SUPPORTING INFORMATION

Isotope Effects and Heavy-Atom Tunneling in the Roush Allylboration of Aldehydes

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Experimental Procedures and NMR Measurements

The Roush allylboronate **4** was synthesized using literature procedures (S1). A solution containing 0.284 g (1 mmol) of **4** in 8 mL of dichloromethane was cooled in a dry ice- acetone bath and maintained at -78 °C. To this solution was added 0.136 g (1 mmol) of **5.** The reaction mixture was stirred for 2 h before the reaction was quenched by the addition of 10 mL of 0.1 N NaOH and 30 mL of diethyl ether. This two phase mixture was stirred vigorously for 30 min at room temperature to hydrolyze the boronate protected alcohol to the homoallylic alcohol **6.** The resulting mixture was extracted with three portions of 10 mL of diethyl ether, and the combined organic layers were dried over Na_2SO_4. The solvent was then removed under reduced pressure to afford 0.2 g of the crude product mixture. The crude mixture was then subjected to flash chromatography using dichloromethane as eluent and 0.170 g (95 % yield) of **6** was isolated. The isolated products characterized by ^{1}H NMR, were found to be free of starting materials or any other impurities. For KIE measurements, a scaled up analog (15 mmol scale and 3 mmol of limiting reagent) of the above mentioned procedure was used. Conversions were determined by the comparison of starting material and product peaks in the NMR spectrum of the crude reaction mixture. The absence of any visible side products and complete consumption of the limiting reagent were confirmed by ^{1}H NMR. As a particular example, for the reaction of **4** and **5**, separate reactions were taken to 18 ± 2% conversion in **4** and 20 ± 2% conversion in **5** by using limiting amounts of the other reagent. The ^{13}C isotopic composition of the two samples of **6,** isolated from these two reactions was compared against each other in order to determine KIEs.

NMR measurements. All samples were prepared using a constant 295 mg of **6** in 5 mm NMR tubes filled to a constant height of 5.0 cm. The ^{13}C spectra were recorded at 125.70 MHz using inverse gated decoupling, 52.5 s delays (5 times T1) between calibrated π/2 pulses, and a 5.0 s acquisition time to collect 195312 points. Integrations were numerically determined using a constant integration region for each peak. A zero-order baseline correction was generally applied, but no first-order correction was applied. Six spectra were recorded for each sample of recovered **6.**

Computational Procedures and Supporting Computational Results

General

All of the M06-2X/6-31+G**, M06-2X/6-31+G**/PCM, B3LYP/6-31+G**, and B3LYP/6-31+G**/PCM calculations of structures, energies, and frequencies employed standard procedures in Gaussian 09 (S2, see the last section for the complete reference) unless otherwise noted. All of the B3LYP/6-31G*, MPW1K, MP2, and M05 calculations of structures, energies, and frequencies employed standard procedures in Gaussian 03 (S3) unless otherwise noted. PCM calcuations in Gaussian 09 were carried out with the solvent being dichloromethane. Complete structures and energetics are provided in a section below.

GAUSSRATE Calculations

General

A number of the calculations in the manuscript made use of the programs GAUSSRATE (reference 17 in the main text) and POLYRATE (reference 18 in the main text, see the last section for the complete reference) (S4). These programs were modified in minor ways. In particular, the subroutine *mepout* was modified to output frequencies with higher precision, and the utility program *shuttle* was modified to save copies of all frequency calculations so that data could be extracted from

them later.

To show the complete set of options selected for these calculations, a sample set of input files for GAUSSRATE / POLYRATE are given in a later section. For the sake of simplicity, the starting material in these calculations was generally taken to be a minimized loose complex of reactants. Such complexes are not kinetically significant but the process employed in the main text of multiplying the TST KIE (not based on a loose complex but rather on separate starting materials) times a CVT/SCT correction avoids having the loose complexes have any effect on the final results.

The Gaussian command int(grid=ultrafine) was used for the calculations, and the starting structures were optimized with tight convergence criteria.

Gaussrate Rate Constants and CVT/SCT Correction Factors

The KIEs that are listed are not directly meaningful, in part because they are for the model system instead of the real system and in part because the formal starting material in this case is the prereactive complex instead of the free separate starting materials.

M06-2X/6-31+G**

	parent	C1-13C	C4-13C	C2-13C	C3-13C
TST	4.1754E-02	4.0227E-02	4.0953E-02	4.0668E-02	4.18E-02
CVT	4.1512E-02	3.9971E-02	4.0683E-02	4.0443E-02	4.05E-02
CVT/SCT	5.5302E-02	5.2832E-02	5.4105E-02	5.3313E-02	5.37E-02*
SCT acceleration	1.32				
KIE					
TST		1.038	1.020	1.027	0.999
CVT		1.039	1.020	1.026	0.999
CVT/SCT		1.047	1.022	1.037	0.999
CVT/SCT correction		1.0085	1.0025	1.0103	1.0006*

*The C3-13C rate constants were calculated with a shorter path link than the others, and the KIEs are based on parent rate constants calculated for the same path link. Considering the low effect of tunneling on the C3-13C KIE, the KIEs were numerically converged at a lower path link, so the calculation was not extended.

M06-2X/6-31+G/PCM**

	parent	C1-13C	C4-13C	C2-13C	C3-13C
TST	3.5428E-01	3.4002E-01	3.4772E-01	3.4572E-01	3.5471E-01
CVT	3.5346E-01	3.3911E-01	3.4674E-01	3.4500E-01	3.5390E-01
CVT/SCT	4.8095E-01	4.5715E-01	4.7120E-01	4.6348E-01	4.8105E-01
SCT acceleration	1.36				
KIE					
TST		1.04194	1.01887	1.02476	0.99879
CVT		1.042	1.019	1.025	0.999
CVT/SCT		1.052	1.021	1.038	1.000
CVT/SCT correction	correction	1.009716	1.0018	1.0126	1.0010

B3LYP/6-31+G**

	parent	C1-13C	C4-13C	C2-13C	C3-13C
TST	1.4120E-11	1.3584E-11	1.3813E-11	1.3764E-11	1.4160E-11
CVT	1.3996E-11	1.3459E-11	1.3683E-11	1.3649E-11	1.4037E-11
CVT/SCT	2.0122E-11	1.9170E-11	1.9606E-11	1.9408E-11	2.0172E-11
SCT acceleration	1.43				
KIE					
TST		1.03946	1.02223	1.02586	0.99718
CVT		1.040	1.023	1.025	0.997
CVT/SCT		1.050	1.026	1.037	0.998
CVT/SCT correction		1.0098	1.0040	1.0106	1.0003

B3LYP/6-31+G/PCM**

	parent	C1-13C	C4-13C	C2-13C	C3-13C
TST	1.0234E-11	9.8090E-12	1.0024E-11	1.0007E-11	1.0277E-11
CVT	1.0179E-11	9.7542E-12	9.9659E-12	9.9569E-12	1.0222E-11
CVT/SCT	1.5540E-11	1.4715E-11	1.5163E-11	1.4966E-11	1.5590E-11
SCT acceleration	1.52				
KIE					
TST		1.04333	1.02095	1.02268	0.996
CVT		1.044	1.021	1.022	0.996
CVT/SCT		1.056	1.025	1.038	0.997
CVT/SCT correction		1.0122	1.0038	1.0153	1.0010

B3LYP KIEs

Method	C1	C2	C3	C4
	Conventional TST KIEs			
Gas phase	1.038	1.026	0.996	1.019
PCM	1.044	1.026	0.997	1.018
	CVT / SCT corrections			
Gas phase	1.010	1.011	1.000	1.004
PCM	1.010	1.015	1.001	1.004
	CVT / SCT KIEs[a]			
Gas phase	1.048	1.037	0.996	1.023
PCM	1.056	1.041	0.998	1.022

The Contributions to the C2 KIE

We describe in the main text the components of the C2 KIE and their percentage contribution to the overall KIE. The reduced isotopic partition function at C2 for the transition state is 1.234252 at 195.15° and it is 1.242288 in the ground state, and the ratio of these contributes 1.0065 to the KIE. The scaled imaginary frequency in the parent isotopomer is -340.4614 and it is -334.36707 in the

labeled compound, contributing 1.0182 to the KIE. The CVT/SCT correction is 1.0126. The multiple of these three components is the isotope effect.

Effect of Scaling Factor on KIEs

The table below shows how the choice of scaling factor influences the size of the KIE predicted from transition state theory for the M06-2X/6-31+G**/PCM calculations. The results show, as described in footnote 13 of the main text, that small changes in the scaling factor have a negligible effect on the predicted isotope effects. It should be noted that there is no perfect or unambiguous choice of scaling factor, as the appropriate scaling factor would vary for high frequencies (which tend to dominate the choice of scaling factor when determined by normal procedures) versus low frequencies (which are more important in carbon KIEs). Luckily, the choice makes little difference, and we have adopted the procedure of using 0.9614 consistently, simply because it was the choice we used in one of our earliest publications of KIE predictions.

Scaling Factor:	0.94	0.9614	0.98	1.00
C1	1.0405	1.0410	1.0416	1.0421
C4	1.0160	1.0164	1.0167	1.0171
C3	0.9986	0.9984	0.9983	0.9981
C2	1.0248	1.0249	1.0249	1.0250

Calculated Structures and Energies

Organization and Structure Names

The data below is organized by structure and method/basis set. For PCM calculations (in dichloromethane using default procedures), the title includes "PCM" at the end. Under each structure title, the first line is the original file names for the computational output files. This lets us use a single code name for structures, energies in tables, and our records. The second line is the description used by the researcher in the calculational input file. The third line is the potential energy. Other lines are self-explanatory.

Exploratory B3LYP / 6-31G* / gas phase calculations were used to delimit the most stable conformers, and only these were considered in later calculations. An exception occurred with anisaldehyde where two conformers are extremely close in energy, and both are listed. The conformers are designated as Conformation A and Conformation B.

Roush allylboronate 4

M062X/6-31+G**
RoushAllylboronateM06
Roush allylboronate
E(RM062X) = -983.975258156

Zero-point correction= 0.341949 (Hartree/Particle)
Thermal correction to Energy= 0.364090
Thermal correction to Enthalpy= 0.365034
Thermal correction to Gibbs Free Energy= 0.287341
Sum of electronic and ZPE= -983.633309
Sum of electronic and thermal Energies= -983.611168
Sum of electronic and thermal Enthalpies= -983.610224
Sum of electronic and thermal Free Energies= -983.687917

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	228.470	79.296	163.518

C,0,-0.6918578101,3.2256244532,-0.3732879523
B,0,-1.500551353,1.8996548396,-0.5588223154
O,0,-1.9560856357,1.1258727796,0.48874846
C,0,-2.8500627484,0.1723798898,-0.0352211819
C,0,-4.285325361,0.6588793567,0.1236583872
O,0,-5.135458447,-0.3636075614,-0.0122558877
C,0,-6.5508316484,-0.0439137114,-0.0338242091
C,0,0.1319892972,3.6122776052,-1.5684479321
C,0,1.4447687049,3.8362469944,-1.5442548599
O,0,-1.890701022,1.38763321,-1.7789649634
C,0,-2.4954017059,0.1347400881,-1.5530297295
C,0,-1.4937951041,-0.9844234873,-1.8143367207
O,0,-2.1353038478,-2.1440278762,-1.9945550027
C,0,-1.3151634571,-3.329156074,-2.1654613426
O,0,-0.2986265038,-0.8420689268,-1.7951123893
O,0,-4.5969458838,1.8112776964,0.285014953

H,0,-3.3746578304,0.0027928368,-2.1893704993
H,0,-2.7265410928,-0.7966204471,0.4543326673
H,0,-0.0715017252,3.1567916192,0.526908661
H,0,-1.441358348,4.0056694886,-0.1674629321
H,0,-0.4026501054,3.6933105973,-2.5143997436
H,0,1.9913783402,4.0990021876,-2.4440615573
H,0,2.0153608094,3.754531929,-0.6220628464
C,0,-2.2049563671,-4.5031740532,-1.8064267521
C,0,-0.7995892324,-3.382904087,-3.5937151484
H,0,-0.4762998766,-3.246234314,-1.4671238708
C,0,-7.2722581319,-1.3308821061,0.3139713164
H,0,-6.7220382939,0.7197941661,0.7308993335
C,0,-6.918259859,0.4983734158,-1.4051511292
H,0,-0.1929313463,-4.2821341475,-3.7339461133
H,0,-1.639681338,-3.4189312883,-4.2941916132
H,0,-0.1806011799,-2.5112604057,-3.8157062731
H,0,-1.638772296,-5.4348668166,-1.8880212352
H,0,-2.5790910262,-4.4102608318,-0.7840281593
H,0,-3.0592488118,-4.5550642089,-2.4879624007
H,0,-8.3509916651,-1.1549450372,0.3403852574
H,0,-7.0636855568,-2.0987059904,-0.4370226114
H,0,-6.9554130759,-1.7024097337,1.2912573758
H,0,-7.9853724711,0.7357075575,-1.4371598167
H,0,-6.3581720001,1.410281556,-1.6248646615
H,0,-6.7079439936,-0.2518731624,-2.1740365613

M062X/6-31+G/PCM**
RoushAllylboronateM06PCM
Roush allylboronate
E(RM062X) = -983.987751142

Zero-point correction= 0.341325 (Hartree/Particle)
Thermal correction to Energy= 0.363552
Thermal correction to Enthalpy= 0.364497
Thermal correction to Gibbs Free Energy= 0.286060
Sum of electronic and ZPE= -983.646426
Sum of electronic and thermal Energies= -983.624199
Sum of electronic and thermal Enthalpies= -983.623255
Sum of electronic and thermal Free Energies= -983.701691

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	228.133	79.466	165.083

C,0,-0.6312441762,3.2085351343,-0.2733741397
B,0,-1.459497186,1.8999143513,-0.4989854572
O,0,-1.9381912401,1.1116267345,0.5270933218
C,0,-2.8234149584,0.1619555883,-0.0292387195
C,0,-4.2634140202,0.6363595207,0.128418409
O,0,-5.1022139679,-0.3718200858,-0.0841344935
C,0,-6.527420785,-0.0698450957,-0.1208719394
C,0,0.0574318247,3.717619729,-1.5073110629
C,0,1.3725010187,3.9036947861,-1.6235517732
O,0,-1.8256851613,1.4083857374,-1.7339474948
C,0,-2.4501220999,0.1554531632,-1.5417923639
C,0,-1.4667303233,-0.9728842678,-1.8340492587
O,0,-2.118241685,-2.1278056121,-1.9265321514
C,0,-1.3289513075,-3.3363207026,-2.1256692261
O,0,-0.2705836712,-0.8274873806,-1.9167754512
O,0,-4.5756857879,1.7807111712,0.3582519202
H,0,-3.3234711784,0.0528331666,-2.1910740776
H,0,-2.6993768073,-0.8143734788,0.4443360869
H,0,0.0874188162,3.0490312113,0.5388148121
H,0,-1.3439527153,3.9615788743,0.0956219365
H,0,-0.5842333007,3.9343920498,-2.3613689536
H,0,1.812555407,4.2653179105,-2.5475257094
H,0,2.0483989067,3.6955377703,-0.7970389706
C,0,-2.1863152153,-4.4782524363,-1.6187740705
C,0,-0.9726414803,-3.4595828509,-3.5968260296
H,0,-0.4235304615,-3.230723046,-1.5214592781
C,0,-7.2352699788,-1.3810676691,0.1526258369
H,0,-6.7237141736,0.6524393938,0.6764267616
C,0,-6.8674285214,0.527344617,-1.4753379268
H,0,-0.3791714229,-4.3642439709,-3.7545364176
H,0,-1.8832674194,-3.5321446096,-4.1990502437
H,0,-0.3874901205,-2.6000023834,-3.9309512678
H,0,-1.6370762499,-5.4180998125,-1.7172977428
H,0,-2.4457000995,-4.3350311556,-0.5671541253
H,0,-3.1075415265,-4.5516179156,-2.2042687398
H,0,-8.3160681468,-1.2185459818,0.1553517133
H,0,-6.9956292642,-2.1124594224,-0.6249725899
H,0,-6.9413576651,-1.7873955782,1.1232115734
H,0,-7.9359926305,0.7537913293,-1.5198921015
H,0,-6.3127051079,1.4532190465,-1.6456720966
H,0,-6.6296051177,-0.1866598298,-2.2698304993

