SUPPORTING INFORMATION

Isotope Effects, Dynamic Matching, and Solvent Dynamics in a Wittig Reaction. Betaines as Bypassed Intermediates

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Experimental Procedures

Reactions of 1 with 2.

Determination of the Isotope Effects in **1**. Example Procedure. A mixture of 25.47 g (80 mmol) of 1-(triphenylphosphoranylidene)-2-propanone (**2**) in 150 mL of THF was heated to

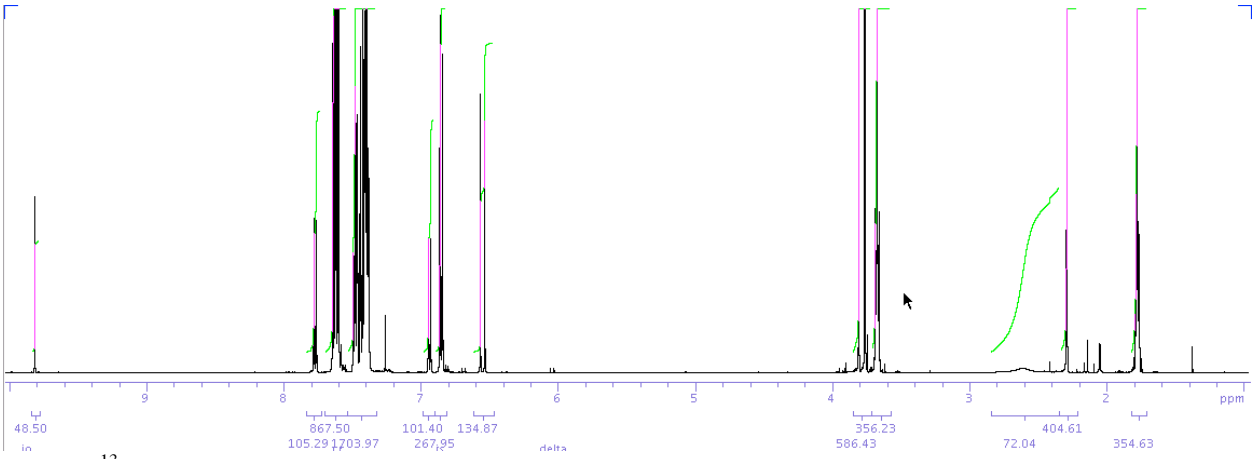
reflux and 13.6 g (100 mmol) of *p*-anisaldehyde (**1**) was added. Refluxing of the mixture with stirring was continued for 24 h, at which time NMR analysis of an aliquot taken from the reaction mixture showed 69 ± 2% conversion of the *p*-anisaldehyde. The cooled solution was then concentrated on a rotary evaporator and 200 mL of pentane was added to precipitate out the triphenylphosphine oxide. After filtration, the filtrate was concentrated on a rotary evaporator again to remove the volatiles. The residue was chromatographed on a 12" × 60 mm silica gel column using 20% ethyl acetate in hexanes as eluent to afford 1.01 g of *p*-anisaldehyde (contaminated by trace amounts of (*Z*)-4-(4-methoxyphenyl)but-3-en-2-one).

A closely analogous procedure using independently prepared **2** was taken to 73 ± 2% conversion, and 2.21 g of purified *p*-anisaldehyde was recovered.

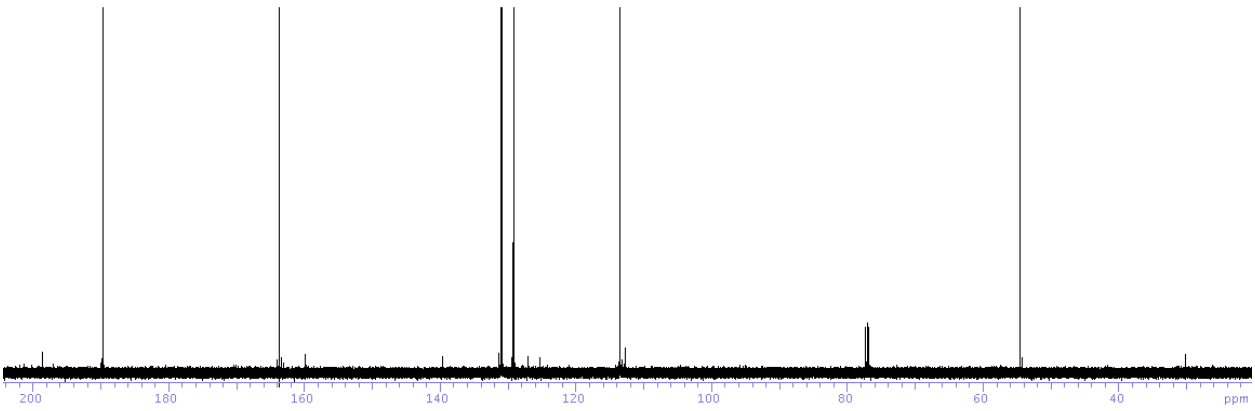
^{1}H NMR Spectrum of Crude Reaction Mixture After Concentration

A note on spectra: we certify that all spectra presented are unaltered screen dumps or pdf printouts of the original spectra. Please note that scales are increased by a factor of 5 from normal to show impurities clearly. The raw electronic files are saved and always available on request.

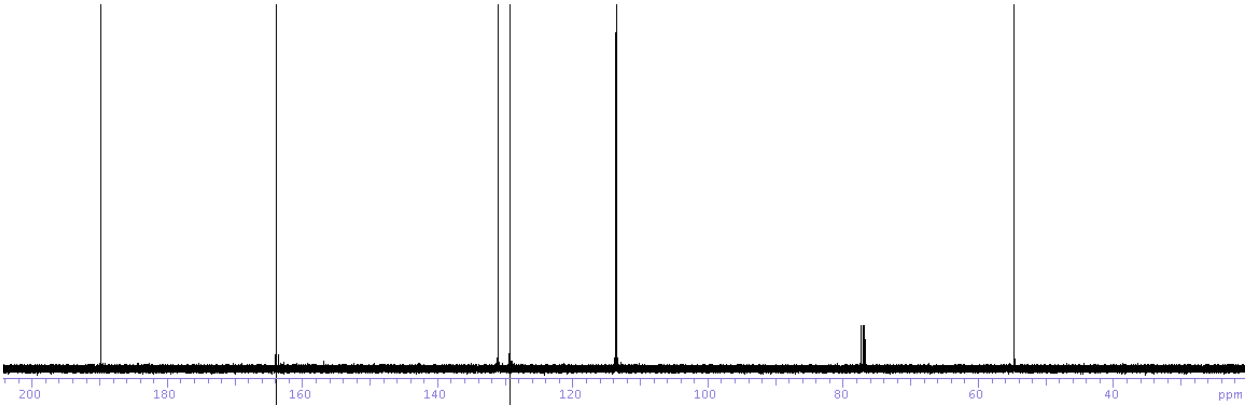
The spectrum below is of the crude reaction mixture from the 73%-conversion reaction above after concentration on a rotary evaporator. The spectrum illustrates the general cleanliness for the reaction. For example, the only peaks showing up in the region from d 4.0 to 3.5 are **1**, **3**, THF, the cis isomer of **3** (≈2%), ^{13}C satellites, and spinning sidebands.



^{13}C NMR Spectrum of Sample



^{13}C NMR Spectrum of Standard



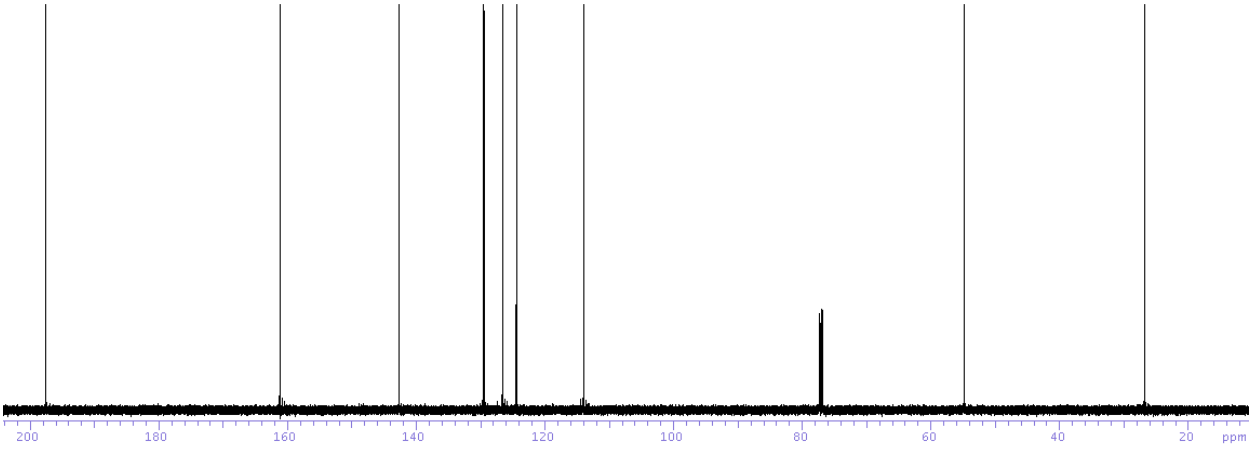
Determination of the Isotope Effects in **2**. Low-conversion Sample. Example Procedure. A mixture of 15.92 g (50 mmol) of 1-(triphenylphosphoranylidene)-2-propanone (**2**) in 75 mL of THF was heated to reflux and 1.36 g (10 mmol) of *p*-anisaldehyde (**1**) was added. Refluxing of the mixture with stirring was continued for 3 days, at which time NMR analysis of an aliquot was consistent with complete conversion of the *p*-anisaldehyde. The cooled solution was then evaporated on a rotary evaporator and 100 mL of 1:1 diethyl ether:hexanes was added to precipitate out the triphenylphosphine oxide. After gravity filtration, the filtrate was concentrated on a rotary evaporator again to remove the volatiles. The residue was chromatographed on a 14" x 40 mm silica gel column using 20% ethyl acetate in hexanes as eluent to afford 1.51 g of (*E*)-4-(4-methoxyphenyl)but-3-en-2-one (**3**) (Sample 2).

In a closely analogous procedure, 15.92 g (50 mmol) of **2** in 150 mL of THF was reacted with 1.36 g of **1** for 24 h, affording after a similar workup 1.26 g of **3** (Sample 1).

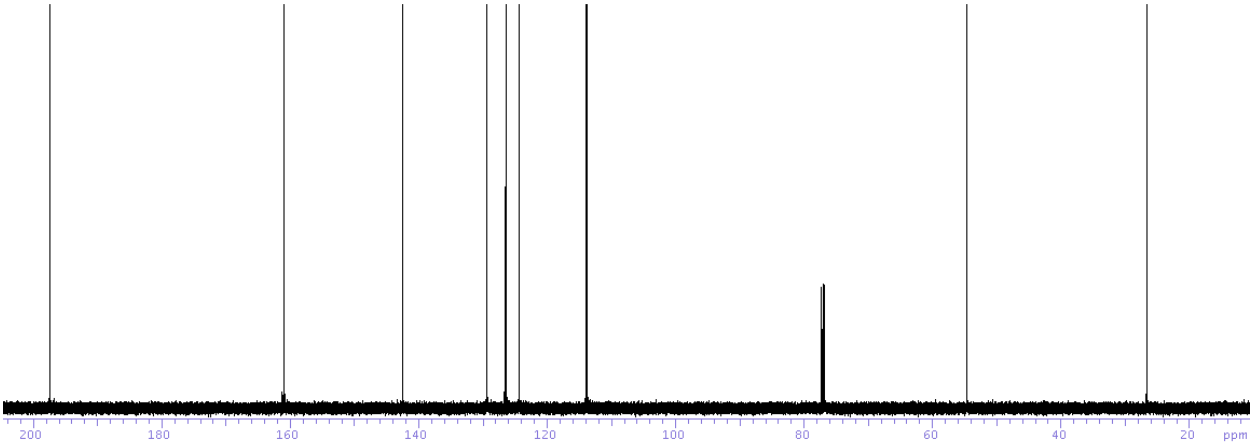
A 100%-conversion standard was prepared by a closely analogous procedure using 3.18 g (10 mmol) of **2** and 6.8 g (50 mmol) of **1**. Silica gel column chromatography as before but using 10% ethyl acetate in hexanes as eluent afforded 1.11 g of **3** (Standard 2). Another 100%-conversion standard was prepared by a closely analogous procedure using 3.18 g (10 mmol) of **2** and 6.8 g (50 mmol) of **1** to afford 1.03 g of **3** (Standard 1). Standard 1 and sample 1 were prepared from a common set of starting materials, and standard 2 and sample 2 were prepared from a different set of common starting materials.

Observations of the *cis*-Isomer of **3**. In the NMR analysis of aliquots taken from reactions of **1** with **2** by the procedures above, the *cis* isomer of **3** was observable based on the presence of a 12.7 Hz doublet at δ 6.0 (1 H) and a corresponding singlet at δ 2.08 (3 H). Measurements of the amount of *cis*-**3** for reactions at 67 °C ranged from 2.1% to 2.7%; these measurements were all considered to be identical within the error of the integrations and there was no suggestion of the ratio changing over the course of the first 4 h of a monitored reaction. Measurements of the amount of *cis*-**3** for reactions at 25 °C ranged from 1.9% to 2.4% and there was no indication of the ratio changing over the course of 26 h. These observations weigh against a significant role for product isomerization in the origin of the *trans* product.

^{13}C NMR Spectrum of 20%-Conversion Sample



^{13}C NMR Spectrum of 100%-Conversion Standard



NMR Measurements

NMR samples of **1** consisted of 300 mg of the *p*-anisaldehyde in 5 mm NMR tubes that were filled to a constant height of 5 cm with $CDCl_3$. Samples of **3** consisted of 250 mg of (E)-4-(4-methoxyphenyl)but-3-en-2-one in 5 mm NMR tubes that were filled to a constant height of 5 cm with $CDCl_3$. The ^{13}C spectra were recorded at 125.70 MHz using inverse gated decoupling. The acquisitions for **1** used a 70 s delay between calibrated $\pi/2$ pulses and a 7 s acquisition time to collect 426,830 points. The acquisitions for **3** used either a 60 s delay (sample/standard 1) or a 30 s delay (sample/standard 2) between calibrated $\pi/2$ pulses and a 5 s acquisition time to collect 271,740 points. Integrations were determined numerically using a macro as exemplified in a later section. A zero-order baseline correction was generally applied, but to avoid any qualitative manipulation no first-order or higher-order baseline correction was ever applied. The integration value of each peak was determined by the average of all measurements. The uncertainty of the measurement was determined by considering a two-side 95% confidence interval in a T-distribution. .

NMR Results and Calculation of KIEs

The raw integrations for anisaldehyde samples are shown in Table S1, along with average values and standard deviations. The integration of peak 5, the carbon meta, was in each case set

to 2000. In the table the labels ortho, meta, and para are relative to the –CHO substituent, and "ipso" refers to the aromatic carbon with the –CHO substituent.

Table S1. Raw integrals, average integrals, standard deviations, and 95% confidence intervals for anisaldehyde NMRs.

	69%-conversion sample							
carbonyl	1053.31	1053.45	1056.80	1057.17	1054.76	1050.80	1055.66	1054.77
para	1004.19	1002.67	1004.53	1007.16	1006.22	1002.56	1008.34	1005.37
ortho	1970.57	1966.02	1961.71	1972.40	1971.47	1965.35	1971.08	1972.72
ipso	1008.26	1006.40	1005.67	1011.59	1007.56	1005.69	1010.24	1011.82
meta	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00
methoxy	976.93	980.61	975.43	976.98	980.82	974.61	976.52	978.45
carbonyl	1052.48	1054.89	1054.07	1051.31	1057.09	1061.34	1057.76	1059.04
para	1005.00	1002.92	1005.20	1005.14	1005.96	1006.99	1004.69	1007.66
ortho	1967.02	1970.84	1968.24	1970.38	1966.03	1971.65	1967.20	1969.56
ipso	1008.51	1008.38	1010.21	1009.13	1004.70	1005.99	1007.50	1009.63
meta	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00
methoxy	976.75	977.11	976.56	978.23	975.43	976.15	974.62	977.35
carbonyl	1058.98	1058.35	1057.06	1058.14	1056.34	1056.31	1055.11	1056.61
para	1009.25	1004.98	1004.61	1004.21	1006.12	1005.35	1001.61	1004.89
ortho	1971.99	1967.75	1972.87	1970.54	1971.63	1972.52	1967.22	1970.61
ipso	1008.13	1005.91	1009.17	1008.22	1007.20	1006.19	1005.45	1007.71
meta	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00
methoxy	976.94	978.04	975.00	978.40	975.84	975.91	975.59	974.98
	Average	Stdev	95% conf.					
carbonyl	1055.90	2.5	1.1					
para	1005.23	1.8	0.8					
ortho	1969.47	2.9	1.2					
ipso	1007.89	1.9	0.8					
meta	2000.00	0.0	0.0					
methoxy	976.80	1.7	0.7					

	73%-conversion sample					
carbonyl	1061.99	1061.15	1061.10	1063.41	1061.46	1061.34
para	1005.23	1007.43	1003.19	1003.60	1004.79	1004.86
ortho	1970.01	1972.74	1969.58	1974.18	1966.55	1969.83
ipso	1007.44	1006.16	1006.43	1008.88	1004.52	1009.51
meta	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00
methoxy	975.90	975.89	972.60	977.57	973.50	977.33
carbonyl	1060.84	1061.57	1059.50	1062.73	1063.07	1064.71
para	1003.89	1005.37	1002.58	1005.66	1005.48	1003.61
ortho	1966.96	1969.84	1968.18	1971.97	1968.64	1969.43
ipso	1006.43	1005.58	1006.56	1008.89	1007.96	1006.52
meta	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00

methoxy	974.23	975.03	974.46	975.30	974.59	974.41		
	Average	Stdev	95% conf.					
carbonyl	1061.91	1.4	0.9					
para	1004.64	1.3	0.8					
ortho	1969.83	2.2	1.4					
ipso	1007.07	1.5	0.9					
meta	2000.00	0.0	0.0					
methoxy	975.07	1.4	0.9					

			standard					
carbonyl	1018.35	1015.42	1017.91	1020.29	1021.15	1020.65	1017.88	1020.33
para	1002.32	997.68	1003.56	1000.46	1002.58	1005.66	1001.07	1000.58
ortho	1967.55	1970.08	1967.26	1964.66	1969.44	1969.35	1967.27	1965.89
ipso	1000.64	998.68	995.58	996.31	999.60	995.50	995.41	998.46
meta	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00
methoxy	977.15	976.31	974.94	975.91	973.08	977.58	978.30	974.95
carbonyl	1018.15	1019.13	1014.37	1016.83	1017.74	1016.46	1018.91	1019.45
para	999.82	1001.21	999.74	1001.05	1001.59	1003.16	1006.42	1003.63
ortho	1967.31	1968.13	1966.61	1964.02	1963.35	1970.51	1971.42	1969.01
ipso	995.79	996.41	996.22	996.65	999.62	1000.02	1001.67	1001.17
meta	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00
methoxy	974.59	975.85	975.47	974.60	976.15	973.00	975.88	974.23
carbonyl	1018.18	1018.74						
para	1000.96	1002.57						
ortho	1967.22	1963.42						
ipso	1002.08	999.82						
meta	2000.00	2000.00						
methoxy	973.68	975.76						
	Average	Stdev	95% conf.					
carbonyl	1018.33	1.8	0.9					
para	1001.89	2.1	1.1					
ortho	1967.36	2.4	1.2					
ipso	998.31	2.3	1.2					
meta	2000.00	0.0	0.0					
methoxy	975.41	1.4	0.7					

The isotope effects in the main text were then calculated from eq 1, and the uncertainties were calculated from eqs 2, 3, 4, and 5. In these eqs, R/R_0 is the ratio of a peak's average integrations for a sample analysis divided by that in the analysis of the standard, F is the fractional conversion, ΔF is the uncertainty in the conversion, IntSample is the average integration for the sample for the carbon peak of interest in the table above, IntStandard is the average integration for standard for the carbon peak of interest in the table above, and ΔIntSample and ΔIntStandard are the 95% confidence ranges in the table above. The uncertainties arising from uncertainties in F were negligible, and the major source of uncertainty

is random variation in the integrations due to noise.

$$KIE_{calcd} = \frac{\ln(1 - F)}{\ln[(1 - F)R/R_0]} \quad (1)$$

$$\Delta KIE_F = \frac{\partial KIE}{\partial F}\Delta F = \frac{-\ln(R/R_0)}{(1 - F)\ln^2[(1 - F)R/R_0]}\Delta F \quad (2)$$

$$\Delta KIE_R = \frac{\partial KIE}{\partial (R/R_0)}\Delta(R/R_0) = \frac{-\ln(1 - F)}{(R/R_0)\ln^2[(1 - F)R/R_0]}\Delta(R/R_0) \quad (3)$$

$$\Delta KIE = KIE^*((\Delta KIE_R/KIE)^2 + (\Delta KIE_F/KIE)^2)^{1/2} \quad (4)$$

$$\Delta(R/R_0) = R/R_0 \times ((\Delta IntSample / IntSample)^2 + (\Delta IntStandard / IntStandard)^2)^{1/2} \quad (5)$$

The raw integrations for (E)-4-(4-methoxylphenyl)but-3-en-2-one (**3**) samples are shown in Table S2, along with average values and standard deviations. The integration of peak 9, the methyl carbon, was in each case set to 1000. In the table the labels ortho, meta, and para are relative to the –CH=CHCOMe substituent, and "ipso" refers to the aromatic carbon with the -CH=CHCOMe substituent. The "olefinic 1" refers to the carbon that was originally the aldehyde carbon in **1**. The "olefinic 2" refers to the carbon that was originally the ylide carbon in **2**. The "solvent" refers to the $CDCl_3$ integration.

The integrations for the carbons derived from anisaldehyde reflect the isotope effects for the anisaldehyde carbons, but by the nature of the experiment the measurement of isotope effects from product integrations is less precise than the measurements above from analyses for the starting anisaldehyde. For this reason, no effort was made to optimize the spectra for measurements on the carbons derived from anisaldehyde. In addition, the measurements on Sample / Standard 2 used the shorter (30 s) delays between pulses, and this was judged to be too short for a reliable measurement of the isotope effect for the carbonyl carbon of **3**. The unreliable KIE of 1.003(3) for this carbon is reasonable but not presented in the main text.

Table S2. Raw integrals, average integrals, standard deviations, and 95% confidence intervals for NMRs of **3**.

Sample 1 from 20% conversion of ylide								
carbonyl	1022.27	1022.18	1017.68	1021.01	1016.76	1023.02	1024.06	1024.12
para	1020.4	1018.56	1017.27	1017.52	1017.82	1026.58	1022.59	1019.6
olefinic 1	1006.7	1009.04	1003.28	1003.64	1008.01	1007.05	1002.07	1006.31
ortho	2028.2	2032.71	2022.75	2017.26	2021.71	2026.93	2027.16	2027.61
ipso	1009.54	1020.64	1010.98	1013.47	1010.23	1011.32	1015.6	1018.55
olefinic 2	979.18	977.962	970.831	975.972	976.837	978.293	973.39	982.475
meta	2017.41	2020.47	2012.95	2017.38	2013.9	2026.4	2017.98	2025.35
solvent	2835.73	2840.43	2799.9	2795.58	2799.04	2780.51	2806.35	2800.4
methoxy	972.984	969.526	973.008	969.902	966.68	972.439	973.076	972.577
methyl	1000	1000	1000	1000	1000	1000	1000	1000
carbonyl	1022.38	1026.57	1021.32	1025.92	1019.26	1020.97	1019.73	1020.26
para	1022.55	1018.04	1014.2	1018.93	1020.19	1023.84	1020.14	1017.84

olefinic 1	1002.51	1011.19	1005.41	1008.49	1002.77	1007.69	1004.65	1009.42
ortho	2027.09	2028.22	2032.44	2024.9	2026.43	2030.15	2031.28	2029.16
ipso	1015.18	1012.39	1016.4	1015.1	1011.29	1019.8	1017.34	1013.39
olefinic 2	974.434	979.124	982.251	978.666	978.943	979.433	977.262	980.871
meta	2024.6	2019.19	2018.8	2024.07	2013.32	2025.04	2024.13	2022.1
solvent	2809.95	2778.94	2784.49	2772.21	2809.79	2782.53	2784.42	2772.55
methoxy	971.845	970.737	969.788	977.589	969.51	971.024	972.082	973.904
methyl	1000	1000	1000	1000	1000	1000	1000	1000

carbonyl	1024.01	1008.89	1025.74	1029.4	1025.67	1028.5	1017.64	1024.57
para	1020.04	1012.81	1023.61	1025.06	1022.54	1025.77	1021.07	1022.73
olefinic 1	1006.96	1002.89	1002.7	1008.1	1006.57	1008.72	998.505	1003.03
ortho	2032.46	2014.62	2024.96	2040.64	2032.22	2039.81	2023.83	2035.71
ipso	1014.84	1008.67	1017.53	1021.86	1016.53	1022.25	1010.91	1016.69
olefinic 2	974.337	973.297	974.163	982.622	976.685	979.764	977.348	974.364
meta	2019.31	2010.38	2021.69	2032.3	2021.94	2035.28	2020.76	2022.56
solvent	2787.07	2741.12	2802.21	2796.96	2768.28	2772.19	2757.88	2765.46
methoxy	971.363	960.908	969.743	974.976	970.983	976.812	968.788	967.271
methyl	1000	1000	1000	1000	1000	1000	1000	1000

carbonyl	1020.83	1023.88	1026.4	1020.51	1030.26	1024.64
para	1022.21	1016.68	1022.63	1019.61	1024.82	1020.34
olefinic 1	1004.14	1000.48	1007.13	1000.02	1006.45	1006.65
ortho	2020.74	2023.91	2022.27	2016.51	2039.8	2028.61
ipso	1013.24	1016.46	1015.68	1003.19	1016.61	1013.51
olefinic 2	975.414	979.327	970.827	967.017	977.194	977.454
meta	2013.72	2022.37	2023.28	2012.55	2026.89	2023.06
solvent	2691.37	2676.13	2683.93	2680.82	2685.54	2670.88
methoxy	975.4	971.541	968.787	963.935	975.41	978.032
methyl	1000	1000	1000	1000	1000	1000

	Average	Stdev	95% conf.
carbonyl	1022.6	4.3	1.6
para	1020.5	3.3	1.2
olefinic 1	1005.4	3.1	1.1
ortho	2027.7	6.5	2.4
ipso	1014.6	4.1	1.5
olefinic 2	976.9	3.6	1.3
meta	2021.0	5.7	2.1
solvent	2767.8	48.5	18.1
methoxy	971.4	3.8	1.4
methyl	1000.0	0.0	0.0

Standard 1 from 100% conversion of ylide, 20% conversion of aldehyde								
carbonyl	1021.06	1020.45	1018.27	1023	1014.15	1017.1	1019.08	1018.92
para	1017.8	1015.04	1020.16	1015.98	1017.39	1021.76	1019.95	1024.67
olefinic 1	980.931	980.849	978.518	984.83	979.023	981.839	980.857	981.666
ortho	2015.46	2027.81	2024.23	2029.57	2017.51	2019.24	2022.51	2036.7
ipso	1013.19	1020.3	1013.26	1017.38	1010.91	1012.32	1008.85	1017.95
olefinic 2	985.665	984.914	982.182	987.417	984.867	982.059	984.165	993.899
meta	2013.16	2024.18	2021.59	2024.24	2014.14	2013.98	2021.44	2022.39
solvent	2477.47	2455.61	2462.51	2464.7	2473.5	2447.8	2432.48	2443.76
methoxy	975.17	978.825	986.19	979.361	976.248	982.268	977.081	980.895
methyl	1000	1000	1000	1000	1000	1000	1000	1000
carbonyl	1020.63	1022.17	1018.7	1016.31	1020.28	1018.22	1023.8	1021.94
para	1024.77	1018.64	1019.08	1016.27	1027.87	1021.16	1023.38	1025.81
olefinic 1	983.082	982.503	983.412	984.63	986.177	978.683	983.861	983.98
ortho	2031.24	2024.71	2024.28	2020.7	2040.11	2027.39	2022.86	2027.53
ipso	1014.52	1015.22	1017.42	1013.18	1021.77	1012.7	1013.09	1012.54
olefinic 2	990.944	991.164	985.19	985.075	990.349	990.607	987.252	987.135
meta	2026.53	2022.63	2019.98	2013.99	2030.27	2020.37	2019.34	2026.58
solvent	2434.97	2441.72	2436.98	2423.95	2413.81	2382.09	2370.89	2379.95
methoxy	978.458	980.824	976.446	975.886	986.031	975.792	978.486	977.366
methyl	1000	1000	1000	1000	1000	1000	1000	1000
			Average	Stdev	95% conf.			
carbonyl	1017.47	1024.93	1019.8	2.8	1.4			
para	1012.51	1017.74	1020.0	4.1	2.0			
olefinic 1	976.586	980.792	981.8	2.5	1.3			
ortho	2019.2	2026.27	2025.4	6.4	3.2			
ipso	1007.11	1008.12	1013.9	4.0	2.0			
olefinic 2	983.912	993.069	987.2	3.6	1.8			
meta	2013.73	2023.77	2020.7	5.1	2.5			
solvent	2363.17	2365.73	2426.2	38.1	19.0			
methoxy	973.255	977.022	978.6	3.5	1.7			
methyl	1000	1000	1000.0	0.0	0.0			

Sample 2 from 20% conversion of ylide								
carbonyl	998.30	995.10	996.66	998.04	1003.40	1000.28	998.191	1005.69
para	991.21	992.14	991.91	993.22	995.97	998.28	995.485	997.186
olefinic 1	986.89	986.86	987.66	986.77	988.12	991.67	987.254	994.339
ortho	1973.31	1975.03	1978.10	1975.31	1978.83	1981.26	1979.83	1983.95
ipso	993.07	995.41	993.62	987.35	994.83	995.51	993.022	995.903
olefinic 2	960.77	963.77	960.23	960.88	962.42	960.15	967.565	965.243
meta	1975.93	1974.54	1975.09	1971.88	1977.53	1980.63	1975.25	1982.61

solvent	2028.77	2000.85	1986.80	1993.66	2056.96	2080.87	2006.84	2005.79
methoxy	947.66	945.08	946.73	944.61	947.47	947.37	947.094	949.95
methyl	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000	1000
					Average	Stdev	95% conf.	
carbonyl	998.684	1000.49	1000.78	1002.09	999.8	2.9	1.9	
para	990.691	994.202	996.051	992.656	994.1	2.5	1.6	
olefinic 1	991.475	986.7	991.421	991.151	989.2	2.6	1.7	
ortho	1979.35	1984.89	1977.73	1973.18	1978.4	3.8	2.4	
ipso	991.599	991.92	995.738	987.572	993.0	3.0	1.9	
olefinic 2	963.055	962.951	966.987	958.938	962.7	2.8	1.8	
meta	1974.98	1974.17	1981.44	1973.78	1976.5	3.4	2.1	
solvent	1998.58	1988.48	1977.7	1965.66	2007.6	33.1	21.0	
methoxy	947.135	952.491	949.718	945.343	947.6	2.2	1.4	
methyl	1000	1000	1000	1000	1000.0	0.0	0.0	

Standard 2 from 100% conversion of ylide, 20% conversion of aldehyde

carbonyl	1003.28	1002.22	1001.23	1004.34	999.917	1003.84
para	998.525	997.106	994.81	993.466	994.934	999.459
olefinic 1	964.718	962.707	961.907	960.55	960.835	965.005
ortho	1981.97	1975.15	1978.36	1971.65	1973.94	1982.77
ipso	995.211	993.625	994.757	993.281	993.946	998.869
olefinic 2	976.824	971.118	976.249	972.128	968.753	976.606
meta	1980.16	1971.25	1969.98	1968.89	1970.45	1977.35
solvent	2102.05	2078.69	2072.69	2068.12	2072.3	2072.8
methoxy	941.073	945.664	944.286	940.363	941.178	940.693
methyl	1000	1000	1000	1000	1000	1000

	Average	Stdev	95% conf.
carbonyl	1002.5	1.7	1.8
para	996.4	2.4	2.5
olefinic 1	962.6	1.9	2.0
ortho	1977.3	4.5	4.7
ipso	994.9	2.1	2.2
olefinic 2	973.6	3.4	3.6
meta	1973.0	4.6	4.8
solvent	2077.8	12.4	13.0
methoxy	942.2	2.2	2.3
methyl	1000.0	0.0	0.0

Computational Procedures and Supporting Computational Results

General

Calculations of structures, energies, and frequencies employed standard procedures in Gaussian09[1,2,3] unless otherwise noted. Complete structures and energetics are provided in sections below. All absolute energies are in Hartrees. All relative energies are presented in kcal/mol.

The program suite PROGDYN used for dynamics is a series of component programs written as either Unix shell scripts or awk programs. Gaussian09 was used to calculate the forces at each point in trajectories. A full description of PROGDYN including listings of the subprograms can be found in a later section. The latest version of this program can be obtained by emailing Daniel Singleton at singleton@mail.chem.tamu.edu. The original version of this program was published in the Supporting Information of a previous paper.[4]

Exploration of DFT Methods

The performance of computational methods for the Wittig reaction of stabilized ylides was evaluated using the model reaction of $Me_3PCHCHO$ with formaldehyde. The evaluation was done by determining relative gas-phase G3B3 potential energies for a series of relevant structures, then determining relative gas-phase single-point energies for these structures using various combinations of DFT methods and basis sets. The structures studied included $Me_3PCHCHO$, formaldehyde, the transition structure for their reaction (in the gas phase the cycloaddition of $Me_3PCHCHO$ with formaldehyde faces a single potential energy saddle point, referred to below as TS1), the oxaphosphetane derived from their reaction (OP1), a transition structure for the cleavage of the oxaphosphetane (OP2), and the products Me_3PO and acrolein.

Because of our particular interest in the energy surface in the area of a possible betaine structure, this list was augmented by three additional structures located in M06-2X/6-31G*/PCM(THF) calculations. These structures corresponded to the transition structure for reaction of $Me_3PCHCHO$ with formaldehyde to afford a betaine (called TS1PCM below), the resulting betaine (betainePCM), and the transition structure for ring closure of the betaine to afford the oxaphosphetane (called TS1.5PCM). The complete geometries for these structures are given in a later section. It should be understood that these last three structures were not reoptimized in carrying out the G3B3 calculations, while the other structures are the ordinary G3B3 stationary points.

Single-point energy calculations were carried out on these ten structures. This provides a series of eight energies to be compared, or seven relative energies. The table below, Table S3, provides for each method/basis set explored the absolute energies obtained for each structure, then shows the energies relative to $Me_3PCHCHO$ + formaldehyde, and finally calculates an average absolute "error" relative to the G3B3 results, assumed to be optimally accurate. The most important observations were that M06-2X, lc-wPBE, and B3P86 provided the best energetics of the DFT methods tried as compared with a 6-31+G** basis set, and that the performance of all three methods improved with large basis sets.

Obviously, this approach applies only to the gas-phase energetics and provides no validation for the solvent models employed. As mentioned in the main text, alternative solvent models and radii were explored with no qualitative difference in the results. See a later section for the detailed energetics found for the alternative methods.

Table S3. Absolute and relative energies for the model reaction of $Me_3PCHCHO$ with formaldehyde, and average absolute errors versus G3B3 energies. Relative energies are versus the reactants and are in kcal/mol. Errors are average absolute errors versus the G3B3 energies.

structure	method & abs. energy	relative energy	method & abs. energy	relative energy	method & abs. energy	relative energy	method & abs. energy	relative energy
			B3LYP		B3LYP		M062X	
	G3B3		6-31G*		6-31+G**		6-31G*	
CH2O	-114.45952		-114.50047		-114.51149		-114.44597	
Me3PCHCHO	-613.49178		-613.71164		-613.74476		-613.53166	
TS1	-727.94497	4.0	-728.20075	7.1	-728.24266	8.5	-727.97489	1.7
OP1	-727.97251	-13.3	-728.22624	-8.9	-728.26252	-3.9	-728.00408	-16.6
TS2	-727.97108	-12.4	-728.22528	-8.3	-728.26346	-4.5	-728.00092	-14.6
Me3PO	-536.17068	-34.5[a]	-536.35299	-31.5[a]	-536.37748	-29.9[a]	-536.20680	-28.8[a]
acrolein	-191.83562		-191.90933		-191.92646		-191.81674	
TS1PCM[b]	-727.94591	3.4	-728.20231	6.2	-728.24438	7.4	-727.97715	0.3
betainePCM[b]	-727.94553	3.6	-728.19853	8.5	-728.24189	9.0	-727.97472	1.8
TS1.5PCM[b]	-727.94893	1.5	-728.19894	8.3	-728.24203	8.9	-727.97559	1.3
				error		error		error
				4.2		6.2		2.6
	M062X		M06		M06		B3LYP	
	6-31+G**		6-31G*		6-31+G**		6-31G*-D2	
CH2O	-114.45458		-114.43499		-114.44418		-114.50097	
Me3PCHCHO	-613.55816		-613.48358		-613.51226		-613.73024	
TS1	-728.00882	2.5	-727.91713	0.9	-727.95394	1.6	-728.22893	1.4
OP1	-728.03267	-12.5	-727.94237	-14.9	-727.97395	-11.0	-728.25479	-14.8
TS2	-728.03149	-11.8	-727.93954	-13.2	-727.97301	-10.4	-728.25279	-13.5
Me3PO	-536.22587	-27.2[a]	-536.18402	-28.2[a]	-536.20509	-26.9[a]	-536.36441	-29.0[a]
acrolein	-191.83014		-191.77952		-191.79414		-191.91306	
TS1PCM[b]	-728.01107	1.0	-727.91964	-0.7	-727.95643	0.0	-728.23211	-0.6
betainePCM[b]	-728.00995	1.8	-727.91636	1.4	-727.95443	1.3	-728.22784	2.1
TS1.5PCM[b]	-728.01059	1.3	-727.91684	1.1	-727.95482	1.0	-728.22773	2.2
		error		error		error		error
		2.1		2.6		2.9		2.4
	B3LYP-D2				M062X		M062X	
	6-31+G**		M062X		6-311++G		6-311++G	
			aug-cc-pvdz		(2df,2p)		(2df,p)	
CH2O	-114.51199		-114.46912		-114.49319		-114.49232	
Me3PCHCHO	-613.76336		-613.59396		-613.67661		-613.67188	
TS1	-728.27084	2.8	-728.06154	1.0	-728.16288	4.3	-728.15724	4.4
OP1	-728.29107	-9.9	-728.08205	-11.9	-728.19047	-13.0	-728.18488	-13.0
TS2	-728.29098	-9.8	-728.08123	-11.4	-728.19038	-12.9	-728.18474	-12.9
Me3PO	-536.38890	-27.5[a]	-536.24905	-23.1[a]	-536.33014	-30.9[a]	-536.32640	-30.9[a]
acrolein	-191.93020		-191.85085		-191.88887		-191.88704	
TS1PCM[b]	-728.27418	0.7	-728.06293	0.1	-728.16628	2.2	-728.16064	2.2
betainePCM[b]	-728.27120	2.6	-728.06270	0.2	-728.16476	3.2	-728.15905	3.2
TS1.5PCM[b]	-728.27081	2.8	-728.06368	-0.4	-728.16561	2.6	-728.15992	2.7
		error		error		error		error
		2.8		3.6		1.1		1.1

	M062X 6-311++G (df,p)		M062X 6-311++G**		M062X 6-31+G (2df,p)		M062X 6-31+G (2d,p)	
CH2O	-114.49016		-114.48695		-114.46438		-114.46151	
Me3PCHCHO	-613.65922		-613.65005		-613.58060		-613.57273	
TS1	-728.14301	4.0	-728.13200	3.1	-728.03885	3.8	-728.02944	3.0
OP1	-728.16873	-12.1	-728.15321	-10.2	-728.06592	-13.1	-728.05381	-12.3
TS2	-728.16855	-12.0	-728.15282	-9.9	-728.06523	-12.7	-728.05242	-11.4
Me3PO	-536.31061	-27.6[a]	-536.29985	-25.3[a]	-536.25059	-30.4[a]	-536.24155	-28.9[a]
acrolein	-191.88276		-191.87749		-191.84289		-191.83872	
TS1PCM[b]	-728.14641	1.9	-728.13505	1.2	-728.04176	2.0	-728.03205	1.4
betainePCM[b]	-728.14465	3.0	-728.13356	2.2	-728.04045	2.8	-728.03098	2.0
TS1.5PCM[b]	-728.14515	2.7	-728.13400	1.9	-728.04133	2.3	-728.03194	1.4
		error		error		error		error
		1.7		2.8		1.1		1.8

	M062X TZVP		M062X Def2TZVP		M062X cc-pvtz		M11 6-31+G**	
CH2O	-114.49336		-114.49880		-114.49631		-114.45249	
Me3PCHCHO	-613.66169		-613.68735		-613.68654		-613.53545	
TS1	-728.15026	3.0	-728.17854	4.8	-728.17674	3.8	-727.98571	1.4
OP1	-728.17230	-10.8	-728.20817	-13.8	-728.20399	-13.3	-728.00497	-10.7
TS2	-728.17203	-10.7	-728.20798	-13.7	-728.20415	-13.4	-728.00419	-10.2
Me3PO	-536.30690	-26.1[a]	-536.33983	-32.3[a]	-536.33597	-30.2[a]	-536.21984	-26.8[a]
acrolein	-191.88970		-191.89781		-191.89501		-191.81079	
TS1PCM[b]	-728.15278	1.4	-728.18188	2.7	-728.17987	1.9	-727.98803	-0.1
betainePCM[b]	-728.15151	2.2	-728.18030	3.7	-728.17810	3.0	-727.98725	0.4
TS1.5PCM[b]	-728.15214	1.8	-728.18138	3.0	-728.17890	2.5	-727.98731	0.4
		error		error		error		error
		2.5		1.0		1.2		3.3

	MP2 6-311+G**		M062X aug-cc-pvtz		M062X jul-cc-pvdz		M062X aug-cc-pvtz	
CH2O	-114.24152		-114.49866		-114.46838		-114.49866	
Me3PCHCHO	-612.47581		-613.69151		-613.58970		-613.69151	
TS1	-726.70988	4.7	-728.18426	3.7	-728.05657	0.9	-728.18426	3.7
OP1	-726.73056	-8.3	-728.21033	-12.7	-728.07689	-11.8	-728.21033	-12.7
TS2	-726.72795	-6.7	-728.21087	-13.0	-728.07583	-11.1	-728.21087	-13.0
Me3PO	-535.33479	-25.7[a]	-536.34026	-29.9[a]	-536.24551	-22.9[a]	-536.34026	-29.9[a]
acrolein	-191.42351		-191.89752		-191.84910		-191.89752	
TS1PCM[b]	-726.71233	3.1	-728.18729	1.8	-728.05775	0.2	-728.18729	1.8
betainePCM[b]	-726.71084	4.1	-728.18606	2.6	-728.05763	0.3	-728.18606	2.6
TS1.5PCM[b]	-726.71269	2.9	-728.18696	2.0	-728.05872	-0.4	-728.18696	2.0
		error		error		error		error
		3.2		1.3		3.7		1.3

	B2PLYP 6-31+G**		M06-2X 6-311+G (2df,p)		wB97 6-31+G**		wB97X 6-31+G**	
CH2O	-114.40251		-114.49223		-114.48593		-114.47646	
Me3PCHCHO	-613.28785		-613.67170		-613.66659		-613.64981	
TS1	-727.68002	6.5	-728.15699	4.4	-728.14943	1.9	-728.12112	3.2
OP1	-727.70049	-6.4	-728.18465	-13.0	-728.16759	-9.5	-728.14075	-9.1
TS2	-727.70063	-6.4	-728.18449	-12.9	-728.16511	-7.9	-728.13904	-8.0
Me3PO	-536.00877	-30.3[a]	-536.32628	-31.0[a]	-536.31246	-26.2[a]	-536.30216	-27.4[a]
acrolein	-191.72980		-191.88699		-191.88187		-191.86782	
TS1PCM[b]	-727.68161	5.5	-728.16039	2.2	-728.14912	2.1	-728.12151	3.0
betainePCM[b]	-727.67963	6.7	-728.15879	3.2	-728.15077	1.1	-728.12199	2.7
TS1.5PCM[b]	-727.68069	6.1	-728.15967	2.7	-728.15252	0.0	-728.12355	1.7
		error		error				
		4.2		1.1		3.4		2.6

	B97D 6-31+G**		wB97XD 6-31+G**		PBE0 6-31+G**		mPW1PW91 6-31+G**	
CH2O	-114.24452		-114.46951		-114.37746		-114.49593	
Me3PCHCHO	-612.81766		-613.63762		-613.27172		-613.69479	
TS1	-727.07364	-7.2	-728.10250	2.9	-727.64597	2.0	-728.18545	3.3
OP1	-727.09078	-17.9	-728.12308	-10.0	-727.66820	-11.9	-728.20509	-9.0
TS2	-727.09405	-20.0	-728.12139	-8.9	-727.66676	-11.0	-728.20455	-8.7
Me3PO	-535.67630	-26.5[a]	-536.29553	-27.3[a]	-535.99691	-27.5[a]	-536.33772	-27.6[a]
acrolein	-191.42805		-191.85507		-191.69613		-191.89694	
TS1PCM[b]	-727.07708	-9.3	-728.10384	2.1	-727.64665	1.6	-728.18638	2.7
betainePCM[b]	-727.07724	-9.5	-728.10300	2.6	-727.64574	2.2	-728.18388	4.3
TS1.5PCM[b]	-727.07768	-9.7	-728.10400	2.0	-727.64711	1.3	-728.18381	4.3
		error		error		error		error
		9.8		2.6		2.2		2.8

	B98 6-31+G**		B971 6-31+G**		B972 6-31+G**		BP86 6-31+G**	
CH2O	-114.46548		-114.47429		-114.46795		-114.50986	
Me3PCHCHO	-613.58187		-613.60474		-613.64808		-613.75194	
TS1	-728.03838	5.6	-728.07173	4.6	-728.10460	7.2	-728.25607	3.6
OP1	-728.05973	-7.8	-728.09274	-8.6	-728.12540	-5.9	-728.27560	-8.7
TS2	-728.05909	-7.4	-728.09162	-7.9	-728.12452	-5.3	-728.27548	-8.6
Me3PO	-536.24767	-29.4[a]	-536.26074	-28.8[a]	-536.30788	-28.4[a]	-536.38533	-27.7[a]
acrolein	-191.84660		-191.86425		-191.85345		-191.92058	
TS1PCM[b]	-728.03958	4.9	-728.07280	3.9	-728.10609	6.2	-728.25693	3.1
betainePCM[b]	-728.03728	6.3	-728.07065	5.3	-728.10434	7.3	-728.25435	4.7
TS1.5PCM[b]	-728.03783	6.0	-728.07123	4.9	-728.10498	6.9	-728.25410	4.8
		error		error		error		error
		3.7		3.0		5.1		2.9

	lc-wPBE 6-31+G**		B3P86 6-31+G**		lc-wPBE 6-31+G (2df,p)		B3P86 6-31+G (2df,p)	
CH2O	-114.43395		-114.79026		-114.44255		-114.79861	
Me3PCHCHO	-613.44768		-614.91186		-613.46824		-614.93172	
TS1	-727.87618	3.4	-729.69731	3.0	-727.90369	4.5	-729.72390	4.0
OP1	-727.89973	-11.4	-729.71937	-10.8	-727.93101	-12.7	-729.74947	-12.0
TS2	-727.89655	-9.4	-729.71888	-10.5	-727.92820	-10.9	-729.74944	-12.0
Me3PO	-536.13835	-27.7[a]	-537.29185	-28.4[a]	-536.16249	-31.1[a]	-537.31450	-31.4[a]
acrolein	-191.78749		-192.45552		-191.79781		-192.46595	
TS1PCM[b]	-727.87523	4.0	-729.69843	2.3	-727.90289	5.0	-729.72537	3.1
betainePCM[b]	-727.87681	3.0	-729.69700	3.2	-727.90449	4.0	-729.72382	4.1
TS1.5PCM[b]	-727.87997	1.0	-729.69793	2.6	-727.90832	1.5	-729.72521	3.2
		error		error		error		error
		2.0		2.0		1.1		1.0

	LC-wPBE 6-311+G (2df,p)		B3P86 6-311+G (2df,p)		lc-wPBE/6-31G*		B3P86/6-31G*	
CH2O	-114.46831		-114.82500		-114.42399		-114.78111	
Me3PCHCHO	-613.54940		-615.01439		-613.41969		-614.88330	
TS1	-728.00974	5.0	-729.83184	4.7	-727.83906	2.9	-729.66067	2.3
OP1	-728.03774	-12.6	-729.85810	-11.7	-727.86890	-15.8	-729.68795	-14.8
TS2	-728.03542	-11.1	-729.85860	-12.1	-727.86364	-12.5	-729.68571	-13.4
Me3PO	-536.23006	-31.7[a]	-537.38327	-32.2[a]	-536.11747	-29.4[a]	-537.27074	-29.9[a]
acrolein	-191.83812		-192.50746		-191.77300		-192.44131	
TS1PCM[b]	-728.00950	5.1	-729.83377	3.5	-727.83812	3.5	-729.66175	1.7
betainePCM[b]	-728.01084	4.3	-729.83200	4.6	-727.83808	3.5	-729.65908	3.3
TS1.5PCM[b]	-728.01471	1.9	-729.83346	3.7	-727.84163	1.3	-729.66020	2.6
		error		error		error		error
		1.3		1.2		1.3		1.7

	M11L 6-31+G**		MN12L 6-31+G**		B3PW91 6-31+G**	
CH2O	-114.46400		-114.39678		-114.46323	
Me3PCHCHO	-613.62064		-613.37521		-613.59374	
TS1	-728.07903	3.5	-727.76624	3.6	-728.04813	5.5
OP1	-728.09466	-6.3	-727.78960	-11.1	-728.06980	-8.1
TS2	-728.09481	-6.4	-727.78782	-9.9	-728.06898	-7.5
Me3PO	-536.27158	-27.9[a]	-536.08313	-27.4[a]	-536.25598	-28.4[a]
acrolein	-191.85749		-191.73261		-191.84627	
TS1PCM[b]	-728.08121	2.2	-727.76949	1.6	-728.04918	4.9
betainePCM[b]	-728.08092	2.3	-727.76794	2.5	-728.04757	5.9
TS1.5PCM[b]	-728.08118	2.2	-727.76826	2.3	-728.04844	5.4
		error		error		error
		3.3		2.3		3.6

[a]Relative energy of Me_3PO + acrolein. [b]All energies are gas phase. The PCM only refers to the origin of the geometry used for the calculation, as described in at the beginning of the section.

KIE Predictions

For the various transition structures versus the lowest-energy conformations of **1** and **2**, conventional TST isotope effects were calculated by the method of Bigeleisen and Mayer[5] using the program QUIVER,[6] modified for easier use with Gaussian 09 and compilation on modern compilers. The conventional TST isotope effects were then corrected by a one-dimensional infinite-parabola tunneling correction.[7] The modified QUIVER program, macros that aid in running the program, and a spreadsheet that carries out the isotope effect calculations is available on request, and we have supplied this material to over 20 groups. A single scaling factor of 0.9614 in all cases. The choice of scaling factor has a negligible effect on the predicted isotope effects except for those at the carbonyl carbon of anisaldehyde, and for this carbon the choice of scaling factor within a reasonable range affected the predicted KIE by no more than 0.002.

In the table the labels ortho, meta, and para are relative to the –CHO substituent, and "ipso" refers to the aromatic carbon with the –CHO substituent.

Table S4. Complete KIE Predictions (67 °C, k_{12C}/k_{13C}).

	M06-2X 6-31G* **4‡**	M06-2X 6-31G* **6‡**	M06-2X 6-31+G** **4‡**	M06-2X 6-31+G** **6‡**	lc-wPBE 6-31+G** concerted	B3PW86 6-31+G** **4‡**	B3PW86 6-31+G** **6‡**
ylide carbon	1.019	0.996	1.022	0.994	1.024	1.020	0.998
carbonyl CHO	1.040	1.018	1.043	1.015	1.045	1.042	1.017
ipso	1.001	1.001	0.999	0.999	0.999	1.001	1.000
ortho	0.999	1.002	1.001	1.001	1.001	1.001	1.001
meta	0.998	1.001	1.000	1.000	1.000	1.000	1.001
para	1.001	1.001	1.000	1.001	1.001	1.001	1.002
meta	1.000	1.001	1.000	1.001	1.000	1.000	1.001
ortho	1.001	1.002	1.001	1.001	1.001	1.001	1.001
carbonyl of ketone	0.999	0.999	0.998	0.999	0.999	1.000	1.001
methyl on ketone	0.998	1.003	1.000	1.002	1.000	1.000	1.005
methoxy	0.998	1.002	1.000	1.000	1.000	1.000	1.002
Aldehyde oxygen (k_{16O}/k_{18O})	1.018	1.022	1.016	1.045	1.013	1.017	1.028
				1.031[a]			
				1.027[b]			

[a]Weighted by the difference in harmonic free-energies at 67 °C in M06-2X/6-31+G(2df,p)//M06-2X/6-31+G** calculations. [b]Weighted from recrossings in trajectories.

Initialization of Trajectories and Additional Details on Trajectories

An initial structure for trajectories in the presence of THF was generated by first creating an 8 x 8 x 8 box of THF molecules spaced at 5 Å. The THF molecules were then constricted to a 24 Å cubic box using a classical equilibration in PM3 calculations at 2000 K for 3 ps and employing the "box" facility in PROGDYN. (The constriction of the atoms into the box works by an algorithm that reverses the momentum of atoms moving away from the boundary of the box.) Structure **4**‡ was then placed in the middle of this box and 11 overlapping THF molecules were deleted. A series of six new trajectories were then started in PM3 calculations giving each

of the atoms a Boltzmann-random motion for 1000 K, except that the ylide carbon, aldehyde carbon, phosphorous atom, and oxygen atom of the aldehyde were fixed in their positions. These six trajectories were then equilibrated for 5 ps at 1000 K after reducing the box size to 20.4 Å, then they were slowly cooled to 340 K using the thermostat facility in PROGDYN with thermostatmult set at 0.999 (removing 0.1% of the energy per fs), and equilibration at 340 K was continued for 10 ps. The method for force calculation was then switched to ONIOM using M06-2X/6-31G* for all of the atoms of **4**‡ and using PM3 for the THF molecules, and the trajectories were continued for 1 ps.

The six trajectories were then continued and at 250 fs intervals the helper program *prodynsam* (listed in a later section) was used to create a *geoPlusVel* file for use in PROGDYN. The *progdynsam* program continues all atoms along their current trajectories, with the exception of atoms that were fixed in position. For the latter atoms, *progdynsam* gives them independent Boltzmann-random velocities based on the temperature. The resulting unconstrained trajectories were integrated forward and backward in time using direct dynamics until either **7** was formed or **1 + 2** were reformed.

The starting points for independent trajectories equilibrated in the area of **5** were taken from trajectories started from **4**‡ above as they passed through the area of **5**, selecting trajectories in which the C-C and P-O distances were 1.641 and 2.912, 1.636 and 2.921, 1.645 and 2.921, and 1.643 and 2.871. These four sets of trajectories had their ylide carbon, aldehyde carbon, phosphorous atom, and oxygen atom of the aldehyde fixed in their positions and were equilibrated for 5 ps at 340 K in PM3 calculations. The method for force calculation was then switched to the ONIOM described above, and the equilibration was continued for 2 ps. The four trajectories were then continued with the constraints on the ylide and aldehyde carbons removed, and at 250 fs intervals the helper program *prodynsam* as above was used to create a *geoPlusVel* file for use in PROGDYN. The resulting unconstrained trajectories were integrated forward and backward in time using direct dynamics until either **7** was formed or **1 + 2** were reformed.

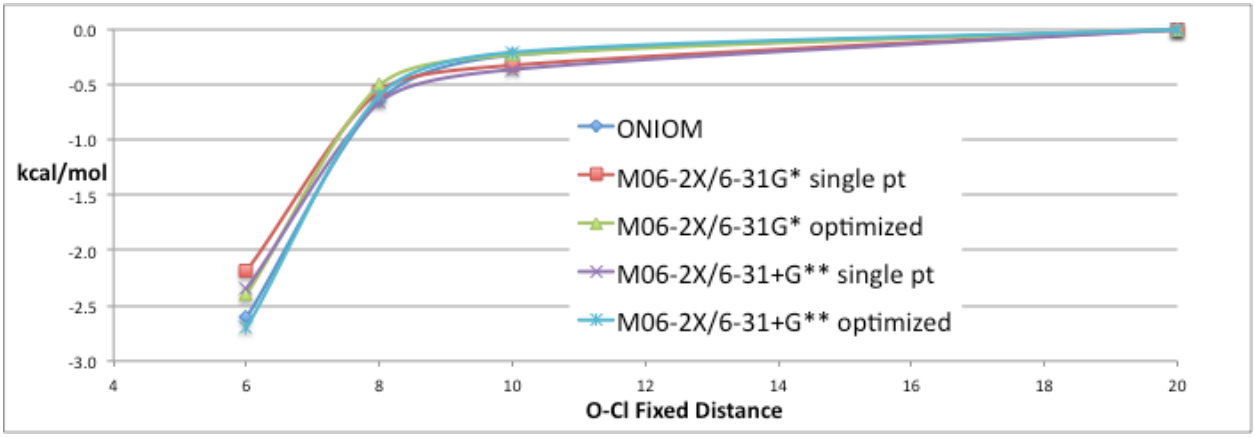
On the Choice of PM3 in ONIOM Trajectories

THF has a dipole moment of 1.63 D in the gas phase. The initial consideration of PM3 calculations for the ONIOM trajectories was based on the reasonable accuracy of the PM3 dipole moment for THF, at 1.668. For comparison, the M06-2X/6-31+G** gas phase dipole moment of THF is 1.79 D, a 10% overestimate. The PM3 THF structure is significantly flatter than that predicted by DFT methods. It was judged that this was unimportant for the purpose at hand. As is true of any semiempirical method, PM3 underestimates the polarizability of THF by about 35% (Bosque, R.; Sales, J. *J. Chem. Inf. Comput. Sci.* **2002**, *42*, 1154-1163), It should be recognized that this limitation is still much better than the use of a molecular mechanics solvent with fixed charges, which would include no polarizability.

The dipole moment of TS1 (**4**) in M06-2X/6-31+G**/PCM calculations is 8.8387. In single point calculations on this structure, PM3 finds a dipole moment of 8.36 in the gas phase and 9.73 in PCM calculations. From these values and the THF dipole moment, it was judged that PM3 should adequately reflect the dipolar stabilization of TS1 by THF solvent. By the nature of an ONIOM calculation, it is the PM3 calculation on the whole system that gives rise to the dipolar stabilization.

