

1 Electronic supplementary information to the paper

2 **New theoretical insight into the reaction kinetics of toluene and**
3 **hydroxyl radicals**

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52

53

54 **1) Table S1.** Structure and frequency of all stationary points shown on the toluene+OH PES

55 optimized by the B2PLYPD3/6-311++G(d,p) method.

56

57 C6H5CH3

58	C	-0.00763900	-1.19953600	1.20517200
59	C	-0.00763900	0.19581200	1.20217500
60	C	-0.00388100	0.91356100	0.00000000
61	C	-0.00763900	0.19581200	-1.20217500
62	C	-0.00763900	-1.19953600	-1.20517200
63	C	-0.00648200	-1.90320000	0.00000000
64	H	-0.01220200	-1.73580100	2.14733200
65	H	-0.01234000	0.73486900	2.14413000
66	H	-0.01234000	0.73486900	-2.14413000
67	H	-0.01220200	-1.73580100	-2.14733200
68	H	-0.00930500	-2.98687900	0.00000000
69	C	0.02927600	2.42117200	0.00000000
70	H	1.05986700	2.78965500	0.00000000
71	H	-0.46581000	2.82728400	-0.88435100
72	H	-0.46581000	2.82728400	0.88435100

73 Frequencies[1/cm]

74 44.69 202.96 341.60 398.43 447.41

75 526.70 537.82 634.09 722.96 800.02

76 840.70 882.53 915.15 936.50 967.28

77 977.87 1010.97 1019.50 1070.19 1137.99

78 1159.51 1191.28 1296.73 1310.74 1369.93

79 1417.20 1442.75 1454.09 1472.11 1565.98

80 1586.86 2927.97 2986.81 3009.30 3052.75

81 3054.42 3067.12 3075.29 3087.53

82

83 OH

84	O	0.00000000	0.00000000	0.10800700
85	H	0.00000000	0.00000000	-0.86405300

86 Frequencies[1/cm]

87 3614.32

88

89 OH...C6H5CH3 #pre-reaction complex

90	C	0.98053000	-0.41677600	0.00000300
91	C	0.26374200	-0.47554900	1.20263700
92	C	-1.12900000	-0.58244200	1.20565300
93	C	-1.83124600	-0.63613400	0.00000700
94	C	-1.12900000	-0.58246600	-1.20564000
95	C	0.26374300	-0.47557500	-1.20262800
96	H	0.80056000	-0.43321500	2.14440900
97	H	-1.66337000	-0.62475800	2.14756700
98	H	-2.91142300	-0.71752500	0.00000700
99	H	-1.66337100	-0.62480100	-2.14755300
100	H	0.80056000	-0.43326100	-2.14440200
101	C	2.47848900	-0.24830700	0.00000100
102	H	2.92678100	-0.70407000	0.88472600
103	H	2.92677900	-0.70407500	-0.88472200
104	H	2.74571400	0.81268200	-0.00000200
105	O	-0.36116300	2.76685000	-0.00002400
106	H	-0.45646600	1.79772300	-0.00003400

107 Frequencies[1/cm]

108	20.81	35.62	60.98	102.21	114.15
109	175.36	219.13	342.17	399.15	460.29
110	527.08	631.74	646.79	735.07	800.12
111	853.75	897.15	955.48	962.99	969.50
112	978.45	1010.64	1024.39	1070.20	1138.41
113	1160.14	1192.36	1295.95	1308.98	1370.17
114	1414.50	1443.95	1453.14	1471.03	1559.81
115	1582.95	2930.84	2991.98	3013.05	3058.03
116	3059.31	3072.02	3079.39	3091.32	3594.43

117

118 m-CH₃C₆H₄•

P1m

119	C	-0.25343300	-1.24974700	-0.00962600
120	C	1.12063000	-1.27682000	0.00330000
121	C	1.95220100	-0.18048800	0.00814000
122	C	1.31803200	1.07076900	0.00208400
123	C	-0.07510300	1.15684400	-0.00917700
124	C	-0.88065700	0.01164900	-0.01092400
125	H	3.03200900	-0.26461200	0.01382700
126	H	1.91641500	1.97551800	0.00091800
127	H	-0.54683600	2.13347500	-0.01759400
128	C	-2.38573500	0.11566100	0.00983300
129	H	-2.71946100	1.06725300	-0.40772900
130	H	-2.84460900	-0.69006400	-0.56654700
131	H	-2.76623800	0.04899600	1.03346600
132	H	-0.84688900	-2.15777400	-0.01812600

133 Frequencies[1/cm]

134	45.17	200.87	344.21	407.23	463.45
135	517.58	576.53	626.64	738.76	793.19

136	836.05	873.07	923.76	996.81	970.24
137	1017.51	1022.06	1060.18	1137.13	1173.96
138	1253.92	1276.21	1367.83	1384.65	1434.92
139	1441.41	1445.14	1513.69	1583.68	2929.90
140	2989.98	3012.02	3054.79	3060.06	3070.22
141	3083.44				
142					
143	H2O	#P			
144	O		0.00000000	0.00000000	0.11747400
145	H		0.00000000	0.75947900	-0.46989500
146	H		0.00000000	-0.75947900	-0.46989500
147	Frequencies[1/cm]				
148	1553.79	3699.35	3805.91		
149					
150	o-CH3C6H4•	#P1o			
151	C		0.14867000	-1.19274800	-0.00000100
152	C		-1.22413800	-1.23410100	-0.00000100
153	C		-1.89314700	0.00117300	0.00000300
154	C		-1.15453200	1.18376100	0.00000400
155	C		0.24221200	1.15341600	-0.00000100
156	C		0.94544000	-0.06409400	-0.00000200
157	H		-1.77397100	-2.16810700	0.00000000
158	H		-2.97702200	0.02887400	0.00000400
159	H		-1.66697400	2.13864500	0.00000600
160	H		0.80285000	2.08338700	0.00000200
161	C		2.45142200	-0.12345000	-0.00000200
162	H		2.87884500	0.88047600	-0.00004600
163	H		2.82035800	-0.65347300	0.88114100
164	H		2.82035100	-0.65354600	-0.88110400
165	Frequencies[1/cm]				
166	15.77	198.31	329.38	402.68	456.67
167	517.13	530.63	631.41	731.66	798.40
168	827.87	898.19	909.03	986.62	968.42
169	1008.80	1017.12	1093.50	1132.82	1184.06
170	1233.02	1288.52	1368.39	1391.00	1423.69
171	1436.09	1453.82	1524.91	1583.80	2936.16
172	2997.04	3014.24	3048.22	3061.97	3074.98
173	3085.53				
174					
175	p-CH3C6H4•	#P1p			
176	C		-0.13092100	1.20604100	-0.00869100
177	C		1.27190700	1.22137000	0.00276700
178	C		1.90400500	-0.00017400	0.00939800
179	C		1.27149500	-1.22163000	0.00271600
180	C		-0.13121100	-1.20591500	-0.00879500
181	C		-0.84250300	0.00021200	-0.01101100

182	H	1.81628900	-2.15837200	0.00207300	
183	H	-0.67249200	-2.14708300	-0.01797400	
184	C	-2.35158600	0.00011300	0.00950600	
185	H	-2.75315000	-0.87818200	-0.49955400	
186	H	-2.72979200	-0.01103200	1.03624300	
187	H	-2.75296000	0.88921700	-0.48047800	
188	H	-0.67190900	2.14735800	-0.01781800	
189	H	1.81690500	2.15799300	0.00217000	
190	Frequencies[1/cm]				
191	51.48	216.70	343.63	395.03	444.07
192	530.64	582.26	615.27	767.29	786.35
193	804.70	888.82	932.70	961.92	973.11
194	1016.78	1021.61	1072.79	1140.64	1185.65
195	1259.22	1285.76	1346.06	1371.89	1429.29
196	1443.45	1449.61	1546.28	1569.65	2929.45
197	2988.59	3010.86	3050.68	3050.92	3076.31
198	3078.08				
199					
200	TS _{abs-m}				
201	C	-1.31246000	-0.41849100	0.01082200	
202	C	-1.50905200	0.96848800	0.05567700	
203	C	-0.43405900	1.85843300	0.02272800	
204	C	0.87852100	1.37826800	-6.67E-021400	
205	C	1.05248400	0.00411000	-0.09929300	
206	C	0.00588600	-0.90158100	-0.06066200	
207	H	-2.52260600	1.35769800	0.12012900	
208	H	-0.61567500	2.92977900	0.06015900	
209	H	1.72584700	2.05701400	-0.07575800	
210	H	2.24578000	-0.46049100	-0.21722000	
211	H	0.19667500	-1.97153300	-0.08975100	
212	C	-2.48278000	-1.37496700	0.01371700	
213	H	-3.35545700	-0.93687500	0.50923000	
214	H	-2.78401000	-1.63537000	-1.00962900	
215	H	-2.23537800	-2.31055900	0.52650800	
216	O	3.34835000	-0.90256800	-0.01580800	
217	H	3.36677500	-0.89466900	0.96054400	
218	Frequencies[1/cm]				
219	-1263.99	49.43	82.01	99.58	108.27
220	203.32	338.00	357.71	422.35	466.97
221	524.13	557.71	644.34	741.77	770.72
222	855.45	860.48	887.81	931.90	1004.59
223	1010.42	1055.49	1058.85	1099.01	1125.31
224	1188.74	1218.87	1270.90	1318.77	1345.62
225	1423.09	1450.60	1498.37	1501.90	1509.93
226	1600.91	1637.56	3045.41	3108.02	3130.74
227	3177.03	3189.49	3193.89	3211.51	3783.29

228				
229	TS _{abs-o}			
230	C	-1.31174500	-0.41955200	0.01115400
231	C	-1.50972600	0.96596000	0.06143600
232	C	-0.43532800	1.85575500	0.02418400
233	C	0.87573700	1.37555800	-0.05560000
234	C	1.05353000	0.00136800	-0.11185400
235	C	0.00384400	-0.90271700	-0.06541600
236	H	-2.52069400	1.35351600	0.13003400
237	H	-0.61578500	2.92400600	0.06578700
238	H	1.72072800	2.05212900	-0.08316800
239	H	2.18564500	-0.43628900	-0.22681400
240	H	0.19384500	-1.96974700	-0.10026500
241	C	-2.48037900	-1.37337400	0.01489300
242	H	-3.33475500	-0.94653200	0.54344200
243	H	-2.80044900	-1.59955200	-1.00658700
244	H	-2.21770900	-2.31753100	0.49565300
245	O	3.35745800	-0.89830100	-0.00666300
246	H	3.35391400	-0.89158700	0.96243200

247 Frequencies[1/cm]

248	-1208.58	60.53	93.95	97.86	127.03
249	199.18	327.13	372.60	431.70	483.99
250	532.09	581.53	646.78	740.84	774.59
251	829.68	846.16	921.85	935.38	970.04
252	986.81	1005.74	1020.96	1049.26	1114.64
253	1138.48	1178.42	1211.77	1255.92	1295.87
254	1371.38	1409.63	1439.97	1444.60	1457.77
255	1543.34	1573.66	2932.36	2993.19	3026.92
256	3053.22	3067.96	3079.73	3089.68	3639.32

257

258	TS _{abs-p}			
259	C	-1.31174500	-0.41955200	0.01115400
260	C	-1.50972600	0.96596000	0.06143600
261	C	-0.43532800	1.85575500	0.02418400
262	C	0.87573700	1.37555800	-0.05560000
263	C	1.05353000	0.00136800	-0.11185400
264	C	0.00384400	-0.90271700	-0.06541600
265	H	-2.52069400	1.35351600	0.13003400
266	H	-0.61578500	2.92400600	0.06578700
267	H	1.72072800	2.05212900	-0.08316800
268	H	2.18564500	-0.43628900	-0.22681400
269	H	0.19384500	-1.96974700	-0.10026500
270	C	-2.48037900	-1.37337400	0.01489300
271	H	-3.33475500	-0.94653200	0.54344200
272	H	-2.80044900	-1.59955200	-1.00658700
273	H	-2.21770900	-2.31753100	0.49565300

274	O		3.35745800	-0.89830100	-0.00666300	
275	H		3.35391400	-0.89158700	0.96243200	
276	Frequencies[1/cm]					
277		-1297.65	43.32	77.79	86.76	118.23
278		218.15	344.20	374.22	398.27	443.13
279		567.43	591.73	627.13	754.08	791.85
280		821.76	822.87	908.30	945.54	967.52
281		982.11	1020.75	1032.33	1032.39	1091.07
282		1149.62	1187.01	1219.70	1278.39	1295.49
283		1365.88	1370.45	1443.19	1447.81	1462.49
284		1556.50	1563.74	2930.76	2990.73	3012.90
285		3056.85	3057.02	3084.51	3085.59	3641.84
286						
287	C6H5CH2•	#P2				
288	C		0.25231700	1.21362000	0.00000600	
289	C		-1.13207900	1.20859100	0.00001700	
290	C		-1.83606400	0.00000200	-0.00002900	
291	C		-1.13208300	-1.20859000	-0.00002600	
292	C		0.25231300	-1.21362000	-0.00003600	
293	C		0.98817300	-0.00000100	0.00001100	
294	H		0.79309900	2.15371800	0.00003900	
295	H		-1.67301500	2.14795900	0.00001200	
296	H		-2.91922800	0.00000200	-0.00001700	
297	H		-1.67302000	-2.14795700	-0.00006000	
298	H		0.79309500	-2.15371900	-0.00003600	
299	C		2.40133200	-0.00000200	0.00004900	
300	H		2.95780500	-0.92793000	0.00002300	
301	H		2.95780600	0.92792800	0.00008600	
302	Frequencies[1/cm]					
303		192.09	355.22	374.93	431.25	456.03
304		472.36	533.82	623.48	630.07	719.79
305		829.95	838.15	876.01	914.62	940.52
306		976.50	963.58	1009.32	1080.72	1133.11
307		1141.75	1232.11	1280.82	1305.32	1429.06
308		1440.71	1448.76	1546.36	1558.84	3047.04
309		3059.70	3062.05	3074.18	3079.56	3092.51
310		3146.51				
311						
312	TS _{abs-CH3}					
313	C		0.29824900	-0.00015600	0.55535900	
314	C		-0.37095900	1.20508500	0.29753800	
315	C		-1.67019700	1.20687600	-0.20752300	
316	C		-2.32409400	0.00016400	-0.46262300	
317	C		-1.67035300	-1.20670800	-0.20788200	
318	C		-0.37111200	-1.20523400	0.29717300	
319	H		0.13233500	2.14541000	0.49653000	

320	H	-2.17336700	2.14781800	-0.39770300	
321	H	-3.33502700	0.00028600	-0.85269400	
322	H	-2.17364200	-2.14753100	-0.39834000	
323	H	0.13206500	-2.14568200	0.49588200	
324	C	1.70121700	-0.00031000	1.06308700	
325	H	1.94873900	0.89581200	1.63325800	
326	H	1.94867400	-0.89666300	1.63292200	
327	H	2.44631700	-0.00016300	0.18343700	
328	O	3.14858400	0.00025500	-1.14261400	
329	H	2.32872700	0.00037400	-1.66315400	
330	Frequencies[1/cm]				
331	-1687.57	76.85	98.75	133.64	217.76
332	339.50	396.69	440.36	490.52	514.99
333	528.22	596.03	632.47	726.29	770.88
334	833.92	841.53	896.25	928.39	945.90
335	997.75	979.95	1012.40	1071.22	1072.80
336	1140.01	1160.47	1187.03	1200.93	1301.59
337	1309.49	1381.04	1423.02	1428.00	1468.18
338	1563.32	1580.02	2979.51	3056.35	3059.99
339	3062.63	3072.71	3081.15	3091.56	3633.74
340					
341					
342	C6H5OH				
343	C	0.24040500	1.21022500	-0.01434700	
344	C	-1.15490900	1.20699800	0.00591300	
345	C	-1.85625000	0.00030700	0.01602100	
346	C	-1.15540600	-1.20666300	0.00606000	
347	C	0.23991700	-1.21049000	-0.01396500	
348	C	0.93254700	-0.00029900	-0.00920900	
349	H	0.79975300	2.13770300	-0.03780300	
350	H	-1.69266800	2.14793200	0.00425000	
351	H	-2.93948400	0.00053700	0.02829300	
352	H	-1.69355000	-2.14737500	0.00464300	
353	H	0.79899500	-2.13812800	-0.03685700	
354	O	2.32049600	-0.00105500	-0.08827700	
355	H	2.68515900	0.00729800	0.80085400	
356	Frequencies[1/cm]				
357	156.12	222.96	405.31	409.85	453.28
358	529.68	533.30	628.39	739.04	823.15
359	830.30	882.52	913.59	936.76	978.39
360	1004.00	1051.70	1133.65	1136.74	1148.69
361	1225.40	1275.53	1307.53	1425.90	1469.04
362	1570.30	1579.22	3063.25	3071.71	3082.77
363	3088.27	3093.65	3709.39		
364					
365	CH3				

366	C	0.00000000	0.00000000	-0.00008100		
367	H	0.00000000	1.07906800	0.00016200		
368	H	-0.93450000	-0.53953400	0.00016200		
369	H	0.93450000	-0.53953400	0.00016200		
370	Frequencies[1/cm]					
371	513.14	1369.86	1369.86	3012.76	3190.07	3190.09
372						
373	ipso-HOC6H5CH3					
374	C	0.03666100	-1.24694500	0.01494200		
375	C	1.39748600	-1.22569600	-0.03284600		
376	C	2.11019800	-0.00000300	-0.07136700		
377	C	1.39748600	1.22569300	-0.03284100		
378	C	0.03666200	1.24695000	0.01495800		
379	C	-0.80174700	0.00000900	0.02675100		
380	H	-0.50761800	-2.18452300	0.05611300		
381	H	1.94977000	-2.15899900	-0.03381000		
382	H	3.19194200	0.00000100	-0.10777300		
383	H	1.94977800	2.15899100	-0.03380600		
384	H	-0.50758400	2.18454700	0.05615000		
385	C	-1.79326700	0.00000300	-1.14188200		
386	H	-2.42709900	0.88757200	-1.08419800		
387	H	-1.26004800	0.00001600	-2.09355000		
388	H	-2.42708400	-0.88757500	-1.08420000		
389	O	-1.64992300	0.00000200	1.21042100		
390	H	-1.06355300	-0.00011200	1.97541100		
391	Frequencies[1/cm]					
392	82.89	228.40	256.73	339.32	342.33	
393	386.17	393.06	454.57	536.45	582.65	
394	586.16	692.09	733.83	772.25	819.87	
395	898.42	961.48	966.98	970.32	980.93	
396	994.23	1020.80	1056.54	1083.45	1099.19	
397	1158.20	1250.17	1272.03	1278.69	1350.94	
398	1351.56	1401.96	1436.99	1445.50	1497.81	
399	1560.77	2935.53	3012.38	3022.72	3056.44	
400	3057.95	3074.17	3075.36	3096.04	3673.71	
401						
402	TS _{elim-ipso}					
403	C	1.39903800	1.21170600	-0.08840500		
404	C	0.02710300	1.21406900	-0.26806800		
405	C	-0.71588100	-0.00042000	-0.30898500		
406	C	0.02735300	-1.21470400	-0.26617000		
407	C	1.39926500	-1.21181400	-0.08659200		
408	C	2.09366800	0.00009700	0.00260400		
409	H	1.93789900	2.15004300	-0.03114500		
410	H	-0.51321200	-2.15117500	-0.34037500		
411	H	1.93833000	-2.14995300	-0.02800700		

412	H	3.16876200	0.00030200	0.13786800
413	O	-1.34603100	0.00187400	1.59411600
414	H	-0.50542900	0.00251800	2.07618900
415	H	-0.51365500	2.15032200	-0.34361900
416	C	-2.11935100	-0.00111900	-0.85695500
417	H	-2.65971300	0.88340700	-0.52045800
418	H	-2.09198900	-0.00296700	-1.95048100
419	H	-2.65991400	-0.88438600	-0.51748300

420 Frequencies[1/cm]

421	-689.5	135.90	180.55	203.45	245.74
422	282.34	398.23	421.77	435.60	520.34
423	612.31	622.99	665.14	672.51	717.01
424	793.18	809.75	867.02	974.17	982.76
425	988.69	974.28	1000.99	1057.84	1125.85
426	1138.32	1146.64	1201.95	1286.75	1317.97
427	1382.98	1383.55	1436.12	1451.93	1536.98
428	1565.81	2963.06	3052.86	3067.37	3074.88
429	3089.86	3096.07	3107.00	3126.80	3704.19

430

431 TS_{add-ipso}

432	C	1.39903800	1.21170600	-0.08840500
433	C	0.02710300	1.21406900	-0.26806800
434	C	-0.71588100	-0.00042000	-0.30898500
435	C	0.02735300	-1.21470400	-0.26617000
436	C	1.39926500	-1.21181400	-0.08659200
437	C	2.09366800	0.00009700	0.00260400
438	H	1.93789900	2.15004300	-0.03114500
439	H	-0.51321200	-2.15117500	-0.34037500
440	H	1.93833000	-2.14995300	-0.02800700
441	H	3.16876200	0.00030200	0.13786800
442	O	-1.34603100	0.00187400	1.59411600
443	H	-0.50542900	0.00251800	2.07618900
444	H	-0.51365500	2.15032200	-0.34361900
445	C	-2.11935100	-0.00111900	-0.85695500
446	H	-2.65971300	0.88340700	-0.52045800
447	H	-2.09198900	-0.00296700	-1.95048100
448	H	-2.65991400	-0.88438600	-0.51748300

449 Frequencies[1/cm]

450	-411.6	106.81	146.65	171.39	218.37
451	265.42	338.04	407.51	408.71	529.67
452	622.56	646.63	739.16	785.77	805.41
453	839.48	920.97	973.90	979.14	968.14
454	971.61	1007.68	1016.53	1080.70	1129.01
455	1156.24	1192.19	1268.01	1299.69	1367.04
456	1407.06	1443.02	1447.98	1450.60	1539.91
457	1567.93	2938.29	3009.51	3036.00	3064.73

458 3070.54 3079.13 3085.37 3093.07 3634.88
459
460 m-HOC6CH4CH3
461 C 0.03828900 -0.98332300 -0.01103200
462 C -1.21419400 -0.36747800 0.00155700
463 C -1.31683100 1.02422600 0.00783400
464 C -0.15108900 1.79118800 0.00251200
465 C 1.10089000 1.18051600 -0.00905900
466 C 1.20539600 -0.21732100 -0.01208300
467 H -2.29153300 1.50193700 0.01367200
468 H -0.22618900 2.87251300 0.00277400
469 H 1.99944500 1.78707000 -0.01692600
470 O -2.31206400 -1.18783600 0.00152300
471 H -3.10835700 -0.64861900 0.00128900
472 H 0.08363700 -2.06635100 -0.01979200
473 C 2.55658700 -0.88788300 0.01051600
474 H 2.91140200 -1.01152500 1.03818800
475 H 2.51470600 -1.87797900 -0.44695700
476 H 3.29911700 -0.29390900 -0.52590100
477 Frequencies[1/cm]
478 50.00 198.61 222.19 244.56 295.05
479 427.33 445.22 521.41 538.70 546.11
480 558.40 741.48 743.99 834.52 847.66
481 912.44 947.09 974.50 988.51 1018.59
482 1071.93 1134.08 1143.48 1165.80 1255.31
483 1287.04 1319.62 1369.79 1428.64 1443.52
484 1462.20 1467.25 1572.12 1598.85 2929.96
485 2989.47 3012.20 3051.32 3063.99 3075.65
486 3081.82 3706.83
487
488 o-HOC6CH4CH3
489 C -0.58741200 -0.62124200 -0.00003100
490 C -0.39709600 0.76973300 -0.00000600
491 C 0.88413500 1.32167300 0.00001700
492 C 1.99797900 0.48646800 0.00001400
493 C 1.83489000 -0.89976800 -0.00004700
494 C 0.54852700 -1.43744100 -0.00007500
495 H 0.98536700 2.40000700 0.00003400
496 H 2.99111300 0.91992900 0.00003400
497 H 2.69768500 -1.55439500 -0.00007200
498 H 0.41480900 -2.51417900 -0.00013200
499 O -1.44958500 1.64859900 0.00011500
500 H -2.27720700 1.15968200 -0.00069600
501 C -1.97801700 -1.20387200 0.00007400
502 H -2.54736500 -0.90051000 0.88608300
503 H -2.54800600 -0.89932200 -0.88512400

504	H		-1.93774900	-2.29330800	-0.00072200
505	Frequencies[1/cm]				
506	94.00	149.91	186.29	259.01	301.30
507	424.19	434.14	512.90	529.95	581.51
508	591.00	746.70	758.39	835.09	850.50
509	903.58	918.78	963.53	1011.53	1018.60
510	1082.58	1134.16	1146.18	1191.56	1239.63
511	1281.99	1328.43	1368.32	1428.31	1438.52
512	1462.05	1470.31	1568.76	1599.29	2908.11
513	2955.21	3014.00	3057.11	3070.55	3085.32
514	3093.61	3713.37			
515					
516	p-HOC6CH4CH3				
517	C		0.72793300	-1.21888100	-0.00140500
518	C		1.43852100	-0.01733900	0.00327400
519	C		0.74887800	1.19466900	-0.00111900
520	C		-0.64762000	1.19870300	-0.00908100
521	C		-1.37951600	0.00884900	-0.00977600
522	C		-0.66342400	-1.19615200	-0.00894900
523	H		1.29558600	2.13295400	-0.00313800
524	H		-1.17062800	2.14924600	-0.01586800
525	O		2.80767300	-0.09363200	0.00788400
526	H		3.17287700	0.79589800	0.00413700
527	H		1.27506500	-2.15356700	-0.00346800
528	H		-1.20434700	-2.13691500	-0.01568900
529	C		-2.88816700	0.01551700	0.01221100
530	H		-3.27078800	-0.15261500	1.02360800
531	H		-3.28284400	0.97204200	-0.33574400
532	H		-3.29593400	-0.77018500	-0.62783500
533	Frequencies[1/cm]				
534	44.94	139.99	242.46	305.27	317.85
535	405.67	425.02	465.80	492.40	539.38
536	655.70	747.07	781.78	814.56	851.84
537	874.72	927.98	1010.00	992.28	1019.39
538	1087.49	1151.12	1152.28	1192.89	1233.22
539	1291.99	1322.85	1371.40	1404.16	1441.86
540	1454.47	1491.65	1576.32	1598.79	2926.43
541	2983.71	3006.69	3045.99	3057.34	3065.82
542	3089.47	3708.61			
543					
544	m-HOC6CH5CH3				
545	C		0.14099700	-0.97869900	-0.32239800
546	C		1.21099700	-0.18524500	-0.03819900
547	C		1.01290600	1.21583700	0.15518800
548	C		-0.28100600	1.78068600	0.06851000
549	C		-1.37041600	1.01057500	-0.21359600

550	C	-1.26403800	-0.46815400	-0.42165900
551	H	1.86322500	1.84760900	0.38399600
552	H	-0.40260700	2.84570600	0.23380800
553	H	-2.36371900	1.44077000	-0.26934000
554	C	2.60530400	-0.74771900	0.08222800
555	H	2.61160600	-1.82600200	-0.08195000
556	H	3.27417400	-0.28656500	-0.64966000
557	H	3.01997100	-0.54980900	1.07447700
558	O	-2.13809300	-1.18196200	0.49153600
559	H	-1.81337900	-0.99991100	1.38073800
560	H	-1.68362200	-0.73293100	-1.40072400
561	H	0.27063700	-2.04685600	-0.46407300

562 Frequencies[1/cm]

563	91.89	121.80	175.96	289.74	330.34
564	371.13	435.12	466.20	495.93	535.98
565	619.64	699.25	762.67	786.67	847.46
566	897.67	950.54	961.86	986.66	989.91
567	1024.75	1040.74	1084.71	1133.73	1161.11
568	1175.99	1272.16	1282.10	1324.70	1344.54
569	1369.46	1389.61	1437.26	1449.26	1515.76
570	1577.37	2898.68	2929.59	2986.09	3014.93
571	3058.36	3060.12	3075.37	3084.80	3670.76

572 T_{Selim-m}

573	C	-0.05072100	-0.97334300	-0.01973500
574	C	-1.22376700	-0.22700800	-0.01481400
575	C	-1.13291700	1.17672500	-0.00966100
576	C	0.11461100	1.81011600	-0.03017800
577	C	1.28954600	1.07397300	-0.02420500
578	C	1.22096500	-0.34003500	0.08041800
579	H	-2.04231800	1.77201500	-0.01640800
580	H	0.16514000	2.89520600	-0.06675600
581	H	2.26645400	1.54472200	-0.05273600
582	C	-2.57297900	-0.90803600	-0.01993900
583	H	-3.04075900	-0.86432200	0.97231300
584	H	-3.26148700	-0.42565600	-0.72290500
585	H	-2.49022500	-1.96356100	-0.29816800
586	O	2.38642900	-1.02527200	-0.17468600
587	H	2.24484800	-1.96376100	0.02515200
588	H	1.29299000	-0.40571800	1.82435600
589	H	-0.09450600	-2.06110000	-0.03868200

590 Frequencies[1/cm]

591	-1207.49	59.18	201.96	207.01	274.54
592	296.67	416.91	453.07	504.34	518.52
593	525.68	583.48	677.41	693.96	752.96
594	802.40	858.55	913.03	950.31	983.14
595	975.51	990.57	1025.98	1069.44	1130.44

596	1144.81	1161.71	1238.16	1287.10	1302.23	
597	1370.47	1405.74	1442.05	1453.30	1475.50	
598	1567.40	1585.66	2932.14	2992.28	3013.28	
599	3051.30	3064.63	3080.30	3101.60	3703.68	
600						
601	TS _{add-m}					
602	C		-1.19598000	-0.12495800	-0.06173800	
603	C		-0.89788600	1.20197800	0.29864400	
604	C		0.38518000	1.72980200	0.13073700	
605	C		1.39686600	0.94537900	-0.39842100	
606	C		1.14714500	-0.41725200	-0.70284300	
607	C		-0.18186600	-0.90615000	-0.59157500	
608	H		-1.68379700	1.82844800	0.70796000	
609	H		0.58112700	2.76118300	0.39933800	
610	H		2.39389000	1.34339000	-0.53688300	
611	H		1.85243700	-0.95737100	-1.31838900	
612	H		-0.38269200	-1.93058600	-0.88288200	
613	C		-2.59072600	-0.66860500	0.12367400	
614	H		-3.33791800	0.01944800	-0.27869300	
615	H		-2.70732800	-1.63015500	-0.37820100	
616	H		-2.81465900	-0.81493000	1.18419500	
617	O		2.02555500	-1.28789100	0.84403100	
618	H		1.51810300	-0.87746300	1.56044800	
619	Frequencies[1/cm]					
620		-449.63	52.35	103.68	133.30	184.01
621		220.51	340.88	393.34	463.09	519.31
622		622.62	655.47	773.11	786.64	836.42
623		885.99	912.04	984.81	997.30	966.60
624		991.57	1019.42	1028.26	1065.89	1137.22
625		1150.17	1189.10	1270.61	1303.34	1370.39
626		1404.16	1440.53	1450.88	1458.91	1543.19
627		1573.47	2931.63	2989.78	3014.34	3058.05
628		3074.73	3078.08	3093.80	3105.29	3632.07
629						
630	o-HOC6CH5CH3					
631	C		0.72707500	-0.56931700	0.11837200	
632	C		-0.23304100	-1.49219200	-0.18886700	
633	C		-1.60934300	-1.16231400	-0.22480300	
634	C		-2.02716900	0.15946600	0.07390800	
635	C		-1.11888800	1.12448100	0.38666100	
636	C		0.35577700	0.86978400	0.37224100	
637	H		0.06630600	-2.51384400	-0.40152900	
638	H		-2.34081200	-1.91973100	-0.47590700	
639	H		-3.08484700	0.39817000	0.05694200	
640	H		-1.43232400	2.13779500	0.61109000	
641	C		2.18409800	-0.90674900	0.19889500	

642	H	2.56334100	-0.72514800	1.21144700	
643	H	2.36617300	-1.95252200	-0.05359700	
644	H	2.76721900	-0.27131000	-0.47271800	
645	O	1.00495600	1.74222300	-0.59603100	
646	H	0.57819900	1.57286500	-1.44396200	
647	H	0.80604800	1.19698700	1.31803800	
648	Frequencies[1/cm]				
649	77.96	149.76	220.62	267.37	323.45
650	377.09	401.02	485.87	507.54	567.10
651	632.51	697.17	766.85	795.22	876.05
652	910.95	962.75	972.28	997.92	984.75
653	1010.78	1025.34	1085.97	1138.84	1162.89
654	1175.05	1263.16	1294.47	1342.65	1364.06
655	1374.74	1383.84	1426.23	1444.83	1504.05
656	1569.86	2902.16	2914.34	2972.35	3012.16
657	3051.22	3060.36	3078.53	3093.82	3667.04
658					
659	TS _{elim-m}				
660	C	0.57534600	-0.66804400	-0.02000100	
661	C	-0.57107100	-1.45073500	-0.01224800	
662	C	-1.84920600	-0.88642800	-0.00578300	
663	C	-1.99427800	0.50136700	-0.03766100	
664	C	-0.87381400	1.31428600	-0.05503100	
665	C	0.41333500	0.74135900	0.08055000	
666	H	-0.46295400	-2.52986600	-0.03341900	
667	H	-2.72330900	-1.52576600	-0.00002100	
668	H	-2.98130500	0.94627900	-0.07947800	
669	H	-0.97040700	2.39450500	-0.08857200	
670	C	1.95781800	-1.24791000	-0.02879400	
671	H	2.53690000	-0.86961700	-0.87442800	
672	H	2.49775400	-0.96016600	0.87872200	
673	H	1.91960800	-2.33642500	-0.08480100	
674	O	1.55225300	1.48958600	-0.13565200	
675	H	1.36508400	2.41059200	0.06877600	
676	H	0.45181400	0.73040100	1.77224700	
677	Frequencies[1/cm]				
678	-1156.69	152.38	163.32	249.66	274.75
679	290.19	408.53	445.67	495.21	536.66
680	565.02	582.06	673.28	717.45	756.64
681	806.77	848.00	880.92	950.43	981.69
682	973.56	1027.50	1033.31	1079.50	1136.20
683	1147.73	1194.93	1215.66	1280.65	1300.48
684	1368.76	1411.86	1429.87	1454.07	1474.94
685	1565.42	1588.92	2928.12	2985.80	3018.19
686	3057.53	3062.49	3077.57	3092.48	3706.17
687					

688	TS _{add-o}				
689	C	-0.15229700	-1.44479400	0.31625700	
690	C	0.75283600	-0.53218700	-0.20946900	
691	C	0.27056900	0.74043100	-0.63358700	
692	C	-1.12431700	0.99162400	-0.64527000	
693	C	-2.00612400	0.06602400	-0.11425200	
694	C	-1.51962900	-1.15512900	0.36657900	
695	H	0.20609500	-2.40216100	0.67823600	
696	H	0.91769200	1.36492800	-1.23496500	
697	H	-1.48198700	1.93856300	-1.03034800	
698	H	-3.06882600	0.27498000	-0.08959600	
699	H	-2.20740600	-1.88583400	0.77632500	
700	C	2.22464800	-0.81304400	-0.27745300	
701	H	2.76195900	-0.07939600	0.32911800	
702	H	2.45820800	-1.81431400	0.08697500	
703	H	2.59174700	-0.72543000	-1.30408100	
704	O	0.86801000	1.83247500	0.92487500	
705	H	0.20432300	1.55131100	1.57250600	
706	Frequencies[1/cm]				
707		-406.00	109.79	129.26	132.58
708		208.50	344.19	395.59	476.62
709		625.48	681.02	753.95	792.87
710		875.91	949.53	980.41	991.43
711		998.24	1013.24	1025.27	1062.32
712		1153.94	1186.92	1277.38	1301.91
713		1403.65	1433.81	1452.92	1469.41
714		1572.15	2929.38	2989.36	3016.66
715		3072.28	3081.24	3087.44	3096.59
716					
717	p-HOC6CH5CH3				
718	C	0.70827100	1.24600900	-0.30063200	
719	C	-0.63855300	1.21997800	-0.10413700	
720	C	-1.36430000	0.00032000	-0.00082100	
721	C	-0.63866600	-1.21968600	-0.10425800	
722	C	0.70800700	-1.24599300	-0.30064900	
723	C	1.53505900	-0.00006800	-0.37954300	
724	H	-1.18469100	-2.15502600	-0.02613300	
725	H	1.24027100	-2.18763800	-0.37457500	
726	O	2.56611500	-0.00021400	0.64458400	
727	H	2.10928400	-0.00002200	1.49352900	
728	H	2.12595000	-0.00014600	-1.30348800	
729	H	1.24070600	2.18755300	-0.37455300	
730	H	-1.18433700	2.15543700	-0.02593900	
731	C	-2.84079900	-0.00008900	0.26276900	
732	H	-3.32083100	-0.88095900	-0.16944000	
733	H	-3.05106300	-0.01072200	1.33947900	

734	H		-3.31831500	0.89040200	-0.15192000
735	Frequencies[1/cm]				
736	15.74	72.37	214.82	268.57	330.97
737	361.72	395.45	453.35	492.38	600.78
738	626.33	748.09	762.53	766.19	871.29
739	953.40	960.88	968.20	986.61	971.90
740	996.28	1019.91	1127.94	1150.12	1177.04
741	1205.34	1223.74	1295.01	1344.94	1365.69
742	1366.55	1419.02	1434.20	1437.59	1485.01
743	1571.82	2905.71	2908.24	2968.89	3005.24
744	3047.94	3048.96	3076.11	3078.07	3669.76
745					
746	TS _{elim-p}				
747	C		0.69740100	-1.22292600	-0.03502200
748	C		-0.68505400	-1.19954000	-0.03932500
749	C		-1.40195500	0.00567400	-0.02000200
750	C		-0.67362900	1.20190200	-0.04259800
751	C		0.71062700	1.20612300	-0.05191700
752	C		1.41917400	-0.01294000	0.08290300
753	H		-1.20475800	2.14685600	-0.08732100
754	H		1.26080600	2.14042400	-0.08507200
755	O		2.77762500	-0.08966600	-0.14790800
756	H		3.19031600	0.73067600	0.13826000
757	H		1.46461900	0.00862900	1.77073400
758	H		1.25091600	-2.15301500	-0.05705100
759	H		-1.22766500	-2.13812000	-0.08112700
760	C		-2.90808000	0.01209500	0.01956800
761	H		-3.32062200	-0.84569100	-0.51582700
762	H		-3.27440100	-0.03614000	1.04992200
763	H		-3.31110500	0.92138900	-0.43089100
764	Frequencies[1/cm]				
765	-1196.85	55.86	131.99	250.17	303.19
766	314.70	393.25	427.27	448.62	510.65
767	531.54	651.35	656.58	709.66	758.72
768	823.29	837.48	881.46	965.16	976.72
769	972.21	988.36	1024.64	1092.88	1142.86
770	1153.44	1198.79	1217.56	1268.16	1310.57
771	1370.56	1412.85	1441.40	1451.98	1473.50
772	1553.42	1597.62	2925.43	2983.17	3008.09
773	3055.98	3061.47	3072.62	3096.32	3705.05
774					
775	TS _{add-p}				
776	C		1.44477800	-0.00000400	-0.62586600
777	C		0.72190000	1.21567800	-0.51618000
778	C		-0.61750100	1.20791700	-0.17197100
779	C		-1.31141800	0.00000500	0.01072000

780	C	-0.61751200	-1.20791500	-0.17197300
781	C	0.72188700	-1.21568100	-0.51617400
782	H	2.41148300	-0.00001100	-1.10829300
783	H	1.24533900	2.15259400	-0.66021300
784	H	-1.14911000	2.14660700	-0.05798800
785	H	-1.14912800	-2.14660200	-0.05799100
786	H	1.24532200	-2.15260000	-0.66020500
787	C	-2.76125500	0.00000500	0.41397200
788	H	-2.85895300	-0.00020900	1.50451400
789	H	-3.27613900	0.88608800	0.03807300
790	H	-3.27622900	-0.88588100	0.03772500
791	O	2.45234200	-0.00000400	1.09048700
792	H	1.70341400	0.00001800	1.70530700

793 Frequencies[1/cm]

794	-427.07	48.02	102.89	124.64	179.49
795	225.81	342.81	406.48	439.23	525.75
796	625.89	679.96	778.49	800.74	819.32
797	841.16	956.33	981.58	994.36	966.87
798	991.07	1015.05	1020.70	1064.71	1135.84
799	1162.07	1200.68	1264.61	1310.03	1368.44
800	1421.19	1441.87	1449.57	1452.36	1530.58
801	1575.81	2926.50	2986.53	3014.14	3061.52
802	3061.82	3088.38	3091.44	3108.45	3633.94

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805 **2). Table S2.** T1 diagnostic values of stationary points.