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)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	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,0,2.0421375634,3.8360354691,-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 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) KCal/Mol	CV Cal/Mol-Kelvin	S 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/6-31+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 PCM solvent model for dichloromethane**
allylDIPEMPW1KPCMPS
E(RmPW+HF-PW91) = -984.112125325

Zero-point correction= 0.347756
(Hartree/Particle)
Thermal correction to Energy= 0.369822
Thermal correction to Enthalpy= 0.370766
Thermal correction to Gibbs Free Energy= 0.292549
Sum of electronic and zero-point Energies= -983.764369
Sum of electronic and thermal Energies= -983.742304
Sum of electronic and thermal Enthalpies= -983.741359
Sum of electronic and thermal Free Energies= -983.819576

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	232.067	78.210	164.621

C,0,3.5562725932,-1.7273178407,-0.4154708991
C,0,4.5744140409,-1.2211207283,0.551396954
C,0,5.7056925787,-0.6134138264,0.2152455396
B,0,2.1168346714,-1.1562980968,-0.2312321814
O,0,1.6581250006,-0.5098957868,0.8840474011
C,0,0.348902262,-0.0710946495,0.6426403726
C,0,0.3308778861,1.4225893142,0.3793074216
O,0,1.2985011917,2.0655431027,0.0722347587
O,0,1.1339627964,-1.2883646538,-1.177159758
C,0,-0.079447752,-0.8559183488,-0.6255393971
C,0,-0.9420283209,-2.047381359,-0.2547887751
O,0,-0.5297255849,-3.1720847361,-0.1522628383
O,0,-2.1801905287,-1.6581607928,-0.0394666751
C,0,-3.1506923102,-2.644140771,0.3832338109
C,0,-3.0551834177,-2.8257176256,1.8793973952
C,0,-4.491206966,-2.1257222255,-0.0715415974
O,0,-0.8962785075,1.883694515,0.4972750892
C,0,-1.1377280926,3.2824235484,0.2196103296
C,0,-0.8616210594,4.0868877097,1.4675876977
C,0,-2.5683566583,3.3728181953,-0.2468942924
H,0,-0.2833840564,-0.2799156808,1.5027919135
H,0,-0.6221097101,-0.2380548523,-1.340082453
H,0,3.8769040596,-1.5595400394,-1.4449939175
H,0,3.4562715265,-2.814445164,-0.3103208785
H,0,4.353336495,-1.3705416461,1.6040720695
H,0,6.4018958546,-0.266603569,0.9657216221
H,0,5.9691434153,-0.4390152735,-0.8203796504
H,0,-0.4557575118,3.5768310762,-0.5770777586
H,0,-2.9070269596,-3.5754682192,-0.1264777813
H,0,-1.0423798363,5.1417809616,1.2705507719
H,0,-1.5177003281,3.7724889478,2.27745082
H,0,0.1717461526,3.9744250452,1.7853576158
H,0,-2.806525337,4.4048718245,-0.495364026
H,0,-2.7285585112,2.7614352498,-1.1316302073
H,0,-3.2505684989,3.0412747819,0.5336344419
H,0,-5.2682265732,-2.8384881556,0.196338718
H,0,-4.7184039895,-1.1744160005,0.4057458187
H,0,-4.5092143812,-1.9880220952,-1.1499377704
H,0,-3.7846184561,-3.5646347995,2.2052310001
H,0,-2.0681806635,-3.1764951338,2.1704126046
H,0,-3.2655585136,-1.8887762023,2.3924416908

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 – 5**

Conformation A, M062X/6-31+G**
anisaldehydeAM06
anisaldehyde conf A
E(RM062X) = -459.924221249

Zero-point correction= 0.144199 (Hartree/Particle)
Thermal correction to Energy= 0.152933
Thermal correction to Enthalpy= 0.153877
Thermal correction to Gibbs Free Energy= 0.110385
Sum of electronic and ZPE= -459.780022
Sum of electronic and thermal Energies= -459.771289
Sum of electronic and thermal Enthalpies= -459.770344
Sum of electronic and thermal Free Energies= -459.813836

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	95.967	32.737	91.536

C,0,-0.0037521555,0.,0.1186513237
C,0,0.0539226945,0.,1.5157940835
C,0,1.3008635493,0.,2.1389002924
C,0,2.4769995815,0.,1.3933944016
C,0,2.4055845275,0.,-0.008959121
C,0,1.1789392333,0.,-0.6417443993
H,0,-0.8476917089,0.,2.1156279629
H,0,1.3549193741,0.,3.2254489302
C,0,3.7828269424,0.,2.0817193968
H,0,3.3306542839,0.,-0.5777416455
H,0,1.0928032377,0.,-1.722975718
O,0,-1.1529133387,0.,-0.5944940574
C,0,-2.3783481722,0.,0.1139100206
H,0,-3.1613103504,0.,-0.6428526441
H,0,-2.4713127034,-0.895949944,0.7380585904
H,0,-2.4713127034,0.895949944,0.7380585904
O,0,4.8559658063,0.,1.519055221
H,0,3.7295429019,0.,3.1908607719

Conformation A, M062X/6-31+G/PCM**
anisaldehydeAM06PCM
anisaldehyde conf A
E(RM062X) = -459.932432920

Zero-point correction= 0.144031 (Hartree/Particle)
Thermal correction to Energy= 0.152802
Thermal correction to Enthalpy= 0.153746
Thermal correction to Gibbs Free Energy= 0.110174
Sum of electronic and ZPE= -459.788402
Sum of electronic and thermal Energies= -459.779631
Sum of electronic and thermal Enthalpies= -459.778687
Sum of electronic and thermal Free Energies= -459.822259

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	95.885	32.838	91.705

C,0,-0.0024249303,0.,0.1165396207
C,0,0.0554694053,0.,1.5148654729
C,0,1.3017680509,0.,2.1373269611
C,0,2.4798626842,0.,1.3902962783
C,0,2.4079513054,0.,-0.0133736443
C,0,1.1810201357,0.,-0.6456212768
H,0,-0.8455904355,0.,2.115194996
H,0,1.3547252653,0.,3.2234590629
C,0,3.7758439197,0.,2.085805219
H,0,3.3282034854,0.,-0.5897540821
H,0,1.0987714766,0.,-1.7273029775
O,0,-1.150768873,0.,-0.5935958611
C,0,-2.3812965352,0.,0.1191530363
H,0,-3.1635307971,0.,-0.6375292849
H,0,-2.4702138331,-0.8960449061,0.7415093652
H,0,-2.4702138331,0.8960449061,0.7415093652

O,0,4.8597403587,0.,1.5305039674
H,0,3.7170641501,0.,3.1917257821

Conformation B, M062X/6-31+G**
anisaldehydeBM06
anisaldehyde conf B
E(RM062X) = -459.924116814

Zero-point correction= 0.143772 (Hartree/Particle)
Thermal correction to Energy= 0.152611
Thermal correction to Enthalpy= 0.153556
Thermal correction to Gibbs Free Energy= 0.109664
Sum of electronic and ZPE= -459.780345
Sum of electronic and thermal Energies= -459.771505
Sum of electronic and thermal Enthalpies= -459.770561
Sum of electronic and thermal Free Energies= -459.814453

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.765	32.884	92.377

C,0,-0.0025165611,0.,0.116468798
C,0,0.0543430715,0.,1.5173381072
C,0,1.2931447998,0.,2.147978541
C,0,2.4733015274,0.,1.4025854906
C,0,2.4030137899,0.,0.0038984919
C,0,1.1778782948,0.,-0.639979427
H,0,-0.8505718772,0.,2.1126055503
H,0,1.3627682804,0.,3.2320107351
C,0,3.7872812202,0.,2.0759046213
H,0,3.3206025231,0.,-0.5802943812
H,0,1.0980264349,0.,-1.721564172
O,0,-1.1522953108,0.,-0.5958387101
C,0,-2.3788641018,0.,0.1115898208
H,0,-3.1604619411,0.,-0.6466267298
H,0,-2.4733076121,-0.8959233956,0.7355471612
H,0,-2.4733076121,0.8959233956,0.7355471612
O,0,3.944387959,0.,3.2773627524
H,0,4.6642001136,0.,1.3948621893

Conformation B, M062X/6-31+G/PCM**
anisaldehydeBM06PCM
anisaldehyde conf B
E(RM062X) = -459.932187405

Zero-point correction= 0.143658 (Hartree/Particle)
Thermal correction to Energy= 0.152521
Thermal correction to Enthalpy= 0.153465
Thermal correction to Gibbs Free Energy= 0.109537
Sum of electronic and ZPE= -459.788529
Sum of electronic and thermal Energies= -459.779666
Sum of electronic and thermal Enthalpies= -459.778722
Sum of electronic and thermal Free Energies= -459.822651

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.708	32.957	92.455

C,0,-0.0013640658,0.,0.116042051
C,0,0.0521638259,0.,1.5185415556
C,0,1.2897465865,0.,2.1501136661
C,0,2.4733095825,0.,1.4061254485
C,0,2.4059915729,0.,0.005585956
C,0,1.1814093891,0.,-0.6391548467
H,0,-0.8535870545,0.,2.1121104867
H,0,1.3488913963,0.,3.2346071802
C,0,3.7867627504,0.,2.0688875787
H,0,3.3235661101,0.,-0.5778027297
H,0,1.1080782896,0.,-1.7213649287
O,0,-1.1492158283,0.,-0.5951452003
C,0,-2.3821803926,0.,0.1139268221
H,0,-3.1615617058,0.,-0.6457521632
H,0,-2.4740699039,-0.8961228929,0.7358676169
H,0,-2.4740699039,0.8961228929,0.7358676169
O,0,3.9551191481,0.,3.2749419227
H,0,4.6586332033,0.,1.3859979675

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)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	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

Conformation A, 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

Conformation B, B3LYP/6-31+G**
panisaldehydeConfBB3PS
anisaldehyde conf B
E(RB3LYP) = -460.129482763

Zero-point correction= 0.142271 (Hartree/Particle)
Thermal correction to Energy= 0.151164
Thermal correction to Enthalpy= 0.152108
Thermal correction to Gibbs Free Energy= 0.108201
Sum of electronic and ZPE= -459.987212
Sum of electronic and thermal Energies= -459.978319
Sum of electronic and thermal Enthalpies= -459.977375
Sum of electronic and thermal Free Energies= -460.021282

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	94.857	33.170	92.410

C,0,-0.0029023209,0.,0.1217643785
C,0,0.0593648757,0.,1.5273311418
C,0,1.2999637323,0.,2.1582227699
C,0,2.4878949799,0.,1.4118971995
C,0,2.4094802181,0.,0.0071411856
C,0,1.1809830004,0.,-0.6367413174
H,0,-0.8442938005,0.,2.1247612056
H,0,1.3660415854,0.,3.2419182894
C,0,3.8032584533,0.,2.0749806811
H,0,3.3246712411,0.,-0.5805425745
H,0,1.1051434352,0.,-1.718933991
O,0,-1.1583713613,0.,-0.5932651483
C,0,-2.4038088373,0.,0.1015700531
H,0,-3.1717865054,0.,-0.6721550459
H,0,-2.5116734877,-0.8964631187,0.7234725743
H,0,-2.5116734877,0.8964631187,0.7234725743
O,0,3.9826957792,0.,3.2827910993
H,0,4.6726355002,0.,1.3817109247

Conformation A, B3LYP/6-31+G/PCM**
panisaldehydeConfAB3PSPCM
anisaldehyde conf A
E(RB3LYP) = -460.138108888

Zero-point correction= 0.142215 (Hartree/Particle)
Thermal correction to Energy= 0.151124
Thermal correction to Enthalpy= 0.152068
Thermal correction to Gibbs Free Energy= 0.108167
Sum of electronic and ZPE= -459.995894
Sum of electronic and thermal Energies= -459.986985
Sum of electronic and thermal Enthalpies= -459.986041
Sum of electronic and thermal Free Energies= -460.029942

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	94.832	33.238	92.398

C,0,-0.0029945149,0.,0.1212937053
C,0,0.0640240908,0.,1.5242173334
C,0,1.3131509101,0.,2.1434286647
C,0,2.4983135887,0.,1.3924528382
C,0,2.4141869571,0.,-0.0167418431
C,0,1.1825698325,0.,-0.6455267685
H,0,-0.8344645428,0.,2.1283625301
H,0,1.3672854174,0.,3.2293025483
C,0,3.7887461372,0.,2.0871163036
H,0,3.3287847313,0.,-0.6011457182
H,0,1.1012333842,0.,-1.7276096938
O,0,-1.1572005412,0.,-0.5888670891
C,0,-2.4072058407,0.,0.112596599
H,0,-3.1756341135,0.,-0.659623127
H,0,-2.5079454971,-0.8969133911,0.7324704079
H,0,-2.5079454971,0.8969133911,0.7324704079
O,0,4.8898590984,0.,1.5427216208
H,0,3.7216173997,0.,3.1937932808

Conformation B, B3LYP/6-31+G/PCM**
panisaldehydeConfBB3PSPCM
anisaldehyde conf B
E(RB3LYP) = -460.137894101

Zero-point correction= 0.142246 (Hartree/Particle)
Thermal correction to Energy= 0.151156
Thermal correction to Enthalpy= 0.152101
Thermal correction to Gibbs Free Energy= 0.108160
Sum of electronic and ZPE= -459.995648
Sum of electronic and thermal Energies= -459.986738
Sum of electronic and thermal Enthalpies= -459.985794
Sum of electronic and thermal Free Energies= -460.029734

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	94.852	33.229	92.480

C,0,-0.0019570808,0.,0.1217069695
C,0,0.0574108322,0.,1.529115139
C,0,1.2962126454,0.,2.160963441
C,0,2.4881719621,0.,1.4163623198
C,0,2.4122342701,0.,0.0091976226
C,0,1.1848804924,0.,-0.6353089128
H,0,-0.8469885155,0.,2.1247148039
H,0,1.3511797984,0.,3.2450668511
C,0,3.8019491494,0.,2.0669728484
H,0,3.3272810859,0.,-0.5777472062
H,0,1.1151556797,0.,-1.7179746957
O,0,-1.1542992222,0.,-0.5918305819
C,0,-2.4079706259,0.,0.1037264814
H,0,-3.1721773687,0.,-0.6726967529
H,0,-2.5126653402,-0.8968518836,0.7229746851
H,0,-2.5126653402,0.8968518836,0.7229746851
O,0,3.9965448474,0.,3.2797988329

H,0,4.6653257308,0.,1.3713794699

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 PCM solvent model for dichloromethane**
anisaldehydeMPW1KPCM+G
E(RmPW+HF-PW91) = -459.991098271

Zero-point correction= 0.146301
(Hartree/Particle)
Thermal correction to Energy= 0.154991
Thermal correction to Enthalpy= 0.155935
Thermal correction to Gibbs Free Energy= 0.112471
Sum of electronic and zero-point Energies= -459.844798
Sum of electronic and thermal Energies= -459.836108
Sum of electronic and thermal Enthalpies= -459.835164
Sum of electronic and thermal Free Energies= -459.878627

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	97.258	32.258	91.476

C,0,0.0001872745,0.,0.1243311077
C,0,0.0636719042,0.,1.5157928884
C,0,1.3044700625,0.,2.1320294068
C,0,2.4777685971,0.,1.3864151788
C,0,2.3989742567,0.,-0.0114751275
C,0,1.1766732577,0.,-0.6366130632
H,0,-0.8293981661,0.,2.1213496542
H,0,1.3581043275,0.,3.2153174975
C,0,3.7608452169,0.,2.0789218424
H,0,3.3114716653,0.,-0.5941214836
H,0,1.095367145,0.,-1.7158617228
O,0,-1.1409623288,0.,-0.5763612353
C,0,-2.3680367215,0.,0.1177582443
H,0,-3.1402494229,0.,-0.6425732374
H,0,-2.4682580493,-0.8910059283,0.7362326053
H,0,-2.4682580493,0.8910059283,0.7362326053
O,0,4.8456340789,0.,1.5330982048
H,0,3.6983765481,0.,3.1802366394