Other explorations of ONIOM calculations supported their ability to reflect dipolar stabilization. The graph below shows the energy of stabilization of an NaCl molecule by a THF molecule with a fixed distance between the O and Cl atoms. The ONIOM is M06-2X/6-31+G**

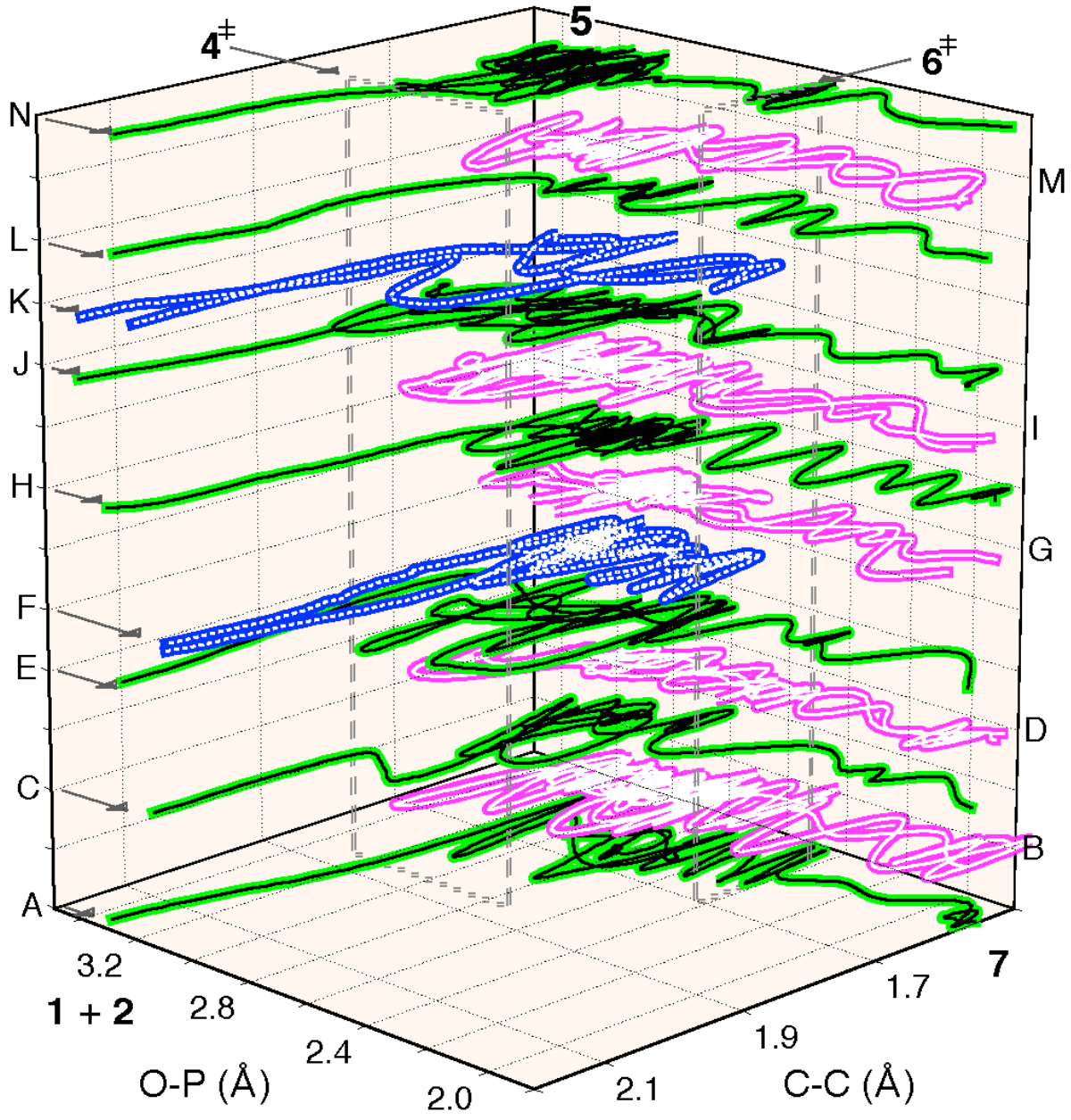
on NaCl and PM3 on the THF, with optimized geometries (except for the fixed distance). The dipolar stabilization by the ONIOM is essentially the same as the full DFT calculations in this range of distances.



Stacked Plots of Trajectory Paths for Trajectories Started from 5

Figure S1 shows selected examples of trajectory paths for trajectories started from **5** in the presence of 53 THF molecules as described above.

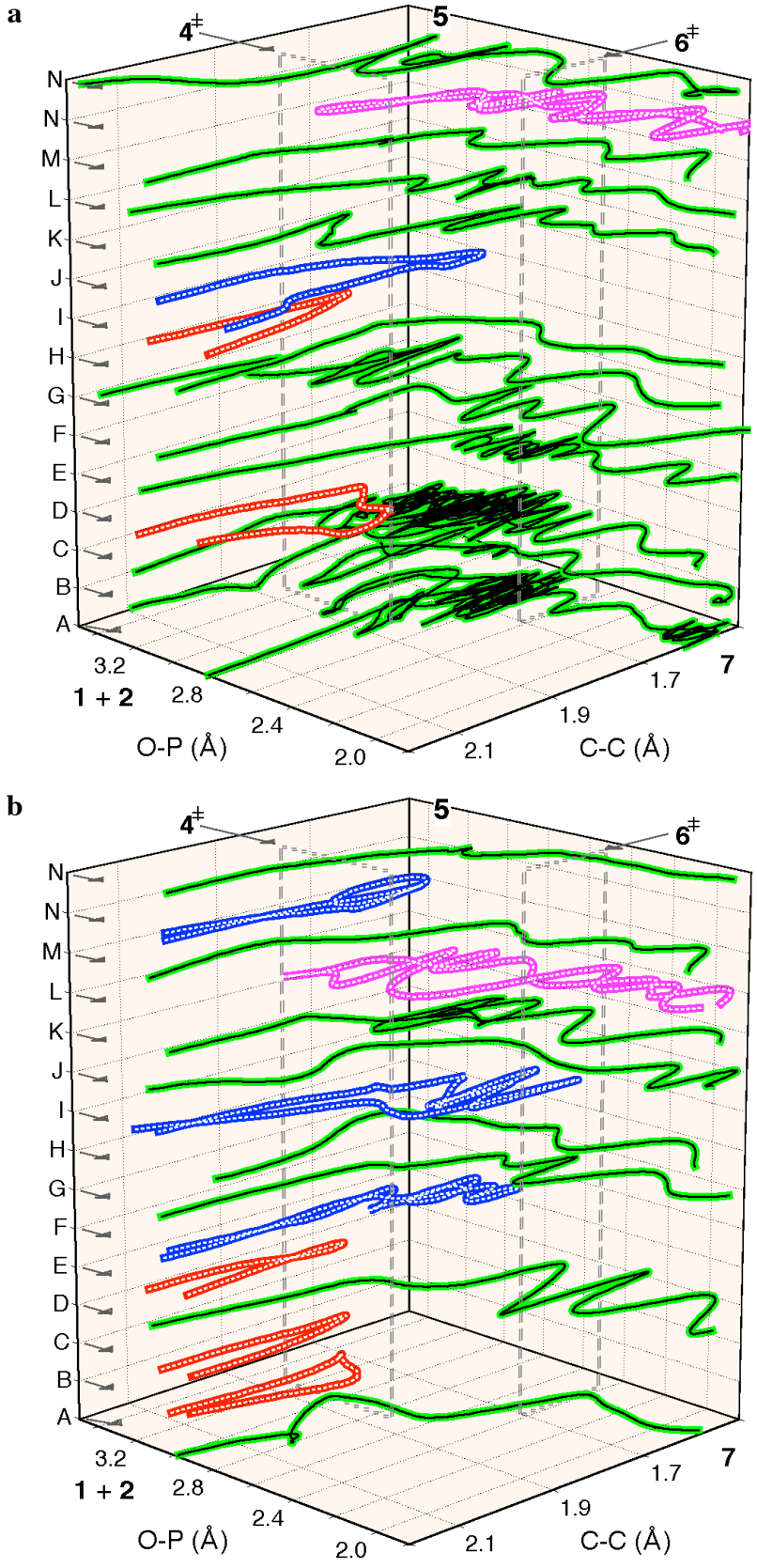
Figure S1

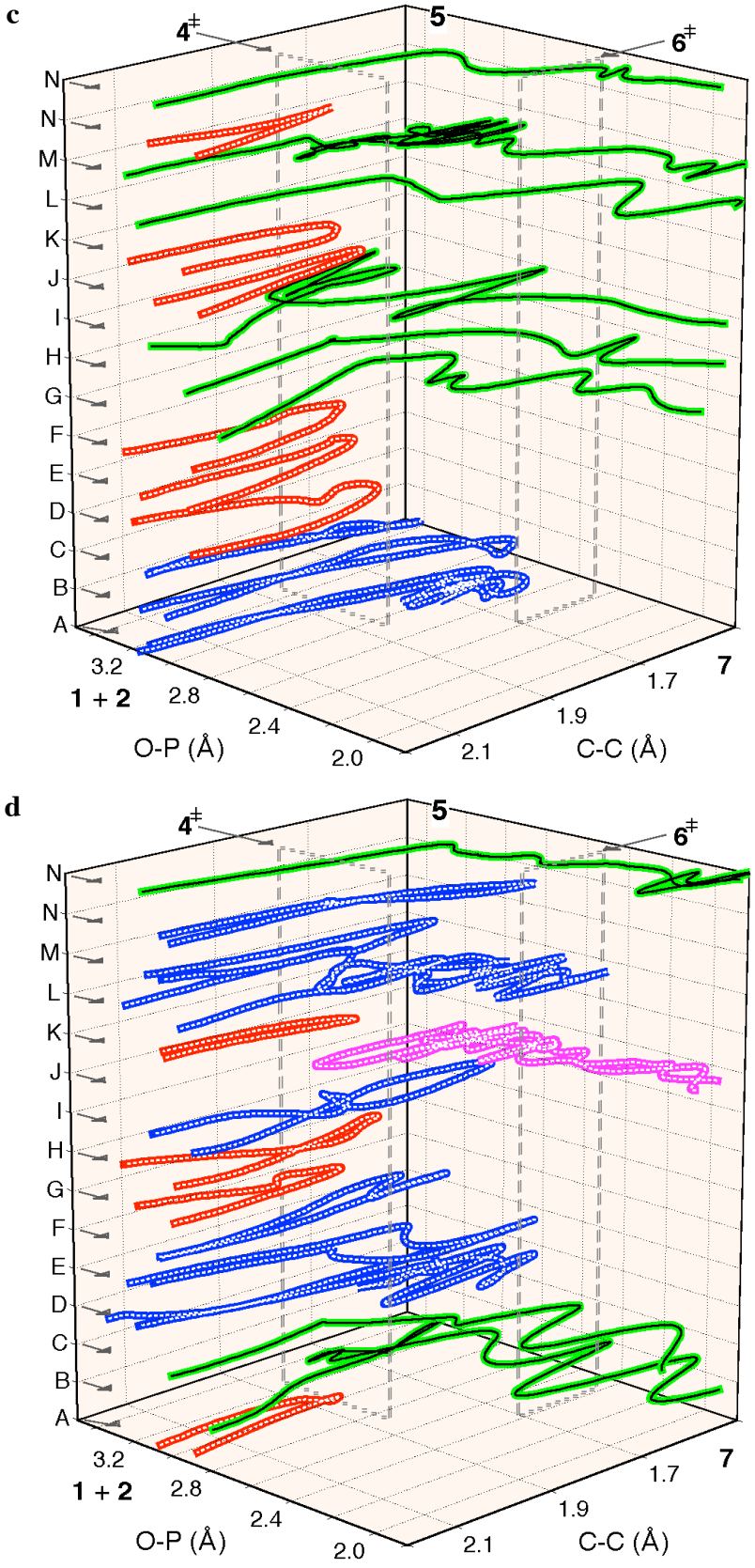


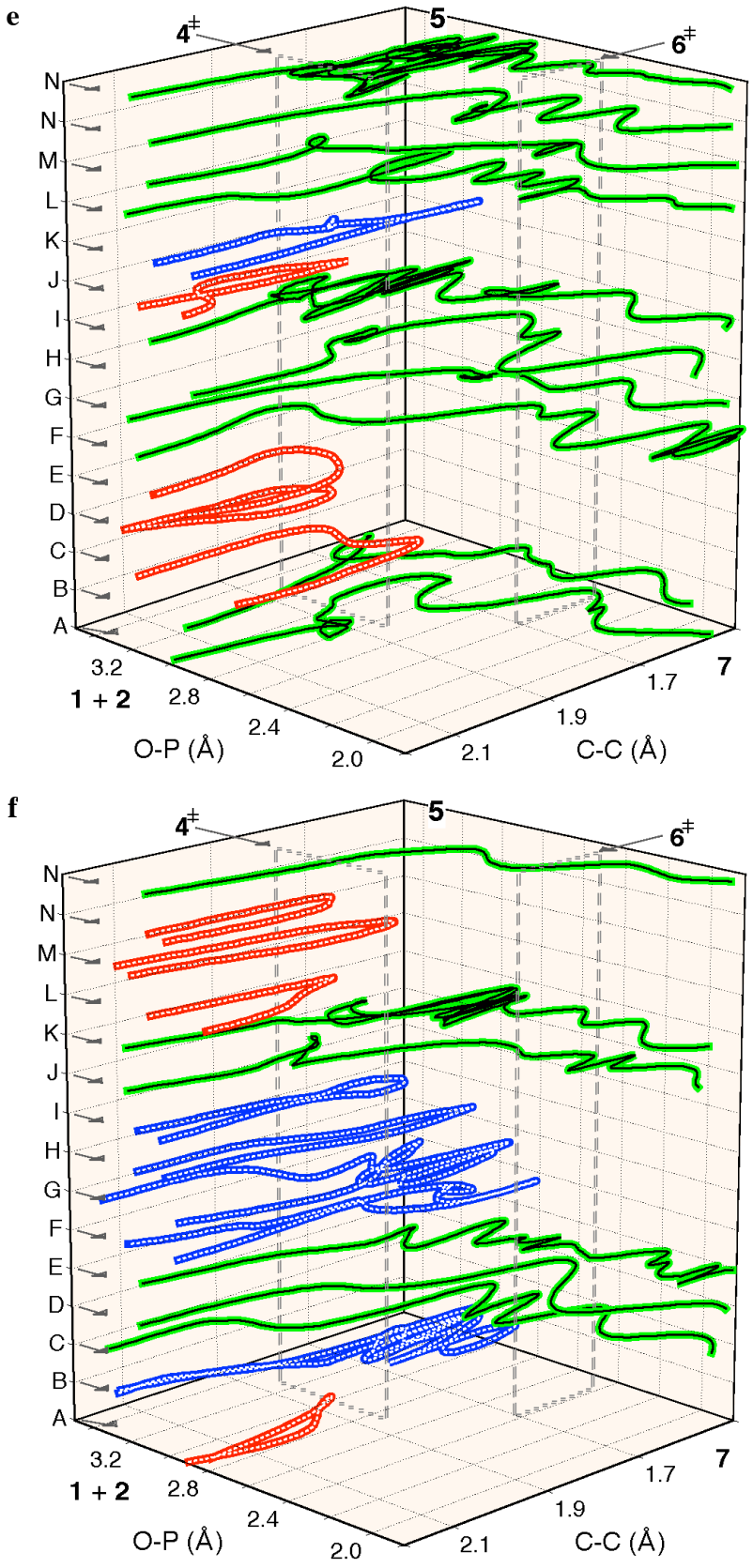
Additional Stacked Plots of Trajectory Paths

The plots below in Figure S2a-m show additional examples of trajectory paths for trajectories started from **4**‡ in the presence of 53 THF molecules as described above. No researcher-selection was involved in the choice of the trajectories below. For a few of the trajectories our program pulling out the paths failed in the middle, and these trajectories show up as incomplete paths in the plots.

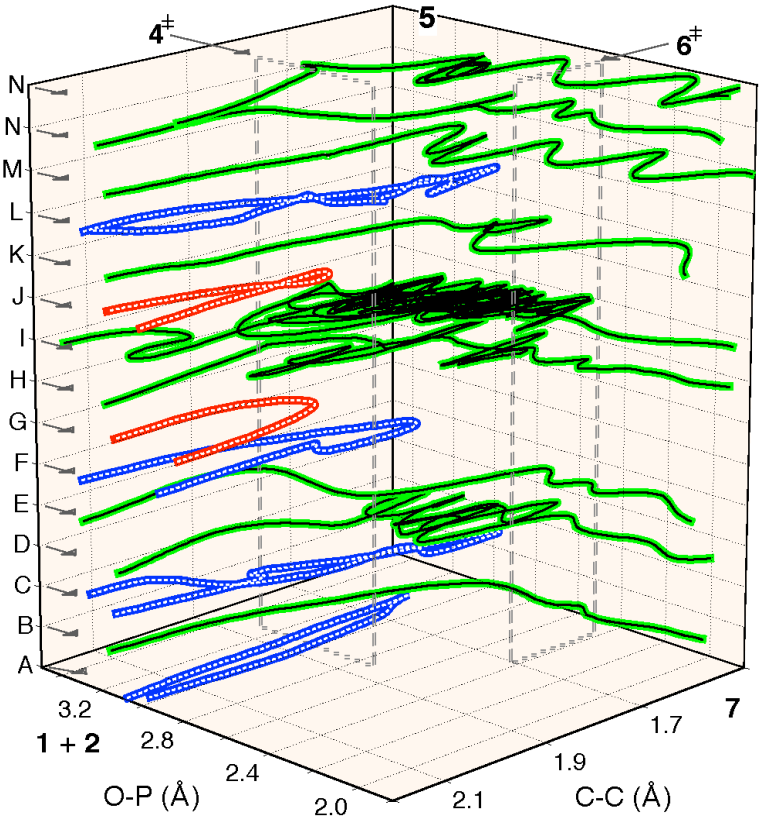
Figure S2


a
4‡
5
6‡
N
N
M
L
K
J
I
H
G
F
E
D
C
B
A
3.2
1 + 2
2.8
2.4
2.0
O-P (Å)
2.1
1.9
1.7
7
C-C (Å)
b
4‡
5
6‡
N
N
M
L
K
J
I
H
G
F
E
D
C
B
A
3.2
1 + 2
2.8
2.4
2.0
O-P (Å)
2.1
1.9
1.7
7
C-C (Å)

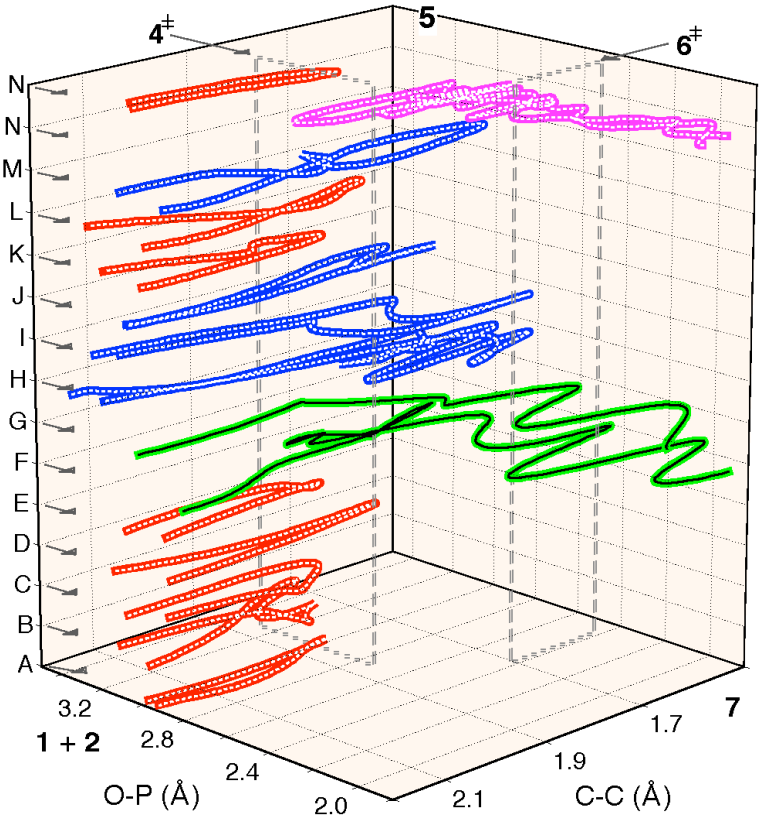

c
4‡
5
6‡
N
N
M
L
K
J
I
H
G
F
E
D
C
B
A
3.2
1 + 2
2.8
2.4
2.0
O-P (Å)
2.1
1.9
1.7
7
C-C (Å)
d
4‡
5
6‡
N
N
M
L
K
J
I
H
G
F
E
D
C
B
A
3.2
1 + 2
2.8
2.4
2.0
O-P (Å)
2.1
1.9
1.7
7
C-C (Å)


e
4‡
5
6‡
N
N
M
L
K
J
I
H
G
F
E
D
C
B
A
3.2
2.8
2.4
2.0
1 + 2
O-P (Å)
2.1
1.9
1.7
7
C-C (Å)
f
4‡
5
6‡
N
N
M
L
K
J
I
H
G
F
E
D
C
B
A
3.2
2.8
2.4
2.0
1 + 2
O-P (Å)
2.1
1.9
1.7
7
C-C (Å)

g


4‡
5
6‡
N
N
M
L
K
J
I
H
G
F
E
D
C
B
A
3.2
1 + 2
2.8
2.4
2.0
O-P (Å)
2.1
1.9
1.7
7
C-C (Å)

h


4‡
5
6‡
N
N
M
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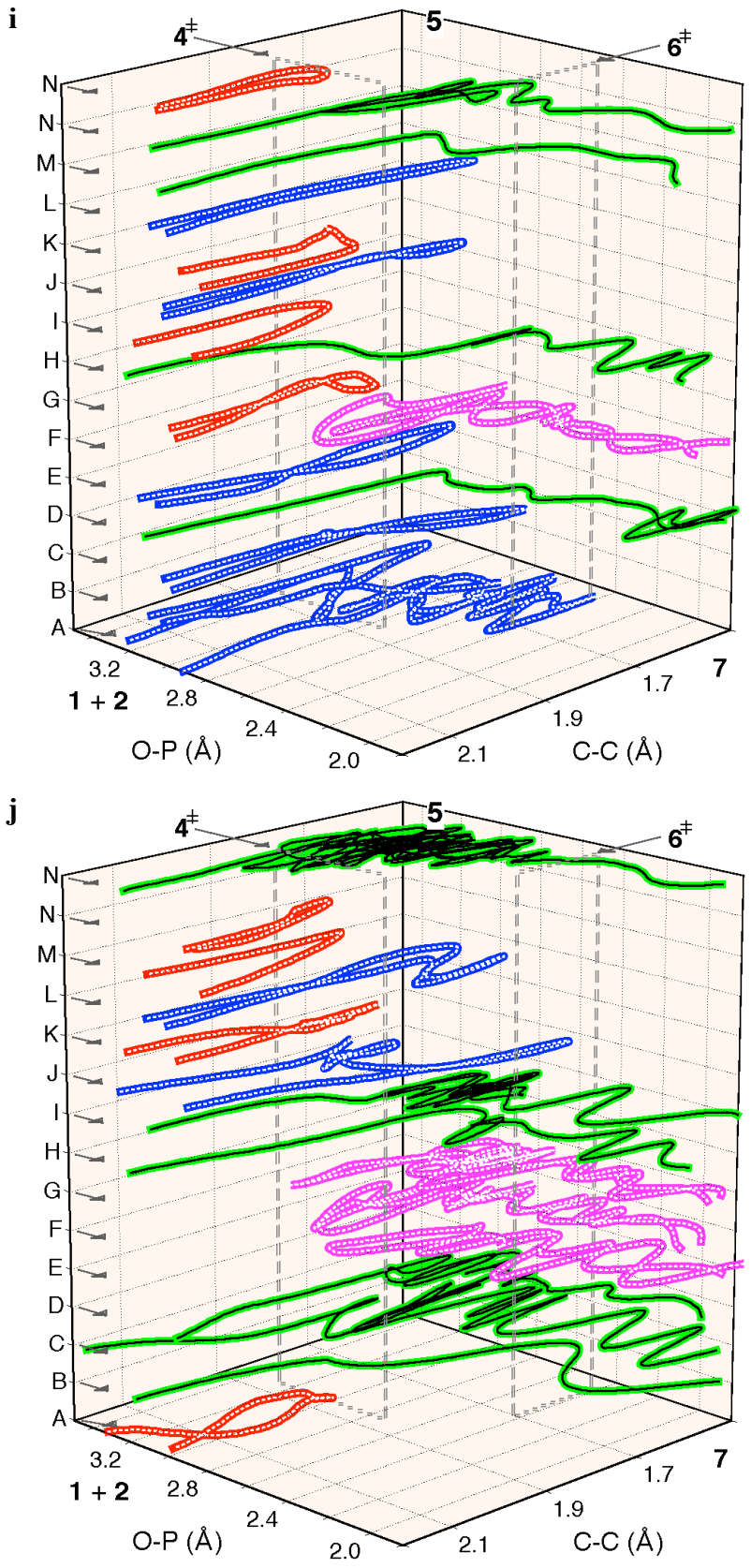
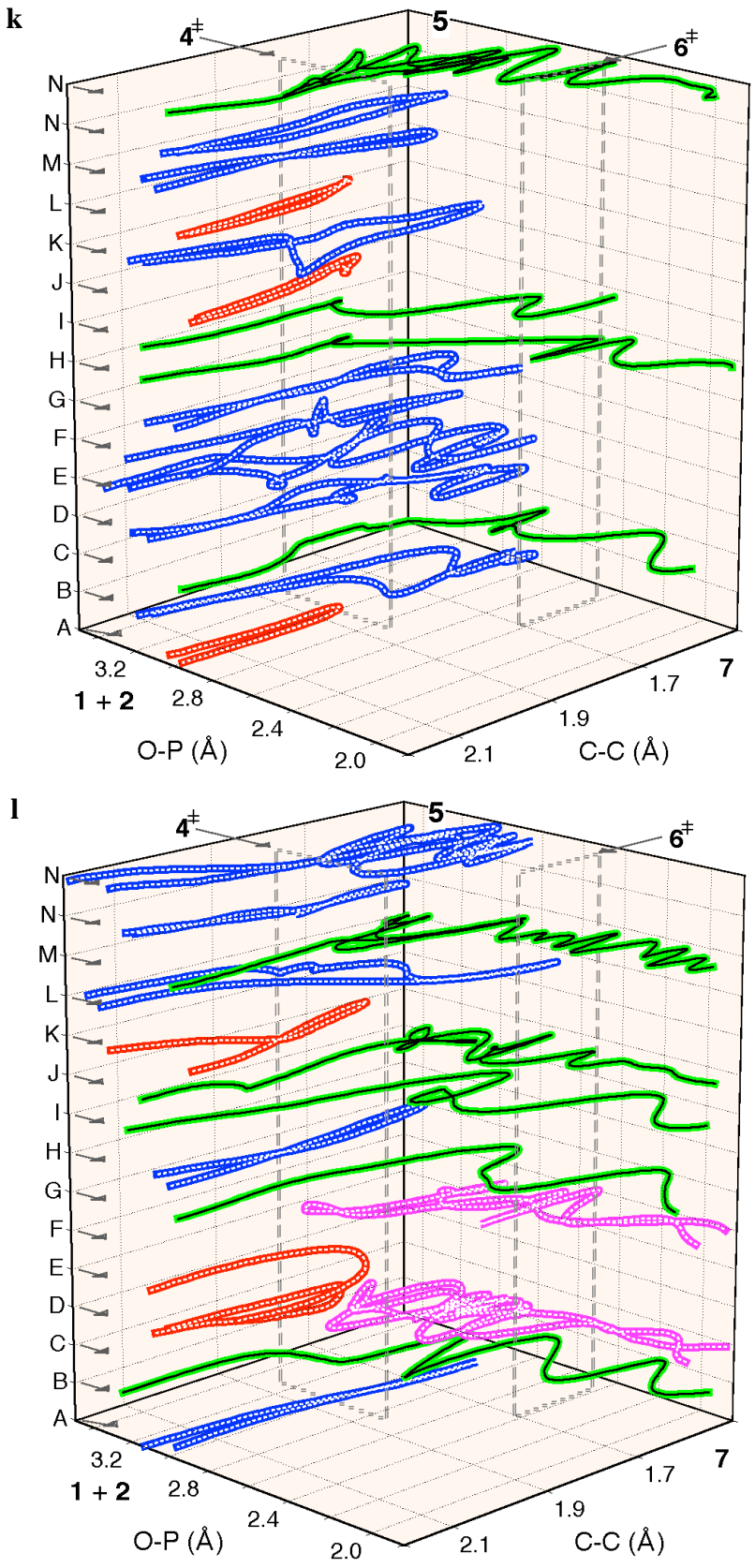
K
J
I
H
G
F
E
D
C
B
A
3.2
1 + 2
2.8
2.4
2.0
O-P (Å)
2.1
1.9
1.7
7
C-C (Å)


i
4‡
5
6‡
N
N
M
L
K
J
I
H
G
F
E
D
C
B
A
3.2
1 + 2
2.8
2.4
2.0
O-P (Å)
2.1
1.9
1.7
7
C-C (Å)
j
4‡
5
6‡
N
N
M
L
K
J
I
H
G
F
E
D
C
B
A
3.2
1 + 2
2.8
2.4
2.0
O-P (Å)
2.1
1.9
1.7
7
C-C (Å)


k
4‡
5
6‡
N
N
M
L
K
J
I
H
G
F
E
D
C
B
A
3.2
1 + 2
2.8
2.4
2.0
O-P (Å)
2.1
1.9
1.7
7
C-C (Å)
l
4‡
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6‡
N
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K
J
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F
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D
C
B
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3.2
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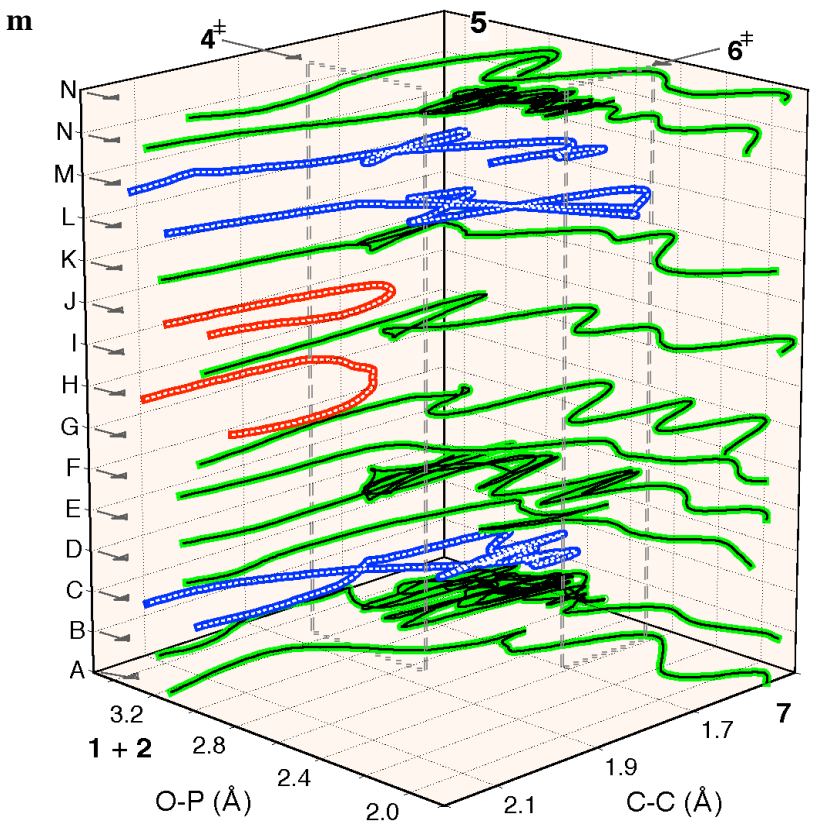
2.8
2.4
2.0
O-P (Å)
2.1
1.9
1.7
7
C-C (Å)



Bimodal Character of Trajectories Started From $4^{‡}$

Figure S3 shows a decay plot of the lifetime of trajectories between $\mathbf{4}^{‡}$ and $\mathbf{6}^{‡}$, for trajectories started from equilibrated $\mathbf{4}^{‡}$, compared with exponential decay. The exponential decay includes a lag time of 50 ps, adjusted to give a best fit of the exponential with the observed decay curve – this lag time allows for a minimal amount of time required for trajectories to pass between the two transition states. Figure S4 show an expansion of the same plot for clarity.

Passage through $\mathbf{4}^{‡}$ was defined by the first time the trajectory crosses a C-C distance of 1.89 Å (see a later section for the detailed algorithm), when the trajectories are viewed in the direction from **1** + **2** to **7**. Passage through $\mathbf{6}^{‡}$ was defined by the last time the trajectory passes through a P-O distance of 2.53 Å when viewed in the same direction. The lifetimes were defined as the time in fs between these two points, and the plots were created by ordering the lifetimes and plotting the times versus the fraction of incomplete trajectories remaining.

Figure S3

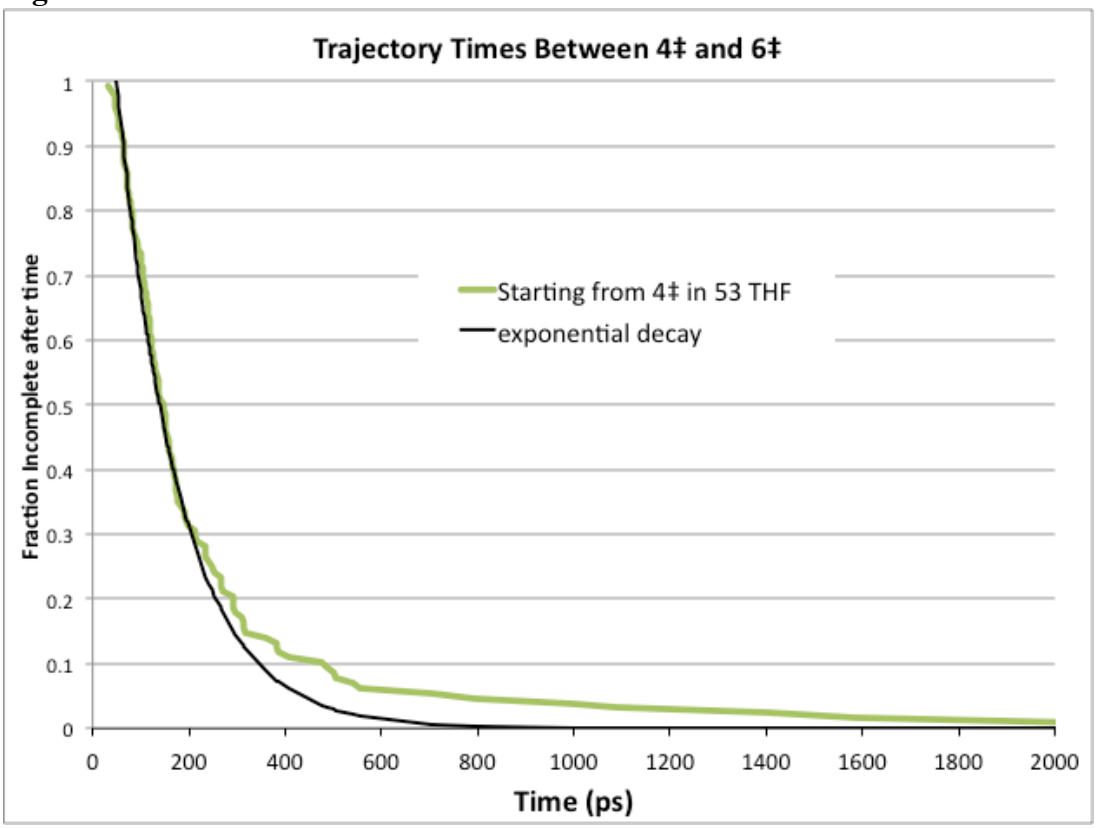
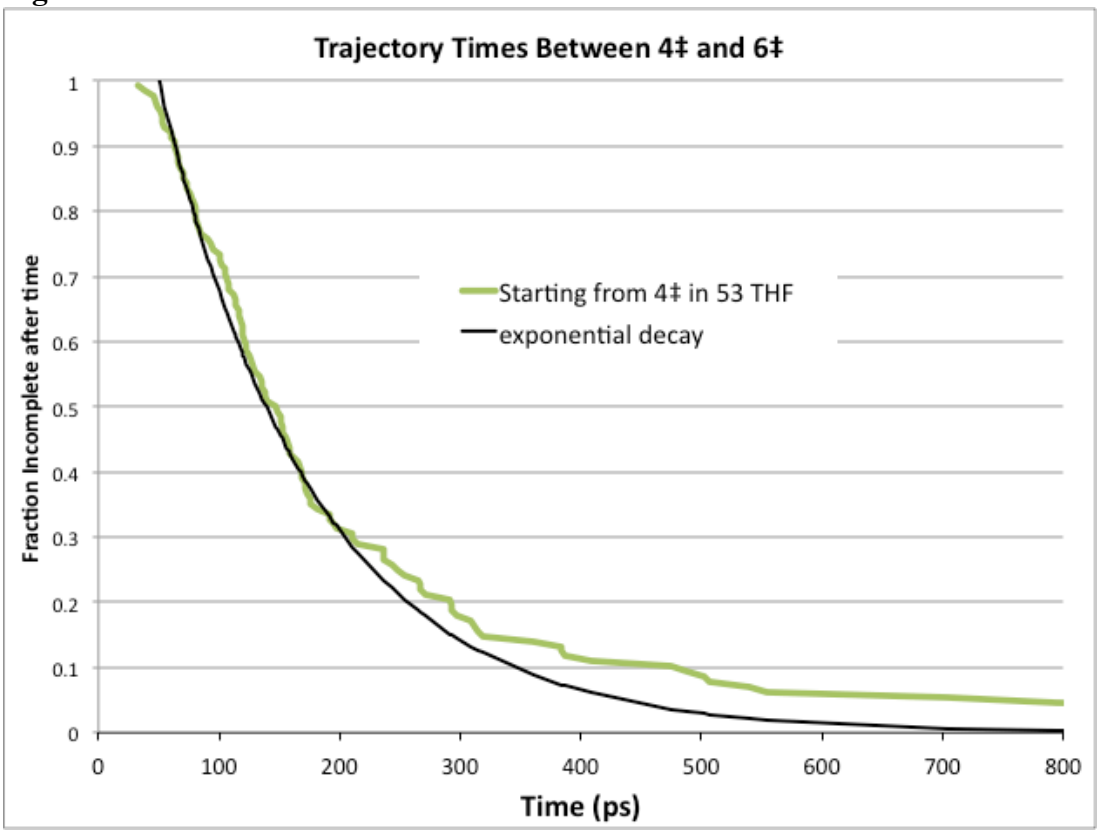


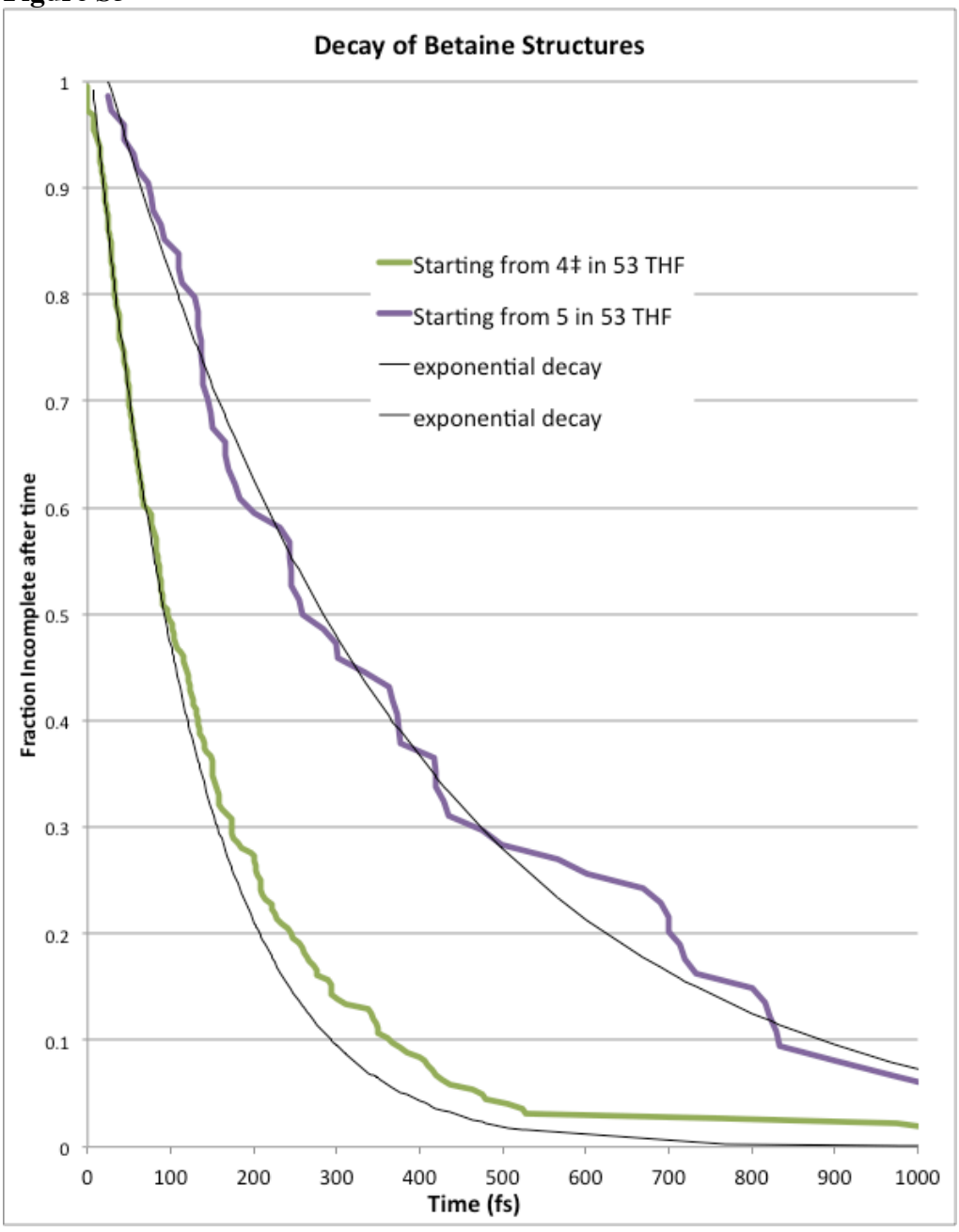
Figure S4



Betaine Lifetimes Started From 4‡ Versus Equilibrated 5

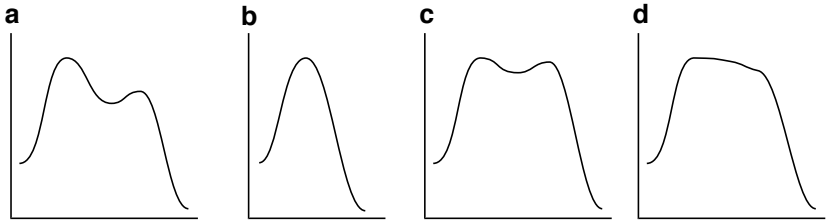
Figure S5 shows a decay plot of betaines for trajectories started from equilibrated **4**‡ versus trajectories started from equilibrated **5**, compared with exponential decay. Passage through **4**‡ was defined by the last time the trajectory crosses a C-C distance of 1.89 Å (see a later section for the detailed algorithm), when the trajectories are viewed in the direction from **5** to **1** + **2**. Passage through **6**‡ was defined by the last time the trajectory passes through a P-O distance of 2.53 Å when viewed in the direction from **5** to **7**. For trajectories started from **5**, the betaine lifetime was defined as the time between the trajectory starting point and passage through **4**‡ or **6**. For trajectories started from **4**‡, the betaine lifetime was defined as the time between the time when the C-C distance first fell below 1.65 Å and passage through **4**‡ or **6**.

Figure S5

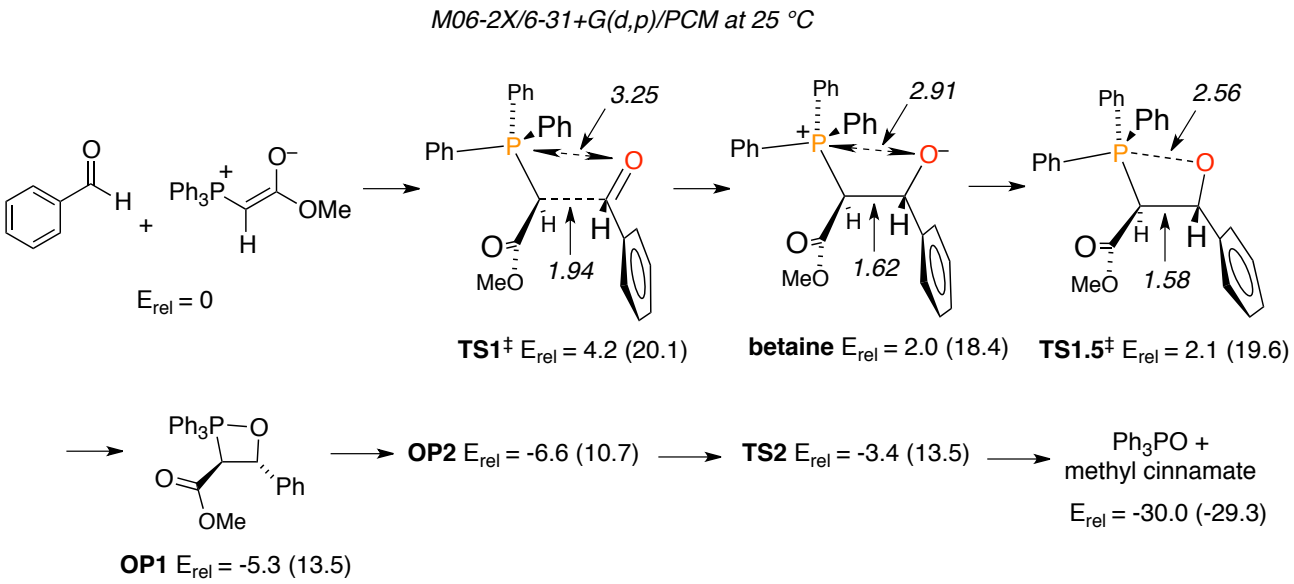


On the Choice of the Experimental System and Its Relationship to Reactions of Ph_3PCHCO_2R.

In general terms, when the reaction coordinate diagram associated with a mechanism looks like **a** below, then it is usually difficult to learn much about the second step in the mechanism. As the difference in energy between the two barriers increases, the second step becomes more hidden from experiment. For the classical question of stepwise versus concerted mechanisms, it is difficult to distinguish **a** from **b** when the barrier height difference is large. (The exception in general terms is when the intermediate has open to it two or more discernable reactions.) In more state-of-the-art considerations, the reaction in **a** may be subject to a variety of interesting dynamic effects such as non-RRKM behavior in the intermediate, but if there is only a single product then the dynamic effects may not show up in experimental observations. One might simply rely on theory, discounting any need for supportive experimental observations, but then one is subject to the non-tender mercies of computational inaccuracy. Even if the computations are right, one ends up talking about effects that make little or no experimental difference in the cases studied. So, in the determination of concerted versus stepwise mechanisms and in the search for some types of interesting dynamic effects (there are several other kinds), it is best to choose reactions that have energy surfaces resembling **c** or **d**.



Our initial exploratory studies were on the reaction of $Ph_3P{=}CHCO_2Me$ with benzaldehyde. Our preliminary experimental results placed the benzaldehyde carbonyl KIE at 25 °C at 1.038 and the ylide carbon KIE at 1.017. M06-2X/6-31+G** calculations predicted a stepwise mechanism, as shown below, and if the first step were rate limiting then the predicted KIEs would be 1.047 and 1.022. The observation of somewhat lower KIEs than predicted supported the stepwise mechanism, the idea being that the KIEs were lowered by the second step (with lower KIEs) being partially rate limiting. Preliminary trajectory studies were also suggesting some of the interesting effects described in the main text. However, we did not consider that the KIE results were sufficiently convincing about the stepwise nature of the reaction, and we also wanted a system with a higher proportion of interesting trajectories. We viewed both issues as arising from the system being more **a** above than like **c**. The second step affects the isotope effects but not enough for the level of argument desired.



The switch to the anisaldehyde / AcCH=PPh_3 was designed to flatten out the surface and make it more like **c** than **a**. This made the experimental isotope effects go further way from those expected for a concerted mechanism or one that was two step with the first step being rate limiting, making their interpretation much more definitive. It also led to a greater number of interesting trajectories. Our preliminary results above suggest that the same features observed for anisaldehyde / AcCH=PPh_3 also apply to benzaldehyde / Ph_3P=$CHCO_2Me$, but that work is not complete.

Programs for Calculations and NMR Integrations

Program Suite PROGDYN

A full listing of the subprograms of PROGDYN is given below. To allow the reader to understand or make use of PROGDYN, we describe here first the overall structure of the program.

The master control program for dynamics, in the form of a Unix Shell Script, is called *progdynstarterHP*. For a user to start to use *progdynstarterHP*, some early lines in it that assign the scratch space and the location of the program files and input files would have to be modified for the local environment. These lines are between lines 29 and 40 and should be apparent. The location of the scratch space is usually passed to *progdynstarterHP* as a parameter.

progdynstarterHP takes as necessary input files:
freqinHP - This is the standard output from a Gaussian 98, 03, or 09 frequency calculation using freq=hpmodes. For isotopically labeled compounds, use freq=(hpmodes,readisotopes).
progdyn.conf – This is a file giving a variety of configuration options, called on by many of the subprograms. progdyn.conf is listed below and contains explanations of the program options.

progdynstarterHP takes optional input the files listed below. These are not needed for basic runs.
isomernumber - A number in file isomernumber provides a start for numbering runs. The default is 1.
detour – A signal file that, by existing, signals the program to do a side calculations
nogo – A signal file that, by existing, signals the program to stop between points

bypassproggen - A signal file that, by existing, signals the program to use a supplied input file *geoPlusVel* instead of generating one for itself. This pathway for initialization is important here because it is used when the program progdynsam, described later, is used to generate the geoPlusVel file.
methodfile – A file that contains lines to be added to the end of each g09.com input file, such as lines that call for an NMR calculation
ZMAT – An input file for the CFOUR (http://www.cfour.de) suite of programs. When ZMAT is supplied, *progdynstarterHP* will automatically run call CFOUR (which must be set up independently by the user) by making use of the script *progcfour*.
cannontraj – A file containing a vector for each atom, used to fire an initial geometry in a particular direction.

progdynstarterHP calls the following programs:
proggenHP - An awk program that starts a trajectory, giving each mode its zero point energy (if a quasiclassical calculation) plus random additional excitations depending on the temperature.
prog1stpoint – Awk program that creates the first Gaussian input file for each run
prog2ndpoint – Awk program that creates the second Gaussian input file for each run. prog2ndpoint also checks the energy of the first point to see if it fits with the desired energy, and aborts the run if it does not by creating appropriate output in file Echeck
progdynb – Creates subsequent Gaussian input files until run is completed, used the awk
proganal – A program to analyze the latest point and see if a run is done. This program must be redone for each new system. Elaborate changes are sometimes programmed into proganal, such as the automatic changing of configuration variables. proganal creates the output to dynfollowfile and NMRlist or NMRlistdis
randgen – A program that generates random numbers between 0 and 1. These are generated all at once and stored in a file for use by proggenHP.
progcfour – A control script to run CFOUR calculations (not needed for most kinds of runs).

progdynstarterHP has the following output files:
isomernumber – A running tab of the trajectory number
runpointnumber – a running tab of the point in the trajectory
Echeck – output form where prog2ndpoint checks the energy of the trajectory to see if it fits with the desired energy
geoRecord – A record of all of the geoPlusVel files.
geoPlusVel – Created by proggen, this gives the starting positions, velocities, isotopic masses, excitations of the normal modes, and initial displacements of the normal modes for current run.
g09.com – Created by prog1stpoint, prog2ndpoint, and progdynb, this is the latest input file for Gaussian09 for current run and latest point.
olddynrun and *olderdynrun* – files containing the last two outputs from Gaussian, for creation of the next point
traj, traj1, traj2, traj3, etc. – files containing the geometries and energies for each trajectory, numbered by the isomernumber, in a format suitable for reading by Molden.
dyn - A record of the Gaussian outputs.
dynfollowfile – A short record of the runs and their results. The data desired for *dynfollowfile* must be programed into the script *proganal* as needed for each system studied.
NMRlist or *NMRlistdis* – output of NMR predictions at each point in a trajectory
skipstart - A signal file that, by existing, tells progdynstarterHP that we are in the middle of a run. For trajectories that are propagated forward and backward in time, skipstart keeps track of whether one is in the forward or reverse part.
diagnostics – optional output that follows which subprograms are running and configuration variables, decided by variable in progdyn.conf
vellist – optional output that lists the velocities of each atom, decided by variable in progdyn.conf, or lists the total kinetic energy in the system and the classical temperature.
A number of files starting with *'temp'* are created then later erased.

The following helper programs were used for the current study.
progdynsam – an awk program that generates a geoPlusVel file based on input from a *traj* file. Typically, the traj file is a trajectory performed with constraints, and the new geoPlusVel will be started without constraints. *progdynsam* must be modified for the desired temperature, and it takes as input the variable pt to decide which points in the traj file are used to define the geoPlusVel. For previously constrained atoms, *progdynsam* gives the atoms a Boltzmann-random velocity and direction of motion appropriate for the desired temperature. The program is invoked with awk –v pt=## –f progdynsam traj where ## is the trajectory point used to start a new geoPlusVel, and traj is the output file from above containing the list of trajectory points.
progtrajlength – an awk program used to analyze the output data in *dynfollowfile*. It is involked with awk –f progtrajlength dynfollowfile where dynfollowfile is a list of one or more of the dynfollowfile output files described above.