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species	T1 value	species	T1 value	807
toluene	0.0100	Tsadd-p	0.0373	808
OH	0.0070	ipso-OHC6H5CH3	0.0293	809
TSabs-m	0.0202	m-OHC6H5CH3	0.0292	810
TSabs-o	0.0200	o-OHC6H5CH3	0.0293	811
TSabs-p	0.0200	p-OHC6H5CH3	0.0295	812
TSabs-CH3	0.0165	TSelimipso	0.0351	813
m-CH3C6H4	0.0427	C6H5OH	0.0106	814
o-CH3C6H4	0.0427	CH3	0.0079	815
p-CH3C6H4	0.0429	TSelimm	0.0350	816
C6H5CH2	0.0374	TSelimo	0.0351	817
H2O	0.0065	Tselimp	0.0352	818
Tsaddipso	0.0374	mOHC6H4CH3	0.0113	819
Tsadd-m	0.0370	oOHC6H4CH3	0.0110	820
Tsadd-o	0.0373	pOHC6H4CH3	0.0108	821

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825 **3).** Detailed information($K(T)$, k_{diss} , f_i) by particle-in-the-box approximation from Multiwell
 826 Package
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Table S3. Equilibrium constants $K(T)$, for the association of the OH radical and toluene into the pre-reaction complex, unimolecular reaction rates for dissociation of the pre-reaction complex k_{diss} , and relative adduct populations f_i (summed for all adducts), calculated with harmonic oscillator and particle-in-the-box models applied to the relative translation of OH radical and toluene in the pre-reaction complex.

T(K)	$k_{\text{diss}}(\text{s}^{-1})$		$K(\text{cm}^3\text{molecule}^{-1})$		f_i		ratio
	Particle in the box	Harmonic oscillator	Particle in the box	Harmonic oscillator	Particle in the box	Harmonic oscillator	$k_{\text{total_box}}/\text{harmo}$
210	2.26E+12	2.94E+12	1.84E-21	3.45E-21	7.08E-04	2.25E-04	1.29
230	2.30E+12	2.99E+12	8.67E-22	1.69E-21	7.78E-04	2.43E-04	1.26
250	2.33E+12	3.04E+12	4.66E-22	9.43E-22	8.46E-04	2.64E-04	1.21
277	2.36E+12	3.08E+12	2.36E-22	4.98E-22	9.32E-04	2.82E-04	1.20
300	2.40E+12	3.13E+12	1.47E-22	3.21E-22	1.06E-03	3.13E-04	1.19
350	2.46E+12	3.21E+12	6.70E-23	1.56E-22	1.29E-03	3.70E-04	1.15
400	2.51E+12	3.28E+12	3.83E-23	9.47E-23	1.54E-03	4.20E-04	1.14
450	2.55E+12	3.34E+12	2.54E-23	6.61E-23	1.81E-03	4.78E-04	1.11
500	2.59E+12	3.40E+12	1.86E-23	5.08E-23	2.08E-03	5.34E-04	1.08
550	2.63E+12	3.45E+12	1.47E-23	4.19E-23	2.36E-03	5.82E-04	1.08
600	2.66E+12	3.49E+12	1.22E-23	3.62E-23	2.64E-03	6.33E-04	1.07
650	2.69E+12	3.53E+12	1.06E-23	3.26E-23	2.90E-03	6.71E-04	1.07
700	2.72E+12	3.56E+12	9.46E-24	3.01E-23	3.15E-03	7.10E-04	1.07
750	2.74E+12	3.60E+12	8.65E-24	2.84E-23	3.42E-03	7.44E-04	1.07
800	2.76E+12	3.63E+12	8.07E-24	2.73E-23	3.67E-03	7.77E-04	1.06
850	2.78E+12	3.65E+12	7.64E-24	2.66E-23	3.91E-03	8.16E-04	1.05
900	2.80E+12	3.68E+12	7.32E-24	2.62E-23	4.16E-03	8.49E-04	1.04
950	2.82E+12	3.70E+12	7.09E-24	2.60E-23	4.39E-03	8.75E-04	1.04
1000	2.83E+12	3.72E+12	6.92E-24	2.60E-23	4.65E-03	9.02E-04	1.05

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830 **4).** **Table S4.** The relative adduct population calculated from Multiwell package. The
 831 uncertainties come from noninfinite number of Monte-Carlo trials.

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T	$f_i(\text{relative adduct populations})$ calculated by particle-in-the-box model				
	ortho-adduct	ipso-adduct	para-adduct	meta-adduct	benzyl radical + H ₂ O
210	4.81E-04	6.69E-05	7.34E-05	7.75E-05	9.92E-06
230	5.08E-04	7.13E-05	8.68E-05	9.92E-05	1.26E-05
250	5.34E-04	7.85E-05	1.02E-04	1.16E-04	1.57E-05
277	5.72E-04	8.31E-05	1.17E-04	1.39E-04	2.03E-05
300	6.16E-04	9.43E-05	1.43E-04	1.77E-04	2.70E-05
350	6.95E-04	1.13E-04	1.92E-04	2.49E-04	4.17E-05

400	7.71E-04	1.32E-04	2.42E-04	3.37E-04	6.11E-05
450	8.43E-04	1.52E-04	2.95E-04	4.37E-04	8.23E-05
500	9.12E-04	1.68E-04	3.54E-04	5.36E-04	1.08E-04
550	9.74E-04	1.85E-04	4.14E-04	6.46E-04	1.38E-04
600	1.03E-03	2.02E-04	4.70E-04	7.56E-04	1.73E-04
650	1.08E-03	2.20E-04	5.27E-04	8.59E-04	2.09E-04
700	1.12E-03	2.34E-04	5.84E-04	9.69E-04	2.45E-04
750	1.18E-03	2.49E-04	6.39E-04	1.07E-03	2.83E-04
800	1.22E-03	2.61E-04	6.89E-04	1.17E-03	3.32E-04
850	1.25E-03	2.76E-04	7.40E-04	1.27E-03	3.75E-04
900	1.29E-03	2.83E-04	7.87E-04	1.37E-03	4.25E-04
950	1.31E-03	2.94E-04	8.36E-04	1.47E-03	4.75E-04
1000	1.33E-03	3.07E-04	8.92E-04	1.61E-03	5.16E-04
fi(relative adduct populations)					
calculated by harmonic oscillator model					
210	1.53E-04	2.05E-05	2.34E-05	2.50E-05	3.04E-06
230	1.60E-04	2.22E-05	2.70E-05	2.92E-05	3.96E-06
250	1.69E-04	2.39E-05	3.17E-05	3.46E-05	4.55E-06
277	1.76E-04	2.46E-05	3.42E-05	4.09E-05	5.85E-06
300	1.83E-04	2.84E-05	4.23E-05	5.13E-05	7.89E-06
350	2.03E-04	3.24E-05	5.33E-05	6.95E-05	1.17E-05
400	2.11E-04	3.57E-05	6.57E-05	9.16E-05	1.62E-05
450	2.25E-04	3.99E-05	7.82E-05	1.13E-04	2.13E-05
500	2.36E-04	4.26E-05	9.01E-05	1.37E-04	2.77E-05
550	2.41E-04	4.66E-05	1.03E-04	1.58E-04	3.38E-05
600	2.51E-04	4.89E-05	1.14E-04	1.79E-04	4.03E-05
650	2.57E-04	5.09E-05	1.22E-04	1.95E-04	4.73E-05
700	2.60E-04	5.27E-05	1.28E-04	2.16E-04	5.33E-05
750	2.58E-04	5.38E-05	1.39E-04	2.32E-04	6.22E-05
800	2.57E-04	5.53E-05	1.46E-04	2.49E-04	6.94E-05
850	2.62E-04	5.68E-05	1.51E-04	2.67E-04	7.91E-05
900	2.65E-04	5.85E-05	1.60E-04	2.78E-04	8.77E-05
950	2.64E-04	5.95E-05	1.66E-04	2.93E-04	9.30E-05
1000	2.69E-04	6.18E-05	1.67E-04	3.00E-04	1.04E-04

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835 **5). Table S5.** The stochastic uncertainties resulting from noninfinite number of Monte-Carlo836 trials. The final uncertainties were calculated by $\sigma = \sqrt{\frac{f_i(1-f_i)}{N_{MC}}}$, where N_{MC} is number of Monte-

837 Carlo trials (1E8). The ortho and meta adducts populations are counted in twice, as there are

838 two ortho and meta positions on toluene.

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σ (stochastic uncertainties)

calculated by particle-in-the-box model					
T	ortho-adduct	ipso-adduct	para-adduct	meta-adduct	benzyl radical + H ₂ O
210	2.19E-06	8.18E-07	8.57E-07	8.80E-07	3.15E-07
230	2.25E-06	8.44E-07	9.31E-07	9.96E-07	3.55E-07
250	2.31E-06	8.86E-07	1.01E-06	1.08E-06	3.96E-07
277	2.39E-06	9.12E-07	1.08E-06	1.18E-06	4.51E-07
300	2.48E-06	9.71E-07	1.20E-06	1.33E-06	5.20E-07
350	2.64E-06	1.06E-06	1.38E-06	1.58E-06	6.46E-07
400	2.78E-06	1.15E-06	1.55E-06	1.84E-06	7.82E-07
450	2.90E-06	1.23E-06	1.72E-06	2.09E-06	9.07E-07
500	3.02E-06	1.30E-06	1.88E-06	2.31E-06	1.04E-06
550	3.12E-06	1.36E-06	2.04E-06	2.54E-06	1.17E-06
600	3.21E-06	1.42E-06	2.17E-06	2.75E-06	1.32E-06
650	3.29E-06	1.48E-06	2.30E-06	2.93E-06	1.45E-06
700	3.35E-06	1.53E-06	2.41E-06	3.11E-06	1.57E-06
750	3.43E-06	1.58E-06	2.53E-06	3.28E-06	1.68E-06
800	3.49E-06	1.62E-06	2.62E-06	3.42E-06	1.82E-06
850	3.54E-06	1.66E-06	2.72E-06	3.56E-06	1.94E-06
900	3.59E-06	1.68E-06	2.80E-06	3.70E-06	2.06E-06
950	3.62E-06	1.72E-06	2.89E-06	3.84E-06	2.18E-06
1000	3.64E-06	1.75E-06	2.99E-06	4.00E-06	2.27E-06
σ (stochastic uncertainties)					
calculated by harmonic oscillator model					
210	1.24E-06	4.52E-07	4.83E-07	5.00E-07	1.74E-07
230	1.27E-06	4.72E-07	5.20E-07	5.40E-07	1.99E-07
250	1.30E-06	4.89E-07	5.63E-07	5.88E-07	2.13E-07
277	1.33E-06	4.96E-07	5.84E-07	6.39E-07	2.42E-07
300	1.35E-06	5.33E-07	6.51E-07	7.16E-07	2.81E-07
350	1.43E-06	5.69E-07	7.30E-07	8.34E-07	3.42E-07
400	1.45E-06	5.98E-07	8.10E-07	9.57E-07	4.03E-07
450	1.50E-06	6.32E-07	8.84E-07	1.06E-06	4.62E-07
500	1.54E-06	6.53E-07	9.49E-07	1.17E-06	5.26E-07
550	1.55E-06	6.83E-07	1.01E-06	1.26E-06	5.82E-07
600	1.58E-06	7.00E-07	1.07E-06	1.34E-06	6.34E-07
650	1.60E-06	7.14E-07	1.10E-06	1.39E-06	6.88E-07
700	1.61E-06	7.26E-07	1.13E-06	1.47E-06	7.30E-07
750	1.61E-06	7.33E-07	1.18E-06	1.52E-06	7.88E-07
800	1.60E-06	7.43E-07	1.21E-06	1.58E-06	8.33E-07
850	1.62E-06	7.54E-07	1.23E-06	1.64E-06	8.89E-07
900	1.63E-06	7.65E-07	1.26E-06	1.67E-06	9.36E-07
950	1.62E-06	7.71E-07	1.29E-06	1.71E-06	9.64E-07
1000	1.64E-06	7.86E-07	1.29E-06	1.73E-06	1.02E-06

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842 **6). Table S6.** The correction ratios between particle-in-the-box approximation and harmonic

T	ortho-adduct	ipso-adduct	para-adduct	meta-adduct	benzyl radical + H ₂ O
210	1.28	1.34	1.28	1.27	1.33
230	1.25	1.26	1.26	1.34	1.25
250	1.20	1.25	1.22	1.27	1.31
277	1.18	1.23	1.25	1.23	1.26
300	1.18	1.17	1.19	1.21	1.20
350	1.12	1.15	1.18	1.18	1.17
400	1.13	1.14	1.14	1.14	1.16
450	1.10	1.11	1.11	1.13	1.13
500	1.08	1.10	1.10	1.09	1.09
550	1.08	1.06	1.08	1.10	1.09
600	1.06	1.06	1.06	1.09	1.10
650	1.05	1.07	1.07	1.09	1.10
700	1.04	1.07	1.09	1.08	1.10
750	1.06	1.07	1.07	1.08	1.06
800	1.06	1.06	1.06	1.06	1.07
850	1.05	1.06	1.07	1.04	1.04
900	1.04	1.03	1.05	1.05	1.03
950	1.03	1.03	1.05	1.05	1.06
1000	1.00	1.01	1.09	1.09	1.00

T(K)	R-> ipso-add	R-> meta-add	R-> ortho-add	R-> para-add	R-> meta-abs	R-> ortho-abs
210	3.53E-13	9.43E-14	3.25E-12	1.26E-13	2.34E-15	4.47E-15
230	3.00E-13	1.13E-13	2.84E-12	1.31E-13	2.95E-15	5.67E-15
250	2.72E-13	1.21E-13	2.49E-12	1.34E-13	3.87E-15	7.45E-15
277	2.44E-13	1.38E-13	2.23E-12	1.49E-13	5.77E-15	1.10E-14
300	2.20E-13	1.54E-13	2.11E-12	1.53E-13	8.17E-15	1.54E-14
350	2.03E-13	1.92E-13	1.84E-12	1.78E-13	1.69E-14	3.08E-14
400	1.98E-13	2.31E-13	1.75E-12	1.98E-13	3.23E-14	5.70E-14
450	1.94E-13	2.72E-13	1.60E-12	2.15E-13	5.73E-14	9.80E-14
500	1.91E-13	2.92E-13	1.44E-12	2.27E-13	9.49E-14	1.58E-13
550	1.79E-13	3.04E-13	1.25E-12	2.22E-13	1.48E-13	2.42E-13
600	1.65E-13	2.91E-13	1.01E-12	2.05E-13	2.20E-13	3.55E-13
650	1.47E-13	2.64E-13	7.94E-13	1.81E-13	3.14E-13	4.99E-13
700	1.25E-13	2.26E-13	6.04E-13	1.53E-13	4.32E-13	6.79E-13
750	1.03E-13	1.87E-13	4.56E-13	1.23E-13	5.77E-13	9.00E-13
800	8.23E-14	1.50E-13	3.35E-13	9.65E-14	7.50E-13	1.16E-12

850	6.73E-14				9.55E-13	1.47E-12
900					1.19E-12	1.83E-12
950					1.45E-12	2.23E-12
1000					1.75E-12	2.69E-12

T(K)	R-> para-abs	R-> methyl-abs	R-> ipso-subs	R-> meta-subs	R-> ortho-subs	R-> para-subs
210	8.90E-16	4.82E-13	1.92E-22	2.86E-24	5.09E-23	2.01E-24
230	1.12E-15	4.10E-13	9.36E-22	1.95E-23	2.47E-22	1.35E-23
250	1.46E-15	4.02E-13	3.94E-21	1.00E-22	1.02E-21	7.41E-23
277	2.20E-15	3.75E-13	2.17E-20	7.46E-22	5.77E-21	6.05E-22
300	3.13E-15	3.58E-13	7.57E-20	3.42E-21	2.17E-20	2.77E-21
350	6.63E-15	3.73E-13	8.23E-19	5.63E-20	2.36E-19	4.83E-20
400	1.30E-14	4.20E-13	5.75E-18	5.24E-19	1.63E-18	4.57E-19
450	2.38E-14	4.72E-13	2.77E-17	3.20E-18	7.44E-18	2.79E-18
500	4.06E-14	5.32E-13	1.00E-16	1.36E-17	2.55E-17	1.21E-17
550	6.53E-14	6.29E-13	2.82E-16	4.48E-17	6.96E-17	4.00E-17
600	9.99E-14	7.50E-13	6.63E-16	1.19E-16	1.58E-16	1.07E-16
650	1.46E-13	8.70E-13	1.33E-15	2.70E-16	3.17E-16	2.45E-16
700	2.07E-13	1.01E-12	2.35E-15	5.39E-16	5.73E-16	4.98E-16
750	2.83E-13	1.11E-12	3.81E-15	9.85E-16	9.65E-16	9.19E-16
800	3.76E-13	1.27E-12	5.74E-15	1.67E-15	1.53E-15	1.58E-15
850	4.89E-13	1.38E-12	8.21E-15	2.74E-15	2.34E-15	2.60E-15
900	6.23E-13	1.51E-12	1.17E-14	4.17E-15	3.40E-15	4.00E-15
950	7.77E-13	1.70E-12	1.53E-14	6.12E-15	4.77E-15	5.92E-15
1000	9.57E-13	1.74E-12	1.96E-14	8.73E-15	6.54E-15	8.52E-15

850

851

852 **8). Table S8.** Final rate coefficients($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) for various channels at 0.1, 0.4, 0.6,
853 0.8, 1.2atm.

854

855 0.1atm

T(K)	R-> ipso-add	R-> meta-add	R-> ortho-add	R-> para-add	R-> meta-abs	R-> ortho-abs
210	3.40E-13	9.46E-14	3.09E-12	1.26E-13	2.29E-15	4.39E-15
230	2.91E-13	1.13E-13	2.73E-12	1.31E-13	2.92E-15	5.63E-15
250	2.66E-13	1.21E-13	2.41E-12	1.34E-13	3.86E-15	7.43E-15
277	2.40E-13	1.36E-13	2.16E-12	1.48E-13	5.77E-15	1.10E-14
300	2.16E-13	1.51E-13	2.02E-12	1.50E-13	8.19E-15	1.55E-14
350	1.95E-13	1.81E-13	1.67E-12	1.67E-13	1.70E-14	3.10E-14
400	1.79E-13	1.99E-13	1.42E-12	1.70E-13	3.27E-14	5.76E-14
450	1.57E-13	2.02E-13	1.09E-12	1.60E-13	5.81E-14	9.95E-14
500	1.32E-13	1.80E-13	7.95E-13	1.39E-13	9.64E-14	1.61E-13

550	1.02E-13	1.51E-13	5.51E-13	1.10E-13	1.50E-13	2.46E-13
600	7.62E-14	1.17E-13	3.62E-13	8.21E-14	2.23E-13	3.59E-13
650	5.52E-14	8.66E-14	2.34E-13	5.92E-14	3.17E-13	5.04E-13
700	3.86E-14	6.15E-14	1.48E-13	4.14E-14	4.35E-13	6.84E-13
750	2.72E-14				5.80E-13	9.05E-13
800					7.53E-13	1.17E-12
850					9.55E-13	1.47E-12
900					1.19E-12	1.83E-12
950					1.45E-12	2.23E-12
1000					1.75E-12	2.69E-12

T(K)	R-> para-abs	R-> methyl-abs	R-> ipso-subst	R-> meta-subst	R-> ortho-subst	R-> para-subst
210	8.69E-16	4.33E-13	1.79E-21	2.56E-23	4.18E-22	1.73E-23
230	1.10E-15	3.84E-13	8.49E-21	1.61E-22	1.85E-21	1.08E-22
250	1.46E-15	3.86E-13	3.41E-20	7.67E-22	6.86E-21	5.37E-22
277	2.20E-15	3.67E-13	1.73E-19	4.97E-21	3.29E-20	3.72E-21
300	3.14E-15	3.54E-13	5.57E-19	1.98E-20	1.05E-19	1.48E-20
350	6.67E-15	3.73E-13	4.72E-18	2.34E-19	8.11E-19	1.83E-19
400	1.32E-14	4.22E-13	2.44E-17	1.56E-18	3.98E-18	1.25E-18
450	2.42E-14	4.77E-13	8.69E-17	7.02E-18	1.39E-17	5.70E-18
500	4.13E-14	5.39E-13	2.37E-16	2.35E-17	3.84E-17	1.96E-17
550	6.63E-14	6.38E-13	5.28E-16	6.38E-17	8.97E-17	5.44E-17
600	1.01E-13	7.60E-13	1.02E-15	1.49E-16	1.85E-16	1.30E-16
650	1.48E-13	8.80E-13	1.78E-15	3.08E-16	3.47E-16	2.75E-16
700	2.08E-13	1.02E-12	2.85E-15	5.85E-16	6.05E-16	5.31E-16
750	2.84E-13	1.12E-12	4.32E-15	1.04E-15	9.97E-16	9.58E-16
800	3.77E-13	1.28E-12	6.28E-15	1.73E-15	1.56E-15	1.62E-15
850	4.90E-13	1.38E-12	8.71E-15	2.74E-15	2.34E-15	2.60E-15
900	6.23E-13	1.51E-12	1.17E-14	4.17E-15	3.39E-15	4.00E-15
950	7.77E-13	1.70E-12	1.53E-14	6.11E-15	4.77E-15	5.92E-15
1000	9.56E-13	1.74E-12	1.96E-14	8.72E-15	6.54E-15	8.51E-15

856

857 0.4atm

T(K)	R-> ipso-add	R-> meta-add	R-> ortho-add	R-> para-add	R-> meta-abs	R-> ortho-abs
210	3.45E-13	9.45E-14	3.16E-12	1.26E-13	2.32E-15	4.43E-15
230	2.96E-13	1.13E-13	2.79E-12	1.31E-13	2.93E-15	5.65E-15
250	2.69E-13	1.21E-13	2.45E-12	1.34E-13	3.86E-15	7.44E-15
277	2.42E-13	1.37E-13	2.21E-12	1.49E-13	5.77E-15	1.10E-14
300	2.18E-13	1.53E-13	2.08E-12	1.52E-13	8.17E-15	1.54E-14
350	2.01E-13	1.90E-13	1.80E-12	1.76E-13	1.69E-14	3.08E-14
400	1.94E-13	2.23E-13	1.66E-12	1.91E-13	3.24E-14	5.72E-14

450	1.84E-13	2.52E-13	1.44E-12	1.99E-13	5.76E-14	9.86E-14
500	1.72E-13	2.54E-13	1.20E-12	1.97E-13	9.55E-14	1.59E-13
550	1.51E-13	2.44E-13	9.58E-13	1.78E-13	1.49E-13	2.44E-13
600	1.29E-13	2.15E-13	7.15E-13	1.51E-13	2.22E-13	3.57E-13
650	1.06E-13	1.80E-13	5.18E-13	1.23E-13	3.16E-13	5.02E-13
700	8.33E-14	1.43E-13	3.66E-13	9.66E-14	4.34E-13	6.82E-13
750	6.39E-14	1.10E-13	2.57E-13	7.22E-14	5.79E-13	9.02E-13
800	4.92E-14				7.52E-13	1.17E-12
850					9.56E-13	1.47E-12
900					1.19E-12	1.83E-12
950					1.45E-12	2.23E-12
1000					1.75E-12	2.69E-12

T(K)	R-> para-abs	R-> methyl-abs	R-> ipso-subst	R-> meta-subst	R-> ortho-subst	R-> para-subst
210	8.79E-16	4.57E-13	4.74E-22	7.00E-24	1.22E-22	8.79E-16
230	1.11E-15	3.97E-13	2.30E-21	4.69E-23	5.80E-22	1.11E-15
250	1.46E-15	3.94E-13	9.58E-21	2.37E-22	2.32E-21	1.46E-15
277	2.19E-15	3.71E-13	5.18E-20	1.70E-21	1.26E-20	2.19E-15
300	3.14E-15	3.56E-13	1.77E-19	7.48E-21	4.49E-20	3.14E-15
350	6.64E-15	3.73E-13	1.79E-18	1.10E-19	4.31E-19	6.64E-15
400	1.31E-14	4.20E-13	1.13E-17	9.03E-19	2.59E-18	1.31E-14
450	2.40E-14	4.74E-13	4.85E-17	4.85E-18	1.05E-17	2.40E-14
500	4.09E-14	5.35E-13	1.56E-16	1.84E-17	3.23E-17	4.09E-14
550	6.58E-14	6.33E-13	3.96E-16	5.52E-17	8.13E-17	6.58E-14
600	1.01E-13	7.55E-13	8.47E-16	1.37E-16	1.75E-16	1.01E-13
650	1.47E-13	8.75E-13	1.58E-15	2.94E-16	3.36E-16	1.47E-13
700	2.07E-13	1.02E-12	2.65E-15	5.69E-16	5.95E-16	2.07E-13
750	2.83E-13	1.11E-12	4.13E-15	1.02E-15	9.87E-16	2.83E-13
800	3.77E-13	1.28E-12	6.06E-15	1.73E-15	1.56E-15	3.77E-13
850	4.90E-13	1.38E-12	8.72E-15	2.74E-15	2.34E-15	4.90E-13
900	6.23E-13	1.51E-12	1.17E-14	4.17E-15	3.40E-15	6.23E-13
950	7.77E-13	1.70E-12	1.53E-14	6.12E-15	4.77E-15	7.77E-13
1000	9.56E-13	1.74E-12	1.96E-14	8.72E-15	6.54E-15	9.56E-13

858

859 0.6atm

T(K)	R-> ipso-add	R-> meta-add	R-> ortho-add	R-> para-add	R-> meta-abs	R-> ortho-abs
210	3.48E-13	9.44E-14	3.20E-12	1.26E-13	2.33E-15	4.45E-15
230	2.97E-13	1.13E-13	2.81E-12	1.31E-13	2.94E-15	5.66E-15
250	2.70E-13	1.21E-13	2.47E-12	1.34E-13	3.87E-15	7.45E-15
277	2.43E-13	1.38E-13	2.22E-12	1.49E-13	5.77E-15	1.10E-14
300	2.19E-13	1.53E-13	2.09E-12	1.53E-13	8.17E-15	1.54E-14

350	2.02E-13	1.91E-13	1.82E-12	1.77E-13	1.69E-14	3.08E-14
400	1.96E-13	2.27E-13	1.71E-12	1.95E-13	3.24E-14	5.71E-14
450	1.89E-13	2.62E-13	1.52E-12	2.07E-13	5.74E-14	9.83E-14
500	1.82E-13	2.72E-13	1.31E-12	2.11E-13	9.52E-14	1.59E-13
550	1.64E-13	2.72E-13	1.09E-12	1.99E-13	1.49E-13	2.43E-13
600	1.46E-13	2.49E-13	8.42E-13	1.75E-13	2.21E-13	3.56E-13
650	1.24E-13	2.16E-13	6.32E-13	1.48E-13	3.15E-13	5.01E-13
700	1.01E-13	1.77E-13	4.61E-13	1.20E-13	4.33E-13	6.81E-13
750	7.97E-14	1.41E-13	3.34E-13	9.22E-14	5.78E-13	9.01E-13
800	6.23E-14	1.11E-13		7.19E-14	7.52E-13	1.16E-12
850					9.56E-13	1.47E-12
900					1.19E-12	1.83E-12
950					1.45E-12	2.23E-12
1000					1.75E-12	2.69E-12

T(K)	R-> para-abs	R-> methyl-abs	R-> ipso-subs	R-> meta-subs	R-> ortho-subs	R-> para-subs
210	8.83E-16	4.67E-13	3.18E-22	4.72E-24	8.33E-23	3.31E-24
230	1.11E-15	4.03E-13	1.55E-21	3.19E-23	4.00E-22	2.21E-23
250	1.46E-15	3.97E-13	6.49E-21	1.63E-22	1.62E-21	1.20E-22
277	2.20E-15	3.73E-13	3.54E-20	1.19E-21	9.01E-21	9.56E-22
300	3.13E-15	3.57E-13	1.22E-19	5.34E-21	3.30E-20	4.28E-21
350	6.63E-15	3.73E-13	1.28E-18	8.31E-20	3.36E-19	7.02E-20
400	1.31E-14	4.20E-13	8.51E-18	7.22E-19	2.15E-18	6.20E-19
450	2.39E-14	4.73E-13	3.85E-17	4.11E-18	9.17E-18	3.52E-18
500	4.08E-14	5.34E-13	1.31E-16	1.64E-17	2.95E-17	1.44E-17
550	6.56E-14	6.32E-13	3.47E-16	5.11E-17	7.68E-17	4.50E-17
600	1.00E-13	7.53E-13	7.71E-16	1.30E-16	1.69E-16	1.16E-16
650	1.47E-13	8.73E-13	1.48E-15	2.85E-16	3.30E-16	2.58E-16
700	2.07E-13	1.02E-12	2.54E-15	5.59E-16	5.88E-16	5.13E-16
750	2.83E-13	1.11E-12	4.01E-15	1.01E-15	9.80E-16	9.36E-16
800	3.77E-13	1.28E-12	5.94E-15	1.70E-15	1.56E-15	1.60E-15
850	4.90E-13	1.38E-12	8.72E-15	2.74E-15	2.34E-15	2.60E-15
900	6.23E-13	1.51E-12	1.17E-14	4.17E-15	3.40E-15	4.00E-15
950	7.77E-13	1.70E-12	1.53E-14	6.12E-15	4.77E-15	5.92E-15
1000	9.56E-13	1.74E-12	1.96E-14	8.72E-15	6.54E-15	8.51E-15

860

861 0.8atm

T(K)	R-> ipso-add	R-> meta-add	R-> ortho-add	R-> para-add	R-> meta-abs	R-> ortho-abs
210	3.51E-13	9.43E-14	3.23E-12	1.26E-13	2.34E-15	4.46E-15
230	2.99E-13	1.13E-13	2.83E-12	1.31E-13	2.94E-15	5.67E-15
250	2.71E-13	1.21E-13	2.48E-12	1.34E-13	3.87E-15	7.45E-15

277	2.44E-13	1.38E-13	2.22E-12	1.49E-13	5.77E-15	1.10E-14
300	2.19E-13	1.53E-13	2.10E-12	1.53E-13	8.17E-15	1.54E-14
350	2.02E-13	1.92E-13	1.83E-12	1.78E-13	1.69E-14	3.08E-14
400	1.97E-13	2.29E-13	1.74E-12	1.97E-13	3.23E-14	5.70E-14
450	1.92E-13	2.68E-13	1.57E-12	2.12E-13	5.73E-14	9.82E-14
500	1.87E-13	2.84E-13	1.38E-12	2.20E-13	9.50E-14	1.59E-13
550	1.73E-13	2.90E-13	1.18E-12	2.12E-13	1.48E-13	2.43E-13
600	1.57E-13	2.73E-13	9.37E-13	1.92E-13	2.21E-13	3.55E-13
650	1.37E-13	2.43E-13	7.21E-13	1.66E-13	3.15E-13	5.00E-13
700	1.14E-13	2.04E-13	5.39E-13	1.38E-13	4.33E-13	6.80E-13
750	9.24E-14	1.66E-13	3.99E-13	1.09E-13	5.78E-13	9.01E-13
800	7.38E-14	1.34E-13		8.68E-14	7.51E-13	1.16E-12
850	5.83E-14				9.55E-13	1.47E-12
900					1.19E-12	1.83E-12
950					1.45E-12	2.23E-12
1000					1.75E-12	2.69E-12

T(K)	R-> para-abs	R-> methyl-abs	R-> ipso-subst	R-> meta-subst	R-> ortho-subst	R-> para-subst
210	8.87E-16	4.76E-13	2.40E-22	3.56E-24	6.31E-23	2.50E-24
230	1.11E-15	4.07E-13	1.17E-21	2.42E-23	3.05E-22	1.68E-23
250	1.46E-15	4.00E-13	4.90E-21	1.24E-22	1.25E-21	9.15E-23
277	2.20E-15	3.74E-13	2.69E-20	9.17E-22	7.03E-21	7.41E-22
300	3.13E-15	3.57E-13	9.35E-20	4.17E-21	2.62E-20	3.36E-21
350	6.63E-15	3.73E-13	1.00E-18	6.70E-20	2.77E-19	5.72E-20
400	1.31E-14	4.20E-13	6.85E-18	6.06E-19	1.85E-18	5.25E-19
450	2.39E-14	4.73E-13	3.21E-17	3.59E-18	8.20E-18	3.11E-18
500	4.07E-14	5.33E-13	1.13E-16	1.48E-17	2.73E-17	1.31E-17
550	6.55E-14	6.30E-13	3.11E-16	4.77E-17	7.29E-17	4.23E-17
600	1.00E-13	7.51E-13	7.11E-16	1.24E-16	1.63E-16	1.11E-16
650	1.47E-13	8.71E-13	1.40E-15	2.77E-16	3.23E-16	2.51E-16
700	2.07E-13	1.02E-12	2.44E-15	5.49E-16	5.80E-16	5.05E-16
750	2.83E-13	1.11E-12	3.91E-15	9.96E-16	9.72E-16	9.27E-16
800	3.76E-13	1.28E-12	5.84E-15	1.68E-15	1.56E-15	1.59E-15
850	4.89E-13	1.38E-12	8.31E-15	2.74E-15	2.34E-15	2.60E-15
900	6.23E-13	1.51E-12	1.17E-14	4.17E-15	3.40E-15	4.00E-15
950	7.77E-13	1.70E-12	1.53E-14	6.12E-15	4.77E-15	5.92E-15
1000	9.57E-13	1.74E-12	1.96E-14	8.73E-15	6.54E-15	8.52E-15

862

863 1.2atm

T(K)	R-> ipso-add	R-> meta-add	R-> ortho-add	R-> para-add	R-> meta-abs	R-> ortho-abs
210	3.55E-13	9.42E-14	3.27E-12	1.26E-13	2.35E-15	4.48E-15

230	3.01E-13	1.13E-13	2.85E-12	1.31E-13	2.95E-15	5.68E-15
250	2.73E-13	1.21E-13	2.50E-12	1.34E-13	3.87E-15	7.46E-15
277	2.45E-13	1.38E-13	2.24E-12	1.49E-13	5.77E-15	1.10E-14
300	2.20E-13	1.54E-13	2.11E-12	1.53E-13	8.17E-15	1.54E-14
350	2.03E-13	1.93E-13	1.84E-12	1.79E-13	1.69E-14	3.08E-14
400	1.99E-13	2.32E-13	1.77E-12	1.99E-13	3.23E-14	5.69E-14
450	1.95E-13	2.75E-13	1.63E-12	2.18E-13	5.72E-14	9.80E-14
500	1.94E-13	2.98E-13	1.48E-12	2.32E-13	9.47E-14	1.58E-13
550	1.83E-13	3.14E-13	1.30E-12	2.30E-13	1.48E-13	2.42E-13
600	1.72E-13	3.06E-13	1.07E-12	2.15E-13	2.20E-13	3.54E-13
650	1.55E-13	2.82E-13	8.55E-13	1.93E-13	3.14E-13	4.98E-13
700	1.34E-13	2.45E-13	6.61E-13	1.66E-13	4.32E-13	6.79E-13
750	1.12E-13	2.06E-13	5.06E-13	1.35E-13	5.77E-13	8.99E-13
800	9.08E-14	1.67E-13	3.77E-13	1.08E-13	7.49E-13	1.16E-12
850	7.54E-14				9.55E-13	1.47E-12
900					1.19E-12	1.83E-12
950					1.45E-12	2.23E-12
1000					1.75E-12	2.69E-12

T(K)	R-> para-abs	R-> methyl-abs	R-> ipso-subs	R-> meta-subs	R-> ortho-subs	R-> para-subs
210	8.92E-16	4.88E-13	1.60E-22	2.39E-24	4.26E-23	1.68E-24
230	1.12E-15	4.13E-13	7.82E-22	1.63E-23	2.07E-22	1.13E-23
250	1.47E-15	4.04E-13	3.29E-21	8.42E-23	8.56E-22	6.23E-23
277	2.20E-15	3.76E-13	1.82E-20	6.29E-22	4.90E-21	5.12E-22
300	3.13E-15	3.58E-13	6.36E-20	2.90E-21	1.86E-20	2.35E-21
350	6.63E-15	3.73E-13	6.98E-19	4.85E-20	2.06E-19	4.19E-20
400	1.30E-14	4.20E-13	4.96E-18	4.62E-19	1.46E-18	4.06E-19
450	2.38E-14	4.72E-13	2.43E-17	2.89E-18	6.83E-18	2.54E-18
500	4.06E-14	5.32E-13	9.03E-17	1.26E-17	2.39E-17	1.13E-17
550	6.52E-14	6.28E-13	2.60E-16	4.24E-17	6.66E-17	3.80E-17
600	9.98E-14	7.49E-13	6.22E-16	1.15E-16	1.54E-16	1.03E-16
650	1.46E-13	8.69E-13	1.27E-15	2.63E-16	3.11E-16	2.40E-16
700	2.06E-13	1.01E-12	2.28E-15	5.30E-16	5.66E-16	4.91E-16
750	2.82E-13	1.11E-12	3.72E-15	9.74E-16	9.58E-16	9.10E-16
800	3.76E-13	1.27E-12	5.64E-15	1.66E-15	1.52E-15	1.57E-15
850	4.89E-13	1.38E-12	8.12E-15	2.74E-15	2.34E-15	2.60E-15
900	6.23E-13	1.51E-12	1.17E-14	4.17E-15	3.40E-15	4.00E-15
950	7.77E-13	1.70E-12	1.53E-14	6.12E-15	4.77E-15	5.92E-15
1000	9.57E-13	1.74E-12	1.96E-14	8.73E-15	6.54E-15	8.52E-15

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866 **9) Table S9.** The computed RRKM/ME rate coefficients ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) in the format of867 $k=A \cdot T^n \cdot \exp(-E_a/RT)$ at 210-1000K, 1atm.