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

MP2/6-31G*
anisaldehydeMP2
E(RHF) = -457.310868765

Zero-point correction= 0.143518
(Hartree/Particle)
Thermal correction to Energy= 0.152612
Thermal correction to Enthalpy= 0.153557
Thermal correction to Gibbs Free Energy= 0.109303
Sum of electronic and zero-point Energies= -458.532401
Sum of electronic and thermal Energies= -458.523307
Sum of electronic and thermal Enthalpies= -458.522363
Sum of electronic and thermal Free Energies= -458.566616

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.766	33.844	93.139

C,0,-0.0049389874,0.,0.1209604005
C,0,0.0530664629,0.,1.5198572363
C,0,1.3005969425,0.,2.1468258107
C,0,2.4794292952,0.,1.398569643
C,0,2.4105699829,0.,-0.0044124132
C,0,1.1794723243,0.,-0.6373610293
H,0,-0.8481655589,0.,2.1230598507
H,0,1.351760233,0.,3.2351549135
C,0,3.7864553798,0.,2.0807407184
H,0,3.3358362067,0.,-0.575009233
H,0,1.0944905782,0.,-1.7205953826
O,0,-1.1571445794,0.,-0.6119846185
C,0,-2.3870276421,0.,0.1110504325
H,0,-3.16725141,0.,-0.6488343907
H,0,-2.4804797107,-0.8953119177,0.7346134554
H,0,-2.4804797107,0.8953119177,0.7346134554
O,0,4.8703423977,0.,1.5029013448
H,0,3.7398477958,0.,3.1905608061

Allylboronate model for 4 lacking ester groups used for POLYRATE calculations
B3LYP/6-31+G**
allylBegB3PS
E(RB+HF-LYP) = -371.349900373

Zero-point correction= 0.140647 (Hartree/Particle)
Thermal correction to Energy= 0.149011
Thermal correction to Enthalpy= 0.149955
Thermal correction to Gibbs Free Energy= 0.106144
Sum of electronic and zero-point Energies= -371.209253
Sum of electronic and thermal Energies= -371.200890
Sum of electronic and thermal Enthalpies= -371.199946
Sum of electronic and thermal Free Energies= -371.243756

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	93.506	29.020	92.207

C,0,-0.5849415633,2.7125040872,-0.1914324753
C,0,-0.1359230902,1.3028889002,-0.4764661648
C,0,-0.916174726,0.3253673436,-0.9489651839
B,0,0.205240456,3.8135313075,-0.9950009859
O,0,1.5576005713,3.755449397,-1.2437115497
C,0,1.9148261621,4.8901259518,-2.0565252165
C,0,0.6539003929,5.7873191474,-2.0484852241
O,0,-0.3823640813,4.9528582139,-1.4948215065
H,0,0.7700187848,6.6688925909,-1.4086942855
H,0,2.7913777616,5.3791058136,-1.622831892
H,0,0.3534336589,6.1134648346,-3.0478392162
H,0,-1.6603123628,2.8237881012,-0.3705869993
H,0,-0.426541983,2.9326393989,0.8777986211
H,0,0.9167078194,1.0919369921,-0.2884839978
H,0,-0.5245567253,-0.6689821648,-1.1432344697
H,0,-1.9719010198,0.4867193104,-1.1574388228
H,0,2.1697379448,4.5326937747,-3.060065631

B3LYP/6-31+G**
allylBegB3PSPCM
allylBeg
E(RB3LYP) = -371.355522058

Zero-point correction= 0.140426 (Hartree/Particle)
Thermal correction to Energy= 0.148821
Thermal correction to Enthalpy= 0.149765
Thermal correction to Gibbs Free Energy= 0.105701
Sum of electronic and ZPE= -371.215096
Sum of electronic and thermal Energies= -371.206701
Sum of electronic and thermal Enthalpies= -371.205757
Sum of electronic and thermal Free Energies= -371.249821

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	93.386	29.146	92.740

C,0,-0.6303163524,2.7188800816,-0.2360144756
C,0,-0.1400468856,1.3076659159,-0.4200552593
C,0,-0.8584262137,0.2981098074,-0.9256271314
B,0,0.1858725413,3.8133079901,-1.0254122303
O,0,1.5150488613,3.6966182294,-1.3590312455
C,0,1.8898998875,4.8640259342,-2.1292134028
C,0,0.6923704647,5.8277543296,-1.9802998024
O,0,-0.3650926833,5.0099457835,-1.4238568552
H,0,0.8978538912,6.646814954,-1.2844736139
H,0,2.8193202722,5.2728171976,-1.7269035273
H,0,0.3573746442,6.242695462,-2.9333913516
H,0,-1.6930636057,2.7986610776,-0.4943368116
H,0,-0.5569658026,2.99309722,0.8297817158
H,0,0.8903958961,1.11725355,-0.1190122995
H,0,-0.4368434762,-0.6967826797,-1.0393951053
H,0,-1.8902962116,0.43490892,-1.2436368514
H,0,2.0530427727,4.5545292269,-3.1659067525

MPW1K/6-31+G**
allylBegMPW1KPS
E(RmPW+HF-PW91) = -371.233287098

Zero-point correction= 0.145239 (Hartree/Particle)
Thermal correction to Energy= 0.153428
Thermal correction to Enthalpy= 0.154372
Thermal correction to Gibbs Free Energy= 0.110988
Sum of electronic and zero-point Energies= -371.088049
Sum of electronic and thermal Energies= -371.079859
Sum of electronic and thermal Enthalpies= -371.078915
Sum of electronic and thermal Free Energies= -371.122299

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	96.277	28.102	91.308

C,0,-0.6060242698,2.7246434632,-0.2179820865
C,0,-0.128478501,1.3317906194,-0.4673867886
C,0,-0.8754695856,0.3429948147,-0.9411625867
B,0,0.1911059011,3.815098933,-1.0093007722
O,0,1.5283238547,3.7391189409,-1.2689367303
C,0,1.8849551833,4.8508812381,-2.0717657251
C,0,0.6651947728,5.7761889275,-2.0088472985
O,0,-0.3708665828,4.9632122689,-1.4853859082
H,0,0.8207209226,6.6207881295,-1.3389149293
H,0,2.7870896397,5.3093920142,-1.6753350671
H,0,0.3692176835,6.1559309612,-2.9831572303
H,0,-1.6700671082,2.8182520425,-0.4306708072
H,0,-0.4837102341,2.964063574,0.8442868424
H,0,0.9164602598,1.1419111953,-0.2526357982
H,0,-0.4643482329,-0.6410850163,-1.1102342132
H,0,-1.9217665381,0.4855865177,-1.1761878325
H,0,2.0877908351,4.5015343763,-3.0831680686

MPW1K/6-31+G PCM solvent model for dichloromethane**
allylBegMPW1KPSPCM
E(RmPW+HF-PW91) = -371.240747612

Zero-point correction= 0.144553 (Hartree/Particle)
Thermal correction to Energy= 0.152776
Thermal correction to Enthalpy= 0.153720
Thermal correction to Gibbs Free Energy= 0.110116
Sum of electronic and zero-point Energies= -371.096194
Sum of electronic and thermal Energies= -371.087972
Sum of electronic and thermal Enthalpies= -371.087027
Sum of electronic and thermal Free Energies= -371.130631

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.868	28.250	91.772

C,0,-0.634865608,2.7255233152,-0.2592882072
C,0,-0.132508205,1.3301683981,-0.429190313
C,0,-0.8420706534,0.3177690065,-0.9143932062
B,0,0.1809811541,3.8112627207,-1.0390062666
O,0,1.5046832883,3.7035883191,-1.3509510196
C,0,1.8692494104,4.8425122329,-2.1243114974
C,0,0.6946450119,5.8069661914,-1.9586565465
O,0,-0.3595030019,4.996586627,-1.4484336767
H,0,0.9064178771,6.5961001051,-1.238707189
H,0,2.8060098656,5.2478448538,-1.7514313798
H,0,0.3817946082,6.2585365104,-2.8962205927
H,0,-1.6891641855,2.7968474934,-0.5283206073
H,0,-0.5721668352,3.008012822,0.7985959751
H,0,0.8977385688,1.1529851864,-0.1349896129
H,0,-0.4144864531,-0.6694285244,-1.0192187619
H,0,-1.8719549601,0.4448306208,-1.2236896556
H,0,2.0053281178,4.5301971215,-3.1585724428

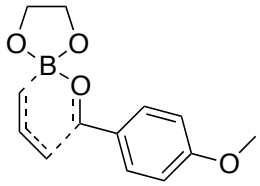
MP2/6-31G*
allylBegMP2
E(RHF) = -369.065970403

Zero-point correction= 0.144062 (Hartree/Particle)
Thermal correction to Energy= 0.152294
Thermal correction to Enthalpy= 0.153238
Thermal correction to Gibbs Free Energy= 0.109608
Sum of electronic and zero-point Energies= -369.986160
Sum of electronic and thermal Energies= -369.977929
Sum of electronic and thermal Enthalpies= -369.976985
Sum of electronic and thermal Free Energies= -370.020615

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.566	28.431	91.828

C,0,-0.4845250621,2.7159821499,0.0029858878
C,0,-0.1132618776,1.3555833357,-0.522831085
C,0,-0.9641405394,0.5105633402,-1.1190924273
B,0,0.2343061898,3.8183331108,-0.8556048199
O,0,1.609220083,3.9258796109,-0.9192565181
C,0,1.9063515424,4.8928318603,-1.9473329476
C,0,0.5757080122,5.6204612407,-2.1886452899
O,0,-0.4261016725,4.7372293364,-1.6420962973
H,0,0.5227570466,6.5759039053,-1.6570565413
H,0,2.702517559,5.5545636727,-1.5980699698
H,0,0.3627881828,5.7906213117,-3.2466059106
H,0,-1.5696321218,2.8554015503,-0.026679905
H,0,-0.1620569715,2.810236867,1.0481827778
H,0,0.9347503285,1.0746409401,-0.4241099186
H,0,-0.6357104005,-0.4505338854,-1.5010757275
H,0,-2.0158706654,0.7543694607,-1.2419618888
H,0,2.2530283663,4.3582351929,-2.8375344188

Allylboronate model for TS 7 lacking ester groups used for POLYRATE calculations



M062X/6-31+G**
This structure was optimized with the Gaussian options int(grid=ultrafine) and nosymm.
anisaldehydeAllylBegTSM062X
ts for allylboration
E(RM062X) = -831.100052631

Zero-point correction= 0.288911 (Hartree/Particle)
Thermal correction to Energy= 0.305120
Thermal correction to Enthalpy= 0.306064
Thermal correction to Gibbs Free Energy= 0.244559
Sum of electronic and ZPE= -830.811141
Sum of electronic and thermal Energies= -830.794933
Sum of electronic and thermal Enthalpies= -830.793989
Sum of electronic and thermal Free Energies= -830.855494

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	191.465	63.095	129.447

C,0,3.4558498119,2.2470743655,-2.522363604
C,0,2.2375466194,2.1117307439,-3.1825147007
C,0,2.1485977843,2.3007950642,-4.5616736832
C,0,3.3049354422,2.6278869048,-5.2841193556
C,0,4.5215108083,2.7667531197,-4.641296171
C,0,4.6024059923,2.5782730951,-3.2536993664
C,0,0.8665322021,2.1428415645,-5.2650887088
O,0,-0.1146681625,1.6051604517,-4.6377364227
B,0,-1.4703689984,1.5843685897,-5.3241908552
C,0,-1.9643416003,3.2310905331,-5.1573549876
C,0,-0.9373056464,3.941622607,-5.8621956044
C,0,0.2763076259,4.2591798598,-5.3065498989
O,0,5.8332804252,2.7340074843,-2.7116114752
O,0,-2.3748211701,0.6948526734,-4.6822679149
C,0,-2.4403945376,-0.4579107901,-5.503375605
C,0,-2.1828488605,0.0830012185,-6.9149448537
O,0,-1.3204202703,1.1892946631,-6.7052013874
H,0,-3.4180674456,-0.9360551058,-5.3943117372
H,0,-3.1175229098,0.4233353034,-7.3827746249
H,0,-1.6587022627,-1.1756338552,-5.2132450015
H,0,-2.0263543865,3.4360916835,-4.0876328686
H,0,-2.9427883345,3.2341866218,-5.6386372544
H,0,-1.0347610169,4.0095450097,-6.9458588705
H,0,1.0559022093,4.7288812043,-5.89859614
H,0,0.3796102596,4.3274639307,-4.2270319486
H,0,0.8871113094,2.0471351658,-6.3531956193
H,0,-1.7043743693,-0.6474770785,-7.5748277891
H,0,3.2438316822,2.7729248344,-6.3601204221

H,0,5.4275817996,3.0160416508,-5.182515778
H,0,3.5012818698,2.0896167516,-1.451789542
H,0,1.3419780752,1.8457553319,-2.6293722742
C,0,5.9736935585,2.5516609723,-1.3154058057
H,0,7.0265462106,2.7220788234,-1.0958960724
H,0,5.3623869173,3.2723824347,-0.7605646176
H,0,5.6984643678,1.5324051732,-1.0216620392

M062X/6-31+G/PCM**
This structure was optimized with the Gaussian options int(grid=ultrafine) and nosymm.
anisaldehydeAllylBegTSM062XPCM
ts for allylboration
E(RM062X) = -831.111740287

Zero-point correction= 0.288645 (Hartree/Particle)
Thermal correction to Energy= 0.304844
Thermal correction to Enthalpy= 0.305788
Thermal correction to Gibbs Free Energy= 0.244287
Sum of electronic and ZPE= -830.823095
Sum of electronic and thermal Energies= -830.806896
Sum of electronic and thermal Enthalpies= -830.805952
Sum of electronic and thermal Free Energies= -830.867454

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	191.292	63.132	129.441

C,0,3.4542717365,2.259391266,-2.525316977
C,0,2.2351275063,2.1392246469,-3.1859878933
C,0,2.1489392723,2.3234376069,-4.5671967858
C,0,3.3087732069,2.6365902782,-5.2914687342
C,0,4.5270078568,2.7604247143,-4.6475743712
C,0,4.605949554,2.5728150768,-3.25885501
C,0,0.8692477417,2.1808564767,-5.2764798816
O,0,-0.1118224102,1.6058077505,-4.6680465244
B,0,-1.463893088,1.5876117937,-5.3465889295
C,0,-1.9696099958,3.2247076709,-5.1973392338
C,0,-0.9241286395,3.9531336652,-5.8612571159
C,0,0.2708668677,4.262914889,-5.2615322771
O,0,5.8368669211,2.7122601837,-2.7155156794
O,0,-2.36225084,0.6941824015,-4.6790511227
C,0,-2.4258203586,-0.4745045586,-5.4858660251
C,0,-2.2056781185,0.0544001007,-6.90484794
O,0,-1.3357905129,1.1637134173,-6.724601818
H,0,-3.3924290882,-0.9675680901,-5.3529453539
H,0,-3.1527208424,0.3911517836,-7.3488837249
H,0,-1.6259128011,-1.1739781011,-5.2034286627
H,0,-2.0640810865,3.429932211,-4.1292735568
H,0,-2.9329667806,3.2406882565,-5.7091896867
H,0,-0.9893560486,4.0510282843,-6.9449365239
H,0,1.0634877627,4.7493062446,-5.8214077238
H,0,0.3387530034,4.3082480309,-4.1777995704
H,0,0.9051629895,2.1055487935,-6.3650858165
H,0,-1.7457960881,-0.6824464804,-7.5697649722
H,0,3.2504257649,2.7829784562,-6.3671312033
H,0,5.4335143895,2.9981736074,-5.1936380801
H,0,3.4964689001,2.1073918176,-1.4540084642
H,0,1.3386474459,1.8936040004,-2.625157547
C,0,5.9736124654,2.5314033587,-1.3124169171
H,0,7.0283722398,2.6865068254,-1.0933138394
H,0,5.372312785,3.2637023005,-0.7642482711
H,0,5.6820632891,1.5177223217,-1.0194667673