Program progdynstarterHP

```
#!/bin/bash
#progdynstarterHP, made to use high-precision modes from Gaussian output with freq=hpmodes
#updated to create a random number file temp811 that is used by proggenHP
#version September 16, 2005, made for workstations
#version August 2007 to allow periodic copying of g09.log to dyn putting it under control of progdynb
#version Feb 2008 moves variables like the scratch directory and location of randgen to the beginning
#version March 2008 added proganal reporting to points 1 and 2
#version Jan 2009 fixed bug generator of having proganal run twice in checking for complete runs
#version May 2009 Echeck catches bad energies after only one point, other lines written simpler, triple while loop, revised comments
#version Aug 2010 isomernumber adds words to ease parsing, increased elements up to bromine, runpointnumber checked for more appropriate restarts
#version Aug 2011 runpointnumber starts better, restart better if died during first few points, awk bug fix
#version Aug 2012 freqinHP reads with only 3 freqs, goingwell and other temp files moved to $scratchdir
#version Aug 2013 adds ability to automatically run a CFOUR program if the file ZMAT exists
#
#version Nov 2013 adds ability to bypass generation of geoPlusVel using the signal file bypassproggen
#LIMITATIONS - standard version only handles elements up to bromine, must change program to do higher atomic numbers
#   only handles up to 4000th excited state for modes - this could start to affect the initialization of classical modes or transition vectors at
#    extremely high temperatures
#   The routine that checks whether the actual energy approximately equals the desired energy checks for lines containing "SCF Done" or "EUMP2 =" or " Energy="
#   This should handle ordinary calculations HF, DFT, ONIOM, and MP2 calculatons but the routine in prog2ndpoint would have to be changed for other calcs.
#
#                                   OUTLINE
# A. initilize to perform Gaussian jobs and know where we are
#    start loop
# B. if no file named "skipstart" then generate a new isomer.  Instructions: Get rid of skipstart to start new isomer.
#    the B loop generates geoPlusVel, adds it to geoRecord, generates and runs first and second points, and sets up for continuous loop
# C. loop over propagation steps
#
#  AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
#origdir, randdir, scratchdir, g09root, logfile all may need varied from system to system and assigned here or by program calling this one
export LC_ALL=C
echo $1
scratchdir=$1
export g09root=/apps/lms/g09_B01_XEON
. $g09root/g09/bsd/g09.profile
origdir=`pwd`
cd $origdir
logfile=docslog
randdir=~/bin
cp /fdata/scratch/d-singleton/binall700/* /tmp/$PBS_JOBID
cp /fdata/scratch/d-singleton/binall700/GENBAS $scratchdir
cp /fdata/scratch/d-singleton/binall700/progcfour $scratchdir
proggramdir=/tmp/$PBS_JOBID
freqfile=/fdata/scratch/d-singleton/binall700/freqinHP
echo ORIGDIR:
echo $origdir
echo SCRATCHDIR:
echo $scratchdir
ls $scratchdir
echo PROGGRAMDIR:
echo $proggramdir
ls $proggramdir

rm -f nogo    # assume that if someone is starting a job, they want it to go.
rm -f diagnostics goingwell tempdone # diagnostics contains extra info from previous runs, other two files are from older versions of progdyn

#### Triple 'while' loop - will have to break multiple times to get out, but advantage is ability to control starting over
while (true)
do

# As long as there is a file "goingwell" the program will not exit entirely by itself
```

```
rm -f $scratchdir/goingwell
while (true)
do
#  BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB
  if (test -f skipstart) then
    echo "skipping start and continuing from previous runs"
  else
#  B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1 generate geoPlusVel and first input file
    if [ `cat runpointnumber` = "1" ]; then
      echo "X did not complete first point so new isomer started" >> dynfollowfile
    fi
    if [ `cat runpointnumber` = "2" ]; then
      echo "X did not complete second point so new isomer started" >> dynfollowfile
    fi
    if [ `cat runpointnumber` = "3" ]; then
      echo "X did not complete third point so new isomer started" >> dynfollowfile
    fi
    cd $origdir
    if (test -f bypassproggen) then
      echo "taking starting conditions from pre-generated geoPlusVel"
    else
      $randdir/randgen > temp811
# the next 8 lines would have to be changed to use low-precision modes
      awk '/        1         2/,/Harmonic frequencies/ {print}' $freqfile > temp401
      awk '/Frequencies --/ {print $3;print $4;print $5;print $6;print $7}' temp401 > tempfreqs
      awk '/Reduced masses/ {print $4;print $5;print $6;print $7;print $8}' temp401 > tempredmass
      awk '/Force constants/ {print $4;print $5;print $6;print $7;print $8}' temp401 > tempfrc
      awk '/0/ && ((length($1) < 2) && ($1 < 4)) {print}' temp401 > tempmodes
      awk '/has atomic number/ {print}' $freqfile > tempmasses
      awk '/Standard orientation:/,/tional const/ {if ($3==0) print}' $freqfile > tempstangeos
      awk '/Input orientation:/,/Stoichiometry/ {if ($3==0) print}' $freqfile > tempinputgeos
      awk -f $proggramdir/proggenHP $freqfile > geoPlusVel
    fi
    if (test -f isomernumber) then
      cp isomernumber temp533
      awk 'BEGIN {getline;i=$1+1;print i,"----trajectory isomer number----"}' temp533 > isomernumber
      rm temp533
    else
      echo "1 ----trajectory isomer number----" > isomernumber
    fi
    echo 1 > runpointnumber
    rm g09.com
    awk -f $proggramdir/prog1stpoint isomernumber > g09.com
#  B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2  if first part successfule then
clean up and run the first input file, otherwise die
    if (test -s g09.com) then
      rm tempfreqs tempredmass tempfrc tempmodes tempstangeos tempmasses temp401 temp811 tempinputgeos
      cat isomernumber >> geoRecord
      cat geoPlusVel >> geoRecord
      rm -f $scratchdir/goingwell
      cd $scratchdir
      cp $origdir/g09.com $scratchdir/g09.com
      $g09root/g09/g09 $scratchdir/g09.com > $scratchdir/g09.log
      cd $origdir
      grep 'Normal termination' $scratchdir/g09.log > $scratchdir/goingwell
      if (test -s $scratchdir/goingwell) then
        cat $scratchdir/g09.log >> dyn
        cp $scratchdir/g09.log olderdynrun
      else
        cp $scratchdir/g09.log $origdir/g09.log
        break
      fi
    else
      break
    fi
#  B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3 if B2 worked then you are here.
create 2nd point, run it, and set up for propagation loop
    rm g09.com
    echo 2 > runpointnumber
    awk -f $proggramdir/prog2ndpoint $scratchdir/g09.log > g09.com
# before we decide to run this, check the energy
    awk -f $proggramdir/proganal $scratchdir/g09.log >> dynfollowfile
```

```
    rm -f $scratchdir/tempdone
    tail -1 dynfollowfile | awk '/XXXX/ {print}' > $scratchdir/tempdone
    if (test  -s $scratchdir/tempdone) then
      rm -f dyn
      rm -f traj
      echo 0 > runpointnumber
      break
    fi
    if (test -s g09.com) then
      rm -f $scratchdir/goingwell
      cd $scratchdir
      cp $origdir/g09.com $scratchdir/g09.com
      $g09root/g09/g09 $scratchdir/g09.com > $scratchdir/g09.log
      cd $origdir
      grep 'Normal termination' $scratchdir/g09.log > $scratchdir/goingwell
      if (test -s $scratchdir/goingwell) then
        cp $scratchdir/g09.log olddynrun
        cat $scratchdir/g09.log >> dyn
        awk -f $proggramdir/proganal $scratchdir/g09.log >> dynfollowfile
        awk '/Input orientation/,/Distance matrix/ {print}' olddynrun | awk '/   0   / {print}' > old
        awk '/Input orientation/,/Distance matrix/ {print}' olderdynrun | awk '/   0   / {print}' > older
        echo 3 > runpointnumber
        awk -f $proggramdir/progdynb olddynrun > g09.com
        rm -f old older
      else
        cp $scratchdir/g09.log $origdir/g09.log
        break
      fi
    else
      break
    fi
# we've just completed a start, so lets skipstart until instructed otherwise
    echo "forward" > skipstart
  fi
# Reverse trajectories starter routine
  if [ `cat skipstart` = "reverserestart" ]; then
    cd $origdir
    rm g09.com
    echo 1 > runpointnumber
    awk -f $proggramdir/prog1stpoint isomernumber > g09.com
    if (test -s g09.com) then
      rm -f $scratchdir/goingwell
      cd $scratchdir
      cp $origdir/g09.com $scratchdir/g09.com
      $g09root/g09/g09 $scratchdir/g09.com > $scratchdir/g09.log
      cd $origdir
      grep 'Normal termination' $scratchdir/g09.log > $scratchdir/goingwell
      if (test -s $scratchdir/goingwell) then
        cp $scratchdir/g09.log olderdynrun
      else
        cp $scratchdir/g09.log $origdir/g09.log
        break
      fi
    else
      break
    fi
    rm g09.com
    echo 2 > runpointnumber
    awk -f $proggramdir/prog2ndpoint $scratchdir/g09.log > g09.com
    awk -f $proggramdir/proganal $scratchdir/g09.log >> dynfollowfile
    rm -f $scratchdir/tempdone
    if (test -s g09.com) then
      rm -f $scratchdir/goingwell
      cd $scratchdir
      cp $origdir/g09.com $scratchdir/g09.com
      $g09root/g09/g09 $scratchdir/g09.com > $scratchdir/g09.log
      cd $origdir
      grep 'Normal termination' $scratchdir/g09.log > $scratchdir/goingwell
      if (test -s $scratchdir/goingwell) then
        cp $scratchdir/g09.log olddynrun
        cat $scratchdir/g09.log >> dyn
        awk -f $proggramdir/proganal $scratchdir/g09.log >> dynfollowfile
```

```
        awk '/Input orientation/,/Distance matrix/ {print}' olddynrun | awk '/   0   / {print}' > old
        awk '/Input orientation/,/Distance matrix/ {print}' olderdynrun | awk '/   0   / {print}' > older
        echo 3 > runpointnumber
        awk -f $proggramdir/progdynb olddynrun > g09.com
        rm -f old older
      else
        cp $scratchdir/g09.log $origdir/g09.log
        break
      fi
    else
      break
    fi
# we've just completed a reversestart, so lets skipstart until instructed otherwise
    echo "reverse" > skipstart
  fi

#  END_of_B___END_of_B___END_of_B___END_of_B___END_of_B___END_of_B___END_of_B___END_of_B___

#  CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC  propagation loop
  while (true)
  do
#increment runpointnumber
    cp runpointnumber $scratchdir/temp533
    awk 'BEGIN {getline;i=$1+1;print i}' $scratchdir/temp533 > runpointnumber
    rm $scratchdir/temp533
    rm -f $scratchdir/goingwell
    cd $scratchdir
    cp $origdir/g09.com $scratchdir/g09.com
    $g09root/g09/g09 $scratchdir/g09.com > $scratchdir/g09.log
    cd $origdir
    grep 'Normal termination' $scratchdir/g09.log > $scratchdir/goingwell
    if (test -s $scratchdir/goingwell) then
      awk -f $proggramdir/proganal $scratchdir/g09.log >> $origdir/dynfollowfile
      mv olddynrun olderdynrun
      awk '/Input orientation/,/Distance matrix/ {print}' $scratchdir/g09.log | awk '/   0   / {print}' > old
      cp $scratchdir/g09.log olddynrun
      awk '/Input orientation/,/Distance matrix/ {print}' olderdynrun | awk '/   0   / {print}' > older
      awk -f $proggramdir/progdynb $scratchdir/g09.log > g09.com
      rm -f old older
    else
      cp $scratchdir/g09.log $origdir/g09.log
      break
    fi
# kludge to do a side calculation of NMR using progcfour.  If ZMAT is there then it gets ran and renamed.
# creation of ZMAT is under the control of progdynb, which is controlled by keyword NMRcc in progdyn.conf
# decisions to be made: erase ZMAT at beginning?  what to do if cfour calc dies?
    if (test  -f ZMAT) then
      cp ZMAT $scratchdir
      cd $scratchdir
      $scratchdir/progcfour $origdir $scratchdir
      cd $origdir
      mv ZMAT temp.ZMAT
      echo "generic one two three" `cat runpointnumber` "runisomer" `cat isomernumber` >> NMRlistcc
      awk '/Nuclear Magnetic Resonance/,/HF-SCF/ {if ($2=="C") print $1,$2,"Isotropic =",$3; if ($2=="H") print
$1,$2,"Isotropic =",$3}' x.log >> NMRlistcc
    fi

# here is a cool link that lets you interupt the dynamics with a short job, then
# it automatically goes back to the dynamics  just make the file 'detour' and it
# will delete detour, run run.com, then go back to dynamics
    if (test  -f detour) then
      rm detour
      date >> $logfile
      cat run.com >> $logfile
      cp run.log temp.log
      cd $scratchdir
      $g09root/g09/g09 $origdir/run.com > $origdir/run.log
      cd $origdir
    fi

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

```
      break
    fi

#figure out if this isomer is done - change in april 2013 is to move proganal call up from here
    rm -f $scratchdir/tempdone
    tail -2 dynfollowfile | awk '/XXXX/ {print}' > $scratchdir/tempdone
    if (test  -s $scratchdir/tempdone) then
      if [ `awk '/reversetraj/ {if ($1=="reversetraj") print $2}' progdyn.conf` = "true" ]; then
        if [ `cat skipstart` = "reverse" ]; then
          rm -f skipstart
          rm -f geoPlusVel
          rm -f olddynrun
          rm -f olderdynrun
          a=`awk '{print $1}' isomernumber`
          mv traj traj$a
          mv dyn dyn$a
        fi
        if [ `cat skipstart` = "forward" ]; then
          echo reverserestart > skipstart
        fi
      else
        rm -f skipstart
        rm -f geoPlusVel
        rm -f olddynrun
        rm -f olderdynrun
        a=`awk '{print $1}' isomernumber`
        mv traj traj$a
        mv dyn dyn$a
      fi
      break
    fi
  done
#
END_of_C_Loop____END_of_C_Loop____END_of_C_Loop____END_of_C_Loop____END_of_C_Loop____END_of_C_L
oop____

# We've got to break a second time to get out of this loop
# if we really want to quit.  Otherwise, it will start over
# at the top
  if (test  -f nogo) then
    break
  fi
  if (test  -s $scratchdir/goingwell) then
    echo "starting a new point or a new direction"
  else
    break
  fi
done

  if (test  -f nogo) then
    break
  fi
  if (test  -s $scratchdir/goingwell) then
    echo "starting a new point or a new direction2"
  else
    break
  fi
done
exit 0
```

Program proggenHP

```
BEGIN {
# aug 2013 summary of changes
#includes molecular rotation, ability to do multiple NMR calculations, ONIOM with link atoms,
#nonstandard routes, handling of linear molecules using geometry linear, fixed but with atoms over 99 but
#bug varies with version of Gaussian, randomization based on PROCINFO (solved many problems), added initialDiss 3 for
random
#phase of normal modes
# Aug 2010 changes classicalSpacing to 2 and upped possible excited states to 4000
# Jan 2009 - a number of little changes to improve reporting, precision, etc, specification of displacement on particular modes
```

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

# default parameters, including quassiclassical, no displacements, transition state, not a DRP
# do not change these - rather, change progdyn.conf to set the parameters
initialDis=0; timestep=1E-15; scaling=1.0; temp=298.15
classical=0; numimag=1; DRP=0; cannonball=0
charge=0; multiplicity=1; method="HF/3-21G"; memory=20000000
diag=1; checkpoint="g09.chk"; searchdir="positive"; boxon=0
boxsize=10; maxAtomMove=0.1; title1="you"; title2="need"
title3="a"; title4="progdyn.conf"; processors=1; highlevel=999
conver1=4.184E26 #dividing by this converts amu angs^2 /s^2 to kcal/mol
geometry="nonlinear";rotationmode=0

#initialization and constants
for (i=1;i<=10000;i++) {disMode[i]=-1}
i=1;j=1;k=1
c=29979245800; h=6.626075E-34; avNum=6.0221415E23
RgasK=0.00198588; RgasJ=8.31447
numAtoms=0; atomnumber=0; classicalSpacing=2
zpeGauss=0; zpeGaussK=0; zpePlusE=0; potentialE=0

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="initialdis") initialDis=$2
  if ($1=="timestep") timestep=$2
  if ($1=="scaling") scaling=$2
  if ($1=="temperature") temp=$2
  if ($1=="searchdir") searchdir=$2
  if ($1=="classical") classical=$2
  if ($1=="numimag") numimag=$2
  if ($1=="geometry") geometry=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="boxon") boxon=$2
  if ($1=="boxsize") boxsize=$2
  if ($1=="DRP") DRP=$2; if (DRP==1) classical=2 #this lets one start a DRP from a point that is not a freq calc
  if ($1=="maxAtomMove") maxAtomMove=$2
  if ($1=="cannonball") cannonball=$2
  if ($1=="displacements") disMode[$2]=$3
  if ($1=="controlphase") controlPhase[$2]=$3
  if ($1=="rotationmode") rotationmode=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }

if (diag>=1) print "***************** starting proggen *****************" >> "diagnostics"
if (diag>=1) print "method,charge,multiplicity,memory" >> "diagnostics"
```

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

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

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

# put in atomic symbols and atomic weights - assigns a default mass but then reads it from tempmasses when possible
for (i=1;i<=numAtoms;i++) {
  getline < "tempmasses"
  if (atNum[i]==1) {atSym[i]="H";atWeight[i]=1.00783}
  if (atNum[i]==2) {atSym[i]="He";atWeight[i]=4.0026}
  if (atNum[i]==3) {atSym[i]="Li";atWeight[i]=6.941}
  if (atNum[i]==4) {atSym[i]="Be";atWeight[i]=9.012}
  if (atNum[i]==5) {atSym[i]="B";atWeight[i]=10.811}
  if (atNum[i]==6) {atSym[i]="C";atWeight[i]=12.}
  if (atNum[i]==7) {atSym[i]="N";atWeight[i]=14.007}
  if (atNum[i]==8) {atSym[i]="O";atWeight[i]=15.9994}
  if (atNum[i]==9) {atSym[i]="F";atWeight[i]=18.9984}
  if (atNum[i]==10) {atSym[i]="Ne";atWeight[i]=20.1797}
  if (atNum[i]==11) {atSym[i]="Na";atWeight[i]=22.989}
  if (atNum[i]==12) {atSym[i]="Mg";atWeight[i]=24.305}
  if (atNum[i]==13) {atSym[i]="Al";atWeight[i]=26.98154}
  if (atNum[i]==14) {atSym[i]="Si";atWeight[i]=28.0855}
  if (atNum[i]==15) {atSym[i]="P";atWeight[i]=30.9738}
  if (atNum[i]==16) {atSym[i]="S";atWeight[i]=32.066}
  if (atNum[i]==17) {atSym[i]="Cl";atWeight[i]=35.4527}
  if (atNum[i]==18) {atSym[i]="Ar";atWeight[i]=39.948}
  if (atNum[i]==19) {atSym[i]="K";atWeight[i]=39.0983}
  if (atNum[i]==20) {atSym[i]="Ca";atWeight[i]=40.078}
  if (atNum[i]==21) {atSym[i]="Sc";atWeight[i]=44.96}
  if (atNum[i]==22) {atSym[i]="Ti";atWeight[i]=47.867}
  if (atNum[i]==23) {atSym[i]="V";atWeight[i]=50.94}
  if (atNum[i]==24) {atSym[i]="Cr";atWeight[i]=51.9961}
  if (atNum[i]==25) {atSym[i]="Mn";atWeight[i]=54.938}
  if (atNum[i]==26) {atSym[i]="Fe";atWeight[i]=55.845}
  if (atNum[i]==27) {atSym[i]="Co";atWeight[i]=58.933}
  if (atNum[i]==28) {atSym[i]="Ni";atWeight[i]=58.693}
  if (atNum[i]==29) {atSym[i]="Cu";atWeight[i]=63.546}
  if (atNum[i]==30) {atSym[i]="Zn";atWeight[i]=65.38}
  if (atNum[i]==31) {atSym[i]="Ga";atWeight[i]=69.723}
  if (atNum[i]==32) {atSym[i]="Ge";atWeight[i]=72.64}
  if (atNum[i]==33) {atSym[i]="As";atWeight[i]=74.9216}
  if (atNum[i]==34) {atSym[i]="Se";atWeight[i]=78.96}
  if (atNum[i]==35) {atSym[i]="Br";atWeight[i]=79.904}
  if (atNum[i]==46) {atSym[i]="Pd";atWeight[i]=106.42}
  if (atNum[i]==53) {atSym[i]="I";atWeight[i]=126.90447}
# gets actual weight from freqinHP when possible so a prior calc with readisotopes gets you isotopic substitution
  if ((i<100) && ($9>0)) atWeight[i]=$9
#  if ((i>99) && ($8>0)) atWeight[i]=$8

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

```
  }

# read in frequencies, scale them, read in Reduced masses, read in force
#constants, replace negative frequencies by 2 wavenumbers
numFreq=3*numAtoms-6
if (geometry=="linear") numFreq=3*numAtoms-5
for (i=1;i<=numFreq;i++) {
  $0=""
  getline < "tempfreqs"
  freq[i]=$0*scaling
  if (freq[i]<0) freq[i]=2
  }
for (i=1;i<=numFreq;i++) {
  $0=""
  getline < "tempredmass"
  redMass[i]=$0
  if (redMass[i]=="") redMass[i]=1.
  }
for (i=1;i<=numFreq;i++) {
  $0=""
  getline < "tempfrc"
  frc[i]=$0
  if (frc[i]=="") frc[i]=0.0001
  if (frc[i]==0) frc[i]=0.0001
  if ((diag>1) && (i==1)) print "freq[i],redMass[i],frc[i]" >> "diagnostics"
  if (diag>1) print freq[i],redMass[i],frc[i] >> "diagnostics"
  }

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

# if doing a cannonball trajectory, read in the vector
if (cannonball>0) {
  for (i=1;i<=numAtoms;i++) {
    getline < "cannontraj"
    cannonArr[i,1]=$1; cannonArr[i,2]=$2; cannonArr[i,3]=$3
    }
  }

# collect a series of random numbers from file temp811, generated from an outside random number generator called by
prodynstarterHP
# read from temp811, starting at a random place
srand(PROCINFO["pid"]); tester=rand()*1000
for (i=1;i<=tester;i++) getline < "temp811"
for (i=1;i<=numFreq;i++) {
  getline < "temp811"; randArr[i]=$1
  getline < "temp811"; randArrB[i]=$1
  getline < "temp811"; randArrC[i]=$1
}
for (i=1;i<=6;i++) {
  getline < "temp811"; randArrR[i]=$1
}

# for a QM distribution for a harmonic oscillator in its ground state, we want to generate a set of random numbers
#between -1 and 1 weighted such that numbers toward the center are properly more common
i=1
while (i<=numFreq) {
  if ((initialDis==2) || (disMode[i]==2)) {
    getline < "temp811"
    tempNum=2*($1-.5)
    prob=exp(-(tempNum^2))
    getline < "temp811"
    if ($1<prob) {
      randArrD[i]=tempNum
```

```
      i++
      }
    }
  if ((initialDis!=2) && (disMode[i]!=2)) i++
  }

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

# determine energy in each normal mode
for (i=1;i<=numFreq;i++) {
  zpeJ[i]=0.5*h*c*freq[i]       #units J per molecule
#if classical, treat as modes spaced by classicalSpacing wavenumbers
  if (classical==1) zpeJ[i]=0.5*h*c*classicalSpacing  # the zpe is not used when classical but the spacing is used to calculate the
E in mode
  zpeK[i]=zpeJ[i]*avNum/4184    #units kcal/mol
  if (temp<10) vibN[i]=0        # avoids working with very small temperatures - if the temp is too low, it just acts like 0 K
  if (temp>=10) {
    zpeRat[i]=exp((-2*zpeK[i])/(RgasK*temp))
    if (zpeRat[i]==1) zpeRat[i]=.99999999999
    Q[i]=1/(1-zpeRat[i])
    newRand=randArr[i]
    vibN[i]=0
    tester=1/Q[i]
#     get up to 4000 excitations of low modes
    for (j=1;j<=(4000*zpeRat[i]+2);j++) {
      if (newRand>tester) vibN[i]++
      tester=tester+((zpeRat[i]^j)/Q[i])
      }
    }
  }

# figure out mode energies and maximum classical shift and then actual shift
# also calculated total energy desired for molecule
desiredModeEnK=0
for (i=1;i<=numFreq;i++) {
  modeEn[i]=(zpeJ[i]*1E18)*(2*vibN[i]+1) # units here are mDyne Ansgroms for compatability with Gaussian force constants
  if (classical==1) modeEn[i]=(zpeJ[i]*1E18)*2*vibN[i]    #no zpe when classical
  modeEnK[i]=zpeK[i]*(2*vibN[i]+1)
  if (classical==1) modeEnK[i]=zpeK[i]*2*vibN[i]          #no zpe when classical
  desiredModeEnK=desiredModeEnK + modeEnK[i]
# no 1/2 hv for imaginary frequencies
# treating modes with frequencies <10 as translations, ignoring their zero point energies
  if (freq[i]<10) modeEn[i]=(zpeJ[i]*1E18)*(2*vibN[i])
  maxShift[i]=(2*modeEn[i]/frc[i])^0.5
# new 2012 initialDis 3 means random phase of normal mode
  if (initialDis==3) shift[i]=maxShift[i]*sin(randArrC[i]*3.141592*2)
  if (initialDis==2) shift[i]=maxShift[i]*randArrD[i]
  if (initialDis==1) shift[i]=maxShift[i]*(2*(randArrC[i]-0.5))
  if (initialDis==0) shift[i]=0
# lines below allow for setting of displacement mode for individual modes
# It used to be necessary to use disMode 10 to turn off displacements for a mode, but hopefully that bug is killed and you can use
disMode 0
  if (disMode[i]==3) shift[i]=maxShift[i]*sin(randArrC[i]*3.141592*2)
  if (disMode[i]==2) shift[i]=maxShift[i]*randArrD[i]
  if (disMode[i]==1) shift[i]=maxShift[i]*(2*(randArrC[i]-0.5))
  if (disMode[i]==10) shift[i]=0 #kept for backward compatability
  if (disMode[i]==0) shift[i]=0
# no displacements along imaginary frequencies and very low ones - it is better to treat these
# as translations - employing a shift can give you initial weird geometries
  if (freq[i]<10) shift[i]=0
  if (numimag==1) shift[1]=0
  if (numimag==2) shift[2]=0
  }
for (i=1;i<=numFreq;i++) {
```

```
  if ((diag>1) && (i==1)) print "zpeJ[i],zpeK[i],zpeRat[i],Q[i],vibN[i],modeEn[i],maxShift[i],shift[i]" >> "diagnostics"
  if (diag>1) print zpeJ[i],zpeK[i],zpeRat[i],Q[i],vibN[i],modeEn[i],maxShift[i],shift[i] >> "diagnostics"
  }

# multiply each of the modes by its shift and add them up
# Do not do this if classical=2
if (classical!=2) {
  for (i=1;i<=numFreq;i++) {
    for (j=1;j<=numAtoms;j++) {
      for (k=1;k<=3;k++) {
        shiftMode[i,j,k]=mode[i,j,k]*shift[i]
        geoArr[j,k]=geoArr[j,k]+shiftMode[i,j,k]
        }
      }
    }
  }

#now start toward velocities
for (i=1;i<=numFreq;i++) {
  kinEn[i]=100000*(modeEn[i]-0.5*frc[i]*shift[i]^2)  # the 100000 converts to g angstrom^2 s^2
  vel[i]=(2*kinEn[i]/(redMass[i]/avNum))^0.5        # in angstrom / s
#use searchdir in progdyn.conf to control the direction for trajectories started from a saddle point
  if (numimag>1) numimag=1  #only the first freq can be sent in the searchdir direction, the rest go in a random direction
  if (i>numimag) {
    if (randArrB[i]<0.5) vel[i]=-vel[i]
    }
  if (i==numimag) {
    if (searchdir=="negative") vel[i]=-vel[i]
    }
  if ((diag>1) && (i==1)) print "vel[i]" >> "diagnostics"
  if (diag>1) print vel[i] >> "diagnostics"
  }

# if controlphase is being used, set the velocity on particular modes as positive or negative as requested
for (i=1;i<=numFreq;i++) {
  if ((controlPhase[i]=="positive") && (vel[i]<0)) vel[i]=-vel[i]
  if ((controlPhase[i]=="negative") && (vel[i]>0)) vel[i]=-vel[i]
  }

# multiply each of the modes by its velocity and add them up
# Do not do this if classical=2
if (classical!=2) {
  for (i=1;i<=numFreq;i++) {
    for (j=1;j<=numAtoms;j++) {
      for (k=1;k<=3;k++) {
        velMode[i,j,k]=mode[i,j,k]*vel[i]*timestep
        velArr[j,k]=velArr[j,k]+velMode[i,j,k]
        }
      }
    }
  }

# to start without normal modes or frequencies we figure out the energy per atom based on 1/2RT in degree of freedom
if (classical==2) {
# to avoid a bug with a box on, starts without modes should use the input geometry, not the standard
  do {
    getline < "tempinputgeos"
    if (oldline==$0) $0=""
    oldline=$0
    atom = $1
    geoArr[atom,1]=$4; geoArr[atom,2]=$5; geoArr[atom,3]=$6
    geoArrOrig[atom,1]=$4; geoArrOrig[atom,2]=$5; geoArrOrig[atom,3]=$6
    }
  while (length($0) > 0)
  degFreedomEnK=temp*RgasK
  degFreedomEnJ=degFreedomEnK/(avNum/4184)
  cartEn=degFreedomEnJ*1E18
  kinEnCart=100000*cartEn
#print degFreedomEnK, degFreedomEnJ, cartEn, kinEnCart
  for (i=1;i<=numAtoms;i++) {
    for (j=1;j<=3;j++) {
      velArr[i,j]=randArrE[i,j]*timestep*(2*kinEnCart/(atWeight[i]/avNum))^0.5
```

```
        if (DRP==1) velArr[i,j]=0
        }
      }
    }

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

# add molecular rotation if requested
if (rotationmode>0) {
#establish three rotation vectors
  for (j=1;j<=numAtoms;j++) {
    rotateX[j,1]=0
    rotateX[j,2]=-geoArrOrig[j,3]
    rotateX[j,3]=geoArrOrig[j,2]
    rotateY[j,1]=-geoArrOrig[j,3]
    rotateY[j,2]=0
    rotateY[j,3]=geoArrOrig[j,1]
    rotateZ[j,1]=-geoArrOrig[j,2]
    rotateZ[j,2]=geoArrOrig[j,1]
    rotateZ[j,3]=0
    }
#figure out how much energy is in the raw vectors
  eRotX=0;eRotY=0;eRotZ=0
  for (j=1;j<=numAtoms;j++) {
    for (k=1;k<=3;k++) {
      eRotX=eRotX + 0.5*atWeight[j]*(rotateX[j,k]^2)/((timestep^2)*conver1)
      eRotY=eRotY + 0.5*atWeight[j]*(rotateY[j,k]^2)/((timestep^2)*conver1)
      eRotZ=eRotZ + 0.5*atWeight[j]*(rotateZ[j,k]^2)/((timestep^2)*conver1)
      }
    }
#  print "rotation energies if raw vector used",eRotX,eRotY,eRotZ
#now deciie how much energy we want in each rotation
  keRx=-0.5*0.001987*temp*log(1-randArrR[1])
  keRy=-0.5*0.001987*temp*log(1-randArrR[2])
  keRz=-0.5*0.001987*temp*log(1-randArrR[3])
  if (eRotX<1) keRx=0;if (eRotY<1) keRy=0;if (eRotZ<1) keRz=0
  rotEdesired=keRx+keRy+keRz
  signX=1;signY=1;signZ=1
  if (randArrR[4]<.5) signX=-1
  if (randArrR[5]<.5) signY=-1
  if (randArrR[6]<.5) signZ=-1

#  print "desired energies",keRx,keRy,keRz,"and random numbers",randArrR[1],randArrR[2],randArrR[3]
#protect against zero rotations
  if (eRotX<1) eRotX=1;if (eRotY<1) eRotY=1;if (eRotZ<1) eRotZ=1
#now scale the rotational vectors
  scaleX=(keRx/eRotX)^.5
  scaleY=(keRy/eRotY)^.5
  scaleZ=(keRz/eRotZ)^.5
#  print "scaling factors" scaleX,scaleY,scaleZ
  for (j=1;j<=numAtoms;j++) {
    for (k=1;k<=3;k++) {
      rotateX[j,k]=rotateX[j,k]*scaleX*signX
      rotateY[j,k]=rotateY[j,k]*scaleY*signY
      rotateZ[j,k]=rotateZ[j,k]*scaleZ*signZ
      }
    }
  for (j=1;j<=numAtoms;j++) {
#     print rotateX[j,1],"   ",rotateX[j,2],"   ",rotateX[j,3]
    }
#  print ""
  for (j=1;j<=numAtoms;j++) {
#     print rotateY[j,1],"   ",rotateY[j,2],"   ",rotateY[j,3]
    }
#  print ""
  for (j=1;j<=numAtoms;j++) {
#     print rotateZ[j,1],"   ",rotateZ[j,2],"   ",rotateZ[j,3]
    }
```

```
# now add the rotational vectors  to velArr
  for (j=1;j<=numAtoms;j++) {
    for (k=1;k<=3;k++) {
      velArr[j,k]=velArr[j,k]+rotateX[j,k]+rotateY[j,k]+rotateZ[j,k]
      }
    }
  }

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

#output the new geometry.
# ****** this section changed for special experiment for cyclopentadiene.  do not use this for other cases
# atWeight[4]=140.0001
# ****** line below added for special experiment switching mass from 12 to 140, keeping momenta the same
#velArr[4,1]=velArr[4,1]/11.66667; velArr[4,2]=velArr[4,2]/11.66667; velArr[4,3]=velArr[4,3]/11.66667
for (j=1;j<=numAtoms;j++) {
  printf("%2s % .7f % .7f % .7f %9.5f \n",atSym[j],geoArr[j,1],geoArr[j,2],geoArr[j,3],atWeight[j])
  }

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

#anything else I add to the file will not affect the trajectories but will keep a record and be good for analysis
for (i=1;i<=numFreq;i++) {
  if (initialDis==0) printf("%.6f   % .6f    %4i    % 1.4e       % .6f %1i\n", randArr[i], randArrB[i], vibN[i], vel[i], shift[i],
disMode[i])
  if (initialDis==1) printf("%.6f   % .6f    %4i    % 1.4e       % .6f %1i\n", randArr[i], randArrC[i], vibN[i], vel[i], shift[i],
disMode[i])
  if (initialDis==2) printf("%.6f   % .6f    %4i    % 1.4e       % .6f %1i\n", randArr[i], randArrD[i], vibN[i], vel[i], shift[i],
disMode[i])
  if (initialDis==3) printf("%.6f   % .6f    %4i    % 1.4e       % .6f %1i % .6f\n", randArr[i], randArrC[i], vibN[i], vel[i], shift[i],
disMode[i], sin(randArrC[i]*3.141592*2))
  }
print "temp ",temp
print "initialDis",initialDis
print "classical",classical
print "timestep",timestep
print "numimag",numimag
OFMT = "%.3f"
print "Total mode energy desired=",desiredModeEnK
print "KE initial from modes=",KEinitmodes,"   KE initial total=",KEinittotal,"   Rotational Energy desired=",rotEdesired
if (cannonball>0) print "cannonball",cannonball,"  cannon Energy=",KEinittotal-KEinitmodes
if (boxon>0) print "boxsize",boxsize
if (DRP>0) print "DRP",DRP,"   maxAtomMove",maxAtomMove
if (DRP>0) print maxAtomMove > "maxMove"
}  # End of BEGIN

/Zero-point correction/ {zpeGauss=$3}
/zero-point Energies/ {zpePlusE=$7}
```

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

Program prog1stpoint

```
BEGIN {
# aug 2013 includes molecular rotation, ability to do multiple NMR calculations, ONIOM with link atoms,
#nonstandard routes,
# aug 2010 changed so that it is more careful in reading in from geoPlusVel
#     removed some default parameters that should always be defined
# Jan 2009 - a number of little changes to improve reporting, precision, etc
# aug 2008 added to atom list so handles H to Cl without change needed
# version Feb 2008 incorporates methodfile, boxon and boxsize, though this point unaffected by box
# version Jan 2008 - allows for ONIOM jobs, fixed atoms
# version Sept 2005 - incorportates meth3, meth4, meth5, meth6, but not yet rotation
# this program creates the first input file for g09
# the title should be changed as appropriate
# the isomer number comes from a file isomernumber

# default parameters, including quassiclassical, no displacements, transition state, not a DRP
# do not change these - rather, change progdyn.conf to set the parameters
initialDis=0; timestep=1E-15; scaling=1.0; temp=298.15
classical=0; numimag=1; DRP=0; cannonball=0
memory=20000000
diag=1; checkpoint="g09.chk"; searchdir="positive"; boxon=0
boxsize=10; maxAtomMove=0.1; title1="you"; title2="need"
title3="a"; title4="progdyn.conf"; processors=1; highlevel=999; linkatoms=0
geometry="nonlinear";nonstandard=0
nmrtype=0;nmrevery=9999999

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

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="method2") meth2=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="timestep") timestep=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="method3") meth3=$2
  if ($1=="method4") meth4=$2
  if ($1=="method5") meth5=$2
  if ($1=="method6") meth6=$2
  if ($1=="method7") meth7=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="linkatoms") linkatoms=$2
  if ($1=="fixedatom1") fixedatom1=$2
  if ($1=="fixedatom2") fixedatom2=$2
  if ($1=="fixedatom3") fixedatom3=$2
  if ($1=="fixedatom4") fixedatom4=$2
  if ($1=="methodfile") methodfilelines=$2
  if ($1=="killcheck") killcheck=$2
  if ($1=="NMRmethod") nmrmethod=$2
```

```
  if ($1=="NMRmethod2") nmrmethod2=$2
  if ($1=="NMRmethod3") nmrmethod3=$2
  if ($1=="NMRtype") nmrtype=$2
  if ($1=="NMRevery") nmrevery=$2
  if ($1=="nonstandard") nonstandard=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }

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

getline < "isomernumber"
isomernum = $1
#read in number of atoms, geometry, masses, and velocity from geoPlusVel
getline < "geoPlusVel"
numAtoms=$1
# geometry
for (i=1;i<=numAtoms;i++) {
  getline < "geoPlusVel"
  weight[i]=$5
  atSym[i]=$1
  for (j=1;j<=3;j++) {
    geoArr[i,j]=$(1+j)
    }
  }
#velocities not needed for 1st point
for (i=1;i<=numAtoms;i++) {
  getline < "geoPlusVel"
  for (j=1;j<=3;j++) {
    velArr[i,j]=$j
    }
  }

print "%nproc=" processors
print "%mem=" memory
if (killcheck!=1) print "%chk=" checkpoint
if (nonstandard==0) {
  print "# " method " force scf=(tight,nosym) "
  if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
  if (length(meth3)>2) print meth3
  if (length(meth4)>2) print meth4
  }
if (nonstandard==1) {
  print "# "
  print "nonstd"
  system("cat nonstandard")
  }
print ""
# make the title four words exactly, leaving out spaces if necessary
print title1,title2,title3,title4
print "runpoint ",runpointnum
print "runisomer ", isomernum
print ""
print charge,multiplicity
}

END {
for (i=1;i<=numAtoms;i++) {
  printf("%s %.7f %.7f %.7f",atSym[i],geoArr[i,1],geoArr[i,2],geoArr[i,3])
  if ((i>highlevel) && (i<=highlevel+linkatoms)) printf(" %s","M H")
  if (i>(highlevel+linkatoms)) printf(" %s","M")
  print ""
  }
```

```
print ""
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
if (methodfilelines>=1) {
   for (i=1;i<=methodfilelines;i++) {
      getline < "methodfile"
      print $0
      }
   }
if ((nmrtype>0) && ((runpointnum % nmrevery)==0)) {
   print "--link1--"
   print "%nproc=" processors
   print "%mem=" memory
   print "%chk=" checkpoint
   print "# " nmrmethod " nmr=giao geom=check"
   if (nmrmethod==method) print "guess=tcheck"
   if (length(meth7)>2) print meth7
   print ""
   print title1,title2,title3,title4
   print "runpoint ",runpointnum
   print "runisomer ",isomernum
   print ""
   print charge,multiplicity
   }
print ""
if ((nmrtype>1) && ((runpointnum % nmrevery)==0)) {
   print "--link1--"
   print "%nproc=" processors
   print "%mem=" memory
   print "%chk=" checkpoint
   print "# " nmrmethod2 " nmr=giao geom=check"
   if (length(meth7)>2) print meth7
   print ""
   print title1,title2,title3,title4
   print "runpoint ",runpointnum
   print "runisomer ",isomernum
   print ""
   print charge,multiplicity
   }
print ""
if ((nmrtype>2) && ((runpointnum % nmrevery)==0)) {
   print "--link1--"
   print "%nproc=" processors
   print "%mem=" memory
   print "%chk=" checkpoint
   print "# " nmrmethod3 " nmr=giao geom=check"
   if (length(meth7)>2) print meth7
   print ""
   print title1,title2,title3,title4
   print "runpoint ",runpointnum
   print "runisomer ",isomernum
   print ""
   print charge,multiplicity
   }
print ""
}
```

Program prog2ndpoint

```
BEGIN {
# aug 2013 includes molecular rotation, ability to do multiple NMR calculations, ONIOM with link atoms,
#nonstandard routes, checks more kinds of energies at point 2
#Aug 2010 added etolerance to make it controllable from progdyn.conf, made it so that DRP does not check energy
# aug 2008 added to atom list so handles 1 to 17 without change needed
# version Feb 2008 incorporates methodfile, boxon and boxsize, though this point unaffected by box
# version Jan 2008 - allows for ONIOM jobs, fixed atoms
# version Sept 9, 2005 - incorportates meth3, meth4, meth5, meth6, but not yet rotation
# read progdyn.conf for configuration info

# default parameters, including quassiclassical, no displacements, transition state, not a DRP
```

```
# do not change these - rather, change progdyn.conf to set the parameters
initialDis=0; timestep=1E-15; scaling=1.0; temp=298.15
classical=0; numimag=1; DRP=0; cannonball=0
memory=20000000
diag=1; checkpoint="g09.chk"; searchdir="positive"; boxon=0
boxsize=10; maxAtomMove=0.1; title1="you"; title2="need"
title3="a"; title4="progdyn.conf"; processors=1; highlevel=999; linkatoms=0
etolerance=1
geometry="nonlinear";nonstandard=0
NMRtype=none;NMRevery=9999999

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

blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="method2") meth2=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="timestep") timestep=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="method3") meth3=$2
  if ($1=="method4") meth4=$2
  if ($1=="method5") meth5=$2
  if ($1=="method6") meth6=$2
  if ($1=="method7") meth7=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="linkatoms") linkatoms=$2
  if ($1=="fixedatom1") fixedatom1=$2
  if ($1=="fixedatom2") fixedatom2=$2
  if ($1=="fixedatom3") fixedatom3=$2
  if ($1=="fixedatom4") fixedatom4=$2
  if ($1=="DRP") DRP=$2
  if ($1=="methodfile") methodfilelines=$2
  if ($1=="killcheck") killcheck=$2
  if ($1=="etolerance") etolerance=$2
  if ($1=="reversetraj") reversetraj=$2
  if ($1=="NMRmethod") nmrmethod=$2
  if ($1=="NMRmethod2") nmrmethod2=$2
  if ($1=="NMRmethod3") nmrmethod3=$2
  if ($1=="NMRtype") nmrtype=$2
  if ($1=="NMRevery") nmrevery=$2
  if ($1=="nonstandard") nonstandard=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }

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

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

```
#get forward or reverse from skipstart if it exists
getline < "skipstart"
trajdirection = $1

print "%nproc=" processors
print "%mem=" memory
if (killcheck!=1) print "%chk=" checkpoint
if (nonstandard==0) {
   print "# " method " force scf=(tight,nosym) "
   if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
   if (meth2=="read") print "guess=tcheck" #for reading orbitals from check, sometimes faster, sometimes not
   if (length(meth3)>2) print meth3
   if (length(meth4)>2) print meth4
   }
if (nonstandard==1) {
   print "# "
   print "nonstd"
   system("cat nonstandard")
   }
print ""
print title1,title2,title3,title4
print "runpoint ",runpointnum
print "runisomer ", isomernum
print ""
print charge,multiplicity

# ok, now we have to figure the second point.  this should be
# x(t) = x + v*t + 1/2*F*t^2/m
# so we need to set up arrays for position, velocity, and force

#read in number of atoms, geometry, masses, and velocity from geoPlusVel
getline < "geoPlusVel"
numAtoms=$1
# geometry
for (i=1;i<=numAtoms;i++) {
   getline < "geoPlusVel"
   weight[i]=$5
   atSym[i]=$1
   for (j=1;j<=3;j++) {
      geoArr[i,j]=$(1+j)
      }
   }
#velocities
for (i=1;i<=numAtoms;i++) {
   getline < "geoPlusVel"
   for (j=1;j<=3;j++) {
      velArr[i,j]=$j
      }
   }

#now we go ahead and add the velocities
for (i=1;i<=numAtoms;i++) {
   for (j=1;j<=3;j++) {
      arr[i,j]=velArr[i,j]+geoArr[i,j]
      if (trajdirection=="reverserestart") arr[i,j]=geoArr[i,j]-velArr[i,j]
      }
   if ((diag>1) && (i==1)) print "geometry after adding velocities" >> "diagnostics"
   if (diag>1) print arr[i,1],arr[i,2],arr[i,3] >> "diagnostics"
   }

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

```
#get initial geometry into file traj
print numAtoms >> "traj"
print potentialE,title1,title2,title3,title4,"runpoint 1 ","runisomer ",isomernum >> "traj"
for (i=1;i<=numAtoms;i++) {
  print atSym[i],geoArr[i,1],geoArr[i,2],geoArr[i,3] >> "traj"
  }
#added by Samae on 102910
scfcount=0
} # end of BEGIN

#pull out the potential energy
/SCF Done/ || /EUMP2 =/ || / Energy=/ {
if (($1=="Energy=") && ($3=="NIter="))  newPotentialE=$2
if (($1=="SCF") && (scfcount==0)) newPotentialE=$5
if ($1=="E2") {
  tempstring=$6
  split(tempstring, arr10, "D")
  newPotentialE=arr10[1]*(10^arr10[2])
  }
newPotentialEK=(newPotentialE-potentialE)*627.509
if ($1=="SCF") {
  if (scfcount==0) {
    pddga=$5
    }
  if (scfcount==1) {
    qm=$5
    }
  if (scfcount==2) {
    pddgb=$5
    pddgc=(pddga-pddgb)
    newPotentialE=(qm+pddgc)
    newPotentialEK=(newPotentialE-potentialE)*627.509
    }
  scfcount++
  }
}

# now we go ahead and translate the forces and add them
(/  1  / || /  2  / || /  3  / || /  4  / || /  5  / || /  6  / || /  7  / || /  8  / || /  9  / || /  10  / || /
11  / || /  12  / || /  13  / || /  14  / || /  15  / || /  16  / || /  17  / || /  18  / || /  19  / || /  20  / || /
21  / || /  22  / || /  23  / || /  24  / || /  25  / || /  26  / || /  27  / || /  28  / || /  29  / || /  30  / || /
31  / || /  32  / || /  33  / || /  34  / || /  35  /) && length($3) > 9 {
i=$1
for (j=1;j<=3;j++) {
  forceArr[i,j]=$(2+j)    #the raw units of the forces are Hartree/Bohr
  }
if ((diag>1) && (i==1)) print "i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]" >> "diagnostics"
if (diag>1) print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3] >> "diagnostics"
}

END {
#put out Echeck but only if not a DRP
if (DRP==0) {
  print "trajectory #",isomernum >> "Echeck"
  print "point 1 potential E=",newPotentialEK,"   point 1 kinetic E=",KEinitmodes,"  Total=",newPotentialEK+KEinitmodes >>
"Echeck"
  print "desired total energy=", desiredModeEnK >> "Echeck"
  if ((newPotentialEK+KEinitmodes)>(desiredModeEnK+etolerance)) print "XXXX bad total Energy" >> "Echeck"
  if ((newPotentialEK+KEinitmodes)<(desiredModeEnK-etolerance)) print "XXXX bad total Energy" >> "Echeck"
  }
# turn the forces into motion
for (i=1;i<=numAtoms;i++) {
  for (j=1;j<=3;j++) {
# conversions here take force to J/angstrom, 1E20 converts to kg angstroms / s^2, then mult time (s^s) and divide by weight in kg
to get angstroms
    forceArr[i,j]=0.5*1E20*forceArr[i,j]*627.509*(4184/(0.529177*avNum))*(timestep^2)/(weight[i]/(avNum*1000))
# for simplicity, DRPs will throw away the forces at the second pont.  This means that if we are not at a saddlepoint, point 2 =
point 1 but this is a minor waste
    if (DRP==1) forceArr[i,j]=0
    arr[i,j]=arr[i,j]+forceArr[i,j]
# if atoms are fixed, replace calcd new position by original position
    if ((i==fixedatom1) || (i==fixedatom2) || (i==fixedatom3) || (i==fixedatom4)) arr[i,j]=geoArr[i,j]
```

```
    }
  if ((diag>1) && (i==1)) print "i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]" >> "diagnostics"
  if (diag>1) print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3] >> "diagnostics"
  printf("%s %.7f %.7f %.7f",atSym[i],arr[i,1],arr[i,2],arr[i,3])
  if ((i>highlevel) && (i<=highlevel+linkatoms)) printf(" %s","M H")
  if (i>(highlevel+linkatoms)) printf(" %s","M")
  print ""
  }
print ""
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
if (methodfilelines>=1) {
  for (i=1;i<=methodfilelines;i++) {
    getline < "methodfile"
    print $0
    }
  }
if ((nmrtype>0) && ((runpointnum % nmrevery)==0)) {
  print "--link1--"
  print "%nproc=" processors
  print "%mem=" memory
  print "%chk=" checkpoint
  print "# " nmrmethod " nmr=giao geom=check"
  if (nmrmethod==method) print "guess=tcheck"
  if (length(meth7)>2) print meth7
  print ""
  print title1,title2,title3,title4
  print "runpoint ",runpointnum
  print "runisomer ",isomernum
  print ""
  print charge,multiplicity
  }
print ""
if ((nmrtype>1) && ((runpointnum % nmrevery)==0)) {
  print "--link1--"
  print "%nproc=" processors
  print "%mem=" memory
  print "%chk=" checkpoint
  print "# " nmrmethod2 " nmr=giao geom=check"
  if (length(meth7)>2) print meth7
  print ""
  print title1,title2,title3,title4
  print "runpoint ",runpointnum
  print "runisomer ",isomernum
  print ""
  print charge,multiplicity
  }
print ""
if ((nmrtype>2) && ((runpointnum % nmrevery)==0)) {
  print "--link1--"
  print "%nproc=" processors
  print "%mem=" memory
  print "%chk=" checkpoint
  print "# " nmrmethod3 " nmr=giao geom=check"
  if (length(meth7)>2) print meth7
  print ""
  print title1,title2,title3,title4
  print "runpoint ",runpointnum
  print "runisomer ",isomernum
  print ""
  print charge,multiplicity
  }
print ""
#get second geometry into file traj
print numAtoms >> "traj"
print newPotentialE,title1,title2,title3,title4,"runpoint ",runpointnum,"runisomer ",isomernum >> "traj"
for (i=1;i<=numAtoms;i++) {
  print atSym[i],arr[i,1],arr[i,2],arr[i,3] >> "traj"
  }
}
BEGIN {
```

Program progdynb

```
BEGIN { #this is the main routine for generating new .com files by the Verlet algorithym
# aug 2013 includes molecular rotation, ability to do multiple NMR calculations, ONIOM with link atoms,
#nonstandard routes, monitoring of loads and randomized NMR calcs, CCSD(T) nmr calculations, making a ZMAT file for
CFOUR
# Aug 2010 increased elements handled automatically but only up to bromine!
# Jan 2009 - a number of little changes to improve reporting, precision, etc
# Nov 2008 added ability to handle DRPs
# Aug 2008 added long list of atoms to handle 1-17 without change
# May 2008 added option to put out velocities in vellist - make diag=3
# version Feb 2008 incorporates methodfile, boxon and boxsize
# version Jan 2008 incorporates fixed atoms, oniom, and velocity damping
# version August 2007 incorporates keepevery to decrease size of dyn file
# version Sept 11, 2005 - incorportates meth3, meth4, meth5, meth6, but not yet rotation

# default parameters, including quassiclassical, no displacements, transition state, not a DRP
# do not change these - rather, change progdyn.conf to set the parameters
initialDis=0; timestep=1E-15; scaling=1.0; temp=298.15
classical=0; numimag=1; DRP=0; cannonball=0
memory=20000000
diag=1; checkpoint="g09.chk"; searchdir="positive"; boxon=0
boxsize=10; maxAtomMove=0.1; title1="you"; title2="need"
title3="a"; title4="progdyn.conf"; processors=1; highlevel=999; linkatoms=0
damping=1;nonstandard=0
nmrtype=0;nmrevery=9999999;nmrcc=0;nmrrand=0;nmrdo=0
thermostat=0;thermostatemult=1.00

#initialization
srand(PROCINFO["pid"])
i=1;j=1;k=1
c=29979245800; h=6.626075E-34; avNum=6.0221415E23
RgasK=0.00198588; RgasJ=8.31447
numAtoms=0; atomnumber=0
conver1=4.184E26 #dividing by this converts amu angs^2 /s^2 to kcal/mol
OFS="     "

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="method2") meth2=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="timestep") timestep=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="temperature") temp=$2
  if ($1=="thermostat") thermostat=$2
  if ($1=="thermostatmult") thermostatmult=$2
  if (thermostatmult>1) thermostatmult=1/thermostatmult
  if ($1=="method3") meth3=$2
  if ($1=="method4") meth4=$2
  if ($1=="method5") meth5=$2
  if ($1=="method6") meth6=$2
  if ($1=="method7") meth7=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="linkatoms") linkatoms=$2
  if ($1=="keepevery") keepevery=$2
  if ($1=="fixedatom1") fixedatom1=$2
  if ($1=="fixedatom2") fixedatom2=$2
  if ($1=="fixedatom3") fixedatom3=$2
  if ($1=="fixedatom4") fixedatom4=$2
  if ($1=="boxon") boxon=$2
  if ($1=="boxsize") boxsize=$2
  if ($1=="DRP") DRP=$2
  if ($1=="maxAtomMove") maxAtomMove=$2
  if ($1=="methodfile") methodfilelines=$2
  if ($1=="killcheck") killcheck=$2
```

```
  if ($1=="damping") damping=$2
  if ($1=="NMRmethod") nmrmethod=$2
  if ($1=="NMRmethod2") nmrmethod2=$2
  if ($1=="NMRmethod3") nmrmethod3=$2
  if ($1=="NMRtype") nmrtype=$2
  if ($1=="NMRevery") nmrevery=$2
  if ($1=="NMRrand") nmrrand=$2
  if ($1=="loadlimit") loadlimit=$2
  if ($1=="NMRcc") nmrcc=$2
  if ($1=="nonstandard") nonstandard=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }

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

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

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

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

#for DRPs read in oldAdjForces and maxAtomMove
if (DRP==1) {
  for (at=1;at<=numAtoms;at++) {
    getline < "oldAdjForces"
    oldForce[at,1]=$1; oldForce[at,2]=$2; oldForce[at,3]=$3
    }
  getline < "maxMove"
  if (($1<maxAtomMove) && ($1>0)) maxAtomMove=$1
  if (maxAtomMove<0.000001) maxAtomMove=0.000001
  }

# record atom velocities for IVR analysis.  This is actually the velocity in the previous run, which is the easiest to calculate.
getline < "isomernumber"
isomernum = $1
getline < "runpointnumber"
runpointnum = $1
# routine to control whether NMR calculations are done.
if ((nmrrand==0) && ((runpointnum % nmrevery)==0)) nmrdo=1
if ((nmrrand==1) && (rand()<(1/nmrevery))) nmrdo=1
getline < "uptimelist"
x=1.0001*substr($10,1,3);if (x<8) x=8
# turn of nmrs if load is too high - this is under control of loadlimit parameter in progdyn.conf and requires proganal to make
uptimelist
if ((nmrrand==1) && (x>loadlimit)) nmrdo=0

if (diag==3) print "runpoint ",runpointnum-1,"runisomer ",isomernum >> "vellist"
for (at=1;at<=numAtoms;at++) {
  atomVel=((oldarr[at,1]-olderarr[at,1])^2 + (oldarr[at,2]-olderarr[at,2])^2 +(oldarr[at,3]-olderarr[at,3])^2)^.5
  KEatomstotal=KEatomstotal+0.5*weight[at]*(atomVel^2)/((timestep^2)*conver1)
```

```
  if (diag==3) print atomVel >> "vellist"
  }
apparentTemp=KEatomstotal*2/(3*RgasK*numAtoms)
if (diag==4) print "KEatomstotal",KEatomstotal,"apparent Temperature",apparentTemp >> "vellist"
if (thermostat==1) {
  if (diag<4) print "KEatomstotal",KEatomstotal,"desired temperature",temp,"apparent Temperature",apparentTemp >> "vellist"
  if (apparentTemp>temp) damping=thermostatmult
  if (apparentTemp<temp) damping=1/thermostatmult
  }
}

#pull out the potential energy
/SCF Done/ || /EUMP2 =/ || / Energy=/ || /ONIOM:/ {
if (($1=="Energy=") && ($3=="NIter="))  newPotentialE=$2
if ($1=="SCF") newPotentialE=$5
if ($2=="extrapolated")  newPotentialE=$5
if ($1=="E2") {
  tempstring=$6
  split(tempstring, arr10, "D")
  newPotentialE=arr10[1]*(10^arr10[2])
  }
}

#must adjust next line for weird atoms
(/      1    / || /      2    / || /      3    / || /      4    / || /      5    / || /      6    / || /      7    / || /      8    / || /      9    / || /      10    / || /
11    / || /      12    / || /      13    / || /      14    / || /      15    / || /      16    / || /      17    / || /      18    / || /      19    / || /      20    / || /
21    / || /      22    / || /      23    / || /      24    / || /      25    / || /      26    / || /      27    / || /      28    / || /      29    / || /      30    / || /
31    / || /      32    / || /      33    / || /      34    / || /      35    /) && length($3) > 9 {
i=$1
for (j=1;j<=3;j++) {
  forceArr[i,j]=$(2+j)    #the raw units of the forces are Hartree/Bohr
  }
if ((diag>1) && (i==1)) print "i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]" >> "diagnostics"
if (diag>1) print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3] >> "diagnostics"
}

END {
#############routine for DRPs##############
if (DRP==1) {
  maxForce=0;oscillTest=0
  for (i=1;i<=numAtoms;i++) {
    for (j=1;j<=3;j++) {
# conversions here take force to J/angstrom, 1E20 converts to kg angstroms / s^2, then mult time (s^s) and divide by weight in kg
to get angstroms
      forceArr[i,j]=1E20*forceArr[i,j]*627.509*(4184/(0.529177*avNum))*(timestep^2)/(weight[i]/(avNum*1000))
      oscillTest=oscillTest+forceArr[i,j]*oldForce[i,j]
      if (forceArr[i,j]>maxForce) maxForce=forceArr[i,j]
      if ((0-forceArr[i,j])>maxForce) maxForce=-forceArr[i,j]
      }
    if (i==1) printf("% .8f % .8f % .8f \n",forceArr[1,1],forceArr[1,2],forceArr[1,3])  > "oldAdjForces"
    if (i>1) printf("% .8f % .8f % .8f \n",forceArr[i,1],forceArr[i,2],forceArr[i,3])  >> "oldAdjForces"
    }
  print "oscillTest ",oscillTest >> "oldAdjForces"
  if (oscillTest<0) {
    maxAtomMove = maxAtomMove*0.5
    print maxAtomMove > "maxMove"
    }
  if (oscillTest>0) {
    maxAtomMove = maxAtomMove*1.2
    print maxAtomMove > "maxMove"
    }
  print "maxAtomMove ",maxAtomMove >> "oldAdjForces"
  forceMult=maxAtomMove/maxForce
  for (i=1;i<=numAtoms;i++) {
    for (j=1;j<=3;j++) {
      newarr[i,j]=oldarr[i,j]+forceMult*forceArr[i,j]
      }
    }
  }
########

#############normal routine for Verlet ##############
```

```
if (DRP==0) {
  for (i=1;i<=numAtoms;i++) {
    for (j=1;j<=3;j++) {
# conversions here take force to J/angstrom, 1E20 converts to kg angstroms / s^2, then mult time (s^s) and divide by weight in kg
to get angstroms
      forceArr[i,j]=1E20*forceArr[i,j]*627.509*(4184/(0.529177*avNum))*(timestep^2)/(weight[i]/(avNum*1000))
      if ((diag>1) && (i==1)) print "i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]" >> "diagnostics"
      if (diag>1) print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3] >> "diagnostics"
      newarr[i,j]=oldarr[i,j]+damping*(oldarr[i,j]-olderarr[i,j])+forceArr[i,j]
      if ((i==fixedatom1) || (i==fixedatom2) || (i==fixedatom3) || (i==fixedatom4)) newarr[i,j]=oldarr[i,j]
#turn around atoms outside the box
      if (boxon==1) {
        if (newarr[i,j]>boxsize) if (oldarr[i,j]>olderarr[i,j]) newarr[i,j]=oldarr[i,j]+damping*(olderarr[i,j]-oldarr[i,j])+forceArr[i,j]
        if (newarr[i,j]<-1*boxsize) if (oldarr[i,j]<olderarr[i,j]) newarr[i,j]=oldarr[i,j]+damping*(olderarr[i,j]-
oldarr[i,j])+forceArr[i,j]
        }
      }
    }
  }
########

if ((runpointnum % keepevery)==0) system("cat g09.log >> dyn")
print "%nproc=" processors
print "%mem=" memory
if (killcheck!=1) print "%chk=" checkpoint
if (nonstandard==0) {
  print "# " method " force scf=(tight,nosym) "
  if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
  if (meth2=="read") print "guess=tcheck" #for reading orbitals from check, sometimes faster, sometimes not
  print "pop=none "
  if (length(meth3)>2) print meth3
  if (length(meth4)>2) print meth4
  }
if (nonstandard==1) {
  print "# "
  print "nonstd"
  system("cat nonstandard")
  }
print ""
print  title1,title2,title3,title4
print "runpoint ",runpointnum
print "runisomer ",isomernum
if (DRP==1) print "maxForce and forceMult and maxAtomMove",maxForce,forceMult,maxAtomMove
print ""
print charge,multiplicity
print numAtoms >> "traj"
print newPotentialE,title1,title2,title3,title4,"runpoint ",runpointnum,"runisomer ",isomernum >> "traj"
for (i=1;i<=numAtoms;i++) {
  printf("%s %.7f %.7f %.7f",atSym[i],newarr[i,1],newarr[i,2],newarr[i,3])
  printf("%s %.7f %.7f %.7f",atSym[i],newarr[i,1],newarr[i,2],newarr[i,3]) >> "traj"
  print "" >> "traj"
  if ((i>highlevel) && (i<=highlevel+linkatoms)) printf(" %s","M H")
  if (i>(highlevel+linkatoms)) printf(" %s","M")
  print ""
  }
print ""
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
if (methodfilelines>=1) {
  for (i=1;i<=methodfilelines;i++) {
    getline < "methodfile"
    print $0
    }
  }
if ((nmrtype>0) && (nmrdo==1)) {
  print "--link1--"
  print "%nproc=" processors
  print "%mem=" memory
  print "%chk=" checkpoint
  print "# " nmrmethod " nmr=giao geom=check"
  if (nmrmethod==method) print "guess=tcheck"
  if (length(meth7)>2) print meth7
```

```
   print ""
   print title1,title2,title3,title4
   print "runpoint ",runpointnum
   print "runisomer ",isomernum
   print ""
   print charge,multiplicity
   }
print ""
if ((nmrtype>1) && (nmrdo==1)) {
   print "--link1--"
   print "%nproc=" processors
   print "%mem=" memory
   print "%chk=" checkpoint
   print "# " nmrmethod2 " nmr=giao geom=check"
   if (length(meth7)>2) print meth7
   print ""
   print title1,title2,title3,title4
   print "runpoint ",runpointnum
   print "runisomer ",isomernum
   print ""
   print charge,multiplicity
   }
print ""
if ((nmrtype>2) && (nmrdo==1)) {
   print "--link1--"
   print "%nproc=" processors
   print "%mem=" memory
   print "%chk=" checkpoint
   print "# " nmrmethod3 " nmr=giao geom=check"
   if (length(meth7)>2) print meth7
   print ""
   print title1,title2,title3,title4
   print "runpoint ",runpointnum
   print "runisomer ",isomernum
   print ""
   print charge,multiplicity
   }
print ""

if ((nmrcc==1) && (nmrdo==1)) {
   print "CCSD(T) NMR calculation" > "ZMAT"
   for (i=1;i<=numAtoms;i++) {
      printf("%s %.7f %.7f %.7f",atSym[i],newarr[i,1],newarr[i,2],newarr[i,3]) >> "ZMAT"
      print "" >> "ZMAT"
      }
   print "" >> "ZMAT"
   print "*ACES2(CALC=CCSD[T],PROP=NMR,BASIS=dzp" >> "ZMAT"
   print "ABCDTYPE=AOBASIS,TREAT_PERT=SEQUENTIAL,CC_PROG=ECC" >> "ZMAT"
   print "COORD=CARTESIAN" >> "ZMAT"
   print "MEM_UNIT=GB,MEMORY=2)" >> "ZMAT"
   print "" >> "ZMAT"
   }
}
```

Program progcfour

The last two lines below would have to be set up for the local environment.

```
#!/bin/bash
origdir=$1
workdir=$2
cd $origdir
echo "starting cfour calculation"
date
mv x.log tempcfour.log
cd $workdir
rm -f -r tempcfour
mkdir tempcfour
mv CSH* tempcfour
mv GRD tempcfour
```

```
mv MOLDEN_NAT tempcfour
mv OPTARC tempcfour
mv AUXMOI tempcfour
mv DERINT tempcfour
mv FILES tempcfour
mv GAMLAM tempcfour
mv IIII tempcfour
mv IIJJ tempcfour
mv IJIJ tempcfour
mv IJKL tempcfour
mv JAINDX tempcfour
mv JMOL.plot tempcfour
mv JOBARC tempcfour
mv MOABCD tempcfour
mv MOINTS tempcfour
mv MOL tempcfour
mv MOLDEN tempcfour
mv MOLECULE.INP tempcfour
mv NEWMOS tempcfour
mv PPPPAA tempcfour
mv PPPHAA tempcfour
mv HHHHAA tempcfour
mv PHPHAA tempcfour
mv PPHHAA tempcfour
mv PHHHAA tempcfour
PATH=/data/d-singleton/cfour/cfour_v1_64bit/bin:$PATH
/data/d-singleton/cfour/cfour_v1_64bit/bin/xcfour > $origdir/x.log
```

Program randgen.c

This is compiled before use to give the service program *randgen*

```
#include <stdio.h>
#include <stdlib.h>

int a,b,c;
double d;

int product(int x, int y);

int main(void)
{
  int count=1;
  srand48(time (0));
  while (count<=100000)
  {
    d = drand48();
    printf ("%.20f\n", d);
    count++;
  }
  return 0;
}
```

