697384,-0.2762629321

C,0,0.1803478518,-0.6742898451,1.116714806

H,0,1.0672917361,-0.785370679,-0.8032755361
C,0,1.4373399644,-0.9049795,1.9465665876
O,0,-0.9201239683,-0.6736456447,1.8257278663
C,0,1.4395387069,0.0295807954,3.1804236137
C,0,1.3667282818,-2.382102073,2.4293101125
C,0,2.7275800553,-0.6989663689,1.1321046874
H,0,2.2629701557,-2.6012041047,3.0183138836
H,0,0.4904509485,-2.5549984302,3.0600096974
H,0,1.3386880592,-3.0816402056,1.586507389
H,0,2.3202294788,-0.1926616927,3.7906451047
H,0,1.4901574453,1.0791350733,2.8858374935
H,0,0.5470688506,-0.1162751232,3.7925828298
H,0,3.5877357353,-0.8297201511,1.79547274
H,0,2.8251738888,-1.4335579151,0.3251374719
H,0,2.7848408578,0.3072025887,0.711384014
Si,0,-2.6418542527,-0.8145827955,1.6083614881
C,0,-3.2613843452,-0.7130475795,3.3696550012
C,0,-3.3093828843,0.5865019102,0.5576704643
C,0,-2.9369029286,-2.5001047468,0.8313719773
H,0,-4.0138247816,-2.6761065781,0.7233229559
H,0,-2.4886195115,-2.5849059381,-0.164090117
H,0,-2.5305337644,-3.302609014,1.4560121006
H,0,-4.3514256853,-0.8241009323,3.4010688679
H,0,-2.82431375,-1.4994411962,3.9936948963
H,0,-3.0092034412,0.254723453,3.8156980916
H,0,-4.4041628897,0.5914862465,0.6284483652
H,0,-2.9483048781,1.5575073525,0.911721003
H,0,-3.0535227385,0.4844364312,-0.5014655956
H,0,-0.7543839069,-0.7096476543,-0.788602089
C,0,0.2160411655,1.4587307258,-0.7318624556
O,0,1.1876191397,2.0664208987,-0.1065144408
H,0,-0.789934803,1.6590470959,-0.3492370778
C,0,0.3185330931,1.3645954748,-2.2170604345
C,0,1.5605309047,1.4844330354,-2.8588845274
C,0,1.6404563807,1.4238954719,-4.2471391843
C,0,0.4915069869,1.2501289913,-5.0373216787
C,0,-0.7463249845,1.1362300149,-4.3871152872
C,0,-0.8331209039,1.1907544226,-2.9965323759
H,0,2.4510503291,1.6478184678,-2.2611328287
H,0,2.609301446,1.5260654908,-4.7295992451
C,0,0.588220992,1.2244511898,-6.5437063413
H,0,-1.651529882,1.0139359225,-4.9761925049
H,0,-1.8069162636,1.1190580198,-2.5178402793
H,0,-0.3168527789,0.8104474738,-6.9971523129
H,0,0.7251709996,2.2373136333,-6.9424484513
H,0,1.4422831894,0.6268565369,-6.8788591983

Ti,0,1.3661991206,3.8036381746,0.8346234219
 Cl,0,3.4254786316,3.1200864642,1.4500099472
 Cl,0,1.188757962,4.8898720638,-1.1128443398
 Cl,0,-0.613534849,3.2250232711,1.8643795947
 Cl,0,1.4755933478,5.6839322159,2.093327761

B3LYP/6-31+G PCM solvent model for dichloromethane**

Re-ptol-syn-clinical-open-TS-1-fullPCM-B3+G

E(RB+HF-LYP) = -3795.25069792

Zero-point correction=	0.415291	(Hartree/Particle)
Thermal correction to Energy=	0.449665	
Thermal correction to Enthalpy=	0.450609	
Thermal correction to Gibbs Free Energy=	0.344934	
Sum of electronic and zero-point Energies=	-3794.835407	
Sum of electronic and thermal Energies=	-3794.801033	
Sum of electronic and thermal Enthalpies=	-3794.800089	
Sum of electronic and thermal Free Energies=	-3794.905764	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	282.169	120.094	222.411

1	6	0	1.448784	1.232256	0.891821
2	6	0	2.221702	0.077793	1.000791
3	1	0	0.974257	1.608544	1.787458
4	6	0	2.202660	-0.864873	2.199755
5	8	0	3.058559	-0.300509	0.057760
6	6	0	2.069189	-2.329862	1.721090
7	6	0	3.573720	-0.689310	2.911260
8	6	0	1.074730	-0.533344	3.193805
9	1	0	3.606306	-1.347801	3.785672
10	1	0	4.402548	-0.955566	2.249681
11	1	0	3.716255	0.340210	3.257562
12	1	0	2.114483	-2.995006	2.589183
13	1	0	1.115312	-2.499459	1.216419
14	1	0	2.876092	-2.597860	1.035714
15	1	0	1.093127	-1.265344	4.007275
16	1	0	1.203828	0.456746	3.643625
17	1	0	0.089619	-0.584558	2.723698
18	14	0	3.922733	0.406573	-1.277945
19	6	0	5.079458	-0.977825	-1.768695
20	6	0	2.721186	0.829075	-2.655965
21	6	0	4.831256	1.914204	-0.627650
22	1	0	5.446423	2.338228	-1.430872
23	1	0	4.153210	2.701593	-0.282497

24	1	0	5.499673	1.650403	0.199146
25	1	0	5.715455	-0.662276	-2.604152
26	1	0	5.731271	-1.265012	-0.936725
27	1	0	4.519566	-1.863977	-2.086933
28	1	0	3.287965	1.033401	-3.572871
29	1	0	2.040618	-0.002744	-2.865885
30	1	0	2.125954	1.722491	-2.440222
31	1	0	1.761869	1.984448	0.176439
32	6	0	-0.384112	0.823860	-0.173057
33	8	0	-0.986659	-0.212635	0.337164
34	1	0	0.177121	0.643313	-1.093022
35	6	0	-1.006107	2.146409	-0.014551
36	6	0	-1.936768	2.397405	1.009867
37	6	0	-2.527247	3.652035	1.122962
38	6	0	-2.217648	4.687355	0.222384
39	6	0	-1.289345	4.426633	-0.800185
40	6	0	-0.687760	3.176582	-0.916874
41	1	0	-2.195591	1.608675	1.710214
42	1	0	-3.244304	3.833198	1.922583
43	6	0	-2.892867	6.031648	0.330142
44	1	0	-1.036903	5.210150	-1.513148
45	1	0	0.019257	2.998273	-1.723684
46	1	0	-2.258467	6.831477	-0.062902
47	1	0	-3.827244	6.039486	-0.246448
48	1	0	-3.149801	6.267114	1.367243
49	22	0	-1.930343	-1.775147	-0.302577
50	17	0	-1.956423	-2.586636	1.797911
51	17	0	-3.659362	-0.488579	-0.944556
52	17	0	-0.210225	-2.037959	-1.785295
53	17	0	-2.919214	-3.696357	-1.144849

Intermediate from TS 51/52

B3LYP/6-31G*

Re-ptol-intermediate-from-anti-periplanar-open-TS-1-B3G

E(RB+HF-LYP) = -3795.16193725

Zero-point correction=	0.422000 (Hartree/Particle)
Thermal correction to Energy=	0.455863
Thermal correction to Enthalpy=	0.456807
Thermal correction to Gibbs Free Energy=	0.353089
Sum of electronic and zero-point Energies=	-3794.739938
Sum of electronic and thermal Energies=	-3794.706075
Sum of electronic and thermal Enthalpies=	-3794.705131
Sum of electronic and thermal Free Energies=	-3794.808848

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	286.058	119.119	218.293

C,0,1.8800222877,3.6175302176,-0.1615348379
C,0,0.879936764,2.6512136659,-0.0535643037
C,0,0.8560484364,1.5574740983,-0.9289561069
C,0,1.844984633,1.4654811744,-1.9148100416
C,0,2.8406970127,2.437578973,-2.0198674484
C,0,2.8745778251,3.5337805777,-1.1467409033
C,0,-0.2525711203,0.5216713171,-0.8421054197
O,0,-1.3512607098,1.0426564307,-0.1868642209
Ti,0,-3.0132007077,0.6332886424,0.4081362154
Cl,0,-4.8351915623,1.5240310053,-0.5603412403
C,0,3.9190478977,4.615649383,-1.2919625601
Cl,0,-3.0653762655,-0.9669996216,2.0236151788
Cl,0,-2.8933144807,2.3225092771,1.9862092297
Cl,0,-3.0210833835,-1.1338329729,-1.2479375077
C,0,0.1499366435,-0.7901054083,-0.0070708155
C,0,1.3602551697,-1.5155500008,-0.4205445081
C,0,1.3584566166,-2.5801935366,-1.4978717137
C,0,2.7788975643,-2.8539484101,-2.0256637066
O,0,2.4702249622,-1.3397698821,0.1823716558
Si,0,3.2273090528,-0.6228527161,1.6413306127
C,0,3.9179181388,-2.1647337846,2.4505321437
C,0,2.008815026,0.2692370946,2.7438752923
C,0,4.5361497331,0.4824106191,0.9006614965
C,0,0.8219944807,-3.8529342034,-0.7604582435
C,0,0.4063052815,-2.251951099,-2.6677819178
H,0,-0.7287805619,-1.43513387,-0.1159384629
H,0,0.2392858654,-0.4635060358,1.0286011386
H,0,0.388928357,-3.1109167,-3.3465245412
H,0,-0.6218327319,-2.0652299299,-2.3451203671
H,0,0.7578803051,-1.3891876624,-3.2434340916
H,0,2.7292556496,-3.6319442145,-2.7933923496
H,0,3.213657647,-1.9577338775,-2.4813230233
H,0,3.4528998648,-3.1969944454,-1.2364604692
H,0,0.8395882298,-4.682379995,-1.475000349
H,0,1.4541824741,-4.1238869391,0.0917127982
H,0,-0.208239812,-3.7242452056,-0.4168276514
H,0,2.5648748292,0.6326461204,3.6190922523
H,0,1.5563763413,1.1403916299,2.26120972
H,0,1.2096745367,-0.3779565352,3.1207760016
H,0,3.1240721334,-2.8489944897,2.7705273553
H,0,4.5908744222,-2.7081932049,1.7788157018
H,0,4.490806306,-1.8881585836,3.3443609982

H,0,5.1331466616,0.9355209693,1.7017690126
H,0,5.2169158754,-0.0827794885,0.255083978
H,0,4.0922630405,1.2915422402,0.3118612419
H,0,-0.5430355266,0.1876082985,-1.8443795192
H,0,1.8275781542,0.64622918,-2.6319767295
H,0,3.5902777793,2.3536434624,-2.8036099933
H,0,1.8742673596,4.4650849686,0.5201458197
H,0,0.088585558,2.7562865455,0.6830141115
H,0,3.5396465787,5.4487814895,-1.897944144
H,0,4.2064685342,5.0299485897,-0.3196360032
H,0,4.8227758331,4.2408138423,-1.7836737643

Elimination of TMSCl from intermediate from *Re* facial attack – TS 53

B3LYP/6-31G*

Re-ptol-TMSCl-elimination-TS-B3G

E(RB+HF-LYP) = -3795.13990837

Zero-point correction=	0.421815 (Hartree/Particle)
Thermal correction to Energy=	0.454839
Thermal correction to Enthalpy=	0.455783
Thermal correction to Gibbs Free Energy=	0.354692
Sum of electronic and zero-point Energies=	-3794.718094
Sum of electronic and thermal Energies=	-3794.685069
Sum of electronic and thermal Enthalpies=	-3794.684125
Sum of electronic and thermal Free Energies=	-3794.785216

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	285.416	117.259	212.764

C,0,-2.0534163642,-0.7368704756,-3.1217754708
C,0,-1.0115297745,-0.2960825545,-2.3004300668
C,0,0.1033553527,0.3093057389,-2.8926421219
C,0,0.1682671852,0.4629176165,-4.2771681193
C,0,-0.8675285503,0.0159806468,-5.1091503282
C,0,-1.9770403197,-0.5907968516,-4.5064825101
C,0,-1.0992243604,-0.4968970297,-0.7962143475
O,0,-0.5498666745,0.5808324686,-0.0847719487
Ti,0,-0.4104918479,2.34202155,0.0907179985
Cl,0,2.1648587096,1.560537929,0.4654943103
Si,0,2.468688435,-0.4517792375,1.8756514791
C,0,2.2444864293,-2.275007651,2.4314212634
C,0,-0.8075180269,0.222787763,-6.604120116
H,0,-2.1588398622,-0.5807675473,-0.5168203695
C,0,-0.4251397401,-1.8128543073,-0.2848800662

C,0,1.0548859349,-1.9466141466,-0.5837335489
 O,0,1.8859055259,-1.2673579764,0.0364734216
 C,0,1.5728253617,-3.0173001051,-1.5534783208
 C,0,1.4326656789,-4.3599333736,-0.774520209
 C,0,0.7607892212,-3.1223187511,-2.8608556108
 C,0,3.0543667449,-2.7691369151,-1.8858220268
 Cl,0,-2.574214425,2.7217672173,-0.4118823674
 Cl,0,0.4609382139,3.6805201835,-1.468789994
 Cl,0,-0.4323295724,3.1667418911,2.1616796511
 C,0,4.3292093834,-0.2286203352,1.7106278779
 C,0,1.5465716998,0.4435606495,3.2570454314
 H,0,-0.9769328201,-2.656420486,-0.7056095614
 H,0,-0.5487080874,-1.8304681071,0.8041912781
 H,0,2.6126218746,-2.3392162397,3.4643489116
 H,0,1.1987139378,-2.6053286185,2.448123329
 H,0,2.8227159971,-2.9852438389,1.8322732167
 H,0,4.8465655678,-0.8888010802,2.4176066664
 H,0,4.6562281425,-0.4914985485,0.6990495715
 H,0,4.6261430259,0.8064188839,1.8967605563
 H,0,1.7181026871,-0.0908168653,4.2000898371
 H,0,1.8635362632,1.4833539079,3.356661595
 H,0,0.4668521794,0.4538000838,3.0743933074
 H,0,1.8204548596,-5.1673806958,-1.4051161834
 H,0,2.005186729,-4.3524992767,0.157666281
 H,0,0.3892988453,-4.5955889118,-0.5385518731
 H,0,1.1326632234,-3.9815364107,-3.4298852025
 H,0,-0.3073857656,-3.2817872848,-2.6893364119
 H,0,0.8732566691,-2.2299596993,-3.4800761526
 H,0,3.4114537626,-3.5533507356,-2.5615469986
 H,0,3.1898479452,-1.8029492119,-2.3821273216
 H,0,3.6806774963,-2.7779102325,-0.9901152516
 H,0,0.9181621069,0.6760203696,-2.2752248601
 H,0,1.0363334987,0.9489047219,-4.7162693674
 H,0,-2.8003407369,-0.9378433669,-5.1265340204
 H,0,-2.9374850358,-1.1911008829,-2.6787578603
 H,0,-1.2042600689,1.2084826039,-6.8804316158
 H,0,0.2217368132,0.1732940247,-6.9752588353
 H,0,-1.3989814682,-0.5281054992,-7.1383129247

Elimination of TMSCl from intermediate from Si facial attack

B3LYP/6-31G*

Si-ptol-TMSCl-elimination-TS-B3G

E(RB+HF-LYP) = -3795.14747757

Zero-point correction= 0.421875 (Hartree/Particle)

Thermal correction to Energy= 0.455018
 Thermal correction to Enthalpy= 0.455962
 Thermal correction to Gibbs Free Energy= 0.353391
 Sum of electronic and zero-point Energies= -3794.725603
 Sum of electronic and thermal Energies= -3794.692460
 Sum of electronic and thermal Enthalpies= -3794.691515
 Sum of electronic and thermal Free Energies= -3794.794086

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	285.528	117.231	215.879

C,0,-2.8359239427,0.7969299629,-0.8719869387
 C,0,-1.7277071353,0.4285180664,-1.6390213765
 C,0,-1.9363713969,-0.0513413826,-2.9378695974
 C,0,-3.2260613496,-0.1572821369,-3.4510179314
 C,0,-4.3440722039,0.2156843365,-2.6901810069
 C,0,-4.1253700007,0.697988132,-1.3947618974
 C,0,-0.3290694335,0.5966901277,-1.0781800326
 O,0,0.4982532563,-0.5153295626,-1.3883211341
 Ti,0,1.1851537673,-1.9376686461,-0.5798433697
 Cl,0,2.3870950721,-1.520643217,1.2731577652
 C,0,-5.7416817345,0.0668717571,-3.2433219625
 C,0,0.3469033864,1.8709113352,-1.6626792934
 C,0,1.8014864883,2.0484805599,-1.2681744956
 O,0,2.7045535678,1.5194344663,-1.9249204847
 Si,0,3.1753212585,0.3799389338,-3.7031550201
 C,0,2.346679858,-1.0192136836,-4.6710478796
 C,0,2.1869619474,2.9377485837,-0.0824159117
 Cl,0,1.3709688934,-3.8102069273,-1.7820536816
 Cl,0,3.4349410174,-1.1526562513,-1.8413475196
 Cl,0,-0.6937858849,-2.4881586113,0.5275091094
 C,0,2.4656993989,1.9230484422,-4.5818875577
 C,0,5.0438561824,0.5702587078,-3.8119974829
 H,0,-0.3933538456,0.6897561366,0.0106296095
 H,0,-0.2456268899,2.7334950831,-1.3456750404
 H,0,0.2940262928,1.8067162646,-2.7517843498
 H,0,2.7992211663,1.8649649018,-5.6276518992
 H,0,1.3708264551,1.9532861045,-4.6083762152
 H,0,2.8288857227,2.8705113714,-4.171124927
 H,0,5.3117790932,1.0672746272,-4.7524443783
 H,0,5.4126927616,1.1882460862,-2.9864604435
 H,0,5.5520828055,-0.3958155259,-3.7573812437
 H,0,2.2187190364,-0.722205425,-5.71965406
 H,0,2.9272036752,-1.9437042984,-4.6178129549
 H,0,1.3545969741,-1.2410783173,-4.2613410879