	A (cm ³ molecule ⁻¹)	n	E _a (kcal mol ⁻¹)
R-> ipso-add	2.45E-09	-1.50	0.36
R-> meta-add	3.19E-11	-0.62	1.07
R-> ortho-add	2.45E-07	-1.88	0.51
R-> para-add	2.82E-09	-1.37	1.12
R-> meta-abs	1.16E-22	3.46	0.92
R-> ortho-abs	5.33E-12	3.29	0.80
R-> para -abs	1.40E-21	3.05	1.43
R-> methyl-abs	4.37E-14	0.53	0.35
R-> ipso-subst	8.42E-13	0.17	9.75
R-> meta-subst	5.94E-18	1.79	10.07
R-> ortho-subst	1.28E-17	1.53	8.64
R-> para-subst	4.45E-17	1.53	10.60

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871 **10) Table S10.** The branching ratios from previous studies at ~300K, 1atm

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Ref.	Branching ratios	Method or technique
this work	ipso-add (7.3%), meta-add (5.1%), ortho-add (69.8%), para-add (5.1%), methyl-abs (11.9%)	CCSD(T)-F12/ccpVQZ-F12//B2PLYP-D3/6-311++G(d,p) μVTST
Suh et al.¹	ipso-add (3%), meta-add (11%), ortho-add (52%), para-add (34%)	B3LYP/6-31G(d,p); TST
Ji et al.²	meta-add (34%), ortho-add (75.8%), para-add (20.8)	QCISD(T)/6-311+G(2d,p) //M06-2X/6-311G(d,p); CVTST
Uc et al.³	ipso-add (13%), meta-add (17%), ortho-add (42%), para-add (17%), methyl-abs (10%)	CBS-QB3; TST
Wu et al.⁴	ipso-add (15%), meta-add (59%), ortho-add (5%), para-add (14%)	ROCBS-QB3//M06-2X/6-311++G(2df,2p); TST
Zhang et al.⁵	ipso-add (4.2%), meta-add (3.4%), ortho-add (59.9%), para-add (3.6%), methyl-abs (30.2%)	M08-SO/MG3S; MSCVT/SCT
Knispel et al.⁶	k _{methyl-abs} /k _{add} < 0.022	FP-RF
Smith et al.⁷	methyl-abs (0.067±0.07)	a
Klotz et al.⁸	methyl-abs (0.067±0.07)	b

873 a: Derived from the measured yield of benzaldehyde [C₆H₅CHO] plus an estimated benzyl nitrate
874 [C₆H₅CH₂ONO₂] yield in irradiated CH₃ONO-NO-toluene-air mixtures at 298 K and atmospheric
875 pressure of air.

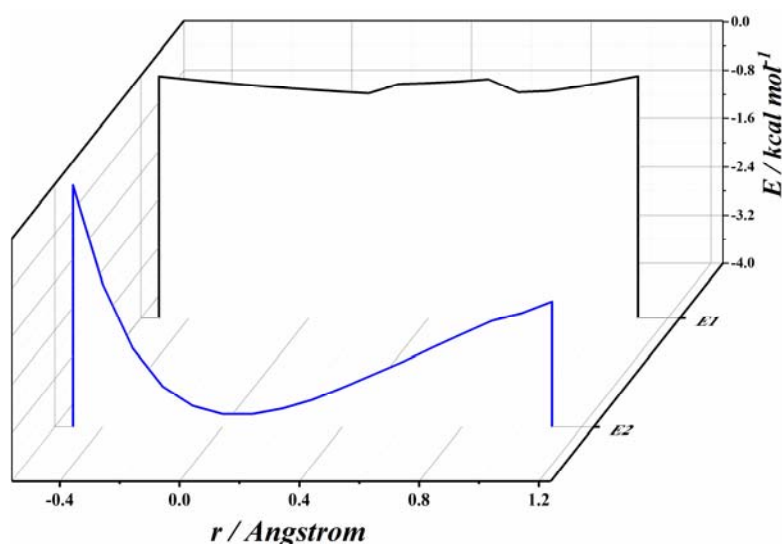
876 b: Derived from the measured yield of benzaldehyde [C₆H₅CHO] plus an estimated benzyl nitrate
877 [C₆H₅CH₂ONO₂] yield in irradiated NO_x-toluene-air mixtures at 298 K and atmospheric pressure of air.

878 1. I. Suh, D. Zhang, R. Y. Zhang, L. T. Molina, M. J. Molina, Chem. Phys. Lett., 2002, 364, 454–462.

- 879 2. Y. M. Ji, J. Zhao, H. Terazono, K. Misawa, N. P. Levitt, Y. Li, Y. Lin, J. Peng, Y. Wang, L. Duan, B. Pan,
 880 F. Zhang, X. Feng, T. An, W. Marrero-Ortiz, J. Secrest, A. L. Zhang, K. Shibuy, M. J. Molina and R.
 881 Zhang, Proc. Natl. Acad. Sci. U.S.A., 2017, 114, 8314-8320
 882 3. V. H. Uc., J. R. Alvarez-Idaboy, A. Galano and A. VivierBunge, J. Phys. Chem. A, 2008, 112, 7608–
 883 7615.
 884 4. R. Wu, S. Pan, Y. Li and L. Wang, J. Phys. Chem. A, 2014, 118, 4533-4547.
 885 5. R. M. Zhang, D. G. Truhlar and X. F. Xu, Research Official Journal of CAST, 2019, 2-62.
 886 6. R. Knispel, R. Koch, M. Siese and C. Zetzsch, Ber. Bunsen Ges. Phys. Chem., 1990, 94.
 887 7. D. F. Smith, C. D. McIver and T. E. Kleindienst, J. Atmos. Chem., 1998, 30, 209–228.
 888 8. B. Klotz, S. Sørensen, I. Barnes and K. H. Becker, J. Phys. Chem. A, 1998, 102, 10289-10299.

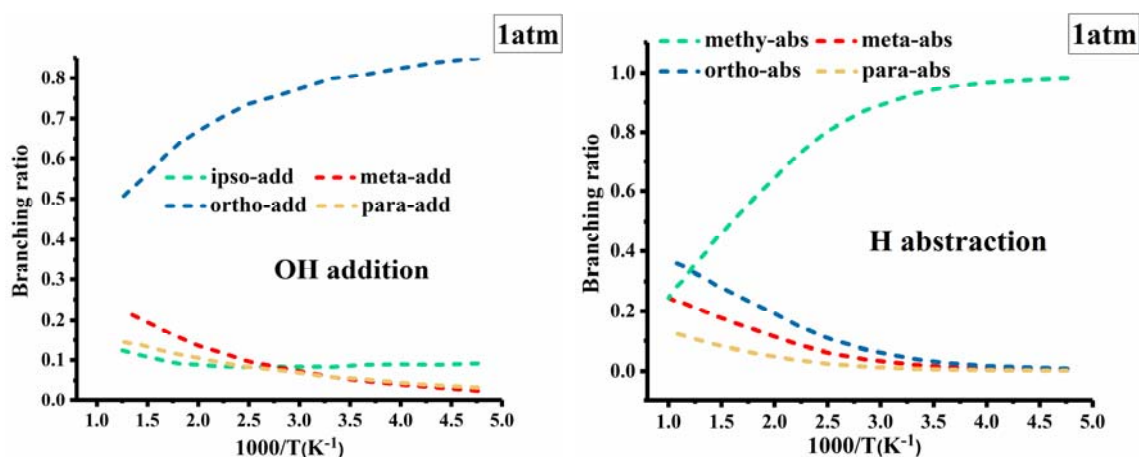
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891 **11). Figure S1.** Potential energy surface of the toluene-OH pre-reaction complex obtained at
 892 the B2PLYPD3/6-311++G(d,p) level. The OH radical was translated in both parallel (E1) and
 893 vertical direction (E2) on the benzene ring.
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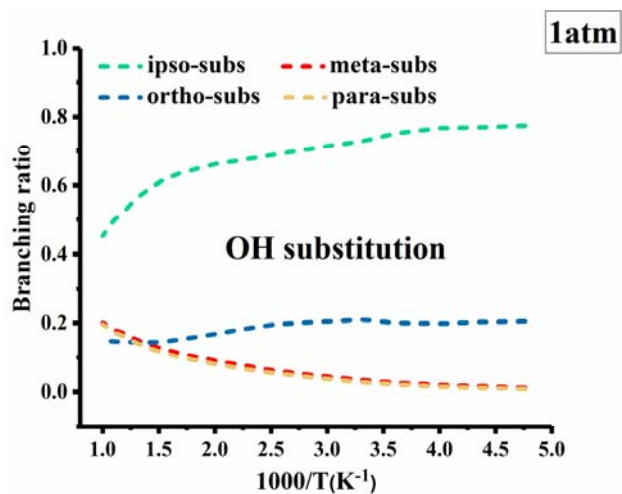


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898 **12). Figure S2.** The detailed branching ratios for some stationary points in OH addition, H
 899 abstraction and OH substitution reaction
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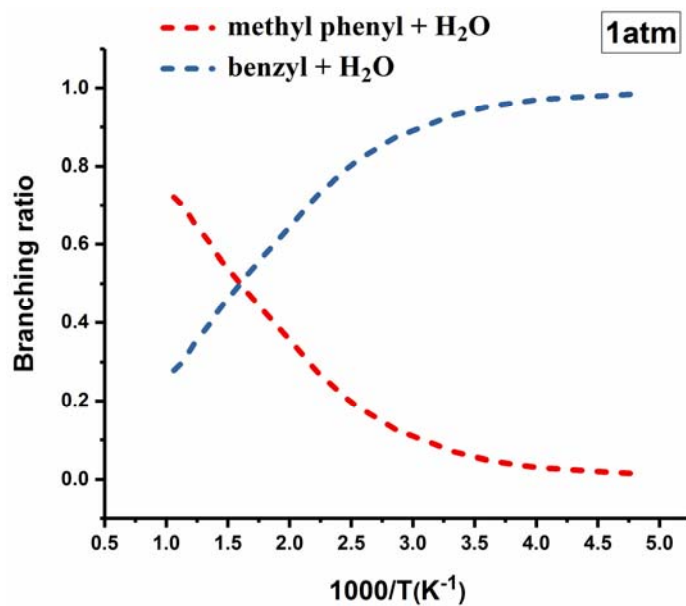


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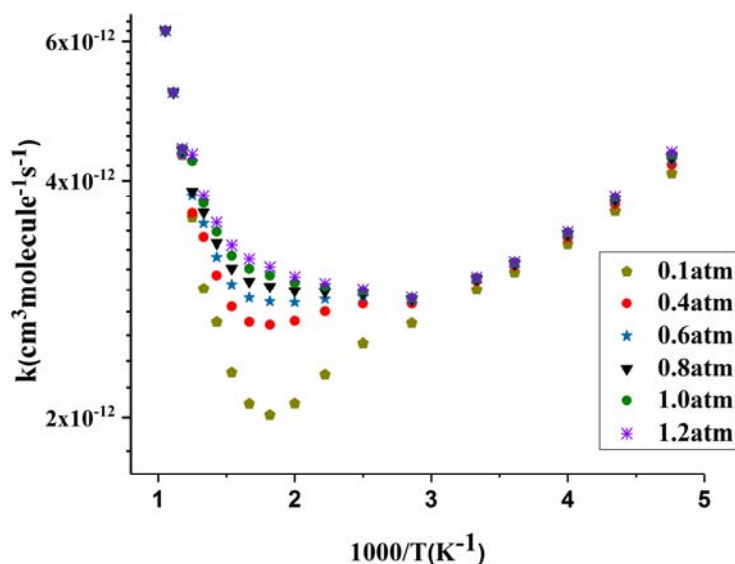
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13). Figure S3. The detailed branching ratios for H-abstraction reaction



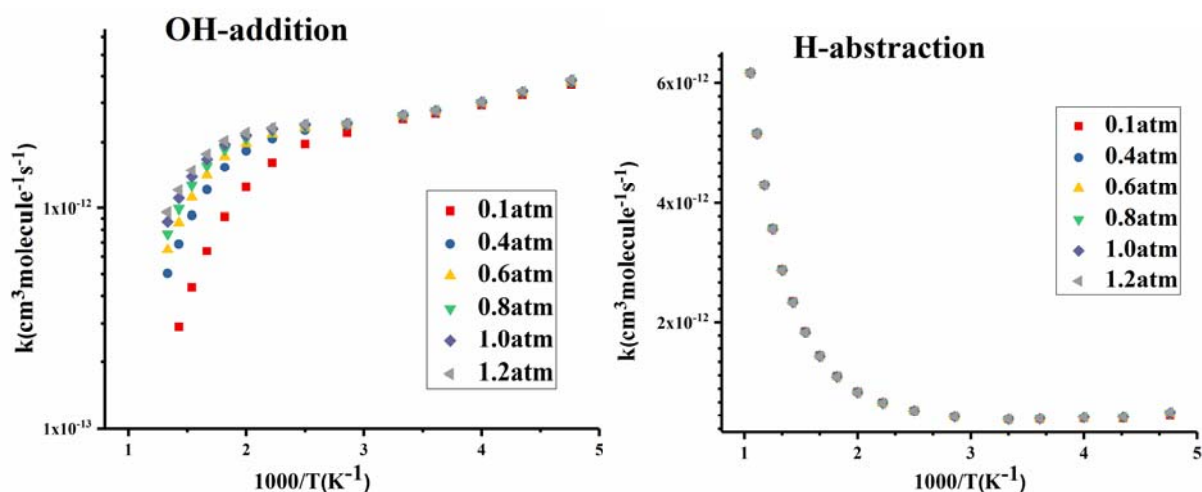
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14). Figure S4. The total rate coefficients at 0.1, 0.4, 0.6, 0.8, 1.0, 1.2 atm

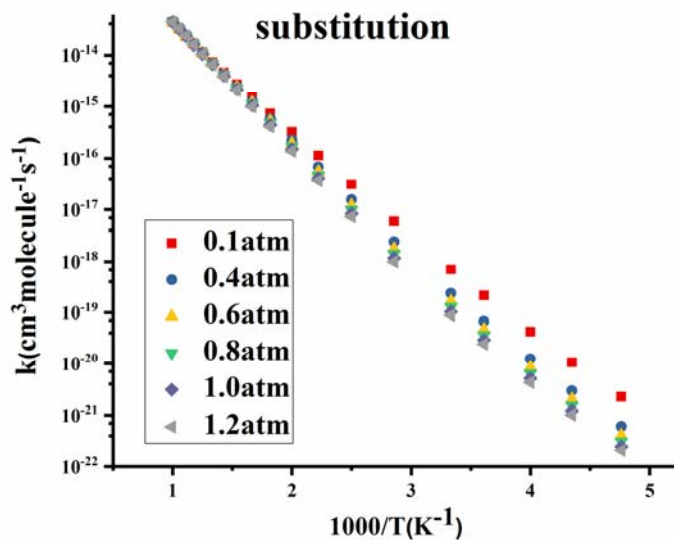


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15). Figure S5. The rate coefficients for OH addition, H abstraction and substitution reaction at 0.1, 0.4, 0.6, 0.8, 1.0, 1.2atm

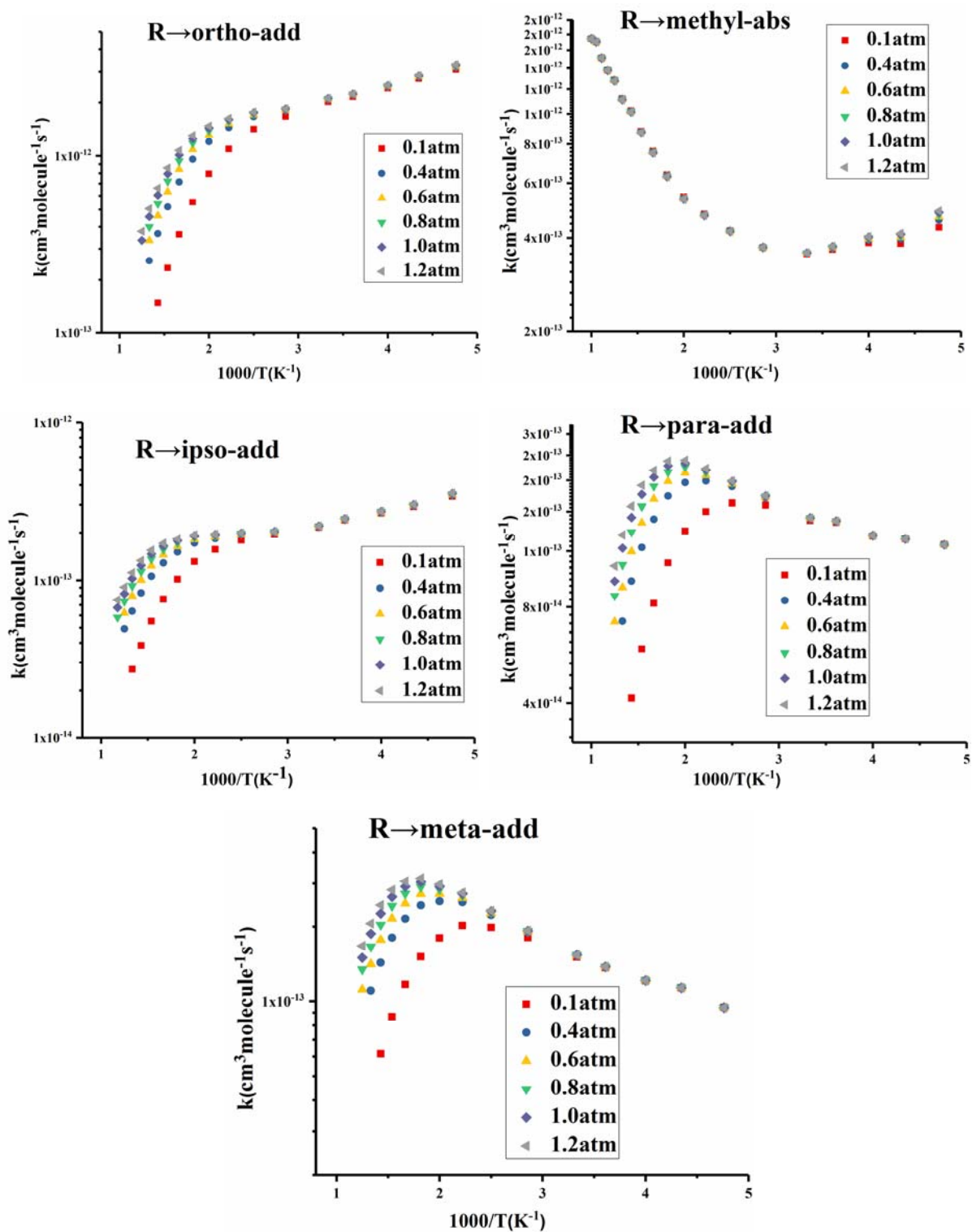


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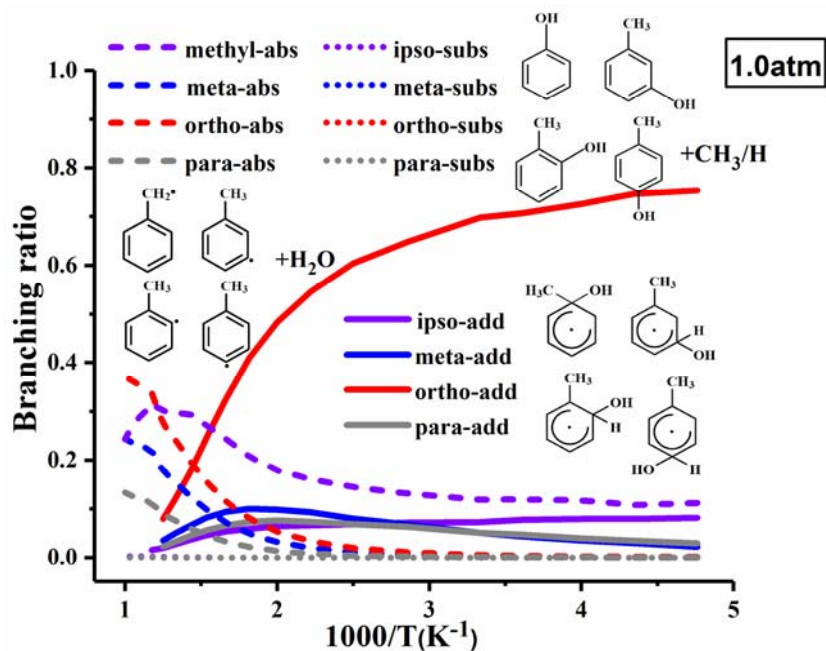


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921 **16). Figure S6.** The rate coefficients for R-> ortho-add, R-> methyl-abs, R-> ipso-add, R->
 922 para-add and R-> meta-add reactions at 0.1, 0.4, 0.6, 0.8, 1.0, 1.2atm
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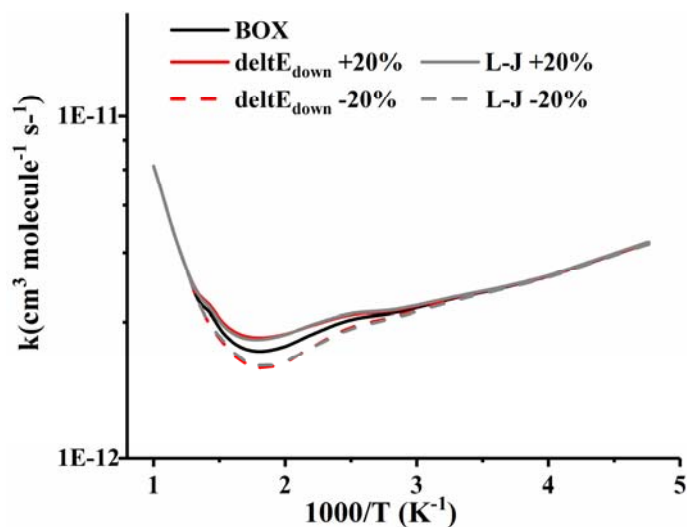


929 **17). Figure S7.** The branching ratio of various channels for OH + toluene.
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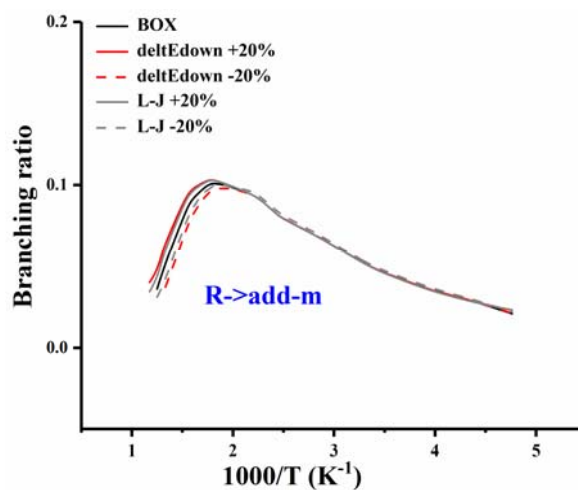
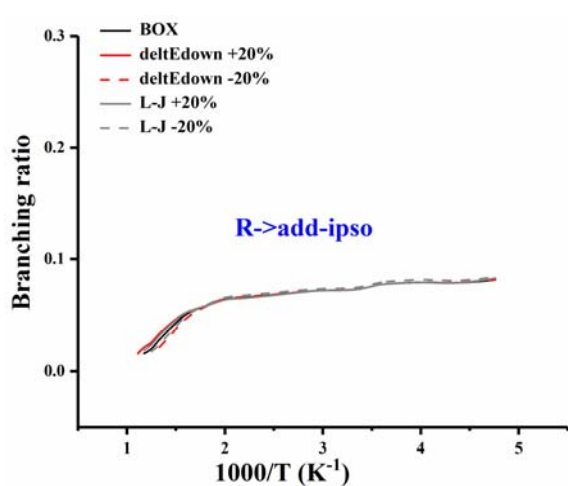
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18). Figure S8. The uncertainty evaluation of the total rate coefficients at 0.1 atm for collisional parameters

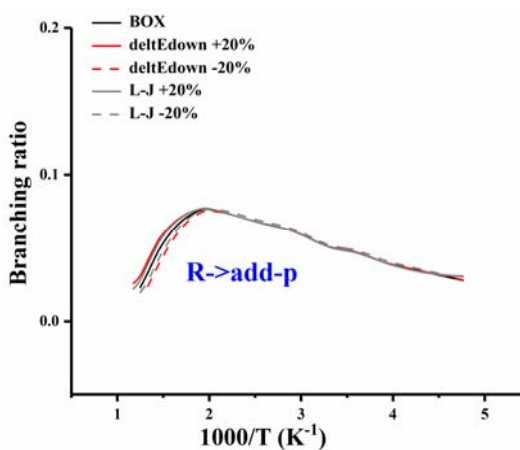
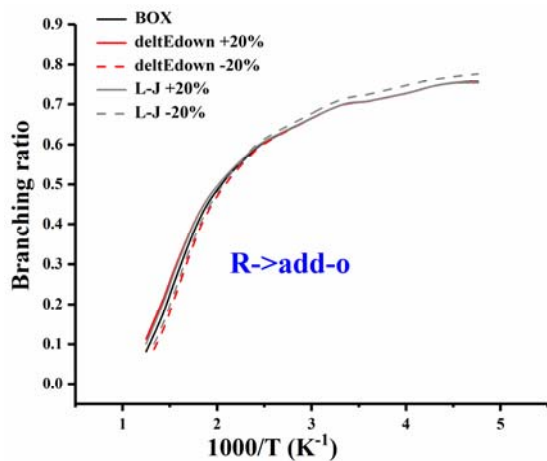


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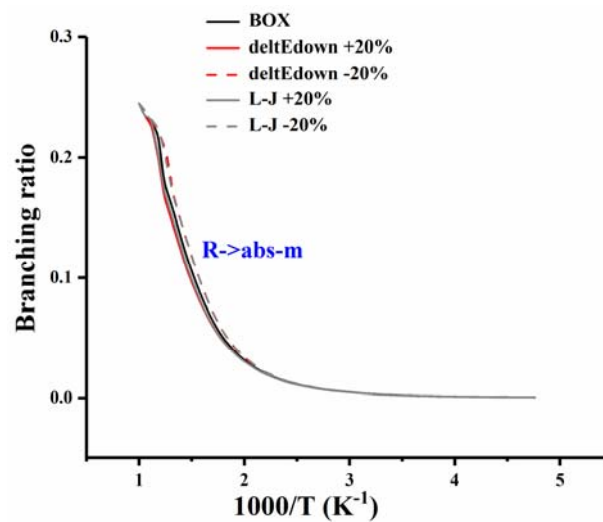
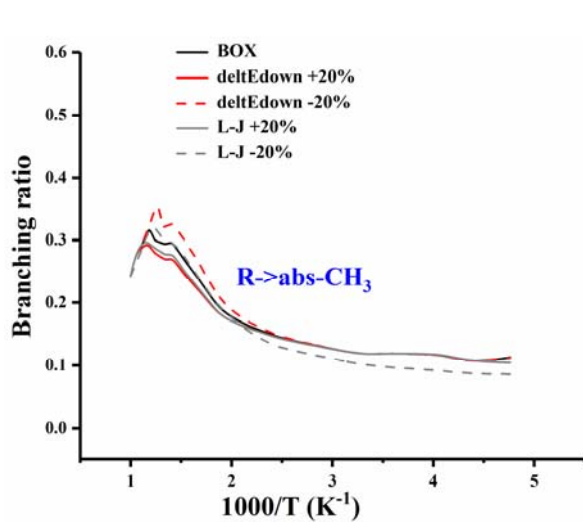
19). Figure S9. The uncertainty evaluation of the branching ratios at 1atm for collisional parameters



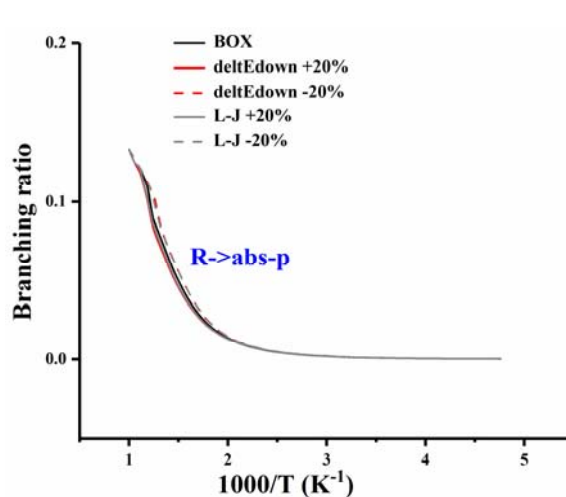
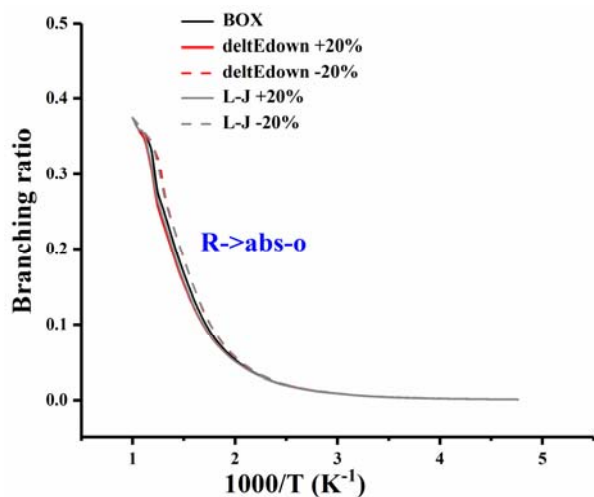
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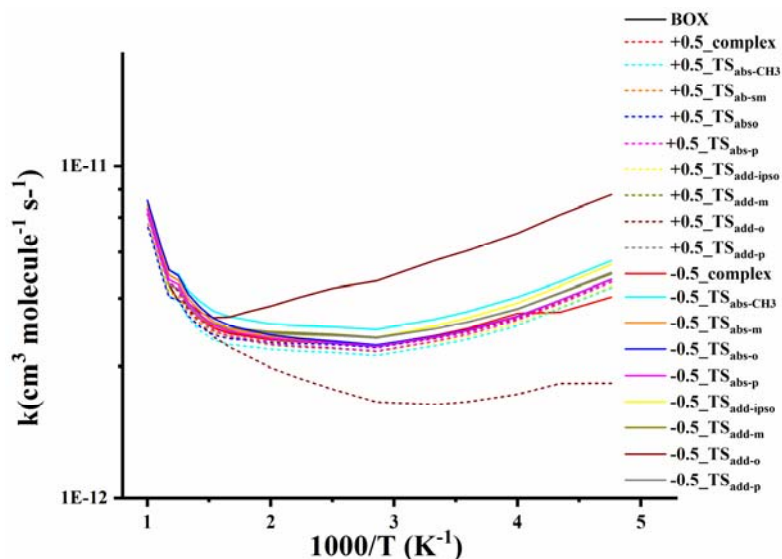


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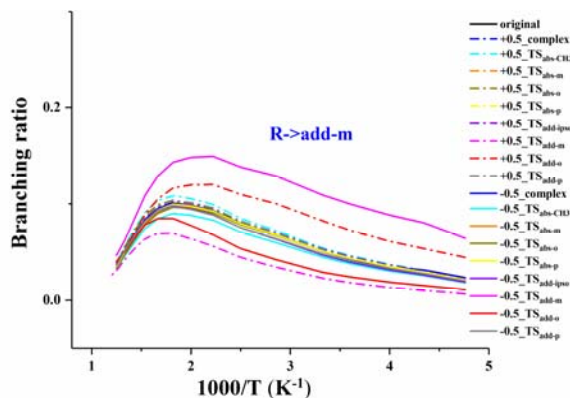
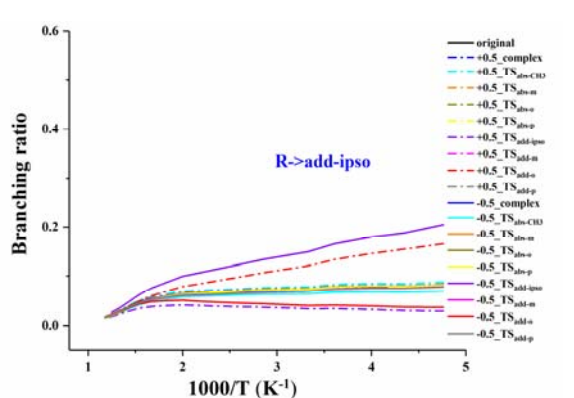
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20). Figure S10. The uncertainty evaluation of the rate coefficients at 1atm for energy

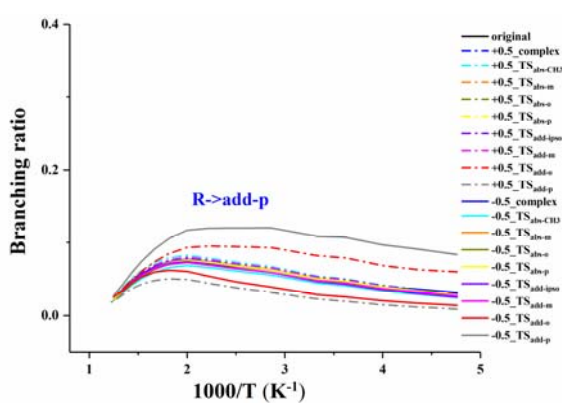
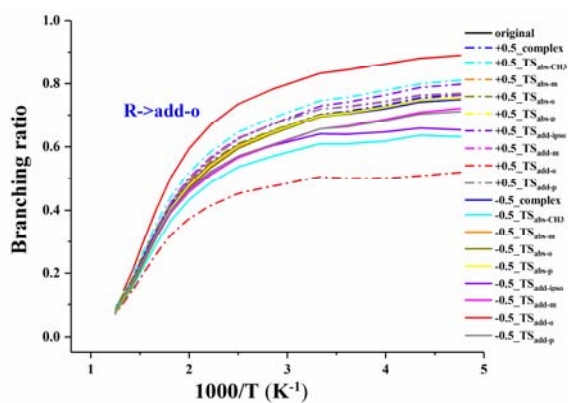