Program proganal

```
BEGIN {
nmrset=0
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="NMRtype") nmrtype=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }
```

```
firsttitle=1
getline < "isomernumber"
isomer=$1
}
/ THF PM3/ {
  if (firsttitle==1) {
    titlestring=$1" " $2" " $3" " $4" " $6" " $7" " $8
    printf("%s %s %s %s %s %s %s  ",$1,$2,$3,$4,$6,$7,$8)
    runpoint=$6
    }
  firsttitle++
  }
/Standard orientation/,/Rotational constants/ {
  if (($1>.5) && ($1<30)) {
    A[$1]=$4;B[$1]=$5;C[$1]=$6
    }
  }
/Isotropic/ {
  if (nmrtype>0) {
    if ($1==1) {
      nmrset++
      if (nmrset==1) print titlestring >> "NMRlist"
      if (nmrset==2) print titlestring >> "NMRlist2"
      if (nmrset==3) print titlestring >> "NMRlist3"
      }
    if (($2=="C") || ($2=="H")) {
      tempstring=$0
      if (nmrset==1) print >> "NMRlist"
      if (nmrset==2) print >> "NMRlist2"
      if (nmrset==3) print >> "NMRlist3"
      }
    }
  }
END {
CC=Distance(2,4)
OP=Distance(3,1)
CO=Distance(2,1)
PC=Distance(3,4)
Ang=Angle(4,3,6)
if (Angle(4,3,12)>Ang) Ang=Angle(4,3,12)
if (Angle(4,3,13)>Ang) Ang=Angle(4,3,13)
printf("%s %.3f %s %.3f %s %.3f %s %.3f %s %.2f ","CC",CC,"OP",OP,"CO",CO,"PC",PC,"Ang",Ang)
  if ((CC<1.6) && (OP<1.8)) {
    print "Formed OP XXXX"
#    system("date > nogo")
    }
  if ((PC)>2.2 && (CO)>2.2) {
    print "Formed Alkene + Ph3PO XXXX"
    }
#  if ((CC)<1.6 && (OP)>3.5){
#    print "Formed Betaine XXXX"
#    }
  if (runpoint>500000) {
    print "   Too many points.  XXXX"
#    system("date > nogo")
    }
  if ((CC>2.2) && (OP>3.0)) {
    print "Returned SM XXXX"
#    system("date > nogo")
    }
  system("date '+%b:%d:%Y %T'")
  system("tail -1 Echeck | grep XXXX")
  #system("uptime > uptimelist")
  }

function Distance(Atom1,Atom2) {
 return sqrt((A[Atom1]-A[Atom2])^2 + (B[Atom1]-B[Atom2])^2 + (C[Atom1]-C[Atom2])^2)
}

function Angle(Atom1,Atom2,Atom3) {
```

```
  value=((-
Distance(Atom1,Atom3)^2+Distance(Atom1,Atom2)^2+Distance(Atom2,Atom3)^2)/(2*Distance(Atom1,Atom2)*Distance(Ato
m2,Atom3)))
  return acos(value)
}

function asin(x) { return (180/3.141592)*atan2(x, sqrt(1-x*x)) }

function acos(x) { return (180/3.141592)*atan2(sqrt(1-x*x), x) }

function atan(x) { return (180/3.141592)*atan2(x,1) }

function Dihedral(Atom1,Atom2,Atom3,Atom4) {
  B1x=A[Atom2]-A[Atom1]
  B1y=B[Atom2]-B[Atom1]
  B1z=C[Atom2]-C[Atom1]
  B2x=A[Atom3]-A[Atom2]
  B2y=B[Atom3]-B[Atom2]
  B2z=C[Atom3]-C[Atom2]
  B3x=A[Atom4]-A[Atom3]
  B3y=B[Atom4]-B[Atom3]
  B3z=C[Atom4]-C[Atom3]
  modB2=sqrt((B2x^2)+(B2y^2)+(B2z^2))
# yAx is x-coord. etc of modulus of B2 times B1
  yAx=modB2*(B1x)
  yAy=modB2*(B1y)
  yAz=modB2*(B1z)
# CP2 is the crossproduct of B2 and B3
  CP2x=(B2y*B3z)-(B2z*B3y)
  CP2y=(B2z*B3x)-(B2x*B3z)
  CP2z=(B2x*B3y)-(B2y*B3x)
  termY=((yAx*CP2x)+(yAy*CP2y)+(yAz*CP2z))
# CP is the crossproduct of B1 and B2
  CPx=(B1y*B2z)-(B1z*B2y)
  CPy=(B1z*B2x)-(B1x*B2z)
  CPz=(B1x*B2y)-(B1y*B2x)
  termX=((CPx*CP2x)+(CPy*CP2y)+(CPz*CP2z))
 dihed4=(180/3.141592)*atan2(termY,termX)
 return dihed4
}

function killdyn(isomer) {
  system("rm -f dyn")
}
```

progdyn.conf

```
#This is the configuration file for PROGDYN.  This file is read by progdynstarterHP and
# the awk programs proggenHP, prog1stpoint, prog2ndpoint, and progdynb.
#The programs won't read anything past the first blank line,
#and this file must end with a blank line.
#The program has a number of default values but they are unlikely to be what you want.
#Do not delete lines - rather, comment out lines for unwanted options.
#The values here are read repeatedly and most can be changed in the middle of running jobs
#***The keywords are case sensitive.  The following keywords should always be defined:***
#***method, charge, multiplicity, memory, processors, title
#*** method --The following word is copied exactly to the gaussian input file.
method ONIOM(M062X/6-31G*:PM3)
#To do a nonstandard route, make nonstandard 1.  For normal calcs, use nonstandard 0 or else leave it out.
#Then make a file called "nonstandard" containing the nonstandard route with no extra lines.
nonstandard 0
# NMRoptions As is NMRtype=1 will add a section for an NMR calc at every NMRevery intervals.  If you want to combine the
two use nonstandard
#NMRtype 1
#NMRmethod2 B97D/6-31G*
#NMRmethod LC-wPBE/6-31G*
#NMRmethod3 B3LYP/cc-pvtz
#NMRevery 4
#NMRrand 1
#NMRcc 1
```

```
#loadlimit 10.0
#geometry linear
rotationmode 0
#*** method2 --The options here are restricted, unrestricted, and read. restricted is the default
#If the method is U..., put unrestricted here and the .com files will have in them guess=mix.
#If you put read here, the .com files will contain guess=tcheck, which sometimes makes things faster, sometimes not.
#The use of read requires a specifically defined checkpoint file name using the keyword checkpoint.
method2 restricted
charge 0
multiplicity 1
processors 8
#*** memory --The following "word" is copied exactly to the gaussian input file after %mem=.
memory 12gb
#*** killcheck and checkpoint -- You can use a specifically defined checkpoint file name by putting
#the name after the keyword checkpoint.  This is necessary if you use the read option with method2.
#Defined checkpoint names are an unnecessary modest hastle and if you do not want to bother, use killcheck 1
#killcheck 1
checkpoint g09.chk
#*** diagnostics -- 0 prints out nothing extra, 1 (default) prints out extra stuff to a
#file "diagnostics", 2 adds more stuff, 3 adds velocities to a file "vellist"
#4 adds the apparent temperature to vellist, but this is meaningless with quasiclassical calculations
diagnostics 0
#*** title -- the title keyword must be followed by exactly four words
title THF PM3ONIOM wittigbetaine dynclassical
#*** initialdis -- 0 (default) turns off displacement of the normal modes, so that all trajectories start from the same place
# and only the energies and signs of the motion in the modes are randomized
# 1 gives a flat distribution of displacements where all of the possible values are equally likely
# 2 (recommended) gives a QM-like gaussian distribution of displacements, so that displacements in the middle are more likely
that
# those at the end by 1/e
initialdis 0
#*** timestep -- this is the time between points in the trajectory.  Typical values would be 1E-15 or 0.5E-15 or 0.25E-15
timestep 1E-15
#*** scaling -- this lets you scale the gaussian frequencies by a constant
scaling 1.0
temperature 340.15
#*** thermostat 1 puts in a damping factor so as to bring the classical temperature toward the desired temperature.
#*** use a thermostatmult between 0.95 and 1, typically 0.995, so the damping happens slowly - otherwise there will be
#*** overadjustment in response to random variation
#*** the thermostat is not exact.  The second traj point ignores this, so it only applies to later points handled by progdynb.
thermostat 1
thermostatmult 0.998
#*** method3, method4, method5, and method6 -- These keywords let you add extra lines to the gaussian input file.
#method3 and method4 add lines at the top of the input after the lines defining the method, and
#this is useful to implement things like the iop for mPW1k
#method5 and method6 add lines after the geometry, after a blank line of course
#only a single term with no spaces can be added, one per method line.  Here are some examples to uncomment if needed
#method3 IOp(3/76=0572004280)
#method3 scrf=(pcm,solvent=ethanol)
#method3 scrf=(pcm,Solvent=dichloromethane)
#add the line below with big structures to get it to put out the distance matrix and the input orientation
method4 iop(2/9=2000)
#method4 iop(3/124=3)
#method4 scrf=(pcm,solvent=dmso,read)
#method5 radii=bondi
#method6
#*** methodfile -- This keyword lets you add more complicated endings to gaussian input files
#such as a gen basis set.  Put after the keyword the number of lines in a file you create called
#methodfile that contains the test you want to add to the end of the gaussian input
methodfile 0
#*** numimag --This tells the program the number of imaginary frequencies in the starting structure.
#if 0, treats as ground state and direction of all modes is random
#if 1, motion along the reaction coordinate will start out in the direction defined by searchdir
#if 2, only lowest freq will go direction of searchdir and other imag mode will go in random direction
numimag 0
#*** searchdir -- This keyword says what direction to follow the mode associated with the imaginary frequency.
#The choices are "negative" and "positive".  Positive moves in the direction defined in the gaussian frequency calculation
#for the imaginary frequency, while negative moves in the opposite direction.  The correct choice can be made either
#by a careful inspection of the normal modes and standard orientation geometry, or by trial and error.
searchdir negative
#*** classical --  for quassiclassical dynamics, the default, use 0.  for classical dynamics, use 1
#if there are no normal modes and the velocities are to be generated from scratch, use classical 2
```

```
classical 2
#*** DRP, saddlepoint, and maxAtomMove --to run a DRP use 'DRP 1' in the line below, otherwise leave it at 0 or comment it
out
#the treatment of starting saddlepoints is not yet implemented so use saddlepoint no
#if DRP shows oscillations then decrease maxAtomMove
#DRP 1
#saddlepoint no
#maxAtomMove 0.01
#*** cannonball -- The program can "fire" a trajectory from a starting position toward a particular target, such as toward
#a ts.  To use this, make a file cannontraj with numAtom lines and three numbers per line that defines the vector
#for firing the trajectory, relative to the starting geometry's standard orientation.  The number following cannonball sets
#the extra energy being put into the structure in kcal/mol
#cannonball 10
#*** keepevery --This tells the program how often to write the gaussian output file to file dyn, after the first two points.
#Use 1 for most dynamics to start with, but use a higher number to save on disk space or molden loading time.
keepevery 99
#*** highlevel --For ONIOM jobs, the following line states the number of highlevel atoms,
#which must come before the medium level atoms.  Use some high value such as 999 if not using ONIOM
highlevel 60
#*** fixedatom1, fixedatom2, fixedatom3, and fixedatom4 - These fix atoms in space.
#Fixing one atom serves no useful purpose and messes things up, while fixing two atoms
#fixes one distance and fixing three has the effect of fixing three distances, not just two
#in current form fixed atoms only are meant to work with no displacements, that is, initialdis=0
#fixedatom1 1
#fixedatom2 3
#fixedatom3 3
#fixedatom4 4
#*** boxon and boxsize - With boxon 1, a cubic box is set such that atoms that reach the edge
#are reflected back toward the middle.  Useful for dynamics with solvent molecules.  This is a crude
#implementation that is ok for a few thousand femtoseconds but will not conserve energy long term.
#Set the box size so as to fit the entire initial molecule but not have too much extra room.
#The dimensions of the box are two times the boxsize, e.g. boxsize 7.5 leads to a box that is 15 x 15 x 15 angstroms
boxon 1
boxsize 10.2
#*** displacements -- This keyword lets you set the initialdis of particular modes by using a series of lines of the format
# displacements NumberOfMode InitialDisForThatMode, as in the example below. You should be able to do as many of these as
you like
# you might consider this for rotations where a straight-line displacement goes wrong at large displacements
# The choices for InitialDisForThatMode are 0, 1, 2, and 10, where 10 does the same thing as 0 but is maintained for now
because
# a previous version of the program had a bug that made 0 not work.
#displacements 2 0
#displacements 3 0
#displacements 4 0
#displacements 5 0
#displacements 6 0
#displacements 7 0
#displacements 8 0
#displacements 9 0
#displacements 10 0
#*** etolerance --This sets the allowable difference between the desired energy in a trajectory and the actual
#energy, known after point 1 from the potential energy + the kinetic energy in the initial velocities.
#The unit is kcal/mol and 1 is a normal value for mid-sized organic systems.  For very large and floppy molecules, a larger value
#may be needed, but the value must stay way below the average thermal energy in the molecule (not counting zpe).
#If initialdis is not 0 and few trajectories are being rejected, decrease the value.
etolerance 9999999999
#*** controlphase --It is sometimes useful to set the phase of particular modes in the initialization of trajectories.
#The format is controlphase numberOfModeToControl positive or controlphase numberOfModeToControl negative.
#controlphase 2 positive
#*** damping -- The damping keyword lets you add or subtract energy from the system at each point, by multiplying the
velocities
#by the damping factor.  A damping of 1 has no effect, and since you mostly want to change the energy slowly, normal values
range
#from 0.95 to 1.05.  The use of damping lets one do simulated annealing - you add energy until the structure is moving enough
#to sample the kinds of possibilities you are interested in, then you take away the energy slowly.
damping 1.000
#at a damping of .9995, the energy is cut in half in 693 points
#*** reversetraj --This keyword sets the trajectories so that both directions from a transition state are explored.
reversetraj true

# reading the file is terminated at a blank line
```

Program progdynsam

```
BEGIN {
temp=340.15
if (pt<1) startpoint=250
if (pt>1) startpoint=pt
line=0
printon=0
pointline=0
secondpoint=0
}

{
line++
if (line==1) numAtoms=$1
pointline++
if (printon==1) {
  if ($1=="H") atWeight[pointline]=1.00783
  if ($1=="C") atWeight[pointline]=12.0000
  if ($1=="O") atWeight[pointline]=15.99940
  if ($1=="P") atWeight[pointline]=30.9738
  if ($1=="N") atWeight[pointline]=14.0030740
  if ($1=="Cl") atWeight[pointline]=35.4527
  if (($1=="C") || ($1=="H") || ($1=="O") || ($1=="P") || ($1=="N") || ($1=="Cl")) {
    Arr0[pointline,0]=$1
    Arr0[pointline,1]=$2
    Arr0[pointline,2]=$3
    Arr0[pointline,3]=$4
    Arr1[pointline,0]=$1
    Arr1[pointline,1]=$2
    Arr1[pointline,2]=$3
    Arr1[pointline,3]=$4
    }
  }
if (secondpoint==1) {
  if (($1=="C") || ($1=="H") || ($1=="O") || ($1=="P") || ($1=="N") || ($1=="Cl")) {
    Arr1[pointline,1]=$2-Arr1[pointline,1]
    Arr1[pointline,2]=$3-Arr1[pointline,2]
    Arr1[pointline,3]=$4-Arr1[pointline,3]
    }
  }
if ($8=="runisomer") {
  pointline=0
  }
if ($7==startpoint) {
  pointline=0
  printon=1
  }
if ($7==startpoint+1) {
  secondpoint=1
  pointline=0
  printon=0
  }
if ($7==startpoint+2) {
  secondpoint=0
  printon=0
  }

}

END {
print numAtoms
for (i=1;i<=numAtoms;i++) {
  print Arr0[i,0],Arr0[i,1],Arr0[i,2],Arr0[i,3],atWeight[i]
  }
conver1=4.184E26
srand()
timestep=1E-15
for (i=1;i<=100;i++) {
  newRand=rand()
  newRand2=rand()
  randArr[i]=newRand
```

```
  sign[i]=1
  if (newRand2<0.5) sign[i]=-1
}
for (i=1;i<=numAtoms;i++) {
  if ((Arr1[i,1]==0) && (Arr1[i,2]==0) && (Arr1[i,3]==0)) {
    for (j=1;j<=3;j++) {
      KE=-0.001987*temp*log(1-randArr[3*i+j])
      Vel=sign[3*i+j]*timestep*(2*KE*conver1/atWeight[i])^0.5
      Arr1[i,j]=Vel
      }
    }
  print Arr1[i,1],Arr1[i,2],Arr1[i,3]
  }
printf("%s %i %i %s ","generated from points",startpoint,startpoint+1,"in a trajectory, so no modes to print out")
system("pwd")
print "Total mode energy desired=",0
for (i=1;i<=700;i++) {
  velsq= Arr1[i,1]^2+Arr1[i,2]^2+Arr1[i,3]^2
  KE=1E30*0.5*atWeight[i]*velsq/conver1
  KE=2.388E3*0.5*atWeight[i]*velsq
  #print i,KE
  }
print ""
}
```

Program progbetalength

#This awk program extracts data from a set of output *dynfollowfile* files from trajectories. The first column gives a symbol for the outcome of the trajectory (SMPO, POSM, SMSM, or POPO), the second column defines the length of time taken to go from transition state to transition state, the third column gives the lifetime of the betaine, and later columns give ancilliary details.

```
BEGIN {
if (pt==0) startpoint=0
if (pt!=0) startpoint=pt
CCdef=1.650001
maxCC=1.89001
minPO=2.53001
maxCCfinal=2.1501
minPOfinal=1.9201
forward=1
oldpoint=0
oldisomer=0
for (i=-2500;i<2502;i++) {
  arrx[i]=0
  arry[i]=0
  }
}
/runisomer/ {
  if (oldfilename!=FILENAME) {
    forward=1
    }
  if ($5==1) {
    if ((oldfilename==FILENAME) && ($7==oldisomer)) forward=-1
    if (($7!=oldisomer) || (oldfilename!=FILENAME)) {
      forward=1
      for (i=-2500;i<2502;i++) {
        arrx[i]=0
        arry[i]=0
        }
      }
    arrx[forward*$5]=$9
    arry[forward*$5]=$11
    }
  if ($5>1) {
    arrx[forward*$5]=$9
    arry[forward*$5]=$11
    }
  oldpoint=$5
  oldisomer=$7
  oldfilename=FILENAME
  }
```

```
/XXX/ {
if (forward==1) {
  if ($19=="OP") resfor="op"
  if ($19=="SM") resfor="sm"
  }
if (forward==-1) {
  if ($19=="OP") resback="op"
  if ($19=="SM") resback="sm"
  }
if (forward==-1) {
  #fill in gaps in numbers
  for (i=-2495;i<2495;i++) {
    if ((arrx[i-5]>0) && (arrx[i+5]>0) && (arrx[i]==0)) {
      arrx[i]=arrx[i-1]
      arry[i]=arry[i-1]
      }
    }

#determine starting number on minus side
  starti=-2500; endi=2502
  for (i=-1;i>-2500;i--) {
    if (arrx[i]>maxCCfinal) {
      resminus="SM"
      }
    if ((arry[i]<minPOfinal) && (arry[i]>0)) {
      resminus="PO"
      }
    if ((arrx[i]>maxCC) && ((arrx[i+1]<maxCC) && (arrx[i+1]>0)i)) {
      starti=i+1
      }
    if ((arry[i]<minPO) && (arry[i+1]>minPO) && (arry[i]>0)) {
      starti=i+1
      }
    }
#determine ending number on plus side
  for (i=1;i<2502;i++) {
    if (arrx[i]>maxCCfinal) {
      resplus="SM"
      }
    if ((arry[i]<minPOfinal) && (arry[i]>0)) {
      resplus="PO"
      }
    if ((arrx[i]>maxCC) && (arrx[i-1]<maxCC) && (arrx[i-1]>0)) {
      endi=i-1
      }
    if ((arry[i]<minPO) && (arry[i-1]>minPO) && (arry[i]>0)) {
      endi=i-1
      }
    }
# determine the point at which the CC bond is first fully formed
  betainestart=0
  if ((resminus=="SM") && (resplus=="PO")) {
    for (i=2500;i>-2500;i--) {
      if ((arrx[i]<CCdef) && (arrx[i-1]>CCdef) && (arrx[i]>0)) {
        betainestart=i
        }
      }
    print resminus resplus,"    ",endi-starti,"     ",endi-betainestart,"     ","starti",starti,"endi",endi,"betainestart",betainestart,
FILENAME" isomer "$7,resfor resbac
    }
  if ((resminus=="PO") && (resplus=="SM")) {
    for (i=-2500;i<2500;i++) {
      if ((arrx[i]<CCdef) && (arrx[i+1]>CCdef) && (arrx[i]>0)) {
        betainestart=i
        }
      }
    print resminus resplus,"    ",endi-starti,"     ",betainestart-starti,"     ","starti",starti,"endi",endi,"betainestart",betainestart,
FILENAME" isomer "$7,resfor resbac
    }
  if ((resminus=="PO") && (resplus=="PO")) {
    betainestart=0
```

```
    print resminus resplus,"    ",endi-starti,"     ",betainestart-starti,"     ","starti",starti,"endi",endi,"betainestart",betainestart,
FILENAME" isomer "$7,resfor resbac
    print "xxxx","    ","xxx","     ",endi-betainestarti,"     ","starti",starti,"endi",endi,"betainestart",betainestart, FILENAME"
isomer "$7,resfor resbac
    }
# for SMSM trajectories, want to report lifetime 0 times if the CC never below CCdef, one time if started at TS and goes <CCdef,
both if started at betaine with CC<CCdef
  if ((resminus=="SM") && (resplus=="SM") && arrx[1]>CCdef) {
    betainestartf=0
    betainestartb=0
    for (i=2500;i>0;i--) {
      if ((arrx[i]<CCdef) && (arrx[i-1]>CCdef) && (arrx[i]>0)) {
        betainestartf=i
        }
      }
    if (betainestartf>0) {
      print resminus resplus,"    ",endi-starti,"     ",endi-betainestartf,"     ","starti",starti,"endi",endi,"betainestartf",betainestartf,
FILENAME" isomer "$7,resfor resbac
      }
    for (i=-2500;i<0;i++) {
      if ((arrx[i]<CCdef) && (arrx[i+1]>CCdef) && (arrx[i]>0)) {
        betainestartb=i
        }
      }
    if ((betainestartf==0) && (betainestartb<0)) {
      print resminus resplus,"    ",endi-starti,"     ",betainestartb-starti,"     ","starti",starti,"endi",endi,"betainestartb",betainestartb,
FILENAME" isomer "$7,resfor resbac
      }
    if ((betainestartf>0) && (betainestartb<0)) {
      print "xxxx","    ",endi-starti,"     ",betainestartb-starti,"     ","starti",starti,"endi",endi,"betainestartb",betainestartb,
FILENAME" isomer "$7,resfor resbac
      }
    if ((betainestartf==0) && (betainestartb==0)) {
      print resminus resplus,"    ",endi-starti,"     ","NoBetaine","     ","starti",starti,"endi",endi,"xxx","xxx", FILENAME" isomer
"$7,resfor resbac
      }
    }
  if ((resminus=="SM") && (resplus=="SM") && arrx[1]<CCdef) {
    betainestart=0
    print resminus resplus,"    ",endi-starti,"     ",betainestart-starti,"     ","starti",starti,"endi",endi,"betainestart",betainestart,
FILENAME" isomer "$7,resfor resbac
    print "xxxx","    ","xxx","     ",endi-betainestarti,"     ","starti",starti,"endi",endi,"betainestart",betainestart, FILENAME"
isomer "$7,resfor resbac
    }



#  print resminus resplus,"    ",endi-starti,"     ","starti",starti,"endi",endi, FILENAME" isomer "$7,resfor resback
  resfor=""
  resback=""
  resminus=""
  resplus=""
  startpoint++
  for (i=-2500;i<2502;i++) {
    arrx[i]=0
    arry[i]=0
    }
  }
oldresult=$14" "$15" "$16
}
```

NMR Integration Macro

The listing below shows a sample macro for the output of NMR integrations. The spectra were first carefully phased by hand and the phases were recorded for use in the macro. The integration cut points shown in the macro were in each case used for both the sample and the standard.

Macro “sam1324doc”

```
$filename='/nmrdata/singleton/chen/081513-OMePhCHO-sample-fid13to24-doc.fid'
$filenameshort='Chen-Anisaldehyde-doc'
rt($filename)

lvl=-0.0
rp=18
lp=8
"my cuts based on biggest 50% linewidth for each peak"
"plus first is increased due to bad peak"
$cut[1]=5
$cut[2]=4.96
$cut[3]=10.96
$cut[4]=7.2
$cut[5]=8
$cut[6]=6

setlimit('fn',2097152,8,2)
fn=1048576
wft('all')
wc=550
axis='p'

"For this program the argument is the number of spectra to be worked up in the array"
if ($#<1) then $numspec=12 else $numspec=$1 endif
$multiplier=1

$spectrum=1
repeat
ds($spectrum)
echo('new spectrum')

"First, I want to get the full spectrum, set some basics and set the shifts"
$totalwidth=0
$sp=sp $wp=wp
vp=12 f intmod='partial' cz vs=160 th=5 nm

"count lines in case something is going wrong and exit if so"
nll('pos',20):$count
echo('here1')
if ($count<5 or $count>15) then
  text
  echo('Problem with wrong number of peaks.')
  return
endif

"----------Setting shifts----------"
"get carbonyl set to 190p then find chlororm and set it at 77.00"
getll(1):$ht,$freq
cr=$freq
rl(190.28p)
sp=76.0p wp=4p
echo('here2')
repeat
  nll('pos',10):$count
  if ($count<3) then th=th-1 endif
  if ($count>3) then th=th+1 endif
```

```
   nll('pos',10):$count
until ($count=3)
getll(2):$ht,$freq
cr=$freq rl(77.00p) f
echo('here3')
"----------------------------------------------------------------"

"-----------------------------Cutting integrations---------------"
"to turn off this section make the next line false, to turn it on make the line true"
if (2>1) then

cz
"1 now focus on carbonyl ono far left and cut it"
sp=187p wp=6p
repeat
   nll('pos',144):$count
   if ($count<1) then th=th-1 endif
   if ($count>1) then th=th+1 endif
   nll('pos',144):$count
until ($count=1)
$i=1
repeat
   getll($i):$ht,$freq
   dres($freq):$lw
   write('file','/home/singleton/dsingle/linewidths1','%.3f ',$lw)
   $totalwidth=$totalwidth+$lw
   z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
   $i=$i+1
until ($i>1)

"2 now focus on second peak from the left"
sp=162p wp=6p
repeat
   nll('pos',20):$count
   if ($count<1) then th=th-1 endif
   if ($count>1) then th=th+1 endif
   nll('pos',20):$count
until ($count=1)
$i=2
repeat
   getll($i-1):$ht,$freq
   dres($freq):$lw
   write('file','/home/singleton/dsingle/linewidths2','%.3f ',$lw)
   $totalwidth=$totalwidth+$lw
   z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
   $i=$i+1
until ($i>2)

"Now focus on cutting the third peak, cut them"
sp=130p wp=6p
repeat
   nll('pos',20):$count
   if ($count<1) then th=th-1 endif
   if ($count>1) then th=th+1 endif
   nll('pos',20):$count
until ($count=1)
```

```
$i=3
repeat
  getll($i-2):$ht,$freq
  dres($freq):$lw
  write('file','/home/singleton/dsingle/linewidths3','%.3f ',$lw)
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
  $i=$i+1
until ($i>3)

"now focus on cutting peaks 4"
sp=128p wp=2p
repeat
  nll('pos',80):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',80):$count
until ($count=1)
$i=4
repeat
  getll($i-3):$ht,$freq
  dres($freq):$lw
  write('file','/home/singleton/dsingle/linewidths4','%.3f ',$lw)
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
  $i=$i+1
until ($i>4)

"Focus on cutting peaks 5 "
sp=111p wp=6p
repeat
  nll('pos',60):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',60):$count
until ($count=1)
$i=5
repeat
  getll($i-4):$ht,$freq
  dres($freq):$lw
  write('file','/home/singleton/dsingle/linewidths5','%.3f ',$lw)
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
  $i=$i+1
until ($i>5)


"Focus on cutting peaks 6 "
sp=52p wp=6p
repeat
  nll('pos',70):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',70):$count
until ($count=1)
$i=6
```

```
repeat
   getll($i-5):$ht,$freq
   dres($freq):$lw
   write('file','/home/singleton/dsingle/linewidths6','%.3f ',$lw)
   $totalwidth=$totalwidth+$lw
   z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
   $i=$i+1
until ($i>6)

endif
"-----------------------------------------------------------------"

echo('The average line width is ',$totalwidth/6)

"--------------------------Output integrals-------------------------"
"to turn off this section make the next line false, to turn it on make the line true"
if (2>1) then
   intmod='partial'
   f
   nll('pos',20):$count
   printon
   shell('date')
   text(file)
   echo('The average line width is ',$totalwidth/6)
   nli
   setint(5,2000)
   printoff('/home/singleton/dsingle/vnmrsys/maclib/temp1')
   shell('cat /home/singleton/dsingle/vnmrsys/maclib/temp1 >>
/home/singleton/dsingle/vnmrsys/maclib/tempsam1324doc')

endif
"-----------------------------------------------------------------"

$spectrum=$spectrum+1
until ($spectrum>$numspec)

sp=$sp wp=$wp
```

Calculated Structures and Complete Energies

Guide to Structures, Structure Titles and Their Organization

The calculated structures provided are divided into large groups by system, then divided by method / basis set / solvent model.

The first section below shows the geometries associated with the reaction of $Me_3PCHCHO$ with formaldehyde. Since the purpose of these calculations was the evaluation of the accuracy of various combinations of functionals and basis sets, and this was done entirely by comparison of single-point (potential) energies versus G3B3 potential energies *for the same geometry*, this section presents only the geometries. The energies are given in a table in a previous section.

The second section below provides structures and a complete set of energies for the reaction of **1** with **2**. For the purpose of ease in record keeping and data retrieval, the listings

here include a file name and complete path for the server on which the calculations are saved. The structure names and file names associated with these structures ended up complicated because our explorations started from structures in the work of Robiette, Richardson, Aggarwal, and Harvey (ref 5 in the main text).

In that work:

"TS1" was the first / only transition state between starting materials and oxaphosphetane

"OP1" was the initially formed oxaphosphetane

"OP2" was a second oxaphosphetane preceding cleavage.

"TS2" was a transition state for cleavage of the oxaphosphetane OP2

Our structure names and file names followed this system initially, but then we found that all calculations including diffuse functions (and an implicit solvent model) located two transition states between the starting materials and the oxaphosphetane (with the exception of the lc-wPBE/6-31+G** calculations). Further, the first-formed oxaphosphetane corresponds to a conformationally different oxaphosphetane from that seen by Robiette et. al. So we ended up using a structure and file-naming system that is kludged on top of the previous system.

In this work:

"TS1" is the initial transition state between starting materials and betaine.

"betaine" is the zwitterionic intermediate.

"TS1.5" is the transition state between the betaine and the initial oxaphosphetane

"OP1direct" is the oxaphosphetane formed from TS1.5. It differs conformationally from OP1 in the cant of the phenyl rings.

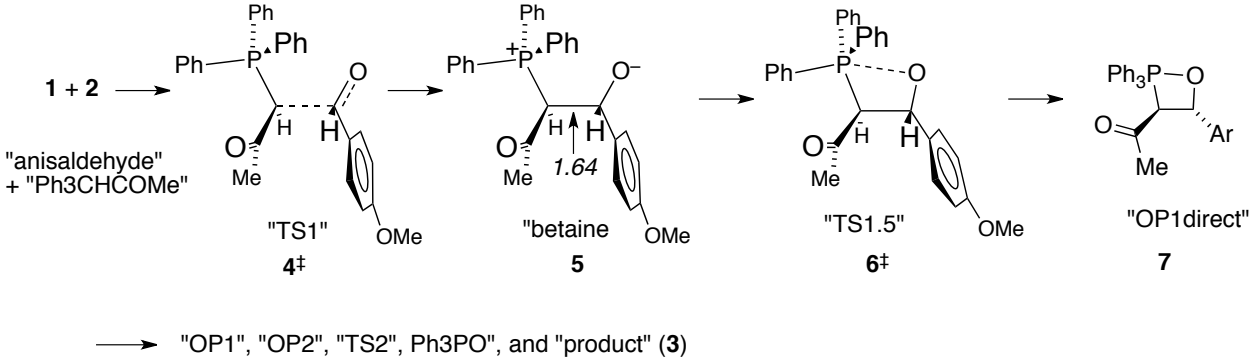
"OP1" is the oxaphosphetane corresponding to OP1 in Robiette et. al.

"OP2" is the oxaphosphetane corresponding to OP2 in Robiette et. al.

"TS2" is still a transition state for cleavage of the oxaphosphetane OP2

"product" refers to the overall product **3**

"Ph3PCHCOMe," "anisaldehyde," and "Ph3PO" are self explanatory



The file names also contain "codes" that denote other aspects of the calculation:

"PS" means 6-31+G**

"SB" means 6-31G*

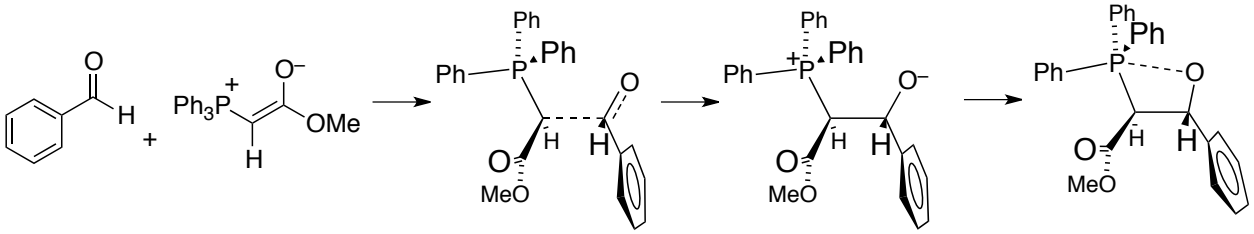
"M062X" is self explanatory.

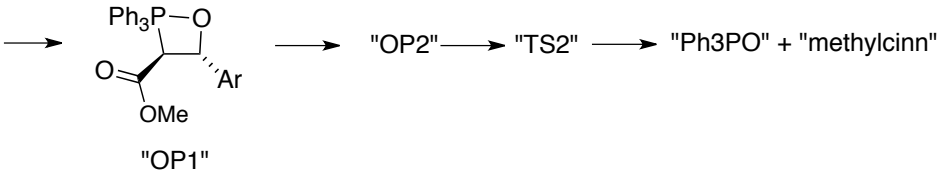
"smd" refers to structures optimized with the SMD solvation model. All other structures were optimized with a PCM model unless otherwise noted.

"UAKS" refers to structures optimized with the UAKS set of radii found in Gaussian09.
"paul" refers to structures optimized with the Pauling set of radii found in Gaussian09.

We carried out both intuition-driven and simulated-annealing searches for lower energy conformations, particularly with regard to other conformations of TS1. Except for rotations about the distal methoxy group, which was considered negligible, the alternative conformers located were significantly higher in energy, and they are not listed here. We were unable to locate a potential-energy minimum for the anti-betaine in M06-2X/6-31+G**/PCM calculations, though our search was not exhaustive.

A final section provides structures and a complete set of energies for the reaction of benzaldehyde with the ester-stabilized ylide Ph_3PCHCO_2Me. The names TS1, betaine, TS1.5, OP1, OP2, and TS2 have analogous meanings to those above for the main-text system, allowing for the difference in ylides and aromatic aldehyde. No structure corresponding to OP1direct was found in this system, though we did not specifically search for it. The name "methylcinn" refers to *trans*-methyl cinnamate, *E*-$PhCH{=}CHCO_2Me$. Other abbreviations retain their meanings from above.





Tabulated Energies for the Full System

Table S5. Absolute and relative energies for the reaction of anisaldehyde (**1**) with Ph3PCHCOMe (**2**). Relative energies are versus the reactants and are in kcal/mol.

	M062X/6-31+G**/ PCM potential energy	E_{rel}	E + zpe	E_{rel}	Free Energy (1 Atm, 298 K)	E_{rel}	H(298)	S(298)
anisaldehyde	-459.931870		-459.788204		-459.822315		-459.778400	92.43
Ph3PCHCOMe	-1227.873970		-1227.533555		-1227.587462		-1227.511575	159.72
TS1	-1687.793615	**7.7**	-1687.307770	**8.8**	-1687.371229	**24.2**	-1687.276725	198.90
betaine	-1687.795865	**6.3**	-1687.307451	**9.0**	-1687.369753	**25.1**	-1687.276561	196.14
TS 1.5	-1687.794726	**7.0**	-1687.307197	**9.1**	-1687.371551	**24.0**	-1687.276750	199.53
OP1direct	-1687.806867	**-0.6**	-1687.317162	**2.9**	-1687.379006	**19.3**	-1687.286993	193.66
OP1	-1687.801374	**2.8**	-1687.311961	**6.1**	-1687.372736	**23.2**	-1687.282279	190.38
OP2	-1687.806484	**-0.4**	-1687.316835	**3.1**	-1687.379531	**19.0**	-1687.286240	196.35
TS2	-1687.806106	**-0.2**	-1687.317226	**2.8**	-1687.379122	**19.2**	-1687.287218	193.43
Ph3PO	-1111.239812	**-26.0**[a]	-1110.958784	**-24.7**[a]	-1111.004915	**-24.6**[a]	-1110.941265	133.96
product	-576.607479		-576.402339		-576.444062		-576.388469	117.01

	Free Energy (1 M, 340 K)[b]		M062X/6-31+G(2df,p)/ PCM//M062X/6-31+G**/ PCM potential energy		Free Energy (1 M, 340 K)[b]	
anisaldehyde	-459.825057		-459.961645		-459.854833	
Ph3PCHCOMe	-1227.594708		-1227.928009		-1227.648747	
TS1	-1687.381097	**24.3**	-1687.874821	**9.3**	-1687.462303	**25.9**
betaine	-1687.379438	**25.3**	-1687.876480	**8.3**	-1687.460053	**27.3**
TS 1.5	-1687.381463	**24.0**	-1687.875453	**8.9**	-1687.462190	**26.0**
OP1direct	-1687.388524	**19.6**	-1687.889849	**-0.1**	-1687.471506	**20.1**
OP1	-1687.382036	**23.7**				
OP2	-1687.389229	**19.2**				
TS2	-1687.388625	**19.5**				
Ph3PO	-1111.010437	**-24.5**[a]	-1111.294007	**-29.0**[a]	-1111.064633	**-27.5**[a]
product	-576.448450		-576.641857		-576.482828	

	M062X/6-31G*/ PCM potential energy		Free Energy (1 Atm, 298 K)	
anisaldehyde	-459.906661		-459.796019	
Ph3PCHCOMe	-1227.819619		-1227.529705	
TS1	-1687.715985	**6.5**	-1687.289704	**22.6**
betaine	-1687.717265	**5.7**	-1687.289225	**22.9**
TS 1.5	-1687.717160	**5.7**	-1687.288410	**23.4**
OP1direct	-1687.734545	**-5.2**	-1687.302911	**14.3**
OP1	-1687.728215	**-1.2**	-1687.300119	**16.1**
OP2	-1687.732856	**-4.1**	-1687.300585	**15.8**
TS2	-1687.730142	**-2.4**	-1687.301906	**14.9**
Ph3PO	-1111.195807	**-27.7**[a]	-1110.960907	**-28.0**[a]
product	-576.574596		-576.409393	

	M062X/6-31+G**/ SMD potential energy	E_{rel}	Free Energy (1 Atm, 298 K)	E_{rel}
anisaldehyde	-459.9384355		-459.829515	
Ph3PCHCOMe	-1227.888892		-1227.600333	
TS1	-1687.813046	9.0	-1687.392213	23.6
betaine	-1687.815419	7.5	-1687.389996	25.0
TS 1.5	-1687.814721	7.9	-1687.389309	25.4

	M062X/6-31+G**/ PCM (Pauling radii) potential energy		Free Energy (1 Atm, 298 K)	
anisaldehyde	-459.938654		-459.830086	
Ph3PCHCOMe	-1227.884363		-1227.596932	
TS1	-1687.811468	**7.2**	-1687.387603	**24.7**
betaine	-1687.816372	**4.2**	-1687.390433	**23.0**
TS 1.5	-1687.812818	**6.4**	-1687.386320	**25.5**
OP1direct	-1687.819833	**2.0**	-1687.391466	**22.3**
Ph3PO	-1111.248888	**-25.7**[a]	-1111.013713	**-23.4**[a]
product	-576.615111		-576.450618	

	M062X/6-31G*/ PCM (Pauling radii) potential energy		Free Energy (1 Atm, 298 K)	
anisaldehyde	-459.912807		-459.802951	
Ph3PCHCOMe	-1227.829340		-1227.538946	
TS1	-1687.733002	**5.7**	-1687.307068	**21.9**
betaine	-1687.736326	**3.7**	-1687.307495	**21.6**
TS 1.5	-1687.734961	**4.5**	-1687.305134	**23.1**
OP1direct	-1687.746658	**-2.8**	-1687.315700	**16.4**
OP1	-1687.740380	**1.1**	-1687.309840	**20.1**
OP2	-1687.744940	**-1.8**	-1687.314188	**17.4**
TS2	-1687.743671	**-1.0**	-1687.312933	**18.2**
Ph3PO	-1111.204908	**-27.9**[a]	-1110.970875	**-28.0**[a]
product	-576.581653		-576.415573	

	lc-wPBE/6-31+G**/ PCM potential energy			
anisaldehyde	-459.811349		-459.700092	
Ph3PCHCOMe	-1227.525492		-1227.23267	
TS1	-1687.312727	**15.1**	-1686.883588	**30.9**
OP1direct	-1687.331753	**3.2**	-1686.899616	**20.8**

	B3P86/6-31+G**/ PCM potential energy	E_{rel}	E + zpe	E_{rel}	Free Energy (1 Atm, 298 K)	E_{rel}	H(298)	S(298)
anisaldehyde	-461.421815		-461.278959		-461.312991		-461.269129	92.32
Ph3PCHCOMe	-1231.338793		-1230.999884		-1231.051832		-1230.977926	155.55
TS1	-1692.735880	**15.5**	-1692.252431	**16.6**	-1692.316293	**30.5**	-1692.221186	200.17
betaine	-1692.737283	**14.6**	-1692.252572	**16.5**	-1692.316962	**30.0**	-1692.221097	201.76
TS 1.5	-1692.737254	**14.7**	-1692.252627	**16.5**	-1692.315078	**31.2**	-1692.222010	195.88

	Free Energy (1 M, 340 K)[b]		B3P86/6-31+G(2df,p)/ PCM//M062X/6-31+G**/ PCM potential energy		Free Energy (1 M, 340 K)[b]	
anisaldehyde	-461.315726		-461.438379		-461.332290	
Ph3PCHCOMe	-1231.058799		-1231.370971		-1231.090978	
TS1	-1692.326247	**30.3**	-1692.783357	**16.3**	-1692.373724	**31.1**
betaine	-1692.327022	**29.8**	-1692.783473	**16.2**	-1692.373212	**31.4**
TS 1.5	-1692.324745	**31.2**	-1692.784594	**15.5**	-1692.372084	**32.1**

[a]Relative energy of Ph_3PO + product. [b]Corrections of the entropy to a 1 M standard state were done by subtracting 6.353 e.u. Corrections of the free energy to 340K use the approximation $G=H_{298}-TS_{298}$; this approximation underestimates the raw entropy so overestimates the raw free energy but leads to negligible errors in relative free energies.

Tabulated Energies for Benzaldehyde + Ph_3PCHCO_2Me

Table S6. Absolute and relative energies for the reaction of benzaldehyde with Ph_3PCHCO_2Me Relative energies are versus the reactants and are in kcal/mol.

	M062X/6-31+G**/ PCM potential energy	E_{rel}	Free Energy (1 Atm, 298 K)	E_{rel}
benzaldehyde	-345.445058		-345.364889	
Ph_3PCHCO_2Me	-1303.079192		-1302.785716	
E-TS1	-1648.517487	**4.2**	-1648.118495	**20.1**
betaine	-1648.521137	**2.0**	-1648.121282	**18.4**
TS 1.5	-1648.520870	**2.1**	-1648.119381	**19.6**
OP1	-1648.532624	**-5.3**	-1648.129097	**13.5**
OP2	-1648.534841	**-6.6**	-1648.133545	**10.7**
TS2	-1648.529735	**-3.4**	-1648.129130	**13.5**
Ph3PO	-1111.239812	**-30.0**[a]	-1111.004915	**-29.3**[a]
product	-537.332222		-537.192312	
Z-TS1	-1648.511487	**8.0**	-1648.112778	**23.7**

[a]Relative energy of Ph_3PO + product.

Model System, G3B3, Gas Phase

CH2O

/home/singletn/wittig/model2/CH2OG3B3
formaldehyde for Wittig high level comp
G3B3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.025762 E(Thermal)= 0.028636
E(QCISD(T))= -114.190832 E(Empiric)= -0.040560
DE(Plus)= -0.009439 DE(2DF)= -0.086333
E(Delta-G3)= -0.132353 E(G3-Empiric)= -0.040560
G3(0 K)= -114.433756 G3 Energy= -114.430881
G3 Enthalpy= -114.429937 G3 Free Energy= -114.455421

C,0,1.226,1.80351,-0.36579
H,0,1.52638,1.22092,0.53039
O,0,1.2209,3.00997,-0.37915
H,0,0.93075,1.19868,-1.24865

Me3PCHCHO

/home/singletn/wittig/model2/Me3PCHCHOG3B3
Me3PCHCHO for Wittig high level comp
G3B3

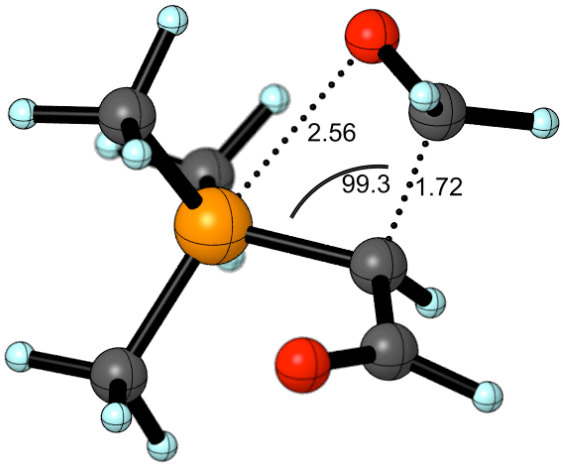
Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.144360 E(Thermal)= 0.154598
E(QCISD(T))= -612.340937 E(Empiric)= -0.141960
DE(Plus)= -0.025199 DE(2DF)= -0.301801
E(Delta-G3)= -0.681877 E(G3-Empiric)= -0.141960
G3(0 K)= -613.347415 G3 Energy= -613.337177
G3 Enthalpy= -613.336233 G3 Free Energy= -613.381737

P,0,0.3450291103,-0.29314921,-1.5851937248
C,0,0.487288457,-0.2005131511,0.1291999901
H,0,0.269174026,0.7221250334,0.655213302
C,0,0.8986125777,-1.3898366687,0.7676600207
H,0,0.9933867705,-1.3395003976,1.8755958032
O,0,1.1554623984,-2.46412802,0.1830500805
C,0,1.9019759829,-0.7184040651,-2.4577327891
H,0,1.7417295692,-0.8630593348,-3.5314647404
H,0,2.6360839419,0.0766960171,-2.2984678326
H,0,2.2726970411,-1.6421720097,-2.0064669013
C,0,-0.8705290362,-1.5302225428,-2.1837836534
H,0,-0.8545518958,-1.6233237533,-3.2749215306
H,0,-0.6014175493,-2.4837217368,-1.7224386452
H,0,-1.8729555719,-1.2435689213,-1.852974914
C,0,-0.1942165625,1.3246121623,-2.2485734569
H,0,-0.2895018447,1.2828955091,-3.3377197768
H,0,-1.1616310073,1.596968796,-1.8167899299
H,0,0.5367125928,2.0943352934,-1.9844233015

TS1

/home/singletn/wittig/model2/TS1G3B3
ts Me3PCHCHO + formaldehyde for Wittig high level comp
G3B3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.174411 E(Thermal)= 0.186552
E(QCISD(T))= -726.523985 E(Empiric)= -0.182520
DE(Plus)= -0.036430 DE(2DF)= -0.392280
E(Delta-G3)= -0.809754 E(G3-Empiric)= -0.182520
G3(0 K)= -727.770558 G3 Energy= -727.758418
G3 Enthalpy= -727.757473 G3 Free Energy= -727.807633



C,0,0.1861502342,-0.1598518717,0.0473795499
O,0,-0.1142757782,-0.1422860083,1.3237104679
P,0,2.4300946338,0.0590450104,1.5426321068
C,0,1.843820234,-0.5990090324,-0.0610673168
C,0,1.9816104218,1.7983290786,1.849646418
C,0,2.0287280569,-1.0490075665,2.9363405975
C,0,4.2698793661,0.0531702558,1.4992555385
H,0,0.153734787,0.8146686757,-0.4974671113
H,0,1.8569816243,-1.6921400143,-0.0240168789
H,0,2.5411737628,2.1763890334,2.7116652497
H,0,0.9049144648,1.8296402462,2.0173529503
H,0,2.2516236432,2.3734764782,0.9597732862
H,0,2.3055228947,-0.5639709375,3.8785661836
H,0,2.6013189253,-1.9773273205,2.8365846474
H,0,0.9563945203,-1.2391904953,2.8901360703
H,0,4.6688138528,0.4214264773,2.4504202179
H,0,4.6176986398,0.6916983748,0.6845648375
H,0,4.6398733821,-0.9640911924,1.3366549685
C,0,2.5170652371,-0.0431285106,-1.246194114
H,0,2.3550450518,-0.6156899523,-2.1853695402
O,0,3.1135209117,1.0288388436,-1.2783589642
H,0,-0.3227488662,-0.913471572,-0.5961931646

OP1

/home/singletn/wittig/model2/OP1G3B3
OP1 for Wittig high level comp
G3B3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.177394 E(Thermal)= 0.189298
E(QCISD(T))= -726.549254 E(Empiric)= -0.182520
DE(Plus)= -0.030737 DE(2DF)= -0.396902
E(Delta-G3)= -0.813096 E(G3-Empiric)= -0.182520
G3(0 K)= -727.795116 G3 Energy= -727.783212
G3 Enthalpy= -727.782267 G3 Free Energy= -727.831888

O,0,0.843860228,1.6365814561,-0.5561213229
C,0,0.5666195748,1.1594580636,0.8045159716
C,0,1.910718742,0.7071532543,1.2850538116
P,0,2.4383172592,1.2719968292,-0.8200385168
H,0,0.1323212495,1.9965287355,1.3593286676
H,0,-0.1520877847,0.3389270056,0.7383629568
H,0,2.4283464926,1.3800385822,1.9724218723
C,0,2.0808047343,-0.6975601352,1.6240922352
H,0,2.9933393957,-0.9271905793,2.224273377
O,0,1.3558091017,-1.6188094676,1.2536667763
C,0,2.9909412466,-0.4270842278,-1.2624252852
H,0,3.2713264394,-0.4898058111,-2.3175022091
H,0,3.8385552501,-0.7081360603,-0.6306943728
H,0,2.1808980337,-1.1306027654,-1.0494285349
C,0,2.3204164502,2.0069447523,-2.5352105112
H,0,3.2751841786,1.9098081117,-3.0638080777
H,0,1.5445107182,1.4955400497,-3.112667444
H,0,2.055259416,3.0674029026,-2.4799594217
C,0,3.8494079666,2.2975765729,-0.2064830236
H,0,4.4945895871,2.6143627491,-1.032681547
H,0,3.4396969635,3.19108357,0.276300933
H,0,4.4255837571,1.7407904121,0.5354976657

TS2

/home/singletn/wittig/model2/TS2G3B3
TS2 for Wittig high level comp
G3B3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.176771 E(Thermal)= 0.188134
E(QCISD(T))= -726.545333 E(Empiric)= -0.182520
DE(Plus)= -0.033409 DE(2DF)= -0.396205
E(Delta-G3)= -0.813611 E(G3-Empiric)= -0.182520
G3(0 K)= -727.794307 G3 Energy= -727.782944
G3 Enthalpy= -727.782000 G3 Free Energy= -727.830597

O,0,0.5903914771,1.4712540472,-0.4824083711
C,0,0.3916614651,0.8122748003,0.8567607488
C,0,1.7149417974,0.5413433138,1.4564783451
P,0,2.143403987,1.3796639552,-0.9260511189
H,0,-0.234506899,1.5214217831,1.4044167209
H,0,-0.1598087804,-0.1078672107,0.6521458641
H,0,2.1049465351,1.2652804233,2.1715268281
C,0,1.8966518112,2.2197861085,-2.5477351835
H,0,2.8355838099,2.2463681248,-3.1109843162
H,0,1.144982542,1.6829924559,-3.1327381241
H,0,1.5454473332,3.2445865788,-2.3949549625
C,0,3.4054094268,2.4692458085,-0.1548661541
H,0,4.0273595746,1.9015125107,0.5368930785
H,0,4.0192539007,2.9437594147,-0.9304690977
H,0,2.8866223315,3.2504136921,0.4085383179
C,0,2.8094550814,-0.2536656282,-1.3882295793
H,0,3.8639889437,-0.3075961055,-1.1004448435
H,0,2.2747581476,-1.0441168251,-0.8447838303
H,0,2.7155289619,-0.4012158224,-2.4684532448
C,0,2.1527254865,-0.8043140678,1.6151883431
O,0,1.6985221948,-1.8018788932,1.0258673891
H,0,3.0266168718,-0.933755464,2.2971261905

Me3PO

/home/singletn/wittig/model2/Me3POG3B3
Me3PO for Wittig high level comp
G3B3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.113376 E(Thermal)= 0.121121
E(QCISD(T))= -535.223841 E(Empiric)= -0.108160
DE(Plus)= -0.017469 DE(2DF)= -0.243515
E(Delta-G3)= -0.577695 E(G3-Empiric)= -0.108160
G3(0 K)= -536.057304 G3 Energy= -536.049558
G3 Enthalpy= -536.048614 G3 Free Energy= -536.088105

O,0,1.7150976947,-0.2571231884,0.3471460797
P,0,1.8911641706,0.4107754918,-0.9858826739
C,0,2.6230532581,-0.6674892069,-2.2777174894
C,0,0.3311456114,1.0211514978,-1.7349613663
C,0,2.9838422013,1.8845141102,-0.951542021
H,0,1.9826288411,-1.5435163821,-2.4202410011
H,0,3.6053970562,-1.0149148768,-1.9426985024
H,0,2.7351487186,-0.1467385945,-3.2349170798
H,0,0.500089222,1.500811093,-2.7052231995
H,0,-0.1362444005,1.741734735,-1.0565834864
H,0,-0.358085104,0.1811864943,-1.866718179
H,0,3.0874726365,2.3439591695,-1.9405596924
H,0,3.9735899705,1.5909080941,-0.5881330612
H,0,2.5709891237,2.6221615627,-0.2563103274

acrolein

/home/singletn/wittig/model2/acroleinG3B3
acrolein for wittig high level comp
G3B3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.059220 E(Thermal)= 0.063663
E(QCISD(T))= -191.360583 E(Empiric)= -0.074360
DE(Plus)= -0.013917 DE(2DF)= -0.146788
E(Delta-G3)= -0.239973 E(G3-Empiric)= -0.074360
G3(0 K)= -191.776401 G3 Energy= -191.771958
G3 Enthalpy= -191.771013 G3 Free Energy= -191.802884

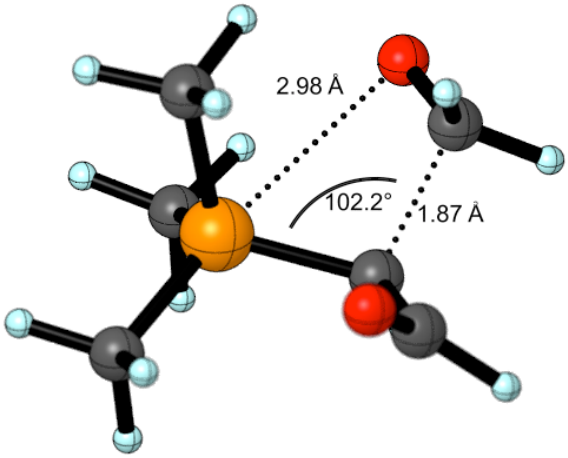
C,0,0.0045373505,0.,-0.0171400839
O,0,-0.0085836686,0.,1.1991504629
H,0,0.9690009928,0.,-0.5698827467
C,0,-1.2099511998,0.,-0.8710709742
C,0,-2.4378583218,0.,-0.339998796
H,0,-1.0543904541,0.,-1.9483967778
H,0,-3.3336523307,0.,-0.9538178429
H,0,-2.5639983683,0.,0.7394877585

TS1 from M06-2X PCM optimization

/home/singletn/wittig/model2/TS1fromM062XPCMdoneG3B3gasphase
Me3PCHCHO TS1 geo from M062XPCM calc
G3B3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.174911 E(Thermal)= 0.187179

E(QCISD(T))= -726.523438 E(Empiric)= -0.182520
DE(Plus)= -0.035931 DE(2DF)= -0.391557
E(Delta-G3)= -0.812468 E(G3-Empiric)= -0.182520
G3(0 K)= -727.771003 G3 Energy= -727.758736
G3 Enthalpy= -727.757792 G3 Free Energy= -727.808302

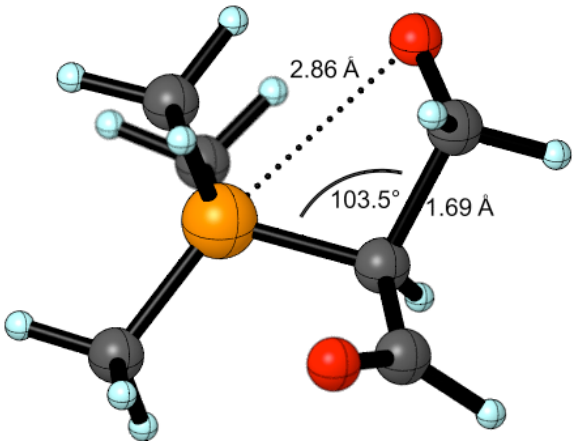


O,0,-2.3221273408,-0.2859272454,0.3648378861
C,0,-1.8030150736,-0.1253808489,-0.7890843057
C,0,-0.0446485167,-0.7696185277,-0.8421555347
P,0,0.6347112473,-0.1341088999,0.6814486063
C,0,0.5737987666,-0.2340781156,-2.0392217539
C,0,2.4476389775,-0.1106140844,0.6676781807
C,0,0.0717959736,1.5509412376,1.0181131129
C,0,0.0887413036,-1.214589779,2.0210897433
H,0,-2.1918825723,-0.71767885,-1.6436823198
H,0,-1.5626431993,0.906732061,-1.1320980164
H,0,-0.173291546,-1.8511436137,-0.8126934128
H,0,0.4374744545,-0.8276727496,-2.9639751229
H,0,2.7849541249,0.5134876412,-0.1622019134
H,0,2.8248668085,-1.1275366236,0.5374028482
H,0,2.8169550317,0.2967203347,1.612494463
H,0,0.371123525,2.1922695142,0.186731709
H,0,0.5261012642,1.9039897709,1.9473806687
H,0,-1.0166510733,1.5117938653,1.1078766179
H,0,0.3874822248,-0.796883751,2.9856765176
H,0,-0.9996119636,-1.2743687746,1.9418919225
H,0,0.5349467357,-2.2043426002,1.8953992468
O,0,1.1294428478,0.8591920387,-2.0934321434

Betaine from M06-2X PCM optimization

/home/singletn/wittig/model2/betainefromM062XPCMdoneG3B3gasphase
Me3PCHCHO betaine from M062XPCM calc
G3B3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.175153 E(Thermal)= 0.188070
E(QCISD(T))= -726.522043 E(Empiric)= -0.182520
DE(Plus)= -0.037639 DE(2DF)= -0.391626
E(Delta-G3)= -0.811699 E(G3-Empiric)= -0.182520
G3(0 K)= -727.770373 G3 Energy= -727.757457
G3 Enthalpy= -727.756512 G3 Free Energy= -727.808781