H,0,-1.0881585071,-0.359633434,-3.5430306477
H,0,-3.3693994423,-0.5400512249,-4.4589278803
H,0,-4.9744931942,0.9879420538,-0.7804408421
H,0,-2.6953398128,1.1574776177,0.144689334
H,0,-5.7785774962,0.3086699064,-4.3112014789
H,0,-6.1018841698,-0.9643246102,-3.1323488106
H,0,-6.4508613821,0.7184432604,-2.722766904
C,0,3.6711390427,2.7405039886,0.2709024413
C,0,1.9480518682,4.4063812544,-0.5271728488
C,0,1.3132279025,2.6223018861,1.152737915
H,0,2.2480157647,5.0753681422,0.286721651
H,0,2.5475201202,4.6589590548,-1.4087269672
H,0,0.8961216257,4.6103352674,-0.7539091846
H,0,1.6083542637,3.2852036877,1.9732672775
H,0,0.2466455823,2.7896936827,0.9690251769
H,0,1.4560212906,1.5907696235,1.4921397096
H,0,3.9290704948,3.3766570816,1.1243293522
H,0,3.8797292996,1.7004730792,0.5386023143
H,0,4.3226974899,3.0088136814,-0.5652269175

p-tolualdehyde-TiCl₄ complex

B3LYP/6-31G*

ptol-TiCl4-complex-B3G

E(RB+HF-LYP) = -3075.39097186

Zero-point correction=	0.145302 (Hartree/Particle)
Thermal correction to Energy=	0.162283
Thermal correction to Enthalpy=	0.163227
Thermal correction to Gibbs Free Energy=	0.096152
Sum of electronic and zero-point Energies=	-3075.245670
Sum of electronic and thermal Energies=	-3075.228689
Sum of electronic and thermal Enthalpies=	-3075.227744
Sum of electronic and thermal Free Energies=	-3075.294820

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.834	56.281	141.171

C,0,1.054175484,-0.3996831014,2.3818922827
C,0,-0.033937485,-0.1057214207,1.5361007311
C,0,-1.202550473,0.426608461,2.1001932584
C,0,-1.2885659265,0.6584604038,3.4682048662
C,0,-0.1986793247,0.3610684837,4.3039234923
C,0,0.9805380376,-0.1730293904,3.7459402012
C,0,0.0634128441,-0.3706034321,0.0553108371

C,0,-0.3156500548,0.613953791,5.7258593107
 O,0,0.5902497599,0.3851452118,6.5388553105
 H,0,0.9588192842,0.0963187175,-0.371271925
 H,0,0.1378228102,-1.4471313535,-0.1441796187
 H,0,-0.8094139047,0.0106412653,-0.4819873063
 H,0,-2.0478054013,0.6596429354,1.458666029
 H,0,-2.198609265,1.0718416352,3.8964447097
 H,0,1.8182712735,-0.3986789247,4.3979252776
 H,0,1.9646176647,-0.8103270323,1.9528853791
 H,0,-1.266823992,1.0322044827,6.0912299203
 Ti,0,0.8800216597,0.5914527991,8.7085374115
 Cl,0,1.2120901275,0.7835486389,10.8924008928
 Cl,0,1.1569309195,-1.6088630758,8.5813215008
 Cl,0,-1.2101390552,1.3913629926,8.7181026521
 Cl,0,2.5156000174,1.9482029129,8.0617507871

B3LYP/6-31G* PCM solvent model for dichlormethane

ptol-TiCl4-complex-PCM-B3G

E(RB+HF-LYP) = -3075.40439552

Zero-point correction=	0.144331 (Hartree/Particle)
Thermal correction to Energy=	0.161436
Thermal correction to Enthalpy=	0.162380
Thermal correction to Gibbs Free Energy=	0.095082
Sum of electronic and zero-point Energies=	-3075.260065
Sum of electronic and thermal Energies=	-3075.242960
Sum of electronic and thermal Enthalpies=	-3075.242015
Sum of electronic and thermal Free Energies=	-3075.309314

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.303	56.605	141.641

C,0,1.0553492868,-0.3981734156,2.4144977547
 C,0,-0.0265312177,-0.1053521663,1.5560266831
 C,0,-1.2045786171,0.4305142202,2.1020807351
 C,0,-1.307754042,0.6679542116,3.4661037927
 C,0,-0.222980417,0.3719238571,4.3175264712
 C,0,0.9668815378,-0.1666999158,3.774917916
 C,0,0.0887113321,-0.3758471674,0.0795447199
 C,0,-0.3681627789,0.6327958313,5.7204241853
 O,0,0.5297380684,0.4079507661,6.56328138
 H,0,0.9940791909,0.0843373842,-0.333814441
 H,0,0.1650713476,-1.4544678048,-0.1100535232
 H,0,-0.776393351,0.0048546938,-0.4702210456
 H,0,-2.0434513544,0.6618821761,1.4484962708

H,0,-2.2239979486,1.0840791836,3.8840738299
H,0,1.8036571191,-0.3934036128,4.4312679857
H,0,1.9720307296,-0.8115370158,1.9966688044
H,0,-1.3245238072,1.0535745328,6.0684808912
Ti,0,0.8862363838,0.5727944925,8.5978349109
Cl,0,1.2982032463,0.7441304379,10.8141474284
Cl,0,1.1674065165,-1.6425185336,8.5296659478
Cl,0,-1.1954616212,1.3816071643,8.7690316807
Cl,0,2.5268473963,1.9660166807,7.998122622

***p*-tolualdehyde-TiCl₄ radical anion complex**

UB3LYP/6-31G*

ptol-TiCl4-radical-anion-complex-UB3G

E(UB+HF-LYP) = -3075.48377593

Zero-point correction=	0.143319 (Hartree/Particle)
Thermal correction to Energy=	0.160852
Thermal correction to Enthalpy=	0.161796
Thermal correction to Gibbs Free Energy=	0.092370
Sum of electronic and zero-point Energies=	-3075.340457
Sum of electronic and thermal Energies=	-3075.322924
Sum of electronic and thermal Enthalpies=	-3075.321980
Sum of electronic and thermal Free Energies=	-3075.391406

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	100.936	57.293	146.121

C,0,0.8416208834,-0.759218145,2.4370980992
C,0,-0.0651481431,-0.149791423,1.5501549272
C,0,-0.9902096039,0.7651016697,2.0705609019
C,0,-1.014770614,1.0632996569,3.4302255773
C,0,-0.1078247743,0.4504186376,4.3104659178
C,0,0.8264331496,-0.4699723946,3.7932836079
C,0,-0.0409423929,-0.4857304487,0.0779037538
C,0,-0.1421554257,0.7707059792,5.7306062488
O,0,0.6391527544,0.2561806987,6.5513465933
H,0,0.961839931,-0.3532379217,-0.3475470032
H,0,-0.3265145127,-1.53135158,-0.0991623153
H,0,-0.7320794335,0.1466709036,-0.4889544363
H,0,-1.6980548464,1.2481697813,1.4002620955
H,0,-1.7378812627,1.7760790488,3.8203611543
H,0,1.5261231671,-0.9393184747,4.477959443
H,0,1.5682207205,-1.4704391593,2.0488193996
H,0,-0.8919246991,1.4954998937,6.0747580161

Ti,0,0.8396061883,0.5032642499,8.6222950202
 Cl,0,1.0941981195,0.7499270124,10.9275087813
 Cl,0,2.5584576558,-1.0368926278,8.4173609228
 Cl,0,-1.4176715638,-0.0820576371,8.69657516
 Cl,0,1.0699017025,2.7691092799,8.1162231347

UB3LYP/6-31G* PCM solvent model for dichloromethane
 ptol-TiCl4-radical-anion-complex-PCM-UB3G
 E(UB+HF-LYP) = -3075.56856578

Zero-point correction=	0.143219	(Hartree/Particle)
Thermal correction to Energy=	0.160957	
Thermal correction to Enthalpy=	0.161901	
Thermal correction to Gibbs Free Energy=	0.091496	
Sum of electronic and zero-point Energies=	-3075.425347	
Sum of electronic and thermal Energies=	-3075.407609	
Sum of electronic and thermal Enthalpies=	-3075.406665	
Sum of electronic and thermal Free Energies=	-3075.477070	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.002	57.402	148.180

C,0,0.8472720604,-0.7686035929,2.4034088524
 C,0,-0.0715748911,-0.1471644909,1.5334337135
 C,0,-0.997070625,0.7623676211,2.0662495768
 C,0,-1.011322182,1.0458314453,3.4283421968
 C,0,-0.0927075878,0.4203106739,4.2897661207
 C,0,0.8416276757,-0.4942648061,3.7614543479
 C,0,-0.0539849001,-0.4652700379,0.0595929078
 C,0,-0.1324301871,0.7425728731,5.7025476732
 O,0,0.6349455655,0.2450401728,6.544509329
 H,0,0.9487672596,-0.3257030416,-0.3618664545
 H,0,-0.3311674258,-1.512614728,-0.1169247297
 H,0,-0.7518150684,0.1669573383,-0.4969145504
 H,0,-1.7104620428,1.2520915344,1.4057327687
 H,0,-1.7328641921,1.7549503945,3.8332499085
 H,0,1.5533563666,-0.9759413265,4.426442047
 H,0,1.5725528748,-1.4737357826,1.9997995026
 H,0,-0.8899072675,1.47517221,6.0258354074
 Ti,0,0.8399480345,0.510976333,8.6452602121
 Cl,0,1.0672083059,0.8158579676,11.0111117196
 Cl,0,2.5612422027,-1.0406225222,8.5362561385
 Cl,0,-1.4338998583,-0.0644052433,8.7664554198
 Cl,0,1.1026628823,2.7926160081,8.1543638923

TMS enol ether of pinacolone radical cation complex**UB3LYP/6-31G***

TMSenolether-radical-cation-pinacolone-UB3G

E(UB+HF-LYP) = -719.508166032

Zero-point correction=	0.270944 (Hartree/Particle)
Thermal correction to Energy=	0.287925
Thermal correction to Enthalpy=	0.288869
Thermal correction to Gibbs Free Energy=	0.226065
Sum of electronic and zero-point Energies=	-719.237222
Sum of electronic and thermal Energies=	-719.220241
Sum of electronic and thermal Enthalpies=	-719.219297
Sum of electronic and thermal Free Energies=	-719.282102

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	180.676	61.275	132.183

C,0,0.3653208719,-0.6791309603,3.8293220773
 Si,0,-0.2806583139,-1.5884635473,2.3399037269
 C,0,-2.1179474534,-1.3762597372,2.052394721
 C,0,0.3537630888,-3.339820027,2.1647423107
 O,0,0.5359615077,-0.6656881265,1.0014655578
 C,0,0.5788659858,-0.6354731894,-0.2782944279
 C,0,1.4885375041,0.3759786998,-0.9411377835
 C,0,0.6166144448,1.2920325721,-1.8484331309
 C,0,-0.2156414865,-1.5387224784,-1.0511034674
 C,0,2.2282083603,1.2251625751,0.1043983277
 C,0,2.5148767303,-0.3974356509,-1.8193284947
 H,0,-0.8721495803,-2.2570953424,-0.5743214188
 H,0,-0.1796381196,-1.5222059059,-2.1332114595
 H,0,1.2755687612,2.0195029006,-2.3326297456
 H,0,0.0991809768,0.7400020173,-2.639394241
 H,0,-0.1261748991,1.8446788672,-1.2643042343
 H,0,2.873292794,1.9433067472,-0.4095314771
 H,0,1.5328933075,1.7866703598,0.7355772805
 H,0,2.8578908329,0.6098443908,0.7540516025
 H,0,3.1702933559,0.3341258819,-2.302166097
 H,0,3.1388388694,-1.0633130766,-1.2146287012
 H,0,2.0402643904,-0.9860288895,-2.6107718062
 H,0,-0.0218305831,-3.9404153157,3.0028414973
 H,0,0.0236635628,-3.8316868311,1.2433594343
 H,0,1.4478233644,-3.3786920138,2.2044868231
 H,0,-0.0183232103,-1.1416762241,4.7469592966
 H,0,1.4590671224,-0.708352974,3.8778211027

H,0,0.049777174,0.3697021048,3.8323116418
H,0,-2.6561105097,-1.7547563576,2.9307728812
H,0,-2.3914541431,-0.3211941615,1.9401145733
H,0,-2.496753706,-1.9267483075,1.1847106305

UB3LYP/6-31G* PCM solvent model for dichloromethane

TMSenolether-radical-cation-pinacolone-PCM-UB3G

E(UB+HF-LYP) = -719.565901851

Zero-point correction=	0.270642 (Hartree/Particle)
Thermal correction to Energy=	0.287531
Thermal correction to Enthalpy=	0.288475
Thermal correction to Gibbs Free Energy=	0.226139
Sum of electronic and zero-point Energies=	-719.295260
Sum of electronic and thermal Energies=	-719.278371
Sum of electronic and thermal Enthalpies=	-719.277427
Sum of electronic and thermal Free Energies=	-719.339762

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	180.428	61.148	131.197

C,0,0.3581664117,-0.6672683067,3.8194156825
Si,0,-0.2787455604,-1.5868080025,2.3306104467
C,0,-2.1142759404,-1.3807195497,2.0380879396
C,0,0.3631556379,-3.3358273366,2.1770688489
O,0,0.5417082026,-0.6710469465,1.0021311742
C,0,0.5773557565,-0.6423505275,-0.279132605
C,0,1.4882641078,0.3712816887,-0.9382137067
C,0,0.6143772391,1.2980463545,-1.8297754514
C,0,-0.2194379618,-1.5387791239,-1.0524056386
C,0,2.2357218502,1.207768155,0.1115114654
C,0,2.5069072108,-0.3950651035,-1.8279754867
H,0,-0.877999623,-2.2624806562,-0.5836925267
H,0,-0.1865338892,-1.5169393257,-2.136741387
H,0,1.2733297351,2.0292734471,-2.3096024453
H,0,0.0915465981,0.7512119087,-2.621050659
H,0,-0.124795046,1.8431170964,-1.2332630008
H,0,2.8816292608,1.9267435403,-0.4015031422
H,0,1.5437133791,1.7658366058,0.7497793264
H,0,2.8640989159,0.581900778,0.7528275738
H,0,3.1601403455,0.3404760451,-2.3090025252
H,0,3.1312272392,-1.0674387798,-1.2300881557
H,0,2.0225824714,-0.9772529963,-2.6184772629
H,0,-0.0052065392,-3.9231296543,3.0280765978
H,0,0.0263285555,-3.8371997684,1.2629904849

H,0,1.4582429199,-3.3633752761,2.2063511283
H,0,-0.035596916,-1.124203006,4.7358119817
H,0,1.4519727293,-0.7008282422,3.8714112849
H,0,0.0440596608,0.3822822365,3.8067428012
H,0,-2.6513758821,-1.7548922801,2.9192908342
H,0,-2.383613576,-0.3255269931,1.914158402
H,0,-2.482926293,-1.9389559811,1.1706380206

Pinacolone radical

UB3LYP/6-31G*

TMS-lost-pinacolone-radical-UB3G

E(UB+HF-LYP) = -310.435371271

Zero-point correction=	0.156458 (Hartree/Particle)
Thermal correction to Energy=	0.165044
Thermal correction to Enthalpy=	0.165988
Thermal correction to Gibbs Free Energy=	0.123428
Sum of electronic and zero-point Energies=	-310.278913
Sum of electronic and thermal Energies=	-310.270327
Sum of electronic and thermal Enthalpies=	-310.269383
Sum of electronic and thermal Free Energies=	-310.311943

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	103.567	32.090	89.576

C,0,-0.0533107338,0.1763374296,-0.0102845704
O,0,-0.0201219023,0.3788528008,1.2185220773
C,0,1.2790170345,0.0550581858,-0.7865834052
C,0,1.0895318808,-0.1940167287,-2.292155421
C,0,2.0563609388,1.3721662836,-0.5704193191
C,0,2.0687985274,-1.1154332556,-0.1604844044
H,0,2.0669039544,-0.2700565389,-2.7823029578
H,0,0.5521881177,-1.1296109689,-2.4884098424
H,0,0.5436860441,0.6239872622,-2.7774623585
H,0,3.0636008179,-1.1888345085,-0.6154179673
H,0,2.1862083804,-0.9646691953,0.9162288977
H,0,1.5549620808,-2.0716956212,-0.3175422627
H,0,3.0509592977,1.3055464912,-1.026838869
H,0,1.5332798034,2.2225100995,-1.0247686016
H,0,2.1739026685,1.5757636795,0.4975524891
C,0,-1.3283431554,0.0637296186,-0.6561341955
H,0,-1.4518188238,-0.1117696332,-1.7180627214
H,0,-2.2144419311,0.1612995996,-0.0375195677

TS 54 – Variational TS for radical coupling**UB3LYP/6-31G***

vartsreal

E(UB+HF-LYP) = -2925.59566229

Zero-point correction=	0.300050	(Hartree/Particle)
Thermal correction to Energy=	0.325261	
Thermal correction to Enthalpy=	0.326205	
Thermal correction to Gibbs Free Energy=	0.238477	
Sum of electronic and zero-point Energies=	-2925.295613	
Sum of electronic and thermal Energies=	-2925.270401	
Sum of electronic and thermal Enthalpies=	-2925.269457	
Sum of electronic and thermal Free Energies=	-2925.357185	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	204.104	86.985	184.639

C,0,0.1486719571,2.1103205535,0.0548228311
C,0,0.3180088024,1.2723032376,-1.06147998
C,0,1.3527352288,1.4727572268,-1.9631316935
C,0,2.2584875872,2.5393391452,-1.7724649009
C,0,2.1002095281,3.3822871434,-0.6490330502
C,0,1.0627516626,3.1606329947,0.2449667447
C,0,3.3329064437,2.8048614584,-2.6906301029
O,0,3.5336840566,2.0848985655,-3.7494437656
Ti,0,3.8744564138,1.1274931308,-5.2421587369
Cl,0,4.3501808331,2.5398107694,-6.8851119817
C,0,-0.9987546889,1.9002345827,1.0100187035
Cl,0,5.6734055199,-0.085921633,-4.7091439145
Cl,0,2.1292143568,-0.180250418,-5.6660179026
C,0,5.4856872419,2.1700370891,-1.1897876544
C,0,6.0083207469,3.5170765424,-1.078511872
O,0,5.3667491887,4.3713408311,-0.4468606417
C,0,7.3463047956,3.8746347212,-1.7620359311
C,0,7.6841262429,5.3464894388,-1.4776628568
C,0,8.4642317325,2.9667032422,-1.1997087816
C,0,7.2202195626,3.6553509737,-3.2873436115
H,0,5.9644336789,1.4000551912,-1.7853444414
H,0,4.6970295225,1.8726803665,-0.5094776595
H,0,8.6332753353,5.6107422456,-1.957624517
H,0,6.9056510597,6.0138026029,-1.8594931054
H,0,7.7752289338,5.532528455,-0.4032843537
H,0,9.4238969482,3.2305195428,-1.6595192546
H,0,8.5663295645,3.0895572406,-0.1152843977