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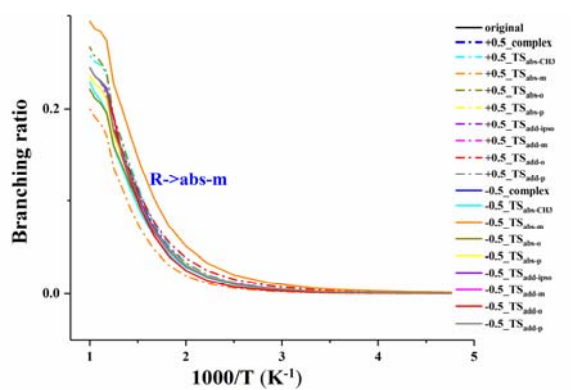
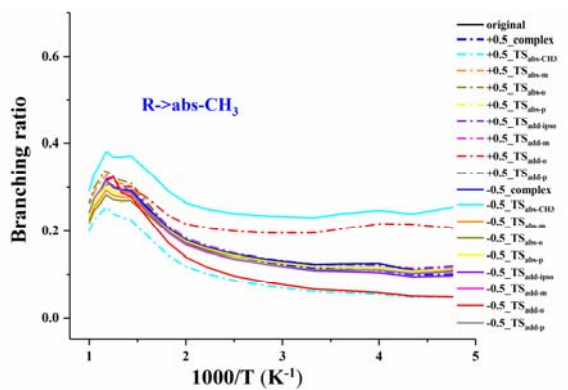
21). Figure S11. The uncertainty evaluation of the branching ratios at 1atm for energy



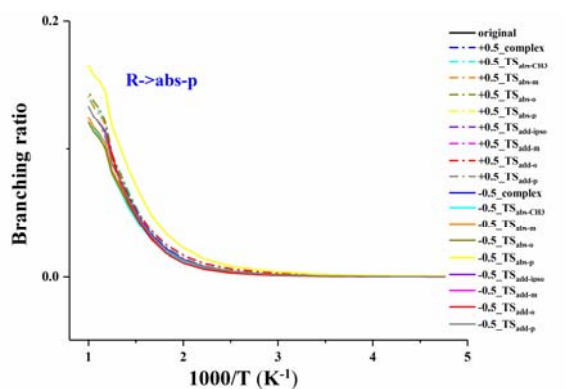
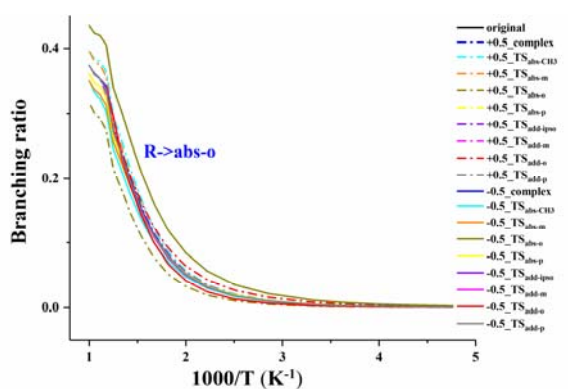
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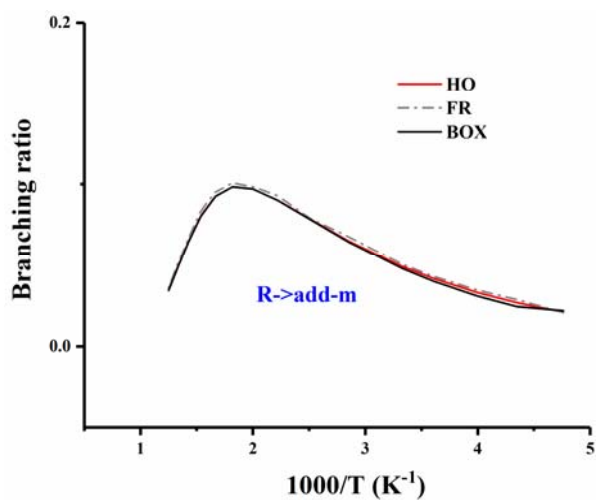
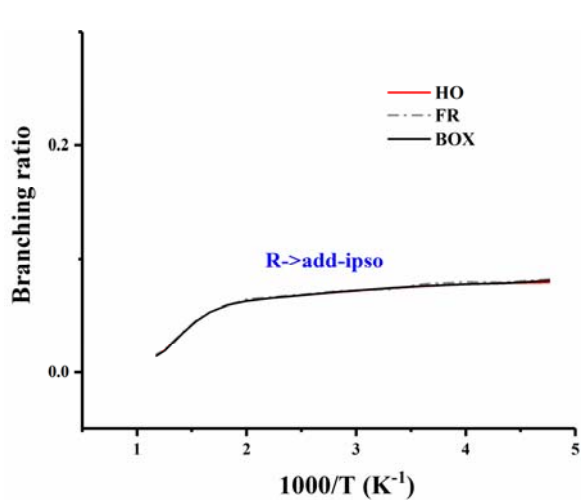
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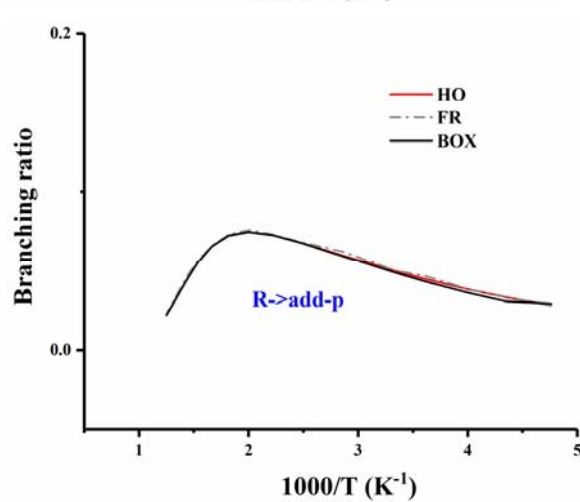
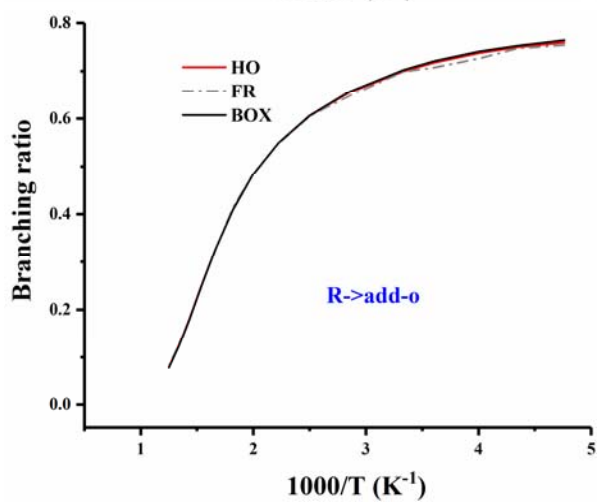
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965 **22). Figure S12.** The uncertainty evaluation of the branching ratios at 1atm for anharmonic
 966 treatment

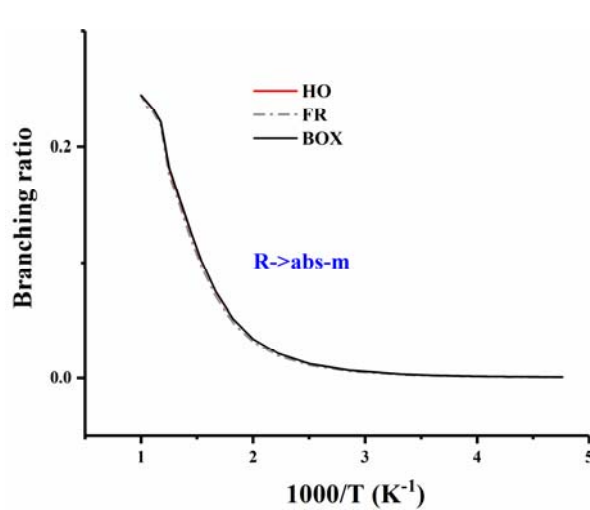
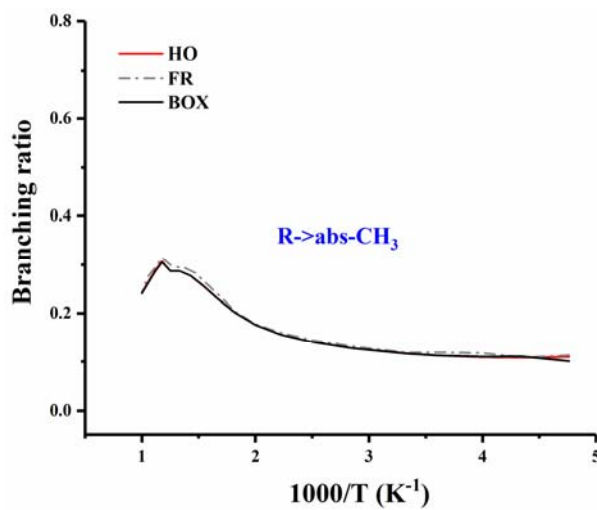
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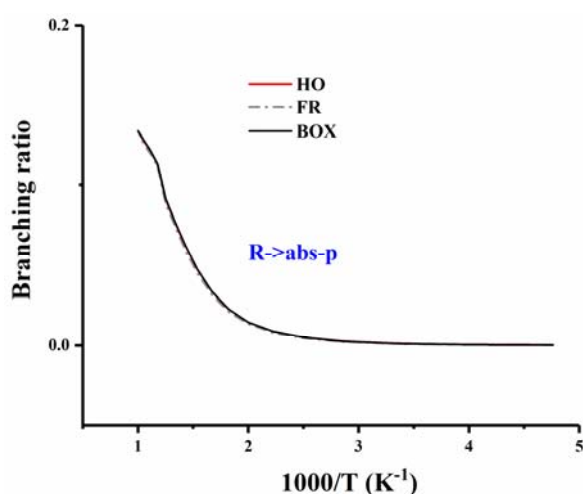
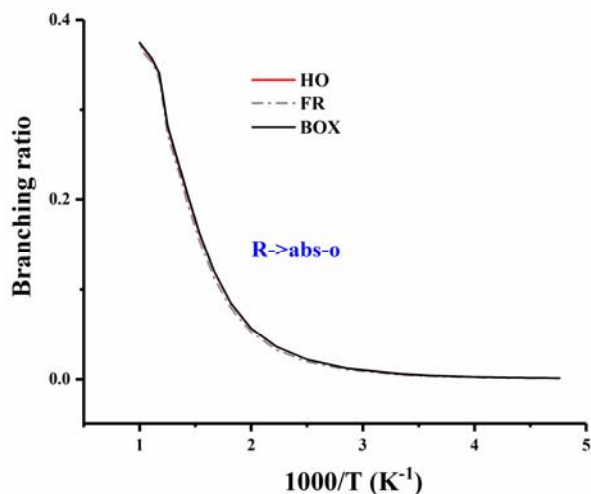


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975 **23). Table S11.** The input for final rate coefficients for each channels at 300K.

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GLOBAL SECTION

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!*****

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983 TemperatureList[K]

300

984 PressureList[atm]

0.1 0.4 0.6 0.8 1.0 1.2

985

!

986

!

987 EnergyStepOverTemperature

.2

! [Discretization energy step

988 (global relax matrix)] / T

989 ExcessEnergyOverTemperature

50

! [Highest barrier in the model

990 (global relax matrix)] / T

991 ModelEnergyLimit[kcal/mol]

400

! Highest reference energy used

992 in the calculation (or ReferenceEnergy[kcal/mol])

993

!

994 CalculationMethod

direct

! direct or low-eigenvalue

995

!

996 WellCutoff

20

! well truncation parameter :

997 Max { dissociation limit (min barrier rel. to bottom of the well) / T }

998 ChemicalEigenvalueMax

0.2

! Max chemical eigenvalue /

999 Lowest Collision relaxation eigenvalue

1000

!

1001 ReductionMethod

diagonalization ! [low eigenvalue method

1002 only] diagonalization or projection (default)

1003

!

1004 !!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!!!!


```

1005 !EnergyStepOverTemperature          0.3          #Ratio of discretization energy
1006 step to T
1007 !ExcessEnergyOverTemperature        40
1008 !WellCutoff                          10
1009 !ChemicalEigenvalueMin              1.e-6          #only for direct
1010 diagonalization method
1011 !!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!
1012 RateOutput
1013 rate_toluene+OH.out                  ! -0.5kcal/mol output file name for rate
1014 coefficients
1015 !LogOutput
1016 thf_pyro.log                          ! log file name
1017 !EigenvalueOutput
1018 thf_pyro_eigval.out                  ! eigenvalue output file name
1019 !EigenvectorOutput
1020 thf_pyro_eigvect.out                 ! eigenvector output file name
1021 !PEDOutput
1022 thf_pyro_ped.out                      ! Product energy distributions file name
1023 !
1024 !
1025 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
1026 !*****
1027 !                MODEL SECTION
1028 !*****
1029 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
1030 !
1031 !
1032 Model
1033 !
1034     EnergyRelaxation                  !
1035     Default collisional energy relaxation kernel
1036         Exponential                    !
1037     Currently the only possible energy relaxation model
1038         Factor[1/cm]                   260                    !
1039     (Delta_E_down)^(0) @ standard T (300 K)
1040         Power                          0.875                    !
1041     Power n in the expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
1042         ExponentCutoff                  10                        ! if
1043     (Delta_E) / (Delta_E_down) > value  transition probability is zero
1044     End
1045 !
1046     CollisionFrequency                  !
1047     Collision frequency model
1048         LennardJones                    !
1049     Currently the only possible collisional frequency model based on LJ potential

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```

1050      Epsilons[K]                48      561.62      !
1051  Epsilon_1 and Epsilon_2 N2 and 2-methylphenol
1052      Sigmas[angstrom]          3.9      6.36      !
1053  Sigma_1 and Sigma_2
1054      Masses[amu]                28.01   109.15      !
1055  Masses of the buffer gas molecule and of the complex (check order)
1056      End
1057  !
1058  !*****
1059  !
1060  !*****
1061  !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
1062  !*****
1063  ! REACTANTS
1064  !*****
1065  !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
1066  !*****
1067
1068
1069  Bimolecular      R      # C6H5CH3 + OH
1070  Fragment REACT1
1071  RRHO
1072  Geometry[angstrom]          15
1073  C      -0.00763900   -1.19953600   1.20517200
1074  C      -0.00763900   0.19581200   1.20217500
1075  C      -0.00388100   0.91356100   0.00000000
1076  C      -0.00763900   0.19581200   -1.20217500
1077  C      -0.00763900   -1.19953600   -1.20517200
1078  C      -0.00648200   -1.90320000   0.00000000
1079  H      -0.01220200   -1.73580100   2.14733200
1080  H      -0.01234000   0.73486900   2.14413000
1081  H      -0.01234000   0.73486900   -2.14413000
1082  H      -0.01220200   -1.73580100   -2.14733200
1083  H      -0.00930500   -2.98687900   0.00000000
1084  C      0.02927600   2.42117200   0.00000000
1085  H      1.05986700   2.78965500   0.00000000
1086  H      -0.46581000   2.82728400   -0.88435100
1087  H      -0.46581000   2.82728400   0.88435100
1088  Core      RigidRotor
1089      SymmetryFactor      1.0000000000000000
1090  End
1091  Rotor      Hindered
1092  Group      13  14  15
1093  Axis      12      1
1094  Symmetry      6

```

```

1095 Potential[kcal/mol]          6
1096 0.0000
1097 -0.0070
1098 0.0023
1099 0.0044
1100 0.0007
1101 -0.0072
1102 End
1103   Frequencies[1/cm]          38
1104   202.96   341.60   398.43   447.41   526.70   537.82   634.09
1105 722.96
1106   800.02   840.70   882.53   915.15   936.50   967.28   977.87
1107 1010.97
1108   1019.50   1070.19   1137.99   1159.51   1191.28   1296.73   1310.74
1109 1369.93
1110   1417.20   1442.75   1454.09   1472.11   1565.98   1586.86   2927.97
1111 2986.81
1112   3009.30   3052.75   3054.42   3067.12   3075.29   3087.53
1113 ZeroEnergy[kcal/mol]          0.
1114 ElectronicLevels[1/cm]          1
1115 0.0000000000000000E+000  1.0000000000000000
1116 End
1117 !*****
1118 Fragment REACT2
1119 RRHO
1120 Geometry[angstrom]            2
1121 O                0.00000000  0.00000000  0.10800700
1122 H                0.00000000  0.00000000 -0.86405300
1123 Core RigidRotor
1124 SymmetryFactor  1.0000000000000000
1125 End
1126   Frequencies[1/cm]            1
1127   3614.32
1128 ZeroEnergy[kcal/mol]          0.
1129 ElectronicLevels[1/cm]          1
1130 0.0000000000000000E+000  2.0000000000000000
1131 End
1132 GroundEnergy[kcal/mol] 0.0
1133 End
1134 !*****
1135 Well W # OHC6H5CH3
1136 Species
1137 RRHO
1138 Geometry[angstrom]            17
1139 C                0.98053000 -0.41677600  0.00000300

```

```

1140  C          0.26374200  -0.47554900   1.20263700
1141  C         -1.12900000  -0.58244200   1.20565300
1142  C         -1.83124600  -0.63613400   0.00000700
1143  C         -1.12900000  -0.58246600  -1.20564000
1144  C          0.26374300  -0.47557500  -1.20262800
1145  H          0.80056000  -0.43321500   2.14440900
1146  H         -1.66337000  -0.62475800   2.14756700
1147  H         -2.91142300  -0.71752500   0.00000700
1148  H         -1.66337100  -0.62480100  -2.14755300
1149  H          0.80056000  -0.43326100  -2.14440200
1150  C          2.47848900  -0.24830700   0.00000100
1151  H          2.92678100  -0.70407000   0.88472600
1152  H          2.92677900  -0.70407500  -0.88472200
1153  H          2.74571400   0.81268200  -0.00000200
1154  O         -0.36116300   2.76685000  -0.00002400
1155  H         -0.45646600   1.79772300  -0.00003400
1156  Core  RigidRotor
1157      SymmetryFactor    0.5          ! chiral (similarly as below)
1158  End
1159      Rotor  Hindered          !freq=60.98
1160      Group                13 14 15
1161      Axis                  12 1
1162      Symmetry              3
1163  Potential[kcal/mol]      12
1164      -0.060 0.732 1.627 2.378 2.749 2.609 2.005 1.135 0.261 -0.389 -0.667 -0.525
1165  End
1166      Rotor  Hindered          !freq=35.62
1167      Group                17
1168      Axis                  16 1
1169      Symmetry              1
1170  Potential[kcal/mol]      36
1171      0.000 0.134 0.512 1.079 1.747 2.403 2.958 3.341 3.521 3.520 3.404 3.256
1172      3.151 3.143 3.254 3.465 3.712 3.914 3.997 3.937 3.752 3.508 3.286 3.155
1173      3.141 3.230 3.374 3.505 3.533 3.382 3.015 2.459 1.788 1.101 0.520 0.135
1174  End
1175  Frequencies[1/cm]        43
1176  20.81 102.21 114.15 175.36 219.13 342.17 399.15
1177  460.29 527.08 631.74 646.79 735.07 800.12 853.75 897.15
1178  955.48 962.99 969.50 978.45 1010.64 1024.39 1070.20 1138.41
1179  1160.14 1192.36 1295.95 1308.98 1370.17 1414.50 1443.95 1453.14
1180  1471.03 1559.81 1582.95 2930.84 2991.98 3013.05 3058.03 3059.31
1181  3072.02 3079.39 3091.32 3594.43
1182  ZeroEnergy[kcal/mol]      -3.45
1183  ElectronicLevels[1/cm]    1
1184  0.0000000000000000E+000  2.000000000000000

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1185 End
1186 End
1187 !*****
1188 Barrier B R W # WR-TS
1189 Variational
1190 RRHO 1
1191 Geometry[angstrom] 17
1192 C 0.00000000 0.00000000 0.00000000
1193 C 0.00000000 0.00000000 1.40127400
1194 C 1.19728500 0.00000000 2.12076900
1195 C 2.42052300 0.00356300 1.44750100
1196 C 2.43484200 0.00754900 0.05129400
1197 C 1.23446300 0.00753300 -0.66302900
1198 H -0.94549900 -0.00407300 1.93317100
1199 H 1.17391800 -0.00163700 3.20428000
1200 H 3.35021200 0.00206200 2.00345300
1201 H 3.37832000 0.01181100 -0.48197700
1202 H 1.25566400 0.00935800 -1.74767100
1203 C -1.29282800 -0.05335400 -0.77331300
1204 H -2.10136800 0.43261200 -0.22420000
1205 H -1.19322600 0.43813900 -1.74281700
1206 H -1.58951400 -1.09077900 -0.95450900
1207 O 0.94431800 -3.27694000 0.55275800
1208 H 1.08798500 -2.31795200 0.64214700
1209 Core RigidRotor
1210 SymmetryFactor 0.5
1211 End
1212 Rotor Hindered
1213 Group 13 14 15
1214 Axis 12 1
1215 Symmetry 3
1216 Potential[kcal/mol] 12
1217 -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
1218 End
1219 Rotor Hindered
1220 Group 17
1221 Axis 16 1
1222 Symmetry 1
1223 Potential[kcal/mol] 36
1224 0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
1225 2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
1226 0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
1227 End
1228 Frequencies[1/cm] 42
1229 30.74 156.68 157.92 208.66 342.34 400.75 460.03 527.11 635.03

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1230 646.75 735.09 800.37 852.23 898.21 954.38 964.33 969.35 978.58 1011.23
1231 1025.49 1070.28 1140.10 1160.63 1192.79 1296.37 1310.10 1371.27 1416.65 1444.66
1232 1453.53 1471.14 1565.20 1582.71 2930.50 2991.63 3013.39 3058.18 3059.94 3072.00
1233 3079.45 3091.28 3594.39
1234 ZeroEnergy[kcal/mol] -3.44
1235 ElectronicLevels[1/cm] 1
1236 0 2
1237 End
1238 !*****
1239 RRHO 5
1240 Geometry[angstrom] 17
1241 C 0.00000000 0.00000000 0.00000000
1242 C 0.00000000 0.00000000 1.40127400
1243 C 1.19728500 0.00000000 2.12076900
1244 C 2.42052300 0.00356300 1.44750100
1245 C 2.43484200 0.00754900 0.05129400
1246 C 1.23446300 0.00753300 -0.66302900
1247 H -0.94549900 -0.00407300 1.93317100
1248 H 1.17391800 -0.00163700 3.20428000
1249 H 3.35021200 0.00206200 2.00345300
1250 H 3.37832000 0.01181100 -0.48197700
1251 H 1.25566400 0.00935800 -1.74767100
1252 C -1.29282800 -0.05335400 -0.77331300
1253 H -2.10136800 0.43261200 -0.22420100
1254 H -1.19322600 0.43813900 -1.74281700
1255 H -1.58951400 -1.09077900 -0.95450900
1256 O 0.92255800 -3.67608700 0.53828700
1257 H 1.06622500 -2.71709900 0.62767600
1258 Core RigidRotor
1259 SymmetryFactor 0.5
1260 End
1261 Rotor Hindered
1262 Group 13 14 15
1263 Axis 12 1
1264 Symmetry 3
1265 Potential[kcal/mol] 12
1266 -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
1267 End
1268 Rotor Hindered
1269 Group 17
1270 Axis 16 1
1271 Symmetry 1
1272 Potential[kcal/mol] 36
1273 0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
1274 2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230

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1275      0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
1276      End
1277      Frequencies[1/cm]                42
1278      16.98 37.93 182.89 206.63 341.89 398.36 456.69 527.02 617.96
1279      634.11 730.87 800.27 848.70 892.70 946.92 949.68 968.57 977.85 1010.57
1280      1023.82 1069.76 1138.86 1159.98 1192.58 1295.80 1309.37 1371.02 1416.01 1444.36
1281      1453.29 1471.00 1563.51 1583.28 2929.98 2990.99 3013.18 3057.39 3059.14 3071.37
1282      3078.92 3090.89 3589.75
1283      ZeroEnergy[kcal/mol]            -3.08
1284      ElectronicLevels[1/cm]          1
1285      0      2
1286      End
1287      !*****
1288      RRHO                                7
1289      Geometry[angstrom]                17
1290      C      0.00000000      0.00000000      0.00000000
1291      C      0.00000000      0.00000000      1.40127400
1292      C      1.19728500      0.00000000      2.12076900
1293      C      2.42052300      0.00356300      1.44750100
1294      C      2.43484200      0.00754900      0.05129400
1295      C      1.23446300      0.00753300      -0.66302900
1296      H      -0.94549900     -0.00407300      1.93317100
1297      H      1.17391800     -0.00163700      3.20428000
1298      H      3.35021200      0.00206200      2.00345300
1299      H      3.37832000      0.01181100     -0.48197700
1300      H      1.25566400      0.00935800     -1.74767100
1301      C      -1.29282800     -0.05335400     -0.77331300
1302      H      -2.10136800      0.43261200     -0.22420100
1303      H      -1.19322600      0.43813900     -1.74281700
1304      H      -1.58951400     -1.09077900     -0.95450900
1305      O      0.91167800     -3.87566000      0.53105100
1306      H      1.05534500     -2.91667100      0.62044000
1307      Core      RigidRotor
1308      SymmetryFactor      0.5
1309      End
1310      Rotor      Hindered
1311      Group                13 14 15
1312      Axis                12 1
1313      Symmetry            3
1314      Potential[kcal/mol]      12
1315      -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
1316      End
1317      Rotor      Hindered
1318      Group                17
1319      Axis                16 1

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1320           Symmetry                      1
1321   Potential[kcal/mol]          36
1322       0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
1323       2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
1324       0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
1325           End
1326   Frequencies[1/cm]              42
1327   14.96 23.77  193.03 206.46 341.70 398.06 454.57 526.97 598.76
1328   633.99 728.89 800.22 847.13 890.10 941.38 944.25 968.25 977.62 1010.34 1022.90
1329   1069.54 1138.48 1159.70 1192.50 1295.51 1309.06 1370.86 1415.84 1444.17 1453.24
1330   1470.92 1563.24 1583.32 2929.79 2990.74 3013.09 3057.07 3058.81 3071.10
1331   3078.68 3090.72 3589.23
1332   ZeroEnergy[kcal/mol]          -2.67
1333   ElectronicLevels[1/cm]        1
1334           0           2
1335   End
1336   !*****
1337           RRHO                      8
1338   Geometry[angstrom]            17
1339   C           0.00000000    0.00000000    0.00000000
1340   C           0.00000000    0.00000000    1.40127400
1341   C           1.19728500    0.00000000    2.12076900
1342   C           2.42052300    0.00356300    1.44750100
1343   C           2.43484200    0.00754900    0.05129400
1344   C           1.23446300    0.00753300   -0.66302900
1345   H           -0.94549900   -0.00407300    1.93317100
1346   H           1.17391800   -0.00163700    3.20428000
1347   H           3.35021200    0.00206200    2.00345300
1348   H           3.37832000    0.01181100   -0.48197700
1349   H           1.25566400    0.00935800   -1.74767100
1350   C           -1.29282800   -0.05335400   -0.77331300
1351   H           -2.10136800    0.43261200   -0.22420100
1352   H           -1.19322600    0.43813900   -1.74281700
1353   H           -1.58951400   -1.09077900   -0.95450900
1354   O           0.90623800   -3.97544600    0.52743300
1355   H           1.04990500   -3.01645800    0.61682200
1356   Core   RigidRotor
1357           SymmetryFactor          0.5
1358   End
1359           Rotor   Hindered
1360           Group                      13 14 15
1361           Axis                      12 1
1362           Symmetry                   3
1363   Potential[kcal/mol]          12
1364       -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558

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```

1365      End
1366                      Rotor  Hindered
1367      Group                      17
1368      Axis                        16 1
1369      Symmetry                    1
1370      Potential[kcal/mol]        36
1371      0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
1372      2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
1373      0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
1374      End
1375      Frequencies[1/cm]          42
1376      15.09 24.11 197.19 206.26 341.62 397.98 453.48 526.94 588.73
1377      633.94 727.99 800.18 846.42 888.91 937.43 943.10 968.09 977.52 1010.24
1378      1022.45 1069.44 1138.31 1159.56 1192.46 1295.37 1308.93 1370.77 1415.77 1444.07
1379      1453.22 1470.87 1563.15 1583.32 2929.70 2990.63 3013.05 3056.91 3058.66 3070.97
1380      3078.57 3090.64 3589.21
1381      ZeroEnergy[kcal/mol]      -2.44
1382      ElectronicLevels[1/cm]    1
1383      0      2
1384      End
1385      !*****
1386      RRHO                      10
1387      Geometry[angstrom]        17
1388      C      0.00000000      0.00000000      0.00000000
1389      C      0.00000000      0.00000000      1.40127400
1390      C      1.19728500      0.00000000      2.12076900
1391      C      2.42052300      0.00356300      1.44750100
1392      C      2.43484200      0.00754900      0.05129400
1393      C      1.23446300      0.00753300      -0.66302900
1394      H      -0.94549900      -0.00407300      1.93317100
1395      H      1.17391800      -0.00163700      3.20428000
1396      H      3.35021200      0.00206200      2.00345300
1397      H      3.37832000      0.01181100      -0.48197700
1398      H      1.25566400      0.00935800      -1.74767100
1399      C      -1.29282800      -0.05335400      -0.77331300
1400      H      -2.10136800      0.43261200      -0.22420100
1401      H      -1.19322600      0.43813900      -1.74281700
1402      H      -1.58951400      -1.09077900      -0.95450900
1403      O      0.89535800      -4.17501900      0.52019700
1404      H      1.03902500      -3.21603100      0.60958600
1405      Core      RigidRotor
1406      SymmetryFactor            0.5
1407      End
1408      Rotor  Hindered
1409      Group                      13 14 15

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```

1410      Axis                      12 1
1411      Symmetry                    3
1412      Potential[kcal/mol]        12
1413      -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
1414      End
1415      Rotor Hindered
1416      Group                        17
1417      Axis                          16 1
1418      Symmetry                      1
1419      Potential[kcal/mol]          36
1420      0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
1421      2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
1422      0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
1423      End
1424      Frequencies[1/cm]           42
1425      15.51 24.32 204.84 205.50 341.48 397.99 451.46 526.83 569.93
1426      633.89 726.43 800.13 845.20 886.86 930.51 941.19 967.83 977.35 1010.09
1427      1021.62 1069.28 1138.05 1159.32 1192.38 1295.12 1308.67 1370.56 1415.69 1443.86
1428      1453.24 1470.79 1563.03 1583.30 2929.56 2990.43 3012.98 3056.64 3058.38 3070.76
1429      3078.38 3090.51 3589.69
1430      ZeroEnergy[kcal/mol]        -2.02
1431      ElectronicLevels[1/cm]      1
1432      0 2
1433      End
1434      !*****
1435      RRHO                          12
1436      Geometry[angstrom]          17
1437      C 0.00000000 0.00000000 0.00000000
1438      C 0.00000000 0.00000000 1.40127400
1439      C 1.19728500 0.00000000 2.12076900
1440      C 2.42052300 0.00356300 1.44750100
1441      C 2.43484200 0.00754900 0.05129400
1442      C 1.23446300 0.00753300 -0.66302900
1443      H -0.94549900 -0.00407300 1.93317100
1444      H 1.17391800 -0.00163700 3.20428000
1445      H 3.35021200 0.00206200 2.00345300
1446      H 3.37832000 0.01181100 -0.48197700
1447      H 1.25566400 0.00935800 -1.74767100
1448      C -1.29282800 -0.05335400 -0.77331300
1449      H -2.10136800 0.43261200 -0.22420100
1450      H -1.19322600 0.43813900 -1.74281700
1451      H -1.58951400 -1.09077900 -0.95450900
1452      O 0.88447900 -4.37459200 0.51296100
1453      H 1.02814600 -3.41560300 0.60235000
1454      Core RigidRotor

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```

1455      SymmetryFactor      0.5
1456      End
1457      Rotor  Hindered
1458      Group                13 14 15
1459      Axis                12 1
1460      Symmetry           3
1461      Potential[kcal/mol]  12
1462      -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
1463      End
1464      Rotor  Hindered
1465      Group                17
1466      Axis                16 1
1467      Symmetry           1
1468      Potential[kcal/mol]  36
1469      0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
1470      2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
1471      0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
1472      End
1473      Frequencies[1/cm]    42
1474      15.78 24 197.35 217.04 341.49 399.57 448.98 526.58 553.99
1475      633.67 725.34 800.01 844.86 885.80 923.90 942.75 967.78 977.19 1009.90
1476      1020.84 1069.13 1137.73 1158.97 1192.22 1294.78 1308.40 1370.31 1415.26 1443.52
1477      1452.92 1470.67 1562.95 1583.22 2929.66 2990.49 3012.76 3056.33 3057.86 3070.58
1478      3078.15 3090.40 3590.32
1479      ZeroEnergy[kcal/mol] -1.71
1480      ElectronicLevels[1/cm] 1
1481      0      2
1482      End
1483      !*****
1484      RRHO                14
1485      Geometry[angstrom]  17
1486      C      0.00000000    0.00000000    0.00000000
1487      C      0.00000000    0.00000000    1.40127400
1488      C      1.19728500    0.00000000    2.12076900
1489      C      2.42052300    0.00356300    1.44750100
1490      C      2.43484200    0.00754900    0.05129400
1491      C      1.23446300    0.00753300   -0.66302900
1492      H      -0.94549900   -0.00407300    1.93317100
1493      H      1.17391800   -0.00163700    3.20428000
1494      H      3.35021200    0.00206200    2.00345300
1495      H      3.37832000    0.01181100   -0.48197700
1496      H      1.25566400    0.00935800   -1.74767100
1497      C      -1.29282800   -0.05335400   -0.77331300
1498      H      -2.10136800    0.43261200   -0.22420100
1499      H      -1.19322600    0.43813900   -1.74281700

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1500 H          -1.58951400  -1.09077900  -0.95450900
1501 O           0.87359900  -4.57416500   0.50572500
1502 H           1.01726600  -3.61517600   0.59511400
1503 Core      RigidRotor
1504      SymmetryFactor          0.5
1505 End
1506      Rotor  Hindered
1507      Group                13 14 15
1508      Axis                  12 1
1509      Symmetry              3
1510 Potential[kcal/mol]      12
1511   -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
1512 End
1513      Rotor  Hindered
1514      Group                17
1515      Axis                  16 1
1516      Symmetry              1
1517 Potential[kcal/mol]      36
1518   0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
1519   2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
1520   0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
1521 End
1522 Frequencies[1/cm]          42
1523 15.87 24.02 198.72 215.03 341.38 399.62 447.98 526.36 544.29
1524 633.71 724.51 799.98 844.03 884.74 920.69 941.27 967.59 977.08 1009.82
1525 1020.51 1069.02 1137.55 1158.81 1192.17 1294.61 1308.23 1370.19 1415.22 1443.43
1526 1452.86 1470.62 1562.89 1583.17 2929.53 2990.31 3012.72 3056.15 3057.69 3070.42
1527 3078.02 3090.31 3590.81
1528 ZeroEnergy[kcal/mol]          -1.37
1529 ElectronicLevels[1/cm]          1
1530      0      2
1531 End
1532 !*****
1533 RRHO                                16
1534 Geometry[angstrom]              17
1535 C           0.00000000   0.00000000   0.00000000
1536 C           0.00000000   0.00000000   1.40127400
1537 C           1.19728500   0.00000000   2.12076900
1538 C           2.42052300   0.00356300   1.44750100
1539 C           2.43484200   0.00754900   0.05129400
1540 C           1.23446300   0.00753300  -0.66302900
1541 H          -0.94549900  -0.00407300   1.93317100
1542 H           1.17391800  -0.00163700   3.20428000
1543 H           3.35021200   0.00206200   2.00345300
1544 H           3.37832000   0.01181100  -0.48197700

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1545  H           1.25566400   0.00935800  -1.74767100
1546  C          -1.29282800  -0.05335400  -0.77331300
1547  H          -2.10136800   0.43261200  -0.22420100
1548  H          -1.19322600   0.43813900  -1.74281700
1549  H          -1.58951400  -1.09077900  -0.95450900
1550  O           0.86271900  -4.77373700   0.49848900
1551  H           1.00638600  -3.81474900   0.58787800
1552      Core   RigidRotor
1553      SymmetryFactor           0.5
1554      End
1555      Rotor  Hindered
1556      Group                13 14 15
1557      Axis                 12 1
1558      Symmetry              3
1559      Potential[kcal/mol]      12
1560      -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
1561      End
1562      Rotor  Hindered
1563      Group                17
1564      Axis                 16 1
1565      Symmetry              1
1566      Potential[kcal/mol]      36
1567      0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
1568      2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
1569      0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
1570      End
1571      Frequencies[1/cm]          42
1572      16.00 24.33  199.41 211.94 341.29 399.79 447.60 526.16 539.30
1573      633.73 723.98 799.96 843.44 884.05 918.88 940.34 967.46 976.98 1009.76
1574      1020.32 1068.93 1137.40 1158.69 1192.13 1294.47 1308.07 1370.04 1415.19
1575      1443.36 1452.83 1470.58 1562.85 1583.12 2929.44 2990.18 3012.67 3056.00 3057.55
1576      3070.29 3077.91 3090.22 3591.51
1577      ZeroEnergy[kcal/mol]          -1.09
1578      ElectronicLevels[1/cm]          1
1579      0      2
1580      End
1581      !*****
1582      RRHO                               19
1583      Geometry[angstrom]              17
1584      C           0.00000000   0.00000000   0.00000000
1585      C           0.00000000   0.00000000   1.40127400
1586      C           1.19728500   0.00000000   2.12076900
1587      C           2.42052300   0.00356300   1.44750100
1588      C           2.43484200   0.00754900   0.05129400
1589      C           1.23446300   0.00753300  -0.66302900

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1590  H          -0.94549900  -0.00407300   1.93317100
1591  H           1.17391800  -0.00163700   3.20428000
1592  H           3.35021200   0.00206200   2.00345300
1593  H           3.37832000   0.01181100  -0.48197700
1594  H           1.25566400   0.00935800  -1.74767100
1595  C          -1.29282800  -0.05335400  -0.77331300
1596  H          -2.10136800   0.43261200  -0.22420100
1597  H          -1.19322600   0.43813900  -1.74281700
1598  H          -1.58951400  -1.09077900  -0.95450900
1599  O           0.84639900  -5.07309600   0.48763600
1600  H           0.99006600  -4.11410800   0.57702500
1601  Core      RigidRotor
1602  SymmetryFactor          0.5
1603  End
1604  Rotor      Hindered
1605  Group                      13 14 15
1606  Axis                      12 1
1607  Symmetry                    3
1608  Potential[kcal/mol]       12
1609  -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
1610  End
1611  Rotor      Hindered
1612  Group                      17
1613  Axis                      16 1
1614  Symmetry                    1
1615  Potential[kcal/mol]       36
1616  0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
1617  2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
1618  0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
1619  End
1620  Frequencies[1/cm]         42
1621  4.16 6.31 200.10 207.33 341.20 400.12 447.77 526.07 536.79
1622  633.76 723.46 799.93 842.82 883.43 917.63 939.51 967.31 976.85 1009.68
1623  1020.25 1068.83 1137.22 1158.52 1192.07 1294.28 1307.88 1369.83 1415.14 1443.30
1624  1452.79 1470.53 1562.78 1583.06 2929.32 2990.01 3012.60 3055.80 3057.36 3070.13
1625  3077.78 3090.11 3592.05
1626  ZeroEnergy[kcal/mol]      -0.73
1627  ElectronicLevels[1/cm]    1
1628  0      2
1629  End
1630  !*****
1631  RRHO                      23
1632  Geometry[angstrom]        17
1633  C           0.00000000   0.00000000   0.00000000
1634  C           0.00000000   0.00000000   1.40127400

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1635  C          1.19728500   0.00000000   2.12076900
1636  C          2.42052300   0.00356300   1.44750100
1637  C          2.43484200   0.00754900   0.05129400
1638  C          1.23446300   0.00753300  -0.66302900
1639  H          -0.94549900  -0.00407300   1.93317100
1640  H          1.17391800  -0.00163700   3.20428000
1641  H          3.35021200   0.00206200   2.00345300
1642  H          3.37832000   0.01181100  -0.48197700
1643  H          1.25566400   0.00935800  -1.74767100
1644  C          -1.29282800  -0.05335400  -0.77331300
1645  H          -2.10136800   0.43261200  -0.22420100
1646  H          -1.19322600   0.43813900  -1.74281700
1647  H          -1.58951400  -1.09077900  -0.95450900
1648  O          0.82463900  -5.47224200   0.47316400
1649  H          0.96830600  -4.51325300   0.56255300
1650          Core   RigidRotor
1651          SymmetryFactor           0.5
1652          End
1653          Rotor   Hindered
1654          Group                13 14 15
1655          Axis                  12 1
1656          Symmetry              3
1657          Potential[kcal/mol]    12
1658          -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
1659          End
1660          Rotor   Hindered
1661          Group                17
1662          Axis                  16 1
1663          Symmetry              1
1664          Potential[kcal/mol]    36
1665          0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
1666          2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
1667          0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
1668          End
1669          Frequencies[1/cm]      42
1670          9.81 12.62 197.39 202.91 341.11 400.47 448.14 526.18 536.11
1671          633.78 722.95 799.90 842.17 882.82 916.77 938.70 967.18 976.70 1009.62
1672          1020.23 1068.72 1137.03 1158.35 1192.01 1294.10 1307.68 1369.55 1415.09 1443.22
1673          1452.76 1470.46 1562.70 1582.99 2929.22 2989.83 3012.51 3055.59 3057.17 3069.94
1674          3077.63 3090.01 3592.43
1675          ZeroEnergy[kcal/mol]   -0.38
1676          ElectronicLevels[1/cm] 1
1677          0      2
1678          End
1679          !*****

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1680          RRHO                               28
1681          Geometry[angstrom]                17
1682  C              0.00000000    0.00000000    0.00000000
1683  C              0.00000000    0.00000000    1.40127400
1684  C              1.19728500    0.00000000    2.12076900
1685  C              2.42052300    0.00356300    1.44750100
1686  C              2.43484200    0.00754900    0.05129400
1687  C              1.23446300    0.00753300   -0.66302900
1688  H              -0.94549900   -0.00407300    1.93317100
1689  H              1.17391800   -0.00163700    3.20428000
1690  H              3.35021200    0.00206200    2.00345300
1691  H              3.37832000    0.01181100   -0.48197700
1692  H              1.25566400    0.00935800   -1.74767100
1693  C              -1.29282800   -0.05335400   -0.77331300
1694  H              -2.10136800    0.43261200   -0.22420100
1695  H              -1.19322600    0.43813900   -1.74281700
1696  H              -1.58951400   -1.09077900   -0.95450900
1697  O              0.79744000   -5.97117400    0.45507400
1698  H              0.94110700   -5.01218500    0.54446300
1699          Core   RigidRotor
1700          SymmetryFactor                0.5
1701          End
1702          Rotor   Hindered
1703          Group                                13 14 15
1704          Axis                                12 1
1705          Symmetry                            3
1706          Potential[kcal/mol]                12
1707          -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
1708          End
1709          Rotor   Hindered
1710          Group                                17
1711          Axis                                16 1
1712          Symmetry                            1
1713          Potential[kcal/mol]                36
1714          0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
1715          2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
1716          0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
1717          End
1718          Frequencies[1/cm]                  42
1719          11.74 15.17 188.86 202.62 341.04 400.63 448.25 526.28 535.56
1720          633.78 722.42 799.86 841.51 882.17 915.82 937.80 967.05 976.59 1009.54
1721          1020.23 1068.62 1136.86 1158.21 1191.93 1293.95 1307.50 1369.27 1415.05 1443.14
1722          1452.75 1470.40 1562.62 1582.91 2929.14 2989.68 3012.42 3055.37 3056.99 3069.77
1723          3077.50 3089.90 3592.48
1724          ZeroEnergy[kcal/mol]                -0.11

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1725      ElectronicLevels[1/cm]          1
1726          0          2
1727      End
1728      End
1729      !*****
1730      Bimolecular      P1m      # mCH3Phenyl + H2O
1731      Fragment PROD1
1732      RRHO
1733      Geometry[angstrom]          14
1734      C      -0.25343300      -1.24974700      -0.00962600
1735      C      1.12063000      -1.27682000      0.00330000
1736      C      1.95220100      -0.18048800      0.00814000
1737      C      1.31803200      1.07076900      0.00208400
1738      C      -0.07510300      1.15684400      -0.00917700
1739      C      -0.88065700      0.01164900      -0.01092400
1740      H      3.03200900      -0.26461200      0.01382700
1741      H      1.91641500      1.97551800      0.00091800
1742      H      -0.54683600      2.13347500      -0.01759400
1743      C      -2.38573500      0.11566100      0.00983300
1744      H      -2.71946100      1.06725300      -0.40772900
1745      H      -2.84460900      -0.69006400      -0.56654700
1746      H      -2.76623800      0.04899600      1.03346600
1747      H      -0.84688900      -2.15777400      -0.01812600
1748      Core      RigidRotor
1749          SymmetryFactor      1
1750      End
1751          Rotor          Hindered
1752      Group      11 12 13
1753      Axis          10          6
1754      Symmetry          3
1755      Potential[kcal/mol]          12
1756          0.000 0.009 0.021 0.032 0.033 0.023 0.011 0.001 -0.004 -0.007 -0.008 -0.004
1757      End
1758          Frequencies[1/cm]          35
1759      200.87  344.21  407.23  463.45  517.58  576.53  626.64  738.76
1760      793.19  836.05  873.07  923.76  996.81  970.24  1017.51  1022.06
1761      1060.18 1137.13 1173.96 1253.92 1276.21 1367.83 1384.65 1434.92
1762      1441.41 1445.14 1513.69 1583.68 2929.90 2989.98 3012.02 3054.79
1763      3060.06 3070.22 3083.44
1764      ZeroEnergy[kcal/mol]          0.
1765      ElectronicLevels[1/cm]          1
1766      0.0000000000000000E+000  1.0000000000000000
1767      End
1768      !*****
1769      Fragment PROD2

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1770 RRHO
1771     Geometry[angstrom]           3
1772 O           0.00000000    0.00000000    0.11747400
1773 H           0.00000000    0.75947900   -0.46989500
1774 H           0.00000000   -0.75947900   -0.46989500
1775     Core   RigidRotor
1776         SymmetryFactor    2.0000000000000000
1777     End
1778     Frequencies[1/cm]           3
1779     1553.79 3699.35 3805.91
1780     ZeroEnergy[kcal/mol]         0.
1781     ElectronicLevels[1/cm]           1
1782     0.0000000000000000E+000    1.0000000000000000
1783     End
1784     GroundEnergy[kcal/mol]   -6.07
1785     End
1786     !*****
1787     Bimolecular   P1o   # oCH3Phenyl + H2O
1788     Fragment PROD1
1789     RRHO
1790     Geometry[angstrom]           14
1791 C           0.14867000   -1.19274800   -0.00000100
1792 C          -1.22413800   -1.23410100   -0.00000100
1793 C          -1.89314700    0.00117300    0.00000300
1794 C          -1.15453200    1.18376100    0.00000400
1795 C           0.24221200    1.15341600   -0.00000100
1796 C           0.94544000   -0.06409400   -0.00000200
1797 H          -1.77397100   -2.16810700    0.00000000
1798 H          -2.97702200    0.02887400    0.00000400
1799 H          -1.66697400    2.13864500    0.00000600
1800 H           0.80285000    2.08338700    0.00000200
1801 C           2.45142200   -0.12345000   -0.00000200
1802 H           2.87884500    0.88047600   -0.00004600
1803 H           2.82035800   -0.65347300    0.88114100
1804 H           2.82035100   -0.65354600   -0.88110400
1805     Core   RigidRotor
1806         SymmetryFactor    1
1807     End
1808     Rotor                               Hindered
1809     Group   12 13 14
1810     Axis           11           6
1811     Symmetry           3
1812     Potential[kcal/mol]           12
1813     0.000 0.007 0.031 0.068 0.104 0.131 0.138 0.130 0.102 0.067 0.031 0.008
1814     End

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1815      Frequencies[1/cm]          35
1816      198.31 329.38 402.68 456.67 517.13 530.63 631.41
1817      731.66 798.40 827.87 898.19 909.03 986.62 968.42 1008.80
1818      1017.12 1093.50 1132.82 1184.06 1233.02 1288.52 1368.39 1391.00
1819      1423.69 1436.09 1453.82 1524.91 1583.80 2936.16 2997.04 3014.24
1820      3048.22 3061.97 3074.98 3085.53
1821      ZeroEnergy[kcal/mol]          0.
1822      ElectronicLevels[1/cm]          1
1823      0.0000000000000000E+000  1.0000000000000000
1824      End
1825      !*****
1826      Fragment PROD2
1827      RRHO
1828      Geometry[angstrom]          3
1829      O          0.00000000  0.00000000  0.11747400
1830      H          0.00000000  0.75947900 -0.46989500
1831      H          0.00000000 -0.75947900 -0.46989500
1832      Core  RigidRotor
1833      SymmetryFactor  2.0000000000000000
1834      End
1835      Frequencies[1/cm]          3
1836      1553.79 3699.35 3805.91
1837      ZeroEnergy[kcal/mol]          0.
1838      ElectronicLevels[1/cm]          1
1839      0.0000000000000000E+000  1.0000000000000000
1840      End
1841      GroundEnergy[kcal/mol]  -6.28
1842      End
1843      !*****
1844      Bimolecular  P1p  # pCH3Phenyl + H2O
1845      Fragment PROD1
1846      RRHO
1847      Geometry[angstrom]          14
1848      C          -0.13092100  1.20604100 -0.00869100
1849      C          1.27190700  1.22137000  0.00276700
1850      C          1.90400500 -0.00017400  0.00939800
1851      C          1.27149500 -1.22163000  0.00271600
1852      C          -0.13121100 -1.20591500 -0.00879500
1853      C          -0.84250300  0.00021200 -0.01101100
1854      H          1.81628900 -2.15837200  0.00207300
1855      H          -0.67249200 -2.14708300 -0.01797400
1856      C          -2.35158600  0.00011300  0.00950600
1857      H          -2.75315000 -0.87818200 -0.49955400
1858      H          -2.72979200 -0.01103200  1.03624300
1859      H          -2.75296000  0.88921700 -0.48047800

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1860 H -0.67190900 2.14735800 -0.01781800
1861 H 1.81690500 2.15799300 0.00217000
1862 Core RigidRotor
1863 SymmetryFactor 1
1864 End
1865 Rotor Hindered
1866 Group 10 11 12
1867 Axis 9 5
1868 Symmetry 3
1869 Potential[kcal/mol] 12
1870 0.000 0.002 0.010 0.013 0.010 0.002 0.000 0.002 0.011 0.013 0.010 0.002
1871 End
1872 Frequencies[1/cm] 35
1873 216.70 343.63 395.03 444.07 530.64 582.26 615.27
1874 767.29 786.35 804.70 888.82 932.70 961.92 973.11 1016.78
1875 1021.61 1072.79 1140.64 1185.65 1259.22 1285.76 1346.06 1371.89
1876 1429.29 1443.45 1449.61 1546.28 1569.65 2929.45 2988.59 3010.86
1877 3050.68 3050.92 3076.31 3078.08
1878 ZeroEnergy[kcal/mol] 0.
1879 ElectronicLevels[1/cm] 1
1880 0.0000000000000000E+000 1.0000000000000000
1881 End
1882 !*****
1883 Fragment PROD2
1884 RRHO
1885 Geometry[angstrom] 3
1886 H 0.00000000 0.76170000 -0.47894200
1887 O 0.00000000 0.00000000 0.11973600
1888 H 0.00000000 -0.76170000 -0.47894200
1889 Core RigidRotor
1890 SymmetryFactor 2.0000000000000000
1891 End
1892 Frequencies[1/cm] 3
1893 1553.79 3699.35 3805.91
1894 ZeroEnergy[kcal/mol] 0.
1895 ElectronicLevels[1/cm] 1
1896 0.0000000000000000E+000 1.0000000000000000
1897 End
1898 GroundEnergy[kcal/mol] -5.56
1899 End
1900 !*****
1901 Barrier B1m W P1m # TS1m
1902 RRHO
1903 Geometry[angstrom] 17
1904 C -1.31246000 -0.41849100 0.01082200