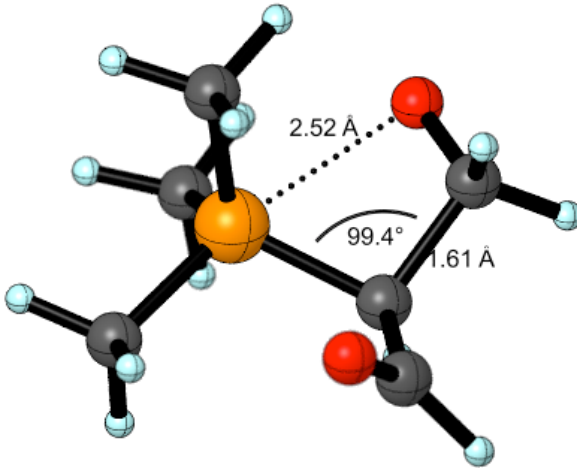


C,0,-1.8360350452,-0.101742198,-0.8326863909
O,0,-2.3917604713,-0.2723077736,0.3401340511
P,0,0.4383968102,-0.0634032392,0.7078978469
C,0,-0.2512265299,-0.6812247181,-0.8457807869
C,0,-0.1093727538,1.6248294489,1.0425281429
C,0,-0.0793292461,-1.1662797494,2.0400093019
C,0,2.2513747892,-0.0662939219,0.6676162823
H,0,-1.6764109651,0.9547893731,-1.1682607848
H,0,-0.3228446355,-1.7706448491,-0.7997110466
H,0,0.3228739466,1.9650076459,1.9870013199
H,0,-1.2001354539,1.5869193519,1.0971751186
H,0,0.2202805369,2.2708582359,0.2260548704
H,0,0.2164758594,-0.7480650051,3.005448214
H,0,0.3922401715,-2.1431075616,1.9038805022
H,0,-1.1649189433,-1.2461200859,1.9531749777
H,0,2.6324319828,0.2716271901,1.6348620216
H,0,2.5990883905,0.603060811,-0.1208745267
H,0,2.6126660414,-1.0791402747,0.4732298727
C,0,0.4572175362,-0.1881758027,-2.0410128031
H,0,0.3438466792,-0.7961888972,-2.9584503498
O,0,1.0489429779,0.8775367596,-2.0821992657
H,0,-2.2864766778,-0.6397317399,-1.6995125676

TS1.5 from M06-2X PCM optimization

/home/singletn/wittig/model2/TS1.5fromM062XPCMdoneG3B3gasphase
Me3PCHCHO TS1.5 geo from M062XPCM calc
G3B3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.174765 E(Thermal)= 0.186344
E(QCISD(T))= -726.524822 E(Empiric)= -0.182520
DE(Plus)= -0.037738 DE(2DF)= -0.393167
E(Delta-G3)= -0.810679 E(G3-Empiric)= -0.182520
G3(0 K)= -727.774161 G3 Energy= -727.762582
G3 Enthalpy= -727.761638 G3 Free Energy= -727.811626



C,0,0.2728544999,-0.1499458696,0.0164631777
O,0,-0.0935262428,-0.2525450734,1.2950464927
P,0,2.3904648864,0.0484877302,1.5542025569
C,0,1.8152692041,-0.6068451105,-0.051007101
C,0,1.9211229773,1.7732133843,1.8336261563
C,0,2.0608801349,-1.0306005699,2.9715522851
C,0,4.2155580118,0.0725046141,1.4815029038
H,0,0.2749068657,0.8844405579,-0.4103147464
H,0,1.8475845656,-1.699601907,-0.0011399663
H,0,2.4259962211,2.1354729821,2.7333516134
H,0,0.8379950366,1.805558947,1.9411905026
H,0,2.2487918869,2.3576642982,0.9705622457
H,0,2.6622325068,-0.693170794,3.8204252853
H,0,2.362130946,-2.0485202844,2.7079136901
H,0,0.9966954373,-1.0046406671,3.187737021
H,0,4.61275085,0.443139517,2.4304884329
H,0,4.5485407074,0.7219324013,0.6703768121
H,0,4.5941902521,-0.9394739983,1.3127070029
C,0,2.5315010256,-0.0737961786,-1.2403791757
H,0,2.4625326979,-0.6883839275,-2.1581932776
O,0,3.0758302166,1.0130611099,-1.2740680935
H,0,-0.2773626872,-0.7804331613,-0.7160278182

Full System, M06-2X/6-31+G**/PCM(THF) with Default Radii

Anisaldehyde 1

/home/singletn/wittig/methoxyketone/M062Xps/anisaldehyde M062XPS
anisaldehde for Wittig anisaldehyde and ketone
M062X/6-31+G**
E(RM062X) = -459.931869643

Zero-point correction= 0.143666 (Hartree/Particle)
Thermal correction to Energy= 0.152525
Thermal correction to Enthalpy= 0.153469
Thermal correction to Gibbs Free Energy= 0.109554
Sum of electronic and ZPE= -459.788204
Sum of electronic and thermal Energies= -459.779345
Sum of electronic and thermal Enthalpies= -459.778400
Sum of electronic and thermal Free Energies= -459.822315

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.711	32.954	92.426

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

Ph3PCHCOMe 2

/home/singletn/wittig/methoxyketone/M062Xps/Ph3PCHCOMeM062XPS
Ph3PCHCOMe for Wittig anisaldehyde and ketone
M062X/6-31+G**
E(RM062X) = -1227.87396966

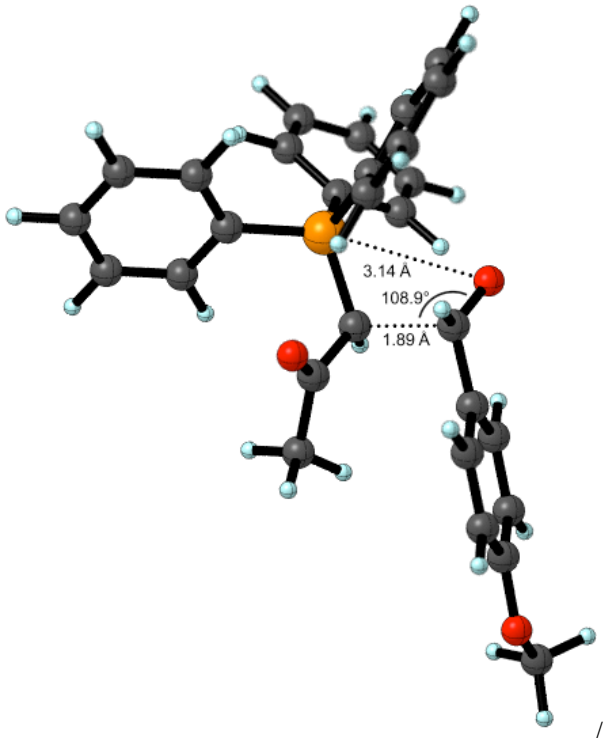
Zero-point correction= 0.340415 (Hartree/Particle)
Thermal correction to Energy= 0.361450
Thermal correction to Enthalpy= 0.362394
Thermal correction to Gibbs Free Energy= 0.286508
Sum of electronic and ZPE= -1227.533555
Sum of electronic and thermal Energies= -1227.512520
Sum of electronic and thermal Enthalpies= -1227.511575
Sum of electronic and thermal Free Energies= -1227.587462

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	226.813	80.224	159.716

C,0,0.3940928673,0.1446599875,0.4188664096
P,0,0.4339366656,-0.1266168487,2.1266935761
H,0,-0.2933816759,0.8962840058,0.0524987633
C,0,4.3209634101,1.1083726773,4.2798873919
C,0,3.0982574515,1.2474618773,4.9357072645
C,0,1.9168889283,0.881983157,4.2918393398
C,0,1.9611626191,0.3719833541,2.9891110439
C,0,3.1886107044,0.2341704322,2.3299958872
C,0,4.3647275152,0.6032889851,2.9799871088
H,0,5.2400498754,1.3966598587,4.7805842261
H,0,3.061266192,1.6434271496,5.9454451586
H,0,0.9649179896,1.0021666597,4.8027335484
H,0,3.212592375,-0.1730443145,1.3231247497
H,0,5.3166191513,0.4976547868,2.4694630823
C,0,-0.5229530696,-4.4704397964,3.3197781208
C,0,0.2538551091,-3.6835960621,4.1691522943
C,0,0.5768166451,-2.3758423464,3.8087761795
C,0,0.1145743566,-1.8549901734,2.5969121145

C,0,-0.6565947079,-2.6468001817,1.7416470153
C,0,-0.9752314326,-3.9529745337,2.1053647276
H,0,-0.7697344684,-5.4898165249,3.5995567255
H,0,0.6146427239,-4.0870355384,5.1097702805
H,0,1.1915908529,-1.7711021023,4.469565276
H,0,-0.9936645091,-2.2390824083,0.7923567174
H,0,-1.5690880379,-4.5687120048,1.4374704024
C,0,-2.8974752437,2.5014769649,3.9162148428
C,0,-1.8223503529,3.0784794996,3.2369259797
C,0,-0.8181650764,2.2716147652,2.7115309582
C,0,-0.8866473124,0.8803998525,2.8636521437
C,0,-1.9603558225,0.3043840895,3.5465651615
C,0,-2.9652843406,1.1187727939,4.0705597018
H,0,-3.6806216933,3.132036329,4.3253098612
H,0,-1.7655029552,4.1556907964,3.1186750423
H,0,0.0221752657,2.7221986823,2.1888856533
H,0,-2.0181249474,-0.7731894875,3.6700823758
H,0,-3.7999479871,0.6691344774,4.5985494579
C,0,1.1609582006,-0.676605509,-0.4298121722
C,0,1.0094029358,-0.4957353294,-1.9306134624
O,0,1.9510634438,-1.5591988986,-0.0128435181
H,0,1.9926762028,-0.2980087672,-2.3667353211
H,0,0.6407655357,-1.4315128141,-2.3617760348
H,0,0.3265796161,0.3141814597,-2.1947210736

TS1 4



/home/singletn/wittig/methoxyketone/M062Xps/TS1M062XPCMPS2
TS1 for Wittig anisaldehyde and ketone
M062X/6-31+G**
E(RM062X) = -1687.79361546

Zero-point correction= 0.485845 (Hartree/Particle)
Thermal correction to Energy= 0.515944
Thermal correction to Enthalpy= 0.516889
Thermal correction to Gibbs Free Energy= 0.422372
Sum of electronic and ZPE= -1687.307770
Sum of electronic and thermal Energies= -1687.277671
Sum of electronic and thermal Enthalpies= -1687.276727
Sum of electronic and thermal Free Energies= -1687.371243

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	323.760	115.482	198.926

O,0,1.0622354854,1.3611509586,1.6251018877
C,0,1.3708468669,0.2022348135,1.1777730313
P,0,-1.3199308016,0.1405142383,-0.0248527823
C,0,0.4113698257,-0.1107193547,-0.4193206255
C,0,2.7947894799,-0.0437995595,0.7249337668
C,0,-2.3783545629,-0.9027575369,-1.0702514072
C,0,-2.1112610337,-0.9319325718,-2.4446660889
C,0,-2.9229093281,-1.6749094355,-3.2946639943
C,0,-4.0039430357,-2.3910913928,-2.7762862086
C,0,-4.2733583896,-2.3583206958,-1.4103619719
C,0,-3.4634786533,-1.6122913524,-0.5526997783
C,0,-1.7689113052,1.8554070142,-0.4065223837
C,0,-1.753635321,-0.2075442881,1.69867522
C,0,-0.8692366907,2.8864459614,-0.1077103703
C,0,-1.2295618327,4.2050364911,-0.3795121718
C,0,-2.4728085557,4.4953025193,-0.9406500672
C,0,-3.3679605741,3.4658660198,-1.2313351853
C,0,-3.0196279122,2.1430543983,-0.9663571341
C,0,-2.3621511573,0.7736963395,2.4855317924
C,0,-2.7217858551,0.4779359159,3.7991347918
C,0,-2.4744774748,-0.7897514221,4.3226189871
C,0,-1.8667440253,-1.7683664043,3.5346349175
C,0,-1.5043282534,-1.4832359413,2.2207650346
C,0,3.3923816959,-1.298380824,0.8862841429
C,0,4.6849439625,-1.5364025153,0.4372700265
C,0,5.4062316762,-0.512455357,-0.1876518175
C,0,4.8280847612,0.7519449683,-0.3443033896
C,0,3.5297670063,0.9717193865,0.1198725106
H,0,0.9848898885,-0.6910910705,1.7145067901
H,0,0.7703322639,0.6969612702,-1.0599404531
H,0,-1.2724074069,-0.3712796911,-2.8515256242
H,0,-2.7121490962,-1.6972083152,-4.3588662315
H,0,-4.6346400111,-2.9741459667,-3.4399050807
H,0,-5.1130676139,-2.9144492672,-1.0065056852
H,0,-3.6798284773,-1.5906737459,0.5110823825
H,0,0.0836732597,2.6461699561,0.36310802
H,0,-0.5363162666,5.0069999573,-0.1469512056
H,0,-2.7451941413,5.5247526774,-1.1518379733
H,0,-4.3360557872,3.6892464819,-1.6676752644
H,0,-3.7182439877,1.3449078554,-1.1999163212
H,0,-2.5466060766,1.7652471915,2.083183107
H,0,-3.1914914638,1.2404938339,4.4116613402
H,0,-2.753864858,-1.0163057212,5.3468291228
H,0,-1.6728145722,-2.7549761744,3.9429718064
H,0,-1.0299210616,-2.237443432,1.5977573488
H,0,2.8338032025,-2.100888394,1.3642074227
H,0,5.1565980664,-2.5061482926,0.5616278685
O,0,6.6626441034,-0.8362733834,-0.6030264932
H,0,5.3721126971,1.5622692176,-0.8152509389
H,0,3.0729547844,1.9522017326,0.0098227972

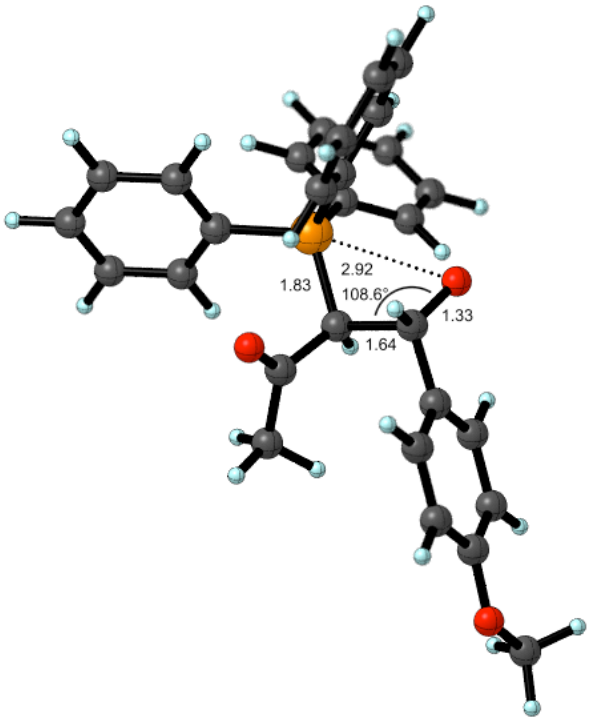
C,0,0.7333009563,-1.4674937563,-0.8816159144
C,0,1.7694898046,-1.6142989036,-1.9700980369
O,0,0.2047985577,-2.4550089225,-0.3708100582
H,0,2.2100016141,-2.6116414794,-1.930486855
H,0,1.2670488391,-1.4864971297,-2.9368766013
H,0,2.5485071756,-0.8513894002,-1.890490465
C,0,7.4256383035,0.1723261422,-1.2439269903
H,0,8.3789625377,-0.287605085,-1.5002316308
H,0,6.930082322,0.5194926031,-2.1574947772
H,0,7.5972644459,1.0221228381,-0.5741201385

Betaine 5

/home/singletn/wittig/methoxyketone/M062Xps/betaineM062XPS
betaiene product from anisaldehyde and ketone
E(RM062X) = -1687.79586467

Zero-point correction= 0.488414 (Hartree/Particle)
Thermal correction to Energy= 0.518360
Thermal correction to Enthalpy= 0.519304
Thermal correction to Gibbs Free Energy= 0.426112
Sum of electronic and zero-point Energies= -1687.307451
Sum of electronic and thermal Energies= -1687.277505
Sum of electronic and thermal Enthalpies= -1687.276561
Sum of electronic and thermal Free Energies= -1687.369753

E (Thermal) CV S
KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin
Total 325.276 115.919 196.140



O,0,0.8259422835,1.5792633085,1.2689167757
C,0,1.2507041824,0.3504831008,0.9994930203
P,0,-1.3133160301,0.0944001518,-0.0457361275
C,0,0.4698822449,-0.1900476919,-0.3374500023
C,0,2.7415249822,0.1953453437,0.7012454905
C,0,-2.2520036803,-1.1768063556,-0.944386415
C,0,-1.9665074391,-1.3762464843,-2.3015876028
C,0,-2.6784144193,-2.323603404,-3.0297243643
C,0,-3.6809011924,-3.0714095048,-2.4081964501
C,0,-3.9719177356,-2.8668282802,-1.0620959135
C,0,-3.2595262141,-1.9187218666,-0.3263034058
C,0,-1.8566187427,1.6767360232,-0.7480152871
C,0,-1.7901548173,-0.0104455384,1.6932988556
C,0,-1.0486654014,2.8157070261,-0.6403399346
C,0,-1.5016181565,4.0225546935,-1.1714161988
C,0,-2.7479916245,4.0986772729,-1.7922952355
C,0,-3.5541728711,2.964390153,-1.8864047038
C,0,-3.1112180605,1.7496510386,-1.3689057799
C,0,-2.5369204898,1.0168150285,2.2754584138
C,0,-2.9475214633,0.8996062728,3.6015711927
C,0,-2.6118485504,-0.2345210194,4.3403031956
C,0,-1.8668677278,-1.2584132848,3.7549621599
C,0,-1.455770841,-1.1543664466,2.4282009462
C,0,3.447505072,-0.9544829487,1.0731167118
C,0,4.7865479032,-1.1145064603,0.7381898186
C,0,5.4506560077,-0.1134196445,0.0197674101
C,0,4.7662350256,1.0495124835,-0.3465356249
C,0,3.4205466213,1.1890858937,0.0018635818
H,0,0.9996833238,-0.4220641208,1.7640967871
H,0,0.7710096836,0.4873590475,-1.1449235941
H,0,-1.1960945957,-0.7872556742,-2.7952352253
H,0,-2.4527938819,-2.4782095293,-4.0796698352
H,0,-4.2343567167,-3.8121008967,-2.9764250406
H,0,-4.7533643506,-3.443183568,-0.5779609827
H,0,-3.4920243169,-1.7639385,0.7224679092
H,0,-0.0974823494,2.7305226556,-0.1147367154
H,0,-0.8782131806,4.9076510154,-1.0943909996
H,0,-3.0941989763,5.0428141808,-2.201478497
H,0,-4.5262270791,3.0218653012,-2.3651939046
H,0,-3.7420691031,0.8696147641,-1.4512975595
H,0,-2.7878134422,1.9061560771,1.7054137515
H,0,-3.5236504624,1.6978102387,4.057932639
H,0,-2.9304814251,-0.3199499501,5.3744252727
H,0,-1.6046800508,-2.1407517032,4.3294550871
H,0,-0.884061892,-1.9520413973,1.96042541
H,0,2.9378007547,-1.7402535027,1.6279127879
H,0,5.3394982602,-2.0037237044,1.0248838938
O,0,6.7609051095,-0.3564136612,-0.2690347851
H,0,5.2634943666,1.8448144597,-0.8895484495
H,0,2.8802528842,2.0936472114,-0.2663382006
C,0,0.8086123056,-1.6252911821,-0.6380361439
C,0,1.8006049619,-1.8836672978,-1.7408804451
O,0,0.3309158731,-2.5258046549,0.0343440919
H,0,2.1655090861,-2.9095649116,-1.6836231564
H,0,1.2996895329,-1.7273043766,-2.7039066852
H,0,2.6334680132,-1.1764038249,-1.6820838141
C,0,7.4684320705,0.6319865221,-0.9979761492
H,0,8.4768331548,0.2429966029,-1.1323078712
H,0,7.0086306756,0.803261131,-1.9776714543
H,0,7.5107759008,1.5761403879,-0.4436976483

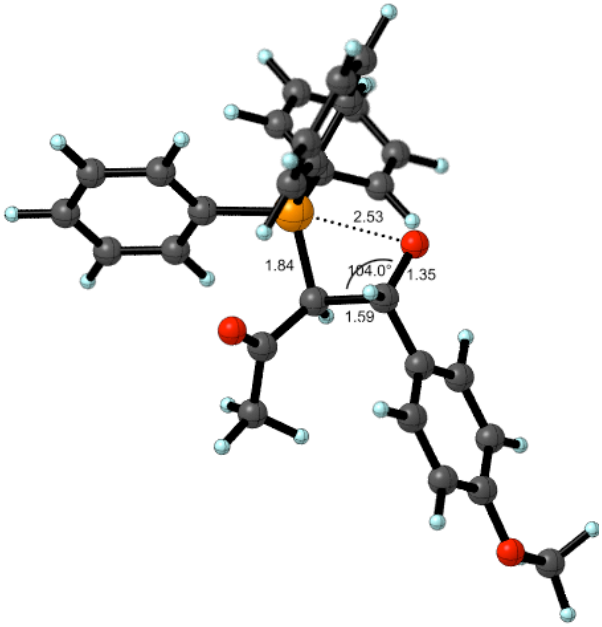
TS1.5 6

/home/singletn/wittig/methoxyketone/M062Xps/TS1.5M062XPS
betaiene product from anisaldehyde and ketone

M062X/6-31+G**
E(RM062X) = -1687.79472605

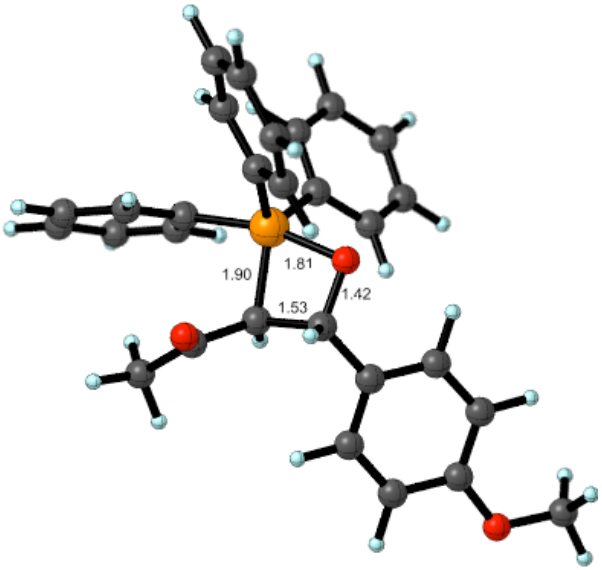
Zero-point correction= 0.487529 (Hartree/Particle)
Thermal correction to Energy= 0.517032
Thermal correction to Enthalpy= 0.517976
Thermal correction to Gibbs Free Energy= 0.423175
Sum of electronic and ZPE= -1687.307197
Sum of electronic and thermal Energies= -1687.277694
Sum of electronic and thermal Enthalpies= -1687.276750
Sum of electronic and thermal Free Energies= -1687.371551

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	324.443	114.104	199.527



O 0.721071 0.995953 1.380383
C 1.239097 -0.144224 0.879627
P-1.244968 0.133193 0.035706
C 0.447592 -0.361778 -0.482467
C 2.735143 -0.143763 0.596031
C -2.346201 -0.763451 -1.122990
C -2.096086 -0.622880 -2.495136
C -2.895522 -1.277210 -3.426253
C -3.956626 -2.075532 -2.993660
C -4.215065 -2.210258 -1.632384
C -3.412916 -1.555166 -0.695587
C -1.675200 1.875550 -0.282763
C -1.734824 -0.392397 1.693868
C -0.749257 2.910910 -0.111787
C -1.131430 4.225857 -0.373845
C -2.432343 4.516388 -0.780900
C -3.360234 3.486282 -0.933815
C -2.983479 2.166772 -0.697135
C -2.316722 0.530182 2.567244
C -2.722030 0.116243 3.833352
C -2.539837 -1.209441 4.229043
C -1.957003 -2.125721 3.355198
C -1.558048 -1.724396 2.080655
C 3.488508 -1.321524 0.665185
C 4.843402 -1.326365 0.358496
C 5.476327 -0.136915 -0.021478
C 4.742288 1.050780 -0.087828
C 3.380104 1.031955 0.222780
H 1.028823 -1.055734 1.485513
H 0.794985 0.420914 -1.168204
H -1.279770 0.008437 -2.842060
H -2.692832 -1.163942 -4.486366
H -4.580349 -2.588079 -3.719115
H -5.041615 -2.826177 -1.293038
H -3.624492 -1.667752 0.363094
H 0.241991 2.661207 0.253798
H -0.408603 5.025533 -0.247497
H -2.725024 5.543378 -0.976707
H -4.376574 3.705593 -1.244483
H -3.711841 1.373699 -0.836247
H -2.437018 1.567346 2.268450
H -3.171350 0.832154 4.513875
H -2.851634 -1.526972 5.219055
H -1.813331 -3.157177 3.660688
H -1.114459 -2.436174 1.389748
H 3.006147 -2.249986 0.967035
H 5.433029 -2.236197 0.414362
O 6.808056 -0.232669 -0.298474
H 5.214100 1.985375 -0.368147
H 2.801803 1.952017 0.192915
C 0.591142 -1.738303 -1.085379
C 1.531218 -1.865865 -2.253344
O 0.021580 -2.698084 -0.594984
H 1.722900 -2.916185 -2.472734
H 1.075199 -1.383064 -3.125945
H 2.468344 -1.340425 -2.041015
C 7.487395 0.952902 -0.674644
H 8.524562 0.666179 -0.843248
H 7.069285 1.371073 -1.597118
H 7.440243 1.703685 0.121910

OP1direct



/home/singletn/wittig/methoxyketone/M062Xps/OP1directM062XPCMPS

OP1 direct for Wittig anisaldehyde and ketone for polyrate
M062X/6-31+G**
E(RM062X) = -1687.80686728

Zero-point correction= 0.489706 (Hartree/Particle)
Thermal correction to Energy= 0.518930
Thermal correction to Enthalpy= 0.519874
Thermal correction to Gibbs Free Energy= 0.427861
Sum of electronic and ZPE= -1687.317162
Sum of electronic and thermal Energies= -1687.287937
Sum of electronic and thermal Enthalpies= -1687.286993
Sum of electronic and thermal Free Energies= -1687.379006

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	325.634	114.931	193.658

O,0,0.9049070255,0.9001795991,1.1164902508
C,0,1.7178983463,-0.2554776447,1.0235526006
P,0,-0.5915921416,0.164736521,0.4052027081
C,0,0.7922748475,-1.1140758489,0.1604534248
C,0,3.0831436926,0.0251228952,0.4400668696
C,0,-1.8678950998,-0.9630732779,-0.4769282395
C,0,-1.9156784164,-0.9946306033,-1.8783114332
C,0,-2.6422353125,-1.9727825942,-2.5591755785
C,0,-3.3357296095,-2.9516651552,-1.8480556718
C,0,-3.2902228156,-2.9452907154,-0.4547534279
C,0,-2.5598177298,-1.9652830025,0.2191895155
C,0,-0.789869983,1.6016338895,-0.73162622
C,0,-1.5051718985,0.3484903116,1.9961674036
C,0,0.3283180196,2.228537883,-1.2888501482
C,0,0.1697559668,3.294356302,-2.1753169834
C,0,-1.104333836,3.7641887125,-2.4857153341
C,0,-2.2244212586,3.1498542798,-1.924453487
C,0,-2.0675705059,2.0621344202,-1.0694381356
C,0,-2.896284141,0.5172033304,2.0019571834
C,0,-3.5844936751,0.7126027939,3.1964604712
C,0,-2.8956923529,0.7053848139,4.4087566065
C,0,-1.5154207525,0.5180342163,4.4159621563
C,0,-0.8212746325,0.3579809425,3.21715216
C,0,3.9043278849,-1.0307027685,0.0206417222
C,0,5.1727154582,-0.7917766003,-0.485605722
C,0,5.6522482165,0.5219154939,-0.5812313556
C,0,4.8502413696,1.5842083681,-0.1631399042
C,0,3.5733977431,1.323052386,0.3460866367
H,0,1.8380034628,-0.7329947574,2.009594201
H,0,1.0583781238,-1.0991909469,-0.9042082979
H,0,-1.3761822441,-0.2488631967,-2.4582854886
H,0,-2.6635829982,-1.9696914237,-3.644989006
H,0,-3.9028806115,-3.7125797005,-2.3752175656
H,0,-3.8188509596,-3.7056617196,0.1122929101
H,0,-2.5268788415,-1.9953267238,1.3053013623
H,0,1.3225837575,1.8858367869,-1.0249482011
H,0,1.0456585305,3.7626876564,-2.6133229312
H,0,-1.2259965626,4.6034294588,-3.1635252996
H,0,-3.2212920561,3.5082748348,-2.1608587347
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H,0,-3.433380632,0.8428944432,5.3418773706
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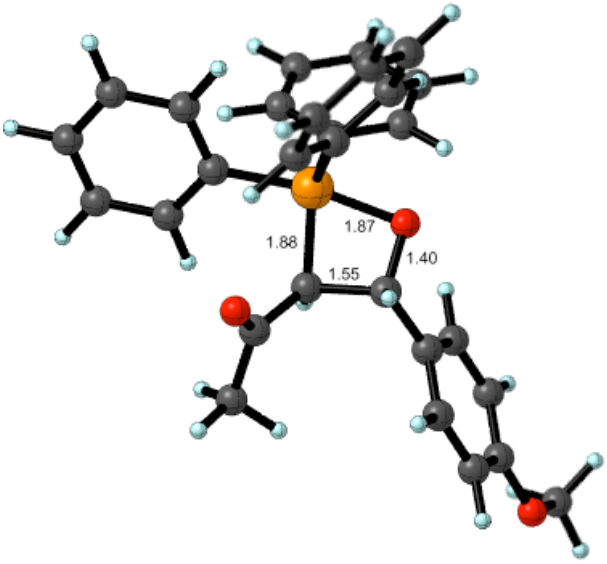
H,0,0.2556998403,0.2489404583,3.2324466769
H,0,3.5483198995,-2.0569351177,0.0932676261
H,0,5.8116997715,-1.6053529619,-0.8138512161
O,0,6.9067294144,0.6598514231,-1.0925408303
H,0,5.1977645487,2.6087628122,-0.2219127086
H,0,2.9460441467,2.1451359285,0.6774675342
C,0,0.4842989238,-2.5212168616,0.6293030003
C,0,0.2914231972,-3.5768405463,-0.425430959
O,0,0.4187022019,-2.7676251084,1.8202689549
H,0,-0.0613431785,-4.5036474229,0.027451833
H,0,-0.4162519321,-3.2294212335,-1.1857940564
H,0,1.2508549478,-3.7500811193,-0.9270539831
C,0,7.4318706154,1.9725318172,-1.2003238084
H,0,8.4307699208,1.8635934128,-1.6202533569
H,0,6.8186338329,2.5873366054,-1.8682711076
H,0,7.4973920615,2.4517255053,-0.2173720461

OP1

/home/singletn/wittig/methoxyketone/M062Xps/OP1M062XPS
OP1 for Wittig anisaldehyde and ketone
M062X/6-31+G**
E(RM062X) = -1687.80137367

Zero-point correction= 0.489413 (Hartree/Particle)
Thermal correction to Energy= 0.518151
Thermal correction to Enthalpy= 0.519095
Thermal correction to Gibbs Free Energy= 0.428637
Sum of electronic and ZPE= -1687.311961
Sum of electronic and thermal Energies= -1687.283223
Sum of electronic and thermal Enthalpies= -1687.282279
Sum of electronic and thermal Free Energies= -1687.372736

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	325.145	113.159	190.384



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C,0,1.788113766,-0.2586053641,0.5855660241
P,0,-0.5199423093,0.3322590741,0.1516847244
C,0,0.8336838584,-0.7965213747,-0.5065919483
C,0,3.2179124182,-0.0759058485,0.1428366949
C,0,-1.9878251096,-0.5290780776,-0.6909467352
C,0,-1.8216000439,-1.1352095821,-1.9421817608
C,0,-2.8971741503,-1.6960339546,-2.6313565439
C,0,-4.1751166784,-1.6552808428,-2.0767823305
C,0,-4.3648002194,-1.0445212614,-0.8375557753
C,0,-3.2824990252,-0.4856771086,-0.1575431098
C,0,-0.8463102299,2.0201783878,-0.5537017312
C,0,-1.1083073689,0.1321795257,1.8820947306
C,0,-0.106446172,3.1266552151,-0.1000699587
C,0,-0.3709946445,4.4075014513,-0.5788365362
C,0,-1.3596546277,4.6115040291,-1.540350611
C,0,-2.0869124217,3.5228643228,-2.0121814349
C,0,-1.8407860129,2.2415524839,-1.5183357754
C,0,-1.1445725465,1.2520805396,2.7190098801
C,0,-1.5928974902,1.1319993533,4.0320336273
C,0,-1.977392939,-0.1141105498,4.5285274791
C,0,-1.9221305831,-1.2351694092,3.7026829484
C,0,-1.5025103295,-1.1131675564,2.3772496997
C,0,4.1753898014,-1.0642803479,0.3973825604
C,0,5.4797849844,-0.9288971358,-0.0592580637
C,0,5.8525021817,0.2131056585,-0.7778679967
C,0,4.9096459592,1.2133920814,-1.0328853186
C,0,3.6014471956,1.0570916019,-0.570482892
H,0,1.7603063995,-0.936972963,1.4565093249
H,0,1.1507636445,-0.3786425724,-1.4703501827
H,0,-0.8443850457,-1.1539796033,-2.4197869265
H,0,-2.7361476446,-2.1594473588,-3.6000676067
H,0,-5.0161931225,-2.0906778475,-2.6073889358
H,0,-5.3572094432,-0.9987934627,-0.3989886734
H,0,-3.4589680525,-0.0012173022,0.799192515
H,0,0.6864063663,2.9783569985,0.6209744811
H,0,0.2085049628,5.245626276,-0.2042003146
H,0,-1.5577107258,5.6091069224,-1.9203507752
H,0,-2.8562710346,3.6630465196,-2.7648884621
H,0,-2.4357105673,1.4229553209,-1.9022689972
H,0,-0.8221090201,2.2204532712,2.3483557417
H,0,-1.6319120061,2.0102888439,4.6688449046
H,0,-2.3159221487,-0.2095957576,5.55569571
H,0,-2.2131578375,-2.2089039825,4.0843505958
H,0,-1.4745665831,-1.9842786068,1.7310888894
H,0,3.8978341698,-1.9500719344,0.9654867912
H,0,6.22824134,-1.6897866022,0.1374362972
O,0,7.1522124116,0.2659363882,-1.1796917375
H,0,5.1781561863,2.1104705208,-1.5779185461
H,0,2.8639215616,1.8339633524,-0.7561091949
C,0,0.6946300893,-2.2987507633,-0.5816002159
C,0,1.4795174958,-2.9835195933,-1.6703947526
O,0,0.0496294549,-2.9191540797,0.2426525376
H,0,1.4098914671,-4.0661488774,-1.5666009985
H,0,1.0988520009,-2.6775520035,-2.6509275638
H,0,2.5265992333,-2.6618988171,-1.6195302418
C,0,7.5689240144,1.4026704854,-1.9177810865
H,0,8.6230092234,1.2457486785,-2.1421492228
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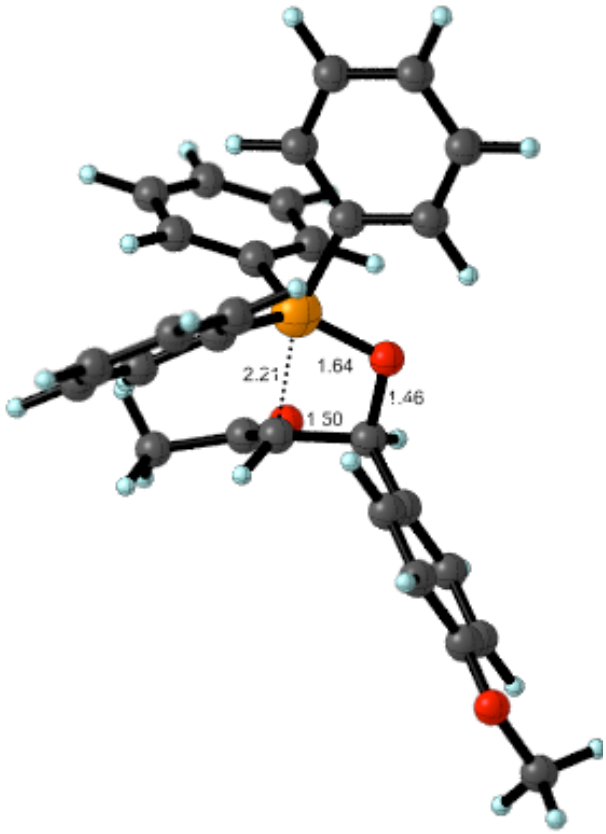
H,0,7.4524530944,2.3191979044,-1.3291936615

OP2

/home/singletn/wittig/methoxyketone/M062Xps/OP2M062XP
CMPS
OP2 for Wittig anisaldehyde and ketone
M062X/6-31+G**
E(RM062X) = -1687.80648383

Zero-point correction= 0.489648 (Hartree/Particle)
Thermal correction to Energy= 0.519299
Thermal correction to Enthalpy= 0.520244
Thermal correction to Gibbs Free Energy= 0.426953
Sum of electronic and ZPE= -1687.316835
Sum of electronic and thermal Energies= -1687.287184
Sum of electronic and thermal Enthalpies= -1687.286240
Sum of electronic and thermal Free Energies= -1687.379531

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	325.865	115.155	196.347



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P,0,0.4345610235,-0.258265838,-0.186488885
H,0,-1.6330166786,1.410281034,-1.9113367815
H,0,-1.5460878404,1.2004271038,1.0944789303
C,0,2.612635411,-4.1265707039,-1.7005597735
C,0,1.3286989733,-3.8481127496,-2.1616942802
C,0,0.6612794023,-2.6954689352,-1.7386622542
C,0,1.2720507799,-1.8025574109,-0.8513996314
C,0,2.5640931079,-2.0969370138,-0.3943627764

C,0,3.2307444771,-3.2456540211,-0.8110676273
H,0,3.1307110699,-5.0217468396,-2.0306247267
H,0,0.8395226883,-4.5268914554,-2.8538821567
H,0,-0.3400478727,-2.4926592103,-2.1006447056
H,0,3.0614669421,-1.4242131126,0.3012991916
H,0,4.2313728696,-3.4522619554,-0.4439885429
C,0,3.8572242708,2.6743747534,-1.1486675847
C,0,3.7255655475,2.2103874786,0.1594407699
C,0,2.7005330553,1.324493657,0.4913998528
C,0,1.8050439387,0.8995484314,-0.4940788976
C,0,1.9396077387,1.3618756148,-1.8067728947
C,0,2.9641923811,2.2471311831,-2.1310171349
H,0,4.6546789989,3.3655341937,-1.4025144573
H,0,4.4237836824,2.5320331029,0.9257894505
H,0,2.6184779767,0.9607605698,1.5115133675
H,0,1.2392600995,1.0354888563,-2.5716922154
H,0,3.0610710376,2.6062773214,-3.1505801391
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C,0,-0.0326436949,-2.585106849,3.1827211979
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C,0,0.347039654,0.1132179289,2.6118288919
C,0,0.2537381306,-0.3097211439,3.9333735914
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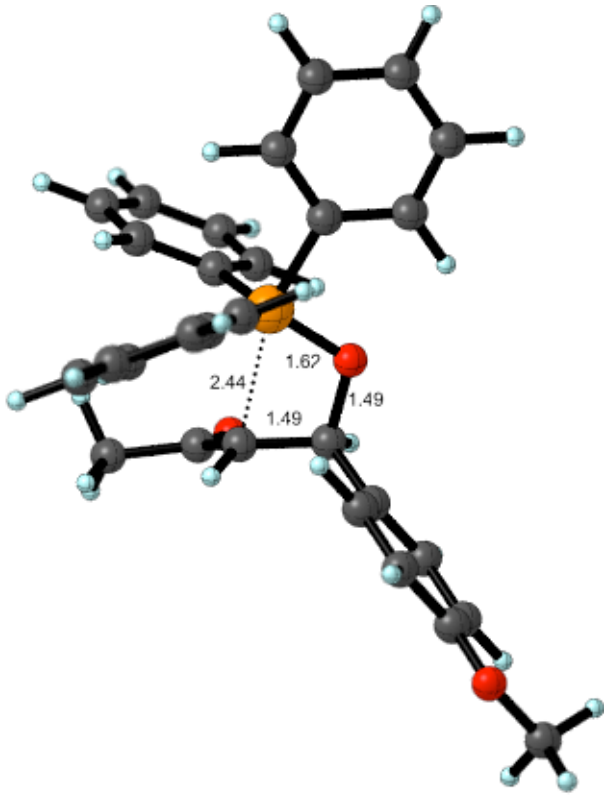
H,0,-0.1983147897,-3.6358879711,3.3976366595
H,0,0.069762517,-2.9022965724,1.0595434927
H,0,0.4567384447,1.1716518713,2.3963024312
H,0,0.3189858287,0.4166763525,4.7371449427
C,0,-5.6612315919,-0.7561441073,-0.4254849263
C,0,-5.4431964818,0.3162084772,-1.2908559647
C,0,-4.1379027778,0.77363469,-1.4975282419
C,0,-3.0519866507,0.1912356954,-0.8527168381
C,0,-3.2901303651,-0.8851364406,0.0144513927
C,0,-4.5750854414,-1.3575169364,0.2265636715
O,0,-6.8837124482,-1.2884508926,-0.1544993977
H,0,-6.2630099535,0.7960211814,-1.8116640505
H,0,-3.9731906999,1.6049513434,-2.1785303859
H,0,-2.4580792774,-1.3628534378,0.5282282669
H,0,-4.7659161233,-2.1921807972,0.8935456436
C,0,-0.5319640614,2.738919665,-0.0048223081
C,0,-0.1419164853,3.5051166812,1.2445315382
O,0,-0.3629559797,3.2648404245,-1.106235111
H,0,-0.2992992043,4.5722935415,1.0772652986
H,0,-0.6971199391,3.1799468976,2.1275694449
H,0,0.9291223507,3.3508800777,1.4259453049
C,0,-8.0097625682,-0.710406347,-0.7943247174
H,0,-8.8744664069,-1.2762859832,-0.4510516209
H,0,-8.1245957692,0.3420668643,-0.5124880566
H,0,-7.9274665668,-0.7917678904,-1.8836930863

TS2

/home/singletn/wittig/methoxyketone/M062Xps/TS2M062XP
CMPS
TS2 for Wittig anisaldehyde and ketone
M062X/6-31+G**
E(RM062X) = -1687.80610634

Zero-point correction= 0.488880 (Hartree/Particle)
Thermal correction to Energy= 0.517944
Thermal correction to Enthalpy= 0.518888
Thermal correction to Gibbs Free Energy= 0.426984
Sum of electronic and ZPE= -1687.317226
Sum of electronic and thermal Energies= -1687.288163
Sum of electronic and thermal Enthalpies= -1687.287218
Sum of electronic and thermal Free Energies= -1687.379122

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	325.015	113.629	193.428



O,0,0.2357799994,0.0691487315,-1.1787336888
C,0,1.0752610493,-1.1134788204,-0.8511933405
C,0,0.4392091209,-1.7164842201,0.3504041153
P,0,-0.9893150036,0.1980474583,-0.1337076663
H,0,0.9818150929,-1.780454747,-1.7130294186
H,0,0.9067316134,-1.5124979189,1.3105272798
C,0,-2.8320476536,4.0790299752,-1.9152411082
C,0,-1.6670806722,3.5648874819,-2.4783237331
C,0,-1.0881057582,2.402102063,-1.9635558322
C,0,-1.6768325112,1.7445052157,-0.8799589555
C,0,-2.8512974301,2.2674612249,-0.3220577385
C,0,-3.4255738452,3.4267569755,-0.8325311986
H,0,-3.2786004739,4.9835472735,-2.3162751291
H,0,-1.2011145041,4.0678174943,-3.3199535783
H,0,-0.1789263754,2.0089419519,-2.4036033952
H,0,-3.3225308675,1.7715193647,0.5239885828
H,0,-4.3340311693,3.8203157255,-0.3878110131
C,0,-4.5736192787,-2.5681407434,-0.9043462772
C,0,-4.4616972507,-1.9460951436,0.3393642107
C,0,-3.3747970383,-1.1192137223,0.616234319
C,0,-2.3913224476,-0.9196829198,-0.3597246669
C,0,-2.503588747,-1.5411579279,-1.6072533139
C,0,-3.5952680785,-2.363097809,-1.8756792346

H,0,-5.4218123552,-3.2116906481,-1.1150682156
H,0,-5.2237861303,-2.0985308778,1.0969224707
H,0,-3.3099705379,-0.6281439672,1.5825197157
H,0,-1.7379181204,-1.3894819146,-2.3631167686
H,0,-3.6746923951,-2.8486011527,-2.8428843083
C,0,-0.2944845304,1.6756602867,4.184511546
C,0,-0.071106311,2.521809556,3.1013561197
C,0,-0.3051196179,2.0714176148,1.8019362629
C,0,-0.7275519446,0.7555884956,1.5828336539
C,0,-0.9216956682,-0.0999939891,2.6730554882
C,0,-0.7285256429,0.3654155496,3.9689300611
H,0,-0.1264009188,2.0321115449,5.195790153
H,0,0.2761476448,3.5371941074,3.2618582107
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H,0,-0.900613335,-0.2986861889,4.809731406
C,0,5.1687734148,0.1476785132,-0.348901983
C,0,4.8462031838,-0.8088058306,-1.3112410733
C,0,3.5106180078,-1.1909953176,-1.4746082711
C,0,2.4972230079,-0.648629884,-0.6916112713
C,0,2.8410332157,0.3108569,0.2725214794
C,0,4.1563218631,0.7095528214,0.4431074782
O,0,6.4294456967,0.5987869758,-0.1062792653
H,0,5.6082652637,-1.2573701769,-1.937008322
H,0,3.2652877516,-1.9335671423,-2.2297130639
H,0,2.0667617894,0.7516772754,0.8976086816
H,0,4.428206168,1.4541876806,1.1846449997
C,0,-0.2102760063,-2.986887976,0.2136221431
C,0,-0.7410400089,-3.6482936027,1.4742392999
O,0,-0.437834243,-3.5353982173,-0.8797939359
H,0,-1.8184720969,-3.4482376233,1.5378252454
H,0,-0.6089440272,-4.7303810913,1.4025195614
H,0,-0.2599523366,-3.2785835949,2.3833221347
C,0,7.4806601063,0.0705432924,-0.8982924703
H,0,8.3906389307,0.5628404014,-0.5584641001
H,0,7.574490574,-1.0116691448,-0.7563038999
H,0,7.3197397619,0.2888831934,-1.9596728731

Product 3

/home/singletn/wittig/methoxyketone/M062Xps/productM062XPS
product for Wittig anisaldehyde and ketone
M062X/6-31+G**
E(RM062X) = -576.607478758

Zero-point correction= 0.205139 (Hartree/Particle)
Thermal correction to Energy= 0.218066
Thermal correction to Enthalpy= 0.219010
Thermal correction to Gibbs Free Energy= 0.163417
Sum of electronic and ZPE= -576.402339
Sum of electronic and thermal Energies= -576.389413
Sum of electronic and thermal Enthalpies= -576.388469
Sum of electronic and thermal Free Energies= -576.444062

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	136.838	46.769	117.005

C,0,0.1859351766,-0.4634789854,0.
C,0,-0.4421031955,0.786359587,0.
C,0,-1.8303418454,0.9144922265,0.
C,0,-2.6189316122,-0.238556756,0.
C,0,-2.0078013859,-1.504052946,0.
C,0,-0.6308054919,-1.6114753056,0.
H,0,0.1680903127,1.6856682195,0.
H,0,-2.2747263816,1.9022212729,0.
O,0,-3.9724398428,-0.2404165579,0.
H,0,-2.6411496603,-2.3850667555,0.
H,0,-0.1827631802,-2.6001960682,0.
C,0,2.4225101339,-1.6210128711,0.
C,0,1.6464787816,-0.5225413835,0.
H,0,2.1625875049,0.4380001081,0.
H,0,2.0081718416,-2.6257454217,0.
C,0,3.9004048537,-1.5014943455,0.
C,0,4.672676045,-2.7976000706,0.
O,0,4.4695102506,-0.4184307614,0.
H,0,5.7442093365,-2.5994568964,0.
H,0,4.4022361874,-3.389232711,0.880797575
H,0,4.4022361874,-3.389232711,-0.880797575
C,0,-4.6410186385,1.012741404,0.
H,0,-5.7053871812,0.7836724363,0.
H,0,-4.3887495941,1.5898076468,0.8957544078
H,0,-4.3887495941,1.5898076468,-0.8957544078

Ph3PO

/home/singletn/wittig/methoxyketone/M062Xps/Ph3POM062XPCMPS
Ph3PO for Wittig
M062X/6-31+G**
E(RM062X) = -1111.23981163

Zero-point correction= 0.281028 (Hartree/Particle)
Thermal correction to Energy= 0.297602
Thermal correction to Enthalpy= 0.298546
Thermal correction to Gibbs Free Energy= 0.234897
Sum of electronic and ZPE= -1110.958784
Sum of electronic and thermal Energies= -1110.942210
Sum of electronic and thermal Enthalpies= -1110.941265
Sum of electronic and thermal Free Energies= -1111.004915

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	186.748	65.236	133.962

8 0.071909 -0.146016 2.434033
15 0.019463 -0.031467 0.932221
6 -2.731192 -3.258317 -0.870994
6 -2.453012 -2.114013 -1.619405
6 -1.641032 -1.114615 -1.088718
6 -1.099886 -1.260306 0.193707
6 -1.385699 -2.404965 0.943703
6 -2.200832 -3.402635 0.410787
1 -3.366848 -4.034617 -1.285504
1 -2.873790 -1.996597 -2.612948
1 -1.445050 -0.216840 -1.669886
1 -0.973836 -2.501787 1.944272
1 -2.423997 -4.288891 0.996311
6 4.194868 -0.774307 -0.866341
6 3.120515 -0.529112 -1.724743
6 1.851494 -0.298194 -1.202106

6 1.653058 -0.310517 0.183421
6 2.728083 -0.556396 1.039959
6 3.999659 -0.787836 0.513256
1 5.183700 -0.954339 -1.276734
1 3.273184 -0.517625 -2.799155
1 1.021024 -0.102903 -1.876424
1 2.558426 -0.565024 2.112786
1 4.833811 -0.978646 1.181003
6 -1.491230 4.095084 -0.459791
6 -2.388298 3.132164 0.006299
6 -1.923382 1.878254 0.391896
6 -0.556834 1.578377 0.312586
6 0.338373 2.549002 -0.148425
6 -0.130330 3.804403 -0.534983
1 -1.854872 5.071687 -0.763878
1 -3.448069 3.357932 0.066886
1 -2.625481 1.130332 0.752277
1 1.400431 2.328463 -0.209767
1 0.568201 4.552559 -0.895457

Full System, M06-2X/6-31G*/PCM(THF) with Default Radii

Anisaldehyde 1

/home/singletn/wittig/methoxyketone/M062Xsb/anisaldehyde M062XSB
anisaldehde for Wittig anisaldehyde and ketone
M062X/6-31G*
E(RM062X) = -459.906660548

Zero-point correction= 0.144632 (Hartree/Particle)
Thermal correction to Energy= 0.153407
Thermal correction to Enthalpy= 0.154351
Thermal correction to Gibbs Free Energy= 0.110642
Sum of electronic and ZPE= -459.762029
Sum of electronic and thermal Energies= -459.753253
Sum of electronic and thermal Enthalpies= -459.752309
Sum of electronic and thermal Free Energies= -459.796019

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	96.264	32.707	91.995

C,0,-0.002304967,0.,0.115423561
C,0,0.053661733,0.,1.5165341416
C,0,1.2911426661,0.,2.1452694641
C,0,2.4726916651,0.,1.4009479483
C,0,2.4045985333,0.,0.0022556682
C,0,1.1801959934,0.,-0.6396337283
H,0,-0.852186681,0.,2.1106152126
H,0,1.3557625158,0.,3.2294761694
C,0,3.7820433207,0.,2.0739170626
H,0,3.3222369997,0.,-0.5814070811
H,0,1.10267611,0.,-1.7215739204
O,0,-1.1483139111,0.,-0.5969611352
C,0,-2.3756464696,0.,0.1149831871
H,0,-3.1598066231,0.,-0.6407185647
H,0,-2.4675354851,-0.8948839618,0.7396217542
H,0,-2.4675354851,0.8948839618,0.7396217542
O,0,3.9385782193,0.,3.2780398477
H,0,4.6573648656,0.,1.3929846592

Ph3PCHCOMe 2

/home/singletn/wittig/methoxyketone/M062Xsb/Ph3PCHCOMeM062XSB
Ph3PCHCOMe for Wittig anisaldehyde and ketone
M062X/6-31G*
E(RM062X) = -1227.81961930

Zero-point correction= 0.342552 (Hartree/Particle)
Thermal correction to Energy= 0.363409
Thermal correction to Enthalpy= 0.364354
Thermal correction to Gibbs Free Energy= 0.289915
Sum of electronic and ZPE= -1227.477068
Sum of electronic and thermal Energies= -1227.456210
Sum of electronic and thermal Enthalpies= -1227.455266
Sum of electronic and thermal Free Energies= -1227.529705

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	228.043	79.768	156.670

C,0,0.3638574851,0.1511402154,0.4174080639
P,0,0.4277253682,-0.1289951458,2.1171096169
H,0,-0.3362755598,0.8950927364,0.0596904329
C,0,4.3300946014,1.0963136958,4.24854634
C,0,3.1105870861,1.2651652388,4.8999468349
C,0,1.9255165335,0.9025011366,4.2639330523
C,0,1.9617272401,0.3617062298,2.9739679782
C,0,3.1881688702,0.1915165389,2.3206715885
C,0,4.3670606247,0.560801654,2.9621370022
H,0,5.2527570704,1.3838871639,4.7432448921
H,0,3.078958972,1.6834570233,5.9009940278
H,0,0.9751763541,1.048002001,4.7708849194
H,0,3.2054997371,-0.2454097934,1.3264104269
H,0,5.3181322181,0.4293606273,2.455641433
C,0,-0.5164160494,-4.4651383477,3.3369890269
C,0,0.1785024034,-3.6409876083,4.2199047693
C,0,0.4978156125,-2.3370140778,3.8504282694
C,0,0.1133159909,-1.855611173,2.5961562025
C,0,-0.5788273697,-2.6841263135,1.7100192861
C,0,-0.8929206093,-3.9877383412,2.0827287963
H,0,-0.7599451011,-5.4833836378,3.6241070322
H,0,0.4775627321,-4.0137653092,5.1943504561
H,0,1.0478379292,-1.699483192,4.5373432259
H,0,-0.8596050191,-2.3021880674,0.7325279871
H,0,-1.4247246279,-4.6336074884,1.3913031453
C,0,-2.8888421579,2.4917948472,3.9380209569
C,0,-1.8002943473,3.0735675028,3.2874575672
C,0,-0.7983571734,2.2703737627,2.7553739987
C,0,-0.8831350612,0.8769503403,2.8715487463
C,0,-1.9713269704,0.2969617994,3.5258564709
C,0,-2.9734037534,1.1075937394,4.0569151006
H,0,-3.6704989994,3.1207198559,4.3526400151
H,0,-1.7319113841,4.1528345756,3.1969948302
H,0,0.0530276536,2.7240282804,2.2538877478
H,0,-2.0405810575,-0.7827375353,3.6189002435
H,0,-3.8197434792,0.6539552745,4.562562458
C,0,1.1462465214,-0.6553692068,-0.4318963028
C,0,0.9932144325,-0.4688965184,-1.9346717679

O,0,1.9485333176,-1.52304584,-0.0203047737
H,0,1.9666141451,-0.2120785675,-2.3633460123
H,0,0.6841796014,-1.41982606,-2.3795062705
H,0,0.2687592191,0.3038569839,-2.2001408143

TS1 4

/home/singletn/wittig/methoxyketone/M062Xsb/TS1M062XP
CMSB2
TS1 for Wittig anisaldehyde and ketone
M062X/6-31G*
E(RM062X) = -1687.71598521

Zero-point correction= 0.489217 (Hartree/Particle)
Thermal correction to Energy= 0.518866
Thermal correction to Enthalpy= 0.519810
Thermal correction to Gibbs Free Energy= 0.426294
Sum of electronic and ZPE= -1687.226768
Sum of electronic and thermal Energies= -1687.197119
Sum of electronic and thermal Enthalpies= -1687.196175
Sum of electronic and thermal Free Energies= -1687.289691

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	325.593	114.535	196.821

O,0,1.3507408163,1.9349795977,0.8589063331
C,0,1.748747789,0.7219246483,0.7729691945
P,0,-0.9390909008,0.2004884085,-0.0896656201
C,0,0.766058009,-0.1253489453,-0.5423790373
C,0,3.1799223259,0.4609705111,0.3410979223
C,0,-2.0153986716,-1.1612697657,-0.6229101756
C,0,-1.8163896714,-1.7035354222,-1.8979234435
C,0,-2.6673753929,-2.6938830736,-2.3732858588
C,0,-3.7229096163,-3.1446568493,-1.58064999
C,0,-3.9274872349,-2.601877556,-0.3158034429
C,0,-3.0769722237,-1.6082214466,0.1661302192
C,0,-1.5269038988,1.6679414869,-0.9770337818
C,0,-1.2111858748,0.4198921819,1.6858572721
C,0,-0.6739558804,2.7651657455,-1.1474547528
C,0,-1.1398058455,3.8902216563,-1.8226203806
C,0,-2.4405057911,3.9250604946,-2.3212582968
C,0,-3.2882653023,2.8335735233,-2.1440432518
C,0,-2.8353234001,1.7013668905,-1.4736099169
C,0,-1.7195669301,1.621617015,2.1814591002
C,0,-1.9523988249,1.7587308326,3.5468090093
C,0,-1.673470274,0.7031184728,4.4118475966
C,0,-1.1597659516,-0.4940474187,3.9157511499
C,0,-0.9268666096,-0.6427442692,2.5518556903
C,0,3.8656601606,-0.6909231111,0.7408414715
C,0,5.1654180219,-0.9282744684,0.3197489978
C,0,5.8094746862,-0.0065993704,-0.5143957563
C,0,5.1419906465,1.1548145083,-0.9122829687
C,0,3.8362580937,1.3761414761,-0.4741321695
H,0,1.4801962249,0.0162375024,1.5937669354
H,0,1.0305081614,0.4420530534,-1.4361881458
H,0,-0.9969619539,-1.3499232596,-2.5197527465
H,0,-2.5071135867,-3.1145891884,-3.3606135456
H,0,-4.3864255144,-3.9194520187,-1.9516022854
H,0,-4.7492865623,-2.9499823748,0.3015668263
H,0,-3.2425308844,-1.1881642132,1.1534298067
H,0,0.3270458548,2.7277804836,-0.7201508599
H,0,-0.4830612136,4.7437536741,-1.957473912
H,0,-2.795679685,4.8047809684,-2.8492606608
H,0,-4.3018100073,2.8604677898,-2.5308798235
H,0,-3.4970147408,0.8500376477,-1.3446297126
H,0,-1.9250907194,2.4473507366,1.5072527507
H,0,-2.3464919923,2.6927930304,3.9336232067
H,0,-1.8539321835,0.8138573652,5.4766206438
H,0,-0.9363950128,-1.3135279883,4.5913558539
H,0,-0.5190968841,-1.5684576539,2.153634814
H,0,3.3669069555,-1.4145754717,1.3836314607
H,0,5.7085917664,-1.8174406363,0.6244909974
O,0,7.082358357,-0.3251450003,-0.877124387
H,0,5.6262193219,1.8881667038,-1.5469480061
H,0,3.3091287933,2.2832487056,-0.7576452309
C,0,1.1305059632,-1.5492315177,-0.5674654487
C,0,2.0972352041,-2.0058648548,-1.6366273589
O,0,0.7043864696,-2.3283591295,0.28041984
H,0,2.6130686917,-2.9101874797,-1.3090233535
H,0,1.524256228,-2.2360642467,-2.5436410501
H,0,2.8225627599,-1.2262314967,-1.8833867836
C,0,7.7657623352,0.582982246,-1.7188118069
H,0,8.7508535403,0.1514299182,-1.8943689278
H,0,7.2451659569,0.7053144618,-2.675652318
H,0,7.876392102,1.5629754912,-1.2405038852

Betaine 5

/home/singletn/wittig/methoxyketone/M062Xsb/betaineM062
XSB
Gaussian calculation: first derivatives
M062X/6-31G*
E(RM062X) = -1687.71726481