H,0,8.2799136117,1.9067518094,-1.4056916118
H,0,8.1615141304,3.9269742066,-3.7794293954
H,0,7.0058785674,2.6125426553,-3.5438632597
H,0,6.4317759418,4.2848986002,-3.7179861439
H,0,3.8793688295,3.7423969081,-2.6315580993
H,0,2.8244972767,4.1721067015,-0.469942372
H,0,0.9571679672,3.8095520022,1.1105835498
H,0,-0.3762426626,0.4512304813,-1.221600608
H,0,1.4603951657,0.8181122998,-2.8218051414
H,0,-1.8917113992,2.4443475731,0.6733874714
H,0,-1.2724096768,0.8425933637,1.0824256486
H,0,-0.7568770072,2.2627021587,2.0141977895

TS 55 – Formation of titanium enolate by O-attack

B3LYP/6-31G*

Concerted-TMSCl-elim-Ti-O-bond-forming-TS-B3G
E(RB+HF-LYP) = -3410.21186129

Zero-point correction=	0.279984 (Hartree/Particle)
Thermal correction to Energy=	0.303765
Thermal correction to Enthalpy=	0.304710
Thermal correction to Gibbs Free Energy=	0.227472
Sum of electronic and zero-point Energies=	-3409.931877
Sum of electronic and thermal Energies=	-3409.908096
Sum of electronic and thermal Enthalpies=	-3409.907152
Sum of electronic and thermal Free Energies=	-3409.984389

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	190.616	84.580	162.560

C,0,-0.7218420775,-1.2862782126,1.0325332419
C,0,-0.270004647,-0.3719250315,0.1723593135
C,0,-1.0874089044,0.3300437882,-0.9192032027
O,0,1.0753947065,0.0276265552,0.2650248345
Si,0,2.7193500928,-1.2049844887,-0.8345198444
Cl,0,3.403058267,1.2062844405,-0.5130362817
Ti,0,1.8055387445,1.4605792379,1.3601828455
Cl,0,0.0972963953,1.4473759919,2.799909561
Cl,0,1.7756347708,3.6427429387,0.954375731
Cl,0,3.3851704141,0.9455054027,2.8239343354
H,0,-0.0808128474,-1.6814723183,1.8128907376
H,0,-1.7422806279,-1.6442945544,0.9997842742
C,0,3.2531215099,-0.9598013051,-2.6290461381
C,0,4.0412489061,-1.7426616522,0.3881862975

C,0,1.4851089714,-2.6345186571,-0.9025989526
 C,0,-2.4265761916,-0.401371517,-1.1404971809
 C,0,-1.3914441949,1.7858140473,-0.4906043315
 C,0,-0.3199888663,0.3709488346,-2.2587735975
 H,0,4.224862386,-2.8142129181,0.2356236609
 H,0,4.9748879651,-1.1921640697,0.2517971289
 H,0,3.7206074262,-1.6067252665,1.425540885
 H,0,3.2648720905,-1.9329529943,-3.1358387054
 H,0,2.5596076304,-0.3101002361,-3.1717120935
 H,0,4.2468683872,-0.5078451695,-2.6896249507
 H,0,2.0773278977,-3.4523242082,-1.340972723
 H,0,1.1271369017,-2.9649227498,0.0736651851
 H,0,0.6198409514,-2.47510658,-1.5488137324
 H,0,-2.9790801321,0.0860867074,-1.9509998109
 H,0,-2.2731623236,-1.4499490378,-1.41914159
 H,0,-3.0607019596,-0.3712152715,-0.2483203642
 H,0,-0.9206066931,0.9004466409,-3.0065094833
 H,0,0.6298472466,0.9048090309,-2.1626886081
 H,0,-0.1220844347,-0.6339398729,-2.6476433548
 H,0,-2.0078915282,2.2718135652,-1.2559141291
 H,0,-1.9312964213,1.817951459,0.4602427492
 H,0,-0.4806308117,2.383713471,-0.3859387063

B3LYP/gen (SDD on Ti , 6-31G* on Si,Cl,H,C) PCM solvent model for dichloromethane
 Concerted-TMSCl-elim-Ti-O-bond-forming-TS-PCM-B3G-SDD
 E(RB+HF-LYP) = -2619.11588118

Zero-point correction=	0.278358 (Hartree/Particle)
Thermal correction to Energy=	0.302798
Thermal correction to Enthalpy=	0.303743
Thermal correction to Gibbs Free Energy=	0.224461
Sum of electronic and zero-point Energies=	-2618.837523
Sum of electronic and thermal Energies=	-2618.813083
Sum of electronic and thermal Enthalpies=	-2618.812139
Sum of electronic and thermal Free Energies=	-2618.891421

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	190.009	85.371	166.863

C,0,-0.7285500704,-1.273031961,1.0272322465
 C,0,-0.2899631068,-0.3431782196,0.1753685196
 C,0,-1.1006282144,0.3480462365,-0.925998268
 O,0,1.0490149609,0.0734311319,0.2856701778
 Si,0,2.7652394381,-1.3481727811,-0.8610976696
 Cl,0,3.4779883838,1.2857357692,-0.4446445399

Ti,0,1.8199293782,1.4516230863,1.3251286756
 Cl,0,0.1113600418,1.5000441187,2.7971072662
 Cl,0,1.7524142845,3.6630398501,0.953231333
 Cl,0,3.3470046665,0.8720873411,2.8424674091
 H,0,-0.0825629398,-1.6666663742,1.8058394744
 H,0,-1.7408324872,-1.6538749664,0.980803641
 C,0,3.2369093216,-0.932572086,-2.6251187461
 C,0,4.0962891113,-1.7715621752,0.3778731739
 C,0,1.484936316,-2.7122915889,-0.8765801815
 C,0,-2.4352145517,-0.3904541383,-1.1519160376
 C,0,-1.4128565674,1.8054759174,-0.5092802239
 C,0,-0.3204330719,0.3773912682,-2.2585852339
 H,0,4.3141460556,-2.8421509383,0.2552834005
 H,0,5.0083903225,-1.1924214738,0.2184479707
 H,0,3.7628961993,-1.6179792664,1.4085641531
 H,0,3.2233928802,-1.8677554001,-3.2016364639
 H,0,2.5280543168,-0.2425432104,-3.0913387976
 H,0,4.2333164849,-0.4859733261,-2.6747312235
 H,0,2.0398799868,-3.5551238301,-1.3210001356
 H,0,1.1458828584,-3.0182231386,0.1144980726
 H,0,0.6143574602,-2.523105281,-1.5066086457
 H,0,-2.984640438,0.0954922749,-1.9654537597
 H,0,-2.2750644129,-1.4380510046,-1.4305355517
 H,0,-3.0728189352,-0.3634124891,-0.2619041882
 H,0,-0.9145477161,0.8986009526,-3.0173403725
 H,0,0.6289446862,0.9122510422,-2.159197372
 H,0,-0.1203670902,-0.6319604894,-2.6354837786
 H,0,-2.0118373571,2.2879829178,-1.2905277146
 H,0,-1.975167596,1.8390878007,0.4289437693
 H,0,-0.5038945985,2.4031904312,-0.3838273792

TS 56 – Formation of titanium enolate by C-attack

B3LYP/6-31G*

Concerted-TMSCl-elim-Ti-C-bond-forming-TS-B3G
 E(RB+HF-LYP) = -3410.20817398

Zero-point correction=	0.279413 (Hartree/Particle)
Thermal correction to Energy=	0.303630
Thermal correction to Enthalpy=	0.304574
Thermal correction to Gibbs Free Energy=	0.223690
Sum of electronic and zero-point Energies=	-3409.928761
Sum of electronic and thermal Energies=	-3409.904544
Sum of electronic and thermal Enthalpies=	-3409.903600
Sum of electronic and thermal Free Energies=	-3409.984484

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	190.531	84.444	170

C,0,-0.2048868499,0.0063687085,1.0020832338
 Ti,0,-0.8093880411,-1.4709805361,2.512403966
 Cl,0,0.3321964536,-1.4232923021,4.4058442559
 C,0,-0.14086953,-0.4579908608,-0.3723425058
 O,0,0.856155625,-1.0661272496,-0.8351865356
 Si,0,2.719857491,-1.7071587221,-0.1250797569
 Cl,0,1.1168602963,-2.7140937248,1.439981073
 C,0,-1.3076079792,-0.2578559574,-1.3593301458
 Cl,0,-2.4749432256,-0.1117132723,3.1367864427
 Cl,0,-2.0601237878,-3.2471031894,2.0842059448
 H,0,0.7828368584,0.1965777443,1.4343504098
 H,0,-0.8773655812,0.8443197585,1.1518282999
 C,0,-0.7488976277,0.5001407654,-2.5876132058
 C,0,-1.7929668693,-1.6615157465,-1.7989659244
 C,0,-2.4878671252,0.5306507387,-0.7676394558
 C,0,3.2357442267,0.1131307597,-0.0732653653
 C,0,4.0318781023,-2.5336290976,0.983713414
 C,0,2.8109234938,-2.6374249988,-1.7590350686
 H,0,3.8359379815,-2.9861946996,-1.9286014744
 H,0,2.162860788,-3.520885827,-1.7275657097
 H,0,2.4926055083,-2.0218706006,-2.6041262114
 H,0,5.01746906,-2.3488866596,0.5314653316
 H,0,4.0448994154,-2.1239145753,1.9989994089
 H,0,3.8946130718,-3.6167751008,1.0617978422
 H,0,4.3195927558,0.159975349,-0.2391988612
 H,0,2.7374444393,0.7300496869,-0.8249751372
 H,0,3.0564512587,0.5556040111,0.9139022801
 H,0,-2.5770829991,-1.5545195434,-2.5566105078
 H,0,-0.9725444606,-2.2434835837,-2.2266241987
 H,0,-2.2119193977,-2.2224303309,-0.9562726837
 H,0,-1.5456932924,0.6343260642,-3.3273226713
 H,0,-0.3791381392,1.4944611302,-2.3099154012
 H,0,0.0688795658,-0.0544013863,-3.054882318
 H,0,-3.2865816367,0.5942653428,-1.5144529357
 H,0,-2.9070493806,0.0500843254,0.1217136284
 H,0,-2.2077124686,1.5568445801,-0.5038394571

B3LYP/gen (SDD on Ti , 6-31G* on Si,Cl,H,C) PCM solvent model for dichloromethane
 Concerted-TMSCl-elim-Ti-C-bond-forming-TS-PCM-B3G-SDD
 E(RB+HF-LYP) = -2619.11003727

Zero-point correction= 0.278528 (Hartree/Particle)

Thermal correction to Energy= 0.302950
 Thermal correction to Enthalpy= 0.303894
 Thermal correction to Gibbs Free Energy= 0.223236
 Sum of electronic and zero-point Energies= -2618.831509
 Sum of electronic and thermal Energies= -2618.807087
 Sum of electronic and thermal Enthalpies= -2618.806143
 Sum of electronic and thermal Free Energies= -2618.886801

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	190.104	84.883	169.759

C,0,-0.1150190696,0.1749548097,0.8371838147
 Ti,0,-0.6443196922,-0.9324565788,2.6033577683
 Cl,0,0.7215233897,-0.6277867612,4.3255989505
 C,0,-0.1349054927,-0.5001241553,-0.4683613659
 O,0,0.7984465149,-1.234645566,-0.8508549448
 Si,0,2.6983860553,-1.9108645266,-0.0779767356
 Cl,0,1.0263663988,-2.5508749964,1.6386530038
 C,0,-1.3138222362,-0.281195256,-1.4283537317
 Cl,0,-2.1370323214,0.6430519594,3.1790092671
 Cl,0,-2.0746434165,-2.6323547601,2.6347426839
 H,0,0.9061532419,0.4181140834,1.1568654173
 H,0,-0.7402502453,1.065021402,0.8615447467
 C,0,-1.1766742128,1.1543233628,-2.0019279033
 C,0,-1.2579222509,-1.2984482164,-2.5815336173
 C,0,-2.6600756053,-0.4170731107,-0.6832488372
 C,0,3.3012458704,-0.1404657832,-0.3262208243
 C,0,3.964127522,-2.6399916487,1.1390321348
 C,0,2.633467513,-3.0891073763,-1.5392110396
 H,0,3.625811809,-3.5307383273,-1.6893067516
 H,0,1.9321444927,-3.9081547234,-1.3416450144
 H,0,2.3145603756,-2.5889061236,-2.4568349661
 H,0,4.9509529997,-2.5925540277,0.65535318
 H,0,4.0204594944,-2.0738075923,2.0749358927
 H,0,3.7583015032,-3.6868168968,1.3850118659
 H,0,4.3793661602,-0.1892527567,-0.5294149702
 H,0,2.8098289783,0.3774061256,-1.153250662
 H,0,3.185195638,0.4601993233,0.5840616683
 H,0,-2.0989364751,-1.1220313648,-3.2607637332
 H,0,-0.3294610851,-1.2087720121,-3.1518569884
 H,0,-1.3278453587,-2.326271614,-2.2099943246
 H,0,-1.9864575773,1.3304966523,-2.7186389827
 H,0,-1.245631201,1.9200685164,-1.2221159623
 H,0,-0.2245439923,1.2816623885,-2.5294733809
 H,0,-3.4788781156,-0.2549902823,-1.3931561536

H,0,-2.7820152351,-1.4190259778,-0.2563454889
H,0,-2.7733353738,0.3159648112,0.1213699844

TS 57 – Formation of titanium enolate by migration of TiCl₄ from C to O

B3LYP/6-31G* Onsager solvent model for dichloromethane

Carbon-to-oxygen-TiCl₄-migration-TS-Ons-B3G

E(RB+HF-LYP) = -3410.24255670

Zero-point correction=	0.279459 (Hartree/Particle)
Thermal correction to Energy=	0.303763
Thermal correction to Enthalpy=	0.304707
Thermal correction to Gibbs Free Energy=	0.225775
Sum of electronic and zero-point Energies=	-3409.963097
Sum of electronic and thermal Energies=	-3409.938794
Sum of electronic and thermal Enthalpies=	-3409.937850
Sum of electronic and thermal Free Energies=	-3410.016781

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	190.614	84.940	166.126

C,0,1.1682674146,-0.5558949586,3.0435463796
Si,0,0.1781820768,-1.7541365951,1.9841761635
C,0,0.5125873949,-3.4899781614,2.5966819877
O,0,0.7466102749,-1.7557101681,0.3173969087
C,0,0.5715353381,-0.9646294001,-0.7733348805
C,0,-0.2922727258,-1.4215953653,-1.7339776827
C,0,1.3704234108,0.3340707723,-0.8730819648
C,0,0.5014446295,1.4195270078,-0.1721152842
C,0,2.7457219428,0.2412323685,-0.1827015001
C,0,1.5671396045,0.7691553316,-2.3417759071
C,0,-1.6411949182,-1.3006518404,1.9290991319
H,0,-1.1275424409,-2.0534987489,-1.4560625033
H,0,-0.3548122436,-0.9222956338,-2.6919226948
H,0,2.1735167048,1.6805059345,-2.3588388334
H,0,2.0869855273,0.0035154793,-2.9237197608
H,0,0.6182449533,1.0048755574,-2.8343161703
H,0,1.0249353222,2.3801126917,-0.2244496788
H,0,-0.4684335301,1.5324256274,-0.6672068378
H,0,0.3255631406,1.1981319874,0.883571555
H,0,3.2332982797,1.2206432566,-0.2278659765
H,0,2.6624766049,-0.0403402213,0.8679341384
H,0,3.3913654532,-0.4856605993,-0.6812323887
H,0,0.3130046237,-3.528460671,3.6752363923
H,0,-0.1127433141,-4.2380178182,2.1036548232

H,0,1.5608450746,-3.7691996268,2.4441320243
H,0,0.8090654484,-0.6591465108,4.0764200042
H,0,2.2356838297,-0.802927426,3.0489220778
H,0,1.0625716047,0.49819829,2.7728596723
H,0,-2.0478867903,-1.2888290356,2.9479926621
H,0,-1.8132552129,-0.3067846557,1.5008835382
H,0,-2.2144342625,-2.0299285584,1.3475521488
Ti,0,0.8397986299,-3.6706223661,-1.541958552
Cl,0,2.7484538319,-2.656262186,-2.2631398779
Cl,0,-1.1503116619,-4.2990152539,-0.5369486589
Cl,0,0.3064599369,-4.5161777065,-3.5120691801
Cl,0,1.9865160476,-5.2168467972,-0.4006922757

B3LYP/gen (SDD on Ti , 6-31G* on Si,Cl,H,C) PCM solvent model for dichloromethane

Carbon-to-oxygen-TiCl4-migration-TS-PCM-B3G-SDD

E(RB+HF-LYP) = -2619.14066494

Zero-point correction=	0.278760 (Hartree/Particle)
Thermal correction to Energy=	0.303146
Thermal correction to Enthalpy=	0.304090
Thermal correction to Gibbs Free Energy=	0.225257
Sum of electronic and zero-point Energies=	-2618.861905
Sum of electronic and thermal Energies=	-2618.837519
Sum of electronic and thermal Enthalpies=	-2618.836575
Sum of electronic and thermal Free Energies=	-2618.915408

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	190.227	85.222	165.919

C,0,1.1970457112,-0.5734595738,3.0285851695
Si,0,0.1822976191,-1.7623564379,1.9829711075
C,0,0.4931440818,-3.4977479896,2.6037212518
O,0,0.7381992734,-1.770897782,0.2995263753
C,0,0.5746991979,-0.9721433515,-0.7842270212
C,0,-0.2778927054,-1.4401805702,-1.7563066706
C,0,1.3679060944,0.3279158569,-0.8738899773
C,0,0.4877376851,1.4000985693,-0.1637663324
C,0,2.7431489842,0.2388242736,-0.1829389945
C,0,1.5593490068,0.7795132904,-2.3382076151
C,0,-1.6306632145,-1.2843963325,1.9236075764
H,0,-1.1380867771,-2.0370132499,-1.4709500266
H,0,-0.3240031088,-0.9575216578,-2.7250118344
H,0,2.1531551211,1.6995232186,-2.3434099063
H,0,2.0916875125,0.0281155892,-2.9273915795
H,0,0.6072931533,1.0040067289,-2.8298180931