```

1905	C	-1.50905200	0.96848800	0.05567700
1906	C	-0.43405900	1.85843300	0.02272800
1907	C	0.87852100	1.37826800	-6.67E-021400
1908	C	1.05248400	0.00411000	-0.09929300
1909	C	0.00588600	-0.90158100	-0.06066200
1910	H	-2.52260600	1.35769800	0.12012900
1911	H	-0.61567500	2.92977900	0.06015900
1912	H	1.72584700	2.05701400	-0.07575800
1913	H	2.24578000	-0.46049100	-0.21722000
1914	H	0.19667500	-1.97153300	-0.08975100
1915	C	-2.48278000	-1.37496700	0.01371700
1916	H	-3.35545700	-0.93687500	0.50923000
1917	H	-2.78401000	-1.63537000	-1.00962900
1918	H	-2.23537800	-2.31055900	0.52650800
1919	O	3.34835000	-0.90256800	-0.01580800
1920	H	3.36677500	-0.89466900	0.96054400
1921	Core	RigidRotor		
1922		SymmetryFactor	0.5	
1923	End			
1924	Rotor		Hindered	
1925	Group	13 14 15		
1926	Axis	12	1	
1927	Symmetry	3		
1928	Potential[kcal/mol]		12	
1929		0.000 -0.100 -0.175 -0.212 -0.205 -0.146 -0.056 0.040 0.110 0.149 0.141 0.082		
1930	End			
1931	Rotor		Hindered	
1932	Group	17		
1933	Axis	16	2	
1934	Symmetry	1		
1935	Potential[kcal/mol]		36	
1936		0.000 -0.060 -0.099 -0.111 -0.092 -0.038 0.063 0.217 0.430 0.701 0.998 1.306		
1937		1.601 1.858 2.072 2.242 2.373 2.473 2.548 2.604 2.643 2.666 2.673 2.648		
1938		0.621 0.657 0.734 0.841 0.972 0.966 0.972 1.005 0.435 0.293 0.176 0.079		
1939	End			
1940	Tunneling	Eckart		
1941		ImaginaryFrequency[1/cm]	1264	
1942		WellDepth[kcal/mol]	7.62	
1943		WellDepth[kcal/mol]	10.23	
1944	End			
1945	Frequencies[1/cm]		42	
1946		99.58 108.27 203.32 338.00 357.71 422.35 466.97 524.13		
1947		557.71 644.34 741.77 770.72 855.45 860.48 887.81 931.90		
1948		1004.59 1010.42 1055.49 1058.85 1099.01 1125.31 1188.74 1218.87		
1949		1270.90 1318.77 1345.62 1423.09 1450.60 1498.37 1501.90 1509.93		

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1950      1600.91 1637.56 3045.41 3108.02 3130.74 3177.03 3189.49 3193.89
1951      3211.51 3783.29
1952          ZeroEnergy[kcal/mol]                4.17
1953          ElectronicLevels[1/cm]              1
1954              0      2
1955      End
1956      !*****
1957      Barrier      B1o  W   P1o      # TS1o
1958      RRHO
1959      Geometry[angstrom]                17
1960      C              -1.31174500   -0.41955200   0.01115400
1961      C              -1.50972600   0.96596000   0.06143600
1962      C              -0.43532800   1.85575500   0.02418400
1963      C              0.87573700    1.37555800   -0.05560000
1964      C              1.05353000    0.00136800   -0.11185400
1965      C              0.00384400   -0.90271700  -0.06541600
1966      H              -2.52069400    1.35351600   0.13003400
1967      H              -0.61578500    2.92400600   0.06578700
1968      H              1.72072800    2.05212900   -0.08316800
1969      H              2.18564500   -0.43628900  -0.22681400
1970      H              0.19384500   -1.96974700  -0.10026500
1971      C              -2.48037900   -1.37337400   0.01489300
1972      H              -3.33475500   -0.94653200   0.54344200
1973      H              -2.80044900   -1.59955200  -1.00658700
1974      H              -2.21770900   -2.31753100   0.49565300
1975      O              3.35745800   -0.89830100  -0.00666300
1976      H              3.35391400   -0.89158700   0.96243200
1977      Core      RigidRotor
1978      SymmetryFactor                0.5
1979      End
1980      Rotor                                Hindered
1981      Group      13 14 15
1982      Axis              12              1
1983      Symmetry              3
1984      Potential[kcal/mol]                12
1985      0.000 0.018 0.028 0.023 0.009 -0.015 -0.079 -0.098 -0.088 -0.050 -0.072 -0.044
1986      End
1987      Rotor                                Hindered
1988      Group      17
1989      Axis              16              6
1990      Symmetry              1
1991      Potential[kcal/mol]                36
1992      0.000 0.089 0.205 0.352 0.532 0.746 0.996 1.274 1.558 0.765 0.646 0.658
1993      0.691 0.737 0.795 0.863 0.921 0.979 0.984 0.987 0.997 1.002 1.031 0.471
1994      0.324 0.185 0.062 -0.034 -0.083 -0.058 0.060 0.270 0.539 0.812 1.036 1.227

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1995 End
1996 Tunneling Eckart
1997 ImaginaryFrequency[1/cm] 1209
1998 WellDepth[kcal/mol] 7.30
1999 WellDepth[kcal/mol] 10.12
2000 End
2001 Frequencies[1/cm] 42
2002 97.86 127.03 199.18 327.13 372.60 431.70 483.99 532.09 581.53 646.78
2003 740.84 774.59 829.68 846.16 921.85 935.38 970.04 986.81 1005.74 1020.96
2004 1049.26 1114.64 1138.48 1178.42 1211.77 1255.92 1295.87 1371.38 1409.63 1439.97
2005 1444.60 1457.77 1543.34 1573.66 2932.36 2993.19 3026.92 3053.22 3067.96 3079.73
2006 3089.68 3639.32
2007 ZeroEnergy[kcal/mol] 3.85
2008 ElectronicLevels[1/cm] 1
2009 0 2
2010 End
2011 !*****
2012 Barrier B1p W P1p # TS1p
2013 RRHO
2014 Geometry[angstrom] 17
2015 C -1.31174500 -0.41955200 0.01115400
2016 C -1.50972600 0.96596000 0.06143600
2017 C -0.43532800 1.85575500 0.02418400
2018 C 0.87573700 1.37555800 -0.05560000
2019 C 1.05353000 0.00136800 -0.11185400
2020 C 0.00384400 -0.90271700 -0.06541600
2021 H -2.52069400 1.35351600 0.13003400
2022 H -0.61578500 2.92400600 0.06578700
2023 H 1.72072800 2.05212900 -0.08316800
2024 H 2.18564500 -0.43628900 -0.22681400
2025 H 0.19384500 -1.96974700 -0.10026500
2026 C -2.48037900 -1.37337400 0.01489300
2027 H -3.33475500 -0.94653200 0.54344200
2028 H -2.80044900 -1.59955200 -1.00658700
2029 H -2.21770900 -2.31753100 0.49565300
2030 O 3.35745800 -0.89830100 -0.00666300
2031 H 3.35391400 -0.89158700 0.96243200
2032 Core RigidRotor
2033 SymmetryFactor 1
2034 End
2035 Rotor Hindered
2036 Group 13 14 15
2037 Axis 12 1
2038 Symmetry 3
2039 Potential[kcal/mol] 12

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2040      0.000 -0.002 0.000 0.002 0.004 0.003 -0.001 0.002 0.004 0.002 0.000 -0.002
2041      End
2042      Rotor                      Hindered
2043      Group      17
2044      Axis              16              4
2045      Symmetry              1
2046      Potential[kcal/mol]              36
2047      0.000 0.011 0.039 0.088 0.159 0.241 0.387 0.339 0.390 -0.535 -0.647 -0.711
2048      -0.733 -0.721 -0.682 -0.617 -0.530 -0.420 -0.286 -0.128 0.061 0.269 0.504 0.773
2049      1.076 1.390 1.674 1.872 1.981 2.030 2.049 2.050 2.037 2.014 1.976 1.921
2050      End
2051      Tunneling      Eckart
2052      ImaginaryFrequency[1/cm]      1298
2053      WellDepth[kcal/mol]      7.88
2054      WellDepth[kcal/mol]      9.99
2055      End
2056      Frequencies[1/cm]      42
2057      86.76 118.23 218.15 344.20 374.22 398.27 443.13 567.43 591.73 627.13
2058      754.08 791.85 821.76 822.87 908.30 945.54 967.52 982.11 1020.75 1032.33
2059      1032.39 1091.07 1149.62 1187.01 1219.70 1278.39 1295.49 1365.88 1370.45 1443.19
2060      1447.81 1462.49 1556.50 1563.74 2930.76 2990.73 3012.90 3056.85 3057.02 3084.51
2061      3085.59 3641.84
2062      ZeroEnergy[kcal/mol]      4.43
2063      ElectronicLevels[1/cm]      1
2064      0      2
2065      End
2066      !*****
2067      Bimolecular      P2      # C6H5CH2 + H2O
2068      Fragment PROD1
2069      RRHO
2070      Geometry[angstrom]      14
2071      C      0.25231700      1.21362000      0.00000600
2072      C      -1.13207900      1.20859100      0.00001700
2073      C      -1.83606400      0.00000200      -0.00002900
2074      C      -1.13208300      -1.20859000      -0.00002600
2075      C      0.25231300      -1.21362000      -0.00003600
2076      C      0.98817300      -0.00000100      0.00001100
2077      H      0.79309900      2.15371800      0.00003900
2078      H      -1.67301500      2.14795900      0.00001200
2079      H      -2.91922800      0.00000200      -0.00001700
2080      H      -1.67302000      -2.14795700      -0.00006000
2081      H      0.79309500      -2.15371900      -0.00003600
2082      C      2.40133200      -0.00000200      0.00004900
2083      H      2.95780500      -0.92793000      0.00002300
2084      H      2.95780600      0.92792800      0.00008600

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2085   Core   RigidRotor
2086       SymmetryFactor   1
2087   End
2088       Rotor Hindered           ! freq=375
2089       Group             13 14
2090       Axis              1 12
2091       Symmetry          2
2092   Potential[kcal/mol]   18
2093       0.000 0.295 1.165 2.555 4.373 6.493 8.752 10.949 12.838 14.049 12.809 10.859
2094       8.594 6.299 4.190 2.421 1.094 0.276
2095   End
2096       Frequencies[1/cm]           35
2097       192.09 355.22 431.25 456.03 472.36 533.82 623.48 630.07 719.79 829.95
2098       838.15 876.01 914.62 940.52 976.50 963.58 1009.32 1080.72 1133.11 1141.75
2099       1232.11 1280.82 1305.32 1429.06 1440.71 1448.76 1546.36 1558.84 3047.04 3059.70
2100       3062.05 3074.18 3079.56 3092.51 3146.51
2101   ZeroEnergy[kcal/mol]           0.
2102   ElectronicLevels[1/cm]           1
2103       0.0000000000000000E+000   2.0000000000000000
2104   End
2105   !*****
2106   Fragment PROD2
2107   RRHO
2108       Geometry[angstrom]           3
2109   O           0.00000000   0.00000000   0.11747400
2110   H           0.00000000   0.75947900  -0.46989500
2111   H           0.00000000  -0.75947900  -0.46989500
2112   Core   RigidRotor
2113       SymmetryFactor   2.0000000000000000
2114   End
2115       Frequencies[1/cm]           3
2116       1553.79 3699.35 3805.91
2117   ZeroEnergy[kcal/mol]           0.
2118   ElectronicLevels[1/cm]           1
2119       0.0000000000000000E+000   1.0000000000000000
2120   End
2121   GroundEnergy[kcal/mol]   -28.76
2122   End
2123   !*****
2124   Barrier   B2   W   P2           # TS2
2125   Variational
2126   RRHO           !           1
2127   Geometry[angstrom]           17
2128   C           0.31169200   0.00053800   0.60447400
2129   C           -0.35961900   1.21539200   0.31234400

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2130  C          -1.64554000   1.20955000  -0.20059300
2131  C          -2.30030700  -0.00051400  -0.45234400
2132  C          -1.64505900  -1.21007300  -0.19937600
2133  C          -0.35913700  -1.21486200   0.31358800
2134  H           0.14191200   2.15460000   0.51794200
2135  H          -2.14870400   2.14787500  -0.40260200
2136  H          -3.31003500  -0.00091200  -0.84448900
2137  H          -2.14783900  -2.14880400  -0.40044300
2138  H           0.14277200  -2.15365900   0.52013900
2139  C           1.58440400   0.00117000   1.22399800
2140  H           2.05887900   0.93007400   1.51371900
2141  H           2.05965800  -0.92768700   1.51419600
2142  H           2.73551600   0.00014800  -0.36123600
2143  O           3.18568600  -0.00093200  -1.21533300
2144  H           2.46025300  -0.00113400  -1.84483800
2145  Core   RigidRotor
2146          SymmetryFactor   0.831548565
2147  End
2148  Rotor                               Hindered
2149  Group   13   14   15   16   17
2150  Axis              12              1
2151  Symmetry              2
2152  Potential[kcal/mol]              18
2153  0.000 0.302 1.140 2.508 4.336 6.509 8.874 11.201 13.222 14.572 13.350 11.324
2154  9.051 6.688 4.548 2.744 1.404 0.611
2155  End
2156  Rotor                               Hindered
2157  Group   17
2158  Axis              16              15
2159  Symmetry              1
2160  Potential[kcal/mol]              36
2161  0.000 -0.014 -0.011 -0.015 -0.014 -0.009 0.000 0.012 0.022 0.025 0.028 0.032
2162  0.035 0.035 0.030 0.026 0.024 0.025 0.041 0.025 0.024 0.026 0.031 0.036
2163  0.035 0.032 0.028 0.025 0.022 0.012 0.000 -0.009 -0.014 -0.015 -0.011 -0.014
2164  End
2165  Frequencies[1/cm]              42
2166  141.24 191.60 213.51 301.96 350.73 384.72 412.49 441.87
2167  523.56 535.39 630.24 659.89 722.83 835.40 838.16 889.04
2168  926.71 949.71 980.20 967.38 1010.95 1081.94 1135.80 1144.49
2169  1228.28 1284.63 1307.39 1430.29 1440.77 1451.49 1550.42 1558.48
2170  1566.23 3037.39 3062.17 3064.85 3075.81 3082.15 3093.43 3138.95
2171  3568.48 3751.44
2172  ZeroEnergy[kcal/mol]   -28.62
2173  ElectronicLevels[1/cm]              1
2174  0.000000000000000000   2.0000000000000000

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2175 End
2176 !*****
2177 RRHO ! 2
2178 Geometry[angstrom] 17
2179 C 0.32029000 0.00054100 0.58667700
2180 C -0.35655100 1.21434400 0.30768800
2181 C -1.64649500 1.20886300 -0.19630600
2182 C -2.30165100 -0.00052600 -0.44876700
2183 C -1.64599100 -1.20937200 -0.19511000
2184 C -0.35604800 -1.21384400 0.30891900
2185 H 0.14554500 2.15389900 0.51039000
2186 H -2.15115800 2.14765300 -0.39229700
2187 H -3.31248900 -0.00092400 -0.83805500
2188 H -2.15026600 -2.14856500 -0.39018200
2189 H 0.14642600 -2.15299300 0.51255200
2190 C 1.60878200 0.00111900 1.17531600
2191 H 2.08420800 0.93086700 1.46553600
2192 H 2.08450600 -0.92812600 1.46673300
2193 H 2.73019700 -0.00010600 -0.30501500
2194 O 3.15884900 -0.00088500 -1.17020300
2195 H 2.41386900 -0.00104100 -1.77535200
2196 Core RigidRotor
2197 SymmetryFactor 0.831548565
2198 End
2199 Rotor Hindered
2200 Group 13 14 15 16 17
2201 Axis 12 1
2202 Symmetry 2
2203 Potential[kcal/mol] 18
2204 0.000 0.373 1.265 2.682 4.551 6.751 9.123 11.433 13.404 14.658 13.177 11.113
2205 8.790 6.473 4.360 2.597 1.310 0.574
2206 End
2207 Rotor Hindered
2208 Group 17
2209 Axis 16 15
2210 Symmetry 1
2211 Potential[kcal/mol] 36
2212 0.000 -0.014 -0.012 -0.016 -0.014 -0.009 0.000 0.011 0.021 0.025 0.028 0.032
2213 0.037 0.037 0.032 0.027 0.024 0.025 0.015 0.026 0.024 0.027 0.032 0.037
2214 0.036 0.032 0.028 0.025 0.021 0.011 0.000 -0.009 -0.014 -0.016 -0.012 -0.014
2215 End
2216 Frequencies[1/cm] 42
2217 131.41 194.57 199.39 317.79 350.06 386.39 418.85 442.98
2218 531.83 535.05 630.38 683.17 723.83 835.92 837.58 890.02
2219 926.92 950.06 980.66 968.17 1011.54 1081.64 1135.86 1145.02

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2220      1226.30 1284.56 1307.44 1429.85 1440.20 1452.07 1551.07 1557.07
2221      1564.38 3035.56 3062.03 3064.67 3075.66 3082.08 3093.39 3136.97
2222      3554.05 3750.72
2223      ZeroEnergy[kcal/mol]   -27.44
2224      ElectronicLevels[1/cm]                               1
2225      0.000000000000000000      2.0000000000000000
2226      End
2227      !*****
2228      RRHO      !      3
2229      Geometry[angstrom]      17
2230      C      0.32963200      0.00052700      0.57357900
2231      C      -0.35562800      1.21119100      0.30716800
2232      C      -1.64865400      1.20718100      -0.19387300
2233      C      -2.30435900      -0.00052200      -0.44940700
2234      C      -1.64815400      -1.20770100      -0.19269100
2235      C      -0.35513700      -1.21068900      0.30838100
2236      H      0.14588300      2.15222200      0.50488000
2237      H      -2.15282600      2.14716300      -0.38536200
2238      H      -3.31418900      -0.00092000      -0.84145600
2239      H      -2.15193600      -2.14807800      -0.38326700
2240      H      0.14676200      -2.15131900      0.50701200
2241      C      1.64442000      0.00108300      1.12127400
2242      H      2.08856900      0.92910100      1.46413200
2243      H      2.08875600      -0.92631400      1.46558500
2244      H      2.71573900      -0.00012600      -0.25678200
2245      O      3.13187800      -0.00085000      -1.12830000
2246      H      2.37845000      -0.00098600      -1.72361400
2247      Core      RigidRotor
2248      SymmetryFactor      0.831548565
2249      End
2250      Rotor      Hindered
2251      Group      13      14      15      16      17
2252      Axis      12      1
2253      Symmetry      2
2254      Potential[kcal/mol]      18
2255      0.000 0.544 1.614 3.189 5.180 7.458 9.836 12.071 13.870 128.213 13.631 22.593
2256      8.744 5.696 3.683 2.063 0.949 0.404
2257      End
2258      Rotor      Hindered
2259      Group      17
2260      Axis      16      15
2261      Symmetry      1
2262      Potential[kcal/mol]      36
2263      0.000 -0.014 -0.012 -0.016 -0.015 -0.009 -0.001 0.011 0.020 0.025 0.028 0.033
2264      0.037 0.038 0.033 0.028 0.024 0.026 0.044 0.024 0.025 0.030 0.034 0.037

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2265      0.037 0.032 0.028 0.025 0.020 0.010 0.000 -0.009 -0.015 -0.016 -0.012 -0.014
2266      End
2267      Frequencies[1/cm]          42
2268      134.58 189.30 211.30 349.31 350.26 393.19 444.43 456.82 533.97 552.31
2269      630.75 722.71 766.78 834.07 837.83 893.89 927.86 951.69 983.19 971.00
2270      1013.08 1080.54 1136.27 1145.79 1215.79 1283.70 1307.33 1428.38 1437.07 1453.07
2271      1550.32 1553.32 1562.26 3026.04 3061.50 3064.02 3075.06 3081.78 3093.09 3125.73
2272      3485.41 3746.84
2273      ZeroEnergy[kcal/mol]    -24.71
2274      ElectronicLevels[1/cm]          1
2275      0.000000000000000000      2.0000000000000000
2276      End
2277      !*****
2278      RRHO          !          4
2279      Geometry[angstrom]          17
2280      C          0.33049100      0.00052000      0.57033800
2281      C          -0.35601300      1.20935000      0.30793900
2282      C          -1.65064800      1.20689900      -0.19387500
2283      C          -2.30545500      -0.00052000      -0.45009200
2284      C          -1.65015100      -1.20742200      -0.19269500
2285      C          -0.35552700      -1.20884400      0.30914200
2286      H          0.14670100      2.15039600      0.50302000
2287      H          -2.15440700      2.14706700      -0.38548700
2288      H          -3.31490200      -0.00092100      -0.84334300
2289      H          -2.15351800      -2.14798600      -0.38339200
2290      H          0.14758200      -2.14949000      0.50514100
2291      C          1.66847700      0.00106200      1.09419200
2292      H          2.07338200      0.92611000      1.49486100
2293      H          2.07352900      -0.92325100      1.49641900
2294      H          2.70434200      -0.00012600      -0.24085400
2295      O          3.12090600      -0.00083600      -1.11170500
2296      H          2.36977300      -0.00097100      -1.70758200
2297      Core      RigidRotor
2298      SymmetryFactor      0.831548565
2299      End
2300      Rotor          Hindered
2301      Group      13      14      15      16      17
2302      Axis          12          1
2303      Symmetry          2
2304      Potential[kcal/mol]          18
2305      0.000 0.928 2.377 4.270 6.486 8.862 11.160 13.097 14.288 12.649 10.562 8.230
2306      5.921 3.827 2.090 0.835 0.136 0.039
2307      End
2308      Rotor          Hindered
2309      Group      17

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2310 Axis          16          15
2311 Symmetry      1
2312 Potential[kcal/mol]          36
2313   0.000 -0.014 -0.012 -0.016 -0.014 -0.009 0.000 0.011 0.021 0.025 0.028 0.032
2314   0.037 0.038 0.032 0.027 0.024 0.025 0.102 0.027 0.025 0.028 0.032 0.038
2315   0.037 0.032 0.028 0.025 0.021 0.011 0.000 -0.009 -0.015 -0.016 -0.012 -0.014
2316 End
2317   Frequencies[1/cm]          42
2318   149.28 202.18 228.00 349.10 364.94 397.03 450.20 476.22 533.14 559.54
2319   631.08 724.78 802.71 831.96 839.39 896.80 928.85 952.39 985.63 973.46
2320   1013.90 1079.68 1136.80 1145.59 1205.55 1284.04 1307.19 1427.91 1433.20 1453.66
2321   1546.82 1555.85 1562.53 3017.64 3061.26 3063.77 3074.66 3081.72 3092.83 3115.11
2322   3419.17 3742.86
2323 ZeroEnergy[kcal/mol]  -22.73
2324   ElectronicLevels[1/cm]          1
2325   0.000000000000000000          2.0000000000000000
2326 End
2327 !*****
2328 RRHO          !          5
2329 Geometry[angstrom]          17
2330 C          0.32635200          0.00052000          0.56881600
2331 C          -0.35595200          1.20807900          0.30857100
2332 C          -1.65208800          1.20696600          -0.19435400
2333 C          -2.30594400          -0.00052000          -0.45045500
2334 C          -1.65159100          -1.20749000          -0.19317500
2335 C          -0.35546500          -1.20757300          0.30976700
2336 H          0.14894600          2.14813400          0.50259300
2337 H          -2.15567600          2.14713400          -0.38647200
2338 H          -3.31556400          -0.00091800          -0.84357500
2339 H          -2.15479000          -2.14805300          -0.38437600
2340 H          0.14982400          -2.14722800          0.50470600
2341 C          1.69351900          0.00104100          1.07100500
2342 H          2.04504000          0.91825800          1.53823900
2343 H          2.04516200          -0.91530900          1.53985500
2344 H          2.68173000          -0.00012500          -0.24003000
2345 O          3.11363500          -0.00082600          -1.09949800
2346 H          2.35296100          -0.00095400          -1.69088400
2347   Core   RigidRotor
2348         SymmetryFactor  0.831548565
2349 End
2350   Rotor          Hindered
2351   Group   13   14   15   16   17
2352   Axis          12          1
2353   Symmetry      2
2354   Potential[kcal/mol]          18