Zero-point correction= 0.490540 (Hartree/Particle)
Thermal correction to Energy= 0.520474
Thermal correction to Enthalpy= 0.521418
Thermal correction to Gibbs Free Energy= 0.428040
Sum of electronic and ZPE= -1687.226725
Sum of electronic and thermal Energies= -1687.196791
Sum of electronic and thermal Enthalpies= -1687.195847
Sum of electronic and thermal Free Energies= -1687.289225

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	326.602	115.540	196.530

8 0.815571 1.398039 1.246614
6 1.250000 0.187970 0.941228
15 -1.290317 0.111918 -0.020946
6 0.449344 -0.294825 -0.401523
6 2.741548 0.052034 0.635995
6 -2.330308 -1.055069 -0.954869
6 -2.085144 -1.198028 -2.327038
6 -2.869282 -2.055008 -3.089556
6 -3.907196 -2.768901 -2.489589
6 -4.159752 -2.620920 -1.129750
6 -3.374016 -1.764026 -0.359409
6 -1.772479 1.743593 -0.652068
6 -1.731404 -0.061010 1.720246
6 -0.878955 2.819947 -0.620006

6 -1.286821 4.057201 -1.112481
6 -2.573540 4.226603 -1.619128
6 -3.464637 3.155408 -1.639046
6 -3.066716 1.910363 -1.163165
6 -2.331984 1.003825 2.394721
6 -2.720130 0.844037 3.720788
6 -2.503932 -0.369483 4.371405
6 -1.898616 -1.428023 3.697388
6 -1.511719 -1.281559 2.367865
6 3.427753 -1.154720 0.810818
6 4.770191 -1.269193 0.479448
6 5.460305 -0.163900 -0.031963
6 4.793951 1.051868 -0.199825
6 3.443069 1.143972 0.139241
1 0.999279 -0.621665 1.672766
1 0.773002 0.388738 -1.193805
1 -1.287720 -0.632491 -2.805322
1 -2.673216 -2.164613 -4.151181
1 -4.519635 -3.437143 -3.086509
1 -4.969043 -3.171122 -0.660879
1 -3.577648 -1.653124 0.700775
1 0.101591 2.659598 -0.176182
1 -0.596263 4.894437 -1.093849
1 -2.885279 5.195122 -1.998125
1 -4.467946 3.285007 -2.031442
1 -3.761928 1.076679 -1.193217
1 -2.485792 1.953305 1.891207
1 -3.187468 1.670000 4.246948
1 -2.806329 -0.489508 5.407078
1 -1.725996 -2.371583 4.204864
1 -1.040427 -2.101041 1.831693
1 2.899331 -2.019320 1.210807
1 5.310548 -2.201009 0.615030
8 6.774863 -0.369335 -0.326805
1 5.311698 1.924784 -0.581219
1 2.910496 2.085260 0.034681
6 0.688838 -1.736552 -0.743062
6 1.624826 -2.025675 -1.889052
8 0.188577 -2.624942 -0.073601
1 1.929399 -3.072944 -1.869343
1 1.099245 -1.818898 -2.829532
1 2.501169 -1.371884 -1.847981
6 7.506298 0.729153 -0.833479
1 8.521005 0.367631 -0.999267
1 7.086581 1.084393 -1.781916
1 7.527035 1.558041 -0.116362

TS1.5 6

/home/singletn/wittig/methoxyketone/M062Xsb/TS1.5M062XSB
betaiene product from anisaldehyde and ketone
M062X/6-31G*
E(RM062X) = -1687.71716032

Zero-point correction= 0.490268 (Hartree/Particle)
Thermal correction to Energy= 0.519484
Thermal correction to Enthalpy= 0.520429
Thermal correction to Gibbs Free Energy= 0.428750
Sum of electronic and ZPE= -1687.226893
Sum of electronic and thermal Energies= -1687.197676
Sum of electronic and thermal Enthalpies= -1687.196732
Sum of electronic and thermal Free Energies= -1687.288410

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	325.981	113.560	192.953

OP1direct

/home/singletn/wittig/methoxyketone/M062Xsb/OP1directM062XPCMSB
OP1 direct for Wittig anisaldehyde and ketone for polyrate
M062X/6-31G*
E(RM062X) = -1687.73454468

Zero-point correction= 0.492474 (Hartree/Particle)
Thermal correction to Energy= 0.521469
Thermal correction to Enthalpy= 0.522413
Thermal correction to Gibbs Free Energy= 0.431633
Sum of electronic and ZPE= -1687.242070
Sum of electronic and thermal Energies= -1687.213076
Sum of electronic and thermal Enthalpies= -1687.212131
Sum of electronic and thermal Free Energies= -1687.302911

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	327.227	114.256	191.062

O,0,0.9116224325,0.860562129,1.1509457514
C,0,1.727813131,-0.2888129184,1.0218517163
P,0,-0.5744649566,0.1527942305,0.4170550295
C,0,0.7885990702,-1.1471891391,0.1749612828
C,0,3.0748681985,0.0101654077,0.406219943
C,0,-1.8513981811,-0.9696540244,-0.4707287558
C,0,-1.8599578852,-1.0284892416,-1.8712383913
C,0,-2.5768398616,-2.0095674817,-2.5542468796
C,0,-3.3011989746,-2.9663801506,-1.8459482456
C,0,-3.2933854449,-2.9359826429,-0.454072822
C,0,-2.5722772231,-1.9526899085,0.2225262362
C,0,-0.7544354422,1.5907033862,-0.7218995978
C,0,-1.5064991004,0.349523813,1.9944534899
C,0,0.3707463241,2.2652972226,-1.2033394687
C,0,0.2263571131,3.3440399732,-2.0738481412
C,0,-1.0419023058,3.7796727178,-2.4457656751
C,0,-2.1697835301,3.1172791407,-1.9638852426
C,0,-2.0253693587,2.0179727412,-1.1244626397
C,0,-2.891789177,0.5532413524,1.9788566954
C,0,-3.5927539058,0.761955574,3.1622069432
C,0,-2.9232979083,0.7315583253,4.3835495928
C,0,-1.5500739271,0.5061817194,4.4119946688
C,0,-0.8419486391,0.3327542275,3.2250897402
C,0,3.8557547896,-1.0159617201,-0.1391207811
C,0,5.1078009,-0.7540106053,-0.6708586516
C,0,5.6120787203,0.5527413625,-0.6675750342
C,0,4.8488389312,1.5857116301,-0.1233406686
C,0,3.5900665159,1.3019191975,0.4112238547
H,0,1.8736206236,-0.7712720512,2.0016751073
H,0,1.0515365196,-1.1691540243,-0.8899177437
H,0,-1.2973409678,-0.2968063456,-2.4470346418
H,0,-2.5694355069,-2.0250458407,-3.6403501567
H,0,-3.8624476196,-3.7305804578,-2.3750825378

H,0,-3.8454824704,-3.6820026939,0.1100346833
H,0,-2.5649721696,-1.9650800352,1.3093617226
H,0,1.3584906079,1.9462645551,-0.8912512621
H,0,1.1094633105,3.8494582209,-2.452339974
H,0,-1.1529886985,4.6297579307,-3.1120518897
H,0,-3.162979865,3.4472184324,-2.251715858
H,0,-2.9124090712,1.4862170539,-0.7962324461
H,0,-3.4380039113,0.5347389065,1.04177785
H,0,-4.663526722,0.9363552334,3.1279611529
H,0,-3.4713575221,0.8815471899,5.308706445
H,0,-1.0218084367,0.4756161812,5.3598615796
H,0,0.2315248603,0.1946817012,3.253846133
H,0,3.4786834552,-2.0371008018,-0.14904828
H,0,5.7167880921,-1.543546314,-1.0995042448
O,0,6.846179703,0.712045778,-1.2161664246
H,0,5.2156201968,2.6053132294,-0.1052166264
H,0,2.9918405843,2.1013735811,0.8385185461
C,0,0.4396945869,-2.5255047349,0.6963314449
C,0,0.2572048278,-3.6233392278,-0.319347199
O,0,0.3256822456,-2.7131624402,1.8919234404
H,0,-0.1472759823,-4.5160738338,0.1587443028
H,0,-0.4029433359,-3.2902190427,-1.1276250329
H,0,1.2316191467,-3.855154634,-0.7673357495
C,0,7.385373543,2.0200144827,-1.2352148379
H,0,8.3626651165,1.9377606388,-1.7099921213
H,0,6.7530177706,2.700494222,-1.8168895982
H,0,7.5040667841,2.4150658227,-0.2198357326

OP1

/home/singletn/wittig/methoxyketone/M062Xsb/OP1M062XSB
OP1 for Wittig anisaldehyde and ketone
M062X/6-31G*
E(RM062X) = -1687.72821480

Zero-point correction= 0.491851 (Hartree/Particle)
Thermal correction to Energy= 0.521413
Thermal correction to Enthalpy= 0.522357
Thermal correction to Gibbs Free Energy= 0.428096
Sum of electronic and ZPE= -1687.236364
Sum of electronic and thermal Energies= -1687.206802
Sum of electronic and thermal Enthalpies= -1687.205858
Sum of electronic and thermal Free Energies= -1687.300119

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	327.192	114.644	198.389

O,0,1.1068311897,0.8986320561,0.8609998302
C,0,1.7919970935,-0.2931095144,0.5918365196
P,0,-0.5057463993,0.3091506599,0.1658504904
C,0,0.8353722001,-0.83259359,-0.4969864675
C,0,3.2134205764,-0.082777339,0.135842253
C,0,-1.9789762251,-0.5325130438,-0.68758469
C,0,-1.8131263251,-1.1644538667,-1.9251466941
C,0,-2.8943711885,-1.7015129893,-2.6220282277
C,0,-4.1773955272,-1.6117101485,-2.0895364177
C,0,-4.3676813016,-0.9750845768,-0.8649882536
C,0,-3.2803587355,-0.4396147159,-0.1775944548
C,0,-0.8087116074,1.9978811502,-0.5492369535
C,0,-1.1189646369,0.1106087551,1.8889149998
C,0,-0.0612957469,3.096619568,-0.0897860697
C,0,-0.3015717733,4.3776126431,-0.5768614449
C,0,-1.2721244479,4.589568633,-1.5528499186
C,0,-2.0052329026,3.5093364745,-2.0316445987
C,0,-1.7845083804,2.2282286624,-1.5294025721
C,0,-1.1045602697,1.2199726219,2.7401921924
C,0,-1.5639541478,1.106653526,4.048184116
C,0,-2.009779141,-0.1239401219,4.5275273387
C,0,-2.004544717,-1.2358437726,3.6897405631
C,0,-1.5736137248,-1.1195722414,2.3689086166
C,0,4.1880529433,-1.0616345923,0.3532733888
C,0,5.4822314429,-0.8952896579,-0.1174377609
C,0,5.8286666381,0.2682590315,-0.8132710998
C,0,4.8664116654,1.257352795,-1.0326085088
C,0,3.5690170423,1.0706354316,-0.5572949903
H,0,1.7802200284,-0.9828560667,1.4542941325
H,0,1.1564863486,-0.4331755887,-1.4669621975
H,0,-0.8282028736,-1.2247952799,-2.3834729581
H,0,-2.733251929,-2.1870757881,-3.5799270601
H,0,-5.022920143,-2.0302679093,-2.6267322866
H,0,-5.36528058,-0.892323712,-0.4436673774
H,0,-3.4545990232,0.0651962936,0.7689453201
H,0,0.7190534149,2.9404277765,0.6430570459
H,0,0.2828495966,5.2102876972,-0.1976338753
H,0,-1.4514710499,5.5879910014,-1.9401479887
H,0,-2.7599343199,3.657203369,-2.797827167
H,0,-2.3815385589,1.4141418915,-1.9195359873
H,0,-0.7352857866,2.1760060961,2.3809344379
H,0,-1.563419465,1.9778807332,4.6959035868
H,0,-2.3573360472,-0.2149599968,5.5522120872
H,0,-2.3427269518,-2.1989467718,4.0598875402
H,0,-1.5808357235,-1.9840134659,1.7138779586
H,0,3.9314680676,-1.9635583195,0.905692286
H,0,6.2461914437,-1.6475375225,0.050376051
O,0,7.121093195,0.3489128913,-1.2284308494
H,0,5.1145500624,2.1699659135,-1.5617919431
H,0,2.8161925939,1.8383251216,-0.7167564219
C,0,0.6714090141,-2.3321632308,-0.5391903558
C,0,1.4732280982,-3.057165622,-1.5919323976
O,0,-0.0051286456,-2.9198858449,0.2803501711
H,0,1.3864937841,-4.1356996283,-1.4581103442
H,0,1.1174856881,-2.7775826239,-2.5901476212
H,0,2.5236333472,-2.7484449995,-1.5282411306
C,0,7.5041808172,1.5060554524,-1.9468506279
H,0,8.5586967754,1.3766742577,-2.1889876351
H,0,6.9267640374,1.6071975668,-2.8729834399
H,0,7.3772831906,2.4103024712,-1.3407111383

OP2

/home/singletn/wittig/methoxyketone/M062Xsb/OP2M062XSB
OP2 for Wittig anisaldehyde and ketone
M062X/6-31G*
E(RM062X) = -1687.73285637

Zero-point correction= 0.492316 (Hartree/Particle)
Thermal correction to Energy= 0.520834
Thermal correction to Enthalpy= 0.521778
Thermal correction to Gibbs Free Energy= 0.432271

Sum of electronic and ZPE= -1687.240540
Sum of electronic and thermal Energies= -1687.212022
Sum of electronic and thermal Enthalpies= -1687.211078
Sum of electronic and thermal Free Energies= -1687.300585

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	326.828	112.586	188.384

8 0.281288 -0.019191 -1.269187
6 1.123063 -1.109836 -0.785050
6 0.384385 -1.496390 0.467798
15 -0.924869 0.103502 -0.156264
1 1.074615 -1.912272 -1.526735
1 0.887199 -1.226918 1.397831
6 -2.863052 3.785682 -2.330331
6 -1.623438 3.325259 -2.761231
6 -1.022871 2.228285 -2.140364
6 -1.655945 1.573286 -1.078988
6 -2.903898 2.051462 -0.656392
6 -3.504382 3.144496 -1.270613
1 -3.329115 4.638312 -2.814865
1 -1.116089 3.818870 -3.584883
1 -0.055872 1.881413 -2.484577
1 -3.418247 1.564648 0.169645
1 -4.471484 3.496111 -0.924173
6 -4.498278 -2.752671 -0.734357
6 -4.426971 -2.006651 0.439821
6 -3.365544 -1.128302 0.650916
6 -2.370288 -0.994659 -0.322152
6 -2.446990 -1.740201 -1.501987
6 -3.507810 -2.616947 -1.704699
1 -5.324138 -3.438961 -0.892864
1 -5.199513 -2.104470 1.196173
1 -3.326387 -0.546828 1.567970
1 -1.671131 -1.641715 -2.257158
1 -3.557202 -3.197272 -2.620536
6 -0.580043 2.156616 3.986675
6 -0.368706 2.892028 2.824573
6 -0.502042 2.284272 1.576748
6 -0.807940 0.922806 1.486906
6 -0.984749 0.183554 2.661450
6 -0.898555 0.800938 3.903328
1 -0.490676 2.634701 4.957113
1 -0.110621 3.944628 2.882987
1 -0.365837 2.872350 0.673886
1 -1.191380 -0.881410 2.603778
1 -1.063186 0.221925 4.806478
6 5.195077 0.199968 -0.253224
6 4.922580 -0.964462 -0.970363
6 3.596226 -1.362927 -1.147999
6 2.539192 -0.633176 -0.616884
6 2.830591 0.532603 0.104106
6 4.138371 0.948645 0.283172
8 6.442146 0.688839 -0.023652
1 5.719447 -1.560547 -1.399020
1 3.389373 -2.267420 -1.714675
1 2.021282 1.123261 0.529752
1 4.373873 1.851799 0.836903
6 -0.159215 -2.867542 0.487910
6 -0.708173 -3.390666 1.802118
8 -0.245120 -3.561937 -0.518760
1 -0.652634 -4.480844 1.811540
1 -0.182377 -2.981099 2.668496
1 -1.766400 -3.107274 1.871243
6 7.534280 -0.042206 -0.548622
1 8.431224 0.506873 -0.263961
1 7.574459 -1.052741 -0.126043
1 7.478089 -0.108916 -1.641130

TS2

/home/singletn/wittig/methoxyketone/M062Xsb/TS2M062XPCMSB
TS2 for Wittig anisaldehyde and ketone
M062X/6-31G*
E(RM062X) = -1687.73014173

Zero-point correction= 0.490643 (Hartree/Particle)
Thermal correction to Energy= 0.519877
Thermal correction to Enthalpy= 0.520821
Thermal correction to Gibbs Free Energy= 0.428236
Sum of electronic and ZPE= -1687.239499
Sum of electronic and thermal Energies= -1687.210264
Sum of electronic and thermal Enthalpies= -1687.209320
Sum of electronic and thermal Free Energies= -1687.301906

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	326.228	113.711	194.863

8 0.207072 0.029330 -1.137807
6 1.035531 -1.213185 -0.812152
6 0.419209 -1.922493 0.317428
15 -1.025556 0.303112 -0.168459
1 0.939854 -1.804106 -1.726716
1 0.823410 -1.766720 1.312162
6 -2.623557 4.229473 -1.985672
6 -1.486340 3.642312 -2.531816
6 -0.977987 2.460408 -1.993140
6 -1.615605 1.864318 -0.903205
6 -2.759676 2.458183 -0.357014
6 -3.260548 3.637223 -0.894997
1 -3.015958 5.149331 -2.407810
1 -0.989171 4.102666 -3.379650
1 -0.091167 2.000995 -2.414931
1 -3.263613 2.001109 0.491657
1 -4.147420 4.092584 -0.466478
6 -4.657667 -2.408704 -0.789796
6 -4.546062 -1.693745 0.403208
6 -3.433907 -0.892247 0.636086
6 -2.422182 -0.814012 -0.331348
6 -2.534993 -1.528638 -1.527170
6 -3.655096 -2.323617 -1.750871
1 -5.527810 -3.032929 -0.967436
1 -5.328089 -1.756731 1.153145
1 -3.361628 -0.329713 1.562510
1 -1.743594 -1.477896 -2.267638
1 -3.734950 -2.885032 -2.675961
6 -0.090169 1.512802 4.168420
6 0.135572 2.399365 3.119676
6 -0.174152 2.026281 1.813519
6 -0.681331 0.748073 1.554235

6 -0.891699 -0.146282 2.610356
6 -0.612407 0.243558 3.913822
1 0.143133 1.807158 5.186829
1 0.545495 3.385159 3.313262
1 -0.013944 2.728051 0.999869
1 -1.257051 -1.147887 2.402584
1 -0.787178 -0.448618 4.730892
6 5.106427 0.083583 -0.234530
6 4.774816 -0.712344 -1.330147
6 3.447097 -1.105700 -1.512719
6 2.446820 -0.734537 -0.621365
6 2.798675 0.068014 0.473954
6 4.106560 0.476172 0.666227
8 6.361245 0.526397 0.043966
1 5.526872 -1.029488 -2.042980
1 3.195044 -1.723457 -2.370891
1 2.035507 0.374051 1.186828
1 4.386526 1.096531 1.511617
6 -0.336867 -3.088012 0.055369
6 -0.952338 -3.803019 1.251411
8 -0.607443 -3.520256 -1.085422
1 -2.022318 -3.557411 1.280257
1 -0.867571 -4.885917 1.124206
1 -0.501228 -3.510637 2.204216
6 7.396191 0.142125 -0.841186
1 8.311439 0.583697 -0.448106
1 7.502914 -0.948108 -0.876676
1 7.212952 0.520753 -1.853268

Product 3

/home/singletn/wittig/methoxyketone/M062Xsb/productM062XSB
product for Wittig anisaldehyde and ketone
M062X/6-31G*
E(RM062X) = -576.574595639

Zero-point correction= 0.206518 (Hartree/Particle)
Thermal correction to Energy= 0.219345
Thermal correction to Enthalpy= 0.220289
Thermal correction to Gibbs Free Energy= 0.165203
Sum of electronic and ZPE= -576.368077
Sum of electronic and thermal Energies= -576.355251
Sum of electronic and thermal Enthalpies= -576.354307
Sum of electronic and thermal Free Energies= -576.409393

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	137.641	46.467	115.939

C,0,0.1824181965,-0.4687530511,0.
C,0,-0.4431313838,0.7815643809,0.
C,0,-1.8290785745,0.9121391509,0.
C,0,-2.6208048179,-0.238365995,0.
C,0,-2.0117161916,-1.5036983384,0.
C,0,-0.6359746033,-1.6137773505,0.
H,0,0.1700289668,1.67901438,0.
H,0,-2.2725536916,1.9005079367,0.
O,0,-3.9728776474,-0.2392285437,0.
H,0,-2.6482454065,-2.382341807,0.
H,0,-0.1881047948,-2.6028383949,0.
C,0,2.4172214778,-1.6281076301,0.
C,0,1.6419448907,-0.531552777,0.
H,0,2.1614474185,0.4270726426,0.
H,0,2.00539227,-2.6340312302,0.
C,0,3.8949456582,-1.4974344891,0.
C,0,4.6765070465,-2.7907783409,0.
O,0,4.4533688463,-0.4127762191,0.
H,0,5.746682365,-2.5828607887,0.
H,0,4.4131040499,-3.3859171329,0.8810694519
H,0,4.4131040499,-3.3859171329,-0.8810694519
C,0,-4.6338208166,1.0142687123,0.
H,0,-5.7003161224,0.7921904348,0.
H,0,-4.3797310883,1.5932007921,0.8946587821
H,0,-4.3797310883,1.5932007921,-0.8946587821

Ph3PO

/home/singletn/wittig/c28/full2X/Ph3POM062XPCMSB
Ph3PO for Wittig
M062X/6-31G*
E(RM062X) = -1111.19580668

Zero-point correction= 0.281698 (Hartree/Particle)
Thermal correction to Energy= 0.298314
Thermal correction to Enthalpy= 0.299258
Thermal correction to Gibbs Free Energy= 0.234900
Sum of electronic and ZPE= -1110.914108
Sum of electronic and thermal Energies= -1110.897492
Sum of electronic and thermal Enthalpies= -1110.896548
Sum of electronic and thermal Free Energies= -1110.960907

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	187.195	65.166	135.454

8 0.151077 0.028161 2.424869
15 0.017495 -0.001485 0.927748
6 2.775029 -3.220540 -0.865638
6 1.743668 -2.709048 -1.652841
6 0.876879 -1.753740 -1.130348
6 1.040809 -1.307011 0.185303
6 2.071206 -1.826661 0.972209
6 2.937150 -2.782587 0.446525
1 3.450349 -3.964982 -1.275990
1 1.612479 -3.057973 -2.672256
1 0.064095 -1.371527 -1.743366
1 2.180830 -1.479916 1.995727
1 3.735750 -3.185850 1.061276
6 1.541564 3.946691 -0.882818
6 0.910242 3.021972 -1.715591
6 0.427932 1.828508 -1.189105
6 0.574815 1.556275 0.175563
6 1.205408 2.484022 1.005959
6 1.688718 3.678895 0.475439
1 1.916335 4.878234 -1.295566
1 0.791803 3.233282 -2.773636
1 -0.073008 1.116963 -1.841613
1 1.308452 2.261424 2.064033
1 2.177099 4.399749 1.123678
6 -4.326961 -0.705844 -0.421271
6 -3.493681 -1.791965 -0.159082

6 -2.168134 -1.578934 0.206883
6 -1.667126 -0.275681 0.308570
6 -2.510996 0.809806 0.050329
6 -3.836704 0.593987 -0.315336
1 -5.360437 -0.873578 -0.708443
1 -3.876175 -2.804323 -0.241182
1 -1.520657 -2.427864 0.410978
1 -2.131430 1.824645 0.132103
1 -4.485434 1.439834 -0.519435

Full System, M06-2X/6-31+G**/PCM(THF) with Pauling Radii

Anisaldehyde 1

/home/singletn/wittig/pauling/m062XPS/anisaldehydeM062XPSpaul
anisaldehyde
M062X/6-31+G**
E(RM062X) = -459.938654144

Zero-point correction= 0.143383 (Hartree/Particle)
Thermal correction to Energy= 0.152393
Thermal correction to Enthalpy= 0.153337
Thermal correction to Gibbs Free Energy= 0.108568
Sum of electronic and ZPE= -459.795271
Sum of electronic and thermal Energies= -459.786262
Sum of electronic and thermal Enthalpies= -459.785317
Sum of electronic and thermal Free Energies= -459.830086

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.628	33.057	94.223

C,0,-0.0003367874,0.,0.1160713773
C,0,0.0513153061,0.,1.5187612855
C,0,1.2880641367,0.,2.1517090815
C,0,2.4732281724,0.,1.4089134559
C,0,2.4069233611,0.,0.0079773713
C,0,1.183023801,0.,-0.6381677552
H,0,-0.8548831991,0.,2.111677176
H,0,1.3404716151,0.,3.2362928925
C,0,3.7874848802,0.,2.0637828517
H,0,3.3257883519,0.,-0.5727317049
H,0,1.1127109458,0.,-1.7206559789
O,0,-1.1492021218,0.,-0.5954903849
C,0,-2.3849119013,0.,0.1145668835
H,0,-3.1631587049,0.,-0.646032252
H,0,-2.4738672173,-0.8964644624,0.7352691211
H,0,-2.4738672173,0.8964644624,0.7352691211
O,0,3.9633476899,0.,3.2726082411
H,0,4.6554918887,0.,1.3795752183

Ph3PCHCOMe 2

/home/singletn/wittig/pauling/m062XPS/Ph3PCHCOMeM062XPSpaul
Ph3PCHCOMe
M062X/6-31+G**
E(RM062X) = -1227.88436274

Zero-point correction= 0.339960 (Hartree/Particle)
Thermal correction to Energy= 0.360930
Thermal correction to Enthalpy= 0.361874
Thermal correction to Gibbs Free Energy= 0.287431
Sum of electronic and ZPE= -1227.544403
Sum of electronic and thermal Energies= -1227.523433
Sum of electronic and thermal Enthalpies= -1227.522488
Sum of electronic and thermal Free Energies= -1227.596932

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	226.487	80.318	156.679

C,0,0.4386106657,0.1169872578,0.4158552475
P,0,0.4361182649,-0.1363375506,2.1329560455
H,0,-0.2169075726,0.8896179722,0.0339719124
C,0,4.2850631222,1.1267617834,4.3296733531
C,0,3.0633634116,1.1560380836,5.0035981449
C,0,1.8948052495,0.7818125858,4.3428409829
C,0,1.9505127766,0.3752460952,3.0045147191
C,0,3.1733772852,0.3533363478,2.3269257111
C,0,4.3388250116,0.7280424689,2.9939588633
H,0,5.1948001428,1.4198955778,4.8442231555
H,0,3.0186702217,1.4744034153,6.0400728807
H,0,0.9427389661,0.8131459361,4.8667781129
H,0,3.2098042221,0.0384199394,1.2886433974
H,0,5.28837475,0.708824361,2.4689913268
C,0,-0.5387395911,-4.4785274854,3.3154738742
C,0,0.3736891249,-3.7530412195,4.0798643423
C,0,0.6996043808,-2.4436327564,3.7256386341
C,0,0.1062104545,-1.8619240432,2.6024373421
C,0,-0.8022834299,-2.5931566136,1.8297029782
C,0,-1.1248650494,-3.8990938989,2.1888991876
H,0,-0.7879960291,-5.4982108159,3.5917174556
H,0,0.8387554082,-4.2057205431,4.9496229369
H,0,1.4193387167,-1.8883940576,4.3193507372
H,0,-1.2446486726,-2.1411943431,0.9457983655
H,0,-1.8269145186,-4.4661388458,1.5861185163
C,0,-2.8875580804,2.5283491515,3.8776770648
C,0,-1.8491619119,3.0839019512,3.1266617995
C,0,-0.8516700676,2.2650325462,2.6059649155
C,0,-0.8929417448,0.8831790643,2.8334384969
C,0,-1.9297046123,0.3278799648,3.5866495665
C,0,-2.9267598676,1.1547142716,4.1067625224
H,0,-3.6645179317,3.1680288832,4.284262714
H,0,-1.8151394216,4.1539097219,2.9493869249
H,0,-0.0386191148,2.698704698,2.0289379791
H,0,-1.9654399156,-0.7421467237,3.7685028542
H,0,-3.7326141816,0.7218113123,4.6907129388
C,0,1.1877322785,-0.7192652639,-0.4245539735
C,0,1.0664308231,-0.522352046,-1.9244644579
O,0,1.9518265164,-1.6354376912,-0.0081975239
H,0,2.0612386731,-0.3411243066,-2.3416680939
H,0,0.6843459414,-1.4455254844,-2.3708138132
H,0,0.4063083053,0.3053592997,-2.1901511375

TS1 4

/home/singletn/wittig/pauling/m062XPS/TS1M062XPSpaul
TS1

M062X/6-31+G**
E(RM062X) = -1687.81146827

Zero-point correction= 0.486148 (Hartree/Particle)
Thermal correction to Energy= 0.516038
Thermal correction to Enthalpy= 0.516982
Thermal correction to Gibbs Free Energy= 0.423865
Sum of electronic and ZPE= -1687.325320
Sum of electronic and thermal Energies= -1687.295430
Sum of electronic and thermal Enthalpies= -1687.294486
Sum of electronic and thermal Free Energies= -1687.387603

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	323.819	115.487	195.981

O,0,0.9775209093,1.7899770503,1.2424484678
C,0,1.3486560511,0.5775322544,1.080953392
P,0,-1.3336417999,0.0452982884,-0.141261823
C,0,0.4115283363,-0.1528644356,-0.4765425154
C,0,2.7863794732,0.2999575757,0.7211587147
C,0,-2.3253875488,-1.2732308388,-0.9044519992
C,0,-2.0124193559,-1.6801183401,-2.2069339281
C,0,-2.8102358021,-2.6226885405,-2.8490689476
C,0,-3.9213558545,-3.1595991771,-2.1950548913
C,0,-4.2341967997,-2.7520315248,-0.9002318732
C,0,-3.4386467143,-1.8071691214,-0.2514929898
C,0,-1.906062068,1.5977247618,-0.882472327
C,0,-1.7583736003,0.0685523498,1.6225988265
C,0,-1.0644317754,2.7153846256,-0.9065739117
C,0,-1.5329151232,3.9162549163,-1.4369652453
C,0,-2.8320752208,4.0050099776,-1.936160983
C,0,-3.6706838303,2.8904510686,-1.9075280329
C,0,-3.211314691,1.6845045905,-1.3826767336
C,0,-2.3367448444,1.2012243907,2.2008880638
C,0,-2.6835661969,1.1847589821,3.551725456
C,0,-2.4530611053,0.044523333,4.3192364066
C,0,-1.8709576798,-1.0849243413,3.740786168
C,0,-1.5216770573,-1.0775681945,2.3932447742
C,0,3.4160876929,-0.8680736647,1.1664179423
C,0,4.738199696,-1.1347628688,0.836428164
C,0,5.4566988196,-0.227763761,0.048174825
C,0,4.8441322314,0.9475353073,-0.3994627203
C,0,3.5158204494,1.1999645734,-0.0516097956
H,0,0.9581780594,-0.1935483445,1.7733072268
H,0,0.7405186345,0.5292249307,-1.2608007939
H,0,-1.1488462952,-1.26218078,-2.7190660459
H,0,-2.5646005358,-2.9392027482,-3.8574223925
H,0,-4.5410370644,-3.896357076,-2.6960687551
H,0,-5.0973835951,-3.166281771,-0.389910304
H,0,-3.6898128388,-1.4922012582,0.7562538356
H,0,-0.0646603249,2.6498310424,-0.4863149436
H,0,-0.8810886886,4.7837285393,-1.4547180143
H,0,-3.1915715111,4.9430190269,-2.3475727891
H,0,-4.68194978,2.9564972052,-2.2951066262
H,0,-3.8681805363,0.8195989462,-1.3664648329
H,0,-2.5096690543,2.0943323118,1.6083974102
H,0,-3.1305228013,2.065094739,4.0017130732
H,0,-2.7242051865,0.0351636066,5.3702623839
H,0,-1.6889513364,-1.9721160844,4.3385006964
H,0,-1.0666600996,-1.9517950371,1.9357199235
H,0,2.8612105103,-1.577820109,1.7762398477
H,0,5.2347079439,-2.0355133359,1.1832579234
O,0,6.747976088,-0.5679237039,-0.2255770469
H,0,5.3860799002,1.6653398483,-1.0035957964
H,0,3.0376911778,2.1161842295,-0.3883399803
C,0,0.8575698874,-1.5343786373,-0.6209915258
C,0,1.9491368607,-1.8210283137,-1.6225074802
O,0,0.385831279,-2.4428392147,0.0734660529
H,0,2.4900509685,-2.7248299624,-1.3370782171
H,0,1.472277659,-1.9851044259,-2.5965658442
H,0,2.6394949518,-0.9793587886,-1.7195026066
C,0,7.5179910624,0.3326775208,-1.0107640267
H,0,8.5045337691,-0.1187295689,-1.1036329538
H,0,7.0767223352,0.4594574471,-2.004811784
H,0,7.6036319699,1.3062775286,-0.5174290985

Betaine 5

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l
betaine
M062X/6-31+G**
E(RM062X) = -1687.81637229

Zero-point correction= 0.488603 (Hartree/Particle)
Thermal correction to Energy= 0.518576
Thermal correction to Enthalpy= 0.519520
Thermal correction to Gibbs Free Energy= 0.425939
Sum of electronic and ZPE= -1687.327770
Sum of electronic and thermal Energies= -1687.297796
Sum of electronic and thermal Enthalpies= -1687.296852
Sum of electronic and thermal Free Energies= -1687.390433

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	325.411	115.771	196.959

8 0.854034 1.603946 1.265016
6 1.256419 0.350114 1.002031
15 -1.333550 0.086356 -0.040410
6 0.459674 -0.220011 -0.285682
6 2.745422 0.188862 0.692171
6 -2.264514 -1.236075 -0.864821
6 -1.952683 -1.523579 -2.200291
6 -2.662753 -2.506424 -2.881369
6 -3.686998 -3.201537 -2.232940
6 -4.000375 -2.910737 -0.907348
6 -3.290595 -1.925902 -0.217854
6 -1.833302 1.621406 -0.867651
6 -1.829759 0.124797 1.695935
6 -1.007601 2.751632 -0.828423
6 -1.426137 3.925834 -1.452163
6 -2.658705 3.977971 -2.102943
6 -3.483194 2.852983 -2.131695
6 -3.073850 1.671517 -1.517384
6 -2.582541 1.195686 2.185239
6 -3.000299 1.189600 3.514650
6 -2.665525 0.123206 4.348739
6 -1.915424 -0.944868 3.855584
6 -1.498002 -0.951980 2.527079
6 3.463363 -0.928146 1.133410
6 4.805126 -1.094373 0.810432

6 5.459561 -0.131765 0.033536
6 4.761946 0.995103 -0.410996
6 3.413692 1.140819 -0.074662
1 1.023332 -0.386175 1.802604
1 0.756039 0.400126 -1.139298
1 -1.156841 -0.979486 -2.704170
1 -2.418940 -2.730690 -3.914546
1 -4.238791 -3.970151 -2.764388
1 -4.796553 -3.448711 -0.403717
1 -3.536686 -1.703421 0.815646
1 -0.065450 2.696659 -0.287628
1 -0.787270 4.802568 -1.424595
1 -2.978636 4.895602 -2.586859
1 -4.443581 2.891511 -2.635144
1 -3.718718 0.798684 -1.548960
1 -2.832237 2.033404 1.541405
1 -3.581085 2.022031 3.897955
1 -2.988162 0.124984 5.385095
1 -1.653443 -1.775187 4.503047
1 -0.921537 -1.785446 2.135850
1 2.961774 -1.682430 1.736634
1 5.365321 -1.958247 1.155147
8 6.776544 -0.372749 -0.233416
1 5.250815 1.758705 -1.004361
1 2.870970 2.021142 -0.411434
6 0.789846 -1.673959 -0.526197
6 1.742719 -1.987226 -1.644935
8 0.327162 -2.541300 0.199981
1 2.102228 -3.013011 -1.558698
1 1.207430 -1.863713 -2.593730
1 2.580658 -1.283810 -1.644497
6 7.484541 0.597246 -0.992465
1 8.502174 0.220972 -1.085709
1 7.043922 0.714639 -1.988110
1 7.494280 1.563776 -0.477942

TS1.5 6

/home/singletn/wittig/pauling/m062XPS/TS1.5M062XPSpaul
TS1.5
M062X/6-31+G**
E(RM062X) = -1687.81281765

Zero-point correction= 0.488245 (Hartree/Particle)
Thermal correction to Energy= 0.517453
Thermal correction to Enthalpy= 0.518397
Thermal correction to Gibbs Free Energy= 0.426498
Sum of electronic and ZPE= -1687.324572
Sum of electronic and thermal Energies= -1687.295365
Sum of electronic and thermal Enthalpies= -1687.294421
Sum of electronic and thermal Free Energies= -1687.386320

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	324.707	113.865	193.419

8 0.672853 0.610277 1.474485
6 1.243087 -0.417324 0.770837
15 -1.189814 0.115704 0.086237
6 0.456896 -0.363455 -0.584045
6 2.739966 -0.321934 0.530975
6 -2.354233 -0.453246 -1.226538
6 -2.076795 -0.077084 -2.548747
6 -2.929419 -0.448581 -3.583774
6 -4.074623 -1.199314 -3.308168
6 -4.360236 -1.570403 -1.996965
6 -3.503761 -1.198713 -0.957594
6 -1.566304 1.899762 0.103661
6 -1.750641 -0.734701 1.584907
6 -0.571787 2.878054 0.184600
6 -0.924548 4.227531 0.165612
6 -2.264369 4.604274 0.092538
6 -3.259048 3.628211 0.022083
6 -2.912579 2.279658 0.010488
6 -2.278118 0.009435 2.644605
6 -2.736410 -0.645202 3.785192
6 -2.656683 -2.035586 3.875872
6 -2.123524 -2.773495 2.820228
6 -1.675938 -2.128353 1.667389
6 3.517929 -1.478308 0.393369
6 4.878756 -1.401804 0.124561
6 5.494374 -0.151309 -0.005990
6 4.736869 1.014307 0.134492
6 3.368323 0.913973 0.400277
1 1.049640 -1.419063 1.209814
1 0.816199 0.519305 -1.127795
1 -1.192968 0.515995 -2.776353
1 -2.702581 -0.152226 -4.603038
1 -4.739899 -1.490404 -4.114827
1 -5.249781 -2.151150 -1.774803
1 -3.740792 -1.492966 0.059941
1 0.464170 2.578720 0.284332
1 -0.147764 4.983266 0.221571
1 -2.534752 5.655515 0.090384
1 -4.304221 3.914339 -0.033614
1 -3.693660 1.528596 -0.068203
1 -2.319077 1.093013 2.589196
1 -3.146545 -0.066741 4.606656
1 -3.007634 -2.542292 4.769379
1 -2.057504 -3.854574 2.887677
1 -1.272678 -2.701272 0.837981
1 3.049696 -2.454950 0.501629
1 5.483473 -2.297503 0.021505
8 6.834329 -0.168743 -0.263949
1 5.193623 1.993065 0.047761
1 2.782050 1.820746 0.521333
6 0.538674 -1.602652 -1.444333
6 1.466311 -1.535798 -2.623378
8 -0.077990 -2.614217 -1.150931
1 1.602048 -2.524761 -3.060933
1 1.031443 -0.856063 -3.365529
1 2.428959 -1.112250 -2.317750
6 7.503374 1.080823 -0.364852
1 8.549291 0.846594 -0.556878
1 7.101751 1.674404 -1.192664
1 7.417910 1.645970 0.569001

OP1direct

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l
OP1 direct

M062X/6-31+G**
E(RM062X) = -1687.81983261

Zero-point correction= 0.489327 (Hartree/Particle)
Thermal correction to Energy= 0.518581
Thermal correction to Enthalpy= 0.519525
Thermal correction to Gibbs Free Energy= 0.428366
Sum of electronic and ZPE= -1687.330506
Sum of electronic and thermal Energies= -1687.301251
Sum of electronic and thermal Enthalpies= -1687.300307
Sum of electronic and thermal Free Energies= -1687.391466

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	325.415	115.057	191.860

O,0,0.8868206849,0.9433337741,1.1243823598
C,0,1.7029817497,-0.2085671292,1.0216388281
P,0,-0.622641218,0.1776721806,0.405248185
C,0,0.7794845223,-1.0693641027,0.1581031937
C,0,3.0677459195,0.0666799268,0.4328664646
C,0,-1.8977031083,-0.956772665,-0.4589346051
C,0,-1.9881489762,-0.9834221419,-1.8577144442
C,0,-2.716572364,-1.974229572,-2.5201241653
C,0,-3.36861788,-2.9688195776,-1.7920491622
C,0,-3.2844303919,-2.9630655982,-0.4001586219
C,0,-2.5531757139,-1.9714690749,0.2546511154
C,0,-0.796834289,1.5945444982,-0.7549906808
C,0,-1.5220679862,0.3534389015,2.0031422916
C,0,0.3298513269,2.1223462463,-1.392203869
C,0,0.1939587564,3.1613346924,-2.3136294523
C,0,-1.0630514403,3.7014540329,-2.5797836513
C,0,-2.1894208853,3.1842677003,-1.9388281291
C,0,-2.0591216288,2.1222394883,-1.0466048365
C,0,-2.910709723,0.5418653721,2.0197174193
C,0,-3.5895881191,0.7107039722,3.2243664319
C,0,-2.8955704915,0.6518553469,4.4328092304
C,0,-1.5188353466,0.4388951927,4.4274281403
C,0,-0.8328184306,0.308063024,3.2202389861
C,0,3.8661390321,-0.9913869536,-0.0243494558
C,0,5.1393400038,-0.7621096162,-0.5255413376
C,0,5.645511143,0.5439601156,-0.5773070143
C,0,4.8648264167,1.6088431231,-0.1276736444
C,0,3.5830134716,1.3578703254,0.3745286008
H,0,1.8301929546,-0.6882321578,2.0052661352
H,0,1.0370485767,-1.0337041632,-0.9083269611
H,0,-1.4799576235,-0.2271828416,-2.451691961
H,0,-2.7702500174,-1.9681705861,-3.6048999942
H,0,-3.9343678293,-3.7414272053,-2.3035155615
H,0,-3.7817648343,-3.7344807519,0.1802399499
H,0,-2.4886498398,-2.0032472517,1.3393032737
H,0,1.3144859262,1.7247339316,-1.168534557
H,0,1.0738401085,3.554330334,-2.8133911344
H,0,-1.1659510208,4.5202231401,-3.2850723017
H,0,-3.172071644,3.5980136797,-2.1414250137
H,0,-2.9500778637,1.7036241161,-0.5905694582
H,0,-3.4785695518,0.5402335553,1.095693512
H,0,-4.6624845959,0.8743508601,3.2164647872
H,0,-3.4258335338,0.768039775,5.3728627667
H,0,-0.9698801375,0.3832002418,5.361929512
H,0,0.2412732709,0.1737722796,3.2312246769
H,0,3.4876615472,-2.0114314363,0.0149587249
H,0,5.7591702403,-1.5789955182,-0.8815742316
O,0,6.9047554791,0.675534524,-1.0840304471
H,0,5.2337691556,2.6268595927,-0.1587698022
H,0,2.9755535082,2.186727629,0.7247305457
C,0,0.5120136199,-2.4912181118,0.599189347
C,0,0.3292442258,-3.524562031,-0.4752738822
O,0,0.4760892844,-2.7731872654,1.7869037894
H,0,-0.0188330229,-4.4648730706,-0.0472947375
H,0,-0.3726061239,-3.1632354144,-1.2338411855
H,0,1.2961384034,-3.6780709585,-0.9698405469
C,0,7.4701923163,1.9793863816,-1.1125052637
H,0,8.4675302018,1.8643026965,-1.5338117059
H,0,6.8782953711,2.6493871491,-1.7446571085
H,0,7.5409484147,2.3943543954,-0.1017753446

Full System, M06-2X/6-31G*/PCM(THF) with Pauling Radii

Anisaldehyde 1

/home/singletn/wittig/pauling/m062XSB/anisaldehydeM062XSBpaul
anisaldehyde
M062X/6-31G*
E(RM062X) = -459.912806908

Zero-point correction= 0.144358 (Hartree/Particle)
Thermal correction to Energy= 0.153266
Thermal correction to Enthalpy= 0.154210
Thermal correction to Gibbs Free Energy= 0.109856
Sum of electronic and ZPE= -459.768449
Sum of electronic and thermal Energies= -459.759541
Sum of electronic and thermal Enthalpies= -459.758597
Sum of electronic and thermal Free Energies= -459.802951

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	96.176	32.823	93.350

C,0,-0.001519557,0.,0.1151864841
C,0,0.0529100644,0.,1.516677917
C,0,1.2898439209,0.,2.1464639378
C,0,2.472910484,0.,1.4030966948
C,0,2.4057123183,0.,0.003979994
C,0,1.181613241,0.,-0.6391562251
H,0,-0.8532347325,0.,2.1102052965
H,0,1.3484690599,0.,3.2307788831
C,0,3.7829265103,0.,2.0693997652
H,0,3.3243854292,0.,-0.5772681453
H,0,1.107036849,0.,-1.721336069
O,0,-1.1482670565,0.,-0.597218452
C,0,-2.3784645333,0.,0.1159858221
H,0,-3.1614955597,0.,-0.6405368558
H,0,-2.4676180282,-0.895201031,0.7392158031
H,0,-2.4676180282,0.895201031,0.7392158031
O,0,3.9448873709,0.,3.2763629719
H,0,4.6551452475,0.,1.3883423752

Ph3PCHCOMe 2

/home/singletn/wittig/pauling/m062XSB/Ph3PCHCOMeM062XSBpaul
Ph3PCHCOMe
M062X/6-31G*
E(RM062X) = -1227.82933969

Zero-point correction= 0.342237 (Hartree/Particle)
Thermal correction to Energy= 0.363040
Thermal correction to Enthalpy= 0.363984
Thermal correction to Gibbs Free Energy= 0.290394
Sum of electronic and ZPE= -1227.487103
Sum of electronic and thermal Energies= -1227.466300
Sum of electronic and thermal Enthalpies= -1227.465355
Sum of electronic and thermal Free Energies= -1227.538946

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	227.811	79.826	154.884

C,0,0.3992612645,0.1281862753,0.4254109356
P,0,0.4303091912,-0.1393613026,2.1341918293
H,0,-0.2637755094,0.9021962264,0.0596698528
C,0,4.3175987783,1.1244513779,4.2623614966
C,0,3.1033528048,1.2076853602,4.9421766587
C,0,1.9226605226,0.8303597561,4.3072488682
C,0,1.9589168149,0.3611180307,2.9893412175
C,0,3.1774239119,0.2819749459,2.3069792844
C,0,4.3533990959,0.6632223653,2.9474175327
H,0,5.2366682639,1.4223362187,4.7573482448
H,0,3.074285908,1.572308384,5.9639148506
H,0,0.9754612821,0.9062901795,4.8347615856
H,0,3.1987753109,-0.0885915401,1.2870275372
H,0,5.2983725421,0.6006166481,2.4175843095
C,0,-0.5338860467,-4.4779618146,3.3250619404
C,0,0.214423193,-3.6814963614,4.1898514351
C,0,0.5376256069,-2.3749560601,3.8313548057
C,0,0.105389963,-1.8645743578,2.6041765815
C,0,-0.6438182261,-2.6645810298,1.736818371
C,0,-0.9614165089,-3.9702285952,2.0990740972
H,0,-0.7808943136,-5.4972844794,3.6046791865
H,0,0.5524318713,-4.0778257088,5.141885558
H,0,1.1287881695,-1.7603457931,4.5040362608
H,0,-0.9670120356,-2.2635144357,0.7804208038
H,0,-1.5364170022,-4.5935625249,1.4220225087
C,0,-2.8805952096,2.5130649392,3.9135968247
C,0,-1.8086957212,3.0804259904,3.2231421318
C,0,-0.8102358462,2.2666400746,2.69960861
C,0,-0.8837024333,0.8776712983,2.8640804561
C,0,-1.9544066675,0.311107987,3.5580616973
C,0,-2.952339619,1.1329051738,4.0807456961
H,0,-3.6589309114,3.1495647844,4.3225471311
H,0,-1.7501200817,4.1564494523,3.0951685464
H,0,0.0279176232,2.7084138067,2.1667178218
H,0,-2.014658495,-0.7650912914,3.6901843066
H,0,-3.7856142565,0.6911241871,4.6175272186
C,0,1.1502685692,-0.7000609808,-0.4242554345
C,0,1.0202095139,-0.4885969095,-1.924514785
O,0,1.918591703,-1.6105893407,-0.0216948613
H,0,2.004925182,-0.2458241451,-2.3358217958
H,0,0.696679445,-1.4259301963,-2.3874568594
H,0,0.3168453525,0.3044424052,-2.1857154568

TS1 4

/home/singletn/wittig/pauling/m062XSB/TS1M062XSBpaul
TS1
M062X/6-31G*
E(RM062X) = -1687.73300158

Zero-point correction= 0.488680 (Hartree/Particle)
Thermal correction to Energy= 0.518529
Thermal correction to Enthalpy= 0.519473
Thermal correction to Gibbs Free Energy= 0.425934
Sum of electronic and ZPE= -1687.244322
Sum of electronic and thermal Energies= -1687.214473
Sum of electronic and thermal Enthalpies= -1687.213528
Sum of electronic and thermal Free Energies= -1687.307068

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	325.382	114.916	196.871

O,0,0.929227219,1.761444474,1.1998066311
C,0,1.3085375913,0.5532028595,1.0387173332
P,0,-1.3369991187,0.0351151874,-0.1448658453
C,0,0.405208291,-0.174354105,-0.4901954871
C,0,2.7580275356,0.2875717637,0.7005334258
C,0,-2.3364933857,-1.2821337323,-0.897125145
C,0,-2.0107479146,-1.7208931734,-2.1856862513
C,0,-2.8113193415,-2.6647031786,-2.8198682633
C,0,-3.940594818,-3.1692317374,-2.1741727729
C,0,-4.2703378466,-2.7270723978,-0.8961042404
C,0,-3.4717112767,-1.7821818122,-0.2545609852
C,0,-1.9038768105,1.5873858564,-0.8878939516
C,0,-1.7417908676,0.0599414789,1.6219433119
C,0,-1.054313064,2.6990568199,-0.9141807671
C,0,-1.512822257,3.89747072,-1.4550250122
C,0,-2.8068078279,3.9897431337,-1.9638906288
C,0,-3.6523516838,2.8820743764,-1.9327110932
C,0,-3.2047796596,1.6781643813,-1.396561098
C,0,-2.2398736304,1.2182712925,2.2220402329
C,0,-2.5614092597,1.2069186329,3.5775032627
C,0,-2.3832229072,0.047703656,4.3284593585
C,0,-1.8778332445,-1.1064126998,3.729946401
C,0,-1.5542310373,-1.1049479866,2.3770727743
C,0,3.381043411,-0.9048447098,1.0847284475
C,0,4.7073266899,-1.1508825686,0.762188018
C,0,5.4404313939,-0.1976655037,0.0448201752
C,0,4.8350332236,1.0027794357,-0.3370241189
C,0,3.5013126774,1.2329223594,0.000983694
H,0,0.9315673528,-0.2228866486,1.7385644583
H,0,0.7284766123,0.5032258722,-1.2806613954
H,0,-1.1331703487,-1.326566041,-2.6924968331
H,0,-2.5535766717,-3.007240475,-3.8165820134
H,0,-4.563378271,-3.9071740887,-2.6695771108
H,0,-5.1492451799,-3.1160647809,-0.3928764836
H,0,-3.7359590094,-1.4396249345,0.7407282664
H,0,-0.0587145542,2.6246094844,-0.4843127489
H,0,-0.8561445794,4.7612691878,-1.4757096868
H,0,-3.1573599749,4.9267777798,-2.3852302029
H,0,-4.660355473,2.9523470282,-2.3280577487

H,0,-3.8660182816,0.816718542,-1.3784935142
H,0,-2.3745249108,2.1234941366,1.6386007744
H,0,-2.9490900251,2.1057184802,4.0454133277
H,0,-2.6351479253,0.0430472514,5.3842819788
H,0,-1.7335111943,-2.0072741794,4.317274407
H,0,-1.1513577294,-1.9957057617,1.9036694197
H,0,2.8129198071,-1.6517101477,1.6356679689
H,0,5.2005629297,-2.071073555,1.0591318553
O,0,6.7337286846,-0.5242528786,-0.2281623668
H,0,5.3894157231,1.7585551419,-0.8810620444
H,0,3.0271994961,2.1696853209,-0.2789580156
C,0,0.8412093443,-1.5620245907,-0.6352957369
C,0,1.9218394688,-1.8530268033,-1.6502967539
O,0,0.3768447184,-2.46136822,0.068421754
H,0,2.4573505744,-2.7632962957,-1.3742771541
H,0,1.4377158471,-2.0074379994,-2.6226723742
H,0,2.6201791136,-1.0176108316,-1.7470002986
C,0,7.5130690108,0.4296153795,-0.9306065988
H,0,8.5002632428,-0.015448367,-1.0496921551
H,0,7.0853353819,0.6405028007,-1.9167057268
H,0,7.5969847401,1.3628543708,-0.3634556534

Betaine 5

/home/singletn/wittig/pauling/m062XSB/betaineM062XSBpaul
betaine
M062X/6-31G*
E(RM062X) = -1687.73632649

Zero-point correction= 0.491134 (Hartree/Particle)
Thermal correction to Energy= 0.520919
Thermal correction to Enthalpy= 0.521863
Thermal correction to Gibbs Free Energy= 0.428832
Sum of electronic and ZPE= -1687.245193
Sum of electronic and thermal Energies= -1687.215407
Sum of electronic and thermal Enthalpies= -1687.214463
Sum of electronic and thermal Free Energies= -1687.307495

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	326.882	115.269	195.801

O,0,0.8169230886,1.548386463,1.2276818058
C,0,1.2435692767,0.3172653503,0.9562234678
P,0,-1.3171255903,0.075372665,-0.0460875485
C,0,0.4597156333,-0.2300885357,-0.3578436886
C,0,2.7392194865,0.1751883622,0.6657655838
C,0,-2.2723189573,-1.1905897465,-0.9312985937
C,0,-1.9820932461,-1.4037246797,-2.285578625
C,0,-2.7124496033,-2.3360485534,-3.0126500387
C,0,-3.7377624199,-3.0539795583,-2.3949726321
C,0,-4.0325356468,-2.8364729563,-1.0525625245
C,0,-3.3024576663,-1.903444851,-0.3168012454
C,0,-1.8559146664,1.6507014667,-0.7651693182
C,0,-1.7702048905,-0.0124668829,1.6996207418
C,0,-1.0044605529,2.7605893594,-0.7843993968
C,0,-1.4540541197,3.9557482573,-1.3403960235
C,0,-2.7426768546,4.0488328679,-1.8621995911
C,0,-3.5926178124,2.9442667165,-1.8311258389
C,0,-3.1523699091,1.7409640787,-1.2887519226
C,0,-2.4394826052,1.0536829034,2.3050927833
C,0,-2.8275018063,0.95051764,3.6379688049
C,0,-2.5461860066,-0.2067688753,4.3613687892
C,0,-1.8758275442,-1.2681282165,3.7551214449
C,0,-1.4863212408,-1.1774911428,2.4219840514
C,0,3.4355447228,-1.0048055688,0.9517650588
C,0,4.7804875359,-1.1385159101,0.637440475
C,0,5.4644279078,-0.0788821143,0.0293783674
C,0,4.7893193887,1.111020797,-0.2515620537
C,0,3.4361430285,1.2232805329,0.0739454925
H,0,1.0011779222,-0.4532723158,1.7276314284
H,0,0.7497987604,0.4309663162,-1.181364281
H,0,-1.1870697645,-0.8422245642,-2.7719035808
H,0,-2.483672681,-2.5028533713,-4.059992747
H,0,-4.3065248436,-3.7820578698,-2.9644123288
H,0,-4.8312274796,-3.3912238758,-0.5714537497
H,0,-3.5368469387,-1.7376452667,0.7296103689
H,0,-0.0191021002,2.6684647223,-0.3349887815
H,0,-0.795255028,4.817890948,-1.3594742615
H,0,-3.0879335738,4.98409003,-2.2919689134
H,0,-4.5971798376,3.0164113769,-2.2347315205
H,0,-3.8151137457,0.8807444476,-1.2771164716
H,0,-2.650975236,1.9582044176,1.7435671425
H,0,-3.3455792754,1.7776274654,4.1118011452
H,0,-2.848781493,-0.2809782735,5.4011269512
H,0,-1.6524770769,-2.1679365393,4.3186353933
H,0,-0.9651411928,-2.0005299213,1.941542796
H,0,2.911637325,-1.8332622414,1.4250679512
H,0,5.326204871,-2.049992047,0.8609233329
O,0,6.7821686095,-0.2988493129,-0.2419503073
H,0,5.3021945509,1.9490617792,-0.7094857246
H,0,2.9072990273,2.1517781246,-0.1223777442
C,0,0.7822412328,-1.6690432197,-0.6600180206
C,0,1.7289856444,-1.9311929657,-1.7999853901
O,0,0.3275309286,-2.5681231407,0.0295551084
H,0,2.0796194158,-2.9636547248,-1.7704236836
H,0,1.1925080127,-1.7529714789,-2.7398595472
H,0,2.5742994226,-1.2373893262,-1.7652704807
C,0,7.513323057,0.7636038007,-0.829682335
H,0,8.532049209,0.3971911868,-0.9523510793
H,0,7.1011227856,1.0329470117,-1.8085427622
H,0,7.5159235616,1.6469349596,-0.1821307325

TS1.5 6

/home/singletn/wittig/pauling/m062XSB/TS1.5M062XSBpaul
TS1.5
M062X/6-31G*
E(RM062X) = -1687.73496109

Zero-point correction= 0.491032 (Hartree/Particle)
Thermal correction to Energy= 0.520022
Thermal correction to Enthalpy= 0.520966
Thermal correction to Gibbs Free Energy= 0.429827
Sum of electronic and ZPE= -1687.243929
Sum of electronic and thermal Energies= -1687.214939
Sum of electronic and thermal Enthalpies= -1687.213995
Sum of electronic and thermal Free Energies= -1687.305134

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 326.319 113.236 191.818

8 0.750875 1.059857 1.255261
6 1.257325 -0.106324 0.798868
15 -1.231963 0.136191 0.043793
6 0.434535 -0.396626 -0.520589
6 2.751869 -0.126609 0.501024
6 -2.390681 -0.802074 -1.024559
6 -2.185378 -0.738284 -2.409801
6 -3.040578 -1.404877 -3.279382
6 -4.114732 -2.137715 -2.773167
6 -4.328331 -2.197965 -1.399714
6 -3.469435 -1.532583 -0.524088
6 -1.668988 1.855405 -0.359744
6 -1.673161 -0.303964 1.742402
6 -0.705921 2.861980 -0.464036
6 -1.094254 4.152322 -0.817073
6 -2.437175 4.446792 -1.040248
6 -3.400841 3.446467 -0.917831
6 -3.019646 2.148961 -0.592175
6 -2.173354 0.676408 2.603251
6 -2.547144 0.328314 3.897275
6 -2.412802 -0.988525 4.335353
6 -1.908523 -1.962544 3.476894
6 -1.541380 -1.627015 2.175230
6 3.442353 -1.338568 0.366368
6 4.798054 -1.365330 0.076867
6 5.503542 -0.164572 -0.075902
6 4.835455 1.051737 0.065250
6 3.467318 1.055829 0.351921
1 1.056697 -0.985222 1.455379
1 0.750925 0.343707 -1.264781
1 -1.355409 -0.161045 -2.813294
1 -2.871230 -1.351342 -4.349989
1 -4.783718 -2.658675 -3.450851
1 -5.164502 -2.764445 -1.002327
1 -3.647746 -1.587373 0.544884
1 0.324904 2.621934 -0.234029
1 -0.343470 4.930551 -0.908083
1 -2.734762 5.456086 -1.306988
1 -4.448665 3.672106 -1.086237
1 -3.773041 1.369874 -0.519593
1 -2.259308 1.705752 2.268875
1 -2.935989 1.088596 4.566699
1 -2.699656 -1.254076 5.347929
1 -1.799713 -2.987299 3.816933
1 -1.153500 -2.382955 1.499363
1 2.906344 -2.278015 0.495481
1 5.336263 -2.302697 -0.024350
8 6.832837 -0.287605 -0.351251
1 5.363027 1.993141 -0.036165
1 2.950714 2.001731 0.482243
6 0.529617 -1.801844 -1.062937
6 1.353749 -1.994766 -2.305562
8 0.001712 -2.734234 -0.480424
1 1.466315 -3.056987 -2.525031
1 0.853795 -1.491744 -3.141428
1 2.334639 -1.524954 -2.178842
6 7.581167 0.906858 -0.499998
1 8.604622 0.598237 -0.710914
1 7.201946 1.509648 -1.332492
1 7.560609 1.503120 0.418628