H,0,1.0059313921,2.3639984628,-0.2131732784
H,0,-0.4833552858,1.5067543596,-0.6583401092
H,0,0.3161359168,1.1706909471,0.8907962997
H,0,3.2195395557,1.2244884239,-0.2130523841
H,0,2.6633950841,-0.0619960507,0.8624767972
H,0,3.397057831,-0.4720637346,-0.6940229828
H,0,0.256671004,-3.5264506064,3.6756133818
H,0,-0.1201609026,-4.2459863666,2.0961559481
H,0,1.5455118366,-3.7789881393,2.4883662002
H,0,0.8403489732,-0.677129975,4.0628094191
H,0,2.2605048348,-0.8385959917,3.0264726324
H,0,1.1028799556,0.4819869054,2.7582592122
H,0,-2.0339449992,-1.2750860157,2.9443858275
H,0,-1.7910085679,-0.2867269271,1.4994524634
H,0,-2.2132558697,-2.0049173229,1.3397342512
Ti,0,0.825016207,-3.6228239594,-1.5297292277
Cl,0,2.7388910936,-2.6366749481,-2.2950525639
Cl,0,-1.1640447637,-4.3016757183,-0.5459647807
Cl,0,0.3299469066,-4.5387056867,-3.4685105108
Cl,0,1.9967321627,-5.1065962382,-0.3265230246

Titanium enolate-aldehyde pre-reactive complex

B3LYP/6-31G*

Ti-enolate-aldehyde-complex-B3G
E(RB+HF-LYP) = -2925.66579047

Zero-point correction=	0.303809 (Hartree/Particle)
Thermal correction to Energy=	0.328905
Thermal correction to Enthalpy=	0.329850
Thermal correction to Gibbs Free Energy=	0.241900
Sum of electronic and zero-point Energies=	-2925.361981
Sum of electronic and thermal Energies=	-2925.336885
Sum of electronic and thermal Enthalpies=	-2925.335941
Sum of electronic and thermal Free Energies=	-2925.423891

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	206.391	87.078	185.106

C,0,4.204184102,-0.8315166413,3.2650151953
C,0,3.7579363685,0.2862931565,2.5336481885
C,0,2.4874767085,0.3190743418,1.9817285729
C,0,1.6211423547,-0.7781611285,2.1518882896
C,0,2.0567116773,-1.8965547843,2.8813017403
C,0,3.3334941808,-1.918285072,3.4317836229

C,0,0.2839985602,-0.7853828469,1.5822145186
 O,0,-0.1919401234,0.1571788288,0.9397661423
 C,0,5.5995832954,-0.8601342048,3.8356430658
 Ti,0,-2.0825921834,0.4775218195,-0.2243708847
 Cl,0,-3.9309695151,0.7279475624,-1.4709581649
 Cl,0,-0.6381954607,0.286062469,-1.9402349059
 Cl,0,-2.839941119,-1.3041646035,0.9638942002
 O,0,-2.1289402467,2.0116781809,0.6102249986
 C,0,-2.1993374521,3.3159075567,1.0114431075
 C,0,-3.092055313,3.526820132,2.2309796408
 C,0,-2.5773774454,2.6435767411,3.3914250202
 C,0,-1.5073139431,4.2341486364,0.3256078376
 C,0,-3.0787039218,5.0010772217,2.6707173442
 C,0,-4.5387742499,3.1155067663,1.8712997637
 H,0,-1.5295497533,5.2792308741,0.6041612169
 H,0,-0.912941636,3.9496373809,-0.5360119
 H,0,-3.2187111055,2.7718288741,4.2708512351
 H,0,-2.5859270991,1.5837813454,3.1195191961
 H,0,-1.5543084615,2.9192537861,3.6726822135
 H,0,-5.1890024671,3.2369607418,2.7454339338
 H,0,-4.9338169715,3.738068214,1.0611461645
 H,0,-4.5930512209,2.0714143967,1.5503725235
 H,0,-3.7219995829,5.1268724319,3.5484221813
 H,0,-2.0708072968,5.3335826282,2.9434513126
 H,0,-3.4590732997,5.6609648046,1.8833462807
 H,0,-0.3282659252,-1.6874178222,1.7409044851
 H,0,1.3895859098,-2.7448372587,3.0150526552
 H,0,3.6629754327,-2.7859760842,3.9968680312
 H,0,4.4244545319,1.1347547658,2.4006993622
 H,0,2.1447575488,1.178614317,1.4145978281
 H,0,5.8600840188,0.0976056887,4.2994247161
 H,0,5.7127201716,-1.6476966105,4.5862380573
 H,0,6.338232932,-1.0461436054,3.0449222133

Titanium enolate

B3LYP/6-31G*

Ti-pinacolone-enolate-B3G

E(RB+HF-LYP) = -2540.75743324

Zero-point correction=	0.164397 (Hartree/Particle)
Thermal correction to Energy=	0.179615
Thermal correction to Enthalpy=	0.180559
Thermal correction to Gibbs Free Energy=	0.118054
Sum of electronic and zero-point Energies=	-2540.593037
Sum of electronic and thermal Energies=	-2540.577819

Sum of electronic and thermal Enthalpies= -2540.576874
 Sum of electronic and thermal Free Energies= -2540.639380

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	112.710	51.673	131.553

Ti,0,-1.1281385097,-5.4227770606,2.1872170713
 O,0,-2.2493044104,-4.1429527429,2.5122964596
 C,0,-3.1233612039,-3.0828886399,2.6161797227
 C,0,-3.2020999619,-2.237512641,1.5840231038
 Cl,0,-2.2048602771,-7.3491839177,2.2408228319
 Cl,0,-0.2516002556,-5.1031553865,0.1898479232
 Cl,0,0.4563847277,-5.396592087,3.7242279945
 C,0,-3.8799084104,-3.0499552131,3.9384775768
 C,0,-4.7057230006,-4.3499595871,4.0812465603
 C,0,-2.8638527186,-2.9475644277,5.100168677
 C,0,-4.8285510342,-1.839183045,3.9867664187
 H,0,-3.8697815451,-1.3867717194,1.6079737325
 H,0,-2.5966408568,-2.3854123884,0.6961911606
 H,0,-3.3950017879,-2.9378726162,6.0584709003
 H,0,-2.1711279948,-3.7945671504,5.1082756121
 H,0,-2.2745783188,-2.0265683593,5.0280484097
 H,0,-5.243036355,-4.3460887489,5.0361776536
 H,0,-5.4432966561,-4.4384252579,3.2757488236
 H,0,-4.0687375624,-5.2393495466,4.0577820804
 H,0,-5.3612586695,-1.8327159488,4.9436439051
 H,0,-4.2820515885,-0.8934985503,3.9028415197
 H,0,-5.5776356103,-1.8798289652,3.1884868626

Boat TS 58 – Si facial attack

B3LYP/6-31G*

Si-ptol-Ti-enolate-boat-TS-B3G
 E(RB+HF-LYP) = -2925.64851986

Zero-point correction= 0.304982 (Hartree/Particle)
 Thermal correction to Energy= 0.328206
 Thermal correction to Enthalpy= 0.329151
 Thermal correction to Gibbs Free Energy= 0.249830
 Sum of electronic and zero-point Energies= -2925.343538
 Sum of electronic and thermal Energies= -2925.320314
 Sum of electronic and thermal Enthalpies= -2925.319369
 Sum of electronic and thermal Free Energies= -2925.398690

E (Thermal)	CV	S
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	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	205.953	83.709	166.945

C,0,2.4984476067,0.1505027338,6.2646963621
C,0,1.10321179,0.2293163118,6.3817638299
C,0,0.4979472525,-0.1649133307,7.5850123635
C,0,1.2785393189,-0.6137685698,8.6451713088
C,0,2.6772100726,-0.6799380689,8.5430992785
C,0,3.2717690955,-0.2947189871,7.3325270933
C,0,0.2924491639,0.6661753709,5.2271898309
O,0,-0.9924084974,0.5409801158,5.2687589639
Ti,0,-2.4338407614,1.4703833115,4.3052672119
Cl,0,-3.7790344758,2.9753699072,3.2852143111
C,0,3.5157794447,-1.1414174619,9.7101137362
H,0,0.7625113279,0.5502270732,4.244951367
Cl,0,-1.523190475,0.7057435211,2.3945059977
Cl,0,-3.9992524604,0.199956598,5.2384833897
O,0,-1.6778919527,2.9050458662,5.3220858252
C,0,-0.4809226694,3.2196494575,5.7147338129
C,0,-0.4031947901,3.9941346273,7.0300507344
C,0,-1.2454578393,3.279143832,8.1096973812
C,0,0.6032870249,2.7803175829,4.9567043751
C,0,1.0463194825,4.1523456598,7.5213818408
C,0,-1.0103435685,5.3929476336,6.7475926765
H,0,1.6141828148,3.0220139439,5.2601290181
H,0,0.4407158345,2.6618778363,3.8898089364
H,0,-1.2448037832,3.8762872332,9.028180837
H,0,-2.2812066449,3.1504682033,7.785218768
H,0,-0.8326165812,2.2935368129,8.3487666496
H,0,-0.9944731421,5.9894511645,7.666685493
H,0,-0.4361853981,5.9297822072,5.983957639
H,0,-2.0456627733,5.3109205233,6.4046831258
H,0,1.049783997,4.7070281335,8.4658093052
H,0,1.522887012,3.1829106779,7.7035181032
H,0,1.6611098428,4.7137654398,6.8091207437
H,0,-0.5839928256,-0.1405577737,7.6665312434
H,0,0.7960135709,-0.9284311034,9.567471758
H,0,4.3519166641,-0.3538651063,7.2246280724
H,0,2.9784768756,0.4338245973,5.330393739
H,0,4.4982064923,-1.4964881541,9.3836289644
H,0,3.6829105534,-0.3228341508,10.4229031759
H,0,3.0251614009,-1.9520266689,10.2593737368

B3LYP/6-31+G**Si-ptol-Ti-enolate-boat-TS-B3+G
E(RB+HF-LYP) = -2925.70405903

Zero-point correction= 0.303025 (Hartree/Particle)
 Thermal correction to Energy= 0.326437
 Thermal correction to Enthalpy= 0.327382
 Thermal correction to Gibbs Free Energy= 0.245556
 Sum of electronic and zero-point Energies= -2925.401034
 Sum of electronic and thermal Energies= -2925.377622
 Sum of electronic and thermal Enthalpies= -2925.376677
 Sum of electronic and thermal Free Energies= -2925.458503

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	204.843	84.159	172.216

C,0,2.5146625584,0.1416751671,6.2612238057
 C,0,1.1196441637,0.2283005423,6.3804683111
 C,0,0.5140220126,-0.1660411553,7.584258578
 C,0,1.2941752913,-0.6215730275,8.6434334977
 C,0,2.6939357617,-0.6949349731,8.5400963564
 C,0,3.2888521926,-0.309749397,7.3285540459
 C,0,0.3080768693,0.6703431149,5.2265515014
 O,0,-0.9766586073,0.5393132132,5.2699368437
 Ti,0,-2.4464972938,1.4483879879,4.3162559726
 Cl,0,-3.8254000548,2.9403143873,3.3224942915
 C,0,3.5291844697,-1.1684938611,9.7050332813
 H,0,0.7795978268,0.5582936677,4.2448183461
 Cl,0,-1.5571947313,0.6953102665,2.3919848942
 Cl,0,-3.9844902076,0.1547651882,5.265294882
 O,0,-1.6783838944,2.9027085375,5.323060759
 C,0,-0.4854758421,3.2245302211,5.71741131
 C,0,-0.4144680156,4.0098198339,7.0283434395
 C,0,-1.2889545505,3.3220611228,8.1007024841
 C,0,0.605149272,2.7876052894,4.9631896394
 C,0,1.0297476257,4.1459694488,7.5437441902
 C,0,-0.9904160191,5.4178416954,6.7223531938
 H,0,1.6130941849,3.0344288346,5.271162996
 H,0,0.4451908478,2.6685862012,3.8965764102
 H,0,-1.2842350565,3.9246701036,9.0147890866
 H,0,-2.3223240405,3.2179090925,7.7630163859
 H,0,-0.9048011928,2.3285170962,8.35079908
 H,0,-0.9748518203,6.0221792457,7.6356324665
 H,0,-0.3959222027,5.9354611336,5.9619685348
 H,0,-2.0221398732,5.3520346285,6.3671130851
 H,0,1.0245584031,4.7045513966,8.4851652947
 H,0,1.4864648388,3.170341319,7.7389638586
 H,0,1.6661142634,4.6945141853,6.8415420301

H,0,-0.5674350232,-0.135134024,7.6671223164
H,0,0.8104205072,-0.9356475773,9.5649998055
H,0,4.3680065236,-0.3741782226,7.2179220744
H,0,2.995906054,0.4244451188,5.3278087169
H,0,4.5394015344,-1.4426538469,9.3887580577
H,0,3.6215710217,-0.3830209428,10.4655096646
H,0,3.0762292031,-2.0383020119,10.1917505123

B3LYP/6-31+G PCM solvent model for dichloromethane**

Si-ptol-Ti-enolate-boat-TS-fullPCM-B3+G

E(RB+HF-LYP) = -2925.71909908

Zero-point correction=	0.301890	(Hartree/Particle)
Thermal correction to Energy=	0.325399	
Thermal correction to Enthalpy=	0.326343	
Thermal correction to Gibbs Free Energy=	0.245882	
Sum of electronic and zero-point Energies=	-2925.417209	
Sum of electronic and thermal Energies=	-2925.393700	
Sum of electronic and thermal Enthalpies=	-2925.392756	
Sum of electronic and thermal Free Energies=	-2925.473217	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	204.191	84.486	169.344

1	6	0	3.104239	-0.995094	-1.438948
2	6	0	2.070504	-0.922752	-0.490561
3	6	0	2.396415	-0.880896	0.877541
4	6	0	3.727985	-0.901029	1.278198
5	6	0	4.771440	-0.955388	0.334475
6	6	0	4.436178	-1.006719	-1.028200
7	6	0	0.675425	-0.944550	-0.950172
8	8	0	-0.281677	-1.126391	-0.086885
9	22	0	-2.122929	-0.626508	0.128341
10	17	0	-4.197832	0.378463	0.023714
11	6	0	6.210849	-0.950735	0.786655
12	1	0	0.507987	-1.340901	-1.958076
13	17	0	-2.659452	-2.121206	-1.494690
14	17	0	-2.297097	-1.420025	2.213256
15	8	0	-1.349281	1.094594	-0.077860
16	6	0	-0.288746	1.590721	-0.657115
17	6	0	0.358112	2.776880	0.054943
18	6	0	0.495272	2.483800	1.565732
19	6	0	0.170858	0.978892	-1.819364
20	6	0	1.737727	3.117309	-0.538218
21	6	0	-0.602763	3.979555	-0.148408

22	1	0	1.055932	1.349271	-2.321277
23	1	0	-0.563516	0.484606	-2.448564
24	1	0	0.910804	3.363994	2.066627
25	1	0	-0.473239	2.258395	2.018375
26	1	0	1.170324	1.642838	1.750308
27	1	0	-0.182870	4.861103	0.347555
28	1	0	-0.729683	4.213581	-1.210768
29	1	0	-1.586883	3.775916	0.283036
30	1	0	2.162351	3.964162	0.010017
31	1	0	2.436550	2.279309	-0.450273
32	1	0	1.671595	3.407149	-1.591881
33	1	0	1.604342	-0.855689	1.619826
34	1	0	3.965619	-0.879314	2.341155
35	1	0	5.226174	-1.064818	-1.775261
36	1	0	2.864330	-1.045098	-2.501047
37	1	0	6.891933	-1.156780	-0.043067
38	1	0	6.481670	0.024715	1.210225
39	1	0	6.382186	-1.697796	1.569430

Boat TS – Re facial attack

B3LYP/6-31G*

Re-ptol-Ti-enolate-boat-TS-B3G

E(RB+HF-LYP) = -2925.64411524

Zero-point correction=	0.304375 (Hartree/Particle)
Thermal correction to Energy=	0.327845
Thermal correction to Enthalpy=	0.328789
Thermal correction to Gibbs Free Energy=	0.247904
Sum of electronic and zero-point Energies=	-2925.339741
Sum of electronic and thermal Energies=	-2925.316270
Sum of electronic and thermal Enthalpies=	-2925.315326
Sum of electronic and thermal Free Energies=	-2925.396211

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	205.726	84.103	170.237

C,0,1.9713689546,-0.0933650881,1.2430276006
C,0,1.0472376483,0.2241998679,2.2516624924
C,0,1.5029095308,0.4071335809,3.5659284996
C,0,2.8555494188,0.282177463,3.8649241461
C,0,3.7879837866,-0.0334125223,2.8655592319
C,0,3.3203865704,-0.2173786864,1.5540641938
C,0,-0.3951664894,0.3365165898,1.9604541335
O,0,-0.8819648969,-0.1237083555,0.8617190173

Ti,0,-1.9130093208,0.2661959325,-0.7571886374
 Cl,0,-3.1147575831,-1.596237773,-0.4578852346
 C,0,5.251154331,-0.2018987294,3.1939774164
 O,0,-2.2273581526,1.8674802981,0.2202240836
 C,0,-1.8552584626,2.434270154,1.3338776007
 C,0,-2.9944407148,2.9057072051,2.2379651608
 C,0,-3.731614664,4.0348197685,1.473082081
 C,0,-0.5038044492,2.4773624393,1.6420423713
 C,0,-3.974475851,1.73593171,2.4865429171
 C,0,-2.4815823733,3.4486275611,3.5827028409
 Cl,0,-3.2231782404,1.11622272,-2.3932820718
 Cl,0,-0.0994930958,0.0094559174,-2.0494628982
 H,0,-0.1550618668,2.957202364,2.5477304534
 H,0,0.211528549,2.3969450291,0.8315020491
 H,0,-4.8185023268,2.0869997474,3.0902131075
 H,0,-4.3690083404,1.3393088904,1.5477416058
 H,0,-3.4951021554,0.9143458242,3.0322482592
 H,0,-4.5754629814,4.3925135443,2.0736024886
 H,0,-3.0663519148,4.8842753806,1.2811873991
 H,0,-4.1140659673,3.6733682664,0.5146835036
 H,0,-3.3308645819,3.7841832435,4.1871689267
 H,0,-1.9507334731,2.6820961435,4.1596554135
 H,0,-1.8118419822,4.3052513485,3.4496494119
 H,0,-1.0467400965,0.3075836816,2.8416696473
 H,0,0.7940163678,0.6481846645,4.3554287982
 H,0,3.1950064657,0.4262557561,4.8876363088
 H,0,4.0275722672,-0.4656172179,0.766411868
 H,0,1.621953363,-0.247514697,0.2270435002
 H,0,5.8877177639,0.1396876057,2.3710070557
 H,0,5.5281178661,0.3546386687,4.0949366078
 H,0,5.4932950972,-1.2578632965,3.3737126504