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2355 0.000 1.252 2.984 5.091 7.431 9.786 11.906 13.453 12.842 10.914 8.672 6.304
2356 4.107 2.215 0.761 -0.162 -0.498 -0.220
2357 End
2358 Rotor Hindered
2359 Group 17
2360 Axis 16 15
2361 Symmetry 1
2362 Potential[kcal/mol] 36
2363 0.000 -0.014 -0.011 -0.016 -0.014 -0.009 0.000 0.012 0.022 0.025 0.028 0.032
2364 0.036 0.036 0.031 0.026 0.024 0.025 0.045 0.016 0.024 0.026 0.031 0.036
2365 0.036 0.032 0.028 0.025 0.022 0.012 0.000 -0.008 -0.014 -0.016 -0.011 -0.015
2366 End
2367 Frequencies[1/cm] 42
2368 60.94 217.64 247.73 349.43 381.58 398.4 455.17 495.19 531.1 550.45
2369 631.8 727.51 817.1 841.63 872.65 902.42 931.04 952.42 991.65 977.8
2370 1014.84 1078.07 1137.7 1143.22 1187.19 1287.89 1306.79 1426.71 1428.13 1455.09
2371 1546.77 1561.97 1564.39 2996.16 3061.34 3063.99 3074.34 3081.81 3087.27 3092.47
2372 3484.28 3716.41
2373 ZeroEnergy[kcal/mol] -19.81
2374 ElectronicLevels[1/cm] 1
2375 0.0000000000000000 2.0000000000000000
2376 End
2377 !*****
2378 RRHO ! 6
2379 Geometry[angstrom] 17
2380 C 0.32302500 0.00051900 0.56859800
2381 C -0.35573500 1.20754800 0.30893200
2382 C -1.65265700 1.20697900 -0.19462300
2383 C -2.30616700 -0.00052000 -0.45058300
2384 C -1.65216000 -1.20750400 -0.19344400
2385 C -0.35525000 -1.20704100 0.31012600
2386 H 0.14932500 2.14750200 0.50290300
2387 H -2.15605300 2.14720900 -0.38678800
2388 H -3.31591200 -0.00091800 -0.84353000
2389 H -2.15516700 -2.14812900 -0.38469100
2390 H 0.15020300 -2.14659500 0.50501300
2391 C 1.70387100 0.00103300 1.06248300
2392 H 2.03183400 0.91298700 1.55521400
2393 H 2.03194600 -0.91000100 1.55684000
2394 H 2.64347000 -0.00009100 -0.20459300
2395 O 3.11388100 -0.00082600 -1.09824800
2396 H 2.34149500 -0.00094000 -1.67673000
2397 Core RigidRotor
2398 SymmetryFactor 0.831548565
2399 End

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2400 Rotor                               Hindered
2401 Group   13   14   15   16   17
2402 Axis                12           1
2403 Symmetry            2
2404 Potential[kcal/mol]                18
2405 0  1.376  3.21  5.387  7.754  10.078  12.091  13.427  13.146  10.159  7.821
2406 5.494
2407 3.359  1.561  0.229  -0.555  -0.743  -0.318
2408 End
2409 Rotor                               Hindered
2410 Group   17
2411 Axis                16           15
2412 Symmetry            1
2413 Potential[kcal/mol]                36
2414 0.000 -0.014 -0.011 -0.015 -0.014 -0.009 0.000 0.013 0.023 0.026 0.028 0.031
2415 0.034 0.034 0.030 0.025 0.024 0.025 0.052 0.026 0.023 0.025 0.029 0.033
2416 0.034 0.031 0.028 0.026 0.023 0.013 0.000 -0.009 -0.014 -0.015 -0.011 -0.015
2417 End
2418 Frequencies[1/cm]                42
2419 155.16 248.58 283.22 347.65 382.38 401.45 455.56 496.33 531.45 564.85
2420 631.86 727.66 816.37 841.84 873.22 902.82 931.31 952.48 989.68 978.13
2421 1014.9 1077.77 1137.81 1143.39 1186.34 1288.29 1306.79 1424.62 1428.17 1455.41
2422 1556.46 1562.42 1565.38 3004.19 3061.41 3064.09 3074.36 3081.89 3092.47 3095.29
2423 3312.26 3716.93
2424 ZeroEnergy[kcal/mol] -17.14
2425 ElectronicLevels[1/cm]                1
2426 0.000000000000000000 2.0000000000000000
2427 End
2428 !*****
2429 RRHO ! 7
2430 Geometry[angstrom] 17
2431 C 0.32128400 0.00051900 0.56850600
2432 C -0.35556400 1.20726800 0.30912600
2433 C -1.65293600 1.20697800 -0.19477400
2434 C -2.30628400 -0.00052000 -0.45065300
2435 C -1.65244000 -1.20750200 -0.19359600
2436 C -0.35507900 -1.20676100 0.31031800
2437 H 0.14938500 2.14729800 0.50314700
2438 H -2.15621500 2.14724800 -0.38691900
2439 H -3.31610700 -0.00091800 -0.84349400
2440 H -2.15532800 -2.14816800 -0.38482200
2441 H 0.15026200 -2.14639100 0.50525700
2442 C 1.70869000 0.00103000 1.05872700
2443 H 2.02532000 0.91074600 1.56399800
2444 H 2.02542800 -0.90774200 1.56562900

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2445 H 2.60183400 -0.00003800 -0.14310800
2446 O 3.11565100 -0.00082800 -1.10070200
2447 H 2.33578700 -0.00093500 -1.67143900
2448 Core RigidRotor
2449 SymmetryFactor 0.831548565
2450 End
2451 Rotor Hindered
2452 Group 13 14 15 16 17
2453 Axis 12 1
2454 Symmetry 2
2455 Potential[kcal/mol] 18
2456 0 1.432 3.313 5.521 7.895 10.199 12.154 13.378 11.821 9.746 7.537
2457 5.105
2458 3.001 1.251 -0.021 -0.739 -0.857 -0.363
2459 End
2460 Rotor Hindered
2461 Group 17
2462 Axis 16 15
2463 Symmetry 1
2464 Potential[kcal/mol] 36
2465 0.000 -0.015 -0.008 -0.014 -0.013 -0.009 0.000 0.013 0.024 0.025 0.025 0.026
2466 0.027 0.026 0.025 0.023 0.023 0.030 0.036 0.034 0.023 0.025 0.025 0.026
2467 0.027 0.027 0.025 0.025 0.024 0.014 0.000 -0.009 -0.013 -0.014 -0.007 -0.015
2468 End
2469 Frequencies[1/cm] 42
2470 197.48 292.79 342.7 397.06 456.08 497.02 526.02 533.24 632.44 665.92
2471 732.09 802.84 842.5 867.96 903.43 932.47 951.35 957.57 975.84 980.89
2472 1015.27 1077.2 1138.93 1145.79 1177.15 1293.04 1306.86 1416.26 1428.43 1429.03
2473 1463.79 1566.62 1567.34 1762.09 2995.95 3061.81 3064.51 3074.34 3081.35 3082.72
2474 3092.47 3668.97
2475 ZeroEnergy[kcal/mol] -13.05
2476 ElectronicLevels[1/cm] 1
2477 0.000000000000000000 2.0000000000000000
2478 End
2479 !*****
2480 RRHO ! 8
2481 Geometry[angstrom] 17
2482 C 0.31994800 0.00051800 0.56845200
2483 C -0.35541900 1.20705300 0.30927100
2484 C -1.65315600 1.20697700 -0.19490600
2485 C -2.30640600 -0.00052000 -0.45071800
2486 C -1.65266000 -1.20750200 -0.19372700
2487 C -0.35493400 -1.20654600 0.31046300
2488 H 0.14938400 2.14717800 0.50341300
2489 H -2.15635100 2.14728500 -0.38701600

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2490  H          -3.31628700  -0.00091800  -0.84343900
2491  H          -2.15546500  -2.14820600  -0.38491800
2492  H           0.15026200  -2.14626900   0.50552200
2493  C           1.71224100   0.00102800   1.05616700
2494  H           2.02010500   0.90900800   1.57106800
2495  H           2.02020900  -0.90598900   1.57270400
2496  H           2.56170100   0.00001600  -0.07847300
2497  O           3.11766500  -0.00083100  -1.10391000
2498  H           2.33172300  -0.00093100  -1.66812200
2499  Core  RigidRotor
2500          SymmetryFactor  0.831548565
2501  End
2502  Rotor                      Hindered
2503  Group  13  14  15  16  17
2504  Axis          12          1
2505  Symmetry          2
2506  Potential[kcal/mol]          18
2507  0.000 1.474 3.388 5.618 7.995 10.282 12.191 13.325 13.035 9.451 7.113 4.811
2508  2.732 1.018 -0.208 -0.877 -0.942 -0.397
2509  End
2510  Rotor                      Hindered
2511  Group  17
2512  Axis          16          15
2513  Symmetry          1
2514  Potential[kcal/mol]          36
2515  0.000 -0.015 -0.009 -0.012 -0.013 -0.009 -0.003 0.007 0.019 0.021 0.021 0.022
2516  0.022 0.023 0.024 0.026 0.030 0.023 0.027 0.023 0.030 0.025 0.024 0.023
2517  0.023 0.022 0.021 0.021 0.020 0.007 -0.003 -0.010 -0.013 -0.012 -0.008 -0.015
2518  End
2519  Frequencies[1/cm]          42
2520  167.35  223.1  342.06 398.21 444.75 485.22 528.56 558.15 561.74 632.76
2521  717.27 743.85 822.47 842.93 900.73 931.76 951.23 988.26 980.65 1014.62
2522  1048.79 1053.1 1081.44 1139.52 1155.76 1189.42 1295.3 1307.29 1419.93 1428.4
2523  1462.3 1541.29 1566.75 1574.32 2990.87 3061.69 3064.22 3074.14 3074.47 3082.43
2524  3092.43 3653.4
2525  ZeroEnergy[kcal/mol] -8.49
2526  ElectronicLevels[1/cm]          1
2527  0.000000000000000000 2.0000000000000000
2528  End
2529  !*****
2530  RRHO          !          9
2531  Geometry[angstrom]          17
2532  C           0.31578600   0.00051800   0.56835900
2533  C          -0.35515500   1.20625100   0.30949000
2534  C          -1.65391400   1.20688600  -0.19555000

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2535  C          -2.30706000  -0.00052100  -0.45097500
2536  C          -1.65341400  -1.20741300  -0.19437000
2537  C          -0.35466700  -1.20574100   0.31067700
2538  H           0.14887400   2.14671000   0.50532200
2539  H          -2.15707900   2.14738200  -0.38739000
2540  H          -3.31728200  -0.00092100  -0.84281000
2541  H          -2.15619000  -2.14830300  -0.38529000
2542  H           0.14975600  -2.14579900   0.50742600
2543  C           1.71917800   0.00102800   1.05732300
2544  H           1.99481200   0.90248700   1.60506100
2545  H           1.99488800  -0.89938600   1.60674900
2546  H           2.46649700   0.00014700   0.11132600
2547  O           3.12707100  -0.00084500  -1.12104500
2548  H           2.31814500  -0.00092200  -1.65715100
2549  Core      RigidRotor
2550          SymmetryFactor    0.831548565
2551  End
2552  Rotor                                Hindered
2553  Group    13    14    15    16    17
2554  Axis              12          1
2555  Symmetry          2
2556  Potential[kcal/mol]          18
2557  0.000 -1.744 -3.009 -3.719 -3.828 -3.326 -2.251 -0.664 1.326 3.580 5.937 8.128
2558  9.911 10.433 8.888 6.745 4.405 2.108
2559  End
2560  Rotor                                Hindered
2561  Group    17
2562  Axis              16          15
2563  Symmetry          1
2564  Potential[kcal/mol]          36
2565  0.000 -0.015 -0.009 -0.012 -0.013 -0.009 -0.003 0.007 0.019 0.021 0.021 0.022
2566  0.023 0.023 0.023 0.025 0.030 0.024 0.027 0.023 0.030 0.025 0.023 0.023
2567  0.023 0.022 0.022 0.021 0.020 0.008 -0.003 -0.009 -0.013 -0.012 -0.008 -0.015
2568  End
2569  Frequencies[1/cm]          42
2570  158.56 223.21 341.92 398.17 438.86 481.95 530.31 540.68 566.18 632.82
2571  722.91 755.69 825.35 842.79 900.11 931.36 950.12 993.22 980.84 1014.12
2572  1047.2 1071.05 1106    1139.82 1158.01 1191.66 1297.16 1307.71 1419.5 1428.32
2573  1463.28 1487.04 1566.19 1575.34 2987.53 3061.36 3063.62 3069.57 3073.85 3082.16
2574  3092.26 3645.28
2575  ZeroEnergy[kcal/mol]    0.75
2576  ElectronicLevels[1/cm]          1
2577  0.000000000000000000    2.0000000000000000
2578  End
2579  !*****

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2580 RRHO ! 10
2581 Geometry[angstrom] 17
2582 C 0.31345584 0.00052263 0.56897532
2583 C -0.35569416 1.20558463 0.30952832
2584 C -1.65460616 1.20666663 -0.19662668
2585 C -2.30794316 -0.00052037 -0.45161068
2586 C -1.65410116 -1.20719137 -0.19544368
2587 C -0.35519716 -1.20507937 0.31071232
2588 H 0.14740384 2.14610463 0.50798632
2589 H -2.15779816 2.14731963 -0.38806668
2590 H -3.31850716 -0.00092237 -0.84259568
2591 H -2.15690516 -2.14823837 -0.38596468
2592 H 0.14829684 -2.14519537 0.51007832
2593 C 1.71693584 0.00103863 1.07511732
2594 H 1.96572684 0.89800263 1.64334432
2595 H 1.96574884 -0.89478337 1.64514132
2596 H 2.45931984 0.00012463 0.19259932
2597 O 3.13805784 -0.00086037 -1.14354268
2598 H 2.30888884 -0.00091937 -1.64913268
2599 Core RigidRotor
2600 SymmetryFactor 0.831548565
2601 End
2602 Rotor Hindered
2603 Group 13 14 15 16 17
2604 Axis 12 1
2605 Symmetry 2
2606 Potential[kcal/mol] 18
2607 0.000 1.552 3.526 5.794 8.172 10.421 12.233 13.177 11.036 8.882 6.528 4.251
2608 2.222 0.580 -0.560 -1.134 -1.099 -0.459
2609 End
2610 Rotor Hindered
2611 Group 17
2612 Axis 16 15
2613 Symmetry 1
2614 Potential[kcal/mol] 36
2615 0.000 -0.015 -0.008 -0.012 -0.013 -0.009 -0.002 0.010 0.021 0.022 0.022 0.023
2616 0.023 0.024 0.024 0.024 0.028 0.027 0.028 0.027 0.028 0.025 0.024 0.024
2617 0.023 0.023 0.022 0.022 0.021 0.010 -0.002 -0.009 -0.013 -0.013 -0.004 -0.015
2618 End
2619 Frequencies[1/cm] 42
2620 133.64 217.76 339.5 396.69 440.35 490.51 514.99 528.22 596.03 632.47
2621 726.29 770.88 833.92 841.53 896.25 928.39 945.9 997.75 979.96 1012.4
2622 1071.22 1072.8 1140.01 1160.47 1187.03 1200.93 1301.59 1309.49 1381.04 1423.02
2623 1428 1468.18 1563.32 1580.02 2979.51 3056.35 3059.99 3062.63 3072.71 3081.15
2624 3091.56 3633.74

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2625 ZeroEnergy[kcal/mol]      1.16
2626   ElectronicLevels[1/cm]                      1
2627   0.000000000000000000      2.0000000000000000
2628 End
2629 !*****
2630 RRHO      !      11
2631 Geometry[angstrom]      17
2632 C          0.31159000    0.00051100    0.57079800
2633 C          -0.35645300    1.20474800    0.30947700
2634 C          -1.65515700    1.20627100   -0.19878900
2635 C          -2.30912100   -0.00051100   -0.45300100
2636 C          -1.65467300   -1.20679000   -0.19761500
2637 C          -0.35598300   -1.20424600    0.31066500
2638 H          0.14474600    2.14552500    0.51198000
2639 H          -2.15823100    2.14719800   -0.38959700
2640 H          -3.32008800   -0.00090300   -0.84297000
2641 H          -2.15736900   -2.14810500   -0.38750400
2642 H          0.14559500   -2.14462300    0.51409100
2643 C          1.70989700    0.00105900    1.10880100
2644 H          1.92449000    0.89348600    1.69889000
2645 H          1.92452000   -0.89020400    1.70064200
2646 H          2.46649200    0.00023500    0.28381400
2647 O          3.15353300   -0.00088700   -1.17931400
2648 H          2.29821900   -0.00093500   -1.64170200
2649   Core   RigidRotor
2650         SymmetryFactor    0.831548565
2651 End
2652 Rotor      Hindered
2653 Group    13   14   15   16   17
2654 Axis          12       1
2655 Symmetry      2
2656 Potential[kcal/mol]      18
2657 0.000 1.500 3.432 5.674 8.053 10.328 12.208 13.286 11.395 9.274 6.930 4.635
2658 2.572 0.880 -0.319 -0.958 -0.991 -0.416
2659 End
2660 Rotor      Hindered
2661 Group    17
2662 Axis          16       15
2663 Symmetry      1
2664 Potential[kcal/mol]      36
2665 0.000 -0.015 -0.008 -0.012 -0.013 -0.009 -0.002 0.010 0.021 0.022 0.022 0.023
2666 0.023 0.024 0.024 0.024 0.028 0.028 0.027 0.028 0.028 0.025 0.024 0.024
2667 0.024 0.023 0.022 0.022 0.021 0.009 -0.002 -0.009 -0.013 -0.013 -0.004 -0.015
2668 End
2669 Frequencies[1/cm]      42

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2670 133.63 217.76 339.50 396.69 440.36 490.51 514.98 528.22 596.03 632.47
2671 726.29 770.88 833.92 841.53 896.25 928.39 945.90 997.75 979.96 1012.40
2672 1071.22 1072.80 1140.01 1160.47 1187.03 1200.93 1301.59 1309.49 1381.04 1423.02
2673 1428.00 1468.18 1563.32 1580.02 2979.51 3056.35 3059.99 3062.62 3072.71 3081.15
2674 3091.56 3633.74
2675 ZeroEnergy[kcal/mol] 0.91
2676 ElectronicLevels[1/cm] 1
2677 0.0000000000000000 2.0000000000000000
2678 End
2679 !*****
2680 RRHO ! 12
2681 Geometry[angstrom] 17
2682 C 0.31116200 0.00051900 0.57216000
2683 C -0.35663700 1.20449800 0.30959000
2684 C -1.65507800 1.20612200 -0.19974600
2685 C -2.30927600 -0.00051400 -0.45375700
2686 C -1.65459200 -1.20664100 -0.19857000
2687 C -0.35616100 -1.20399300 0.31077900
2688 H 0.14381100 2.14540800 0.51344100
2689 H -2.15799600 2.14715200 -0.39053800
2690 H -3.32030200 -0.00090400 -0.84358400
2691 H -2.15713400 -2.14805900 -0.38844300
2692 H 0.14466400 -2.14450200 0.51555600
2693 C 1.70677900 0.00106400 1.12127800
2694 H 1.91173000 0.89246300 1.71649200
2695 H 1.91175100 -0.88918000 1.71821800
2696 H 2.47009700 0.00026300 0.30912000
2697 O 3.15810900 -0.00089800 -1.19175000
2698 H 2.29561500 -0.00095000 -1.64095500
2699 Core RigidRotor
2700 SymmetryFactor 0.831548565
2701 End
2702 Rotor Hindered
2703 Group 13 14 15 16 17
2704 Axis 12 1
2705 Symmetry 2
2706 Potential[kcal/mol] 18
2707 0.000 1.444 3.333 5.547 7.922 10.222 12.165 13.366 11.752 9.669 7.338 5.027
2708 2.930 1.189 -0.071 -0.776 -0.880 -0.372
2709 End
2710 Rotor Hindered
2711 Group 17
2712 Axis 16 15
2713 Symmetry 1
2714 Potential[kcal/mol] 36

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2715      0.000 -0.015 -0.009 -0.012 -0.013 -0.010 -0.003 0.006 0.018 0.021 0.021 0.021
2716      0.022 0.023 0.024 0.026 0.028 0.021 0.008 0.022 0.029 0.025 0.024 0.023
2717      0.022 0.021 0.021 0.021 0.018 0.005 -0.003 -0.009 -0.013 -0.012 -0.008 -0.015
2718      End
2719      Frequencies[1/cm]          42
2720      59.49 184.96 195.45 343.13 398.94 435.38 509.81 526.71 587.21 633.61
2721      726.76 805.71 842.92 888.61 922.58 942.28 997.78 975.79 988.66 1010.59
2722      1070.14 1139.15 1159.64 1193.34 1291.56 1311.59 1361.94 1371.59 1425.92
2723      1430.52
2724      1470.77 1563.46 1584.46 2470.37 2964.87 3022.83 3055.58 3057.47 3069.20
2725      3077.47
2726      3088.87 3606.84
2727      ZeroEnergy[kcal/mol]      0.57
2728      ElectronicLevels[1/cm]          1
2729      0.000000000000000000      2.000000000000000000
2730      End
2731      !*****
2732      RRHO          !          13
2733      Geometry[angstrom]          17
2734      C          0.31022100      0.00052600      0.57606700
2735      C          -0.35687800      1.20405600      0.31024200
2736      C          -1.65446600      1.20584800      -0.20197500
2737      C          -2.30902000      -0.00052100      -0.45588300
2738      C          -1.65396800      -1.20636600      -0.20079000
2739      C          -0.35638300      -1.20354800      0.31143500
2740      H          0.14201600      2.14523600      0.51682500
2741      H          -2.15690100      2.14707500      -0.39320300
2742      H          -3.31994200      -0.00091900      -0.84599400
2743      H          -2.15602100      -2.14798400      -0.39109500
2744      H          0.14289000      -2.14432200      0.51894700
2745      C          1.69990700      0.00108300      1.14682200
2746      H          1.88753400      0.89078600      1.75039700
2747      H          1.88754500      -0.88746900      1.75209400
2748      H          2.47611100      0.00031300      0.35646200
2749      O          3.16623500      -0.00091800      -1.21707600
2750      H          2.29081800      -0.00098400      -1.64114000
2751      Core      RigidRotor
2752      SymmetryFactor      0.831548565
2753      End
2754      Rotor          Hindered
2755      Group      13      14      15      16      17
2756      Axis          12          1
2757      Symmetry          2
2758      Potential[kcal/mol]          18
2759      0.000 -2.252 -4.619 -6.808 -8.688 -10.125 -11.029 -11.345 -11.047 -10.160 -8.737 -6.868

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2760 -4.687 -2.344 -0.067 1.889 3.275 2.013
2761 End
2762 Rotor Hindered
2763 Group 17
2764 Axis 16 15
2765 Symmetry 1
2766 Potential[kcal/mol] 36
2767 0.000 -0.015 -0.009 -0.012 -0.013 -0.010 -0.003 0.007 0.018 0.021 0.021 0.022
2768 0.022 0.023 0.024 0.026 0.029 0.022 0.021 0.021 0.029 0.026 0.023 0.023
2769 0.022 0.022 0.021 0.021 0.018 0.006 -0.003 -0.009 -0.013 -0.012 -0.007 -0.015
2770 End
2771 Frequencies[1/cm] 42
2772 197.48 292.79 342.70 397.06 456.08 497.02 526.02 533.24 632.44 665.92
2773 732.09 802.84 842.50 867.96 903.43 932.47 951.35 957.57 975.84 980.89
2774 1015.27 1077.20 1138.93 1145.79 1177.15 1293.04 1306.86 1416.26 1428.43 1429.03
2775 1463.79 1566.62 1567.34 1762.09 2995.95 3061.81 3064.51 3074.34 3081.35 3082.72
2776 3092.47 3668.97
2777 ZeroEnergy[kcal/mol] -0.10
2778 ElectronicLevels[1/cm] 1
2779 0.000000000000000000 2.000000000000000000
2780 End
2781 !*****
2782 RRHO ! 14
2783 Geometry[angstrom] 17
2784 C 0.30900400 0.00052700 0.58154200
2785 C -0.35704800 1.20377000 0.31199700
2786 C -1.65302200 1.20556200 -0.20487000
2787 C -2.30790500 -0.00052000 -0.45890700
2788 C -1.65252700 -1.20608400 -0.20368400
2789 C -0.35656000 -1.20325900 0.31319000
2790 H 0.14057500 2.14518300 0.52079500
2791 H -2.15484800 2.14694100 -0.39689100
2792 H -3.31815500 -0.00091900 -0.85080300
2793 H -2.15397100 -2.14785600 -0.39477800
2794 H 0.14144500 -2.14426400 0.52292000
2795 C 1.69234800 0.00110100 1.17259200
2796 H 1.86511400 0.88951900 1.78256100
2797 H 1.86512500 -0.88615700 1.78425000
2798 H 2.47995500 0.00035400 0.39976200
2799 O 3.17277900 -0.00093600 -1.24293200
2800 H 2.28594100 -0.00102000 -1.64306400
2801 Core RigidRotor
2802 SymmetryFactor 0.831548565
2803 End
2804 Rotor Hindered

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2805  Group   13   14   15   16   17
2806  Axis                12           1
2807  Symmetry                2
2808  Potential[kcal/mol]                18
2809  0.000 -1.129 -1.680 -1.616 -0.942 0.298  2.030 3.092 5.369 7.747 9.983 11.766
2810  12.147 10.409 8.243 5.885 3.617 1.602
2811  End
2812  Rotor                                Hindered
2813  Group   17
2814  Axis                16           15
2815  Symmetry                1
2816  Potential[kcal/mol]                36
2817  0.000 -0.015 -0.008 -0.012 -0.013 -0.009 -0.002 0.008 0.020 0.022 0.022 0.022
2818  0.023 0.023 0.023 0.025 0.029 0.025 0.021 0.026 0.030 0.024 0.024 0.023
2819  0.023 0.022 0.022 0.022 0.020 0.008 -0.003 -0.010 -0.013 -0.012 -0.007 -0.015
2820  End
2821  Frequencies[1/cm]                42
2822  60.94 217.64 247.73 349.43 381.58 398.40 455.17 495.19 531.10 550.45
2823  631.80 727.51 817.10 841.63 872.65 902.42 931.04 952.42 991.65 977.80
2824  1014.84 1078.07 1137.70 1143.22 1187.19 1287.89 1306.79 1426.71 1428.13 1455.09
2825  1546.77 1561.97 1564.39 2996.16 3061.34 3063.99 3074.34 3081.81 3087.27 3092.47
2826  3484.28 3716.41
2827  ZeroEnergy[kcal/mol]   -1.10
2828  ElectronicLevels[1/cm]                                1
2829  0.000000000000000000  2.0000000000000000
2830  End
2831  !*****
2832  RRHO                !                15
2833  Geometry[angstrom]                17
2834  C                    0.30730700    0.00053300    0.58930100
2835  C                    -0.35711400    1.20347900    0.31461000
2836  C                    -1.65096700    1.20539500   -0.20799100
2837  C                    -2.30540000   -0.00052200   -0.46372800
2838  C                    -1.65047100   -1.20592200   -0.20680300
2839  C                    -0.35662400   -1.20296100    0.31580400
2840  H                    0.13877300    2.14508900    0.52668100
2841  H                    -2.15172000    2.14691800   -0.40225400
2842  H                    -3.31454000   -0.00092400   -0.85846500
2843  H                    -2.15084000   -2.14784000   -0.40013400
2844  H                    0.13964700   -2.14415800    0.52881000
2845  C                    1.68457800    0.00111800    1.19811500
2846  H                    1.84522800    0.88860000    1.81274200
2847  H                    1.84523400   -0.88519900    1.81442600
2848  H                    2.48113200    0.00038500    0.43910100
2849  O                    3.17740400   -0.00095500   -1.26918800

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2850 H                2.28035000  -0.00105600  -1.64626100
2851   Core   RigidRotor
2852         SymmetryFactor    0.831548565
2853 End
2854   Rotor                                Hindered
2855   Group   13   14   15   16   17
2856   Axis                12           1
2857   Symmetry                2
2858   Potential[kcal/mol]                18
2859 0.000 0.928 2.376 4.269 6.484 8.860 11.158 13.097 14.290 12.656 10.570 8.499
2860 5.929 3.834 2.097 0.841 0.140 0.041
2861 End
2862   Rotor                                Hindered
2863   Group   17
2864   Axis                16           15
2865   Symmetry                1
2866   Potential[kcal/mol]                36
2867     0.000 -0.015 -0.008 -0.014 -0.013 -0.008 0.000 0.014 0.024 0.025 0.026 0.027
2868     0.027 0.027 0.025 0.023 0.024 0.024 0.046 0.033 0.023 0.024 0.025 0.027
2869     0.027 0.027 0.026 0.025 0.024 0.014 0.000 -0.009 -0.013 -0.014 -0.008 -0.015
2870 End
2871   Frequencies[1/cm]                42
2872 62.69 84.04 207.77 351.55 365.36 395.88 449.88 475.99 532.91 560.69
2873 631.10 724.98 807.79 832.26 839.36 896.74 928.66 952.25 988.65 973.50
2874 1013.96 1079.89 1136.79 1145.39 1204.86 1284.17 1307.18 1427.85 1434.75 1453.59
2875 1539.50 1556.05 1562.14 3006.84 3061.17 3063.57 3074.59 3081.80 3092.94 3103.92
2876 3485.11 3776.42
2877 ZeroEnergy[kcal/mol]    -2.66
2878   ElectronicLevels[1/cm]                1
2879 0.000000000000000000    2.0000000000000000
2880 End
2881 !*****
2882 RRHO           !                16
2883 Geometry[angstrom]    17
2884 C                0.30491100    0.00054100    0.59923800
2885 C                -0.35731500    1.20324900    0.31868900
2886 C                -1.64822900    1.20524600   -0.21157600
2887 C                -2.30163000   -0.00052600   -0.47038400
2888 C                -1.64773000   -1.20577500   -0.21038500
2889 C                -0.35682200   -1.20272300    0.31988400
2890 H                0.13685200    2.14500600    0.53426000
2891 H                -2.14751600    2.14689400   -0.40906300
2892 H                -3.30876700   -0.00093200   -0.87020100
2893 H                -2.14662900   -2.14782400   -0.40693900
2894 H                0.13773200   -2.14406300    0.53639200

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2895  C          1.67727200   0.00113300   1.22240100
2896  H          1.82897900   0.88793000   1.83987100
2897  H          1.82897500  -0.88449000   1.84156200
2898  H          2.47630800   0.00040300   0.47578900
2899  O          3.18011800  -0.00097500  -1.29540800
2900  H          2.27440600  -0.00108700  -1.65094300
2901  Core  RigidRotor
2902          SymmetryFactor   0.831548565
2903  End
2904  Rotor                               Hindered
2905  Group   13   14   15   16   17
2906  Axis           12           1
2907  Symmetry           2
2908  Potential[kcal/mol]           18
2909  0.000 -1.882 -4.115 -6.412 -8.551 -10.347 -11.685 -12.539 -12.827 -12.545 -11.741 -10.400
2910 -8.630 -6.520 -4.246 -2.018 -0.114 1.058
2911  End
2912  Rotor                               Hindered
2913  Group   17
2914  Axis           16           15
2915  Symmetry           1
2916  Potential[kcal/mol]           36
2917      0.000 -0.014 -0.011 -0.015 -0.014 -0.009 0.000 0.013 0.023 0.026 0.028 0.032
2918      0.035 0.035 0.030 0.026 0.023 0.027 0.285 0.027 0.023 0.026 0.030 0.034
2919      0.035 0.032 0.028 0.025 0.022 0.013 0.000 -0.009 -0.014 -0.015 -0.011 -0.014
2920  End
2921  Frequencies[1/cm]           42
2922  125.92 187.63 205.52 342.27 384.02 401.93 461.91 526.82 630.36 633.96
2923  726.67 799.80 845.37 892.07 945.47 950.94 998.43 977.44 999.72 1011.05
2924  1069.22 1138.84 1159.91 1189.48 1293.92 1311.05 1375.70 1395.03 1435.01 1436.30
2925  1471.15 1564.03 1585.03 2871.37 2973.31 3018.60 3054.54 3056.19 3068.57 3076.62
2926  3088.39 3602.43
2927  ZeroEnergy[kcal/mol]   -3.21
2928  ElectronicLevels[1/cm]           1
2929  0.000000000000000000   2.0000000000000000
2930  End
2931  !*****
2932  RRHO          !           17
2933  Geometry[angstrom]           17
2934  C          0.30500100   0.00054500   0.60393900
2935  C          -0.35664300   1.20309600   0.32176500
2936  C          -1.64534800   1.20518500  -0.21408000
2937  C          -2.29760900  -0.00052900  -0.47590600
2938  C          -1.64484500  -1.20571600  -0.21289000
2939  C          -0.35614800  -1.20256400   0.32296000

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2940  H          0.13546100   2.14478800   0.54255800
2941  H         -2.14207000   2.14708800  -0.41655900
2942  H         -3.30031200  -0.00094100  -0.88648800
2943  H         -2.14117800  -2.14802500  -0.41443400
2944  H          0.13634400  -2.14383400   0.54469300
2945  C          1.67195900   0.00114700   1.24328100
2946  H          1.80554300   0.88576600   1.86938500
2947  H          1.80551800  -0.88227300   1.87108300
2948  H          2.48498500   0.00042400   0.51830700
2949  O          3.17800800  -0.00098800  -1.31721600
2950  H          2.25918100  -0.00117300  -1.64415600
2951  Core  RigidRotor
2952          SymmetryFactor   0.831548565
2953  End
2954  Rotor                               Hindered
2955  Group   13   14   15   16   17
2956  Axis           12           1
2957  Symmetry           2
2958  Potential[kcal/mol]           18
2959  0.000 0.572 1.670 3.270 5.280 7.569  9.945 12.166 13.929 14.137 12.366 10.185
2960  7.824 5.566 3.570 1.974 0.889 0.376
2961  End
2962  Rotor                               Hindered
2963  Group   17
2964  Axis           16           15
2965  Symmetry           1
2966  Potential[kcal/mol]           36
2967  0.000 -0.014 -0.011 -0.015 -0.014 -0.009 0.000 0.012 0.022 0.026 0.028 0.032
2968  0.035 0.035 0.030 0.026 0.023 0.026 0.072 0.026 0.024 0.026 0.030 0.035
2969  0.035 0.032 0.028 0.025 0.022 0.012 0.000 -0.009 -0.014 -0.015 -0.011 -0.015
2970  End
2971  Frequencies[1/cm]           42
2972  124.53 209.75 256.92 343.32 395.69 402.36 462.19 526.49 633.57 634.01
2973  726.90 798.85 845.88 892.81 946.11 951.65 961.11 977.76 1001.71 1011.12
2974  1068.99 1138.69 1159.99 1188.07 1293.77 1311.07 1375.51 1396.92 1436.17 1439.67
2975  1471.06 1564.24 1584.97 2918.60 2980.11 3009.60 3054.37 3055.81 3068.82 3076.81
2976  3088.88 3574.47
2977  ZeroEnergy[kcal/mol]   -3.39
2978  ElectronicLevels[1/cm]           1
2979  0.00000000000000000000  2.00000000000000000000
2980  End
2981  !*****
2982  RRHO          !           18
2983  Geometry[angstrom]           17
2984  C          0.30294800   0.00055400   0.61677800

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2985  C          -0.35588200   1.20306600   0.32681500
2986  C          -1.64040300   1.20509700  -0.21918200
2987  C          -2.29118800  -0.00053400  -0.48498000
2988  C          -1.63989600  -1.20563100  -0.21799200
2989  C          -0.35538200  -1.20252500   0.32800900
2990  H           0.13496900   2.14500900   0.54932500
2991  H          -2.13705900   2.14689100  -0.42252600
2992  H          -3.29407900  -0.00094700  -0.89530800
2993  H          -2.13615900  -2.14783400  -0.42040400
2994  H           0.13586100  -2.14404300   0.55145700
2995  C           1.66428100   0.00116100   1.26604600
2996  H           1.79868400   0.88713400   1.89021800
2997  H           1.79864300  -0.88360000   1.89195000
2998  H           2.48055400   0.00041500   0.53434700
2999  O           3.17279600  -0.00100300  -1.33983500
3000  H           2.24818500  -0.00124800  -1.65029800
3001  Core      RigidRotor
3002          SymmetryFactor    0.831548565
3003  End
3004  Rotor                      Hindered
3005  Group    13   14   15   16   17
3006  Axis          12           1
3007  Symmetry          2
3008  Potential[kcal/mol]          18
3009  0.000 0.462 1.451 2.953 4.889 7.133  9.511 11.785 13.661 14.731 13.669 10.700
3010  8.355 6.062 4.001 2.312 1.116 0.482
3011  End
3012  Rotor                      Hindered
3013  Group    17
3014  Axis          16           15
3015  Symmetry          1
3016  Potential[kcal/mol]          36
3017  0.000 -0.015 -0.009 -0.014 -0.013 -0.008 0.000 0.014 0.024 0.025 0.026 0.028
3018  0.029 0.028 0.026 0.023 0.023 0.028 0.014 0.025 0.023 0.024 0.026 0.028
3019  0.029 0.028 0.027 0.025 0.025 0.015 0.000 -0.009 -0.013 -0.014 -0.008 -0.015
3020  End
3021  Frequencies[1/cm]          42
3022  108.83 184.72 214.71 298.47 352.85 384.10 406.05 440.58 528.93 535.40
3023  630.20 659.75 722.22 835.10 838.40 888.32 926.11 949.18 982.32 967.16
3024  1010.84 1082.16 1135.77 1144.33 1229.14 1284.77 1307.37 1430.37 1442.74 1451.46
3025  1550.32 1559.04 1568.64 3029.90 3062.14 3064.85 3075.81 3082.11 3093.42 3130.72
3026  3571.46 3767.05
3027  ZeroEnergy[kcal/mol]    -3.61
3028  ElectronicLevels[1/cm]          1
3029  0.000000000000000000    2.0000000000000000