B3LYP/6-31+G**
anisaldehydeAllylBegTSB3PS
Saddle point
E(RB3LYP) = -831.458633015

Zero-point correction= 0.285544 (Hartree/Particle)
Thermal correction to Energy= 0.302023
Thermal correction to Enthalpy= 0.302968
Thermal correction to Gibbs Free Energy= 0.240939
Sum of electronic and ZPE= -831.173089
Sum of electronic and thermal Energies= -831.156610
Sum of electronic and thermal Enthalpies= -831.155665
Sum of electronic and thermal Free Energies= -831.217694

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	189.523	64.025	130.551

C,0,3.4850035824,2.2540424043,-2.5078442771
C,0,2.2658095433,2.1364238558,-3.1755671489
C,0,2.176974161,2.3448830051,-4.5585276087
C,0,3.3479826493,2.6728074468,-5.2677344894
C,0,4.5662879766,2.794417867,-4.6163972861
C,0,4.6426386755,2.5877977164,-3.2280737508
C,0,0.9017763718,2.2049700242,-5.2796720854
O,0,-0.0867256157,1.6130665401,-4.6765744346
B,0,-1.4327949475,1.5340475732,-5.3480777358
C,0,-1.9955916935,3.2102445499,-5.1993021683
C,0,-0.9873633885,3.9520522517,-5.8856948286
C,0,0.2402110072,4.2659904985,-5.32855124
O,0,5.8801954188,2.7288070664,-2.677705497
O,0,-2.3308954326,0.6626926103,-4.6647272449
C,0,-2.5189679996,-0.4771474445,-5.5014186143
C,0,-2.2426205832,0.0471433508,-6.9217270076
O,0,-1.3205201109,1.1179481659,-6.7262314971
H,0,-3.5358236632,-0.864100807,-5.3741180969
H,0,-3.1616742415,0.4261877237,-7.3942923972
H,0,-1.8051578502,-1.2688325819,-5.2262791566
H,0,-2.0742117039,3.3865731189,-4.1252754393
H,0,-2.9700218503,3.1763057065,-5.687254113
H,0,-1.0870815815,4.0421957039,-6.9675785668
H,0,0.9955781798,4.7761118584,-5.91914802
H,0,0.3351808,4.3662426815,-4.2513951489
H,0,0.9562840169,2.1031254623,-6.3646041124
H,0,-1.800979307,-0.7093104151,-7.5803284129
H,0,3.2999302607,2.8299653736,-6.3425231409
H,0,5.4737165622,3.0425649851,-5.1567879857
H,0,3.523181848,2.0796439894,-1.4392995486
H,0,1.3711316019,1.8659533405,-2.6242348731
C,0,6.0353532393,2.5313603081,-1.2752343553
H,0,7.0934664472,2.6951091539,-1.0695232898
H,0,5.436650979,3.2508001863,-0.7035988236
H,0,5.7606916482,1.5102777303,-0.9843206047

B3LYP/6-31+G/PCM**
anisaldehydeAllylBegTSB3PSPCM
Saddle point
E(RB3LYP) = -831.470007628

Zero-point correction= 0.285274 (Hartree/Particle)
Thermal correction to Energy= 0.301771
Thermal correction to Enthalpy= 0.302715
Thermal correction to Gibbs Free Energy= 0.240473
Sum of electronic and ZPE= -831.184733
Sum of electronic and thermal Energies= -831.168237

Sum of electronic and thermal Enthalpies= -831.167292
Sum of electronic and thermal Free Energies= -831.229534

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	189.364	64.103	130.999

C,0,3.4854946543,2.2647750972,-2.5098648406
C,0,2.2658232212,2.1603716315,-3.1780314757
C,0,2.1793270278,2.3647102906,-4.5628065943
C,0,3.3532279571,2.6817899776,-5.2734372953
C,0,4.5727350565,2.7906977292,-4.6211543011
C,0,4.6475422518,2.5841025396,-3.2317651903
C,0,0.9063632716,2.2393608658,-5.2901453011
O,0,-0.0805486005,1.6084581983,-4.7094055493
B,0,-1.4286107451,1.538550768,-5.3715479903
C,0,-1.9963678847,3.1989802487,-5.240558008
C,0,-0.9712680598,3.9599118811,-5.8874505639
C,0,0.2376982222,4.2657995765,-5.2866120308
O,0,5.8843017939,2.7114045931,-2.6798007566
O,0,-2.3178562744,0.6606147475,-4.6621542552
C,0,-2.5078600482,-0.4947762293,-5.485746251
C,0,-2.2748492507,0.0234255333,-6.9117519722
O,0,-1.3370713321,1.0900361336,-6.7459563721
H,0,-3.5141972031,-0.897326434,-5.3320325483
H,0,-3.2064039699,0.4081882588,-7.3526605699
H,0,-1.7736512344,-1.2706314916,-5.2222052394
H,0,-2.1069489527,3.3788526553,-4.1691063913
H,0,-2.9568431375,3.1807475919,-5.7577859855
H,0,-1.0405879142,4.07875484,-6.9687722702
H,0,1.0055158198,4.7929532987,-5.8446330055
H,0,0.2974126679,4.343410021,-4.2049201349
H,0,0.9763086986,2.1608474453,-6.3754110524
H,0,-1.8606110361,-0.7377438541,-7.5814053515
H,0,3.3073326247,2.8406875385,-6.3477091982
H,0,5.4802259049,3.0298268205,-5.165817896
H,0,3.5210902089,2.0947526372,-1.4408515473
H,0,1.3705457147,1.9086229439,-2.6191073677
C,0,6.0352782375,2.5162785121,-1.2694549117
H,0,7.0944621474,2.668492118,-1.0637934346
H,0,5.4431913282,3.2454446102,-0.706044319
H,0,5.7474138339,1.4999899062,-0.9797230288

B3LYP/6-31G*
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)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	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

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

Transition structures for reaction of 4 and 5 – *Si* facial attack – 7 in manuscript

M062X/6-31+G**
This structure was optimized with the Gaussian option int(grid=ultrafine).
FullRoushAnisaldehydeTSm06
ts for allylboration with Roush allylboronate and anisaldehyde
E(RM062X) = -1443.90674453

Zero-point correction= 0.488891 (Hartree/Particle)
Thermal correction to Energy= 0.519111
Thermal correction to Enthalpy= 0.520055
Thermal correction to Gibbs Free Energy= 0.424660
Sum of electronic and ZPE= -1443.417853
Sum of electronic and thermal Energies= -1443.387634
Sum of electronic and thermal Enthalpies= -1443.386690
Sum of electronic and thermal Free Energies= -1443.482085

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	325.747	113.534	200.776

C,0,5.1342206722,0.0083298591,-1.1156892069
C,0,3.8071814189,-0.3656755959,-0.920715637
C,0,3.2355131851,-0.3306513268,0.3506660316
C,0,4.0115626697,0.0908053478,1.4390465027
C,0,5.3315704267,0.4638775357,1.2605859742
C,0,5.9005014785,0.4223310036,-0.020307393
C,0,1.8307562383,-0.7133943658,0.5621217461
O,0,1.0697453143,-0.8215200326,-0.4713104124
B,0,-0.3112917094,-1.3601454101,-0.2609047243
O,0,-0.9493531284,-0.8164334506,0.9284506889
C,0,-1.8552182043,0.1487559766,0.4909979082
C,0,-1.1965322557,1.5268135966,0.4208016803
O,0,-0.0594408785,1.7641703303,0.7477906098
O,0,7.1978728622,0.8058404733,-0.0989283626
O,0,-1.1368981215,-1.0247399996,-1.387318367
C,0,-2.2693736744,-0.362203307,-0.919477104
C,0,-3.4430902234,-1.3230827447,-0.7549225872
O,0,-3.3553926223,-2.5242252992,-0.6981306241
C,0,-0.0273049145,-3.041280799,-0.0496828819
C,0,0.7825870873,-3.0365504324,1.1322603196
C,0,2.1340421725,-2.7810371424,1.1166734344
O,0,-4.5921119928,-0.6377369172,-0.6306118996
C,0,-5.784186371,-1.4029528142,-0.3401325356
C,0,-5.805715775,-1.7531130384,1.1394537068
C,0,-6.9525007982,-0.5329206277,-0.7629377543
O,0,-2.0615477157,2.4412066044,-0.0393709448
C,0,-1.5861778213,3.8039506338,-0.151043478
C,0,-1.6254522837,4.4661245919,1.2167779495
C,0,-2.4916655532,4.4774615473,-1.1645235336
H,0,-2.7132382539,0.2257190409,1.1701992556
H,0,-2.5669340183,0.4537531869,-1.5846658914
H,0,0.469640267,-3.3909879426,-0.9556414257
H,0,-1.0375442945,-3.4366620135,0.0587081971
H,0,0.2642299759,-2.9796693946,2.0895919676
H,0,2.6973865793,-2.7130067286,2.0424457268
H,0,2.7092546885,-2.9704118434,0.2145181432
H,0,1.3594049729,-0.425390169,1.5032957676
H,0,-0.5554255235,3.7609564645,-0.5161323024
H,0,-5.7417866095,-2.3172737365,-0.939954999
H,0,3.5684075986,0.1296759722,2.4311148797
H,0,5.9468939386,0.7977333734,2.0888356491
H,0,5.5544400355,-0.0211255158,-2.1134979604
H,0,3.1980769505,-0.6787136459,-1.7631555017
H,0,-1.2835074819,5.5021840462,1.1384219977
H,0,-2.6495154168,4.4669993751,1.602976727
H,0,-0.9753574944,3.9402742294,1.9190938622
H,0,-2.1765925557,5.5137626383,-1.3140103273
H,0,-2.4525312528,3.9581938372,-2.1249910641
H,0,-3.526205335,4.4757384793,-0.8086269064
H,0,-7.8934445756,-1.0610468427,-0.5859970785
H,0,-6.9611143849,0.3967147469,-0.1860458662
H,0,-6.8853508614,-0.283501434,-1.824456486
H,0,-6.7067213729,-2.3264153784,1.3759298739
H,0,-4.9340922425,-2.3551888651,1.4059235579
H,0,-5.8098484206,-0.8377825695,1.7400178591
C,0,7.8205000921,0.7874013401,-1.3688404264
H,0,8.8428572061,1.1254081395,-1.2061124704
H,0,7.831850323,-0.2252965811,-1.7878407222
H,0,7.3164319837,1.467364594,-2.065052142

m062x/6-31+G/PCM**
FullRoushAnisaldehydeTSm06PCM
ts for allylboration with Roush allylboronate and anisaldehyde
E(RM062X) = -1443.92412239

Zero-point correction= 0.488496 (Hartree/Particle)
Thermal correction to Energy= 0.518651
Thermal correction to Enthalpy= 0.519595
Thermal correction to Gibbs Free Energy= 0.424505
Sum of electronic and ZPE= -1443.435626
Sum of electronic and thermal Energies= -1443.405472
Sum of electronic and thermal Enthalpies= -1443.404527
Sum of electronic and thermal Free Energies= -1443.499618

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	325.458	113.514	200.135

C,0,5.1123765586,0.1962155444,-1.116322246
C,0,3.8076622661,-0.2464412188,-0.9186687978
C,0,3.2408873914,-0.2530419111,0.3566433689
C,0,4.0012151546,0.1932860211,1.4473207181
C,0,5.3001645538,0.6339387237,1.2659564741
C,0,5.8643224845,0.6345893448,-0.0187207733
C,0,1.8618596645,-0.7130506306,0.5800739949

O,0,1.0786588859,-0.8224922682,-0.4446873827
B,0,-0.2726924324,-1.4244331527,-0.2236291865
O,0,-0.947815949,-0.8853317326,0.9479981981
C,0,-1.8725397699,0.0545526197,0.4882139587
C,0,-1.2593468137,1.4541088104,0.4197958649
O,0,-0.1391500028,1.730701226,0.7816299333
O,0,7.1407976007,1.0765327804,-0.1016784748
O,0,-1.1090508879,-1.1384407856,-1.3658683985
C,0,-2.2545661572,-0.4740469051,-0.9237274054
C,0,-3.4322603743,-1.4336063664,-0.7830627299
O,0,-3.3442988894,-2.6394827686,-0.7713228352
C,0,0.071026492,-3.0836529605,0.0085177847
C,0,0.9350891237,-3.0491936815,1.1549358897
C,0,2.2740869728,-2.7462013952,1.0719675797
O,0,-4.5706940403,-0.7502507839,-0.6325183136
C,0,-5.7778696537,-1.5070883983,-0.3508384725
C,0,-5.804900381,-1.8597025718,1.1269387205
C,0,-6.9343935938,-0.6242879911,-0.7753806854
O,0,-2.1387673054,2.3267398794,-0.0756233212
C,0,-1.7288265986,3.7174488422,-0.1772635253
C,0,-1.8833200224,4.3818479274,1.1801439899
C,0,-2.6084144134,4.3328055883,-1.2473970383
H,0,-2.7412377521,0.1121813378,1.1551848215
H,0,-2.5398113172,0.3352404301,-1.6025473353
H,0,0.5419262071,-3.4384475126,-0.9101448904
H,0,-0.911911155,-3.5256623961,0.173940029
H,0,0.4660975012,-3.0186305922,2.1386816503
H,0,2.8778760088,-2.6624886059,1.9701915253
H,0,2.8070328085,-2.9119146619,0.1393143963
H,0,1.3997881627,-0.4609414316,1.5358261966
H,0,-0.6798187078,3.7245225685,-0.4868188898
H,0,-5.7409459516,-2.4159972609,-0.9577623611
H,0,3.5663386842,0.193393815,2.4438151902
H,0,5.8993306203,0.984422567,2.0994819783
H,0,5.5276184462,0.1961802065,-2.1164226409
H,0,3.2194234376,-0.5871475114,-1.7651224721
H,0,-1.5800352086,5.4302571612,1.1138615607
H,0,-2.9290138649,4.3420488509,1.5004347439
H,0,-1.2598453406,3.8882649686,1.9290673917
H,0,-2.3402562511,5.383798283,-1.3830076954
H,0,-2.4803604439,3.8145301571,-2.2007638836
H,0,-3.6608759884,4.2775488619,-0.9533720769
H,0,-7.878355058,-1.1480130933,-0.603477018
H,0,-6.9403983324,0.3022249141,-0.1932617819
H,0,-6.8630960576,-0.3736512655,-1.8364807544
H,0,-6.7085983607,-2.4314878609,1.3550070945
H,0,-4.936215256,-2.4638317774,1.3999480899
H,0,-5.8104507197,-0.9461625054,1.7298361847
C,0,7.7653408083,1.0804504634,-1.3782481293
H,0,8.7766416347,1.4483376617,-1.2139008126
H,0,7.8049228432,0.0692566533,-1.7962586953
H,0,7.2390687395,1.7471327889,-2.0690833052

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) KCal/Mol	CV Cal/Mol-Kelvin	S 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/PCM**
FullRoushAnisaldehydeTSAB3PSPCM
ts for allylboration with Roush allylboronate and anisaldehyde with G09 PCM
E(RB3LYP) = -1444.53692178

Zero-point correction= 0.482191 (Hartree/Particle)
Thermal correction to Energy= 0.513097
Thermal correction to Enthalpy= 0.514041
Thermal correction to Gibbs Free Energy= 0.416127
Sum of electronic and ZPE= -1444.054731
Sum of electronic and thermal Energies= -1444.023825
Sum of electronic and thermal Enthalpies= -1444.022881
Sum of electronic and thermal Free Energies= -1444.120795