B3LYP/6-31+G**

Re-ptol-Ti-enolate-boat-TS-B3+G

E(RB+HF-LYP) = -2925.70039648

Zero-point correction=	0.302581 (Hartree/Particle)
Thermal correction to Energy=	0.326153
Thermal correction to Enthalpy=	0.327097
Thermal correction to Gibbs Free Energy=	0.245702
Sum of electronic and zero-point Energies=	-2925.397816
Sum of electronic and thermal Energies=	-2925.374244
Sum of electronic and thermal Enthalpies=	-2925.373300
Sum of electronic and thermal Free Energies=	-2925.454695

E (Thermal)

CV

S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	204.664	84.490	171.311

C,0,1.9808920126,-0.0836216638,1.2411629293
C,0,1.0539242425,0.222666372,2.2513900087
C,0,1.5080254299,0.3912794965,3.5687656737
C,0,2.8624196495,0.2661541347,3.8690720104
C,0,3.7984480298,-0.0360433102,2.8672423361
C,0,3.3316261311,-0.2078892676,1.552550191
C,0,-0.3904312592,0.3306459542,1.959632233
O,0,-0.8714096348,-0.1282257881,0.8567112293
Ti,0,-1.9092455292,0.2529041267,-0.7712319636
Cl,0,-3.0845150559,-1.6270122192,-0.487382523
C,0,5.2615386622,-0.206601953,3.1960101059
O,0,-2.2446622677,1.8559227587,0.2288937401
C,0,-1.8680867969,2.4282747802,1.3362084283
C,0,-3.0038910562,2.9132355916,2.2404399541
C,0,-3.7382826387,4.0398815893,1.4680706008
C,0,-0.513390205,2.4709157572,1.6430896939
C,0,-3.9881288789,1.7492306234,2.5027911901
C,0,-2.4864411606,3.4659807597,3.5802754905
Cl,0,-3.2269941357,1.1048275289,-2.3989175969
Cl,0,-0.093512673,0.0160837843,-2.0627007272
H,0,-0.166722781,2.9547171629,2.5469189979
H,0,0.2003511935,2.3908074133,0.8319378081
H,0,-4.8230367076,2.1082694219,3.1132697989
H,0,-4.3940483188,1.3520824738,1.5699477382
H,0,-3.5080582306,0.9277669203,3.0463955
H,0,-4.5775773691,4.4056449077,2.0690824517
H,0,-3.0701723985,4.8843151873,1.267511271
H,0,-4.1258091025,3.6725236875,0.5147231048
H,0,-3.3343760381,3.8093176853,4.1812513961
H,0,-1.9593020532,2.7029142474,4.1636780127
H,0,-1.814907494,4.319209798,3.4400335092
H,0,-1.0424494073,0.2940412712,2.8398336283
H,0,0.7986744469,0.6197351364,4.3609627492
H,0,3.1985418064,0.3992663361,4.8939976429
H,0,4.0388855673,-0.4475103462,0.7627625898
H,0,1.6330658552,-0.2310347117,0.2239358154
H,0,5.8977398428,0.1437968708,2.377496467
H,0,5.5357719271,0.3414290912,4.1020744093
H,0,5.5015063954,-1.2639556087,3.365276105

B3LYP/6-31+G** PCM solvent model for dichloromethane

Re-ptol-Ti-enolate-boat-TS-fullPCM-B3+G

E(RB+HF-LYP) = -2925.71560809

Zero-point correction= 0.301691 (Hartree/Particle)
 Thermal correction to Energy= 0.325333
 Thermal correction to Enthalpy= 0.326277
 Thermal correction to Gibbs Free Energy= 0.245131
 Sum of electronic and zero-point Energies= -2925.413917
 Sum of electronic and thermal Energies= -2925.390275
 Sum of electronic and thermal Enthalpies= -2925.389331
 Sum of electronic and thermal Free Energies= -2925.470477

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	204.149	84.703	170.785

1	6	0	2.810400	-0.989866	-0.246951
2	6	0	2.400096	0.179733	0.421546
3	6	0	3.367561	1.110111	0.835939
4	6	0	4.718323	0.878998	0.580161
5	6	0	5.137304	-0.280271	-0.091143
6	6	0	4.159405	-1.211095	-0.495110
7	6	0	0.987638	0.434948	0.730283
8	8	0	0.122746	-0.535989	0.700301
9	22	0	-1.567223	-1.166586	0.057579
10	17	0	-2.230260	-1.690030	2.154838
11	6	0	6.596355	-0.534941	-0.376650
12	8	0	-1.651605	0.586994	-0.631728
13	6	0	-0.901027	1.664594	-0.668417
14	6	0	-1.572980	2.944643	-0.178047
15	6	0	-2.726277	3.252106	-1.169745
16	6	0	0.421935	1.532576	-1.061896
17	6	0	-2.160808	2.716882	1.234750
18	6	0	-0.595948	4.133213	-0.148430
19	17	0	-3.662740	-1.524885	-0.849561
20	17	0	-0.615652	-2.865387	-1.079817
21	1	0	1.070909	2.397774	-1.114442
22	1	0	0.698438	0.679291	-1.670956
23	1	0	-2.671237	3.627701	1.563692
24	1	0	-2.887443	1.900870	1.240377
25	1	0	-1.377447	2.491695	1.967248
26	1	0	-3.243311	4.161902	-0.847359
27	1	0	-2.344786	3.417220	-2.183058
28	1	0	-3.449394	2.432947	-1.199086
29	1	0	-1.129235	5.026210	0.192126
30	1	0	0.236457	3.963672	0.543340
31	1	0	-0.185274	4.350192	-1.139820
32	1	0	0.800756	1.233583	1.455370

33	1	0	3.066108	2.011031	1.369416
34	1	0	5.457418	1.606143	0.912536
35	1	0	4.465136	-2.123128	-1.006508
36	1	0	2.070302	-1.721138	-0.555548
37	1	0	6.787522	-0.539740	-1.456770
38	1	0	7.232829	0.229420	0.076559
39	1	0	6.907244	-1.513428	0.006993

B. Listing of Dynamics Programs for Program Suite PROGDYN

version 0.9.3, March, 2009

The end of this section shows program changes used for special experiments.

1. Program progdynstarterHP

```
#!/bin/bash
# This is the master control program for dynamics, in the form of a Unix Shell Script.
#
# Necessary input files:
# freqinHP - This is the standard output from a Gaussian 98 or 03 frequency calculation
# using freq=hpmodes.
# progdyn.conf - This is a file giving a variety of configuration options, called on by many of the
# subprograms.
#
# Optional input:
# isomernumber - A number in file isomernumber provides a start for numbering runs.
# detour - A signal file that, by existing, signals the program to do a side calculations
# nogo - A signal file that, by existing, signals the program to stop between points
# methodfile - a file that contains lines that go at the end of the Gaussian input file
# cannontraj - a file that contains initial x, y, and z velocities to be added to the normal velocities
# generated by proggenHP.
# These are used for shooting a structure toward another structure.
#
# Programs called:
# proggenHP - An awk program that starts a trajectory, giving each mode its zero point
# energy (if a quasiclassical calculation) plus random additional excitations depending on the
# temperature.
# prog1stpoint - Awk program that creates the first Gaussian input file for each run
# prog2ndpoint - Awk program that creates the second Gaussian input file for each run
# progdynb - Awk program that creates subsequent Gaussian input files until trajectory is
# completed.
# proganal - A program to analyze the latest point and see if a trajectory is done. This program
# must be redone for each new system. Elaborate changes are often programmed into proganal,
# such as the automatic changing of configuration variables.
# randgen - A program that generates random numbers between 0 and 1. These are generated all
# at once and stored in a file for use by proggenHP.
#
# Output files
# isomernumber - A running tab of the run number
# geoRecord - A record of all the starting positions and velocities.
# geoPlusVel - Created by proggen, this gives starting position and velocities for current run.
# g03.com - Created by prog1stpoint, prog2ndpoint, and progdynb, this is the latest input
# file for Gaussian03 for current run and latest point.
# olddynrun and olderdynrun - files containing the last two outputs from Gaussian, for creation
# of the next point
# dyn - A record of all of the Gaussian outputs.
# dynfollowfile - A short record of the runs and their results.
# skipstart - A signal file that, by existing, tells progdynstarterHP that we are in the middle of a
# run.
# diagnostics - optional output that follows which subprograms are running and configuration
# variables, decided by variable in progdyn.conf
# vellist - optional output that list the velocities of each atom, decided by variable in
# progdyn.conf
# Echeck - After the first point of a trajectory runs, prog2ndpoint checks to see if the total
# potential energy + kinetic energy is sufficiently close to
```

```
# the energy desired based on the original design that assumed the harmonic approximation. The
output of this check is placed into Echeck, and proganal will start a new run if the energy is too
far off.
```

```
# A number of files starting with 'temp' are created then later erased.
```

```
#progdynstarterHP, made to use high-precision modes from Gaussian freq output
#updated to create a random number file temp811 that is used by proggenHP
#version September 16, 2005, made for workstations
#version August 2007 to allow periodic copying of g03.log to dyn putting it under control of
progdynb
#version Feb 2008 moves variables like the scratch directory and location of randgen to the
beginning
#version March 2008 added proganal reporting to points 1 and 2
#version Jan 2009 fixed bug generator of having proganal run twice in checking for complete
runs
#
#          OUTLINE
# A. initilize to perform Gaussian jobs and know where we are
#   start loop
# B. if no file named "skipstart" then generate a new isomer. Get rid of skipstart to start new
isomer.
#
# AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
#origdir, randdir, scratchdir, g03root, logfile, freqfile, programdir, all may need varied from
system to system and assigned here or by program calling this one
export g03root=/apps/lms/g03_E01_pre
. $g03root/g03/bsd/g03.profile
origdir=`pwd`
cd $origdir
logfile=docslog
randdir=~/bin
scratchdir=/tmp/$PBS_JOBID
programdir=~/bin2
freqfile=~/bin2/freqinHP
```

```
rm -f nogo  # assume that if someone is starting a job, they want it to go.
rm -f diagnostics # contains extra info from start of progFS
```

```
while (true)
do
# BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB
if (test -f skipstart) then
    echo "skipping start and continuing from previous runs"
else
# change from older versions - freqin and most other files are in origdir. Advantage is
compartmentalization.
# Also allows separate configurations for separate runs, so we can move to using config files.
# Disadvantage is multiple copies of files.
    cd $origdir
    echo 3 > runpointnumber
    $randdir/randgen > temp811
# lets keep the next 8 lines as the only difference between progdynstarter and progdynstarterHP
    awk '/      1      2      3      4/,/Harmonic frequencies/ {print}' $freqfile > temp401
    awk '/Frequencies --/ {print $3;print $4;print $5;print $6;print $7}' temp401 > tempfreqs
    awk '/Reduced masses/ {print $4;print $5;print $6;print $7;print $8}' temp401 > tempredmass
    awk '/Force constants/ {print $4;print $5;print $6;print $7;print $8}' temp401 > tempfrc
    awk '/0/ && ((length($1) < 2) && ($1 < 4)) {print}' temp401 > tempmodes
    awk '/has atomic number/ {print}' $freqfile > tempmasses
    awk '/Standard orientation:/ {print}' $freqfile > tempstangeos
    awk -f $programdir/progenHP $freqfile > geoPlusVel
if (test -f isomernumber) then
    cp isomernumber temp533
    awk 'BEGIN {getline;i=$1+1;print i}' temp533 > isomernumber
    rm temp533
else
```

```

echo 1 > isomernumber
fi
rm g03.com
awk -f $programdir/prog1stpoint geoPlusVel > g03.com
# TO DO - put error checking in prog1stpoint, prog2ndpoint, and progdynb so no g03.com
unless things are ok
if (test -s g03.com) then
  rm tempfreqs tempredmass tempfrc tempmodes tempstangeos tempmasses temp401 temp811
  cat isomernumber >> geoRecord
  cat geoPlusVel >> geoRecord
  cat g03.com
  rm -f goingwell
  cd $scratchdir
  $g03root/g03/g03 $origdir/g03.com > $origdir/g03.log
  cd $origdir
  grep 'Normal termination' g03.log > goingwell
  if (test -s goingwell) then
    cat g03.log >> dyn
    awk -f $programdir/proganal g03.log >> dynfollowfile
    cp g03.log olddynrun
  else
    break
  fi
else
  break
fi
rm g03.com
awk -f $programdir/prog2ndpoint g03.log > g03.com
if (test -s g03.com) then
  rm -f goingwell
  cd $scratchdir
  $g03root/g03/g03 $origdir/g03.com > $origdir/g03.log
  cd $origdir
  grep 'Normal termination' g03.log > goingwell
  if (test -s goingwell) then
    cp g03.log olddynrun
    cat g03.log >> dyn
    awk -f $programdir/proganal g03.log >> dynfollowfile
  # old program progdyn replaced here with commands from progdyn
  awk '/Input orientation/./Distance matrix/ {print}' olddynrun > temp101
  awk '/^ / {print}' temp101 > old
  awk '/Input orientation/./Distance matrix/ {print}' olderdynrun > temp102
  awk '/^ / {print}' temp102 > older
  awk -f $programdir/progdynb olddynrun > g03.com
  rm -f temp101 temp102 old older tempchk
  else
    break
  fi
else
  break
fi
# we've just completed a start, so lets skipstart until instructed otherwise
echo "skipping start" > skipstart
fi

while (true)
do
#increment runpointnumber
  if (test -f runpointnumber) then
    cp runpointnumber temp533
    awk 'BEGIN {getline;i=$1+1;print i}' temp533 > runpointnumber
    rm temp533
  else
    echo 4 > runpointnumber

```

```

fi
# this loop always starts with a g03.com in place - because of the loss of former program
progdyn, I
# may have to worry about how each it is to restart from a bad run
rm -f goingwell
cd $scratchdir
$g03root/g03/g03 $origdir/g03.com > $origdir/g03.log
cd $origdir
grep 'Normal termination' g03.log > goingwell
if (test -s goingwell) then
  cp olddynrun olderdynrun
  cp g03.log olddynrun
# old program progdyn replaced here too
  awk '/Input orientation/./Distance matrix/ {print}' olddynrun > temp101
  awk '/ 0 / {print}' temp101 > old
  awk '/Input orientation/./Distance matrix/ {print}' olderdynrun > temp102
  awk '/ 0 / {print}' temp102 > older
  awk -f $programdir/progdynb olddynrun > g03.com
  rm -f temp101 temp102 old older tempchk
# line removed to move the command under control of progdynb      cat g03.log >> dyn
else
  break
fi

# here is a cool link that lets you interupt the dynamics with a short job, then
# it automatically goes back to the dynamics just make the file 'detour' and it
# will delete detour, run run.com, then go back to dynamics
if (test -f detour) then
  rm detour
  date >> $logfile
  cat run.com >> $logfile
  cp run.log temp.log
  cd $scratchdir
  $g03root/g03/g03 $origdir/run.com > $origdir/run.log
  cd $origdir
fi

#stop it all nicely by creating a nogo file
if (test -f nogo) then
  break
fi

#figure out if this isomer is done
awk -f $programdir/proganal g03.log >> dynfollowfile
rm -f tempdone
tail -2 dynfollowfile > temp281
awk '/XXXX/ {print}' temp281 > tempdone
rm temp281
if (test -s tempdone) then
  rm -f skipstart
  rm -f olddynrun
  rm -f olderdynrun
  rm -f geoPlusVel
  break
fi
done

# We've got to break a second time to get out of this loop
# if we really want to quit. Otherwise, it will start over
# at the top
if (test -f nogo) then
  break
fi
if (test -s goingwell) then

```

```

echo "probably starting a new point"
else
break
fi
done
exit 0

```

2. Program proggenHP

```

# Jan 2009 - a number of little changes to improve reporting, precision, etc, specification of
displacement on particular modes
# Jan 2009 cannonball trajectories. adds desired energy to initial velocities based on file
cannonontraj, so one can shoot toward a ts
# updated Nov 2008 to incorporate running DRPs
# updated Nov 2008 to allow for start without an initial freq calc using classical = 2
# updated Aug 2008 added to atom list to handle a large number of atoms without changes
needed
# updated June 2008 to incorporate new method for choosing displacements with initialdis 2
# updated Jan 17 2008 - bug fix for > 99 atoms, 300 excitations of low modes possible
# version August 2007 - incorporates classical trajectory calculation option
#also allows listing of number of imaginary frequencies
# version Sept 16, 2005 - incorporates searchdir but not yet rotation
# now reads random numbers from temp811, starting at a random place
# The input files are generated before this and are tempfreqs, tempredmass,
# tempfrc, tempmodes, and tempstangeos.
# It will count the number of atoms.

# default parameters, including quasiclassical, no displacements, transition state, not a DRP
# do not change these - rather, change progdyn.conf to set the parameters
initialDis=0; timestep=1E-15; scaling=1.0; temp=298.15
classical=0; numimag=1; DRP=0; cannonball=0
charge=0; multiplicity=1; method="HF/3-21G"; memory=20000000
diag=1; checkpoint="g03.chk"; searchdir="positive"; boxon=0
boxsize=10; maxAtomMove=0.1; title1="you"; title2="need"
title3="a"; title4="progdyn.conf"; processors=1; highlevel=999
conver1=4.184E26 #dividing by this converts amu ang^2 /s^2 to kcal/mol

#initialization and constants
i=1;j=1;k=1
c=29979245800; h=6.626075E-34; avNum=6.0221415E23
RgasK=0.00198588; RgasJ=8.31447
numAtoms=0; atomnumber=0; classicalSpacing=4
zpeGauss=0; zpeGaussK=0; zpePlusE=0; potentialE=0

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="initialdis") initialDis=$2
  if ($1=="timestep") timestep=$2
  if ($1=="scaling") scaling=$2
  if ($1=="temperature") temp=$2
  if ($1=="searchdir") searchdir=$2
  if ($1=="classical") classical=$2
  if ($1=="numimag") numimag=$2
  if ($1=="highlevel") highlevel=$2
}