OP1direct

/home/singletn/wittig/pauling/m062XSB/OP1directM062XSB
paul
OP1 direct
M062X/6-31G*
E(RM062X) = -1687.74665849

Zero-point correction= 0.492133 (Hartree/Particle)
Thermal correction to Energy= 0.521231
Thermal correction to Enthalpy= 0.522175
Thermal correction to Gibbs Free Energy= 0.430959
Sum of electronic and ZPE= -1687.254526
Sum of electronic and thermal Energies= -1687.225428
Sum of electronic and thermal Enthalpies= -1687.224483
Sum of electronic and thermal Free Energies= -1687.315700

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	327.077	114.380	191.980

O,0,0.9000076109,0.8760466043,1.1888820332
C,0,1.7216086053,-0.267486267,1.0400240591
P,0,-0.5940359494,0.1498979277,0.4385621136
C,0,0.7851735186,-1.1179005911,0.1812275289
C,0,3.0661447436,0.0386592986,0.4200469245
C,0,-1.8724140762,-0.9681218473,-0.4465557479
C,0,-1.9292291091,-0.999179266,-1.8467112289
C,0,-2.6595718965,-1.9771772666,-2.5230059664
C,0,-3.3482749464,-2.955359123,-1.8086145453
C,0,-3.2958833357,-2.9485422914,-0.4164170725
C,0,-2.5627485306,-1.9693041566,0.2527495054
C,0,-0.7391764236,1.5715609792,-0.7178044919
C,0,-1.5279825955,0.3429867903,2.0137539409
C,0,0.4069381709,2.1165216835,-1.3020732524
C,0,0.3022302931,3.1641679594,-2.2152376546
C,0,-0.9455338372,3.6975440903,-2.5270664245
C,0,-2.0925740345,3.1644782384,-1.9406705643
C,0,-1.991954685,2.0940133308,-1.0570506646
C,0,-2.9148328184,0.5397794442,1.9925561584
C,0,-3.6221533788,0.7348933717,3.1744315347
C,0,-2.9587776453,0.6948515946,4.3995021327
C,0,-1.5848610804,0.4737263376,4.4332064116
C,0,-0.8697751497,0.314225823,3.24792101
C,0,3.8417250392,-0.9835707732,-0.14121541
C,0,5.0903790311,-0.7180361935,-0.6813166174
C,0,5.5958765243,0.5886139131,-0.6695429571
C,0,4.8381751989,1.6176473633,-0.1110269999
C,0,3.5824052621,1.3307320479,0.4297351189
H,0,1.8762526309,-0.7628090608,2.0118189146
H,0,1.0413784502,-1.1077349627,-0.885270528
H,0,-1.3943088895,-0.2522723526,-2.4288270031
H,0,-2.6894474069,-1.9732685885,-3.6086972871
H,0,-3.9180807893,-3.7168834024,-2.3320994682
H,0,-3.8234272223,-3.7076108792,0.1535406319
H,0,-2.5254907866,-1.9971868267,1.3385751382
H,0,1.3824957073,1.7214357052,-1.0398173446
H,0,1.1994917433,3.5684004688,-2.6733953976
H,0,-1.0262101789,4.523308524,-3.2271178298
H,0,-3.0687645291,3.5736294661,-2.1806055501

H,0,-2.8987397262,1.6659344399,-0.6422478011
H,0,-3.4570908245,0.524990572,1.0533109733
H,0,-4.6935694531,0.9042333093,3.1366868239
H,0,-3.5130739481,0.8320222614,5.3228806837
H,0,-1.0619504384,0.4339936094,5.3834402306
H,0,0.2034012168,0.1755354605,3.2817594202
H,0,3.4623443183,-2.0038074016,-0.1556559207
H,0,5.6937020448,-1.5055264993,-1.121735094
O,0,6.8263009212,0.7541780278,-1.2277682313
H,0,5.2061237158,2.6364512894,-0.0903781903
H,0,2.989338608,2.1320251725,0.8597863081
C,0,0.4720424294,-2.5169490445,0.6631512819
C,0,0.3028665148,-3.5865467202,-0.380310902
O,0,0.3745752547,-2.7453245506,1.8560708444
H,0,-0.0547007692,-4.5097587254,0.0771808609
H,0,-0.3922067365,-3.2477301464,-1.1562214902
H,0,1.2720543631,-3.7609073668,-0.8630485234
C,0,7.3823123891,2.0587397806,-1.2046557202
H,0,8.3574845345,1.9792242927,-1.6835524929
H,0,6.7567139046,2.764637959,-1.7616526184
H,0,7.5045684461,2.4151241667,-0.1762395933

OP1

/home/singletn/wittig/pauling/m062XSB/OP1M062XSBpaul
OP1
M062X/6-31G*
E(RM062X) = -1687.74038040

Zero-point correction= 0.492322 (Hartree/Particle)
Thermal correction to Energy= 0.521686
Thermal correction to Enthalpy= 0.522630
Thermal correction to Gibbs Free Energy= 0.430541
Sum of electronic and ZPE= -1687.248058
Sum of electronic and thermal Energies= -1687.218694
Sum of electronic and thermal Enthalpies= -1687.217750
Sum of electronic and thermal Free Energies= -1687.309840

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	327.363	114.453	193.819

O,0,1.1104715857,0.9533765623,0.8620572087
C,0,1.7913990417,-0.2457879751,0.6013792966
P,0,-0.5180640079,0.3334373295,0.1690604301
C,0,0.8376445834,-0.7883538347,-0.4855899374
C,0,3.2166033694,-0.0566126202,0.1481053248
C,0,-1.9810848455,-0.5197293845,-0.6828988525
C,0,-1.8063729259,-1.1451489122,-1.9226333969
C,0,-2.8834945015,-1.6866554465,-2.6238138562
C,0,-4.1684905478,-1.6087191545,-2.0929465574
C,0,-4.3659775616,-0.9784637746,-0.8657142109
C,0,-3.2838210297,-0.4374458037,-0.1741780439
C,0,-0.8394944721,2.0199640413,-0.5421109239
C,0,-1.1160031313,0.1170057598,1.894054447
C,0,-0.1439073537,3.1382404321,-0.0501574303
C,0,-0.4061252471,4.4148473352,-0.5386663013
C,0,-1.3469422945,4.6037442618,-1.5483952795
C,0,-2.0281614169,3.5041783471,-2.0594215499
C,0,-1.7860499018,2.2271661736,-1.5558657234
C,0,-1.1136890596,1.2121575285,2.7633741884
C,0,-1.567970275,1.0707782316,4.0714094894
C,0,-1.9980638212,-0.1728770275,4.5321307467
C,0,-1.9836706479,-1.2702875663,3.6752366363
C,0,-1.55797905,-1.1255584089,2.3557787722
C,0,4.1854777056,-1.0236875081,0.4332909978
C,0,5.4854273116,-0.8919824255,-0.0341709106
C,0,5.8435610866,0.2266537623,-0.7945062299
C,0,4.8884077039,1.205296001,-1.0822471246
C,0,3.5852802156,1.052470467,-0.6092411046
H,0,1.7738466025,-0.9280717877,1.4685486273
H,0,1.1468655451,-0.3788275541,-1.4543078684
H,0,-0.8197814263,-1.1937795105,-2.3786681412
H,0,-2.7171364639,-2.1659923407,-3.5838524419
H,0,-5.0099604515,-2.0318139616,-2.6326915957
H,0,-5.3648835308,-0.9046560343,-0.4461165042
H,0,-3.4640720985,0.0628272967,0.773703978
H,0,0.6124638545,3.0090306159,0.7119630208
H,0,0.1375768776,5.261750475,-0.1319857766
H,0,-1.5429841408,5.5986025786,-1.9361131723
H,0,-2.7578252991,3.6327076982,-2.8526936824
H,0,-2.3430296273,1.3987937638,-1.9736926528
H,0,-0.761623431,2.1804436418,2.4215477637
H,0,-1.5765778204,1.9313771664,4.7329939253
H,0,-2.3410717013,-0.2851784367,5.5560217755
H,0,-2.3116868765,-2.2432881603,4.027479629
H,0,-1.5656122267,-1.9790340496,1.6870306607
H,0,3.9162058618,-1.8913859661,1.0316870359
H,0,6.2424226341,-1.638002245,0.1854384699
O,0,7.1404010731,0.2767349826,-1.2047838014
H,0,5.1463460168,2.0827289592,-1.6634975776
H,0,2.8416377639,1.8139747559,-0.82952849
C,0,0.7100089229,-2.2909127121,-0.5437084794
C,0,1.5200531506,-2.9812690929,-1.609298425
O,0,0.0544480658,-2.9078505014,0.2753749382
H,0,1.4638746306,-4.0635034491,-1.4885203549
H,0,1.1469801035,-2.6961848103,-2.5993669163
H,0,2.561215274,-2.6434684401,-1.547010372
C,0,7.5344007419,1.3855468195,-1.996018995
H,0,8.5890974154,1.2338820118,-2.2229851871
H,0,6.9612561846,1.4275736592,-2.9285120619
H,0,7.4090658628,2.3262162374,-1.449256433

OP2

/home/singletn/wittig/pauling/m062XSB/OP2M062XSBpaul
OP2
M062X/6-31G*
E(RM062X) = -1687.74493997

Zero-point correction= 0.492485 (Hartree/Particle)
Thermal correction to Energy= 0.521916
Thermal correction to Enthalpy= 0.522860
Thermal correction to Gibbs Free Energy= 0.430752
Sum of electronic and ZPE= -1687.252455
Sum of electronic and thermal Energies= -1687.223024
Sum of electronic and thermal Enthalpies= -1687.222080
Sum of electronic and thermal Free Energies= -1687.314188

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	327.507	114.578	193.856

O,0,0.28459946,-0.0520158875,-1.2377671106
C,0,1.1282954521,-1.1425042477,-0.7350405991
C,0,0.3985313939,-1.5190643518,0.5217691991
P,0,-0.9350049101,0.0888425557,-0.1478185139
H,0,1.0809841167,-1.9469327981,-1.4739402267
H,0,0.8801155089,-1.2105043702,1.4494375427
C,0,-2.9476508164,3.6749707528,-2.4042492593
C,0,-1.7543279264,3.1573449749,-2.8974023732
C,0,-1.1245291337,2.0923223168,-2.2488197214
C,0,-1.6816447639,1.5289139599,-1.0967776279
C,0,-2.8859935407,2.0608253628,-0.6141034695
C,0,-3.5148340872,3.1219209539,-1.2555893624
H,0,-3.4357235451,4.5024034469,-2.910068214
H,0,-1.3053284323,3.5804844224,-3.7910797524
H,0,-0.1938558442,1.7034478419,-2.6447774989
H,0,-3.3395400308,1.6438481791,0.2828517623
H,0,-4.4462097896,3.5171330894,-0.8616937258
C,0,-4.4817702388,-2.8034851657,-0.6969770472
C,0,-4.4227477799,-2.0366453173,0.4649260163
C,0,-3.3687133613,-1.1473600151,0.6693058981
C,0,-2.3661032313,-1.0276125049,-0.2983043716
C,0,-2.4328138702,-1.7887753888,-1.4691215309
C,0,-3.4872647445,-2.6756268482,-1.6645584828
H,0,-5.3021218339,-3.4976926576,-0.8489648916
H,0,-5.2002868725,-2.1259258365,1.2171215367
H,0,-3.3432669353,-0.5474594919,1.5742616433
H,0,-1.6584246331,-1.6912263549,-2.2258449246
H,0,-3.5283130659,-3.268646648,-2.5724437012
C,0,-0.4784041548,2.2340122852,3.927873359
C,0,-0.234613501,2.9207976778,2.7417756917
C,0,-0.4049664002,2.2808542612,1.5145652547
C,0,-0.7836732074,0.9355820559,1.4718373197
C,0,-0.9920652872,0.2411940706,2.668162192
C,0,-0.8658007824,0.8939395748,3.8891707475
H,0,-0.3604440142,2.7373214921,4.8822160919
H,0,0.0779323129,3.9597709689,2.7655530311
H,0,-0.2372127712,2.8301060859,0.5927508743
H,0,-1.2486366176,-0.8142339645,2.6443870725
H,0,-1.0535538727,0.3533450834,4.8112463584
C,0,5.1918375217,0.2248529849,-0.2869486139
C,0,4.9073495309,-0.8576609049,-1.1182765264
C,0,3.5836134924,-1.2807741379,-1.2592762181
C,0,2.542535652,-0.6540790774,-0.5829676278
C,0,2.8468993589,0.432398816,0.2497511765
C,0,4.1516739856,0.8704573432,0.3971831761
O,0,6.4386480216,0.7262707467,-0.0779000435
H,0,5.6933160389,-1.3717879855,-1.6583054855
H,0,3.3664070845,-2.121516931,-1.9130621373
H,0,2.0498245715,0.942571814,0.7875406763
H,0,4.3954159541,1.7136205661,1.0356316246
C,0,-0.1465840202,-2.8755991063,0.5829228412
C,0,-0.6890489537,-3.3569504486,1.9139674705
O,0,-0.2509614624,-3.6054915177,-0.4052800263
H,0,-0.6162593756,-4.4450625184,1.9686951888
H,0,-0.1735154156,-2.9021526238,2.7632021752
H,0,-1.7515951673,-3.0870252904,1.9671610535
C,0,7.5107041309,0.124552957,-0.7856793623
H,0,8.4065706116,0.6751644107,-0.5013845358
H,0,7.6237872576,-0.9290882484,-0.5088572848
H,0,7.3591143408,0.202006232,-1.867532774

TS2

/home/singletn/wittig/pauling/m062XSB/TS2M062XSBpaul
TS2
M062X/6-31G*
E(RM062X) = -1687.74367070

Zero-point correction= 0.491684 (Hartree/Particle)
Thermal correction to Energy= 0.520460
Thermal correction to Enthalpy= 0.521404
Thermal correction to Gibbs Free Energy= 0.430737
Sum of electronic and ZPE= -1687.251987
Sum of electronic and thermal Energies= -1687.223211
Sum of electronic and thermal Enthalpies= -1687.222267
Sum of electronic and thermal Free Energies= -1687.312933

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	326.593	112.806	190.824

O,0,0.2867488057,-0.0844809056,-1.2332017034
C,0,1.1268677586,-1.1712864007,-0.7210524386
C,0,0.3485288077,-1.5794063375,0.4997580493
P,0,-0.9294659102,0.0581957289,-0.1341883115
H,0,1.1147839136,-1.9572887475,-1.4803155573
H,0,0.8266681031,-1.366142373,1.4560888778
C,0,-2.9741889831,3.602925802,-2.4322221179
C,0,-1.7641158375,3.1072989584,-2.9066646093
C,0,-1.1278503477,2.0505746904,-2.2507486505
C,0,-1.6962386201,1.4715902339,-1.1122639464
C,0,-2.9190654292,1.9791459441,-0.6502081697
C,0,-3.553067407,3.0342138377,-1.2969306748
H,0,-3.4667919438,4.4248918734,-2.9425750866
H,0,-1.3068814488,3.5418861212,-3.7906305453
H,0,-0.1827465451,1.6806616696,-2.6305971337
H,0,-3.3830275679,1.5443800288,0.2335433542
H,0,-4.4983533994,3.4115636758,-0.9188219917
C,0,-4.5487764315,-2.7799533316,-0.4929120904
C,0,-4.2770188602,-2.1996082176,0.7442621168
C,0,-3.2035853815,-1.3223425115,0.8896174512
C,0,-2.4034439933,-1.0174517941,-0.2142388757
C,0,-2.6874793222,-1.5855873585,-1.4591740565
C,0,-3.7530279876,-2.4707815866,-1.5944620712
H,0,-5.3810114383,-3.4686224429,-0.5985064669
H,0,-4.9018721764,-2.4276380867,1.6021904462
H,0,-3.0090588106,-0.8717637072,1.8580862082
H,0,-2.0719960941,-1.3420893756,-2.3220448136
H,0,-3.9611967366,-2.9173134612,-2.5615117431
C,0,-0.2102159,2.4020763365,3.804194539
C,0,-0.1120654093,3.0383732241,2.57000073
C,0,-0.3699341205,2.3334771523,1.3958987968
C,0,-0.6951046377,0.9723933938,1.4442284941
C,0,-0.7542552943,0.3332891148,2.6879434669
C,0,-0.5393501429,1.0483450683,3.8615923166
H,0,-0.0224693698,2.9552588965,4.7189357785
H,0,0.1574805578,4.0882023152,2.5159788609
H,0,-0.3061458377,2.8453523273,0.4411749631
H,0,-0.9574542432,-0.7306728509,2.7449896235
H,0,-0.6105191466,0.5429663522,4.8192801688
C,0,5.1699048318,0.2102314604,-0.1352314543
C,0,4.9084390301,-0.8378491752,-1.0167209773
C,0,3.5910531005,-1.2655516852,-1.1964830494

C,0,2.5326914989,-0.6793138935,-0.5099027185
C,0,2.8153723269,0.3703287254,0.3761546981
C,0,4.1136912084,0.8133462754,0.5621237214
O,0,6.4079214082,0.7158043969,0.1119762651
H,0,5.7071969393,-1.3203707323,-1.567062966
H,0,3.3925449978,-2.0773526175,-1.8916718436
H,0,2.0080239064,0.8499395579,0.9254296888
H,0,4.3392766573,1.6287985716,1.2420707677
C,0,-0.2654044133,-2.9127799718,0.4472559985
C,0,-0.7265541374,-3.5345395561,1.7488639747
O,0,-0.4332603582,-3.5284068325,-0.6056021159
H,0,-1.040834657,-2.7877686575,2.4815153772
H,0,-1.5464410892,-4.2282193315,1.5527032054
H,0,0.1113687083,-4.0939235748,2.1813197808
C,0,7.496512667,0.1552964123,-0.604114874
H,0,8.3818949482,0.7039338863,-0.2851465725
H,0,7.6182953195,-0.9072312902,-0.3683981849
H,0,7.3591679194,0.2745402402,-1.6840541696

Full System, M06-2X/6-31+G**/SMD(THF)

Anisaldehyde 1

/home/singletn/wittig/methoxyketone/SMD/smd/anisaldehyde
M062XpsSMD
anisaldehyde smd
M062X/6-31+G**
E(RM062X) = -459.938435544

Zero-point correction= 0.143526 (Hartree/Particle)
Thermal correction to Energy= 0.152469
Thermal correction to Enthalpy= 0.153413
Thermal correction to Gibbs Free Energy= 0.108920
Sum of electronic and ZPE= -459.794910
Sum of electronic and thermal Energies= -459.785967
Sum of electronic and thermal Enthalpies= -459.785023
Sum of electronic and thermal Free Energies= -459.829515

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.675	32.982	93.642

C,0,-0.001756808,0.,0.1136134217
C,0,0.0509603378,0.,1.5164371717
C,0,1.2877869036,0.,2.1500292541
C,0,2.4724693189,0.,1.4078683694
C,0,2.4064341114,0.,0.0072144345
C,0,1.1826928602,0.,-0.6396578988
H,0,-0.8560537351,0.,2.1087846241
H,0,1.3420322457,0.,3.2352686537
C,0,3.7879562513,0.,2.0683643152
H,0,3.326222681,0.,-0.5735442068
H,0,1.1136607353,0.,-1.7227395607
O,0,-1.1485706533,0.,-0.5963029145
C,0,-2.3807105635,0.,0.1162059185
H,0,-3.1631616202,0.,-0.6419336032
H,0,-2.4741508758,-0.8968708553,0.7376804493
H,0,-2.4741508758,0.8968708553,0.7376804493
O,0,3.9592517123,0.,3.2734220908
H,0,4.6567109739,0.,1.381005032

Ph3PCHCOMe 2

/home/singletn/wittig/methoxyketone/SMD/smd/Ph3PCHCO
MeM062XpsSMD
Ph3PCHCOMe smd
M062X/6-31+G**
E(RM062X) = -1227.88889189

Zero-point correction= 0.340550 (Hartree/Particle)
Thermal correction to Energy= 0.361429
Thermal correction to Enthalpy= 0.362373
Thermal correction to Gibbs Free Energy= 0.288559
Sum of electronic and ZPE= -1227.548342
Sum of electronic and thermal Energies= -1227.527463
Sum of electronic and thermal Enthalpies= -1227.526519
Sum of electronic and thermal Free Energies= -1227.600333

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	226.800	80.174	155.354

C,0,0.4094937714,0.1313686606,0.420173729
P,0,0.4357557298,-0.1396268737,2.1288058497
H,0,-0.288836267,0.8718473589,0.0493449409
C,0,4.3053233088,1.1315291714,4.2951542587
C,0,3.0814408751,1.229313358,4.9573594948
C,0,1.9065991984,0.8481509652,4.3106528774
C,0,1.9580324038,0.3643372582,2.9980568109
C,0,3.185903124,0.2687558275,2.3328820108
C,0,4.3560912927,0.652173573,2.9858613479
H,0,5.2197014417,1.4313610044,4.7987321992
H,0,3.038950019,1.6061414956,5.9747066363
H,0,0.9541099827,0.9327713846,4.8280803613
H,0,3.2173379137,-0.1179812547,1.3180575978
H,0,5.3084492924,0.5777182373,2.4697586928
C,0,-0.5400953795,-4.4816887437,3.3240195749
C,0,0.3183979103,-3.7303552037,4.125149431
C,0,0.6455740596,-2.4225554193,3.7662172378
C,0,0.1077776123,-1.8669587971,2.6022572628
C,0,-0.7464784978,-2.6239150918,1.7942366073
C,0,-1.0703548205,-3.9289235443,2.1573730236
H,0,-0.7908386606,-5.5005430729,3.6039177766
H,0,0.740064629,-4.1612012075,5.0281983874
H,0,1.3230980299,-1.847729216,4.3915847456
H,0,-1.1477917162,-2.1921960729,0.8805916229
H,0,-1.73083866,-4.5152393311,1.5256863099
C,0,-2.891344508,2.5134454465,3.8930236373
C,0,-1.8224756853,3.0785900249,3.1940704993
C,0,-0.8218255664,2.2631147436,2.6745053423
C,0,-0.8881124766,0.8746323895,2.852071155
C,0,-1.9549946703,0.3102219811,3.5551556465
C,0,-2.9561319926,1.1336093435,4.0730218119
H,0,-3.6721079421,3.1507954882,4.2974330684
H,0,-1.7668954193,4.1540003214,3.0556624749
H,0,0.0139772934,2.7050120129,2.1366370998
H,0,-2.013122345,-0.7648626515,3.7005417271
H,0,-3.7860018703,0.6925351237,4.6167033628
C,0,1.19006517,-0.682302293,-0.4276059833
C,0,1.0431896938,-0.4935097298,-1.927953813
O,0,1.9910046466,-1.5519838847,-0.0120910906
H,0,2.0185151573,-0.23440608,-2.3521383559
H,0,0.7341434842,-1.4436483076,-2.3755953745

H,0,0.3193134379,0.280380605,-2.1935629953

TS1 4

/home/singletn/wittig/methoxyketone/SMD/smd/TS1M062XpsSMD
TS1 checking smd single point energy
M062X/6-31+G**
E(RM062X) = -1687.81304609

Zero-point correction= 0.485507 (Hartree/Particle)
Thermal correction to Energy= 0.515652
Thermal correction to Enthalpy= 0.516596
Thermal correction to Gibbs Free Energy= 0.420833
Sum of electronic and ZPE= -1687.327539
Sum of electronic and thermal Energies= -1687.297394
Sum of electronic and thermal Enthalpies= -1687.296450
Sum of electronic and thermal Free Energies= -1687.392213

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	323.577	115.565	201.551

O,0,1.0873454142,1.3419157564,1.6357128642
C,0,1.3889368637,0.1869718004,1.1820661151
P,0,-1.3221304203,0.135116973,-0.0158001784
C,0,0.4070583891,-0.1252903194,-0.4117503962
C,0,2.8090339849,-0.057682354,0.7130758153
C,0,-2.3875259624,-0.9000279827,-1.0644507052
C,0,-2.1157666419,-0.9328562892,-2.4380598623
C,0,-2.9314931176,-1.6699089306,-3.2899077982
C,0,-4.020165098,-2.3768450632,-2.774677899
C,0,-4.2930353626,-2.3410218983,-1.4093292289
C,0,-3.4798610756,-1.6005438687,-0.5496093724
C,0,-1.760556602,1.8555258627,-0.3953467223
C,0,-1.7639842492,-0.2088718345,1.708351883
C,0,-0.8656427146,2.8804394806,-0.0621409562
C,0,-1.2105188392,4.2032151748,-0.333771182
C,0,-2.435085307,4.5046272894,-0.929648074
C,0,-3.3258676441,3.4816601104,-1.2544505807
C,0,-2.9929756004,2.1544620362,-0.9883616745
C,0,-2.4415745169,0.7477196213,2.4697417992
C,0,-2.81379774,0.4492361384,3.779411317
C,0,-2.5106917242,-0.7965474003,4.3259217118
C,0,-1.8357015379,-1.7510143332,3.5633657494
C,0,-1.4619359752,-1.4635534328,2.2528040797
C,0,3.4062002313,-1.3154532353,0.8516349376
C,0,4.6987395188,-1.5469567283,0.3980149157
C,0,5.4223429108,-0.5128980042,-0.2085996347
C,0,4.8450400343,0.7551788324,-0.3414732508
C,0,3.5462356645,0.9671795563,0.1259527349
H,0,1.0101212366,-0.7094626416,1.7187851994
H,0,0.763395925,0.6827305839,-1.0534952713
H,0,-1.2699672504,-0.3803656356,-2.8426000324
H,0,-2.7169260694,-1.6946654753,-4.3538572531
H,0,-4.6536577192,-2.9556532812,-3.4401991658
H,0,-5.1381991246,-2.8910703336,-1.0071589076
H,0,-3.7009665352,-1.5778972648,0.5136848679
H,0,0.0738904063,2.6308790405,0.4314244082
H,0,-0.5198585955,4.9998401232,-0.0745408715
H,0,-2.6955850965,5.537426464,-1.1418358721
H,0,-4.2797337408,3.713108947,-1.7181782798
H,0,-3.6909607321,1.3635369123,-1.2474690597
H,0,-2.6728766515,1.7235335031,2.0523303152
H,0,-3.3365085138,1.1942065436,4.3711033965
H,0,-2.7989593251,-1.0248651782,5.3478129638
H,0,-1.5975975915,-2.7213706103,3.988312486
H,0,-0.9418570216,-2.2036386957,1.6496151225
H,0,2.8488475287,-2.1258015021,1.3183753319
H,0,5.1679222553,-2.5202885673,0.5071923454
O,0,6.6764653085,-0.8296973442,-0.6294361475
H,0,5.3910808816,1.5743269101,-0.795760898
H,0,3.0925318573,1.9513960171,0.0354427946
C,0,0.7205526064,-1.4801245056,-0.8848548526
C,0,1.7439269794,-1.6192025226,-1.9860646906
O,0,0.1940526146,-2.4722155963,-0.3812483918
H,0,2.2172990156,-2.6019308693,-1.9373964464
H,0,1.2170249466,-1.5320646312,-2.9451934734
H,0,2.5001692857,-0.8304873689,-1.9449801812
C,0,7.4425719085,0.1934399511,-1.2449046735
H,0,8.3948262116,-0.262836869,-1.5158775014
H,0,6.9501967526,0.5675473918,-2.1498132615
H,0,7.6218433642,1.024613547,-0.5532344074

Betaine 5

/home/singletn/wittig/methoxyketone/SMD/smd/betaineM062XpsSMD
betaine checking smd single point energy
M062X/6-31+G**
E(RM062X) = -1687.81541898

Zero-point correction= 0.488169 (Hartree/Particle)
Thermal correction to Energy= 0.518203
Thermal correction to Enthalpy= 0.519148
Thermal correction to Gibbs Free Energy= 0.425423
Sum of electronic and ZPE= -1687.327250
Sum of electronic and thermal Energies= -1687.297216
Sum of electronic and thermal Enthalpies= -1687.296271
Sum of electronic and thermal Free Energies= -1687.389996

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	325.178	115.996	197.259

8 0.840547 1.562461 1.219163
6 1.258804 0.330037 0.964944
15 -1.309158 0.099178 -0.042386
6 0.464263 -0.225506 -0.353848
6 2.751146 0.167944 0.667987
6 -2.280307 -1.160633 -0.924333
6 -1.963974 -1.420128 -2.264318
6 -2.703666 -2.352201 -2.984971
6 -3.764254 -3.024544 -2.373432
6 -4.085796 -2.759186 -1.044602
6 -3.346768 -1.825403 -0.316507
6 -1.836466 1.686370 -0.754693
6 -1.777743 0.009929 1.701521
6 -1.013100 2.816157 -0.669193
6 -1.454573 4.023347 -1.209492
6 -2.706013 4.110019 -1.819053
6 -3.527471 2.985261 -1.892081

6 -3.095420 1.769951 -1.365558
6 -2.493674 1.055093 2.290913
6 -2.903740 0.943732 3.617851
6 -2.598865 -0.202694 4.351298
6 -1.884858 -1.244440 3.759056
6 -1.475174 -1.145990 2.431010
6 3.447466 -0.997636 1.010637
6 4.790617 -1.153674 0.690318
6 5.472129 -0.132095 0.016870
6 4.797601 1.045493 -0.321072
6 3.446507 1.179772 0.011421
1 1.011174 -0.431898 1.743170
1 0.760588 0.428837 -1.181566
1 -1.144591 -0.892225 -2.748258
1 -2.453581 -2.554680 -4.021828
1 -4.338678 -3.754384 -2.935984
1 -4.911689 -3.277296 -0.567387
1 -3.605453 -1.622270 0.718331
1 -0.058191 2.723079 -0.151118
1 -0.818015 4.900920 -1.147873
1 -3.044298 5.054748 -2.234594
1 -4.504035 3.050070 -2.361753
1 -3.741149 0.899151 -1.432621
1 -2.723723 1.954089 1.726625
1 -3.455832 1.756554 4.079251
1 -2.917322 -0.283604 5.386399
1 -1.645858 -2.137181 4.328614
1 -0.929012 -1.959161 1.959667
1 2.929437 -1.797266 1.537602
1 5.333774 -2.055075 0.958908
8 6.784708 -0.369850 -0.255029
1 5.307153 1.857230 -0.828373
1 2.915415 2.096949 -0.231583
6 0.778314 -1.670601 -0.633316
6 1.739662 -1.963132 -1.753258
8 0.300994 -2.555648 0.059254
1 2.172152 -2.957526 -1.630442
1 1.177291 -1.930703 -2.695720
1 2.527437 -1.206760 -1.812420
6 7.507305 0.638063 -0.942538
1 8.518657 0.250865 -1.068731
1 7.069661 0.837689 -1.927569
1 7.544350 1.566660 -0.361422

TS1.5 6

/home/singletn/wittig/methoxyketone/SMD/smd/TS1.5M062X
psSMD
TS1.5 checking smd single point energy
M062X/6-31+G**
E(RM062X) = -1687.81472058

Zero-point correction= 0.487373 (Hartree/Particle)
Thermal correction to Energy= 0.516725
Thermal correction to Enthalpy= 0.517669
Thermal correction to Gibbs Free Energy= 0.425412
Sum of electronic and ZPE= -1687.327348
Sum of electronic and thermal Energies= -1687.297996
Sum of electronic and thermal Enthalpies= -1687.297052
Sum of electronic and thermal Free Energies= -1687.389309

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	324.250	114.107	194.171

O,0,0.7629964614,0.9877834096,1.3838372451
C,0,1.2630900498,-0.1473385333,0.8687097306
P,0,-1.2426942986,0.1050297503,0.0208473107
C,0,0.4561405141,-0.3731921909,-0.4895077843
C,0,2.7592864753,-0.1468963575,0.5673800386
C,0,-2.3552937844,-0.7966146073,-1.1194280371
C,0,-2.1110005846,-0.6819915745,-2.4951666443
C,0,-2.9369056065,-1.3265842145,-3.4106274971
C,0,-4.0177633855,-2.0872253765,-2.9594762096
C,0,-4.2694318441,-2.1953108731,-1.5942885272
C,0,-3.4414857294,-1.5509636037,-0.6726783436
C,0,-1.6663114696,1.8486053134,-0.3016689813
C,0,-1.7245793088,-0.3901831147,1.6924619571
C,0,-0.7345763323,2.8796075199,-0.1368142735
C,0,-1.1119029341,4.1959080698,-0.4004806882
C,0,-2.4132195049,4.4916741168,-0.8036020565
C,0,-3.345950908,3.4654498403,-0.9516010461
C,0,-2.9745453693,2.1446058473,-0.711566109
C,0,-2.3224550954,0.5457422396,2.5410103277
C,0,-2.7402347374,0.1559753816,3.8103993192
C,0,-2.5542758331,-1.1600358088,4.2364207531
C,0,-1.9539863829,-2.0897235168,3.3886498837
C,0,-1.542920509,-1.712939495,2.1104059605
C,0,3.4928685422,-1.3382746463,0.4933734877
C,0,4.8471207928,-1.3310376774,0.1844143123
C,0,5.5031760755,-0.1157462516,-0.0523640813
C,0,4.7904884253,1.0836065351,0.0271562227
C,0,3.4272850803,1.0521371894,0.3378847464
H,0,1.0624645233,-1.0643594926,1.4722616369
H,0,0.7886818357,0.4058274981,-1.1864639851
H,0,-1.2795731071,-0.0798006193,-2.8577929665
H,0,-2.7384856024,-1.234260745,-4.474054162
H,0,-4.6615533079,-2.5928724429,-3.6728797783
H,0,-5.1111259563,-2.7815726404,-1.2381437158
H,0,-3.6516817444,-1.641587013,0.3886538045
H,0,0.2561276789,2.6262780993,0.2305922257
H,0,-0.3852878398,4.993603408,-0.2772312621
H,0,-2.702591575,5.5201207906,-0.9990234086
H,0,-4.3630320939,3.6882518982,-1.2591508696
H,0,-3.7079692363,1.3541769225,-0.8440237969
H,0,-2.4497186024,1.5757859804,2.2209364316
H,0,-3.2042833079,0.8836375729,4.4690476924
H,0,-2.8753457305,-1.45946665,5.2297166954
H,0,-1.8066980999,-3.1138135415,3.7177799775
H,0,-1.0876036163,-2.4390957265,1.4420048544
H,0,2.9964587784,-2.2887644227,0.6863036937
H,0,5.4186667792,-2.2531387798,0.131599087
O,0,6.8311684507,-0.2008314249,-0.3410985556
H,0,5.2800614712,2.0369803071,-0.136711712
H,0,2.8647830976,1.9783323409,0.423182352
C,0,0.5898720521,-1.7519396772,-1.0898575476
C,0,1.4719058639,-1.8816451401,-2.3000454232
O,0,0.0422682341,-2.7123198926,-0.5749342811
H,0,1.6992271241,-2.9304594911,-2.4962160506
H,0,0.9382428994,-1.4569194097,-3.1598745046
H,0,2.394240532,-1.3056599988,-2.1739456139
C,0,7.5322490027,1.0109360082,-0.5670669349
H,0,8.5671886504,0.7298038229,-0.7633014631

H,0,7.1320656041,1.5459613811,-1.4363329277
H,0,7.4940094433,1.6624947065,0.3136234915

Full System, M06-2X/6-31G* Gas Phase (Concerted, no betaine intermediate)

TS1 4

/home/singletn/wittig/methoxyketone/gasphase/TS1gasphase
M062XSB
TS1
M062X/6-31G*
E(RM062X) = -1687.69776699

Zero-point correction= 0.489348 (Hartree/Particle)
Thermal correction to Energy= 0.518206
Thermal correction to Enthalpy= 0.519151
Thermal correction to Gibbs Free Energy= 0.427876
Sum of electronic and ZPE= -1687.208419
Sum of electronic and thermal Energies= -1687.179561
Sum of electronic and thermal Enthalpies= -1687.178616
Sum of electronic and thermal Free Energies= -1687.269891

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	325.179	112.381	192.105

O,0,0.7761494034,1.7831711013,0.7214425283
C,0,1.2374705866,0.5815873764,0.8262308481
P,0,-1.3056722271,0.0282789925,-0.0959614503
C,0,0.4229078599,-0.3866056681,-0.4052812827
C,0,2.7183780603,0.3574068716,0.570231426
C,0,-2.3529024354,-1.3675674329,-0.6198093886
C,0,-2.048687215,-1.9987577458,-1.8310524291
C,0,-2.8606518975,-3.0166990117,-2.314317832
C,0,-3.9873215031,-3.4098738089,-1.5938327046
C,0,-4.2999002435,-2.7789872431,-0.3943534223
C,0,-3.4877412522,-1.7566914618,0.0934829077
C,0,-1.8578244871,1.4139196138,-1.1383257379
C,0,-1.6887745811,0.3449525898,1.6433113192
C,0,-1.0109000662,2.5017480947,-1.3849988791
C,0,-1.4604646434,3.5421164582,-2.1943274332
C,0,-2.7369376783,3.5080428875,-2.7493242424
C,0,-3.5788523916,2.4278439634,-2.4966852845
C,0,-3.1424614127,1.3776914399,-1.6962451313
C,0,-2.0219843416,1.6324262995,2.0655041378
C,0,-2.3276902689,1.8543380797,3.4037860843
C,0,-2.2836466391,0.8014681841,4.3146057003
C,0,-1.9276002058,-0.4777099212,3.8939615316
C,0,-1.6260376883,-0.7134719038,2.5558601475
C,0,3.3981389956,-0.7438157659,1.1014611404
C,0,4.7385088745,-0.9564314895,0.8205223245
C,0,5.4306355742,-0.0571951577,0.0014961473
C,0,4.7699075683,1.055859981,-0.5218309182
C,0,3.4205252815,1.2521949495,-0.2265379082
H,0,0.941662304,-0.0118614893,1.7253324254
H,0,0.7546615722,0.0777747423,-1.3366406305
H,0,-1.1727411524,-1.6908873339,-2.3978612226
H,0,-2.6139041479,-3.5045717478,-3.2519262842
H,0,-4.6203738858,-4.2076136058,-1.9699352361
H,0,-5.1772164982,-3.0818723673,0.1684569765
H,0,-3.7382288293,-1.2687655669,1.030323674
H,0,-0.0327501266,2.5173659553,-0.904380952
H,0,-0.8064234845,4.3866997049,-2.3874001961
H,0,-3.0786451814,4.3240403501,-3.3793405141
H,0,-4.5747527964,2.3978353319,-2.9271794266
H,0,-3.8005121344,0.5335565611,-1.5148846175
H,0,-2.0190091777,2.4529621743,1.3554869328
H,0,-2.5874019902,2.8538215752,3.7370812172
H,0,-2.5171465565,0.9815039108,5.3597299067
H,0,-1.8743110363,-1.2931739949,4.6082218377
H,0,-1.3215703442,-1.7005417492,2.2173895563
H,0,2.8627280722,-1.4453767876,1.7400449234
H,0,5.2804474744,-1.8040907922,1.2275205134
O,0,6.7436194226,-0.3501779665,-0.2192546652
H,0,5.2919269049,1.7732528144,-1.1451866611
H,0,2.8896586057,2.1240372163,-0.5988812427
C,0,0.7388202283,-1.8248211672,-0.2649620379
C,0,1.7935857006,-2.3991007717,-1.1847410929
O,0,0.2076371684,-2.5051686287,0.6016179276
H,0,2.2453707188,-3.278248092,-0.7222615339
H,0,1.3049669273,-2.7061040099,-2.1186050933
H,0,2.563383984,-1.661941026,-1.4270908249
C,0,7.4838198551,0.5529341455,-1.005649462
H,0,8.4984390247,0.1561253065,-1.0508130341
H,0,7.0772892172,0.6273352927,-2.0224123003
H,0,7.5033351348,1.5533697433,-0.5555170615

Full System, lc-wPBE/6-31+G**/PCM(THF) with Default Radii

Anisaldehyde 1

/home/singletn/wittig/methoxyketone/lcwpbePS/anisaldehydelcwpbePS
anisaldehyde
lc-wpbe/6-31+G**
E(RLC-wPBE) = -459.811349026

Zero-point correction= 0.145234 (Hartree/Particle)
Thermal correction to Energy= 0.154017
Thermal correction to Enthalpy= 0.154961
Thermal correction to Gibbs Free Energy= 0.111257
Sum of electronic and ZPE= -459.666115
Sum of electronic and thermal Energies= -459.657332
Sum of electronic and thermal Enthalpies= -459.656388
Sum of electronic and thermal Free Energies= -459.700092

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	96.647	32.611	91.984

C,0,0.0012778338,0.,0.1201263258
C,0,0.0576214751,0.,1.5165908753
C,0,1.2920047796,0.,2.144614003
C,0,2.4717457354,0.,1.4048198996
C,0,2.4010896457,0.,0.0087579461
C,0,1.1804165996,0.,-0.6323722746
H,0,-0.8461804011,0.,2.1136866375
H,0,1.350070647,0.,3.2290352874
C,0,3.7837442114,0.,2.0666804353
H,0,3.3166849642,0.,-0.5778137644

H,0,1.1088673371,0.,-1.714839281
O,0,-1.1459691471,0.,-0.5890134905
C,0,-2.37927009,0.,0.1129927654
H,0,-3.1567968049,0.,-0.6489378804
H,0,-2.4787341187,-0.8957439287,0.7330478416
H,0,-2.4787341187,0.8957439287,0.7330478416
O,0,3.9531667458,0.,3.2724676799
H,0,4.6566177061,0.,1.3865051528

Ph3PCHCOMe 2

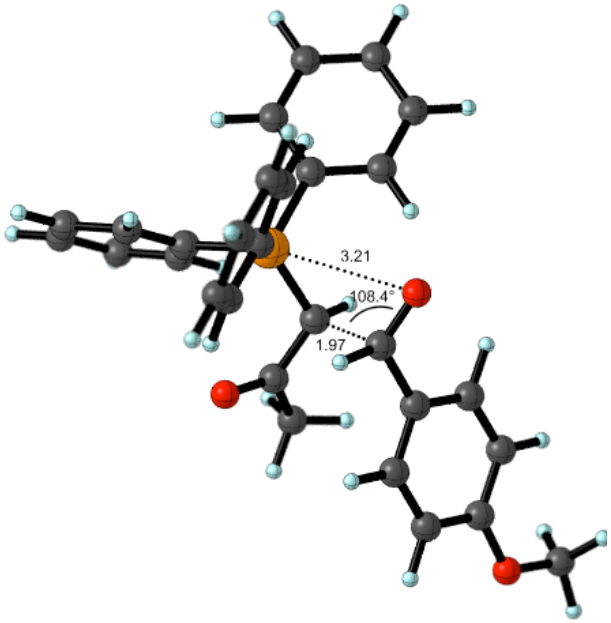
/home/singletn/wittig/methoxyketone/lcwpbePS/Ph3PCHCOMelcwpbePS
ylide
lc-wpbe/6-31+G**
E(RLC-wPBE) = -1227.52549247

Zero-point correction= 0.344761 (Hartree/Particle)
Thermal correction to Energy= 0.365469
Thermal correction to Enthalpy= 0.366413
Thermal correction to Gibbs Free Energy= 0.292822
Sum of electronic and ZPE= -1227.180731
Sum of electronic and thermal Energies= -1227.160024
Sum of electronic and thermal Enthalpies= -1227.159080
Sum of electronic and thermal Free Energies= -1227.232670

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	229.335	79.132	154.885

6 -0.530129 -0.009888 2.083383
15 -0.017809 -0.002934 0.436980
1 0.183117 -0.359808 2.819511
6 0.393135 4.126932 -1.547054
6 1.314393 3.129528 -1.839704
6 1.198097 1.879986 -1.244442
6 0.154963 1.623895 -0.354537
6 -0.770234 2.627372 -0.063391
6 -0.647152 3.874487 -0.660254
1 0.486851 5.104755 -2.010265
1 2.129733 3.323327 -2.529915
1 1.928215 1.108816 -1.472939
1 -1.588462 2.414339 0.618842
1 -1.368381 4.652965 -0.430682
6 -2.609237 -2.641600 -2.284507
6 -2.015438 -1.501448 -2.810338
6 -1.244204 -0.680348 -1.997387
6 -1.065502 -1.002457 -0.654430
6 -1.667966 -2.143509 -0.127802
6 -2.436261 -2.961908 -0.942540
1 -3.214849 -3.280113 -2.920806
1 -2.155927 -1.245258 -3.855906
1 -0.789714 0.214041 -2.412847
1 -1.540806 -2.378909 0.925380
1 -2.907445 -3.847647 -0.527762
6 4.208992 -1.804246 0.420920
6 3.907457 -0.708591 1.223563
6 2.628706 -0.173845 1.215069
6 1.639898 -0.734278 0.402916
6 1.946160 -1.828596 -0.400831
6 3.230271 -2.361756 -0.389366
1 5.211015 -2.222514 0.428346
1 4.671399 -0.268866 1.857172
1 2.400622 0.685471 1.840188
1 1.186117 -2.271584 -1.037126
1 3.462369 -3.216410 -1.017228
6 -1.851487 0.326360 2.418356
6 -2.283213 0.188006 3.863147
8 -2.698544 0.726356 1.581496
1 -2.677755 1.145457 4.211592
1 -3.095246 -0.541329 3.921177
1 -1.472859 -0.128141 4.521980

TS1 4 (Concerted)



/home/singletn/wittig/methoxyketone/lcwpbePS/TS1lcwpbePS
TS1
lc-wpbe/6-31+G**
E(RLC-wPBE) = -1687.31272745

Zero-point correction= 0.491945 (Hartree/Particle)
Thermal correction to Energy= 0.521739
Thermal correction to Enthalpy= 0.522683
Thermal correction to Gibbs Free Energy= 0.429139
Sum of electronic and ZPE= -1686.820782
Sum of electronic and thermal Energies= -1686.790988
Sum of electronic and thermal Enthalpies= -1686.790044
Sum of electronic and thermal Free Energies= -1686.883588

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	327.396	114.140	196.880

O,0,-0.9489120885,-1.9864296586,0.9134407854
C,0,-1.3516266908,-0.7847223565,0.9756324499
P,0,1.3453199032,0.0108786164,-0.1004315277
C,0,-0.3901538583,0.264926727,-0.3887562212
C,0,-2.788790272,-0.4803586406,0.6306346376
C,0,2.318308576,1.4449477033,-0.6299430293

C,0,2.0347341015,2.0096483604,-1.8746013779
C,0,2.7865437635,3.0752758526,-2.3421691379
C,0,3.8268442228,3.5831733668,-1.5705006469
C,0,4.1147418853,3.0204537544,-0.335435539
C,0,3.363873537,1.9498478195,0.1363867653
C,0,1.9048944398,-1.3705008947,-1.1244820301
C,0,1.7916996569,-0.3286816446,1.6175918976
C,0,1.0995704953,-2.5033152303,-1.2499245497
C,0,1.5313287592,-3.5676448776,-2.0297253577
C,0,2.7580334666,-3.5083166551,-2.6798028167
C,0,3.5628853953,-2.3834628049,-2.5479891285
C,0,3.1396908698,-1.3133343488,-1.7719014674
C,0,2.5027006689,-1.4786889872,1.9515744548
C,0,2.864066859,-1.7084115978,3.2724693891
C,0,2.5164871393,-0.794312779,4.2581520749
C,0,1.8069792698,0.3541977474,3.9258295295
C,0,1.4435921843,0.5916078169,2.6084174088
C,0,-3.4841523859,0.5262761119,1.2994550135
C,0,-4.8083410156,0.7962372017,1.0022141872
C,0,-5.4662382806,0.0567846125,0.0191546629
C,0,-4.7891694703,-0.9604661379,-0.6505989291
C,0,-3.4607662369,-1.2207085011,-0.3311536562
H,0,-1.0012692149,-0.1486137593,1.8110522549
H,0,-0.7082383316,-0.246738412,-1.2965761319
H,0,1.2255763322,1.6145667637,-2.4837324704
H,0,2.5601175523,3.5120743646,-3.3097252469
H,0,4.4136766089,4.4205563534,-1.935650823
H,0,4.9262269637,3.4140567999,0.2685646021
H,0,3.5971799997,1.515354559,1.1031932044
H,0,0.1548142941,-2.5501464413,-0.7082270325
H,0,0.9052534207,-4.4493690028,-2.1264259831
H,0,3.0896842941,-4.3427216325,-3.2906915994
H,0,4.5228013411,-2.3351358046,-3.0524757235
H,0,3.7731680406,-0.436674562,-1.6779289428
H,0,2.7710625665,-2.2010897194,1.1873422275
H,0,3.4151189343,-2.6074110983,3.5301126492
H,0,2.7978911144,-0.9777201501,5.2908261051
H,0,1.5332319767,1.0689463551,4.6956906163
H,0,0.8894728212,1.486861953,2.3382756584
H,0,-2.9800231918,1.1088113437,2.0674572327
H,0,-5.3545425454,1.5762484566,1.5234955772
O,0,-6.7634230398,0.3935956959,-0.2120228763
H,0,-5.2813135252,-1.5566504494,-1.4103351356
H,0,-2.9315602545,-2.0234902213,-0.8373617515
C,0,-0.8322755755,1.6463679941,-0.2560891194
C,0,-1.9014539841,2.141921649,-1.1928938853
O,0,-0.3623540983,2.3892019391,0.6102752725
H,0,-2.4322202327,2.9812703596,-0.7433968448
H,0,-1.4157502496,2.488276406,-2.1111604486
H,0,-2.6047849926,1.3518944885,-1.4613226442
C,0,-7.4755377803,-0.3343256435,-1.1947461788
H,0,-8.4783303186,0.0900791377,-1.2183462745
H,0,-7.014207058,-0.2250470308,-2.1816702474
H,0,-7.5389167621,-1.3957762676,-0.9343058815

OP1direct

/home/singletn/wittig/methoxyketone/lcwpbePS/OP1directlcwpbePS
betaine from anisaldehyde and ketone
lc-wpbe/6-31+G**

E(RLC-wPBE) = -1687.33175344

Zero-point correction= 0.495119 (Hartree/Particle)
Thermal correction to Energy= 0.524553
Thermal correction to Enthalpy= 0.525498
Thermal correction to Gibbs Free Energy= 0.432138
Sum of electronic and ZPE= -1686.836634
Sum of electronic and thermal Energies= -1686.807200
Sum of electronic and thermal Enthalpies= -1686.806256
Sum of electronic and thermal Free Energies= -1686.899616

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	329.162	113.794	196.492

O,0,0.5400051933,0.8829341034,0.9316437132
C,0,1.3604857913,-0.2704606688,0.8877414384
P,0,-0.9026749275,0.1062900393,0.144653881
C,0,0.5883631082,-0.9968318482,-0.2069753813
C,0,2.81039857,0.027001927,0.6032339395
C,0,-2.0636293327,-0.9129286941,-0.956351624
C,0,-1.9411852116,-0.7827696159,-2.3449989122
C,0,-2.6657530894,-1.5850352713,-3.2139180695
C,0,-3.5328442436,-2.5503222323,-2.7099130531
C,0,-3.6656824905,-2.6951241252,-1.3376017315
C,0,-2.9379003726,-1.8819691384,-0.470382364
C,0,-1.3698696495,1.7245098192,-0.60937595
C,0,-1.7442931504,-0.1268630538,1.7488793274
C,0,-0.4534302612,2.7627748638,-0.7670292647
C,0,-0.8465927806,3.9788678187,-1.3153066965
C,0,-2.1675908831,4.1846124811,-1.6848499854
C,0,-3.096495989,3.1645580557,-1.5117391478
C,0,-2.6970759891,1.9422260605,-0.9932218048
C,0,-2.6177165255,0.8503471589,2.2240984464
C,0,-3.2351610632,0.7014361158,3.4596035542
C,0,-2.9839507842,-0.4207879502,4.2376660123
C,0,-2.1080746356,-1.3931284766,3.7733108448
C,0,-1.4900583572,-1.2499468775,2.5372669546
C,0,3.8156083339,-0.5941120367,1.3438364824
C,0,5.1530452796,-0.3550153778,1.0805348271
C,0,5.5167998648,0.5258671117,0.0630371297
C,0,4.5275897539,1.1599754008,-0.6847422556
C,0,3.1897947551,0.9013529004,-0.4069588073
H,0,1.2992423782,-0.8398354974,1.8248380832
H,0,0.9342834667,-0.6627704379,-1.1935582506
H,0,-1.2732059131,-0.0315694054,-2.7628558954
H,0,-2.5541060613,-1.4584172119,-4.28702636
H,0,-4.1019875093,-3.1815516022,-3.3859878795
H,0,-4.3421522384,-3.4416395997,-0.9311778598
H,0,-3.0688685554,-2.0127600877,0.5994760255
H,0,0.5680312029,2.6166982406,-0.4409619206
H,0,-0.1143147287,4.7707067136,-1.4416824401
H,0,-2.4762851771,5.1379927861,-2.103621611
H,0,-4.1353126422,3.3171560836,-1.7884062402
H,0,-3.4338099096,1.1525432797,-0.8825784525
H,0,-2.8179336885,1.7421981357,1.6395212794
H,0,-3.9125122647,1.4722719492,3.8150137544
H,0,-3.465961087,-0.5352712806,5.2040170642
H,0,-1.900303263,-2.273311664,4.374595214
H,0,-0.8087654333,-2.0226550952,2.1946180581
H,0,3.546404618,-1.2776234798,2.1454107308
H,0,5.9337758415,-0.8382977389,1.6593739485

O,0,6.8512321023,0.7053091062,-0.1237427221
H,0,4.7803410242,1.8530714853,-1.4786905929
H,0,2.4276573278,1.4037102106,-0.9959644957
C,0,0.5297165197,-2.5076676529,-0.1833448613
C,0,0.449511327,-3.2314368269,-1.4930541684
O,0,0.6042042514,-3.1117045544,0.8733210746
H,0,0.3892973835,-4.3057296453,-1.3231911588
H,0,-0.4173416238,-2.8904430314,-2.0638622621
H,0,1.3394048124,-3.0002063124,-2.0862307212
C,0,7.267287355,1.6000259858,-1.138421207
H,0,8.3561475221,1.5983818506,-1.1154818097
H,0,6.9267467027,1.2679338699,-2.1245237649
H,0,6.9036583465,2.6145589378,-0.9460270625

Full System, B3P86P6-31+G**/PCM(THF) with Default Radii

Anisaldehyde 1

/home/singletn/wittig/methoxyketone/b3p86PS/anisaldehydeb3p86PS
anisaldehyde
B3P86/6-31+G**
E(RB3P86) = -461.421815482

Zero-point correction= 0.142856 (Hartree/Particle)
Thermal correction to Energy= 0.151742
Thermal correction to Enthalpy= 0.152686
Thermal correction to Gibbs Free Energy= 0.108824
Sum of electronic and ZPE= -461.278959
Sum of electronic and thermal Energies= -461.270073
Sum of electronic and thermal Enthalpies= -461.269129
Sum of electronic and thermal Free Energies= -461.312991

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.220	33.138	92.315

C,0,-0.0010872572,0.,0.1193436642
C,0,0.0554818065,0.,1.5231063791
C,0,1.2903663612,0.,2.1545111964
C,0,2.4787237655,0.,1.4121806759
C,0,2.4063516736,0.,0.0092050498
C,0,1.1830495253,0.,-0.6351604303
H,0,-0.8506866833,0.,2.1165132923
H,0,1.3478684133,0.,3.2386624221
C,0,3.7862383643,0.,2.0648777436
H,0,3.3230734442,0.,-0.5752870317
H,0,1.1128042898,0.,-1.7176210909
O,0,-1.1474385061,0.,-0.5905741948
C,0,-2.386855892,0.,0.1099766516
H,0,-3.1593255683,0.,-0.6575770479
H,0,-2.4879994877,-0.8961772502,0.7304778575
H,0,-2.4879994877,0.8961772502,0.7304778575
O,0,3.9732709635,0.,3.2749154842
H,0,4.651787275,0.,1.3713675216

Ph3PCHCOMe 2

/home/singletn/wittig/methoxyketone/b3p86PS/Ph3PCHCOMeb3p86PS
ylide
B3P86/6-31+G**
E(RB3P86) = -1231.33879255

Zero-point correction= 0.338908 (Hartree/Particle)
Thermal correction to Energy= 0.359922
Thermal correction to Enthalpy= 0.360866
Thermal correction to Gibbs Free Energy= 0.286961
Sum of electronic and ZPE= -1230.999884
Sum of electronic and thermal Energies= -1230.978870
Sum of electronic and thermal Enthalpies= -1230.977926
Sum of electronic and thermal Free Energies= -1231.051832

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	225.855	80.717	155.547

C,0,0.3896740806,0.1474617238,0.4338671709
P,0,0.4323379142,-0.1344620855,2.1440158324
H,0,-0.3446730748,0.8649228911,0.0873050358
C,0,4.3361507459,1.0438744245,4.3121911929
C,0,3.108177895,1.4083348398,4.8613426342
C,0,1.9221165036,1.0602030899,4.2157755586
C,0,1.9636490051,0.3421567131,3.0143522146
C,0,3.2002161222,-0.0256046119,2.4635925324
C,0,4.3791680167,0.3282349918,3.1149241462
H,0,5.2584538173,1.3177060871,4.8156788955
H,0,3.0691814944,1.9658869613,5.7921327081
H,0,0.9705084029,1.3525420737,4.6488709421
H,0,3.216710803,-0.5876732357,1.5326693963
H,0,5.3347216353,0.043599639,2.684939742
C,0,-0.5033239204,-4.4994377468,3.2971000365
C,0,0.3044924218,-3.7299467523,4.133737666
C,0,0.6141552534,-2.4151991822,3.7902750485
C,0,0.1099909041,-1.8664134784,2.6063629995
C,0,-0.6946736665,-2.6423560927,1.7658192016
C,0,-1.0011221936,-3.9555582003,2.1126680376
H,0,-0.7390771086,-5.5250587738,3.5643323394
H,0,0.699413477,-4.1536110696,5.051905803
H,0,1.2516675594,-1.8233058959,4.4400133599
H,0,-1.0653048315,-2.2149937061,0.838460553
H,0,-1.6214044865,-4.5561879512,1.4546611451
C,0,-2.9380718392,2.478625232,3.9004372619
C,0,-1.9546382557,3.0424660001,3.08624569
C,0,-0.9371356676,2.2468786428,2.5676747186
C,0,-0.8988814853,0.8759670107,2.8599489782
C,0,-1.8839129853,0.3156056251,3.6788360916
C,0,-2.9008334175,1.117713878,4.1959610812
H,0,-3.7314470628,3.1007542165,4.303116483
H,0,-1.9786178636,4.1027249,2.8548572256
H,0,-0.1728506641,2.6930866943,1.9379698632
H,0,-1.8636854522,-0.7444866702,3.9105343945
H,0,-3.6641539537,0.674970421,4.8280782262
C,0,1.2027484344,-0.5750193289,-0.457887757
C,0,1.0208902635,-0.320856513,-1.9433584284
O,0,2.0640096324,-1.4236296277,-0.1017426699
H,0,1.9778517463,-0.0105409039,-2.3746810092
H,0,0.7338584532,-1.256832824,-2.4335915507