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	321.973	115.443	206.077

6 5.316161 -0.020893 -1.252270
6 4.012491 -0.413954 -0.951576
6 3.522270 -0.350990 0.360627
6 4.374684 0.116499 1.379423
6 5.674591 0.508282 1.094862
6 6.156062 0.440774 -0.225125
6 2.144024 -0.743101 0.695719
8 1.271260 -0.817773 -0.278654
5 -0.108070 -1.317932 -0.014521
8 -0.774489 -0.684096 1.113531
6 -1.807517 0.133602 0.629140
6 -1.403639 1.615705 0.584629
8 -0.306288 2.049960 0.876011
8 7.441681 0.845986 -0.407789
8 -0.932648 -1.095086 -1.180186
6 -2.112273 -0.436565 -0.801823
6 -3.315876 -1.390353 -0.771275
8 -3.252136 -2.602607 -0.843941
6 0.146547 -3.014894 0.304043
6 1.059374 -3.005198 1.407093
6 2.415586 -2.763211 1.258301
8 -4.453084 -0.686556 -0.651780
6 -5.728847 -1.413241 -0.574360
6 -6.008157 -1.778582 0.878593
6 -6.774191 -0.492363 -1.185124
8 -2.447069 2.363639 0.192111
6 -2.270480 3.819674 0.082158
6 -2.574956 4.459428 1.431374
6 -3.198571 4.273601 -1.034221
1 -2.684535 0.066939 1.282931
1 -2.350119 0.365207 -1.508205
1 0.547051 -3.422092 -0.626655

1 -0.853744 -3.389394 0.521910
1 0.638096 -2.926194 2.409313
1 3.056146 -2.702800 2.132884
1 2.907421 -3.025534 0.326148
1 1.772915 -0.416650 1.666943
1 -1.226786 3.994408 -0.190572
1 -5.615902 -2.318803 -1.175614
1 4.010644 0.177286 2.401700
1 6.333125 0.874691 1.875502
1 5.663616 -0.074090 -2.276618
1 3.362833 -0.764718 -1.746620
1 -2.450572 5.544929 1.360324
1 -3.606495 4.250096 1.733652
1 -1.896808 4.089016 2.204830
1 -3.091311 5.352493 -1.184160
1 -2.954728 3.770173 -1.974180
1 -4.243572 4.063078 -0.784018
1 -7.748908 -0.990177 -1.180388
1 -6.859135 0.436648 -0.611745
1 -6.519733 -0.243980 -2.219550
1 -6.955730 -2.323073 0.944998
1 -5.219462 -2.418688 1.283162
1 -6.085511 -0.877114 1.495522
6 7.999061 0.805730 -1.725944
1 9.020739 1.170574 -1.623861
1 8.011926 -0.217491 -2.116593
1 7.442992 1.457477 -2.408323

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) KCal/Mol	CV Cal/Mol-Kelvin	S 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 PCM solvent model for dichloromethane**
panisaldehydeDIPESiTSPCMmpw1k+G
E(RmPW+HF-PW91) = -1444.09535888

Zero-point correction= 0.497144
(Hartree/Particle)
Thermal correction to Energy= 0.527180
Thermal correction to Enthalpy= 0.528124
Thermal correction to Gibbs Free Energy= 0.432279
Sum of electronic and zero-point Energies= -1443.598215
Sum of electronic and thermal Energies= -1443.568179
Sum of electronic and thermal Enthalpies= -1443.567235
Sum of electronic and thermal Free Energies= -1443.663080

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	330.810	111.741	201.724

1	6	0	5.189787	-0.065726	-1.183072
2	6	0	3.881706	-0.452806	-0.946096
3	6	0	3.353646	-0.435060	0.339658
4	6	0	4.164090	-0.022093	1.398898
5	6	0	5.467070	0.364405	1.177551
6	6	0	5.988651	0.343855	-0.116950

7	6	0	1.967139	-0.816224	0.605818
8	8	0	1.141118	-0.849855	-0.379836
9	5	0	-0.233190	-1.379790	-0.141684
10	8	0	-0.872054	-0.796451	1.017455
11	6	0	-1.796148	0.134918	0.573813
12	6	0	-1.230518	1.546698	0.578940
13	8	0	-0.155817	1.849308	1.027088
14	8	0	7.266892	0.738275	-0.240165
15	8	0	-1.052847	-1.053731	-1.275593
16	6	0	-2.167265	-0.353848	-0.845105
17	6	0	-3.401051	-1.239379	-0.802373
18	8	0	-3.406608	-2.426068	-1.000954
19	6	0	0.019562	-3.036893	0.080612
20	6	0	0.932023	-3.080950	1.183588
21	6	0	2.276823	-2.873234	1.044713
22	8	0	-4.472009	-0.516250	-0.520670
23	6	0	-5.745340	-1.183253	-0.415036
24	6	0	-5.909472	-1.722344	0.986826
25	6	0	-6.787819	-0.158252	-0.785080
26	8	0	-2.101058	2.396989	0.063541
27	6	0	-1.768458	3.800193	0.048851
28	6	0	-2.111272	4.408608	1.388680
29	6	0	-2.547988	4.402080	-1.093395
30	1	0	-2.665445	0.159010	1.233138
31	1	0	-2.391959	0.478441	-1.512349
32	1	0	0.424813	-3.419040	-0.852850
33	1	0	-0.967047	-3.439154	0.287920
34	1	0	0.513597	-3.045499	2.185918
35	1	0	2.919274	-2.852348	1.913563
36	1	0	2.755967	-3.061075	0.093820
37	1	0	1.572418	-0.562047	1.585377
38	1	0	-0.697790	3.879942	-0.135437
39	1	0	-5.745134	-2.002843	-1.132555
40	1	0	3.764002	0.001480	2.406013
41	1	0	6.100350	0.692013	1.991216
42	1	0	5.568056	-0.085250	-2.193551
43	1	0	3.260078	-0.765408	-1.774755
44	1	0	-1.864388	5.468625	1.385370
45	1	0	-3.175685	4.305431	1.593159
46	1	0	-1.549848	3.933144	2.188829
47	1	0	-2.321420	5.463216	-1.173775
48	1	0	-2.288640	3.923948	-2.034961
49	1	0	-3.618360	4.290778	-0.930080
50	1	0	-7.777187	-0.609277	-0.744494
51	1	0	-6.764872	0.682239	-0.093766
52	1	0	-6.622516	0.216506	-1.792382
53	1	0	-6.868426	-2.229088	1.077406
54	1	0	-5.125825	-2.437780	1.223512
55	1	0	-5.880692	-0.912319	1.713863
56	6	0	7.852681	0.744166	-1.521047
57	1	0	8.869761	1.092396	-1.383142
58	1	0	7.868716	-0.256802	-1.951038
59	1	0	7.326148	1.422808	-2.191253

M05/6-31G*

panisaldehyeDIPESiTSM05G

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,0,7.3319553118,0.7066282098,-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 4 and 5 with *Re* facial attack

M062X/6-31+G**
FullRoushAnisaldehydeTSReFacem06
ts for addition to the re face with Rouse allylboronate
E(RM062X) = -1443.90400633

Zero-point correction= 0.488395 (Hartree/Particle)
Thermal correction to Energy= 0.518746
Thermal correction to Enthalpy= 0.519690
Thermal correction to Gibbs Free Energy= 0.423599
Sum of electronic and ZPE= -1443.415611
Sum of electronic and thermal Energies= -1443.385260
Sum of electronic and thermal Enthalpies= -1443.384316
Sum of electronic and thermal Free Energies= -1443.480407

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	325.518	113.709	202.241

C,0,-5.3329527164,0.2282002045,-0.7737623388
C,0,-3.9783324596,-0.0924002988,-0.7475669461
C,0,-3.3902392642,-0.6045018832,0.4086982483
C,0,-4.176678429,-0.7890356827,1.5543433889
C,0,-5.5234835915,-0.47656385,1.5416780402
C,0,-6.1096886082,0.031667499,0.3732633414
C,0,-1.9589237671,-0.9370661548,0.4439974578
O,0,-1.2204289064,-0.5648100356,-0.5377532575
B,0,0.1969757812,-1.0430188273,-0.573995581
O,0,1.0102221454,-0.3106374185,-1.5003371359
C,0,1.9222497864,0.4529716161,-0.7750271904
C,0,1.4102235152,1.8692903098,-0.5291273464
O,0,0.2737579347,2.2377197756,-0.6801085168
O,0,-7.4332444571,0.3074967252,0.4545647097
C,0,-8.0800585244,0.814723729,-0.6971769025
O,0,0.8035002038,-0.9125728053,0.7425735359
C,0,2.04186891,-0.2964676807,0.5888702835
C,0,3.1633055646,-1.3274847523,0.5032778993
O,0,3.0062875089,-2.5132189355,0.3441655854
C,0,0.0147982238,-2.6839372097,-1.0603184856
C,0,-0.7610579142,-3.2301942151,0.0145694618
C,0,-2.1250706214,-3.1029453765,0.0986579668
O,0,4.3572082687,-0.7240111366,0.6001013113
C,0,5.5307314842,-1.5506125857,0.4209178721
C,0,5.7475084595,-1.7946014794,-1.0639444706
C,0,6.6742748329,-0.7974729954,1.073250726
O,0,2.4105507383,2.6472580755,-0.0775996749
C,0,2.080616087,4.0156627042,0.252532337
C,0,2.0198710152,4.8423652921,-1.0220809869
C,0,3.1569768309,4.4838990649,1.2133147856
H,0,-3.3602766824,0.0691300285,-1.6255400772
H,0,-3.7229632781,-1.1829300761,2.4608976243
H,0,-6.1488942846,-0.6104248384,2.4176684564
H,0,-5.7659700868,0.6320774927,-1.6806020561
H,0,-1.4863679193,-1.0568875807,1.4211958558
H,0,2.2619536581,0.3856376727,1.4171923201
H,0,5.34555124,-2.4997179986,0.9336275867
H,0,1.0459110531,-3.0347945111,-1.1025178498
H,0,-0.4781340285,-2.6721379363,-2.0339996211
H,0,-0.214243981,-3.535252768,0.9075010211
H,0,-2.6675474568,-3.4598239181,0.969202095
H,0,-2.7111661904,-2.9291577761,-0.7997572476
H,0,2.8849519854,0.5205652415,-1.2934621971
H,0,1.0995169978,4.0090447573,0.7385909081
H,0,2.9599363052,5.5148939014,1.5201901165
H,0,3.1837823539,3.8527387921,2.1049634274
H,0,4.1381398585,4.4455034672,0.730495369
H,0,1.7805197349,5.882463708,-0.7817645101
H,0,2.9889809891,4.8170592647,-1.5302814482
H,0,1.2504367685,4.4565286485,-1.6941642193
H,0,7.5974392479,-1.377809847,0.9910978325
H,0,6.8234547371,0.166824588,0.5782700243
H,0,6.4670186936,-0.6175990748,2.1308239777
H,0,6.6389297728,-2.410079231,-1.2161676534
H,0,4.8911574069,-2.3142814289,-1.499654787
H,0,5.8917760256,-0.8408571052,-1.5815030802
H,0,-9.123108207,0.9554383526,-0.417019851
H,0,-7.6496929472,1.7762717629,-0.999731259
H,0,-8.0166997974,0.1047427395,-1.5297418756

M062X/6-31+G/PCM**
FullRoushAnisaldehydeTSReFacem06PCM
ts for addition to the re face with Rouse allylboronate
E(RM062X) = -1443.92236947

Zero-point correction= 0.487559 (Hartree/Particle)
Thermal correction to Energy= 0.518000
Thermal correction to Enthalpy= 0.518944
Thermal correction to Gibbs Free Energy= 0.422507
Sum of electronic and ZPE= -1443.434811
Sum of electronic and thermal Energies= -1443.404370
Sum of electronic and thermal Enthalpies= -1443.403426
Sum of electronic and thermal Free Energies= -1443.499862

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	325.050	113.938	202.968

C,0,-5.3875508175,0.170421564,-0.7670505913
C,0,-4.0358253963,-0.1587209653,-0.7423934219
C,0,-3.4404998766,-0.6476198237,0.4219440432
C,0,-4.2201292898,-0.8087148551,1.5767615061
C,0,-5.5652976622,-0.4869424406,1.5657797574
C,0,-6.1572070361,0.0029871775,0.3912535322
C,0,-2.0123595826,-0.9869795606,0.4611090393
O,0,-1.2540124508,-0.5705215906,-0.4966637064
B,0,0.1622136578,-1.0447764227,-0.5448920153
O,0,0.9535998838,-0.2940781824,-1.4879916409
C,0,1.8961125638,0.4585198586,-0.786148473
C,0,1.43381198,1.8952735537,-0.5591993094
O,0,0.3186659013,2.3115936851,-0.7682628547
O,0,-7.4764732774,0.2893316151,0.4732704398
C,0,-8.1294762582,0.7807395329,-0.6898868244
O,0,0.7949367433,-0.8994230533,0.7584256945
C,0,2.0274210904,-0.2734865002,0.5853925214
C,0,3.165091636,-1.2890303563,0.5174726598
O,0,3.0196853536,-2.4863886814,0.4267062746
C,0,0.0004076516,-2.6791478141,-1.0322929171
C,0,-0.8185565489,-3.2433166456,0.0058032481
C,0,-2.1840533151,-3.1136672199,0.0356714709
O,0,4.3441637293,-0.6638935083,0.5514898952
C,0,5.5410036078,-1.4723217284,0.3959490143
C,0,5.7446719187,-1.7755674356,-1.0788727056
C,0,6.6716339358,-0.6650063646,1.0020535649
O,0,2.4399609426,2.6242282869,-0.0663045366
C,0,2.172378776,4.0143211441,0.258325262

C,0,2.2282082838,4.8457179931,-1.0120807748
C,0,3.2222658401,4.4117452807,1.2771312725
H,0,-3.431493799,-0.0288670224,-1.6350114429
H,0,-3.7648488001,-1.1897651606,2.4875841933
H,0,-6.181533022,-0.601204903,2.451222638
H,0,-5.825261955,0.5531833807,-1.6805072415
H,0,-1.5586452472,-1.1349395029,1.4429004655
H,0,2.2431797268,0.4228853689,1.4027640525
H,0,5.3826620418,-2.3981748265,0.9563965151
H,0,1.0292164854,-3.040521969,-1.0452953929
H,0,-0.4594914942,-2.669455853,-2.0227581546
H,0,-0.3158262435,-3.5734530672,0.9154736668
H,0,-2.7600847868,-3.4838571118,0.878225364
H,0,-2.731001124,-2.9166524972,-0.8825635724
H,0,2.8505481478,0.4941501689,-1.3229509904
H,0,1.1706824375,4.0584622862,0.695983536
H,0,3.0620108932,5.4480922956,1.5858418554
H,0,3.1682676737,3.7720089428,2.1613573239
H,0,4.2229457095,4.3291001117,0.8424212028
H,0,2.0294393805,5.894568272,-0.7750776871
H,0,3.2223402741,4.7736471275,-1.4638739697
H,0,1.4812291824,4.5059418122,-1.7327939566
H,0,7.6036153283,-1.2326406966,0.938241844
H,0,6.8004629875,0.2768915785,0.4603847838
H,0,6.4700298058,-0.4428459588,2.0526309894
H,0,6.6467754239,-2.3792160316,-1.2114456227
H,0,4.8954174025,-2.3306259221,-1.484393654
H,0,5.8646833183,-0.843217345,-1.6393848657
H,0,-9.168710397,0.9355445323,-0.4054406201
H,0,-7.690732261,1.7307524242,-1.0116825608
H,0,-8.0755090731,0.0518010232,-1.5049611244

B3LYP/6-31G*
panisaldehyeDIPEReTSB3G
E(RB+HF-LYP) = -1444.42728662

Zero-point correction= 0.485997
(Hartree/Particle)
Thermal correction to Energy= 0.516686
Thermal correction to Enthalpy= 0.517630
Thermal correction to Gibbs Free Energy= 0.420630
Sum of electronic and zero-point Energies= -1443.941290
Sum of electronic and thermal Energies= -1443.910600
Sum of electronic and thermal Enthalpies= -1443.909656
Sum of electronic and thermal Free Energies= -1444.006656