```

```

if ($1=="boxon") boxon=$2
if ($1=="boxsize") boxsize=$2
if ($1=="DRP") DRP=$2; if (DRP==1) classical=2 #this lets one start a DRP from a point that
is not a freq calc
if ($1=="maxAtomMove") maxAtomMove=$2
if ($1=="cannonball") cannonball=$2
if ($1=="displacements") disMode[$2]=$3
if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
}
blankLineTester=length($0)
}

if (diag>=1) print "***** starting proggen *****" >>
"diagnostics"
if (diag>=1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag>=1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag>=1) print "processors,checkpoint,title,initialdis,timestep,scaling,temperature" >>
"diagnostics"
if (diag>=1) print processors,checkpoint,title1,title2,title3,title4,initialDis,timestep,scaling,temp
>> "diagnostics"
if (diag>=1) print "classical,numimag,highlevel,boxon,boxsize,DRP,maxAtomMove,cannonball"
>> "diagnostics"
if (diag>=1) print classical,numimag,highlevel,boxon,boxsize,DRP,maxAtomMove,cannonball
>> "diagnostics"

# put geometries into array, also figure out number of atoms
# note that this picks out the last geometry in a file, assuming
# that if there is an optimization followed by a freq, nothing else follows
# kludgy - repeats last line twice - must be a better way
do {
    getline < "tempstangeos"
    if (oldline==$0) $0=""
    oldline=$0
    atom = $1
    if (atom>numAtoms) numAtoms=atom
    atNum[atom]=$2
    geoArr[atom,1]=$4; geoArr[atom,2]=$5; geoArr[atom,3]=$6
    velArr[atom,1]=0; velArr[atom,2]=0; velArr[atom,3]=0
}
while (length($0) > 0)

#output the number of atoms, used in many routines
print numAtoms

# put in atomic symbols and atomic weights - assigns a default mass but then reads it from
tempmasses when possible
for (i=1;i<=numAtoms;i++) {
    getline < "tempmasses"
    if (atNum[i]==1) {atSym[i]="H";atWeight[i]=1.00783}
    if (atNum[i]==2) {atSym[i]="He";atWeight[i]=4.0026}
    if (atNum[i]==3) {atSym[i]="Li";atWeight[i]=6.941}
    if (atNum[i]==4) {atSym[i]="Be";atWeight[i]=9.012}
    if (atNum[i]==5) {atSym[i]="B";atWeight[i]=10.811}
    if (atNum[i]==6) {atSym[i]="C";atWeight[i]=12.}
    if (atNum[i]==7) {atSym[i]="N";atWeight[i]=14.007}
    if (atNum[i]==8) {atSym[i]="O";atWeight[i]=15.9994}
    if (atNum[i]==9) {atSym[i]="F";atWeight[i]=18.9984}
    if (atNum[i]==10) {atSym[i]="Ne";atWeight[i]=20.1797}
    if (atNum[i]==11) {atSym[i]="Na";atWeight[i]=22.989}
    if (atNum[i]==12) {atSym[i]="Mg";atWeight[i]=24.305}
}

```

```

if (atNum[i]==13) {atSym[i]="Al";atWeight[i]=26.98154}
if (atNum[i]==14) {atSym[i]="Si";atWeight[i]=28.0855}
if (atNum[i]==15) {atSym[i]="P";atWeight[i]=30.9738}
if (atNum[i]==16) {atSym[i]="S";atWeight[i]=32.066}
if (atNum[i]==17) {atSym[i]="Cl";atWeight[i]=35.4527}
if (atNum[i]==18) {atSym[i]="Ar";atWeight[i]=39.948}
if (atNum[i]==19) {atSym[i]="K";atWeight[i]=39.0983}
if (atNum[i]==20) {atSym[i]="Ca";atWeight[i]=40.078}
if (atNum[i]==34) {atSym[i]="Se";atWeight[i]=78.96}
if (atNum[i]==35) {atSym[i]="Br";atWeight[i]=79.904}
if (atNum[i]==46) {atSym[i]="Pd";atWeight[i]=106.42}
if (atNum[i]==53) {atSym[i]="I";atWeight[i]=126.90447}
# gets actual weight from freqinHP when possible so a prior calc with readisotopes gets you
isotopic substitution
if ((i<100) && ($9>0)) atWeight[i]=$9
if ((i>99) && ($8>0)) atWeight[i]=$8

if ((diag>1) && (i==1)) print
"atNum[i],atSym[i],atWeight[i],geoArr[i,1],geoArr[i,2],geoArr[i,3]" >> "diagnostics"
if (diag>1) print atNum[i],atSym[i],atWeight[i],geoArr[i,1],geoArr[i,2],geoArr[i,3] >>
"diagnostics"
}

# read in frequencies, scale them, read in Reduced masses, read in force
#constants, replace negative frequencies by 4 wavenumbers
numFreq=3*numAtoms-6
for (i=1;i<=numFreq;i++) {
$0=""
getline < "tempfreqs"
freq[i]=$0*scaling
if (freq[i]<0) freq[i]=4
}
for (i=1;i<=numFreq;i++) {
$0=""
getline < "tempredmass"
redMass[i]=$0
if (redMass[i]== "") redMass[i]=1.
}
for (i=1;i<=numFreq;i++) {
$0=""
getline < "tempfrc"
frc[i]=$0
if (frc[i]== "") frc[i]=0.0001
if (frc[i]== 0) frc[i]=0.0001
if ((diag>1) && (i==1)) print "freq[i],redMass[i],frc[i]" >> "diagnostics"
if (diag>1) print freq[i],redMass[i],frc[i] >> "diagnostics"
}

# read in the modes - note that trajectories always need a freq calc with freq=hpmodes unless
classical=2
for (i=1;i<=numFreq;i+=5) {
for (j=1;j<=(3*numAtoms);j++) {
getline < "tempmodes"
mode[i,$2,$1]=$4; mode[i+1,$2,$1]=$5; mode[i+2,$2,$1]=$6; mode[i+3,$2,$1]=$7;
mode[i+4,$2,$1]=$8
}
}
if (diag>2) {for (i=1;i<=numFreq;i++) {print mode[i,1,1],mode[i,1,2],mode[i,1,3] >>
"modesread"}}

# if doing a cannonball trajectory, read in the vector
if (cannonball>0) {
for (i=1;i<=numAtoms;i++) {
getline < "cannontraj"
}
}

```

```

        cannonArr[i,1] = $1; cannonArr[i,2] = $2; cannonArr[i,3] = $3
    }

# collect a series of random numbers from file temp811, generated from an outside random
# number generator called by prodynstarterHP
# read from temp811, starting at a random place
strand(); tester=rand()*1000
for (i=1;i<=tester;i++) getline < "temp811"
for (i=1;i<=numFreq;i++) {
    getline < "temp811"; randArr[i] = $1
    getline < "temp811"; randArrB[i] = $1
    getline < "temp811"; randArrC[i] = $1
}
# for a QM distribution for a harmonic oscillator in its ground state, we want to generate a set of
# random numbers
# between -1 and 1 weighted such that numbers toward the center are properly more common
i=1
while (i<=numFreq) {
    getline < "temp811"
    tempNum=2*($1-.5)
    prob=exp(-(tempNum^2))
    getline < "temp811"
    if ($1<prob) {
        randArrD[i]=tempNum
        i++
    }
}

# to start without normal modes or frequencies we need to just pick a random direction for the
# motion of each atom, requiring 3N random numbers
for (i=1;i<=numAtoms;i++) {
    for (j=1;j<=3;j++) {
        getline < "temp811"
        if ($1>0.5) randArrE[i,j] = 1
        if ($1<.5) randArrE[i,j] = -1
    }
}

# determine energy in each normal mode
for (i=1;i<=numFreq;i++) {
    zpeJ[i] = 0.5*h*c*freq[i] #units J per molecule
    #if classical, treat as modes spaced by classicalSpacing wavenumbers
    if (classical==1) zpeJ[i] = 0.5*h*c*classicalSpacing # the zpe is not used when classical but the
    spacing is used to calculate the E in mode
    zpeK[i] = zpeJ[i]*avNum/4184 #units kcal/mol
    if (temp<10) vibN[i] = 0 # avoids working with very small temperatures - if the temp is too
    low, it just acts like 0 K
    if (temp>=10) {
        zpeRat[i] = exp((-2*zpeK[i])/(RgasK*temp))
        if (zpeRat[i]==1) zpeRat[i] = .99999999999
        Q[i] = 1/(1-zpeRat[i])
        newRand = randArr[i]
        vibN[i] = 0
        tester = 1/Q[i]
    }
    # get up to 1000 excitations of low modes
    for (j=1;j<=(1000*zpeRat[i]+2);j++) {
        if (newRand>tester) vibN[i]++
        tester = tester + ((zpeRat[i]^j)/Q[i])
    }
}

# figure out mode energies and maximum classical shift and then actual shift

```

```

# also calculated total energy desired for molecule
desiredModeEnK=0
for (i=1;i<=numFreq;i++) {
    modeEn[i]=(zpeJ[i]*1E18)*(2*vibN[i]+1) # units here are mDyne Angstroms for compatibility
    with Gaussian force constants
    if (classical==1) modeEn[i]=(zpeJ[i]*1E18)*2*vibN[i] #no zpe when classical
    modeEnK[i]=zpeK[i]*(2*vibN[i]+1)
    if (classical==1) modeEnK[i]=zpeK[i]*2*vibN[i] #no zpe when classical
    desiredModeEnK=desiredModeEnK + modeEnK[i]
# no 1/2 hv for imaginary frequencies
# treating modes with frequencies <10 as translations, ignoring their zero point energies
if (freq[i]<10) modeEn[i]=(zpeJ[i]*1E18)*(2*vibN[i])
maxShift[i]=(2*modeEn[i]/frc[i])^0.5
if (initialDis==2) shift[i]=maxShift[i]*randArrD[i]
if (initialDis==1) shift[i]=maxShift[i]*(2*(randArrC[i]-0.5))
if (initialDis==0) shift[i]=0
# lines below allow for setting of displacement mode for individual modes; use disMode 10 to
turn off displacements for a mode
if (disMode[i]==2) shift[i]=maxShift[i]*randArrD[i]
if (disMode[i]==1) shift[i]=maxShift[i]*(2*(randArrC[i]-0.5))
if (disMode[i]==10) shift[i]=0
# no displacements along imaginary frequencies and very low ones - it is better to treat these
# as translations - employing a shift can give you initial weird geometries
if (freq[i]<10) shift[i]=0
if (numimag==1) shift[1]=0
if (numimag==2) shift[2]=0
}
for (i=1;i<=numFreq;i++) {
    if ((diag>1) && (i==1)) print
    "zpeJ[i],zpeK[i],zpeRat[i],Q[i],vibN[i],modeEn[i],maxShift[i],shift[i]" >> "diagnostics"
    if (diag>1) print zpeJ[i],zpeK[i],zpeRat[i],Q[i],vibN[i],modeEn[i],maxShift[i],shift[i] >>
    "diagnostics"
}
# multiply each of the modes by its shift and add them up
for (i=1;i<=numFreq;i++) {
    for (j=1;j<=numAtoms;j++) {
        for (k=1;k<=3;k++) {
            shiftMode[i,j,k]=mode[i,j,k]*shift[i]
            geoArr[j,k]=geoArr[j,k]+shiftMode[i,j,k]
        }
    }
}
#output the new geometry.
for (j=1;j<=numAtoms;j++) {
    printf("%2s % .7f % .7f % .7f % 9.5f
\n",atSym[j],geoArr[j,1],geoArr[j,2],geoArr[j,3],atWeight[j])
}
#now start toward velocities
for (i=1;i<=numFreq;i++) {
    kinEn[i]=100000*(modeEn[i]-0.5*frc[i]*shift[i]^2) # the 100000 converts to g angstrom^2
    s^2
    vel[i]=(2*kinEn[i]/(redMass[i]/avNum))^0.5 # in angstrom / s
    #use searchdir in progdyn.conf to control the direction for trajectories started from a saddle point
    if (numimag>1) numimag=1 #only the first freq can be sent in the searchdir direction, the rest
    go in a random direction
    if (i>numimag) {
        if (randArrB[i]<0.5) vel[i]=-vel[i]
    }
    if (i==numimag) {
        if (searchdir=="negative") vel[i]=-vel[i]
    }
}

```

```

if ((diag>1) && (i==1)) print "vel[i]" >> "diagnostics"
if (diag>1) print vel[i] >> "diagnostics"
}
# the next line can be uncommented and set so as to make a particular mode velocity either
positive or negative
# if (vel[2]<0) vel[2]=-vel[2]

# multiply each of the modes by its velocity and add them up
for (i=1;i<=numFreq;i++) {
    for (j=1;j<=numAtoms;j++) {
        for (k=1;k<=3;k++) {
            velMode[i,j,k]=mode[i,j,k]*vel[i]*timestep
            velArr[j,k]=velArr[j,k]+velMode[i,j,k]
        }
    }
}

# to start without normal modes or frequencies we figure out the energy per atom based on
1/2RT in degree of freedom
if (classical==2) {
    degFreedomEnK=temp*RgasK
    degFreedomEnJ=degFreedomEnK/(avNum/4184)
    cartEn=degFreedomEnJ*1E18
    kinEnCart=100000*cartEn
#print degFreedomEnK, degFreedomEnJ, cartEn, kinEnCart
    for (i=1;i<=numAtoms;i++) {
        for (j=1;j<=3;j++) {
            velArr[i,j]=randArrE[i,j]*timestep*(2*kinEnCart/(atWeight[i]/avNum))^0.5
            if (DRP==1) velArr[i,j]=0
        }
    }
}

# calculate the KE in the modes at this point
KEinitmodes=0
for (j=1;j<=numAtoms;j++) {
    KEinitmodes=KEinitmodes + 0.5*atWeight[j]*(velArr[j,1]^2 + velArr[j,2]^2 +
    velArr[j,3]^2)/((timestep^2)*conver1)
}

# if doing a cannonball, adjust multiplier until extra energy is correct
if (cannonball>0) {
    multiplier=1; tester=0; tolerance=.1
    while (tester==0) {
        KEinittotal=0
        for (j=1;j<=numAtoms;j++) {
            cannonvelArr[j,1]=velArr[j,1]+multiplier*cannonArr[j,1];
            cannonvelArr[j,2]=velArr[j,2]+multiplier*cannonArr[j,2];
            cannonvelArr[j,3]=velArr[j,3]+multiplier*cannonArr[j,3];
            KEinittotal=KEinittotal + 0.5*atWeight[j]*(cannonvelArr[j,1]^2 + cannonvelArr[j,2]^2 +
            cannonvelArr[j,3]^2)/((timestep^2)*conver1)
        }
        if (KEinittotal>(KEinitmodes+cannonball+tolerance)) multiplier=multiplier*0.98901364
        if (KEinittotal<(KEinitmodes+cannonball-tolerance)) multiplier=multiplier*1.01
        if ((KEinittotal<(KEinitmodes+cannonball+tolerance)) &&
        (KEinittotal>(KEinitmodes+cannonball-tolerance))) tester=1
    }
    for (j=1;j<=numAtoms;j++) {
        velArr[j,1]=velArr[j,1]+multiplier*cannonArr[j,1];
        velArr[j,2]=velArr[j,2]+multiplier*cannonArr[j,2];
        velArr[j,3]=velArr[j,3]+multiplier*cannonArr[j,3];
    }
}

```

```

#output the velocities and calculate the total kinetic energy overall
KEinittotal=0
for (j=1;j<=numAtoms;j++) {
    KEinittotal=KEinittotal + 0.5*atWeight[j]*(velArr[j,1]^2 + velArr[j,2]^2 +
    velArr[j,3]^2)/((timestep^2)*conver1)
    printf("% .8f % .8f % .8f \n",velArr[j,1],velArr[j,2],velArr[j,3])
}

#anything else I add to the file will not affect the trajectories but will keep a record and be good
for (i=1;i<=numFreq;i++) {
    if (initialDis==0) printf("% .6f % .6f % 4i % 1.4e % .6f % 1i\n", randArr[i],
    randArrB[i], vibN[i], vel[i], shift[i], disMode[i])
    if (initialDis==1) printf("% .6f % .6f % 4i % 1.4e % .6f % 1i\n", randArr[i],
    randArrC[i], vibN[i], vel[i], shift[i], disMode[i])
    if (initialDis==2) printf("% .6f % .6f % 4i % 1.4e % .6f % 1i\n", randArr[i],
    randArrD[i], vibN[i], vel[i], shift[i], disMode[i])
}
print "temp ",temp
print "initialDis",initialDis
print "classical",classical
print "timestep",timestep
print "numimag",numimag
OFMT = "%.3f"
print "Total mode energy desired=",desiredModeEnK
print "KE initial from modes=",KEinitmodes, " KE initial total=",KEinittotal
if (cannonball>0) print "cannonball",cannonball," cannon Energy=",KEinittotal-KEinitmodes
if (boxon>0) print "boxsize",boxsize
if (DRP>0) print "DRP",DRP," maxAtomMove",maxAtomMove
} # End of BEGIN

/Zero-point correction/ {zpeGauss=$3}
/zero-point Energies/ {zpePlusE=$7}
END {
zpeGaussK=zpeGauss*627.509
potentialE=zpePlusE - zpeGauss
OFMT = "%.6f"
print "Gaussian zpe=",zpeGauss,"or",zpeGaussK,"kcal/mol E + zpe=",zpePlusE," potential
E=",potentialE
print "" #will use blank line to mark end of geoPlusVel file
}

```

3. Program prog1stpoint

```

BEGIN {
# Jan 2009 - a number of little changes to improve reporting, precision, etc
# aug 2008 added to atom list so handles H to Cl without change needed
# version Feb 2008 incorporates methodfile, boxon and boxsize, though this point unaffected by
box
# version Jan 2008 - allows for ONIOM jobs, fixed atoms
# version Sept 2005 - incorporates meth3, meth4, meth5, meth6, but not yet rotation
# this program creates the first input file for g03
# the title should be changed as appropriate
# the isomer number comes from a file isomernumber

# default parameters, including quasiclassical, no displacements, transition state, not a DRP
# do not change these - rather, change progdyn.conf to set the parameters
initialDis=0; timestep=1E-15; scaling=1.0; temp=298.15
classical=0; numimag=1; DRP=0; cannonball=0
charge=0; multiplicity=1; method="HF/3-21G"; memory=20000000
diag=1; checkpoint="g03.chk"; searchdir="positive"; boxon=0
boxsize=10; maxAtomMove=0.1; title1="you"; title2="need"