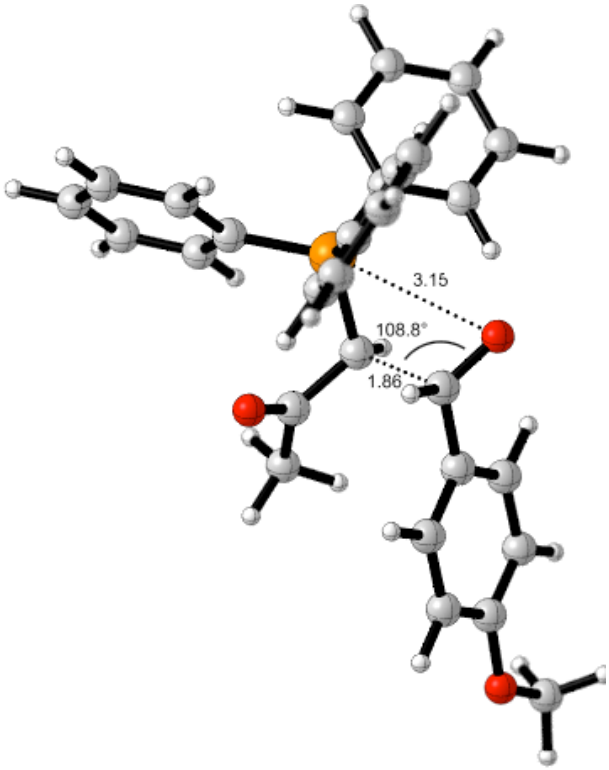
H,0,0.2677263472,0.4396375945,-2.1626557909

TS1 4

/home/singletn/wittig/methoxyketone/b3p86PS/TS1b3p86PS
TS1
B3P86/6-31+G**
E(RB3P86) = -1692.73587964

Zero-point correction= 0.483448 (Hartree/Particle)
Thermal correction to Energy= 0.513750
Thermal correction to Enthalpy= 0.514694
Thermal correction to Gibbs Free Energy= 0.419587
Sum of electronic and ZPE= -1692.252431
Sum of electronic and thermal Energies= -1692.222130
Sum of electronic and thermal Enthalpies= -1692.221186
Sum of electronic and thermal Free Energies= -1692.316293

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	322.383	116.199	200.169



O,0,-0.9442735868,-1.9659049922,0.8072794205
C,0,-1.3366570126,-0.7420307838,0.8841617358
P,0,1.3594091232,-0.0118951909,-0.0960476279
C,0,-0.403923968,0.2672800561,-0.3738288349
C,0,-2.7902365363,-0.4490143405,0.5789814516
C,0,2.3279457226,1.4314851623,-0.6325381687
C,0,2.0709883406,1.9764558803,-1.897755283
C,0,2.8201549088,3.0540305211,-2.3581414952
C,0,3.8309901016,3.5935598019,-1.5610236046
C,0,4.0925698803,3.0500392804,-0.3055724542
C,0,3.3453433989,1.9687072514,0.1605146023
C,0,1.917899199,-1.3953291806,-1.1293679447
C,0,1.7932678863,-0.3463038199,1.6305615976
C,0,1.1193280574,-2.5411508846,-1.2447801329
C,0,1.5585548491,-3.6050620234,-2.0300664671
C,0,2.7832713667,-3.535108066,-2.6936695747
C,0,3.5797567694,-2.3970938106,-2.5708129247
C,0,3.1511896312,-1.3250776924,-1.7915435511
C,0,2.5538492127,-1.4717508218,1.9651584579
C,0,2.9098976297,-1.696056232,3.2928799886
C,0,2.5084762653,-0.8028438428,4.2853655557
C,0,1.7510009247,0.3196038423,3.9513684791
C,0,1.3914570873,0.5544612049,2.6264797639
C,0,-3.4906662481,0.5347136177,1.2868761651
C,0,-4.8317393002,0.7891889903,1.0290692567
C,0,-5.5048601472,0.0566779171,0.0442569153
C,0,-4.8237353271,-0.937615408,-0.6666321652
C,0,-3.4790890881,-1.1821173222,-0.386154943
H,0,-1.0218647834,-0.1547734381,1.7731696663
H,0,-0.7001172872,-0.2207683959,-1.3041675713
H,0,1.2893321469,1.5603327391,-2.5272685039
H,0,2.6141470075,3.4728919378,-3.3379856178
H,0,4.4129012392,4.4367337285,-1.9199922996
H,0,4.8778374308,3.4664556429,0.3173197678
H,0,3.5544480974,1.5517961983,1.1400508591
H,0,0.1792951386,-2.5865222532,-0.6911549705
H,0,0.9404874281,-4.4931516344,-2.119997704
H,0,3.1183265335,-4.3670736617,-3.3057722315
H,0,4.5346976334,-2.3392463006,-3.0835522805
H,0,3.7755309107,-0.4416985865,-1.7060510239
H,0,2.8606218821,-2.1741779451,1.1971547619
H,0,3.4968845372,-2.5719696107,3.5502083448
H,0,2.7849007201,-0.9822609962,5.3198752047
H,0,1.4365126413,1.0154486759,4.7228808758
H,0,0.8059786138,1.4287122301,2.3548626011
H,0,-2.9777375482,1.1078422301,2.0561206636
H,0,-5.3771697193,1.5468042107,1.5833492119
O,0,-6.8155709605,0.3750033903,-0.1449108579
H,0,-5.3274172678,-1.5262245544,-1.4247133016
H,0,-2.9518776421,-1.9683275168,-0.9195095489
C,0,-0.8096226075,1.6746511688,-0.2610250926
C,0,-1.8458507613,2.1896768194,-1.2250605451
O,0,-0.3457998938,2.4034284079,0.6229329453
H,0,-2.3355813529,3.0733889177,-0.8130622325
H,0,-1.3413535259,2.4726018165,-2.1574472985
H,0,-2.5881696648,1.4261121274,-1.4697081284
C,0,-7.5416513088,-0.3453553392,-1.127632978
H,0,-8.5519160193,0.0628684676,-1.1129976669
H,0,-7.1082950258,-0.2060869061,-2.1247190087
H,0,-7.5788557324,-1.4148856841,-0.8914762588

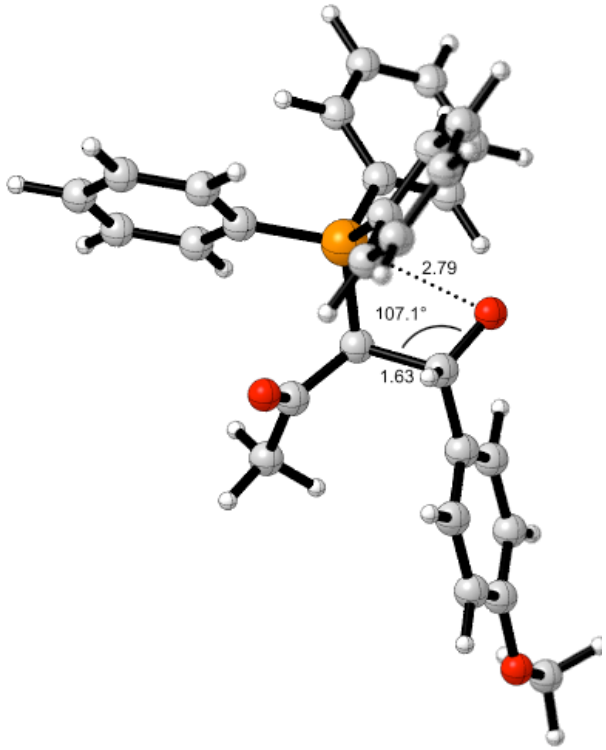
Betaine 5

/home/singletn/wittig/methoxyketone/b3p86PS/betaineb3p86PS
betaine from anisaldehyde and ketone
B3P86/6-31+G**
E(RB3P86) = -1692.73728281

Zero-point correction= 0.484710 (Hartree/Particle)
Thermal correction to Energy= 0.515241
Thermal correction to Enthalpy= 0.516185
Thermal correction to Gibbs Free Energy= 0.420321

Sum of electronic and ZPE= -1692.252572
Sum of electronic and thermal Energies= -1692.222042
Sum of electronic and thermal Enthalpies= -1692.221097
Sum of electronic and thermal Free Energies= -1692.316962

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	323.319	117.109	201.764



O,0,0.7786855431,1.4630356129,1.1696950718
C,0,1.2555199223,0.2431869315,0.9175440606
P,0,-1.3149553295,0.070375221,-0.0434175352
C,0,0.4505833438,-0.3264336497,-0.3761183258
C,0,2.7518953092,0.1567020779,0.6334381564
C,0,-2.3161476877,-1.1505833066,-0.9583791783
C,0,-2.0953145712,-1.3009670283,-2.3351350336
C,0,-2.8459112936,-2.2136987331,-3.0687776215
C,0,-3.8265982446,-2.9799808146,-2.4367630218
C,0,-4.0555536313,-2.8269536871,-1.0717380433
C,0,-3.3037617193,-1.9144165454,-0.3315337829
C,0,-1.8199044642,1.6715422607,-0.7452114968
C,0,-1.7780592108,-0.0488416605,1.6989721577
C,0,-0.9777359022,2.7882976389,-0.6687312238
C,0,-1.3957796919,4.0017703185,-1.2112878025
C,0,-2.6483716376,4.11303449,-1.8134257951
C,0,-3.4920491362,3.0043194119,-1.8766096091
C,0,-3.0811429813,1.7823763661,-1.3502607583
C,0,-2.5126125593,0.9790739002,2.2992731232
C,0,-2.9028325358,0.8620372872,3.630186535
C,0,-2.5589570068,-0.2738405997,4.3635807421
C,0,-1.8304609017,-1.2991327651,3.7625197462
C,0,-1.4419601964,-1.1965253344,2.4281577533
C,0,3.5352327626,-0.8773779943,1.1583867498
C,0,4.8988328685,-0.95547147,0.8992009642
C,0,5.5140109501,0.0135231885,0.0991438168
C,0,4.7503506685,1.0600358254,-0.4290978374
C,0,3.3837623599,1.119820417,-0.1524953048
H,0,1.0424374569,-0.5157604488,1.70587851
H,0,0.7521967406,0.3123039956,-1.2130340479
H,0,-1.3473815048,-0.6983202874,-2.8437001826
H,0,-2.666893235,-2.3248484757,-4.1335158955
H,0,-4.4115317927,-3.6925235611,-3.0099417933
H,0,-4.8194666092,-3.4176873946,-0.5762045975
H,0,-3.4880560212,-1.8036589826,0.7316417192
H,0,-0.024615091,2.668295145,-0.1521966449
H,0,-0.7402361837,4.8655098499,-1.1551435493
H,0,-2.9695703527,5.0625270891,-2.2312344993
H,0,-4.4705061385,3.0860330044,-2.339347378
H,0,-3.7431043351,0.9252299031,-1.4143229947
H,0,-2.7677746129,1.8708738181,1.7361532822
H,0,-3.4689845629,1.662733179,4.0954001825
H,0,-2.8594240304,-0.3593774892,5.4033763367
H,0,-1.5634785034,-2.184904903,4.3304778571
H,0,-0.8860433046,-1.9970031354,1.9483404764
H,0,3.0708137828,-1.6330069782,1.7885772032
H,0,5.505009936,-1.7544257424,1.3152502783
O,0,6.8534151373,-0.1390294693,-0.1023204538
H,0,5.2055770856,1.8294114086,-1.0423303299
H,0,2.7941111639,1.9451051768,-0.5428512771
C,0,0.7313784769,-1.7767399541,-0.6483069882
C,0,1.70088502,-2.0892330135,-1.7520227106
O,0,0.2464818295,-2.6535594405,0.0589813085
H,0,1.9808162236,-3.1427961125,-1.724471798
H,0,1.2351372038,-1.860289371,-2.7178341504
H,0,2.5910763758,-1.4580301193,-1.6677705995
C,0,7.5223726692,0.8293280034,-0.8932718331
H,0,8.5687861441,0.5259270652,-0.9175584609
H,0,7.1275247961,0.8514061669,-1.9156251678
H,0,7.4444742098,1.8287297146,-0.4502533084

TS1.5 6

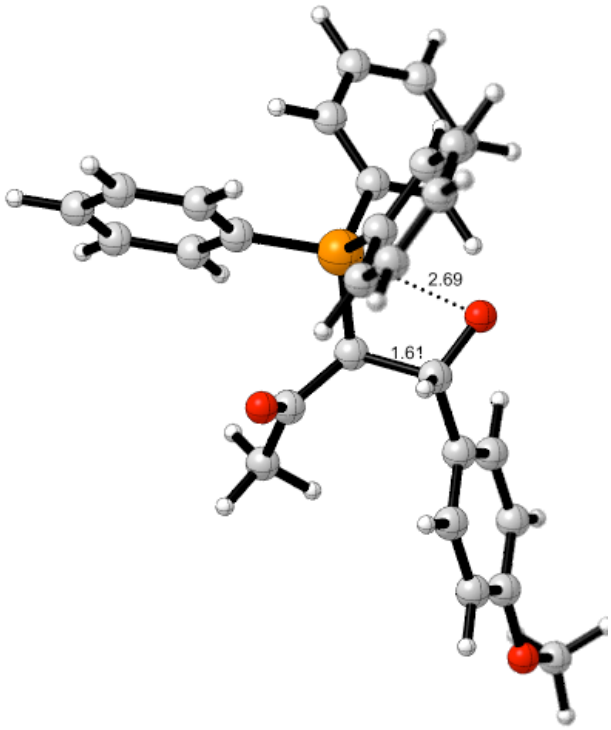
/home/singletn/wittig/methoxyketone/b3p86PS/TS1.5b3p86PS
TS1.5
B3P86/6-31+G**
E(RB3P86) = -1692.73725445

Zero-point correction= 0.484627 (Hartree/Particle)
Thermal correction to Energy= 0.514300
Thermal correction to Enthalpy= 0.515245
Thermal correction to Gibbs Free Energy= 0.422177
Sum of electronic and ZPE= -1692.252627
Sum of electronic and thermal Energies= -1692.222954
Sum of electronic and thermal Enthalpies= -1692.222010
Sum of electronic and thermal Free Energies= -1692.315078

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	322.728	115.118	195.878

O,0,0.8331355909,1.1056360178,1.3663697873
C,0,1.2739141391,-0.0600635006,0.8752790839
P,0,-1.2910865114,0.1493455071,0.0312217248
C,0,0.420046658,-0.3197270213,-0.4672180762
C,0,2.7617646778,-0.1292803333,0.5528092704
C,0,-2.407212911,-0.7889578946,-1.0731621212

C,0,-2.2210410459,-0.6830545683,-2.4591866046
C,0,-3.0549301082,-1.3714259177,-3.3342749826
C,0,-4.0865950739,-2.1679743473,-2.8349037948
C,0,-4.2815894301,-2.2693593026,-1.4598957548
C,0,-3.4458801515,-1.5820828135,-0.5791650289
C,0,-1.7127235569,1.8868277628,-0.3221234862
C,0,-1.7267229773,-0.3072060954,1.7247638964
C,0,-0.8008419495,2.9214729479,-0.0774879861
C,0,-1.1616700422,4.2381278355,-0.3563739586
C,0,-2.4279400711,4.532834091,-0.8596368259
C,0,-3.3415216475,3.50463001,-1.0894265102
C,0,-2.9873106145,2.1831810806,-0.8297035379
C,0,-2.3575964503,0.621684013,2.5589501481
C,0,-2.7254100492,0.2530690226,3.8495180654
C,0,-2.4603942698,-1.0362196084,4.3127482295
C,0,-1.8340648181,-1.9613363326,3.4794385669
C,0,-1.4704619723,-1.6060837013,2.1815860686
C,0,3.5062262953,-1.2901090166,0.7925121529
C,0,4.8622517652,-1.3540656034,0.494451633
C,0,5.5094835367,-0.2413124736,-0.0541359614
C,0,4.7857622064,0.931932014,-0.291903736
C,0,3.425204515,0.9738154002,0.0171617564
H,0,1.0497900842,-0.9476009294,1.5112549343
H,0,0.7461884675,0.4465217946,-1.1789397321
H,0,-1.4327968202,-0.0531368491,-2.863212153
H,0,-2.9007048112,-1.2841494399,-4.4051608446
H,0,-4.7368859311,-2.7054011973,-3.5180933898
H,0,-5.0845931789,-2.8843187778,-1.0659190266
H,0,-3.6059211196,-1.6693198219,0.4901559758
H,0,0.1616916431,2.6516771951,0.3551858318
H,0,-0.4502548448,5.0370209729,-0.1702810001
H,0,-2.7050699406,5.5614756388,-1.0702873015
H,0,-4.3311437363,3.7271086983,-1.4759300487
H,0,-3.7050329223,1.3933224347,-1.0238556792
H,0,-2.5490963826,1.6306808822,2.208480832
H,0,-3.2119105767,0.9769444566,4.495652812
H,0,-2.7426969935,-1.318746482,5.3223357155
H,0,-1.6279819401,-2.9658349351,3.8359111241
H,0,-0.994940759,-2.3266531843,1.5223467347
H,0,3.0175541847,-2.1590322361,1.2285449004
H,0,5.4386268498,-2.2534233249,0.6887899147
O,0,6.839202001,-0.3910035325,-0.3133726068
H,0,5.2678966923,1.8113704379,-0.7035563066
H,0,2.8650166802,1.8912654208,-0.1423347007
C,0,0.5795047581,-1.7057732896,-1.0285347313
C,0,1.4962047972,-1.8579806245,-2.2082124597
O,0,0.0487444288,-2.6691758483,-0.4878412031
H,0,1.6853644833,-2.9127675234,-2.4098937988
H,0,1.0347526282,-1.3935566727,-3.0876780852
H,0,2.4391147359,-1.3322176254,-2.0259993592
C,0,7.5412649162,0.7170636926,-0.8520197403
H,0,8.5732986123,0.388478017,-0.9726777033
H,0,7.1372491171,1.0091830845,-1.8282415193
H,0,7.5110091435,1.576452396,-0.1725494035



Benzaldehyde + Ph3PCHCO2Me, M06-2X/6-31+G**/PCM(THF) with Default Radii

benzaldehyde

/home/singletn/wittig/c28/full2XPS/benzaldehydeM062XPCMPS
benzaldehyde for Wittig
M062X/6-31+G**
E(RM062X) = -345.445058363

Zero-point correction= 0.110776 (Hartree/Particle)
Thermal correction to Energy= 0.117100
Thermal correction to Enthalpy= 0.118044
Thermal correction to Gibbs Free Energy= 0.080170
Sum of electronic and ZPE= -345.334282
Sum of electronic and thermal Energies= -345.327959
Sum of electronic and thermal Enthalpies= -345.327014
Sum of electronic and thermal Free Energies= -345.364889

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	73.481	23.812	79.713

C,0,0.0023657138,0.,0.028396675
C,0,0.0116868247,0.,1.4283689619
C,0,1.2240384561,0.,2.1078721837
C,0,2.4255616493,0.,1.3916926368
C,0,2.4179996262,0.,-0.0027974853
C,0,1.20323253,0.,-0.6857909087
H,0,-0.9338578403,0.,1.9620946017
H,0,1.2394001419,0.,3.1930038546

H,0,3.3706643515,0.,1.9258980197
H,0,3.3532188936,0.,-0.5528005037
H,0,1.1838100962,0.,-1.7731283176
C,0,-1.2761303241,0.,-0.7171745635
O,0,-2.3730203175,0.,-0.1950785026
H,0,-1.1804018013,0.,-1.820056652

Ph3PCHCO2Me

/home/singletn/wittig/c28/full2XPS/Ph3PCHCO2MeM062XPCMPS
Ph3PCHCOOMe for Wittig
M062X/6-31+G**
E(RM062X) = -1303.07919182

Zero-point correction= 0.346538 (Hartree/Particle)
Thermal correction to Energy= 0.368222
Thermal correction to Enthalpy= 0.369166
Thermal correction to Gibbs Free Energy= 0.293475
Sum of electronic and ZPE= -1302.732654
Sum of electronic and thermal Energies= -1302.710970
Sum of electronic and thermal Enthalpies= -1302.710025
Sum of electronic and thermal Free Energies= -1302.785716

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	231.063	82.915	159.305

C,0,0.4229488787,0.1725720433,0.3956946251
P,0,0.4446752522,-0.1056497039,2.0901372465
H,0,-0.2655370166,0.9099729406,0.0067946662
C,0,4.3009976237,1.0748850056,4.3355723991
C,0,3.0620575965,1.3187422417,4.925564882
C,0,1.8889217032,0.9741921441,4.2540518918
C,0,1.958010407,0.3829732881,2.9877562012
C,0,3.203174877,0.1392610802,2.3948566826
C,0,4.3702570808,0.4856077719,3.0723706486
H,0,5.2127840178,1.3458900766,4.8587561191
H,0,3.0054636806,1.7796299557,5.9065154178
H,0,0.9254705609,1.1694268468,4.7176597966
H,0,3.2491673594,-0.3298299776,1.4158473139
H,0,5.3348804421,0.296166434,2.6121628709
C,0,-0.4655825702,-4.4655123443,3.2679430039
C,0,0.3571772776,-3.6957696423,4.0893412389
C,0,0.6662349332,-2.3828575724,3.7355844566
C,0,0.1447034115,-1.8404783263,2.5574992536
C,0,-0.6757066658,-2.6146139121,1.7317541047
C,0,-0.9802192936,-3.925894404,2.0882877392
H,0,-0.7016718665,-5.4883963307,3.5443762955
H,0,0.7634646451,-4.117082581,5.0032761003
H,0,1.3137482209,-1.7886177093,4.3741934131
H,0,-1.0635021261,-2.18710906,0.810730624
H,0,-1.6131621062,-4.52742943,1.4438852446
C,0,-2.9406186766,2.4392111159,3.9001799497
C,0,-1.9652185708,3.0302683255,3.0941627977
C,0,-0.9439313062,2.2545417407,2.5531099701
C,0,-0.8984132953,0.8789527692,2.8149593431
C,0,-1.8726779515,0.2897215415,3.6247066432
C,0,-2.8927401737,1.0727779108,4.1655992523
H,0,-3.7365232749,3.0459041561,4.3203729183
H,0,-1.9996336052,4.0951779326,2.8882522544
H,0,-0.1822803924,2.7185243518,1.9316279943
H,0,-1.8416588234,-0.7756938056,3.8327303052
H,0,-3.6490207659,0.6106582842,4.7916578531
C,0,1.21920254,-0.6250093432,-0.4580342568
O,0,1.0208396776,-0.35306356,-1.7835236269
O,0,2.0241706989,-1.5016007651,-0.1141061291
C,0,1.8014640806,-1.1233603194,-2.6926367413
H,0,1.5265155099,-0.7751134907,-3.6877466411
H,0,2.8689380584,-0.96490965,-2.5203570207
H,0,1.5799499476,-2.1884760294,-2.5918171012

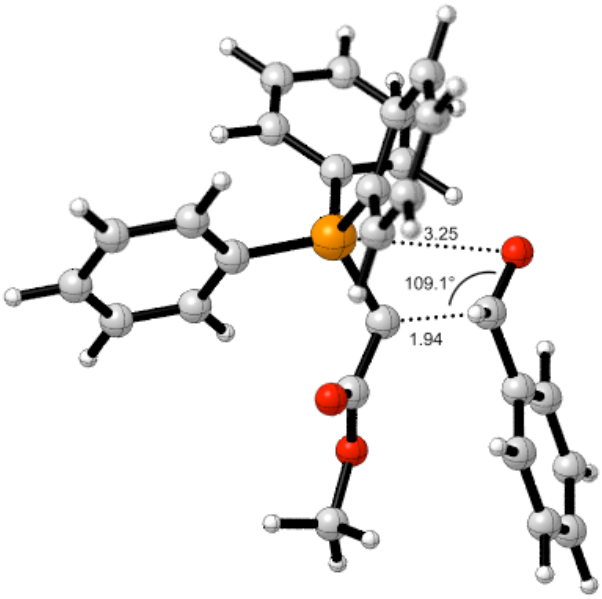
E TS1 for benzaldehyde + Ph3PCHCO2Me

/home/singletn/wittig/c28/full2XPS/TS1EM062XPCMPS
ts Ph3PCHCOOMe + benzaldehyde for Wittig
M062X/6-31+G**
E(RM062X) = -1648.51748729

Zero-point correction= 0.459559 (Hartree/Particle)
Thermal correction to Energy= 0.487809
Thermal correction to Enthalpy= 0.488753
Thermal correction to Gibbs Free Energy= 0.398992
Sum of electronic and ZPE= -1648.057928
Sum of electronic and thermal Energies= -1648.029679
Sum of electronic and thermal Enthalpies= -1648.028734
Sum of electronic and thermal Free Energies= -1648.118495

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	306.105	108.908	188.917

P-C-C-O dihedral is -57.0°



O,0,1.5123694544,1.8150764924,1.5812638953
C,0,1.7310681204,0.6051578576,1.2559198125
P,0,-0.9581392642,0.5483810936,-0.107456407
C,0,0.7712006219,0.2046643263,-0.387525561
C,0,3.1257012371,0.194131494,0.8342137641
C,0,-2.0134427137,-0.542275526,-1.1050684522
C,0,-1.6344627085,-0.7920287275,-2.4297856705

C,0,-2.4407771784,-1.5800861125,-3.2443119499
C,0,-3.6256464001,-2.1197161018,-2.7401410776
C,0,-4.0047664613,-1.8682782653,-1.4231511902
C,0,-3.2005940419,-1.0778975519,-0.6011339167
C,0,-1.3021144311,2.2456720586,-0.6364565251
C,0,-1.4750954989,0.3538614223,1.6176455053
C,0,-0.3816585626,3.253324158,-0.3224393145
C,0,-0.6497550545,4.5646104837,-0.710058599
C,0,-1.8217873884,4.8687282503,-1.4025712282
C,0,-2.7375441958,3.8621568352,-1.7084148852
C,0,-2.4822304239,2.5463469799,-1.3263902692
C,0,-2.075795873,1.4096214813,2.3077986866
C,0,-2.4947184547,1.221753158,3.6242751764
C,0,-2.3130310065,-0.0120892132,4.2457476427
C,0,-1.712377797,-1.0654433902,3.5544118945
C,0,-1.2925558444,-0.8889522023,2.2390581237
C,0,3.5779063328,-1.1056708314,1.0685218915
C,0,4.8535591102,-1.495034842,0.6594337054
C,0,5.6862574429,-0.5816647286,0.0136999098
C,0,5.2426991811,0.7246017325,-0.209482161
C,0,3.9699771517,1.1109990386,0.2043142703
H,0,1.2495344026,-0.2024347488,1.8453386245
H,0,1.2036014266,0.9296598294,-1.0764092512
H,0,-0.7112542096,-0.3733333468,-2.8242465274
H,0,-2.1433467166,-1.7756198926,-4.2692005024
H,0,-4.2513471152,-2.7388023848,-3.3750912091
H,0,-4.9245497714,-2.2888164873,-1.030093298
H,0,-3.4985145411,-0.8863243226,0.4254452559
H,0,0.5172497376,3.0036254525,0.2414325649
H,0,0.0601911082,5.3491403141,-0.4689843596
H,0,-2.0218793062,5.8917240039,-1.7056104868
H,0,-3.6493791814,4.0983421848,-2.2471762646
H,0,-3.1957720767,1.7646641288,-1.5706958912
H,0,-2.2112237315,2.3750493921,1.829132457
H,0,-2.9579956722,2.0417551732,4.1631076879
H,0,-2.638095234,-0.1544036724,5.2716469529
H,0,-1.5690693316,-2.025406478,4.0397790626
H,0,-0.8235688469,-1.703185321,1.6913912662
H,0,2.9220772798,-1.81735109,1.5672829833
H,0,5.1974258618,-2.5085345915,0.8455271407
H,0,6.679103844,-0.8822030239,-0.3072489529
H,0,5.8932906783,1.4395795206,-0.7047449758
H,0,3.6131708103,2.1256527129,0.0463552412
C,0,1.0431011327,-1.1916694352,-0.726074803
O,0,1.9969963807,-1.3255976126,-1.6627732104
O,0,0.5190342806,-2.1529215472,-0.1776219912
C,0,2.436516542,-2.6638086064,-1.914635271
H,0,3.2405870702,-2.5760495071,-2.6429064016
H,0,2.8065288559,-3.117636191,-0.9923602459
H,0,1.61676097,-3.2639238228,-2.3155326658

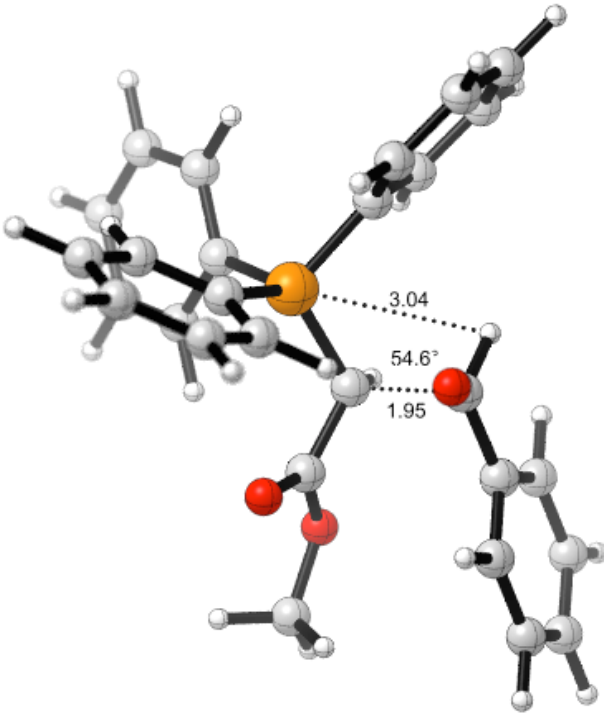
Z TS1 for benzaldehyde + Ph3PCHCO2Me

/home/singletn/wittig/c28/full2XPS/TS1ZM062XPCMPS
ts Ph3PCHCOOMe + benzaldehyde for Wittig cis
M062X/6-31+G**
E(RM062X) = -1648.51148697

Zero-point correction= 0.459577 (Hartree/Particle)
Thermal correction to Energy= 0.487804
Thermal correction to Enthalpy= 0.488748
Thermal correction to Gibbs Free Energy= 0.398709
Sum of electronic and ZPE= -1648.051910
Sum of electronic and thermal Energies= -1648.023683
Sum of electronic and thermal Enthalpies= -1648.022739
Sum of electronic and thermal Free Energies= -1648.112778

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	306.101	108.822	189.503

P-C-C-O dihedral is 54.6°



O,0,1.4662950726,1.3568532156,1.7147667891
C,0,1.7371443091,1.2635966451,0.4776764926
P,0,-0.9792529136,0.0308115107,-0.0696229215
C,0,0.7599366214,-0.1919169046,-0.3816186534
C,0,3.1403083634,0.877487816,0.0554179179
C,0,-1.9443193546,-0.7841307731,-1.3776293999
C,0,-1.4566425209,-1.9735626018,-1.9294248304
C,0,-2.2048144592,-2.6521501108,-2.8886491696
C,0,-3.4363151846,-2.1441695193,-3.2999676172
C,0,-3.9233363935,-0.9566965934,-2.7526672601
C,0,-3.1810682129,-0.2748355107,-1.7909028991
C,0,-1.3474643902,1.8010945051,-0.1999141127
C,0,-1.5819817726,-0.5958059326,1.5172892576
C,0,-1.2290541126,2.4146871423,-1.4542162817
C,0,-1.4477059151,3.7829737182,-1.5781514861
C,0,-1.7835096663,4.5389160115,-0.4531026367
C,0,-1.9007681495,3.9275115797,0.7933357903
C,0,-1.6817788015,2.5564486409,0.9251792633
C,0,-0.8538972981,-0.3514868792,2.6888449951
C,0,-1.363936031,-0.7904823665,3.9077262309
C,0,-2.5810784121,-1.4715189432,3.9618061668
C,0,-3.298172514,-1.7173807886,2.7927626939
C,0,-2.8016588882,-1.2806773112,1.5656348985
C,0,3.9846141275,0.2310211863,0.9586453966
C,0,5.2687156891,-0.1506497,0.5687876543

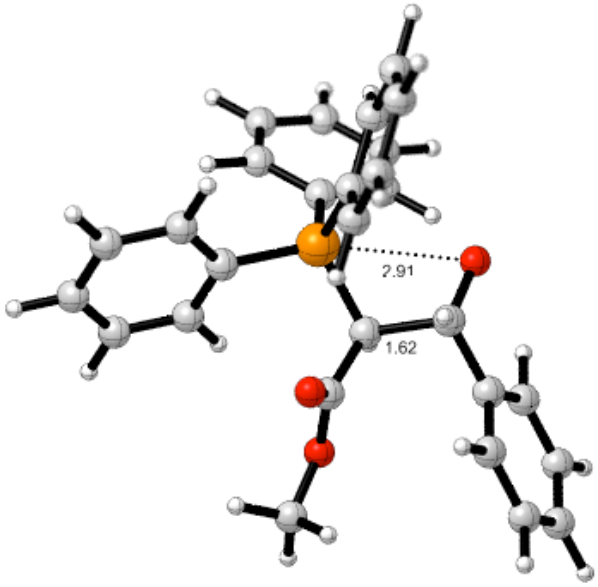
C,0,5.7177028612,0.1199924179,-0.7245045197
C,0,4.8806801534,0.7818517428,-1.6255214982
C,0,3.59742145,1.1572841624,-1.2335818039
H,0,1.3148095039,2.0211165179,-0.2151456269
H,0,0.927177827,-0.0190113805,-1.447668771
H,0,-0.4941866559,-2.3706397387,-1.618141902
H,0,-1.8227880222,-3.5736356797,-3.3152142523
H,0,-4.0156100707,-2.6715502143,-4.0511112748
H,0,-4.8797430694,-0.558846257,-3.0757188096
H,0,-3.5633856272,0.6503780994,-1.3679345415
H,0,-0.9713371368,1.8265288545,-2.3321918063
H,0,-1.3552235583,4.2575995861,-2.5494199134
H,0,-1.9536059431,5.6064505584,-0.5506759456
H,0,-2.160272214,4.5153689416,1.6674377503
H,0,-1.7652416011,2.0845151932,1.8992480605
H,0,0.0971343482,0.1744836601,2.6267935771
H,0,-0.8035447246,-0.6048274467,4.8184041555
H,0,-2.9679469141,-1.815795581,4.9159982579
H,0,-4.2409646037,-2.2531584605,2.8300357004
H,0,-3.3627352853,-1.4841690155,0.6591071177
H,0,3.616226494,0.0389428392,1.9627022019
H,0,5.9215032429,-0.6575920782,1.2739754995
H,0,6.7178615731,-0.1751337868,-1.0273835982
H,0,5.2302067608,1.0052882394,-2.6292575817
H,0,2.9400089635,1.6699794342,-1.9345439205
C,0,1.3766712155,-1.4411155797,0.078035918
O,0,2.2493143703,-1.9205809117,-0.8357202343
O,0,1.2132269272,-1.9742054169,1.1622648929
C,0,3.0575608146,-3.0172062265,-0.4030949872
H,0,3.7162063199,-3.2433780728,-1.2400032706
H,0,3.6427532998,-2.7293607409,0.4731887159
H,0,2.4351421086,-3.8812696965,-0.1603908681

betaine for benzaldehyde + Ph3PCHCO2Me

/home/singletn/wittig/c28/full2XPS/betaineM062XPS
betaine benzaldehyde + ester
M062X/6-31+G**
E(RM062X) = -1648.52113677

Zero-point correction= 0.461269 (Hartree/Particle)
Thermal correction to Energy= 0.489644
Thermal correction to Enthalpy= 0.490588
Thermal correction to Gibbs Free Energy= 0.399855
Sum of electronic and ZPE= -1648.059868
Sum of electronic and thermal Energies= -1648.031493
Sum of electronic and thermal Enthalpies= -1648.030548
Sum of electronic and thermal Free Energies= -1648.121282

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	307.256	109.439	190.965

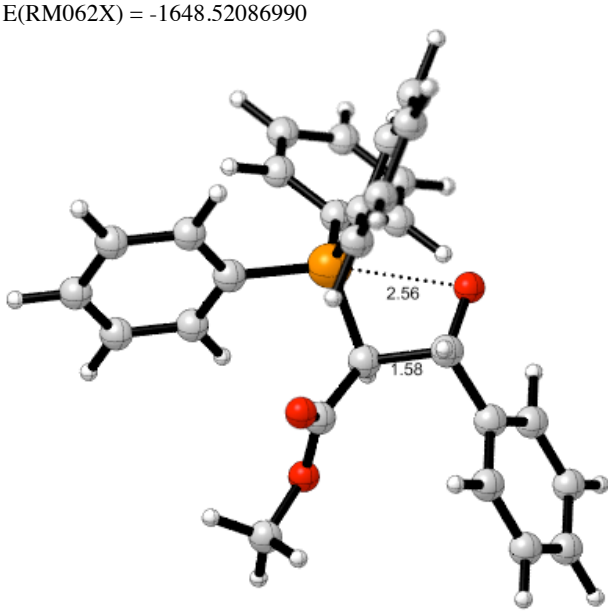


O,0,0.9024837034,1.424042219,1.3222464061
C,0,1.2614416678,0.1867660699,0.983669858
P,0,-1.3416514037,0.1293702355,0.004287402
C,0,0.4220434995,-0.2500240832,-0.3273829679
C,0,2.7354353428,-0.0110992704,0.615077273
C,0,-2.3389894169,-1.0755754776,-0.9204556773
C,0,-2.0210251986,-1.3124862537,-2.2650259252
C,0,-2.7784405327,-2.2118024423,-3.0081116527
C,0,-3.8562883559,-2.8734518603,-2.4156429677
C,0,-4.1777774422,-2.6316435561,-1.0822279684
C,0,-3.4211215557,-1.7319695637,-0.3307973345
C,0,-1.8022763158,1.7596393908,-0.6439088889
C,0,-1.7843237405,-0.0225490885,1.7463830694
C,0,-0.9622642901,2.861341149,-0.4371861771
C,0,-1.3427629446,4.1075414239,-0.9314297974
C,0,-2.5473506092,4.2584812488,-1.6173653232
C,0,-3.3844577097,3.1601383021,-1.8130918199
C,0,-3.0157488365,1.9065090472,-1.3297708045
C,0,-2.4396333235,1.0239037191,2.399795475
C,0,-2.8189327344,0.8694122549,3.731204436
C,0,-2.540685394,-0.3200359326,4.40374915
C,0,-1.886236822,-1.3623846662,3.74719616
C,0,-1.5084440274,-1.2218410985,2.4139924189
C,0,3.3727042884,-1.2440655205,0.7792685746
C,0,4.7057163415,-1.411408237,0.4018742284
C,0,5.4174482445,-0.3401000071,-0.1392404548
C,0,4.7894995281,0.8970404647,-0.2959208374
C,0,3.4569077354,1.0579516084,0.0808557849
H,0,1.0154833175,-0.601346622,1.7336585396
H,0,0.7412157011,0.4140423551,-1.1369120138
H,0,-1.1880562613,-0.7952533432,-2.7365540501
H,0,-2.5278063453,-2.3966427528,-4.0473799599
H,0,-4.4442340912,-3.5775033861,-2.9957236619
H,0,-5.0154739715,-3.1437151986,-0.6206037744
H,0,-3.6754131401,-1.5484725877,0.708418779
H,0,-0.0389990701,2.7089112028,0.122190554
H,0,-0.6936857273,4.963388851,-0.7763324223
H,0,-2.8353786114,5.2327123389,-2.0000899887
H,0,-4.3230929367,3.2751909688,-2.3451752172
H,0,-3.6703851499,1.0556615608,-1.4922050068
H,0,-2.6426154701,1.9555608213,1.8800048006

H,0,-3.3251929381,1.6809094431,4.2435278557
H,0,-2.8343391883,-0.4355046509,5.4423431202
H,0,-1.6703751308,-2.2876689823,4.2713014654
H,0,-1.0057309568,-2.0329603021,1.8924610007
H,0,2.8214598099,-2.0787830173,1.2105432019
H,0,5.1913294126,-2.3735890722,0.5384295703
H,0,6.4567730931,-0.465648226,-0.4278118384
H,0,5.3423736669,1.7374339502,-0.7062370554
H,0,2.9534357826,2.0158660991,-0.0168163625
C,0,0.6431280847,-1.6882875634,-0.6899382222
O,0,1.3877730317,-1.8237666036,-1.788060798
O,0,0.2498507719,-2.625330878,-0.023025155
C,0,1.7726952536,-3.1664233104,-2.115011795
H,0,2.3710381784,-3.0876662724,-3.0197663246
H,0,2.3615950865,-3.5914378468,-1.2993146578
H,0,0.8853831005,-3.7784350509,-2.2876692227

TS1.5 for benzaldehyde + Ph3PCHCO2Me

/home/singletn/wittig/c28/full2XPS/TS1.5M062XPS
betaine benzaldehyde + ester
M062X/6-31+G**
E(RM062X) = -1648.52086990



Zero-point correction= 0.461517 (Hartree/Particle)
Thermal correction to Energy= 0.489117
Thermal correction to Enthalpy= 0.490061
Thermal correction to Gibbs Free Energy= 0.401489
Sum of electronic and ZPE= -1648.059352
Sum of electronic and thermal Energies= -1648.031753
Sum of electronic and thermal Enthalpies= -1648.030809
Sum of electronic and thermal Free Energies= -1648.119381

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	306.925	107.333	186.415

O,0,0.7310783352,0.9959197078,1.4143193692
C,0,1.2327729871,-0.1516323278,0.9140570608
P,0,-1.2547314225,0.131237182,0.0482534091
C,0,0.4487801539,-0.3642162112,-0.4413821307
C,0,2.7283893624,-0.1700161699,0.6130268769
C,0,-2.3470043445,-0.8066644971,-1.0822023914
C,0,-2.0474718735,-0.8031228623,-2.4518137968
C,0,-2.860707188,-1.4897530776,-3.3481517335
C,0,-3.9831612712,-2.1790046685,-2.8849490894
C,0,-4.2901373025,-2.1762491077,-1.5266839673
C,0,-3.4742816984,-1.4921840028,-0.6242099639
C,0,-1.6720125561,1.8678490994,-0.3076571864
C,0,-1.7398829043,-0.3666308426,1.7156191897
C,0,-0.7625061014,2.905706343,-0.0715591287
C,0,-1.1322812073,4.2194983947,-0.3551255084
C,0,-2.4024319869,4.5051568115,-0.8534594507
C,0,-3.3121322345,3.4720552189,-1.0763728321
C,0,-2.9489864115,2.1533281375,-0.8135844522
C,0,-2.3307153311,0.5652304425,2.5724593413
C,0,-2.7475279102,0.1643731669,3.8388876864
C,0,-2.5651845094,-1.15631148,4.2505954917
C,0,-1.9713541786,-2.0813723755,3.3930190622
C,0,-1.5627940506,-1.6943468121,2.1173134683
C,0,3.4181248772,-1.37910219,0.4803743157
C,0,4.7762100975,-1.3912937213,0.1642710095
C,0,5.4605956018,-0.1881381956,-0.015697752
C,0,4.7795710609,1.0217857422,0.1254777684
C,0,3.4200240032,1.0291659945,0.4392251737
H,0,1.02113149,-1.057134657,1.5282304707
H,0,0.8015598939,0.3991548202,-1.1431946635
H,0,-1.1815644544,-0.2606357564,-2.8262012939
H,0,-2.6197654948,-1.4855420488,-4.4062215507
H,0,-4.6168823682,-2.7150078772,-3.5841902126
H,0,-5.1634417258,-2.7077148265,-1.16285999
H,0,-3.7223749359,-1.4964531277,0.4326118613
H,0,0.204868789,2.6543499006,0.3526405236
H,0,-0.4242562115,5.0223999461,-0.176295558
H,0,-2.6846612519,5.5312980425,-1.0677702747
H,0,-4.3029647201,3.6881526174,-1.4621791866
H,0,-3.6619932692,1.3578685349,-1.0058040567
H,0,-2.4519662705,1.5979228409,2.2584340376
H,0,-3.2074051267,0.8856304176,4.5064419492
H,0,-2.8856047575,-1.4638679206,5.2410693607
H,0,-1.8277790429,-3.1085567673,3.712473293
H,0,-1.1108554892,-2.4143628406,1.439719128
H,0,2.8884691197,-2.318314033,0.63674298
H,0,5.302544207,-2.3364599196,0.0672628831
H,0,6.5195973137,-0.1939931487,-0.255842954
H,0,5.3110718744,1.9604035124,-0.0037573868
H,0,2.8731229439,1.9590321168,0.5687854577
C,0,0.5614184054,-1.7380610503,-1.040288643
O,0,1.2561900265,-1.7325863073,-2.1788210238
O,0,0.1293165866,-2.7468310434,-0.5204855683
C,0,1.5028568295,-3.0190240326,-2.765093077
H,0,2.0831310192,-2.8243637905,-3.6640534815
H,0,2.0668519224,-3.6426563793,-2.0688314829
H,0,0.5563837008,-3.5044639214,-3.0112623803

OP1 for benzaldehyde + Ph3PCHCO2Me

/home/singletn/wittig/c28/full2XPS/OP1EM062XPS
OP1 for Wittig
M062X/6-31+G**
E(RM062X) = -1648.53262356

Zero-point correction= 0.462923 (Hartree/Particle)
Thermal correction to Energy= 0.490541
Thermal correction to Enthalpy= 0.491485
Thermal correction to Gibbs Free Energy= 0.403526
Sum of electronic and ZPE= -1648.069701
Sum of electronic and thermal Energies= -1648.042082
Sum of electronic and thermal Enthalpies= -1648.041138
Sum of electronic and thermal Free Energies= -1648.129097

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	307.819	108.490	185.125

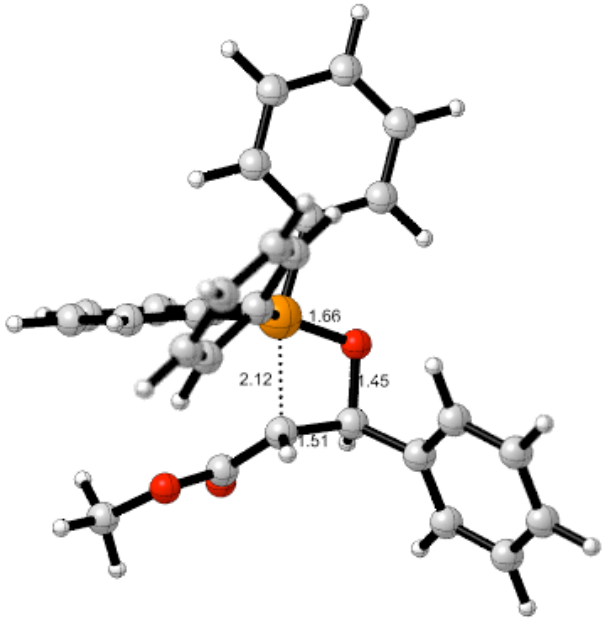
8 -1.102008 0.646013 1.214764
6 -1.658862 -0.636076 0.995955
6 -0.708573 -1.111501 -0.101154
15 0.376648 0.424577 0.181624
1 -1.121723 -1.052692 -1.113508
6 3.134943 0.977347 3.877549
6 1.900476 0.346112 4.015952
6 1.064469 0.189106 2.911226
6 1.470934 0.630899 1.648225
6 2.721882 1.245806 1.513941
6 3.540730 1.435164 2.624004
1 3.779398 1.111778 4.740841
1 1.577999 -0.016816 4.986649
1 0.093679 -0.275085 3.034843
1 3.072969 1.572201 0.540635
1 4.500024 1.928826 2.505419
6 3.343683 -1.656371 -2.839656
6 3.565788 -1.761963 -1.468696
6 2.752789 -1.069656 -0.568650
6 1.709525 -0.247901 -1.016085
6 1.492396 -0.167830 -2.399275
6 2.299486 -0.856122 -3.303284
1 3.975127 -2.194118 -3.540381
1 4.369712 -2.388629 -1.092850
1 2.939074 -1.187276 0.495900
1 0.677446 0.440672 -2.786388
1 2.110170 -0.769048 -4.369156
6 -0.440819 4.395896 -2.091847
6 0.865600 3.932016 -1.935245
6 1.104995 2.730985 -1.273225
6 0.046101 1.996178 -0.723694
6 -1.259737 2.472721 -0.877675
6 -1.501651 3.658486 -1.571909
1 -0.628879 5.325703 -2.619715
1 1.699407 4.496618 -2.340364
1 2.123498 2.363590 -1.206048
1 -2.085741 1.918732 -0.448104
1 -2.522012 4.007706 -1.695291
6 -3.724161 -1.688926 -0.011172
6 -3.124105 -0.595081 0.620577
6 -3.905268 0.515362 0.947160
6 -5.266401 0.535711 0.640374
6 -5.858968 -0.556503 0.007858
6 -5.083917 -1.671145 -0.316385
1 -3.126733 -2.561362 -0.269133
1 -3.434504 1.360450 1.440328
1 -5.863354 1.405644 0.897161
1 -6.917572 -0.540842 -0.232074
1 -5.538055 -2.524903 -0.810003
1 -1.541581 -1.272698 1.888082
6 0.003616 -2.414965 0.112226
8 0.219255 -3.067983 -1.030959
8 0.366076 -2.820384 1.197480
6 0.986299 -4.274452 -0.924714
1 1.100453 -4.639120 -1.943317
1 1.960864 -4.054987 -0.483368
1 0.456541 -5.003932 -0.309084

OP2 for benzaldehyde + Ph3PCHCO2Me

/home/singletn/wittig/c28/full2XPS/OP2EM062XPS
OP2 for Wittig
M062X/6-31+G**
E(RM062X) = -1648.53484139

Zero-point correction= 0.462569 (Hartree/Particle)
Thermal correction to Energy= 0.490465
Thermal correction to Enthalpy= 0.491409
Thermal correction to Gibbs Free Energy= 0.401296
Sum of electronic and ZPE= -1648.072273
Sum of electronic and thermal Energies= -1648.044377
Sum of electronic and thermal Enthalpies= -1648.043433
Sum of electronic and thermal Free Energies= -1648.133545

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	307.771	108.660	189.658



O,0,0.791342705,0.3488066998,-1.3551465207
C,0,1.5555889807,-0.8574983469,-1.1021964913
C,0,0.8664551233,-1.3422123225,0.1491081513
P,0,-0.3610983488,0.3522594382,-0.1616203288
H,0,1.3985351401,-1.5411527111,-1.942205259
H,0,1.4569716089,-1.2430730929,1.0596178335
C,0,-2.0886253584,4.4626482021,-1.6455450179
C,0,-0.7878384646,4.1059132185,-1.9930179702
C,0,-0.2624371726,2.8764107994,-1.587455631
C,0,-1.0294296573,1.9845944668,-0.8286963303
C,0,-2.3353325739,2.3588979267,-0.4856411955

C,0,-2.8637530254,3.5831970951,-0.8880427073
H,0,-2.4981570791,5.4170821057,-1.9622266963
H,0,-0.1762065314,4.7831596226,-2.5817585469
H,0,0.7526111343,2.6114573319,-1.862638369
H,0,-2.954196984,1.6871936292,0.1057739352
H,0,-3.8797957756,3.8494862977,-0.6127707396
C,0,-4.0356973989,-2.2493528858,-1.184337245
C,0,-3.7633302357,-1.9778677374,0.1556890084
C,0,-2.6720228105,-1.1820122191,0.5050526434
C,0,-1.854973872,-0.6470385022,-0.4935388575
C,0,-2.1318169315,-0.9155528123,-1.8374585848
C,0,-3.2185155399,-1.7156194242,-2.1808327991
H,0,-4.8834679937,-2.8725369317,-1.4514409892
H,0,-4.4000823625,-2.3841861101,0.9356757714
H,0,-2.474854227,-0.9760328907,1.5524982908
H,0,-1.4958395548,-0.4997057267,-2.6158083651
H,0,-3.4253347482,-1.9229813577,-3.2259445176
C,0,0.0076075983,1.6975524871,4.2816217097
C,0,0.090367404,2.6401890607,3.2605331395
C,0,-0.0387270964,2.2461821133,1.9281311078
C,0,-0.2172259527,0.8958260471,1.6024476412
C,0,-0.2623971532,-0.050971921,2.6363549943
C,0,-0.1767735019,0.3504441264,3.9660362981
H,0,0.0934516985,2.007656586,5.3183851327
H,0,0.2460921713,3.6884775076,3.4948022105
H,0,0.0013797831,2.9989903745,1.1481079244
H,0,-0.3587015085,-1.1084475934,2.4077558019
H,0,-0.2355518317,-0.3924571147,4.7552926058
C,0,5.7455543583,-0.0286038087,-0.5488606508
C,0,5.3362622263,-1.2053970143,-1.1754719419
C,0,3.9790372207,-1.4547869695,-1.3750419733
C,0,3.0196069548,-0.5352550272,-0.9453076065
C,0,3.4343535723,0.6441913807,-0.320480894
C,0,4.7908679026,0.8962658669,-0.1234642937
H,0,6.8019734685,0.1699577874,-0.397251367
H,0,6.0736760083,-1.9267441065,-1.5140983685
H,0,3.6605653491,-2.3705523874,-1.8674270727
H,0,2.6929787277,1.3704868706,0.0044299805
H,0,5.1032156763,1.8172527382,0.3593765292
C,0,0.2052378614,-2.6560539422,0.0622980771
O,0,-0.1781614975,-3.108216232,1.2773368405
O,0,-0.0400038163,-3.2720975586,-0.9593943239
C,0,-0.9426494802,-4.316629725,1.2775739706
H,0,-1.1880809529,-4.5102154642,2.3204612894
H,0,-1.8526632623,-4.186523344,0.686469636
H,0,-0.3545269744,-5.1386734999,0.864985131

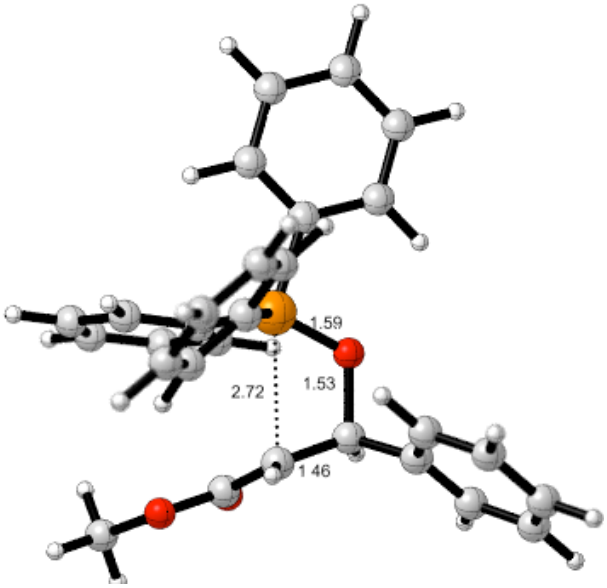
TS2 for benzaldehyde + Ph3PCHCO2Me

/home/singletn/wittig/c28/full2XPS/TS2M062XPCMPS
TS2 for Wittig
M062X/6-31+G**
E(RM062X) = -1648.52973489

Zero-point correction= 0.461265 (Hartree/Particle)
Thermal correction to Energy= 0.489004
Thermal correction to Enthalpy= 0.489948
Thermal correction to Gibbs Free Energy= 0.400606
Sum of electronic and ZPE= -1648.068470
Sum of electronic and thermal Energies= -1648.040731
Sum of electronic and thermal Enthalpies= -1648.039787

Sum of electronic and thermal Free Energies= -1648.129128

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	306.855	107.787	188.036



O,0,0.720597707,0.335966323,-1.1920341729
C,0,1.5854329981,-0.9095174966,-1.0130320474
C,0,1.0795141295,-1.6943671366,0.1147232213
P,0,-0.5090320917,0.4880598952,-0.187723933
H,0,1.4516562459,-1.4326330982,-1.9633085117
H,0,1.5293675889,-1.5630038894,1.0909844079
C,0,-2.1603539682,4.5615113719,-1.5848998822
C,0,-0.8936682578,4.1579186588,-2.0022028067
C,0,-0.3837691549,2.9218850231,-1.6034100848
C,0,-1.1492843652,2.0864167608,-0.7846942788
C,0,-2.4215684667,2.4942468205,-0.3667909763
C,0,-2.924926044,3.7287102771,-0.7657264226
H,0,-2.5542786079,5.5231203233,-1.8983510966
H,0,-0.2983933134,4.8034315177,-2.6398841801
H,0,0.6010929966,2.6040779363,-1.927869317
H,0,-3.0240624825,1.8493216922,0.2684276946
H,0,-3.9125271995,4.0387160099,-0.44032672
C,0,-4.0097906952,-2.3278462504,-1.0766673088
C,0,-3.8587738602,-1.8320041377,0.2189830798
C,0,-2.7855781839,-1.0007135083,0.5304624008
C,0,-1.8524420271,-0.675626258,-0.461948915
C,0,-2.0013076599,-1.1757919421,-1.7598525689
C,0,-3.0848035962,-1.9952808611,-2.0645171418
H,0,-4.8491413195,-2.973232586,-1.3155124969
H,0,-4.5806977413,-2.0844479738,0.9890229471
H,0,-2.6912762061,-0.601411452,1.5352022025
H,0,-1.2672750435,-0.9345242092,-2.5237220386
H,0,-3.1946146844,-2.3866493571,-3.0704411301
C,0,0.317064629,1.3169104476,4.2674992395
C,0,0.42629991,2.3355139143,3.3245165909
C,0,0.15955963,2.0735720949,1.9807373768
C,0,-0.1863423603,0.7783252436,1.5758515188
C,0,-0.2799192863,-0.2489488884,2.5257849975
C,0,-0.044184872,0.0277521383,3.8677303072
H,0,0.5152893324,1.5238240009,5.3144683787
H,0,0.7098121421,3.337118513,3.6302220804

H,0,0.2259231372,2.8786251545,1.2547207122
H,0,-0.5119411815,-1.2624918437,2.2096946419
H,0,-0.1265382404,-0.7674140799,4.6013122387
C,0,5.6450928568,0.4591090885,-0.5533955985
C,0,5.3079472896,-0.398819015,-1.5982298557
C,0,3.9874874222,-0.8221484753,-1.7575768739
C,0,2.996089212,-0.4011257888,-0.8699966127
C,0,3.3405752578,0.462724966,0.1763327726
C,0,4.6555215311,0.8910096471,0.33349118
H,0,6.6708978336,0.7920340993,-0.4293405263
H,0,6.0699083778,-0.7367492454,-2.2939627231
H,0,3.7260880551,-1.4885394492,-2.5755983902
H,0,2.57414221,0.7992017979,0.8719523987
H,0,4.9110879516,1.5602948613,1.1494924189
C,0,0.3003763107,-2.84773169,-0.119447239
O,0,-0.0874910106,-3.4607511823,1.0555117131
O,0,-0.0812689681,-3.3028834169,-1.2050264429
C,0,-0.9790765188,-4.5581620352,0.9069198856
H,0,-1.1750858943,-4.9231550806,1.9155757955
H,0,-1.9137627487,-4.2374022827,0.4357923955
H,0,-0.5310767045,-5.3512239471,0.3026156958

E-methyl cinnamate

/home/singletn/wittig/c28/full2XPS/methylcinnM062XPSPC
M
methyl cinnamate for Wittig
M062X/6-31+G**
E(RM062X) = -537.332221621

Zero-point correction= 0.178438 (Hartree/Particle)
Thermal correction to Energy= 0.189463
Thermal correction to Enthalpy= 0.190408
Thermal correction to Gibbs Free Energy= 0.139909
Sum of electronic and ZPE= -537.153783
Sum of electronic and thermal Energies= -537.142758
Sum of electronic and thermal Enthalpies= -537.141814
Sum of electronic and thermal Free Energies= -537.192312

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	118.890	40.271	106.283

C,0,0.1465456408,-0.5038989168,0.
C,0,-0.5057661361,0.7368686376,0.
C,0,-1.8968232921,0.81272114,0.
C,0,-2.655737143,-0.3561956439,0.
C,0,-2.0172582905,-1.5994991404,0.
C,0,-0.6293898654,-1.6746131884,0.
H,0,0.0867649114,1.6479064137,0.
H,0,-2.3859713398,1.7816467464,0.
H,0,-3.7398774768,-0.3025924609,0.
H,0,-2.6054003481,-2.5117479745,0.
H,0,-0.1485492194,-2.6480600384,0.
C,0,2.4101758058,-1.5995750457,0.
C,0,1.6142659837,-0.5206922457,0.
H,0,2.1021561761,0.4538249089,0.
H,0,2.0414117925,-2.6195699597,0.
C,0,3.8779570214,-1.4257795894,0.
O,0,4.5072286811,-2.6113137665,0.
O,0,4.4696840667,-0.3640730544,0.
C,0,5.9375105251,-2.5579483212,0.
H,0,6.2705496832,-3.593499572,0.
H,0,6.2956014134,-2.0388744648,-0.8912803112
H,0,6.2956014134,-2.0388744648,0.8912803112

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