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3030 End
3031 Tunneling Eckart
3032 ImaginaryFrequency[1/cm] 1192.8499999999999
3033 WellDepth[kcal/mol] 4.62
3034 WellDepth[kcal/mol] 29.93
3035 End
3036 End
3037 !*****
3038 Bimolecular P3 # C6H5OH + CH3
3039 Fragment PROD1
3040 RRHO
3041 Geometry[angstrom] 13
3042 C 0.24040500 1.21022500 -0.01434700
3043 C -1.15490900 1.20699800 0.00591300
3044 C -1.85625000 0.00030700 0.01602100
3045 C -1.15540600 -1.20666300 0.00606000
3046 C 0.23991700 -1.21049000 -0.01396500
3047 C 0.93254700 -0.00029900 -0.00920900
3048 H 0.79975300 2.13770300 -0.03780300
3049 H -1.69266800 2.14793200 0.00425000
3050 H -2.93948400 0.00053700 0.02829300
3051 H -1.69355000 -2.14737500 0.00464300
3052 H 0.79899500 -2.13812800 -0.03685700
3053 O 2.32049600 -0.00105500 -0.08827700
3054 H 2.68515900 0.00729800 0.80085400
3055 Core RigidRotor
3056 SymmetryFactor 1.0000000000000000
3057 End
3058 Rotor Hindered
3059 Group 13
3060 Axis 6 12
3061 Symmetry 1
3062 Potential[kcal/mol] 36
3063 0.000 -0.116 -0.453 -0.953 -1.549 -2.171 -2.740 -3.185 -3.446 -3.512 -3.386 -
3064 3.062
3065 -2.572 -1.977 -1.356 -0.783 -0.327 -0.053 -0.015 -0.216 -0.607 -1.129 -1.718 -
3066 2.307
3067 -2.829 -3.225 -3.454 -3.512 -3.401 -3.117 -2.676 -2.127 -1.530 -0.955 -0.467 -
3068 0.129
3069 End
3070 Frequencies[1/cm] 32
3071 223.27 405.88 409.85 453.28 529.68 533.30 628.39 739.04
3072 823.15 830.30 882.52 913.59 936.76 978.39 1004.00 1051.70
3073 1133.65 1136.74 1148.69 1225.40 1275.53 1307.53 1425.90 1469.04
3074 1570.30 1579.22 3063.25 3071.71 3082.77 3088.27 3093.65 3709.39

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3075 ZeroEnergy[kcal/mol] 0.
3076 ElectronicLevels[1/cm] 1
3077 0.0000000000000000E+000 1.0000000000000000
3078 End
3079 !*****
3080 Fragment PROD2
3081 RRHO
3082 Geometry[angstrom] 4
3083 C 0.00000000 0.00000000 -0.00008100
3084 H 0.00000000 1.07906800 0.00016200
3085 H -0.93450000 -0.53953400 0.00016200
3086 H 0.93450000 -0.53953400 0.00016200
3087 Core RigidRotor
3088 SymmetryFactor 6.0000000000000000
3089 End
3090 Frequencies[1/cm] 6
3091 513.14 1369.86 1369.86 3012.76 3190.07 3190.09
3092 ZeroEnergy[kcal/mol] 0.
3093 ElectronicLevels[1/cm] 1
3094 0.0000000000000000E+000 2.0000000000000000
3095 End
3096 GroundEnergy[kcal/mol] -5.56
3097 End
3098 !*****
3099 Well W32 # ipsoOHC6H5CH3
3100 Species
3101 RRHO
3102 Geometry[angstrom] 17
3103 C 0.03666100 -1.24694500 0.01494200
3104 C 1.39748600 -1.22569600 -0.03284600
3105 C 2.11019800 -0.00000300 -0.07136700
3106 C 1.39748600 1.22569300 -0.03284100
3107 C 0.03666200 1.24695000 0.01495800
3108 C -0.80174700 0.00000900 0.02675100
3109 H -0.50761800 -2.18452300 0.05611300
3110 H 1.94977000 -2.15899900 -0.03381000
3111 H 3.19194200 0.00000100 -0.10777300
3112 H 1.94977800 2.15899100 -0.03380600
3113 H -0.50758400 2.18454700 0.05615000
3114 C -1.79326700 0.00000300 -1.14188200
3115 H -2.42709900 0.88757200 -1.08419800
3116 H -1.26004800 0.00001600 -2.09355000
3117 H -2.42708400 -0.88757500 -1.08420000
3118 O -1.64992300 0.00000200 1.21042100
3119 H -1.06355300 -0.00011200 1.97541100

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3120 Core RigidRotor
3121 SymmetryFactor 1
3122 End
3123 Rotor Hindered !freq=257
3124 Group 13 14 15
3125 Axis 6 12
3126 Symmetry 3
3127 Potential[kcal/mol] 12
3128 0.000 0.215 0.806 1.639 2.509 3.177 3.427 3.167 2.495 1.622 0.798 0.217
3129 End
3130 Rotor Hindered !freq=340
3131 Group 17
3132 Axis 6 16
3133 Symmetry 1
3134 Potential[kcal/mol] 36
3135 0.000 0.106 0.413 0.878 1.435 1.994 2.485 2.849 3.053 3.106 3.058 2.977
3136 2.914 2.907 2.980 3.105 3.255 3.383 3.437 3.401 3.285 3.135 3.002 2.925
3137 2.907 2.960 3.041 3.102 3.075 2.898 2.549 2.057 1.486 0.911 0.429 0.113
3138 End
3139 Frequencies[1/cm] 43
3140 82.89 228.40 342.33 386.17 393.06 454.57 536.45 582.65
3141 586.16 692.09 733.83 772.25 819.87 898.42 961.48 966.98
3142 970.32 980.93 994.23 1020.80 1056.54 1083.45 1099.19 1158.20
3143 1250.17 1272.03 1278.69 1350.94 1351.56 1401.96 1436.99 1445.50
3144 1497.81 1560.77 2935.53 3012.38 3022.72 3056.44 3057.95 3074.17
3145 3075.36 3096.04 3673.71
3146 ZeroEnergy[kcal/mol] -18.38
3147 ElectronicLevels[1/cm] 1
3148 0 2
3149 End
3150 End
3151 !*****
3152 Barrier B33 W32 P3 # TS33
3153 RRHO
3154 Geometry[angstrom] 17
3155 C 1.39903800 1.21170600 -0.08840500
3156 C 0.02710300 1.21406900 -0.26806800
3157 C -0.71588100 -0.00042000 -0.30898500
3158 C 0.02735300 -1.21470400 -0.26617000
3159 C 1.39926500 -1.21181400 -0.08659200
3160 C 2.09366800 0.00009700 0.00260400
3161 H 1.93789900 2.15004300 -0.03114500
3162 H -0.51321200 -2.15117500 -0.34037500
3163 H 1.93833000 -2.14995300 -0.02800700
3164 H 3.16876200 0.00030200 0.13786800

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3165 O -1.34603100 0.00187400 1.59411600
3166 H -0.50542900 0.00251800 2.07618900
3167 H -0.51365500 2.15032200 -0.34361900
3168 C -2.11935100 -0.00111900 -0.85695500
3169 H -2.65971300 0.88340700 -0.52045800
3170 H -2.09198900 -0.00296700 -1.95048100
3171 H -2.65991400 -0.88438600 -0.51748300
3172 Core RigidRotor
3173 SymmetryFactor 1
3174 End
3175 Tunneling Eckart
3176 ImaginaryFrequency[1/cm] 411.60
3177 WellDepth[kcal/mol] 24.77
3178 WellDepth[kcal/mol] 11.94
3179 End
3180 Frequencies[1/cm] 44
3181 106.81 146.65 171.39 218.37 265.42 338.04 407.51 408.71 529.67 622.56
3182 646.63 739.16 785.77 805.41 839.48 920.97 973.90 979.14 968.14 971.61
3183 1007.68 1016.53 1080.70 1129.01 1156.24 1192.19 1268.01 1299.69 1367.04 1407.06
3184 1443.02 1447.98 1450.60 1539.91 1567.93 2938.29 3009.51 3036.00 3064.73 3070.54
3185 3079.13 3085.37 3093.07 3634.88
3186 ZeroEnergy[kcal/mol] 6.38
3187 ElectronicLevels[1/cm] 1
3188 0 2
3189 End
3190 !*****
3191 Barrier B32 W W32
3192 Variational
3193 RRHO ! 1
3194 Geometry[angstrom] 17
3195 C 1.37576800 1.20658100 -0.09419400
3196 C 0.01683500 1.20342600 -0.40859100
3197 C -0.68587100 -0.00089600 -0.56928200
3198 C 0.01719300 -1.20462000 -0.40593600
3199 C 1.37617400 -1.20672400 -0.09125000
3200 C 2.06111000 0.00016800 0.06515600
3201 H 1.89739400 2.14827200 0.03049900
3202 H -0.51153100 -2.14497600 -0.51738800
3203 H 1.89803800 -2.14800700 0.03584800
3204 H 3.11574900 0.00061800 0.31444800
3205 O -1.38465100 0.00278100 1.96078100
3206 H -0.44175100 -0.00109100 2.18192000
3207 H -0.51219300 2.14337400 -0.52230300
3208 C -2.13975400 -0.00118200 -0.96697100
3209 H -2.65464900 0.87510200 -0.57123500

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3210 H -2.23719900 0.01123200 -2.05655300
3211 H -2.64758600 -0.89000400 -0.59167400
3212 Core RigidRotor
3213 SymmetryFactor 0.856940376
3214 End
3215 Rotor Hindered
3216 Group 15 16 17
3217 Axis 14 3
3218 Symmetry 3
3219 Potential[kcal/mol] 12
3220 0.000 -0.691 -0.632 -0.626 -0.663 -0.728 -0.820 -0.910 -0.975 -0.988 -0.953 -0.879
3221 End
3222 Rotor Hindered
3223 Group 12
3224 Axis 11 3
3225 Symmetry 1
3226 Potential[kcal/mol] 36
3227 0.000 0.011 -0.874 -0.961 -0.989 -0.955 -0.864 -0.731 -0.566 -0.377 -0.170 0.049
3228 0.276 0.079 0.010 -0.090 -0.164 -0.213 -0.243 -0.257 -0.253 -0.232 -0.194 -0.130
3229 -0.037 0.093 0.980 0.136 -0.746 -0.876 -0.960 -0.990 -0.962 -0.883 -0.760 -0.606
3230 End
3231 Frequencies[1/cm] 42
3232 79.80 101.23 205.52 338.44 341.33 401.59 452.43 526.62
3233 631.87 638.80 728.25 798.80 844.75 896.86 956.02 959.69
3234 969.58 978.23 1009.73 1024.03 1070.67 1137.09 1159.01 1190.78
3235 1295.56 1307.20 1369.72 1413.01 1442.81 1449.80 1467.67 1558.96
3236 1581.68 2934.74 2999.46 3025.66 3059.12 3062.56 3071.25 3079.73
3237 3089.22 3657.23
3238 ZeroEnergy[kcal/mol] -3.56
3239 ElectronicLevels[1/cm] 1
3240 0.000000000000000000 2.0000000000000000
3241 End
3242 !*****
3243 RRHO ! 2
3244 Geometry[angstrom] 17
3245 C 1.38193000 1.20707600 -0.09955700
3246 C 0.01903400 1.20442600 -0.39015700
3247 C -0.68679000 -0.00071300 -0.54053400
3248 C 0.01937900 -1.20540200 -0.38822600
3249 C 1.38226200 -1.20721000 -0.09758800
3250 C 2.06962500 0.00014900 0.04865300
3251 H 1.90631000 2.14880800 0.01535600
3252 H -0.51185300 -2.14485300 -0.49530300
3253 H 1.90690400 -2.14861100 0.01884500
3254 H 3.12859400 0.00048200 0.27922400

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3255 O -1.40419800 0.00237000 1.90855800
3256 H -0.47859000 0.00197400 2.19152500
3257 H -0.51246300 2.14355500 -0.49873000
3258 C -2.13804700 -0.00124600 -0.93944400
3259 H -2.64918100 0.88180900 -0.55636700
3260 H -2.23384100 -0.00085600 -2.02970500
3261 H -2.64820500 -0.88513900 -0.55706900
3262 Core RigidRotor
3263 SymmetryFactor 0.856940376
3264 End
3265 Rotor Hindered
3266 Group 15 16 17
3267 Axis 14 3
3268 Symmetry 3
3269 Potential[kcal/mol] 12
3270 0.000 -0.690 -0.632 -0.627 -0.665 -0.731 -0.823 -0.913 -0.976 -0.988 -0.952 -0.877
3271 End
3272 Rotor Hindered
3273 Group 12
3274 Axis 11 3
3275 Symmetry 1
3276 Potential[kcal/mol] 36
3277 0.000 -0.741 -0.876 -0.962 -0.989 -0.954 -0.861 -0.727 -0.561 -0.372 -0.165 0.054
3278 0.281 0.079 0.614 -0.093 -0.166 -0.214 -0.243 -0.257 -0.253 -0.231 -0.193 -0.128
3279 -0.034 0.097 0.089 0.137 -0.750 -0.879 -0.962 -0.990 -0.961 -0.881 -0.757 -0.602
3280 End
3281 Frequencies[1/cm] 42
3282 82.84 115.27 208.24 340.34 363.52 401.33 452.19 527.99
3283 631.41 638.55 729.12 800.04 845.20 898.48 957.37 960.11
3284 970.30 978.37 1009.23 1024.20 1072.08 1137.15 1159.59 1193.86
3285 1294.92 1307.12 1370.63 1413.89 1441.61 1450.53 1467.19 1557.24
3286 1583.54 2934.09 3000.86 3032.19 3058.13 3062.17 3071.10 3078.13
3287 3087.89 3664.29
3288 ZeroEnergy[kcal/mol] -3.36
3289 ElectronicLevels[1/cm] 1
3290 0.0000000000000000 2.0000000000000000
3291 End
3292 !*****
3293 RRHO ! 3
3294 Geometry[angstrom] 17
3295 C 1.38627900 1.20743200 -0.09997800
3296 C 0.02045200 1.20526800 -0.37447700
3297 C -0.69022400 -0.00067100 -0.51364900
3298 C 0.02078400 -1.20620300 -0.37259400
3299 C 1.38659500 -1.20756100 -0.09808000

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3345  C          1.38683800   1.20713300  -0.09906300
3346  C          0.01763700   1.20456300  -0.35870100
3347  C         -0.69072900  -0.00065000  -0.50327000
3348  C          0.01795900  -1.20545200  -0.35683900
3349  C          1.38713800  -1.20726300  -0.09719200
3350  C          2.07833500   0.00012800   0.02533800
3351  H          1.91396500   2.14837900   0.00468000
3352  H         -0.51637200  -2.14493100  -0.44582200
3353  H          1.91451400  -2.14820700   0.00800600
3354  H          3.14425500   0.00041300   0.22070300
3355  O         -1.41035100   0.00217200   1.82178400
3356  H         -0.50299000   0.00243400   2.17096300
3357  H         -0.51693800   2.14376200  -0.44912900
3358  C         -2.14111000  -0.00117700  -0.90912300
3359  H         -2.65333700   0.88175100  -0.52653300
3360  H         -2.22775100  -0.00251100  -1.99950900
3361  H         -2.65329700  -0.88320400  -0.52438600
3362  Core  RigidRotor
3363      SymmetryFactor  0.856940376
3364  End
3365  Rotor                      Hindered
3366  Group  15 16 17
3367  Axis          14          3
3368  Symmetry          3
3369  Potential[kcal/mol]          12
3370  0.000 -0.693 -0.633 -0.625 -0.661 -0.726 -0.817 -0.908 -0.973 -0.988 -0.955 -0.881
3371  End
3372  Rotor                      Hindered
3373  Group  12
3374  Axis          11          3
3375  Symmetry          1
3376  Potential[kcal/mol]          36
3377  0.000 0.022 0.034 -0.962 -0.989 -0.953 -0.861 -0.727 -0.560 -0.371 -0.164 0.055
3378  0.282 0.079 0.006 -0.093 -0.166 -0.214 -0.243 -0.257 -0.253 -0.231 -0.192 -0.128
3379  -0.034 0.098 0.321 0.615 0.367 -0.879 -0.962 -0.990 -0.961 -0.880 -0.756 -0.601
3380  End
3381  Frequencies[1/cm]          42
3382  83.54 207.76 217.83 339.93 402.60 446.19 504.08 530.51
3383  630.89 637.58 728.95 799.81 844.21 901.60 958.35 960.46
3384  970.71 979.41 1010.26 1025.70 1072.10 1136.97 1159.42 1192.18
3385  1294.13 1305.20 1370.02 1412.56 1442.54 1449.75 1466.48 1558.35
3386  1582.38 2936.73 3003.21 3030.00 3059.90 3063.88 3072.50 3080.01
3387  3089.58 3608.29
3388  ZeroEnergy[kcal/mol]  -2.55
3389  ElectronicLevels[1/cm]          1

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3390      0.0000000000000000      2.0000000000000000
3391      End
3392      !*****
3393      RRHO      !      5
3394      Geometry[angstrom]      17
3395      C      1.38705400      1.20748900      -0.09864800
3396      C      0.01656800      1.20527900      -0.34752400
3397      C      -0.69408800      -0.00063100      -0.48607000
3398      C      0.01688100      -1.20614500      -0.34565300
3399      C      1.38734500      -1.20761800      -0.09677000
3400      C      2.07961700      0.00012100      0.01865000
3401      H      1.91519600      2.14850100      0.00302600
3402      H      -0.51853800      -2.14519800      -0.43188400
3403      H      1.91573200      -2.14833300      0.00637500
3404      H      3.14721800      0.00039700      0.20602900
3405      O      -1.40651600      0.00212700      1.78911800
3406      H      -0.51089000      0.00242300      2.16427100
3407      H      -0.51909200      2.14405800      -0.43521600
3408      C      -2.14182300      -0.00115800      -0.90122700
3409      H      -2.65538000      0.88172800      -0.52007300
3410      H      -2.22399500      -0.00247600      -1.99259900
3411      H      -2.65533300      -0.88315000      -0.51794900
3412      Core      RigidRotor
3413      SymmetryFactor      0.856940376
3414      End
3415      Rotor      Hindered
3416      Group      15 16 17
3417      Axis      14      3
3418      Symmetry      3
3419      Potential[kcal/mol]      12
3420      0.000 -0.697 -0.635 -0.623 -0.658 -0.721 -0.811 -0.902 -0.970 -0.988 -0.957 -0.886
3421      End
3422      Rotor      Hindered
3423      Group      12
3424      Axis      11      3
3425      Symmetry      1
3426      Potential[kcal/mol]      36
3427      0.000 -0.742 -0.877 -0.962 -0.989 -0.953 -0.861 -0.726 -0.560 -0.371 -0.164 0.056
3428      0.282 0.079 0.006 -0.093 -0.166 -0.214 -0.243 -0.257 -0.253 -0.231 -0.192 -0.128
3429      -0.034 0.098 0.089 0.138 -0.750 -0.879 -0.962 -0.990 -0.961 -0.880 -0.756 -0.601
3430      End
3431      Frequencies[1/cm]      42
3432      88.39 176.06 222.57 339.58 402.87 445.66 513.93 533.70
3433      630.46 637.81 730.28 799.75 844.38 903.91 959.63 961.93
3434      971.31 979.61 1010.16 1026.72 1072.85 1137.07 1159.59 1192.24

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3435      1292.45 1304.38 1370.59 1412.64 1442.61 1450.02 1465.63 1557.45
3436      1582.84 2933.19 3001.07 3029.42 3059.41 3064.21 3072.18 3079.74
3437      3088.53 3622.43
3438 ZeroEnergy[kcal/mol]   -2.20
3439   ElectronicLevels[1/cm]                               1
3440      0.000000000000000000      2.0000000000000000
3441 End
3442 !*****
3443 RRHO          !          6
3444 Geometry[angstrom]      17
3445 C              1.38689900    1.20769900   -0.09807900
3446 C              0.01478000    1.20566600   -0.33485600
3447 C             -0.69712300   -0.00061000   -0.46930500
3448 C              0.01508500   -1.20650100   -0.33298500
3449 C              1.38718000   -1.20782700   -0.09620700
3450 C              2.08027600    0.00011300    0.01097200
3451 H              1.91624600    2.14847500   -0.00151500
3452 H             -0.52164400   -2.14519400   -0.41398000
3453 H              1.91676600   -2.14831800    0.00181700
3454 H              3.14986100    0.00037500    0.18614100
3455 O             -1.40206000    0.00208400    1.75758500
3456 H             -0.51540900    0.00244000    2.15340000
3457 H             -0.52218100    2.14409600   -0.41730600
3458 C             -2.14153400   -0.00114800   -0.89511700
3459 H             -2.65798000    0.88194100   -0.51870300
3460 H             -2.21213200   -0.00255700   -1.98708100
3461 H             -2.65798000   -0.88326700   -0.51643000
3462   Core   RigidRotor
3463         SymmetryFactor    0.856940376
3464 End
3465   Rotor                               Hindered
3466   Group   15 16 17
3467   Axis           14           3
3468   Symmetry           3
3469   Potential[kcal/mol]           12
3470   0.000 -0.827 -0.919 -0.973 -0.989 -0.952 -0.873 -0.777 -0.691 -0.638 -0.622 -0.660
3471 End
3472   Rotor                               Hindered
3473   Group   12
3474   Axis           11           3
3475   Symmetry           1
3476   Potential[kcal/mol]           36
3477   0.000 -0.461 -0.877 -0.963 -0.989 -0.953 -0.861 -0.726 -0.560 -0.370 -0.163 0.056
3478   0.283 0.079 0.006 -0.093 -0.166 -0.214 -0.244 -0.257 -0.253 -0.231 -0.192 -0.128
3479   -0.033 0.098 0.089 0.138 -0.751 -0.879 -0.962 -0.990 -0.960 -0.880 -0.756 -0.601

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3480 End
3481   Frequencies[1/cm]           42
3482   94.77 187.48 226.29 339.06 403.29 443.47 525.97 552.67
3483   630.12 637.58 730.65 800.15 844.17 905.88 960.65 962.67
3484   971.31 980.14 1010.60 1026.60 1073.37 1136.93 1159.67 1192.66
3485   1291.55 1303.64 1370.06 1412.55 1442.47 1449.88 1465.28 1558.02
3486   1583.31 2934.69 3002.69 3030.82 3060.34 3065.15 3073.13 3080.62
3487   3089.41 3621.73
3488 ZeroEnergy[kcal/mol]   -1.74
3489   ElectronicLevels[1/cm]           1
3490   0.000000000000000000          2.0000000000000000
3491 End
3492 !*****
3493 RRHO           !           7
3494 Geometry[angstrom]           17
3495 C               1.38647800    1.20803800   -0.09776700
3496 C               0.01318300    1.20632600   -0.32296800
3497 C              -0.70081200   -0.00058900   -0.45065900
3498 C               0.01348000   -1.20713300   -0.32109400
3499 C               1.38675000   -1.20816500   -0.09590100
3500 C               2.08037900    0.00010700    0.00425800
3501 H               1.91712500    2.14854100   -0.00578100
3502 H              -0.52441700   -2.14537800   -0.39832200
3503 H               1.91763100   -2.14839300   -0.00245900
3504 H               3.15156200    0.00035700    0.16939800
3505 O              -1.39662700    0.00204200    1.72605100
3506 H              -0.51952400    0.00245100    2.14174300
3507 H              -0.52494100    2.14431600   -0.40165200
3508 C              -2.14116200   -0.00114000   -0.88951800
3509 H              -2.66059400    0.88211300   -0.51769800
3510 H              -2.20039000   -0.00261000   -1.98230500
3511 H              -2.66062700   -0.88337100   -0.51532400
3512   Core   RigidRotor
3513         SymmetryFactor   0.856940376
3514 End
3515   Rotor           Hindered
3516   Group   15 16 17
3517   Axis           14           3
3518   Symmetry           3
3519   Potential[kcal/mol]           12
3520   0.000 -0.705 -0.639 -0.623 -0.653 -0.713 -0.801 -0.893 -0.965 -0.990 -0.962 -0.895
3521 End
3522   Rotor           Hindered
3523   Group   12
3524   Axis           11           3

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3525 Symmetry 1
3526 Potential[kcal/mol] 36
3527 0.000 -0.100 0.064 -0.963 -0.989 -0.953 -0.860 -0.726 -0.559 -0.370 -0.163 0.057
3528 0.283 0.079 0.006 -0.093 -0.166 -0.215 -0.244 -0.257 -0.253 -0.231 -0.192 -0.128
3529 -0.033 0.099 0.090 0.138 -0.751 -0.880 -0.962 -0.990 -0.960 -0.880 -0.755 -0.600
3530 End
3531 Frequencies[1/cm] 42
3532 96.80 188.30 231.15 338.58 403.86 440.52 528.29 580.63
3533 629.65 638.09 731.82 800.28 844.29 908.58 962.37 964.29
3534 971.53 980.47 1010.93 1026.80 1074.19 1136.81 1159.77 1193.04
3535 1289.71 1302.89 1369.89 1412.57 1442.47 1449.88 1464.58 1558.15
3536 1583.73 2934.00 3002.77 3031.37 3060.78 3065.96 3073.88 3081.10
3537 3089.67 3625.02
3538 ZeroEnergy[kcal/mol] -1.27
3539 ElectronicLevels[1/cm] 1
3540 0.0000000000000000 2.0000000000000000
3541 End
3542 !*****
3543 RRHO ! 8
3544 Geometry[angstrom] 17
3545 C 1.38582500 1.20841200 -0.09781600
3546 C 0.01159700 1.20705800 -0.31165300
3547 C -0.70498100 -0.00056500 -0.43026000
3548 C 0.01188600 -1.20783700 -0.30977700
3549 C 1.38608900 -1.20853900 -0.09596100
3550 C 2.07988000 0.00010100 -0.00147100
3551 H 1.91792200 2.14859600 -0.01183500
3552 H -0.52704500 -2.14564500 -0.38392000
3553 H 1.91841500 -2.14846100 -0.00853600
3554 H 3.15244800 0.00034000 0.15403700
3555 O -1.39055600 0.00200200 1.69503500
3556 H -0.52214500 0.00246800 2.12799300
3557 H -0.52755500 2.14462100 -0.38724700
3558 C -2.14042100 -0.00113500 -0.88452800
3559 H -2.66357600 0.88235300 -0.51871200
3560 H -2.18503900 -0.00268400 -1.97801800
3561 H -2.66365100 -0.88353800 -0.51620700
3562 Core RigidRotor
3563 SymmetryFactor 0.856940376
3564 End
3565 Rotor Hindered
3566 Group 15 16 17
3567 Axis 14 3
3568 Symmetry 3
3569 Potential[kcal/mol] 12

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3570 0.000 -0.096 -0.189 -0.249 -0.271 -0.242 -0.167 -0.072 0.017 0.074 0.097 0.067
3571 End
3572 Rotor Hindered
3573 Group 12
3574 Axis 11 3
3575 Symmetry 1
3576 Potential[kcal/mol] 36
3577 0.000 -0.501 -0.878 -0.963 -0.989 -0.953 -0.860 -0.725 -0.559 -0.369 -0.162 0.058
3578 0.284 0.079 0.005 -0.094 -0.166 -0.215 -0.244 -0.257 -0.253 -0.231 -0.192 -0.127
3579 -0.033 0.099 0.090 0.138 -0.752 -0.880 -0.962 -0.990 -0.960 -0.879 -0.755 -0.600
3580 End
3581 Frequencies[1/cm] 42
3582 101.69 193.80 236.49 338.08 404.64 436.23 529.50 614.80
3583 629.10 639.24 733.22 800.18 844.48 911.75 964.52 966.29
3584 971.58 980.59 1011.36 1026.60 1075.11 1136.53 1159.77 1193.40
3585 1287.38 1302.23 1369.43 1412.55 1442.51 1449.79 1463.72 1558.32
3586 1583.71 2934.13 3003.54 3032.29 3061.59 3066.94 3074.83 3081.95
3587 3090.38 3626.87
3588 ZeroEnergy[kcal/mol] -0.80
3589 ElectronicLevels[1/cm] 1
3590 0.000000000000000000 2.0000000000000000
3591 End
3592 !*****
3593 RRHO ! 9
3594 Geometry[angstrom] 17
3595 C 1.38494800 1.20878400 -0.09849400
3596 C 0.01027000 1.20813500 -0.30156400
3597 C -0.70995500 -0.00054000 -0.40736200
3598 C 0.01055400 -1.20888300 -0.29968800
3599 C 1.38520500 -1.20891500 -0.09665100
3600 C 2.07901600 0.00009700 -0.00567000
3601 H 1.91861600 2.14869400 -0.01897200
3602 H -0.52918800 -2.14626900 -0.37180800
3603 H 1.91909900 -2.14857500 -0.01570000
3604 H 3.15259400 0.00032700 0.14233300
3605 O -1.38397200 0.00196400 1.66459600
3606 H -0.52381300 0.00248400 2.11303100
3607 H -0.52968700 2.14528100 -0.37513100
3608 C -2.13947700 -0.00113300 -0.88003600
3609 H -2.66680700 0.88255400 -0.52084500
3610 H -2.16771500 -0.00276300 -1.97414000
3611 H -2.66692600 -0.88367200 -0.51820900
3612 Core RigidRotor
3613 SymmetryFactor 0.856940376
3614 End

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3615 Rotor                               Hindered
3616 Group    15 16 17
3617 Axis              14              3
3618 Symmetry          3
3619 Potential[kcal/mol]              12
3620 0.000 -0.094 -0.189 -0.253 -0.279 -0.256 -0.184 -0.091 0.001 0.061 0.089 0.065
3621 End
3622 Rotor                               Hindered
3623 Group    12
3624 Axis              11              3
3625 Symmetry          1
3626 Potential[kcal/mol]              36
3627 0.000 -0.744 -0.879 -0.963 -0.989 -0.952 -0.859 -0.724 -0.558 -0.368 -0.161 0.059
3628 0.285 0.079 0.193 -0.078 -0.155 -0.212 -0.244 -0.258 -0.252 -0.228 -0.184 -0.114
3629 -0.014 0.126 0.090 0.139 -0.752 -0.881 -0.963 -0.990 -0.960 -0.879 -0.754 -0.599
3630 End
3631 Frequencies[1/cm]              42
3632 104.36 199.28 242.65 337.67 405.69 430.93 530.24 628.32
3633 640.90 653.95 735.32 799.33 844.92 915.41 967.59 969.35
3634 971.51 980.09 1011.67 1025.93 1076.26 1136.04 1159.65 1193.52
3635 1284.11 1301.67 1368.99 1412.44 1442.70 1449.68 1462.31 1557.59
3636 1582.82 2933.87 3004.10 3032.94 3062.02 3067.68 3075.95 3082.37
3637 3090.69 3629.17
3638 ZeroEnergy[kcal/mol]    -0.67
3639 ElectronicLevels[1/cm]              1
3640 0.000000000000000000 2.0000000000000000
3641 End
3642 !*****
3643 RRHO          !              10
3644 Geometry[angstrom]              17
3645 C              1.38400900    1.20963200    -0.09849600
3646 C              0.00955400    1.20917900    -0.29365000
3647 C             -0.71621300    -0.00051600    -0.38163700
3648 C              0.00982000    -1.20992500    -0.29177500
3649 C              1.38424500    -1.20974300    -0.09667200
3650 C              2.07771400    0.00009600    -0.00935000
3651 H              1.91952400    2.14906900    -0.02790500
3652 H             -0.53029300    -2.14705400    -0.36379400
3653 H              1.91998800    -2.14894700    -0.02467800
3654 H              3.15213100    0.00030500    0.13248000
3655 O             -1.37703300    0.00193000    1.63509500
3656 H             -0.52421600    0.00250300    2.09673000
3657 H             -0.53077400    2.14607000    -0.36709900
3658 C             -2.13873000    -0.00113100    -0.87591200
3659 H             -2.67052100    0.88295700    -0.52462700

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3660 H -2.14810500 -0.00285800 -1.97027500
3661 H -2.67068800 -0.88400300 -0.52183500
3662 Core RigidRotor
3663 SymmetryFactor 0.856940376
3664 End
3665 Rotor Hindered
3666 Group 15 16 17
3667 Axis 14 3
3668 Symmetry 3
3669 Potential[kcal/mol] 12
3670 0.000 -0.090 -0.188 -0.257 -0.288 -0.272 -0.206 -0.114 -0.020 0.044 0.077 0.061
3671 End
3672 Rotor Hindered
3673 Group 12
3674 Axis 11 3
3675 Symmetry 1
3676 Potential[kcal/mol] 36
3677 0.000 -0.745 -0.879 -0.964 -0.989 -0.952 -0.859 -0.724 -0.557 -0.367 -0.160 0.060
3678 0.286 0.079 0.004 -0.095 -0.167 -0.215 -0.244 -0.257 -0.253 -0.230 -0.191 -0.127
3679 -0.032 0.100 0.090 0.139 -0.753 -0.881 -0.963 -0.990 -0.960 -0.878 -0.753 -0.598
3680 End
3681 Frequencies[1/cm] 42
3682 109.02 206.41 249.32 337.46 407.10 424.63 530.51 627.23
3683 644.69 698.51 737.69 797.26 844.85 919.68 971.24 973.50
3684 971.08 978.89 1011.54 1024.08 1077.68 1134.92 1159.12 1193.05
3685 1279.81 1301.37 1368.27 1411.83 1442.88 1449.48 1459.95 1555.48
3686 1579.99 2934.52 3005.40 3034.21 3062.94 3068.70 3076.53 3083.47
3687 3091.44 3630.78
3688 ZeroEnergy[kcal/mol] -0.55
3689 ElectronicLevels[1/cm] 1
3690 0.000000000000000000 2.000000000000000000
3691 End
3692 !*****
3693 RRHO ! 11
3694 Geometry[angstrom] 17
3695 C 1.38290200 1.21043400 -0.10022500
3696 C 0.00936400 1.21117600 -0.28688500
3697 C -0.72396000 -0.00047100 -0.35320300
3698 C 0.00962500 -1.21186700 -0.28501100
3699 C 1.38313600 -1.21057700 -0.09842000
3700 C 2.07679300 0.00008100 -0.01064500
3701 H 1.92008000 2.14937500 -0.03661900
3702 H -0.53073200 -2.14868100 -0.35806300
3703 H 1.92052400 -2.14930800 -0.03348200
3704 H 3.15167400 0.00029000 0.12717300

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3705 O -1.37022200 0.00190100 1.60705800
3706 H -0.52394000 0.00253000 2.07980000
3707 H -0.53119000 2.14777200 -0.36128600
3708 C -2.13764100 -0.00114100 -0.87288700
3709 H -2.67379500 0.88320500 -0.52920400
3710 H -2.12847400 -0.00299700 -1.96699500
3711 H -2.67399200 -0.88420200 -0.52621500
3712 Core RigidRotor
3713 SymmetryFactor 0.856940376
3714 End
3715 Rotor Hindered
3716 Group 15 16 17
3717 Axis 14 3
3718 Symmetry 3
3719 Potential[kcal/mol] 12
3720 0.000 -0.086 -0.185 -0.261 -0.298 -0.292 -0.233 -0.143 -0.048 0.023 0.062 0.055
3721 End
3722 Rotor Hindered
3723 Group 12
3724 Axis 11 3
3725 Symmetry 1
3726 Potential[kcal/mol] 36
3727 0.000 -0.745 -0.879 -0.964 -0.989 -0.952 -0.858 -0.723 -0.556 -0.366 -0.159 0.061
3728 0.287 0.079 0.004 -0.095 -0.167 -0.215 -0.244 -0.257 -0.252 -0.230 -0.191 -0.126
3729 -0.031 0.101 0.090 0.139 -0.754 -0.881 -0.963 -0.990 -0.959 -0.878 -0.753 -0.598
3730 End
3731 Frequencies[1/cm] 42
3732 117.67 209.55 256.29 337.14 406.03 415.86 530.42 625.42
3733 647.98 741.00 749.48 793.31 843.65 923.64 971.66 975.94
3734 969.99 975.96 1010.42 1021.39 1079.25 1132.72 1158.04 1192.75
3735 1274.21 1300.72 1367.69 1410.15 1443.15 1448.89 1456.08 1549.61
3736 1575.23 2936.33 3007.40 3035.32 3063.60 3069.47 3077.55 3084.30
3737 3092.11 3633.12
3738 ZeroEnergy[kcal/mol] -0.35
3739 ElectronicLevels[1/cm] 1
3740 0.000000000000000000 2.0000000000000000
3741 End
3742 !*****
3743 RRHO ! 12
3744 Geometry[angstrom] 17
3745 C 1.38170060 1.21168903 -0.10213541
3746 C 0.00976560 1.21405203 -0.28179841
3747 C -0.73321840 -0.00043697 -0.32271541
3748 C 0.01001560 -1.21472097 -0.27990041
3749 C 1.38192760 -1.21183097 -0.10032241