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	324.225	114.590	204.153

C,0,-5.4729347486,0.19631087,-0.6715443294
C,0,-4.1221738527,-0.1424050393,-0.6835250524
C,0,-3.5190045589,-0.7405269898,0.4304831217
C,0,-4.3038573741,-0.9916255678,1.5705826697
C,0,-5.6485825917,-0.6610237018,1.5943329772
C,0,-6.2452213524,-0.0647367665,0.4701460581
C,0,-2.0889857073,-1.0795425353,0.4336463137
O,0,-1.3417195998,-0.5992210518,-0.5128725284
B,0,0.0890999079,-1.0167366662,-0.6107011241
O,0,0.8384737269,-0.2177665057,-1.5339221546
C,0,1.8322886037,0.4743329478,-0.8336612271
C,0,1.4359717008,1.9313319527,-0.5711854301
O,0,0.3131767447,2.3764338611,-0.6230812264
O,0,-7.5686251242,0.22349072,0.5913960203
C,0,-8.2326152395,0.8393662133,-0.5038712244
O,0,0.7527190406,-0.9669274487,0.6777526304
C,0,1.9739095445,-0.3060641676,0.5263747937
C,0,3.1402640334,-1.2990996186,0.4587773825
O,0,3.0367388227,-2.4914695635,0.2701316233
C,0,-0.0512877921,-2.6610870937,-1.2151769997
C,0,-0.8023358213,-3.3065576776,-0.1838513264
C,0,-2.1737573272,-3.1977960027,-0.0605135307
O,0,4.310258995,-0.6451625569,0.621189958
C,0,5.5372058729,-1.4307588923,0.5361821458
C,0,5.9362699399,-1.5917934641,-0.9269878015
C,0,6.5691047287,-0.6863703449,1.371674788
O,0,2.5361850792,2.6465700732,-0.2359389666
C,0,2.3407084102,4.0496800884,0.1079310008
C,0,2.3088193751,4.883643689,-1.1689430206
C,0,3.4823131655,4.415137665,1.0465925945
H,0,-3.515470699,0.0722909015,-1.5571740488
H,0,-3.8488264219,-1.448327877,2.4466181436
H,0,-6.2624905907,-0.8460456379,2.469889596
H,0,-5.9103797703,0.6666337969,-1.5444740044
H,0,-1.6203358365,-1.2480815824,1.4041053371
H,0,2.1617448292,0.3766560869,1.363281684
H,0,5.3232220489,-2.412185714,0.969371636
H,0,0.9890753836,-2.9768138131,-1.2922629249
H,0,-0.5457554409,-2.5855535381,-2.1860794445
H,0,-0.2373132354,-3.6638518483,0.677317864
H,0,-2.6913816924,-3.6492020267,0.7817508901
H,0,-2.7828485988,-3.0126595098,-0.9407341718
H,0,2.7739082867,0.4778250569,-1.3942100366
H,0,1.3773996509,4.1282446996,0.6208155044
H,0,3.384168835,5.4569551665,1.3710912044
H,0,3.4770222652,3.7745944825,1.93420781
H,0,4.4495581703,4.300098941,0.5449835797
H,0,2.1805975311,5.9443050779,-0.9242514119
H,0,3.2447960968,4.7690015481,-1.7272587769
H,0,1.4753835978,4.5748557626,-1.8055077726
H,0,7.5166180375,-1.2362444634,1.3756928033
H,0,6.7522082821,0.3133198963,0.9625771195
H,0,6.227924427,-0.5783335413,2.4060642525
H,0,6.8664107406,-2.1664876778,-1.0025775615
H,0,5.1593840672,-2.1259548412,-1.4809379777
H,0,6.0973260865,-0.6131432308,-1.3930497917
H,0,-9.2679144099,0.9734590038,-0.1862585128
H,0,-7.7950957308,1.8176909685,-0.7401254135
H,0,-8.2061825115,0.2041954871,-1.3984967103

B3LYP/6-31+G**
panisaldehyeDIPEReTSB3+G
E(RB+HF-LYP) = -1444.51745011

Zero-point correction= 0.482770
(Hartree/Particle)
Thermal correction to Energy= 0.513692
Thermal correction to Enthalpy= 0.514636
Thermal correction to Gibbs Free Energy= 0.416547
Sum of electronic and zero-point Energies= -1444.034681
Sum of electronic and thermal Energies= -1444.003758
Sum of electronic and thermal Enthalpies= -1444.002814
Sum of electronic and thermal Free Energies= -1444.100903

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	322.346	115.314	206.445

C,0,-5.4945556552,0.2275411572,-0.5994871673
C,0,-4.1474723584,-0.1322783311,-0.6382120637

C,0,-3.5479505407,-0.7986007611,0.4387278712
C,0,-4.3315454532,-1.0969381695,1.5693972569
C,0,-5.6725311094,-0.7472071414,1.6198840947
C,0,-6.2648717625,-0.0827461411,0.5318339647
C,0,-2.1218742992,-1.1610126803,0.4192400623
O,0,-1.3702239086,-0.634941346,-0.504042551
B,0,0.0551275515,-1.041384342,-0.6315601611
O,0,0.7923077291,-0.2094485524,-1.538918534
C,0,1.8050303457,0.4614717967,-0.8417241484
C,0,1.4361752125,1.9231111023,-0.5591259225
O,0,0.3115339603,2.3689734901,-0.509466227
O,0,-7.5847762295,0.2219633029,0.6739726717
C,0,-8.2503261821,0.9040345388,-0.3850724524
O,0,0.7439564231,-1.0268527852,0.6456184309
C,0,1.9549487721,-0.3402788585,0.5093143107
C,0,3.1441837099,-1.3063716512,0.4351417437
O,0,3.0732848176,-2.485468972,0.1588662289
C,0,-0.0805260319,-2.6704807728,-1.2949469672
C,0,-0.8494533787,-3.3543034769,-0.3050465422
C,0,-2.2235474903,-3.2285400643,-0.1879790817
O,0,4.2916272621,-0.6495119961,0.7047669408
C,0,5.5470466302,-1.3967359375,0.6217443975
C,0,6.0422632568,-1.3958489645,-0.8207683261
C,0,6.5029381845,-0.7207194171,1.5944430544
O,0,2.5601013527,2.6444575616,-0.3404230939
C,0,2.4080808831,4.0583004775,-0.0009194867
C,0,2.3304901618,4.8762364609,-1.2860589482
C,0,3.6001676843,4.4138597761,0.8767022602
H,0,-3.543197022,0.1226573719,-1.5025020189
H,0,-3.8805558641,-1.6050768236,2.418309163
H,0,-6.2823331443,-0.9691641462,2.4893085075
H,0,-5.9269176823,0.7515209923,-1.4433191992
H,0,-1.6556436261,-1.3755617399,1.3818086685
H,0,2.1212537133,0.3299352866,1.3598764232
H,0,5.3325109363,-2.4211444988,0.939295319
H,0,0.9616329893,-2.9797182849,-1.3691958035
H,0,-0.5620213351,-2.5392568907,-2.2658108122
H,0,-0.303287357,-3.774832035,0.5394880378
H,0,-2.7518297086,-3.7205876069,0.623609143
H,0,-2.820321392,-2.9893586059,-1.0632444234
H,0,2.7357172942,0.4586258401,-1.4188023025
H,0,1.4726439791,4.1586948122,0.5571336424
H,0,3.5339018053,5.4614506659,1.1887198796
H,0,3.6258903049,3.7878687996,1.7734442816
H,0,4.5397997556,4.2754282854,0.3315587384
H,0,2.2216099411,5.9395955962,-1.0463628551
H,0,3.242205598,4.7478994758,-1.8793741768
H,0,1.4698161084,4.5718227604,-1.8869474357
H,0,7.4625719752,-1.2479590663,1.6001110223
H,0,6.6825169516,0.3196818867,1.3039399917
H,0,6.0977035988,-0.7314460518,2.6104943991
H,0,6.9860916825,-1.9474085291,-0.8904036106
H,0,5.3184098286,-1.8790386084,-1.4822468115
H,0,6.2155696773,-0.3718287829,-1.1685205456
H,0,-9.2795434574,1.0359544274,-0.0501892171
H,0,-7.7987329915,1.8857518537,-0.5720371525
H,0,-8.2399120964,0.312082313,-1.308255468

B3LYP/6-31+G PCM solvent model for dichloromethane**
panisaldehydeDIPEReTSPCMB3PSalternative
E(RB+HF-LYP) = -1444.54071075

Zero-point correction= 0.481090
(Hartree/Particle)
Thermal correction to Energy= 0.512014
Thermal correction to Enthalpy= 0.512958
Thermal correction to Gibbs Free Energy= 0.415035
Sum of electronic and zero-point Energies= -1444.059621
Sum of electronic and thermal Energies= -1444.028697
Sum of electronic and thermal Enthalpies= -1444.027753
Sum of electronic and thermal Free Energies= -1444.125676

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	321.294	115.483	206.097

1	6	0	-5.474599	0.683741	-0.624833
2	6	0	-4.161601	0.215493	-0.681201
3	6	0	-3.608203	-0.513958	0.380899
4	6	0	-4.405057	-0.772309	1.513240
5	6	0	-5.713395	-0.314955	1.581187
6	6	0	-6.257888	0.415689	0.509815
7	6	0	-2.220193	-1.002283	0.351622
8	8	0	-1.394393	-0.461637	-0.509350
9	5	0	-0.013884	-0.989354	-0.664839
10	8	0	0.789806	-0.157693	-1.531283
11	6	0	1.879467	0.365620	-0.816754
12	6	0	1.687283	1.848873	-0.474514
13	8	0	0.627298	2.444190	-0.504915
14	8	0	-7.548650	0.822345	0.667223
15	6	0	-8.167383	1.576387	-0.379477
16	8	0	0.688455	-1.092706	0.605648
17	6	0	1.956739	-0.507099	0.493230
18	6	0	3.064595	-1.565038	0.385250
19	8	0	2.882647	-2.745589	0.150895
20	6	0	-0.274884	-2.548570	-1.417101
21	6	0	-1.141562	-3.221531	-0.497275
22	6	0	-2.500001	-2.965269	-0.418665
23	8	0	4.261876	-0.995505	0.582012
24	6	0	5.469298	-1.827267	0.482329
25	6	0	5.931475	-1.861891	-0.969702
26	6	0	6.484255	-1.206596	1.430657
27	8	0	2.863440	2.390122	-0.121935
28	6	0	2.897609	3.800128	0.288330
29	6	0	3.030478	4.678233	-0.950820
30	6	0	4.068704	3.926165	1.251307
31	1	0	-3.555805	0.429825	-1.558519
32	1	0	-3.990301	-1.334383	2.349623
33	1	0	-6.331283	-0.506977	2.455729
34	1	0	-5.867629	1.251514	-1.461299
35	1	0	-1.805156	-1.326994	1.309137
36	1	0	2.177825	0.106957	1.375400
37	1	0	5.196134	-2.833624	0.816356
38	1	0	0.730952	-2.963052	-1.490453
39	1	0	-0.713970	-2.324032	-2.392439
40	1	0	-0.676015	-3.756760	0.333960
41	1	0	-3.104597	-3.455879	0.339460
42	1	0	-3.032656	-2.610709	-1.297326
43	1	0	2.797630	0.287212	-1.409881
44	1	0	1.953116	4.011407	0.800820
45	1	0	4.138445	4.957417	1.612599
46	1	0	3.938398	3.266432	2.114155
47	1	0	5.010473	3.669588	0.754860
48	1	0	3.055353	5.732478	-0.654588
49	1	0	3.957230	4.449958	-1.488487
50	1	0	2.183667	4.534560	-1.627279
51	1	0	7.405789	-1.797793	1.421059
52	1	0	6.727456	-0.183093	1.126673
53	1	0	6.099854	-1.184960	2.454772
54	1	0	6.833982	-2.476652	-1.054617

55	1	0	5.164230	-2.295258	-1.617625
56	1	0	6.167682	-0.852926	-1.324482
57	1	0	-9.180472	1.783269	-0.033559
58	1	0	-7.637857	2.520476	-0.551086
59	1	0	-8.207719	0.999188	-1.310279

MPW1K/6-31+G PCM solvent model for dichloromethane**
panisaldehydeDIPEReTSPCMmpw1kPSalternative
E(RmPW+HF-PW91) = -1444.09392090

Zero-point correction= 0.497028 (Hartree/Particle)
Thermal correction to Energy= 0.527115
Thermal correction to Enthalpy= 0.528059
Thermal correction to Gibbs Free Energy= 0.431768
Sum of electronic and zero-point Energies= -1443.596893
Sum of electronic and thermal Energies= -1443.566806
Sum of electronic and thermal Enthalpies= -1443.565861
Sum of electronic and thermal Free Energies= -1443.662153

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	330.770	111.814	202.662

1	6	0	-5.282080	0.431842	-0.759501
2	6	0	-3.968092	-0.004444	-0.760267
3	6	0	-3.399855	-0.559533	0.380631
4	6	0	-4.174894	-0.674538	1.536710
5	6	0	-5.483405	-0.246652	1.550353
6	6	0	-6.046104	0.308664	0.399656
7	6	0	-2.006950	-1.001201	0.405035
8	8	0	-1.219910	-0.604805	-0.529731
9	5	0	0.163354	-1.159229	-0.589823
10	8	0	0.967947	-0.447118	-1.541675
11	6	0	1.897594	0.316203	-0.853917
12	6	0	1.472069	1.771836	-0.735061
13	8	0	0.572184	2.274146	-1.354830
14	8	0	-7.326583	0.699747	0.504329
15	6	0	-7.954972	1.269449	-0.620449
16	8	0	0.820045	-1.029805	0.694140
17	6	0	2.031499	-0.385152	0.515451
18	6	0	3.194330	-1.363172	0.519060
19	8	0	3.092234	-2.558647	0.613469
20	6	0	-0.077119	-2.765966	-1.061982
21	6	0	-0.963712	-3.288223	-0.064092
22	6	0	-2.312010	-3.068017	-0.073913
23	8	0	4.339402	-0.709197	0.420223
24	6	0	5.566435	-1.465318	0.392015
25	6	0	5.847350	-1.902150	-1.026819
26	6	0	6.630643	-0.558408	0.957286
27	8	0	2.265242	2.420968	0.100945
28	6	0	2.078370	3.840581	0.268080
29	6	0	2.842701	4.569544	-0.812152
30	6	0	2.557716	4.165890	1.660588
31	1	0	-3.373174	0.096112	-1.658350
32	1	0	-3.743339	-1.101959	2.434552
33	1	0	-6.090323	-0.327407	2.442275
34	1	0	-5.691620	0.864919	-1.659106
35	1	0	-1.578129	-1.194124	1.385663
36	1	0	2.220174	0.330539	1.315082
37	1	0	5.428332	-2.336324	1.031410
38	1	0	0.915851	-3.204482	-1.044671
39	1	0	-0.497276	-2.738316	-2.064573
40	1	0	-0.518918	-3.674909	0.848901
41	1	0	-2.932227	-3.428766	0.734387
42	1	0	-2.814856	-2.828813	-1.000837
43	1	0	2.848168	0.334757	-1.390893
44	1	0	1.012368	4.043769	0.174342
45	1	0	2.431348	5.229237	1.853643
46	1	0	1.990525	3.613176	2.405919
47	1	0	3.612073	3.919788	1.772674
48	1	0	2.707135	5.643585	-0.699453
49	1	0	3.906501	4.348810	-0.742288
50	1	0	2.487437	4.286009	-1.799724
51	1	0	7.583951	-1.082324	0.983478
52	1	0	6.744820	0.332064	0.341791
53	1	0	6.380286	-0.250658	1.969745
54	1	0	6.772903	-2.473868	-1.060747
55	1	0	5.046974	-2.532070	-1.406904
56	1	0	5.955865	-1.036545	-1.678348
57	1	0	-8.967048	1.503162	-0.310970
58	1	0	-7.451490	2.184413	-0.930706
59	1	0	-7.984670	0.566647	-1.452421

Prereactive Complex Used in Polyrate Calculation
M062X/6-31+G**
This structure was optimized with the Gaussian options int(grid=ultrafine) and nosymm.
anisaldehydeAllylBegPrereactiveM062X
allylboration anisaldehyde prereactive complex
E(RM062X) = -831.115237698