```

```

title3="a"; title4="progdyn.conf"; processors=1; highlevel=999

#initialization
i=1;j=1;k=1
c=29979245800; h=6.626075E-34; avNum=6.0221415E23
RgasK=0.00198588; RgasJ=8.31447
numAtoms=0; atomnumber=0

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
    getline < "progdyn.conf"
    if ($1=="method") method=$2
    if ($1=="method2") meth2=$2
    if ($1=="charge") charge=$2
    if ($1=="multiplicity") multiplicity=$2
    if ($1=="memory") memory=$2
    if ($1=="processors") processors=$2
    if ($1=="checkpoint") checkpoint=$2
    if ($1=="timestep") timestep=$2
    if ($1=="diagnostics") diag=$2
    if ($1=="method3") meth3=$2
    if ($1=="method4") meth4=$2
    if ($1=="method5") meth5=$2
    if ($1=="method6") meth6=$2
    if ($1=="highlevel") highlevel=$2
    if ($1=="fixedatom1") fixedatom1=$2
    if ($1=="fixedatom2") fixedatom2=$2
    if ($1=="fixedatom3") fixedatom3=$2
    if ($1=="fixedatom4") fixedatom4=$2
    if ($1=="methodfile") methodfilelines=$2
    if ($1=="killcheck") killcheck=$2
    if ($1=="title") {
        title1=$2
        title2=$3
        title3=$4
        title4=$5
    }
    blankLineTester=length($0)
}

if (diag==1) print "***** starting prog1stpoint *****" >>
"diagnostics"
if (diag==1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag==1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag==1) print "processors,checkpoint,title" >> "diagnostics"
if (diag==1) print processors,checkpoint,title1,title2,title3,title4 >> "diagnostics"

getline < "isomernumber"
isomernum = $1
print "%nproc=" processors
print "%mem=" memory
if (killcheck!=1) print "%chk=" checkpoint
print "#p " method " force scf=(tight,nosym) "
#print "IOp(3/76=0572004280)" #for mPW1K in g03
if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
if (length(meth3)>2) print meth3
if (length(meth4)>2) print meth4
print ""
# make the title four words exactly, leaving out spaces if necessary
print title1,title2,title3,title4
print "runpoint 1"
print "runisomer ", isomernum
print ""

```

```

print charge,multiplicity
}

(/H / ||/He / ||/Li / ||/Be / ||/B / ||/C / ||/N / ||/O / ||/F / ||/Ne / ||/Na / ||/Mg / ||/Al / ||/Si / ||/P /
||/S / ||/Cl /) {
atomnumber++
printf("%s %.7f %.7f %.7f", $1, $2, $3, $4)
if (atomnumber>highlevel) printf(" %s", "M")
print ""
}

END {
print ""
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
if (methodfilelines>=1) {
  for (i=1;i<=methodfilelines;i++) {
    getline < "methodfile"
    print $0
  }
}
print ""
}

```

4. Program prog2ndpoint

```

BEGIN {
# aug 2008 added to atom list so handles 1 to 17 without change needed
# version Feb 2008 incorporates methodfile, boxon and boxsize, though this point unaffected by
box
# version Jan 2008 - allows for ONIOM jobs, fixed atoms
# version Sept 9, 2005 - incorporates meth3, meth4, meth5, meth6, but not yet rotation
# read progdyn.conf for configuration info

# default parameters, including quasiclassical, no displacements, transition state, not a DRP
# do not change these - rather, change progdyn.conf to set the parameters
initialDis=0; timestep=1E-15; scaling=1.0; temp=298.15
classical=0; numimag=1; DRP=0; cannonball=0
charge=0; multiplicity=1; method="HF/3-21G"; memory=20000000
diag=1; checkpoint="g03.chk"; searchdir="positive"; boxon=0
boxsize=10; maxAtomMove=0.1; title1="you"; title2="need"
title3="a"; title4="progdyn.conf"; processors=1; highlevel=999

#initialization
i=1;j=1;k=1
c=29979245800; h=6.626075E-34; avNum=6.0221415E23
RgasK=0.00198588; RgasJ=8.31447
numAtoms=0; atomnumber=0

blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="method2") meth2=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="timestep") timestep=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="method3") meth3=$2
  if ($1=="method4") meth4=$2
}

```

```

if ($1=="method5") meth5=$2
if ($1=="method6") meth6=$2
if ($1=="highlevel") highlevel=$2
if ($1=="fixedatom1") fixedatom1=$2
if ($1=="fixedatom2") fixedatom2=$2
if ($1=="fixedatom3") fixedatom3=$2
if ($1=="fixedatom4") fixedatom4=$2
if ($1=="DRP") DRP=$2
if ($1=="methodfile") methodfilelines=$2
if ($1=="killcheck") killcheck=$2
if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
}
blankLineTester=length($0)
}

if (diag>=1) print "***** starting prog2ndpoint *****" >>
"diagnostics"
if (diag>=1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag>=1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag>=1) print "processors,checkpoint,title" >> "diagnostics"
if (diag>=1) print processors,checkpoint,title1,title2,title3,title4 >> "diagnostics"

#get the isomer number from file
getline < "isomernumber"
isomernum = $1

print "%nproc=" processors
print "%mem=" memory
if (killcheck!=1) print "%chk=" checkpoint
print "#p " method " force scf=(tight,nosym) "
if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
if (meth2=="read") print "guess=tcheck" #for reading orbitals from check, sometimes faster,
sometimes not
if (length(meth3)>2) print meth3
if (length(meth4)>2) print meth4
print ""
print title1,title2,title3,title4
print "runpoint 2"
print "runisomer ", isomernum
print ""
print charge,multiplicity

# ok, now we have to figure the second point. this should be
#  $x(t) = x + v*t + 1/2*F*t^2/m$ 
# so we need to set up arrays for position, velocity, and force
getline < "geoPlusVel"
numAtoms=$1
# first the geometry
for (i=1;i<=numAtoms;i++) {
    getline < "geoPlusVel"
    weight[i]=$5
    atSym[i]=$1
    for (j=1;j<=3;j++) {
        geoArr[i,j]=$(1+j)
    }
}
#now we go ahead and add the velocities
for (i=1;i<=numAtoms;i++) {
    getline < "geoPlusVel"
    for (j=1;j<=3;j++) {

```

```

arr[i,j]=$j+geoArr[i,j]
}
if ((diag>1) && (i==1)) print "geometry after adding velocities" >> "diagnostics"
if (diag>1) print arr[i,1],arr[i,2],arr[i,3] >> "diagnostics"
}

#pull out other information useful for testing whether total energy is right or bad
blankLineTester=10
while (blankLineTester>1) {
  getline < "geoPlusVel"
  if ($4=="desired") desiredModeEnK=$5
  if ($4=="modes") {
    KEinitmodes=$5
    KEinittotal=$9
  }
  if ($11=="potential") potentialE=$13
  blankLineTester=length($0)
}
} # end of BEGIN

/SCF Done/ {
print "trajectory #",isomernum >> "Echeck"
newPotentialE=$5
newPotentialEK=(newPotentialE-potentialE)*627.509
print "point 1 potential E=",newPotentialEK," point 1 kinetic E=",KEinittotal,"Total=",newPotentialEK+KEinittotal >> "Echeck"
print "desired total energy=", desiredModeEnK >> "Echeck"
if ((newPotentialEK+KEinittotal)>(desiredModeEnK+1)) print "XXXX bad total Energy" >> "Echeck"
if ((newPotentialEK+KEinittotal)<(desiredModeEnK-1)) print "XXXX bad total Energy" >> "Echeck"
}

# now we go ahead and translate the forces and add them
( 1 / / 2 / / 3 / / 4 / / 5 / / 6 / / 7 / /
8 / / 9 / / 10 / / 11 / / 12 / / 13 / / 14 / /
15 / / 16 / / 17 / ) && length($3)>9 {
i=$1
for (j=1;j<=3;j++) {
  forceArr[i,j]=$(2+j) #the raw units of the forces are Hartree/Bohr
}
if ((diag>1) && (i==1)) print "i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]" >> "diagnostics"
if (diag>1) print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3] >> "diagnostics"
}

END {
# turn the forces into motion
for (i=1;i<=numAtoms;i++) {
  for (j=1;j<=3;j++) {
# conversions here take force to J/angstrom, 1E20 converts to kg angstroms / s^2, then mult time (s^s) and divide by weight in kg to get angstroms

forceArr[i,j]=0.5*1E20*forceArr[i,j]*627.509*(4184/(0.529177*avNum))*(timestep^2)/(weight[i]/(avNum*1000))
# for simplicity, DRPs will throw away the forces at the second point. This means that if we are not at a saddlepoint, point 2 = point 1 but this is a minor waste
  if (DRP==1) forceArr[i,j]=0
  arr[i,j]=arr[i,j]+forceArr[i,j]
# if atoms are fixed, replace calcd new position by original position
  if ((i==fixedatom1) || (i==fixedatom2) || (i==fixedatom3) || (i==fixedatom4))
  arr[i,j]=geoArr[i,j]
}
}

```

```

if ((diag>1) && (i==1)) print "i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]" >>
"diagnostics"
if (diag>1) print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3] >> "diagnostics"
printf("%s %.7f %.7f %.7f",atSym[i],arr[i,1],arr[i,2],arr[i,3])
if (i>highlevel) printf(" %s","M")
print ""
}
print ""
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
if (methodfilelines>=1) {
  for (i=1;i<=methodfilelines;i++) {
    getline < "methodfile"
    print $0
  }
}
print ""
}

```

5. Program progdynb

```

BEGIN { #this is the main routine for generating new .com files by the Verlet algorithym
# Jan 2009 - a number of little changes to improve reporting, precision, etc
# Nov 2008 added ability to handle DRPs
# Aug 2008 added long list of atoms to handle 1-17 without change
# May 2008 added option to put out velocities in vellist - make diag=2
# version Feb 2008 incorporates methodfile, boxon and boxsize
# version Jan 2008 incorporates fixed atoms, oniom, and velocity damping
# version August 2007 incorporates keepevery to decrease size of dyn file
# version Sept 11, 2005 - incorportates meth3, meth4, meth5, meth6, but not yet rotation

# default parameters, including quasiclassical, no displacements, transition state, not a DRP
# do not change these - rather, change progdyn.conf to set the parameters
initialDis=0; timestep=1E-15; scaling=1.0; temp=298.15
classical=0; numimag=1; DRP=0; cannonball=0
charge=0; multiplicity=1; method="HF/3-21G"; memory=20000000
diag=1; checkpoint="g03.chk"; searchdir="positive"; boxon=0
boxsize=10; maxAtomMove=0.1; title1="you"; title2="need"
title3="a"; title4="progdyn.conf"; processors=1; highlevel=999

#initialization
i=1;j=1;k=1
c=29979245800; h=6.626075E-34; avNum=6.0221415E23
RgasK=0.00198588; RgasJ=8.31447
numAtoms=0; atomnumber=0
OFS=" "

#allow for damping from file named damping, but limit its range
damping=1
DRP=0
getline < "damping"
if (($1>0.05) && ($1<2.1)) damping=$1

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="method2") meth2=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
}

```

```

if ($1=="processors") processors=$2
if ($1=="checkpoint") checkpoint=$2
if ($1=="timestep") timestep=$2
if ($1=="diagnostics") diag=$2
if ($1=="method3") meth3=$2
if ($1=="method4") meth4=$2
if ($1=="method5") meth5=$2
if ($1=="method6") meth6=$2
if ($1=="highlevel") highlevel=$2
if ($1=="keepevery") keepevery=$2
if ($1=="fixedatom1") fixedatom1=$2
if ($1=="fixedatom2") fixedatom2=$2
if ($1=="fixedatom3") fixedatom3=$2
if ($1=="fixedatom4") fixedatom4=$2
if ($1=="boxon") boxon=$2
if ($1=="boxsize") boxsize=$2
if ($1=="DRP") DRP=$2
if ($1=="maxAtomMove") maxAtomMove=$2
if ($1=="methodfile") methodfilelines=$2
if ($1=="killcheck") killcheck=$2
if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
}
blankLineTester=length($0)
}

if (diag>=1) print "***** starting progdynb *****" >>
"diagnostics"
if (diag>=1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag>=1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag>=1) print "processors,checkpoint,title" >> "diagnostics"
if (diag>=1) print processors,checkpoint,title1,title2,title3,title4 >> "diagnostics"

# get number of atoms and weights from geoPlusVel, and previous geometries from old and
# older
getline < "geoPlusVel"
numAtoms=$1
for (i=1;i<=numAtoms;i++) {
    getline < "geoPlusVel"
    weight[i]=$5; atSym[i]=$1
}

for (at=1;at<=numAtoms;at++) {
    getline < "old"
    oldarr[at,1]=$4; oldarr[at,2]=$5; oldarr[at,3]=$6
}

for (at=1;at<=numAtoms;at++) {
    getline < "older"
    olderarr[at,1]=$4; olderarr[at,2]=$5; olderarr[at,3]=$6
}

#for DRPs read in oldAdjForces and maxAtomMove
if (DRP==1) {
    for (at=1;at<=numAtoms;at++) {
        getline < "oldAdjForces"
        oldForce[at,1]=$1; oldForce[at,2]=$2; oldForce[at,3]=$3
    }
    getline < "maxMove"
    if (($1<maxAtomMove) && ($1>0)) maxAtomMove=$1
}

```

```

# record atom velocities for IVR analysis. This is actually the velocity in the previous run,
which is the easiest to calculate.
getline < "isomernumber"
isomernum = $1
getline < "runpointnumber"
runpointnum = $1
if (diag==3) print "runpoint ",runpointnum-1,"runisomer ",isomernum >> "vellist"
for (at=1;at<=numAtoms;at++) {
    atomVel=((oldarr[at,1]-olderarr[at,1])^2 + (oldarr[at,2]-olderarr[at,2])^2 +(oldarr[at,3]-
    olderarr[at,3])^2)^.5
    if (diag==3) print atomVel >> "vellist"
}
}

#must adjust next line for weird atoms
( / 1 / / 2 / / 3 / / 4 / / 5 / / 6 / / 7 / /
8 / / 9 / / 10 / / 11 / / 12 / / 13 / / 14 / /
15 / / 16 / / 17 / ) && length($3) > 9 {
i=$1
for (j=1;j<=3;j++) {
    forceArr[i,j]=$(2+j) #the raw units of the forces are Hartree/Bohr
}
if ((diag>1) && (i==1)) print "i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]" >>
"diagnostics"
if (diag>1) print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3] >> "diagnostics"
}

END {
#####
routine for DRPs#####
if (DRP==1) {
    maxForce=0;oscillTest=0
    for (i=1;i<=numAtoms;i++) {
        for (j=1;j<=3;j++) {
# conversions here take force to J/angstrom, 1E20 converts to kg angstroms / s^2, then mult time
(s^s) and divide by weight in kg to get angstroms

        forceArr[i,j]=1E20*forceArr[i,j]*627.509*(4184/(0.529177*avNum))*(timestep^2)/(weight[i]/(a
vNum*1000))
        oscillTest=oscillTest+forceArr[i,j]*oldForce[i,j]
        if (forceArr[i,j]>maxForce) maxForce=forceArr[i,j]
        if ((0-forceArr[i,j])>maxForce) maxForce=-forceArr[i,j]
    }
    if (i==1) printf("% .8f % .8f % .8f \n",forceArr[1,1],forceArr[1,2],forceArr[1,3]) >
"oldAdjForces"
    if (i>1) printf("% .8f % .8f % .8f \n",forceArr[i,1],forceArr[i,2],forceArr[i,3]) >>
"oldAdjForces"
}
print "oscillTest ",oscillTest >> "oldAdjForces"
if (oscillTest<0) {
    maxAtomMove = maxAtomMove*0.5
    print maxAtomMove > "maxMove"
}
if (oscillTest>0) {
    maxAtomMove = maxAtomMove*1.2
    print maxAtomMove > "maxMove"
}
print "maxAtomMove ",maxAtomMove >> "oldAdjForces"
forceMult=maxAtomMove/maxForce
for (i=1;i<=numAtoms;i++) {
    for (j=1;j<=3;j++) {
        newarr[i,j]=oldarr[i,j]+forceMult*forceArr[i,j]
    }
}
}

```

```

}
#####
#####normal routine for Verlet #####
if (DRP==0) {
    for (i=1;i<=numAtoms;i++) {
        for (j=1;j<=3;j++) {
# conversions here take force to J/angstrom, 1E20 converts to kg angstroms / s^2, then mult time
(s^s) and divide by weight in kg to get angstroms
forceArr[i,j]=1E20*forceArr[i,j]*627.509*(4184/(0.529177*avNum))*(timestep^2)/(weight[i]/(a
vNum*1000))
        if ((diag>1) && (i==1)) print "i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]" >>
"diagnostics"
        if (diag>1) print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]>> "diagnostics"
        newarr[i,j]=oldarr[i,j]+damping*(oldarr[i,j]-olderarr[i,j])+forceArr[i,j]
        if ((i==fixedatom1) || (i==fixedatom2) || (i==fixedatom3) || (i==fixedatom4))
newarr[i,j]=oldarr[i,j]
#turn around atoms outside the box
        if (boxon==1) {
            if (newarr[i,j]>boxsize) if (oldarr[i,j]>olderarr[i,j])
newarr[i,j]=oldarr[i,j]+damping*(olderarr[i,j]-oldarr[i,j])+forceArr[i,j]
            if (newarr[i,j]<-1*boxsize) if (oldarr[i,j]<olderarr[i,j])
newarr[i,j]=oldarr[i,j]+damping*(olderarr[i,j]-oldarr[i,j])+forceArr[i,j]
        }
    }
}
#####

if ((runpointnum % keepevery)==0) system("cat g03.log >> dyn")
print "%nproc=" processors
print "%mem=" memory
if (killcheck!=1) print "%chk=" checkpoint
print "# " method " force scf=(maxcycle=200)"
if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
if (meth2=="read") print "guess=tcheck" #for reading orbitals from check, sometimes faster,
sometimes not
print "pop=none"
if (length(meth3)>2) print meth3
if (length(meth4)>2) print meth4
print ""
print title1,title2,title3,title4
print "runpoint ",runpointnum
print "runisomer ",isomernum
if (DRP==1) print "maxForce and forceMult and
maxAtomMove",maxForce,forceMult,maxAtomMove
print ""
print charge,multiplicity
for (i=1;i<=numAtoms;i++) {
    printf("%s %.7f %.7f %.7f",atSym[i],newarr[i,1],newarr[i,2],newarr[i,3])
    if (i>highlevel) printf(" %s","M")
    print ""
}
print ""
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
if (methodfilelines>=1) {
    for (i=1;i<=methodfilelines;i++) {
        getline < "methodfile"
        print $0
    }
}
print ""