Zero-point correction= 0.287347 (Hartree/Particle)
Thermal correction to Energy= 0.306160
Thermal correction to Enthalpy= 0.307104
Thermal correction to Gibbs Free Energy= 0.237042
Sum of electronic and ZPE= -830.827890
Sum of electronic and thermal Energies= -830.809078
Sum of electronic and thermal Enthalpies= -830.808134
Sum of electronic and thermal Free Energies= -830.878195

	E KCal/Mol	CV Cal/Mol-K	S Cal/Mol-K
Total	192.118	67.151	147.457

C,0,3.6424102638,2.065315018,-2.4988226407
C,0,2.4306730618,1.6682419196,-3.0533961509
C,0,2.1837346251,1.829733342,-4.4171685046
C,0,3.1682818031,2.4027555375,-5.2326002139
C,0,4.3791742252,2.8042639439,-4.69704983
C,0,4.6202543182,2.6360445344,-3.3255889221
C,0,0.8953473599,1.4191406745,-5.0039975498
O,0,-0.0217117232,0.9367435415,-4.3645597728
B,0,-2.1696342381,1.853193414,-5.6556075716
C,0,-2.0245522869,3.3519327742,-5.1931609117
C,0,-0.8879061184,4.0699169184,-5.8584961473
C,0,0.1797043508,4.562358254,-5.227570734
O,0,5.8299717452,3.0566039859,-2.8889353652
O,0,-2.9584339647,0.9360587918,-5.0128872776
C,0,-2.6684716475,-0.3419273002,-5.5777089736
C,0,-1.9388170277,-0.0245178878,-6.9007905371
O,0,-1.5736775861,1.353060942,-6.7918355331
H,0,-3.6001924611,-0.8926826451,-5.7266606235
H,0,-2.5835094725,-0.1482729275,-7.7769782687
H,0,-2.0248988019,-0.8875790847,-4.8816195441
H,0,-1.912075288,3.3715362832,-4.1033500812
H,0,-2.9722932418,3.8620983912,-5.4181006906
H,0,-0.944875955,4.1583565452,-6.9436055041
H,0,0.9833910794,5.0548612652,-5.7667021312

H,0,0.2845604353,4.4825333197,-4.1473534328
H,0,0.7854875185,1.5755473532,-6.0942714909
H,0,-1.0357439247,-0.6262189395,-7.0345171789
H,0,2.9708765591,2.538445404,-6.2934889176
H,0,5.1564851262,3.2519190793,-5.3064729979
H,0,3.8166719197,1.9312036746,-1.4383165971
H,0,1.6561245777,1.2266630009,-2.4332241819
C,0,6.1296146042,2.9173062331,-1.5127964771
H,0,7.1355982066,3.3138977338,-1.3845685147
H,0,5.4281722208,3.4912944375,-0.8969966153
H,0,6.1095257371,1.8644184724,-1.2098971162

M062X/6-31+G/PCM**
This structure was optimized with the Gaussian options int(grid=ultrafine) and nosymm.
anisaldehydeAllylBegPrereactiveM062XPCM
allylboration anisaldehyde prereactive complex
E(RM062X) = -831.125637421

Zero-point correction= 0.287035 (Hartree/Particle)
Thermal correction to Energy= 0.305888
Thermal correction to Enthalpy= 0.306832
Thermal correction to Gibbs Free Energy= 0.236825
Sum of electronic and ZPE= -830.838602
Sum of electronic and thermal Energies= -830.819750
Sum of electronic and thermal Enthalpies= -830.818806
Sum of electronic and thermal Free Energies= -830.888813

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	191.947	67.301	147.342

C,0,3.653045284,2.142067681,-2.4742340151
C,0,2.4294736035,1.7499852136,-3.0042481707
C,0,2.1896335927,1.8198807779,-4.3789049625
C,0,3.197073007,2.2946156716,-5.230782664
C,0,4.4208507773,2.6897850843,-4.7198400859
C,0,4.6533097487,2.6153382956,-3.3374217474
C,0,0.892260669,1.422665276,-4.9461608241
O,0,-0.0516360168,1.013393991,-4.2893389644
B,0,-2.1687657765,1.8371372892,-5.66193434
C,0,-2.0418206085,3.3248512512,-5.1594221705
C,0,-0.9047122603,4.0698395415,-5.7942788354
C,0,0.1610440551,4.5403165682,-5.1426157248
O,0,5.8737446258,3.0230000551,-2.9257741066
O,0,-2.9749982729,0.9025627101,-5.0593812216
C,0,-2.7001165339,-0.3597839079,-5.6785804111
C,0,-1.9607535389,0.0017813746,-6.9817437952
O,0,-1.5610810478,1.3672139306,-6.8029106406
H,0,-3.6379012618,-0.8894564202,-5.8555130588
H,0,-2.6090125631,-0.0604606261,-7.8604758541
H,0,-2.0708661888,-0.9461236817,-5.0032440247
H,0,-1.9418373839,3.3232056953,-4.0681019028
H,0,-2.9919282839,3.8295317221,-5.3872168851
H,0,-0.9597570374,4.201909549,-6.8751290831
H,0,0.9666347152,5.0504071455,-5.6623647221
H,0,0.2634266545,4.4180041027,-4.0658473796
H,0,0.7958330977,1.5155427516,-6.0439532283
H,0,-1.0736975951,-0.6141789539,-7.1452894377
H,0,3.0103616035,2.3570191261,-6.3002019284
H,0,5.2126130193,3.0614813452,-5.3612314279
H,0,3.8198822893,2.0798523046,-1.4060967953
H,0,1.6432294655,1.3847103695,-2.3503387827
C,0,6.1650591493,2.9776433946,-1.5347736774
H,0,7.1829587582,3.3487767912,-1.4320009398
H,0,5.4803238246,3.6198615027,-0.9721395383
H,0,6.1073924295,1.9518690783,-1.1576056537

B3LYP/6-31+G**
anisaldehydeAllylBegPrereactiveB3PS
allylboration anisaldehyde prereactive complex
E(RB3LYP) = -831.483720493

Zero-point correction= 0.283731 (Hartree/Particle)
Thermal correction to Energy= 0.303288
Thermal correction to Enthalpy= 0.304232
Thermal correction to Gibbs Free Energy= 0.228769
Sum of electronic and ZPE= -831.199989
Sum of electronic and thermal Energies= -831.180433
Sum of electronic and thermal Enthalpies= -831.179488
Sum of electronic and thermal Free Energies= -831.254951

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	190.316	68.036	158.825

C,0,4.3056826503,1.3211330344,-2.4635335018
C,0,3.1296271975,0.8375032242,-3.0285458718
C,0,2.4478436126,1.5704805247,-4.0117827326
C,0,2.970190909,2.8113251513,-4.4228354209
C,0,4.141255203,3.3066861176,-3.8690890309
C,0,4.8161562646,2.5629778081,-2.8849189871
C,0,1.202792981,1.0679395821,-4.612101173
O,0,0.6581680559,0.0111291662,-4.3153602858
B,0,-2.4648880316,2.0903148165,-6.060038934
C,0,-2.5730708585,3.6566444691,-6.2225187486
C,0,-1.3499151922,4.3120773133,-6.8040171965
C,0,-0.6314509666,5.2743720795,-6.2147176659
O,0,5.9532831637,3.1265588562,-2.3995650271
O,0,-3.2286905536,1.3752323553,-5.1705654103
C,0,-2.8028844815,-0.0053618887,-5.2305543887
C,0,-1.8998230199,-0.0802744388,-6.4809642814
O,0,-1.6224337683,1.3017132321,-6.8077804488
H,0,-3.6861770579,-0.6462004431,-5.296721629
H,0,-2.4020439995,-0.5403870096,-7.3392335556
H,0,-2.2500122349,-0.2375692109,-4.3157984934
H,0,-2.8413739283,4.1103565148,-5.2610784314
H,0,-3.4325568287,3.8380465461,-6.8898628273
H,0,-1.0361530736,3.9489825942,-7.7828494664
H,0,0.2442993876,5.7028049652,-6.6943431923
H,0,-0.8992060921,5.6709571405,-5.2373177374
H,0,0.7548919328,1.7222422405,-5.3869132033
H,0,-0.9575723599,-0.5934253898,-6.282614192
H,0,2.4448038094,3.3874913747,-5.1806912485
H,0,4.5558438385,4.2615485458,-4.1744246754
H,0,4.8148900736,0.7376805718,-1.7060132819
H,0,2.7211426693,-0.1181647837,-2.7145259979
C,0,6.6939579891,2.4383161118,-1.3940595686
H,0,7.5463701969,3.0788302402,-1.1669005517
H,0,6.0936645409,2.2937350649,-0.4880751117
H,0,7.0526549713,1.4685475234,-1.7587827312

B3LYP/6-31+G/PCM**
anisaldehydeAllylBegPrereactiveB3PSPCM
allylboration anisaldehyde prereactive complex
E(RB3LYP) = -831.494308967

Zero-point correction= 0.283193 (Hartree/Particle)
Thermal correction to Energy= 0.302949
Thermal correction to Enthalpy= 0.303893

Thermal correction to Gibbs Free Energy= 0.226362
Sum of electronic and ZPE= -831.211116
Sum of electronic and thermal Energies= -831.191360
Sum of electronic and thermal Enthalpies= -831.190416
Sum of electronic and thermal Free Energies= -831.267947

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	190.103	68.272	163.177

C,0,4.7188264259,1.1438433937,-2.4568817163
C,0,3.5705427541,0.5967691444,-3.0188063874
C,0,2.7338351067,1.3644632082,-3.8469485867
C,0,3.075500435,2.7074616095,-4.1033125994
C,0,4.2167425883,3.2672922121,-3.550184223
C,0,5.0465725296,2.4879846323,-2.7220649844
C,0,1.5189956305,0.8035977584,-4.444914117
O,0,1.1178802342,-0.3485303199,-4.2918940999
B,0,-2.7415640203,2.1958768408,-6.2771986822
C,0,-2.9198174589,3.708558241,-6.6883685064
C,0,-1.648397232,4.4248696547,-7.0543805923
C,0,-1.1742689917,5.5204371843,-6.4493955128
O,0,6.1391272779,3.1174636038,-2.2247248544
O,0,-3.7098835569,1.4932029336,-5.5961206791
C,0,-3.1877522836,0.1708890342,-5.3159670824
C,0,-1.9104844963,0.0681681332,-6.1756392909
O,0,-1.6368598957,1.4355212012,-6.5783086016
H,0,-3.9420901078,-0.5737580846,-5.5793444331
H,0,-2.0637858826,-0.5290706937,-7.0799057804
H,0,-2.9767325552,0.1046981461,-4.2441880965
H,0,-3.4530251698,4.244379732,-5.893420837
H,0,-3.6001729813,3.707984272,-7.5565083378
H,0,-1.0789969192,3.9954806959,-7.8791784294
H,0,-0.2430737221,5.9840113266,-6.7634027592
H,0,-1.7018322416,5.988409275,-5.6203328172
H,0,0.9416526846,1.5051264669,-5.0787011093
H,0,-1.0509721511,-0.3173315984,-5.6238024112
H,0,2.4359659279,3.3110663357,-4.7422824114
H,0,4.4887287059,4.3001929258,-3.7403769145
H,0,5.3476679763,0.5322523637,-1.8218639548
H,0,3.3096593338,-0.4378553742,-2.8193059141
C,0,7.0342690282,2.3943943064,-1.3696624682
H,0,7.8179374443,3.102411191,-1.1023998365
H,0,6.521400232,2.0537651733,-0.4643270334
H,0,7.473671351,1.540221075,-1.8949829397

Product Complex Used in Polyrate Calculation

M062X/6-31+G**
This structure was optimized with the Gaussian options
int(grid=ultrafine) and nosymm.
anisaldehydeAllylBegProductM062X
anisaldehyde product complex
E(RM062X) = -831.166579084

Zero-point correction= 0.291575 (Hartree/Particle)
Thermal correction to Energy= 0.308809
Thermal correction to Enthalpy= 0.309753
Thermal correction to Gibbs Free Energy= 0.244477
Sum of electronic and ZPE= -830.875004
Sum of electronic and thermal Energies= -830.857770
Sum of electronic and thermal Enthalpies= -830.856826
Sum of electronic and thermal Free Energies= -830.922102

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	193.781	63.928	137.386

C,0,3.5825297317,2.2249952368,-2.5145094646
C,0,2.3534229131,2.1091159203,-3.1703334908
C,0,2.2204472333,2.446726648,-4.51239109
C,0,3.3485832051,2.9078038625,-5.2020118939
C,0,4.5738970223,3.0317761163,-4.566863221
C,0,4.6958207128,2.6904822405,-3.2143072708
C,0,0.8854251077,2.3820737742,-5.2170348179
O,0,0.0222208157,1.4999250498,-4.5103852791
B,0,-0.9421624025,0.8290143861,-5.1820395496
C,0,-2.2814741806,3.7985200448,-5.427772681
C,0,-1.0850102772,3.7434588578,-6.01362285
C,0,0.2183167018,3.7711417625,-5.269102874
O,0,5.937192342,2.8405039906,-2.6754326022
O,0,-1.9762099242,0.1878030213,-4.5410209457
C,0,-2.6876553379,-0.5457252158,-5.5358569493
C,0,-2.2359929767,0.0872674377,-6.8649201086
O,0,-0.9739114742,0.6751093847,-6.5556631898
H,0,-3.7615792112,-0.4520941915,-5.3610022595
H,0,-2.922124154,0.8788469361,-7.1897242573
H,0,-2.4046039926,-1.602203468,-5.4711808507
H,0,-2.3754988823,3.8977486486,-4.3490723242
H,0,-3.2003548627,3.7503983902,-6.0044190903
H,0,-1.0246909274,3.6223231757,-7.0953562396
H,0,0.91842647,4.4691537601,-5.742962861
H,0,0.0637760322,4.1008750157,-4.2351335023
H,0,1.0303366414,2.0102336596,-6.240355096
H,0,-2.1155961635,-0.6389223986,-7.6713581623
H,0,3.2676500919,3.1671588287,-6.2557094523
H,0,5.4548230431,3.3820237222,-5.0942653021
H,0,3.6528847604,1.9471855059,-1.4696712447
H,0,1.4882872091,1.7376628847,-2.6309845186
C,0,6.1056814602,2.5020846657,-1.3151297761
H,0,7.1533794836,2.6916541228,-1.0844002868
H,0,5.4716462354,3.1226853824,-0.6706152908
H,0,5.8784065544,1.4439278418,-1.1387062069

M062X/6-31+G/PCM**
This structure was optimized with the Gaussian options
int(grid=ultrafine) and nosymm.
anisaldehydeAllylBegProductM062XPCM
anisaldehyde product complex
E(RM062X) = -831.176616703

Zero-point correction= 0.291228 (Hartree/Particle)
Thermal correction to Energy= 0.308525
Thermal correction to Enthalpy= 0.309469
Thermal correction to Gibbs Free Energy= 0.243787
Sum of electronic and ZPE= -830.885389
Sum of electronic and thermal Energies= -830.868092
Sum of electronic and thermal Enthalpies= -830.867148
Sum of electronic and thermal Free Energies= -830.932830

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	193.602	64.096	138.239

C,0,3.5781511914,2.2772874708,-2.5025277111
C,0,2.3469353573,2.1673897107,-3.15551773
C,0,2.2240563764,2.4367452745,-4.5153535175
C,0,3.3660723139,2.8260754914,-5.2262432794
C,0,4.5949505501,2.9450945094,-4.5939143676
C,0,4.7064696966,2.6706457567,-3.2247384103

C,0,0.8864578557,2.3830276527,-5.2153944989
O,0,0.0313616937,1.4708055039,-4.5301425628
B,0,-0.9359015517,0.81573149,-5.2185253573
C,0,-2.2916441497,3.7899672436,-5.3673163778
C,0,-1.0985447084,3.7480697004,-5.962600621
C,0,0.2102774213,3.7678649695,-5.2271837915
O,0,5.9507168459,2.8090078184,-2.6897967563
O,0,-1.9661714333,0.1655447458,-4.5782351507
C,0,-2.6844934303,-0.5586700059,-5.5857068446
C,0,-2.2451826526,0.1010924132,-6.9029724659
O,0,-0.9734347709,0.6828839581,-6.5907333622
H,0,-3.7564823031,-0.4722835223,-5.4026436248
H,0,-2.9298523052,0.901686597,-7.2037232743
H,0,-2.3918019573,-1.612165081,-5.53970875
H,0,-2.3779521249,3.8762898607,-4.2864554943
H,0,-3.2140585061,3.7439233146,-5.9384973147
H,0,-1.0447897898,3.647300437,-7.0466745932
H,0,0.9031785186,4.4780104747,-5.6930795382
H,0,0.0612111729,4.0741601782,-4.1848607731
H,0,1.0310478525,2.0416849814,-6.2483922432
H,0,-2.132180523,-0.6089570692,-7.7231732229
H,0,3.2935226635,3.0350372276,-6.2912790576
H,0,5.483921878,3.2413297531,-5.1413052293
H,0,3.638836879,2.0536393619,-1.4442669809
H,0,1.4721264407,1.8558589382,-2.5935562611
C,0,6.1061432825,2.5380186452,-1.3063490747
H,0,7.1582525893,2.7071883255,-1.0826445329
H,0,5.4898522204,3.212421785,-0.7020458695
H,0,5.8452364069,1.499027089,-1.0777563604

B3LYP/6-31+G**
anisaldehydeAllylBegProductB3PS
anisaldehyde product complex
E(RB3LYP) = -831.522521789

Zero-point correction= 0.288021 (Hartree/Particle)
Thermal correction to Energy= 0.305664
Thermal correction to Enthalpy= 0.306608
Thermal correction to Gibbs Free Energy= 0.239534
Sum of electronic and ZPE= -831.234501
Sum of electronic and thermal Energies= -831.216858
Sum of electronic and thermal Enthalpies= -831.215914
Sum of electronic and thermal Free Energies= -831.282988

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	191.807	64.881	141.169

C,0,3.4795091444,2.2642966388,-2.5280740179
C,0,2.2222338764,2.2622758003,-3.1441126505
C,0,2.081056661,2.5384926406,-4.5055501514
C,0,3.2385327256,2.8173823564,-5.2495887016
C,0,4.4947868141,2.8290639567,-4.6532230274
C,0,4.6221363397,2.552714132,-3.2837183717
C,0,0.7204020967,2.5912058935,-5.1744032329
O,0,-0.1800697835,1.6976077764,-4.501510151
B,0,-0.9467425975,0.8102417775,-5.1763758318
C,0,-2.3492736972,4.4612676727,-5.4290623359
C,0,-1.1536600119,4.145379234,-5.9353090993
C,0,0.1152810095,4.0139732321,-5.1388215336
O,0,5.8971355817,2.58187234,-2.7866187036
O,0,-1.8739349335,0.016209644,-4.532801125
C,0,-2.3831754396,-0.9124724729,-5.5016635922
C,0,-1.9406158963,-0.3345714007,-6.8669073354
O,0,-0.881289189,0.5810335743,-6.5412004548
H,0,-3.4698076239,-0.982977967,-5.4004755325
H,0,-2.7459702209,0.2212376487,-7.3614840452
H,0,-1.9453347135,-1.8995713551,-5.3105235464
H,0,-2.4856395236,4.6471019035,-4.3661136675
H,0,-3.2302954107,4.5460336737,-6.0590753944
H,0,-1.065953844,3.9585299094,-7.0068060375
H,0,0.8738243729,4.7010655266,-5.5375054191
H,0,-0.0547755538,4.290237386,-4.0917064759
H,0,0.8262259698,2.276445172,-6.2197116364
H,0,-1.5621353288,-1.096657903,-7.5537026813
H,0,3.1587730737,3.0223688509,-6.3150403169
H,0,5.3902307991,3.0389555764,-5.2292998826
H,0,3.5498094482,2.0372838207,-1.4708673431
H,0,1.341709521,2.0244537647,-2.5562755597
C,0,6.093876555,2.3041069103,-1.4063775665
H,0,7.1684774224,2.3840458678,-1.2370535707
H,0,5.5709941965,3.0314612935,-0.7724167298
H,0,5.75996716,1.2906421253,-1.1499392784

B3LYP/6-31+G/PCM**
anisaldehydeAllylBegProductB3PSPCM
anisaldehyde product complex
E(RB3LYP) = -831.532730584

Zero-point correction= 0.287795 (Hartree/Particle)
Thermal correction to Energy= 0.305514
Thermal correction to Enthalpy= 0.306458
Thermal correction to Gibbs Free Energy= 0.238232
Sum of electronic and ZPE= -831.244936
Sum of electronic and thermal Energies= -831.227216
Sum of electronic and thermal Enthalpies= -831.226272
Sum of electronic and thermal Free Energies= -831.294499

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	191.713	65.026	143.595

C,0,3.3586279988,2.4170660364,-2.566021469
C,0,2.0949739598,2.5455667245,-3.1518950944
C,0,1.9359621818,2.6059678792,-4.5405670271
C,0,3.0855427719,2.5339300505,-5.3420548902
C,0,4.3528343351,2.4138044651,-4.7769189432
C,0,4.4967000151,2.3546569631,-3.3825902567
C,0,0.5688463912,2.7835212666,-5.1722869342
O,0,-0.3751898898,1.8791889695,-4.5580419832
B,0,-0.9016971832,0.824764552,-5.2273050312
C,0,-2.405830117,4.8576276618,-5.1945544105
C,0,-1.2567051701,4.4628933131,-5.7522411457
C,0,0.0273025113,4.2177291206,-5.0074809006
O,0,5.7773418954,2.2319003172,-2.9173689888
O,0,-1.8260106936,-0.0088762495,-4.6295261633
C,0,-2.0677572797,-1.0994192226,-5.5442798687
C,0,-1.4809819388,-0.615778209,-6.8888979134
O,0,-0.59585688,0.468078544,-6.5270234033
H,0,-3.1408835369,-1.2965630001,-5.5955855449
H,0,-2.251854248,-0.2252381623,-7.5611319304
H,0,-1.5567951541,-1.9917405226,-5.1676109236
H,0,-2.4900291413,5.0249719697,-4.1227829666
H,0,-3.2983729066,5.0280967104,-5.7902737534
H,0,-1.218712119,4.3038582892,-6.8314110054
H,0,0.8040223281,4.8980135089,-5.3821097731
H,0,-0.1006421141,4.4274084036,-3.9391602924
H,0,0.6414938616,2.5515523704,-6.2404055299
H,0,-0.9098185373,-1.3885100152,-7.4079929708
H,0,2.9908120874,2.5693581109,-6.4246731112

H,0,5.2395310728,2.3557110197,-5.4004642647
H,0,3.4396345962,2.3669568892,-1.486871719
H,0,1.2211896353,2.586047638,-2.5082627722
C,0,5.9881735585,2.1700305349,-1.505487858
H,0,7.0660647748,2.079009751,-1.3707047168
H,0,5.6339612404,3.0819656079,-1.0114342064
H,0,5.4904106942,1.297183714,-1.0678972377

Sample input files for POLYRATE calculations

file p.dat

```
*General

 TITLE
allylboration of anisaldehyde parent
calculation of rates parent
pcm
END

 ATOMS
  1       C
  2       C
  3       C
  4       C
  5       C
  6       C
  7       C   13.0033548378
  8       O
  9       B
 10       C
 11       C
 12       C
 13       O
 14       O
 15       C
 16       C
 17       O
 18       H
 19       H
 20       H
 21       H
 22       H
 23       H
 24       H
 25       H
 26       H
 27       H
 28       H
 29       H
 30       H
 31       H
 32       C
 33       H
 34       H
 35       H
END

 NOSUPERMOL

 INPUNIT AU

*OPTIMIZATION

 OPTMIN  OHOOK

 OPTTS   OHOOK

*SECOND

 HESSCAL HHOOK

*REACT1
 SPECIES   NONLINRP
 STATUS 2
 GEOM
  1       6.90325514     4.04792128    -4.67562468
  2       4.59103976     3.30699279    -5.67720628
  3       4.13780782     3.43907626    -8.27493114
  4       6.04159241     4.33619520    -9.88474670
  5       8.35419724     5.08295717    -8.91920515
  6       8.79348104     4.94227312    -6.30681309
  7       1.68612830     2.68844775    -9.34688937
  8      -0.09757793     1.91503711    -8.10567593
  9      -4.09837336     3.47168635   -10.69950530
 10      -3.85848176     6.28305830    -9.74989491
 11      -1.70965840     7.69088214   -10.94960010
 12       0.30432916     8.57995487    -9.71813533
 13      11.09976870     5.71264220    -5.52891179
 14      -5.62193198     1.70559634    -9.56084491
 15      -5.10248078    -0.67989305   -10.73096180
 16      -3.70528720     0.00336631   -13.19358370
 17      -2.95001565     2.58365989   -12.85563800
 18      -6.87463708    -1.68082904   -11.06531600
 19      -4.93031922    -0.11425402   -14.85414660
 20      -3.91336995    -1.78791465    -9.45476098
 21      -3.66954085     6.27994865    -7.68759848
 22      -5.65392507     7.23676617   -10.18036450
 23      -1.81367795     7.94045828   -12.99211110
 24       1.82667488     9.54388636   -10.70031860
 25       0.49780423     8.34881781    -7.68333805
 26       1.50390660     2.86396074   -11.42141640
 27      -2.02899440    -1.16063002   -13.50264020
 28       5.68875899     4.45412064   -11.90565620
 29       9.85041104     5.78536130   -10.13125910
 30       7.21853139     3.93035125    -2.65713786
 31       3.10525366     2.61672337    -4.44149662
 32      11.65027340     5.62693054    -2.90030193
 33      13.57382490     6.32827102    -2.70608960
 34      10.35631110     6.84054688    -1.83707749
 35      11.54129910     3.68849801    -2.18755766
END

*PROD1
 SPECIES   NONLINRP
 STATUS 2
 GEOM
  1       6.76172581     4.30344965    -4.72909201
  2       4.43506508     4.09577298    -5.96306432
  3       4.20285746     4.60478122    -8.53278154
```

```
 4       6.36095482    5.34050871   -9.87616850
 5       8.68319813    5.56542206   -8.68124003
 6       8.89393878    5.04678908   -6.09387245
 7       1.67516258    4.50326963   -9.85566728
 8       0.05926501    2.77941960   -8.56072879
 9      -1.76859762    1.54150911   -9.86158374
10      -4.33057984    7.16200014  -10.14275800
11      -2.07594864    7.08282526  -11.26768220
12       0.39736674    7.12023290   -9.87794581
13      11.24522510    5.30825548   -5.08297922
14      -3.71552554    0.31283423   -8.65161061
15      -5.07295739   -1.05573331  -10.55545620
16      -4.24278033    0.19103697  -13.04472750
17      -1.83952513    1.29046366  -12.45468110
18      -7.09872278   -0.89248651  -10.20951680
19      -5.53661847    1.70394073  -13.61306410
20      -4.51985066   -3.04655048  -10.46853240
21      -4.49367827    7.32512625   -8.10022697
22      -6.07369035    7.07498973  -11.22213360
23      -1.97436657    6.89239895  -13.31628510
24       1.70676005    8.46221342  -10.75836120
25       0.11567235    7.69904696   -7.90824077
26       1.94839807    3.85822546  -11.80775010
27      -4.02923725   -1.15076209  -14.59468230
28       6.22385585    5.73538916  -11.88879440
29      10.36311050    6.12522554   -9.71565885
30       6.87640514    3.88081597   -2.72926906
31       2.78191581    3.50706513   -4.90111104
32      11.53893850    4.79616016   -2.46864199
33      13.52713700    5.11584453   -2.04590167
34      10.37431720    6.07059740   -1.32667443
35      11.04589600    2.83275066   -2.03666436
END

*START
 SPECIES NONLINTS
 STATUS 2
 GEOM
  1       4.44942891    0.32173551    3.92865198
  2       2.14558568    0.09456480    2.68016243
  3       1.98269039    0.44276001    0.07007313
  4       4.17443104    1.03463720   -1.29859636
  5       6.47654967    1.26875598   -0.08181273
  6       6.62574490    0.91419678    2.54248038
  7      -0.43557128    0.17336763   -1.27031422
  8      -2.28952701   -0.91338320   -0.12058890
  9      -4.84458193   -0.94771565   -1.40280248
 10      -5.80019046    2.14601630   -1.12065956
 11      -3.82449264    3.52243003   -2.37531258
 12      -1.56617651    4.10762827   -1.24205192
 13       8.95182717    1.17784981    3.56925052
 14      -6.54227819   -2.63599425   -0.14135971
 15      -6.66262442   -4.84442922   -1.66608678
 16      -6.24657682   -3.84490269   -4.34755308
 17      -4.60261691   -1.74869601   -4.00690138
 18      -8.48933616   -5.77601596   -1.41490468
 19      -8.03619220   -3.20842475   -5.18664798
 20      -5.15113668   -6.16639849   -1.13241453
 21      -5.97860343    2.53374923    0.89771683
 22      -7.62070558    2.17622245   -2.08784478
 23      -3.94777513    3.70740563   -4.42316838
 24      -0.06834006    5.02674182   -2.30009278
 25      -1.43787214    4.19336564    0.80590347
 26      -0.36762201    0.03104691   -3.32747858
 27      -5.37759257   -5.23735835   -5.60409028
 28       4.06414754    1.31122860   -3.33130788
 29       8.18957607    1.71813599   -1.11371838
 30       4.52920200    0.03441684    5.95312115
 31       0.45151893   -0.36975982    3.73995825
 32       9.21023967    0.83612353    6.22072237
 33      11.20342050    1.12938102    6.63478568
 34       8.07382727    2.21988907    7.25658332
 35       8.65943697   -1.07949301    6.77433004
 END

# end of start section

*PATH

 SCALEMASS  1.00

 RODS ON

 INTMU   3
 SSTEP   0.001
 INH     10

 SRANGE
  SLP   0.5
  SLM  -0.5
 END

 RPM       pagem

 SIGN    REACTANT

 IDIRECT   1

 COORD  CART

 FREQSCALE 0.9614

 PRPATH
  COORD 3 4
  INTERVAL 1
  XMOL
 END

 EXFIRST
  EXPROD
  EXNSTEP 200
  EXSTEP 0.005
 END

 EXSECOND
  EXREACT
  EXNSTEP 200
  EXSTEP 0.005
 END

 SPECSTOP
  CURVE vag
  POINT savegrid
  PERCENTDOWN 95.
 END

*TUNNEL

 QUAD
  NQE   40
```

```
 NQTH  40
END

 SCT

*RATE

 FORWARDK

 SIGMAF       1
 CVT

 TEMP
  195.15
  273.15
  298.15
END
```

File p.70

```
*GRGENERAL

 GRRESTART
 RSTTOL 0.00001

*GRSTART

 CHARGE      0
 MULTIPLICITY  1

*GRREACT1

 CHARGE      0
 MULTIPLICITY  1

*GRPROD1

 CHARGE      0
 MULTIPLICITY  1

*GRCOMMON

 GRENER
    #p M062X/6-31+G** UNITS=AU FCHK NOSYMM
    scf=tight int(grid=ultrafine)
    scrf=(pcm,solvent=dichloromethane)
 END

 GRFIRST
    #p M062X/6-31+G** FORCE UNITS=AU FCHK NOSYMM
    scf=tight guess=tcheck
    scrf=(pcm,solvent=dichloromethane) int(grid=ultrafine)
 END

 GRSEC
    #p M062X/6-31+G** FREQ=NORAMAN UNITS=AU FCHK
NOSYMM
    scf=tight guess=tcheck
    scrf=(pcm,solvent=dichloromethane) int(grid=ultrafine)
 END

 GRLINK0
   %chk=g09.chk
   %nproc=8
   %mem=4gb
 END
```

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