```

}

6. Program randgen

```
# c program
# this can be replaced by a more reliable random number
# generator when available on a system
#include <stdio.h>
#include <stdlib.h>

int a,b,c;
double d;

int product(int x, int y);

int main(void)
{
    int count=1;
    srand48(time (0));
    while (count<=10000)
    {
        d = drand48();
        printf ("%,.20f\n", d);
        count++;
    }
    return 0;
}
```

7. Program proganal

```
BEGIN {
getline <"isomernumber"
isomer=$1
}

/ CpDim/
printf("%s %s %s %s %s %s %s ",$1,$2,$3,$4,$6,$8)
runpoint=$6
isomer=$8
}
/ 1 C 0.000000/./ 6 H 0.000000/
if ($1==8) CCset=$4
if ($1==10) CCh=$3
if ($1==12) CCl=$6
}
END {
printf("%s %.3f %s %.3f %s %.3f ","CCset",CCset,CCh,CCh,CCl,CCl)
if (runpoint>500) {
    print "Too many points. XXXX"
    movedyn(isomer)
}
if (CCset>2.2) {
    print "Dead starting material XXXX"
    killdyn(isomer)
}
if ((CCset<1.7) && (CCh<2.2)) {
    print "Heavy carbon reacted XXXX"
    movedyn(isomer)
}
if ((CCset<1.7) && (CCl<2.2)) {
    print "Light carbon reacted XXXX"
    movedyn(isomer)
}
```

```

system("date")
if (runpoint>2) system("tail -1 Echeck | grep XXXX")
}

function movedyn(isomer) {
if (isomer==1) system("mv dyn dyn1")
if (isomer==2) system("mv dyn dyn2")
if (isomer==3) system("mv dyn dyn3")
if (isomer==4) system("mv dyn dyn4")
if (isomer==5) system("mv dyn dyn5")
if (isomer==6) system("mv dyn dyn6")
if (isomer==7) system("mv dyn dyn7")
if (isomer==8) system("mv dyn dyn8")
if (isomer==9) system("mv dyn dyn9")
if (isomer==10) system("mv dyn dyn10")
if (isomer==11) system("mv dyn dyn11")
if (isomer==12) system("mv dyn dyn12")
if (isomer==13) system("mv dyn dyn13")
if (isomer==14) system("mv dyn dyn14")
if (isomer==15) system("mv dyn dyn15")
if (isomer==16) system("mv dyn dyn16")
if (isomer==17) system("mv dyn dyn17")
if (isomer==18) system("mv dyn dyn18")
if (isomer==19) system("mv dyn dyn19")
if (isomer==20) system("mv dyn dyn20")
if (isomer==21) system("mv dyn dyn21")
if (isomer==22) system("mv dyn dyn22")
if (isomer==23) system("mv dyn dyn23")
if (isomer==24) system("mv dyn dyn24")
if (isomer==25) system("mv dyn dyn25")
if (isomer==26) system("mv dyn dyn26")
if (isomer==27) system("mv dyn dyn27")
if (isomer==28) system("mv dyn dyn28")
if (isomer==29) system("mv dyn dyn29")
if (isomer==30) system("mv dyn dyn30")
}

function killdyn(isomer) {
  system("rm -f dyn")
}

function moveold(isomer) {
if (isomer==1) system("cp old* n1")
if (isomer==2) system("cp old* n2")
if (isomer==3) system("cp old* n3")
if (isomer==4) system("cp old* n4")
if (isomer==5) system("cp old* n5")
if (isomer==6) system("cp old* n6")
if (isomer==7) system("cp old* n7")
if (isomer==8) system("cp old* n8")
if (isomer==9) system("cp old* n9")
if (isomer==10) system("cp old* n10")
if (isomer==11) system("cp old* n11")
if (isomer==12) system("cp old* n12")
if (isomer==13) system("cp old* n13")
if (isomer==14) system("cp old* n14")
if (isomer==15) system("cp old* n15")
if (isomer==16) system("cp old* n16")
if (isomer==17) system("cp old* n17")
if (isomer==18) system("cp old* n18")
if (isomer==19) system("cp old* n19")
if (isomer==20) system("cp old* n20")
if (isomer==21) system("cp old* n21")
if (isomer==22) system("cp old* n22")
}

```

```

if (isomer==23) system("cp old* n23")
if (isomer==24) system("cp old* n24")
if (isomer==25) system("cp old* n25")
if (isomer==26) system("cp old* n26")
if (isomer==27) system("cp old* n27")
if (isomer==28) system("cp old* n28")
if (isomer==29) system("cp old* n29")
if (isomer==30) system("cp old* n30")
}

```

8. progdyn.conf

```

#conf file for dynamics. This is read by awk programs prog1stpoint, prog2ndpoint, and
progdynb.

#The programs won't read anything past the first blank line,
#and this file must end with a blank line. You can add to these comments but
#don't use keywords as the first word on a line. Don't delete lines - the program
#has no built in default values if they aren't here.

#values here are read repeatedly and can be changed in the middle of runs
method B3LYP/6-31G*
method2 restricted #The options here are restricted, unrestricted, and read.
#If the method is U..., put unrestricted here and the .com files will have in them guess=mix.
#If you put read here, the .com files will contain guess=tcheck, which sometimes makes things
faster, sometimes not.

charge 0
multiplicity 1
memory 100000000
killcheck 1
#checkpoint dyn20.chk #uses one checkpoint file repeatedly
processors 1
diagnostics 0 # 1 prints out extra stuff to a file "diagnostics", 2 adds velocities to a file "vellist"
title CpDim76C4 B3631Gd 298QC dis=2 # the title must be exactly four words
initialdis 2
timestep 1E-15
scaling 1.0
temperature 298.15
#add extra lines to .com files to implement things like the iop for mPW1k
#Leave the second word blank if you are not going to use them. otherwise any word you put in
will end up in the com file
#only a single term with no spaces can be added, one per method line
#method3 IOp(3/76=0572004280)
#add the line below with big structures to get it to put out the distance matrix and the input
orientation
#method3 iop(2/9=2002)
#method4 scrf=(pcm,solvent=dmso,read)
#method5 and method6 are placed at the end of the file instead of in the keyword section
method5
method6
#for more complicated ends of .com files, it will be necessary to put the ends in a file

```

```

#methodfile 1
#searchdir says what direction to follow the mode associated with the imaginary frequency.
#put as values the words "negative" or "positive"
searchdir negative
#for quasiclassical dynamics, the default, use 0. for classical dynamics, use 1 below
#if there are no normal modes and the velocities are to be generated from scratch, use classical=2
classical 0
#to run a DRP use 'DRP 1' in the line below, otherwise leave it at 0
#treatment of starting saddlepoints not yet implemented
#if DRP shows oscillations then decrease maxAtomMove
#DRP 1
#saddlepoint no
#maxAtomMove 0.01
# to fire a structure toward a ts, make a file cannontraj with initial velocities and set cannonball
to the amount of extra energy you want to put in
#cannonball 10
#line below gives number of negative frequencies - if 0, treats as ground state and direction of all
modes is random
#if 1, negative freq will go direction of searchdir
#if 2, only lowest freq will go direction of searchdir and other imag mode will go in random
direction
numimag 1
# the line below tells progdynb how often to write g03.log to file dyn, after the first two points.
Use 1 for most dynamics
# until excessive, but use a higher integer if doing long term classical dynamics.
keepevery 5
# for ONIOM jobs, the following line states the number of highlevel atoms, which must come
before the medium level atoms
# make this number 999 if not ONIOM
highlevel 999
#use fixedatom1, fixedatom2, fixedatom3, fixedatom4 to fix atoms in space.
#note that fixing one atom serves no useful purpose and messes things up, while
#fixing two atoms fixes one distance, and
#fixing three has the effect of fixing three distances, not just two
#in current form fixed atoms only are meant to work with no displacements, that is, initialdis=0
#fixedatom1 2
#fixedatom2 3
#fixedatom3 19
#dynamics with solvent molecules tends to blast molecules away. Because of this,
#it would be good to have a pressure and periodic boundary conditions, etc, but until
#I learn how to do this, I can just restrict the molecules to a box
#atoms outside this box get bounced. Set box size so as to fit the entire initial molecule but not
have too much extra room
#the box does not affect anything until progdynb
boxon 0
boxsize 7.5

```

```
# you can set the initialdis of particular modes by using a series of lines of the format
# displacements NumberOfMode InitialDisForThatMode, as in the line below. You should be
able to do as many of these as you like
# you might consider this for rotations where a straight-line displacement goes wrong at large
displacements
#displacements 86 2
```

```
#updated Aug 9, 2007 to include the possibility of classical dynamics by the keyword classical
#updated Jan 2008 to include fixed atoms, ONIOM jobs, keepevery, and box size
#update Feb 2008 to include methodfile parameter
# updated Nov 2008 to allow for start without an initial freq calc using classical = 2
```

9. Program modifications used in calculational experiments

Classical trajectories were accessed from the standard code above using classical 1 in progdyn.conf.

To start trajectories with carbon 12 then switch to using carbon 140 with constant momentum, lines as shown below, modified slightly for each carbon, were added to proggenHP at line 335:
***** this section changed for special experiment for cyclopentadiene. do not use this for other cases

```
atWeight[1]=140.0001
# ***** line below added for special experiment switching mass from 12 to 140, keeping
momenta the same
velArr[1,1]=velArr[1,1]/11.66667; velArr[1,2]=velArr[1,2]/11.66667;
velArr[1,3]=velArr[1,3]/11.66667
```

To start trajectories with carbon 140 then switch to using carbon 12 with constant momentum, lines as shown below were added to proggenHP. At line 123, the addition was:

```
# ***** line below is commented out for special experiment switching weights - do not use
for regular runs
# if ((i<100) && ($9>0)) atWeight[i]=$9
at line 340, the addition was:
# ***** line below added for special experiment switching mass from 140 to 12, keeping
momenta the same
velArr[4,1]=11.66667*velArr[4,1]; velArr[4,2]=11.66667*velArr[4,2];
velArr[4,3]=11.66667*velArr[4,3]
```

To equalize the sampling of trajectories with positive and negative signs for the velocities of the lowest-energy real vibrational mode, the line 476 of proggenHP was uncommented, using either:
if (vel[2]<0) vel[2]=-vel[2]
or
if (vel[2]>0) vel[2]=-vel[2]
to obtain trajectories of a desired sign.

C. POLYRATE calculations

Chapter 2 – summary of rate constants

Reaction of acetaldehyde and enamine of acetone – B3LYP/6-31G* - Onsager solvent model for DMSO. Rates calculated with

No Label	¹³ C Label at parent	¹³ C Label at Carbonyl	¹³ C Label at enamine	¹³ C Label at methyl	² H label at carboxylic proton
TST	TST	TST	TST	TST	TST
7.71E+03	7.44E+03	7.57E+03	7.72E+03	3.45E+03	
TST/W	TST/W	TST/W	TST/W	TST/W	TST/W
8.64E+03	8.31E+03	8.46E+03	8.65E+03	3.84E+03	
TST/CAG	TST/CAG	TST/CAG	TST/CAG	TST/CAG	TST/CAG
5.33E+03	5.14E+03	5.21E+03	5.34E+03	2.95E+03	
CVT	CVT	CVT	CVT	CVT	CVT
6.09E+03	5.86E+03	5.96E+03	6.10E+03	3.20E+03	
CVT/CAG	CVT/CAG	CVT/CAG	CVT/CAG	CVT/CAG	CVT/CAG
6.00E+03	5.77E+03	5.86E+03	6.00E+03	3.15E+03	
TST/ZCT	TST/ZCT	TST/ZCT	TST/ZCT	TST/ZCT	TST/ZCT
6.27E+03	6.01E+03	6.09E+03	6.27E+03	3.41E+03	
CVT/ZCT	CVT/ZCT	CVT/ZCT	CVT/ZCT	CVT/ZCT	CVT/ZCT
7.04E+03	6.75E+03	6.85E+03	7.05E+03	3.64E+03	
TST/ZCTnt	TST/ZCTnt	TST/ZCTnt	TST/ZCTnt	TST/ZCTnt	TST/ZCTnt
4.51E+03	4.35E+03	4.41E+03	4.51E+03	2.50E+03	
CVT/ZCTnt	CVT/ZCTnt	CVT/ZCTnt	CVT/ZCTnt	CVT/ZCTnt	CVT/ZCTnt
5.07E+03	4.88E+03	4.96E+03	5.07E+03	2.68E+03	
TST/SCT	TST/SCT	TST/SCT	TST/SCT	TST/SCT	TST/SCT
6.57E+03	6.29E+03	6.38E+03	6.57E+03	3.62E+03	
CVT/SCT	CVT/SCT	CVT/SCT	CVT/SCT	CVT/SCT	CVT/SCT
7.39E+03	7.07E+03	7.17E+03	7.39E+03	3.86E+03	
TST/SCTnt	TST/SCTnt	TST/SCTnt	TST/SCTnt	TST/SCTnt	TST/SCTnt
4.44E+03	4.29E+03	4.35E+03	4.45E+03	2.46E+03	
CVT/SCTnt	CVT/SCTnt	CVT/SCTnt	CVT/SCTnt	CVT/SCTnt	CVT/SCTnt
5.00E+03	4.82E+03	4.89E+03	5.00E+03	2.63E+03	

Chapter 4 – summary of rate constants

Reaction of *p*-nitrobenzaldehyde and **38** – B3LYP/6-31G*

Rates calculated with

No Label	13C Label at parent	13C Label at TST	13C Label at methylene	13C Label at internal	13C Label at terminal
TST	TST	TST	TST	TST	TST
6.64E-07	6.41E-07	6.52E-07	6.66E-07	6.48E-07	
TST/W	TST/W	TST/W	TST/W	TST/W	TST/W
7.71E-07	7.42E-07	7.56E-07	7.73E-07	7.48E-07	
TST/CAG	TST/CAG	TST/CAG	TST/CAG	TST/CAG	TST/CAG
6.53E-07	6.30E-07	6.40E-07	6.55E-07	6.37E-07	
CVT	CVT	CVT	CVT	CVT	CVT
6.37E-07	6.14E-07	6.25E-07	6.40E-07	6.22E-07	
CVT/CAG	CVT/CAG	CVT/CAG	CVT/CAG	CVT/CAG	CVT/CAG
6.34E-07	6.12E-07	6.22E-07	6.37E-07	6.19E-07	
TST/ZCT	TST/ZCT	TST/ZCT	TST/ZCT	TST/ZCT	TST/ZCT
7.89E-07	7.58E-07	7.73E-07	7.91E-07	7.65E-07	
CVT/ZCT	CVT/ZCT	CVT/ZCT	CVT/ZCT	CVT/ZCT	CVT/ZCT
7.66E-07	7.37E-07	7.51E-07	7.69E-07	7.43E-07	
TST/ZCTnt	TST/ZCTnt	TST/ZCTnt	TST/ZCTnt	TST/ZCTnt	TST/ZCTnt
5.45E-07	5.26E-07	5.34E-07	5.47E-07	5.33E-07	
CVT/ZCTnt	CVT/ZCTnt	CVT/ZCTnt	CVT/ZCTnt	CVT/ZCTnt	CVT/ZCTnt
5.29E-07	5.11E-07	5.19E-07	5.31E-07	5.18E-07	
TST/SCT	TST/SCT	TST/SCT	TST/SCT	TST/SCT	TST/SCT
8.16E-07	7.84E-07	8.01E-07	8.19E-07	7.91E-07	
CVT/SCT	CVT/SCT	CVT/SCT	CVT/SCT	CVT/SCT	CVT/SCT
7.93E-07	7.62E-07	7.78E-07	7.96E-07	7.69E-07	
TST/SCTnt	TST/SCTnt	TST/SCTnt	TST/SCTnt	TST/SCTnt	TST/SCTnt
5.39E-07	5.21E-07	5.28E-07	5.41E-07	5.27E-07	
CVT/SCTnt	CVT/SCTnt	CVT/SCTnt	CVT/SCTnt	CVT/SCTnt	CVT/SCTnt
5.24E-07	5.06E-07	5.14E-07	5.26E-07	5.13E-07	

Reaction of *p*-anisaldehyde and **38** – B3LYP/6-31G*

Rates calculated with

No Label parent	13C Label at carbonyl	13C Label at methelene	13C Label at internal	13C Label at terminal
TST	TST	TST	TST	TST
2.62E-08	2.51E-08	2.56E-08	2.62E-08	2.56E-08
TST/W	TST/W	TST/W	TST/W	TST/W
3.33E-08	3.18E-08	3.25E-08	3.34E-08	3.23E-08
TST/CAG	TST/CAG	TST/CAG	TST/CAG	TST/CAG
2.60E-08	2.50E-08	2.54E-08	2.61E-08	2.54E-08
CVT	CVT	CVT	CVT	CVT
2.59E-08	2.48E-08	2.53E-08	2.60E-08	2.53E-08
CVT/CAG	CVT/CAG	CVT/CAG	CVT/CAG	CVT/CAG
2.58E-08	2.48E-08	2.52E-08	2.59E-08	2.53E-08
TST/ZCT	TST/ZCT	TST/ZCT	TST/ZCT	TST/ZCT
3.53E-08	3.36E-08	3.44E-08	3.54E-08	3.41E-08
CVT/ZCT	CVT/ZCT	CVT/ZCT	CVT/ZCT	CVT/ZCT
3.50E-08	3.34E-08	3.41E-08	3.51E-08	3.39E-08
TST/ZCTnt	TST/ZCTnt	TST/ZCTnt	TST/ZCTnt	TST/ZCTnt
2.10E-08	2.02E-08	2.05E-08	2.10E-08	2.06E-08
CVT/ZCTnt	CVT/ZCTnt	CVT/ZCTnt	CVT/ZCTnt	CVT/ZCTnt
2.08E-08	2.00E-08	2.03E-08	2.09E-08	2.04E-08
TST/SCT	TST/SCT	TST/SCT	TST/SCT	TST/SCT
3.72E-08	3.53E-08	3.62E-08	3.72E-08	3.59E-08
CVT/SCT	CVT/SCT	CVT/SCT	CVT/SCT	CVT/SCT
3.69E-08	3.51E-08	3.59E-08	3.70E-08	3.56E-08
TST/SCTnt	TST/SCTnt	TST/SCTnt	TST/SCTnt	TST/SCTnt
2.07E-08	1.99E-08	2.02E-08	2.08E-08	2.03E-08
CVT/SCTnt	CVT/SCTnt	CVT/SCTnt	CVT/SCTnt	CVT/SCTnt
2.06E-08	1.98E-08	2.01E-08	2.06E-08	2.02E-08