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3795  C          1.38049900   1.21294400  -0.10404600
3796  C          0.01016700   1.21692800  -0.27671200
3797  C         -0.74247700  -0.00040300  -0.29222800
3798  C          0.01040600  -1.21757500  -0.27479000
3799  C          1.38071900  -1.21308400  -0.10222500
3800  C          2.07586900   0.00007900  -0.01160800
3801  H          1.92104300   2.15067700  -0.05313200
3802  H         -0.53036700  -2.15370200  -0.35014800
3803  H          1.92146200  -2.15063200  -0.04999200
3804  H          3.15117500   0.00028000   0.12110200
3805  O         -1.35651500   0.00181300   1.55371300
3806  H         -0.52159300   0.00247200   2.04511700
3807  H         -0.53079400   2.15283800  -0.35341300
3808  C         -2.13573500  -0.00113100  -0.86848400
3809  H         -2.68030600   0.88357500  -0.53917300
3810  H         -2.09017900  -0.00297100  -1.96142800
3811  H         -2.68051100  -0.88460400  -0.53621200
3812  Core   RigidRotor
3813          SymmetryFactor   0.856940376
3814  End
3815  Rotor          Hindered
3816  Group   15 16 17
3817  Axis          14          3
3818  Symmetry          3
3819  Potential[kcal/mol]          12
3820  0.000 0.721 1.588 2.389 2.887 2.910 2.440 1.637 0.753 0.016 -0.401 -0.418
3821  End
3822  Rotor          Hindered
3823  Group   12
3824  Axis          11          3
3825  Symmetry          1
3826  Potential[kcal/mol]          36
3827  0.000 0.065 0.341 0.791 1.354 1.933 2.448 2.832 3.046 3.102 3.054 2.972
3828  2.910 2.903 2.975 3.099 3.249 3.377 3.432 3.397 3.282 3.133 2.999 2.921
3829  2.903 2.956 3.037 3.098 3.072 2.903 2.572 2.104 1.555 0.990 0.497 0.153
3830  End
3831  Frequencies[1/cm]          42
3832  169.46 229.70 276.20 339.65 402.26 408.31 528.67 619.08
3833  639.67 734.95 779.61 831.74 862.73 913.61 973.73 978.98
3834  965.94 966.96 1004.31 1013.49 1081.43 1123.93 1153.87 1191.21
3835  1264.64 1297.97 1366.45 1402.36 1441.29 1446.32 1446.70 1530.43
3836  1559.49 2938.31 3010.30 3035.97 3065.42 3071.13 3080.37 3086.04
3837  3093.66 3634.53
3838  ZeroEnergy[kcal/mol]   -1.34
3839  ElectronicLevels[1/cm]          1

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3840      0.0000000000000000      2.0000000000000000
3841      End
3842      !*****
3843      RRHO      !      14
3844      Geometry[angstrom]      17
3845      C      1.37917300      1.21456400      -0.10598100
3846      C      0.01106800      1.22055900      -0.27297300
3847      C      -0.75290500      -0.00036700      -0.26042600
3848      C      0.01128900      -1.22119100      -0.27101800
3849      C      1.37938400      -1.21469800      -0.10413800
3850      C      2.07588900      0.00008100      -0.01158400
3851      H      1.92140200      2.15161300      -0.06096100
3852      H      -0.52970300      -2.15696600      -0.34721600
3853      H      1.92180200      -2.15157200      -0.05775600
3854      H      3.15122300      0.00027800      0.11947300
3855      O      -1.34977900      0.00176000      1.52838600
3856      H      -0.51942700      0.00240900      2.02689900
3857      H      -0.53010600      2.15611200      -0.35057400
3858      C      -2.13482000      -0.00111800      -0.86701400
3859      H      -2.68343600      0.88371600      -0.54450000
3860      H      -2.07163400      -0.00286700      -1.95904000
3861      H      -2.68362500      -0.88480400      -0.54167900
3862      Core      RigidRotor
3863      SymmetryFactor      0.856940376
3864      End
3865      Rotor      Hindered
3866      Group      15 16 17
3867      Axis      14      3
3868      Symmetry      3
3869      Potential[kcal/mol]      12
3870      0.000 0.666 1.518 2.354 2.933 3.067 2.692 1.941 1.053 0.267 -0.227 -0.332
3871      End
3872      Rotor      Hindered
3873      Group      12
3874      Axis      11      3
3875      Symmetry      1
3876      Potential[kcal/mol]      36
3877      0.000 0.066 0.341 0.792 1.355 1.934 2.449 2.833 3.047 3.102 3.054 2.972
3878      2.910 2.903 2.975 3.099 3.249 3.378 3.432 3.397 3.282 3.132 2.998 2.921
3879      2.903 2.956 3.037 3.098 3.072 2.903 2.571 2.103 1.554 0.989 0.497 0.152
3880      End
3881      Frequencies[1/cm]      42
3882      188.50 240.14 288.99 342.86 396.66 409.89 527.88 614.55
3883      630.98 730.48 771.62 820.78 900.52 920.51 972.60 977.78
3884      961.61 962.76 999.07 1012.91 1081.60 1117.27 1151.48 1191.07

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3885      1262.02 1295.26 1365.68 1395.44 1435.96 1445.07 1445.09 1519.98
3886      1551.53 2938.59 3011.23 3035.39 3066.26 3071.67 3081.87 3086.85
3887      3094.59 3635.25
3888 ZeroEnergy[kcal/mol]   -2.61
3889   ElectronicLevels[1/cm]                               1
3890      0.000000000000000000      2.0000000000000000
3891 End
3892 !*****
3893 RRHO           !           15
3894 Geometry[angstrom]           17
3895 C              1.37757600      1.21625800      -0.10790600
3896 C              0.01235000      1.22442100      -0.27006600
3897 C             -0.76408900     -0.00033200     -0.22791100
3898 C              0.01256200     -1.22503800     -0.26807900
3899 C              1.37777800     -1.21638800     -0.10604900
3900 C              2.07632600      0.00008000     -0.01124100
3901 H              1.92154000      2.15259900     -0.06852400
3902 H             -0.52860000     -2.16054000     -0.34515400
3903 H              1.92192500     -2.15256500     -0.06530000
3904 H              3.15156300      0.00027300      0.11872000
3905 O             -1.34318900      0.00171500      1.50380700
3906 H             -0.51682000      0.00236600      2.00825000
3907 H             -0.52898900      2.15970100     -0.34855100
3908 C             -2.13365000     -0.00110900     -0.86585900
3909 H             -2.68618400      0.88385600     -0.54992900
3910 H             -2.05442200     -0.00281800     -1.95653900
3911 H             -2.68636100     -0.88497800     -0.54717500
3912   Core   RigidRotor
3913           SymmetryFactor      0.856940376
3914 End
3915   Rotor                               Hindered
3916   Group   15 16 17
3917   Axis           14           3
3918   Symmetry           3
3919   Potential[kcal/mol]           12
3920   0.000 0.601 1.429 2.289 2.944 3.188 2.919 2.233 1.352 0.526 -0.044 -0.239
3921 End
3922   Rotor                               Hindered
3923   Group   12
3924   Axis           11           3
3925   Symmetry           1
3926   Potential[kcal/mol]           36
3927   0.000 0.066 0.341 0.791 1.355 1.934 2.449 2.833 3.047 3.102 3.054 2.972
3928   2.910 2.903 2.975 3.099 3.249 3.378 3.432 3.397 3.282 3.132 2.998 2.921
3929   2.903 2.956 3.037 3.098 3.072 2.903 2.571 2.103 1.554 0.989 0.497 0.152

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3930 End
3931 Frequencies[1/cm] 42
3932 202.06 248.93 302.52 347.47 391.46 412.26 528.04 609.42
3933 622.02 726.55 763.93 808.08 886.38 970.03 971.36 976.55
3934 994.01 996.17 1031.43 1015.35 1080.72 1110.37 1150.24 1193.00
3935 1260.90 1291.51 1364.84 1386.83 1429.65 1443.50 1445.22 1510.88
3936 1547.57 2939.88 3012.67 3033.96 3066.58 3071.39 3083.01 3087.03
3937 3095.47 3637.14
3938 ZeroEnergy[kcal/mol] -4.66
3939 ElectronicLevels[1/cm] 1
3940 0.0000000000000000 2.0000000000000000
3941 End
3942 !*****
3943 RRHO ! 16
3944 Geometry[angstrom] 17
3945 C 1.37598600 1.21792700 -0.10983600
3946 C 0.01336100 1.22806000 -0.26726900
3947 C -0.77516200 -0.00029700 -0.19530900
3948 C 0.01356500 -1.22866200 -0.26525500
3949 C 1.37618900 -1.21805600 -0.10796700
3950 C 2.07689400 0.00008000 -0.01070200
3951 H 1.92170200 2.15359500 -0.07642100
3952 H -0.52729800 -2.16422900 -0.34386300
3953 H 1.92207900 -2.15357300 -0.07318600
3954 H 3.15202200 0.00027100 0.11830900
3955 O -1.33652500 0.00167200 1.47924900
3956 H -0.51404200 0.00232900 1.98949300
3957 H -0.52767600 2.16340400 -0.34728900
3958 C -2.13232400 -0.00110300 -0.86457200
3959 H -2.68925200 0.88396500 -0.55577800
3960 H -2.03706700 -0.00278400 -1.95368800
3961 H -2.68942500 -0.88511300 -0.55306800
3962 Core RigidRotor
3963 SymmetryFactor 0.856940376
3964 End
3965 Rotor Hindered
3966 Group 15 16 17
3967 Axis 14 3
3968 Symmetry 3
3969 Potential[kcal/mol] 12
3970 0.000 0.533 1.329 2.199 2.918 3.263 3.101 2.488 1.626 0.770 0.133 -0.147
3971 End
3972 Rotor Hindered
3973 Group 12
3974 Axis 11 3

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3975 Symmetry 1
3976 Potential[kcal/mol] 36
3977 0.000 0.066 0.342 0.792 1.356 1.935 2.450 2.833 3.047 3.102 3.053 2.972
3978 2.910 2.903 2.975 3.099 3.249 3.378 3.432 3.397 3.282 3.132 2.998 2.921
3979 2.903 2.956 3.037 3.098 3.072 2.902 2.570 2.102 1.553 0.988 0.496 0.152
3980 End
3981 Frequencies[1/cm] 42
3982 212.26 250.41 303.64 339.72 373.26 400.53 509.61 581.87
3983 591.33 696.03 730.24 766.21 839.19 933.83 938.97 950.28
3984 954.04 973.13 987.45 1021.37 1077.91 1105.17 1150.54 1196.77
3985 1260.18 1286.75 1364.07 1377.80 1423.69 1442.36 1445.83 1504.29
3986 1547.95 2940.38 3013.47 3031.19 3066.04 3070.15 3083.26 3086.29
3987 3096.04 3638.82
3988 ZeroEnergy[kcal/mol] -7.19
3989 ElectronicLevels[1/cm] 1
3990 0.000000000000000000 2.000000000000000000
3991 End
3992 !*****
3993 RRHO ! 17
3994 Geometry[angstrom] 17
3995 C 1.37456300 1.21947800 -0.11181900
3996 C 0.01373300 1.23121500 -0.26406500
3997 C -0.78573800 -0.00025800 -0.16306800
3998 C 0.01392800 -1.23180200 -0.26202500
3999 C 1.37476200 -1.21960500 -0.10993800
4000 C 2.07737100 0.00008000 -0.01005500
4001 H 1.92195100 2.15456400 -0.08533100
4002 H -0.52599300 -2.16789800 -0.34304200
4003 H 1.92232000 -2.15455300 -0.08208600
4004 H 3.15247100 0.00027000 0.11788100
4005 O -1.32965700 0.00162800 1.45432100
4006 H -0.51145500 0.00229700 1.97073600
4007 H -0.52635900 2.16708600 -0.34649500
4008 C -2.13076400 -0.00109600 -0.86293200
4009 H -2.69276100 0.88402800 -0.56236400
4010 H -2.01835200 -0.00275400 -1.95011100
4011 H -2.69293300 -0.88520200 -0.55969100
4012 Core RigidRotor
4013 SymmetryFactor 0.856940376
4014 End
4015 Rotor Hindered
4016 Group 15 16 17
4017 Axis 14 3
4018 Symmetry 3
4019 Potential[kcal/mol] 12

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4020 0.000 0.466 1.223 2.095 2.863 3.295 3.235 2.698 1.865 0.990 0.295 -0.062
4021 End
4022 Rotor Hindered
4023 Group 12
4024 Axis 11 3
4025 Symmetry 1
4026 Potential[kcal/mol] 36
4027 0.000 0.067 0.343 0.794 1.358 1.937 2.452 2.834 3.047 3.102 3.053 2.972
4028 2.910 2.903 2.976 3.100 3.250 3.378 3.432 3.397 3.281 3.132 2.998 2.921
4029 2.903 2.956 3.038 3.098 3.072 2.902 2.569 2.100 1.552 0.986 0.495 0.151
4030 End
4031 Frequencies[1/cm] 42
4032 234.06 274.03 327.50 358.56 386.31 421.82 532.38 600.62
4033 608.71 719.80 756.47 786.56 860.21 969.61 975.22 983.31
4034 986.29 977.31 1005.43 1030.72 1073.64 1102.14 1151.91 1203.37
4035 1258.87 1281.34 1363.38 1369.45 1418.14 1441.73 1446.57 1499.68
4036 1549.88 2940.34 3014.11 3027.60 3064.64 3068.08 3082.26 3084.53
4037 3096.17 3641.49
4038 ZeroEnergy[kcal/mol] -9.97
4039 ElectronicLevels[1/cm] 1
4040 0.0000000000000000 2.0000000000000000
4041 End
4042 !*****
4043 RRHO ! 18
4044 Geometry[angstrom] 17
4045 C 1.37326800 1.22084700 -0.11392200
4046 C 0.01341600 1.23385500 -0.26012400
4047 C -0.79576900 -0.00022100 -0.13154300
4048 C 0.01360300 -1.23442400 -0.25805600
4049 C 1.37346400 -1.22097300 -0.11202900
4050 C 2.07759700 0.00007900 -0.00938900
4051 H 1.92224900 2.15538900 -0.09557700
4052 H -0.52499400 -2.17128400 -0.34231700
4053 H 1.92260800 -2.15539200 -0.09232100
4054 H 3.15277800 0.00026700 0.11716600
4055 O -1.32245100 0.00158300 1.42886000
4056 H -0.50998300 0.00226700 1.95336800
4057 H -0.52534500 2.17049000 -0.34580100
4058 C -2.12883000 -0.00108900 -0.86091200
4059 H -2.69637500 0.88407200 -0.56975800
4060 H -1.99760000 -0.00272300 -1.94567600
4061 H -2.69654700 -0.88527200 -0.56712100
4062 Core RigidRotor
4063 SymmetryFactor 0.856940376
4064 End

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4065 Rotor                               Hindered
4066 Group    15 16 17
4067 Axis              14              3
4068 Symmetry                3
4069 Potential[kcal/mol]                12
4070 0.000 0.401 1.118 1.984 2.789 3.294 3.326 2.864 2.065 1.180 0.439 0.015
4071 End
4072 Rotor                               Hindered
4073 Group    12
4074 Axis              11              3
4075 Symmetry                1
4076 Potential[kcal/mol]                36
4077 0.000 0.068 0.346 0.797 1.361 1.940 2.455 2.836 3.049 3.102 3.053 2.972
4078 2.910 2.903 2.977 3.101 3.251 3.379 3.433 3.397 3.281 3.131 2.998 2.921
4079 2.904 2.957 3.038 3.099 3.071 2.901 2.567 2.098 1.549 0.984 0.493 0.150
4080 End
4081 Frequencies[1/cm]                42
4082 289.78 293.77 344.29 363.54 386.16 428.85 536.76 597.19
4083 604.52 716.36 755.67 778.96 851.19 968.88 974.80 979.16
4084 981.08 972.19 1020.11 1044.48 1069.14 1100.25 1153.60 1215.03
4085 1256.51 1275.86 1362.25 1362.76 1413.17 1441.46 1447.29 1496.28
4086 1550.92 2939.96 3014.94 3024.01 3062.75 3065.63 3080.46 3082.26
4087 3095.98 3645.30
4088 ZeroEnergy[kcal/mol]    -12.39
4089 ElectronicLevels[1/cm]                1
4090 0.00000000000000000000000000000000 2.00000000000000000000000000000000
4091 End
4092 !*****
4093 RRHO          !              19
4094 Geometry[angstrom]                17
4095 C              1.37192500    1.22203800    -0.11623400
4096 C              0.01254800    1.23612500    -0.25525300
4097 C             -0.80528300    -0.00018400    -0.10092600
4098 C              0.01272600    -1.23667400    -0.25315600
4099 C              1.37211400    -1.22216300    -0.11432900
4100 C              2.07748200    0.00007900    -0.00881300
4101 H              1.92248900    2.15598300    -0.10721700
4102 H             -0.52454300    -2.17425700    -0.34124000
4103 H              1.92283400    -2.15600300    -0.10394800
4104 H              3.15284300    0.00026400    0.11588700
4105 O             -1.31492600    0.00153400    1.40293500
4106 H             -0.51013500    0.00224100    1.93802100
4107 H             -0.52487600    2.17348300    -0.34475900
4108 C             -2.12628900    -0.00108100    -0.85860100
4109 H             -2.69959500    0.88415400    -0.57793600

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4110 H -1.97465100 -0.00268900 -1.94040300
4111 H -2.69976600 -0.88538100 -0.57533900
4112 Core RigidRotor
4113 SymmetryFactor 0.856940376
4114 End
4115 Rotor Hindered
4116 Group 15 16 17
4117 Axis 14 3
4118 Symmetry 3
4119 Potential[kcal/mol] 12
4120 0.000 0.342 1.018 1.874 2.704 3.269 3.383 2.990 2.229 1.340 0.563 0.082
4121 End
4122 Rotor Hindered
4123 Group 12
4124 Axis 11 3
4125 Symmetry 1
4126 Potential[kcal/mol] 36
4127 0.000 0.069 0.348 0.801 1.365 1.944 2.458 2.838 3.050 3.102 3.053 2.971
4128 2.910 2.904 2.978 3.102 3.252 3.380 3.433 3.397 3.280 3.131 2.997 2.921
4129 2.904 2.958 3.039 3.099 3.071 2.899 2.565 2.095 1.545 0.980 0.490 0.149
4130 End
4131 Frequencies[1/cm] 42
4132 304.87 340.49 367.44 386.30 436.74 473.15 547.67 594.02
4133 603.23 713.69 756.87 772.95 844.61 968.07 974.01 975.46
4134 975.80 967.57 1028.89 1055.76 1065.06 1098.87 1154.97 1232.49
4135 1252.72 1271.03 1356.18 1362.19 1408.86 1441.41 1447.97 1493.62
4136 1551.23 2939.30 3015.92 3020.69 3060.63 3063.06 3078.38 3079.88
4137 3095.61 3650.55
4138 ZeroEnergy[kcal/mol] -14.72
4139 ElectronicLevels[1/cm] 1
4140 0.0000000000000000 2.0000000000000000
4141 End
4142 !*****
4143 RRHO ! 20
4144 Geometry[angstrom] 17
4145 C 1.37033200 1.22312800 -0.11900500
4146 C 0.01106700 1.23824400 -0.24889000
4147 C -0.81396100 -0.00014600 -0.07162400
4148 C 0.01123500 -1.23876500 -0.24676000
4149 C 1.37051300 -1.22325300 -0.11708500
4150 C 2.07685000 0.00007900 -0.00854600
4151 H 1.92260600 2.15634400 -0.12104400
4152 H -0.52489200 -2.17693600 -0.33903800
4153 H 1.92293300 -2.15638500 -0.11775500
4154 H 3.15252800 0.00025900 0.11336800

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4155 O -1.30734000 0.00147900 1.37676800
4156 H -0.51183500 0.00221500 1.92416600
4157 H -0.52520400 2.17618800 -0.34260400
4158 C -2.12255300 -0.00107100 -0.85609300
4159 H -2.70197700 0.88435900 -0.58751600
4160 H -1.94802200 -0.00264500 -1.93429200
4161 H -2.70214600 -0.88561900 -0.58496800
4162 Core RigidRotor
4163 SymmetryFactor 0.856940376
4164 End
4165 Rotor Hindered
4166 Group 15 16 17
4167 Axis 14 3
4168 Symmetry 3
4169 Potential[kcal/mol] 12
4170 0.000 0.290 0.930 1.773 2.621 3.233 3.413 3.081 2.356 1.469 0.665 0.138
4171 End
4172 Rotor Hindered
4173 Group 12
4174 Axis 11 3
4175 Symmetry 1
4176 Potential[kcal/mol] 36
4177 0.000 0.069 0.348 0.801 1.365 1.944 2.458 2.838 3.050 3.102 3.053 2.971
4178 2.910 2.904 2.978 3.102 3.252 3.380 3.433 3.397 3.280 3.131 2.997 2.921
4179 2.904 2.958 3.039 3.099 3.071 2.899 2.565 2.095 1.545 0.980 0.490 0.149
4180 End
4181 Frequencies[1/cm] 42
4182 318.01 347.40 369.88 387.17 444.88 532.41 589.47 590.86
4183 647.98 714.38 766.58 768.56 840.78 967.05 970.92 971.03
4184 974.48 963.56 1038.47 1061.56 1062.30 1097.88 1155.69 1247.27
4185 1253.61 1267.70 1351.33 1362.03 1405.28 1441.58 1448.62 1491.59
4186 1551.32 2937.75 3015.92 3017.22 3058.16 3060.23 3076.06 3077.29
4187 3095.03 3657.48
4188 ZeroEnergy[kcal/mol] -16.55
4189 ElectronicLevels[1/cm] 1
4190 0.000000000000000000 2.000000000000000000
4191 End
4192 !*****
4193 RRHO ! 21
4194 Geometry[angstrom] 17
4195 C 1.36801300 1.22437600 -0.12319300
4196 C 0.00837200 1.24071100 -0.23866800
4197 C -0.82022000 -0.00010700 -0.04552700
4198 C 0.00852300 -1.24119300 -0.23648600
4199 C 1.36817800 -1.22449700 -0.12124100

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4200 C          2.07488800   0.00007700  -0.00991800
4201 H          1.92260100   2.15651600  -0.14103800
4202 H          -0.52736800  -2.17950600  -0.33217500
4203 H          1.92289300  -2.15658600  -0.13769800
4204 H          3.15129800   0.00024700   0.10589000
4205 O          -1.30102100   0.00140600   1.35222000
4206 H          -0.51547000   0.00218200   1.91193000
4207 H          -0.52764300   2.17880200  -0.33583300
4208 C          -2.11505900  -0.00105500  -0.85447000
4209 H          -2.70170300   0.88496600  -0.60203800
4210 H          -1.91060400  -0.00256600  -1.92796000
4211 H          -2.70185800  -0.88627700  -0.59958000
4212 Core RigidRotor
4213 SymmetryFactor 0.856940376
4214 End
4215 Rotor Hindered
4216 Group 15 16 17
4217 Axis 14 3
4218 Symmetry 3
4219 Potential[kcal/mol] 12
4220 0.000 0.259 0.875 1.710 2.565 3.204 3.423 3.129 2.427 1.543 0.725 0.172
4221 End
4222 Rotor Hindered
4223 Group 12
4224 Axis 11 3
4225 Symmetry 1
4226 Potential[kcal/mol] 36
4227 0.000 0.075 0.358 0.815 1.381 1.959 2.470 2.847 3.054 3.103 3.052 2.970
4228 2.910 2.916 2.981 3.107 3.257 3.383 3.434 3.396 3.278 3.128 2.996 2.921
4229 2.905 2.961 3.042 3.101 3.070 2.894 2.556 2.083 1.532 0.968 0.481 0.143
4230 End
4231 Frequencies[1/cm] 42
4232 325.35 351.03 371.20 387.95 452.49 539.20 587.84 592.08
4233 698.85 731.42 766.43 816.26 851.10 965.35 968.88 969.23
4234 974.73 997.62 1052.03 1059.10 1069.60 1097.57 1155.89 1242.41
4235 1266.58 1274.13 1348.44 1363.51 1402.87 1442.26 1449.39 1490.67
4236 1551.93 2933.18 3011.10 3012.81 3054.64 3056.58 3073.30 3073.98
4237 3093.80 3667.88
4238 ZeroEnergy[kcal/mol] -17.65
4239 ElectronicLevels[1/cm] 1
4240 0.0000000000000000 2.0000000000000000
4241 End
4242 !*****
4243 RRHO ! 22
4244 Geometry[angstrom] 17

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4245  C          1.36554400   1.22581100  -0.12920700
4246  C          0.00469300   1.24326600  -0.22417900
4247  C         -0.81754000  -0.00007900  -0.03811400
4248  C          0.00482300  -1.24369100  -0.22191900
4249  C          1.36568500  -1.22592700  -0.12718300
4250  C          2.07136400   0.00007100  -0.01926200
4251  H          1.92323700   2.15659600  -0.17492800
4252  H         -0.53394700  -2.18136400  -0.31087900
4253  H          1.92346400  -2.15671900  -0.17141600
4254  H          3.14988900   0.00021600   0.07796700
4255  O         -1.30680500   0.00132500   1.35516300
4256  H         -0.52024700   0.00209100   1.90836700
4257  H         -0.53414800   2.18074600  -0.31476900
4258  C         -2.09927100  -0.00102800  -0.86284200
4259  H         -2.69505800   0.88706200  -0.63624300
4260  H         -1.84505700  -0.00235000  -1.93016300
4261  H         -2.69515000  -0.88853300  -0.63406400
4262  Core  RigidRotor
4263      SymmetryFactor    0.856940376
4264  End
4265  Rotor                               Hindered
4266  Group    15 16 17
4267  Axis           14           3
4268  Symmetry           3
4269  Potential[kcal/mol]           12
4270  0.000 0.288 0.927 1.770 2.617 3.231 3.413 3.084 2.360 1.473 0.669 0.141
4271  End
4272  Rotor                               Hindered
4273  Group    12
4274  Axis           11           3
4275  Symmetry           1
4276  Potential[kcal/mol]           36
4277  0.000 0.081 0.370 0.830 1.398 1.975 2.483 2.856 3.058 3.104 3.051 2.969
4278  2.910 2.918 2.985 3.112 3.262 3.387 3.435 3.394 3.274 3.125 2.993 2.921
4279  2.907 2.964 3.045 3.102 3.068 2.887 2.545 2.069 1.517 0.954 0.470 0.138
4280  End
4281  Frequencies[1/cm]           42
4282  294.53 349.31 374.97 388.78 454.94 538.63 587.67 592.75
4283  702.83 734.13 769.74 819.82 856.20 969.38 969.48 973.02
4284  978.27 996.45 1056.23 1060.24 1072.69 1099.67 1156.23 1247.97
4285  1268.82 1273.72 1351.20 1368.66 1403.94 1444.70 1450.64 1492.44
4286  1553.90 2911.13 2985.71 3005.44 3046.49 3048.78 3069.01 3069.67
4287  3090.12 3704.82
4288  ZeroEnergy[kcal/mol]    -17.36
4289  ElectronicLevels[1/cm]           1

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4290      0.0000000000000000      2.0000000000000000
4291      End
4292      !*****
4293          Tunneling      Eckart
4294          ImaginaryFrequency[1/cm]      411.6
4295          WellDepth[kcal/mol]      3.18
4296          WellDepth[kcal/mol]      18.11
4297      End
4298      End
4299      !*****
4300      Bimolecular      P4m      # mOHC6H4CH3 + H
4301      Fragment PROD1
4302      RRHO
4303      Geometry[angstrom]      16
4304      C      0.03828900      -0.98332300      -0.01103200
4305      C      -1.21419400      -0.36747800      0.00155700
4306      C      -1.31683100      1.02422600      0.00783400
4307      C      -0.15108900      1.79118800      0.00251200
4308      C      1.10089000      1.18051600      -0.00905900
4309      C      1.20539600      -0.21732100      -0.01208300
4310      H      -2.29153300      1.50193700      0.01367200
4311      H      -0.22618900      2.87251300      0.00277400
4312      H      1.99944500      1.78707000      -0.01692600
4313      O      -2.31206400      -1.18783600      0.00152300
4314      H      -3.10835700      -0.64861900      0.00128900
4315      H      0.08363700      -2.06635100      -0.01979200
4316      C      2.55658700      -0.88788300      0.01051600
4317      H      2.91140200      -1.01152500      1.03818800
4318      H      2.51470600      -1.87797900      -0.44695700
4319      H      3.29911700      -0.29390900      -0.52590100
4320      Core      RigidRotor
4321          SymmetryFactor      0.5
4322      End
4323          Rotor      Hindered      ! freq=50
4324          Group      14 15 16
4325          Axis      6 13
4326          Symmetry      3
4327      Potential[kcal/mol]      12
4328          0.000 0.005 0.012 0.021 0.018 0.008 0.001 0.001 0.008 0.015 0.012 0.004
4329      End
4330          Rotor      Hindered      !freq=244
4331          Group      11
4332          Axis      2 10
4333          Symmetry      1
4334      Potential[kcal/mol]      36

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4335      0.000 0.092 0.389 0.864 1.452 2.084 2.683 3.172 3.487 3.568 3.400 3.028
4336      2.516 1.924 1.325 0.786 0.367 0.116 0.040 0.136 0.405 0.837 1.382 1.980
4337      2.565 3.067 3.426 3.574 3.472 3.122 2.616 2.009 1.378 0.800 0.343 0.070
4338      End
4339      Frequencies[1/cm]          40
4340      198.61  222.19  295.05  427.33  445.22  521.41  538.70  546.11
4341      558.40  741.48  743.99  834.52  847.66  912.44  947.09  974.50
4342      988.51 1018.59 1071.93 1134.08 1143.48 1165.80 1255.31 1287.04
4343      1319.62 1369.79 1428.64 1443.52 1462.20 1467.25 1572.12 1598.85
4344      2929.96 2989.47 3012.20 3051.32 3063.99 3075.65 3081.82 3706.83
4345      ZeroEnergy[kcal/mol]          0.
4346      ElectronicLevels[1/cm]          1
4347      0.0000000000000000E+000  1.0000000000000000
4348      End
4349      !*****
4350      Fragment PROD2
4351      RRHO
4352      Geometry[angstrom]          1
4353      H          0.00000000  0.00000000  0.00000000
4354      Core  RigidRotor
4355      SymmetryFactor  1.0000000000000000
4356      End
4357      ZeroEnergy[kcal/mol]          0.
4358      ElectronicLevels[1/cm]          1
4359      0.0000000000000000E+000  2.0000000000000000
4360      End
4361      GroundEnergy[kcal/mol]  1.02
4362      End
4363      !*****
4364      Bimolecular  P4o  # oOHC6H4CH3 + H
4365      Fragment PROD1
4366      RRHO
4367      Geometry[angstrom]          16
4368      C          -0.58741200  -0.62124200  -0.00003100
4369      C          -0.39709600   0.76973300  -0.00000600
4370      C           0.88413500   1.32167300   0.00001700
4371      C           1.99797900   0.48646800   0.00001400
4372      C           1.83489000  -0.89976800  -0.00004700
4373      C           0.54852700  -1.43744100  -0.00007500
4374      H           0.98536700   2.40000700   0.00003400
4375      H           2.99111300   0.91992900   0.00003400
4376      H           2.69768500  -1.55439500  -0.00007200
4377      H           0.41480900  -2.51417900  -0.00013200
4378      O          -1.44958500   1.64859900   0.00011500
4379      H          -2.27720700   1.15968200  -0.00069600

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4380  C          -1.97801700  -1.20387200   0.00007400
4381  H          -2.54736500  -0.90051000   0.88608300
4382  H          -2.54800600  -0.89932200  -0.88512400
4383  H          -1.93774900  -2.29330800  -0.00072200
4384  Core  RigidRotor
4385      SymmetryFactor  0.5
4386  End
4387  Rotor  Hindered          ! freq=94
4388      Group              14 15 16
4389      Axis                1 13
4390      Symmetry            3
4391  Potential[kcal/mol]      12
4392      0.000 0.071 0.296 0.643 1.024 1.322 1.445 1.347 1.064 0.686 0.330 0.089
4393  End
4394  Rotor  Hindered          !freq=150
4395      Group              12
4396      Axis                2 11
4397      Symmetry            1
4398  Potential[kcal/mol]      36
4399      0.000 0.053 0.246 0.591 1.055 1.583 2.124 2.609 2.963 3.155 3.106 2.798
4400      2.296 1.666 0.998 0.368 -0.128 -0.445 -0.548 -0.447 -0.133 0.362 0.991 1.659
4401      2.289 2.794 3.104 3.156 2.966 2.614 2.130 1.589 1.061 0.596 0.249 0.054
4402  End
4403  Frequencies[1/cm]        40
4404      186.29  259.01  301.30  424.19  434.14  512.90  529.95  581.51
4405      591.00  746.70  758.39  835.09  850.50  903.58  918.78  963.53
4406      1011.53 1018.60 1082.58 1134.16 1146.18 1191.56 1239.63 1281.99
4407      1328.43 1368.32 1428.31 1438.52 1462.05 1470.31 1568.76 1599.29
4408      2908.11 2955.21 3014.00 3057.11 3070.55 3085.32 3093.61 3713.37
4409  ZeroEnergy[kcal/mol]    0.
4410  ElectronicLevels[1/cm]  1
4411  0.0000000000000000E+000  1.0000000000000000
4412  End
4413  !*****
4414  Fragment PROD2
4415  RRHO
4416      Geometry[angstrom]  1
4417  H          0.00000000  0.00000000  0.00000000
4418  Core  RigidRotor
4419      SymmetryFactor  1.0000000000000000
4420  End
4421  ZeroEnergy[kcal/mol]    0.
4422  ElectronicLevels[1/cm]  1
4423  0.0000000000000000E+000  2.0000000000000000
4424  End

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4425 GroundEnergy[kcal/mol] 0.71
4426 End
4427 !*****
4428 Bimolecular P4p # pOHC6H4CH3 + H
4429 Fragment PROD1
4430 RRHO
4431 Geometry[angstrom] 16
4432 C 0.72793300 -1.21888100 -0.00140500
4433 C 1.43852100 -0.01733900 0.00327400
4434 C 0.74887800 1.19466900 -0.00111900
4435 C -0.64762000 1.19870300 -0.00908100
4436 C -1.37951600 0.00884900 -0.00977600
4437 C -0.66342400 -1.19615200 -0.00894900
4438 H 1.29558600 2.13295400 -0.00313800
4439 H -1.17062800 2.14924600 -0.01586800
4440 O 2.80767300 -0.09363200 0.00788400
4441 H 3.17287700 0.79589800 0.00413700
4442 H 1.27506500 -2.15356700 -0.00346800
4443 H -1.20434700 -2.13691500 -0.01568900
4444 C -2.88816700 0.01551700 0.01221100
4445 H -3.27078800 -0.15261500 1.02360800
4446 H -3.28284400 0.97204200 -0.33574400
4447 H -3.29593400 -0.77018500 -0.62783500
4448 Core RigidRotor
4449 SymmetryFactor 1
4450 End
4451 Rotor Hindered ! freq=45
4452 Group 14 15 16
4453 Axis 5 13
4454 Symmetry 3
4455 Potential[kcal/mol] 12
4456 0.000 0.001 0.032 0.054 0.061 0.051 0.016 -0.002 -0.001 -0.004 -0.005 -0.003
4457 End
4458 Rotor Hindered !freq=242.8
4459 Group 10
4460 Axis 2 9
4461 Symmetry 1
4462 Potential[kcal/mol] 36
4463 0.000 0.079 0.323 0.750 1.287 1.862 2.405 2.853 3.145 3.228 3.086 2.758
4464 2.297 1.761 1.211 0.709 0.315 0.083 0.000 0.070 0.302 0.674 1.170 1.721
4465 2.254 2.723 3.064 3.224 3.161 2.884 2.447 1.910 1.335 0.792 0.353 0.078
4466 End
4467 Frequencies[1/cm] 40
4468 139.99 305.27 317.85 405.67 425.02 465.80 492.40 539.38
4469 655.70 747.07 781.78 814.56 851.84 874.72 927.98 971.97

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4470      992.28  1019.39 1087.49 1151.12 1152.28 1192.89 1233.22 1291.99
4471      1322.85 1371.40 1404.16 1441.86 1454.47 1491.65 1576.32 1598.79
4472      2926.43 2983.71 3006.69 3045.99 3057.34 3065.82 3089.47 3708.61
4473      ZeroEnergy[kcal/mol]          0.
4474      ElectronicLevels[1/cm]                1
4475      0.0000000000000000E+000  1.0000000000000000
4476      End
4477      !*****
4478      Fragment PROD2
4479      RRHO
4480      Geometry[angstrom]          1
4481      H          0.00000000  0.00000000  0.00000000
4482      Core  RigidRotor
4483      SymmetryFactor  1.0000000000000000
4484      End
4485      ZeroEnergy[kcal/mol]          0.
4486      ElectronicLevels[1/cm]                1
4487      0.0000000000000000E+000  2.0000000000000000
4488      End
4489      GroundEnergy[kcal/mol]  1.61
4490      End
4491      !*****
4492      Well  W4m2          # mHOC6CH5CH3
4493      Species
4494      RRHO
4495      Geometry[angstrom]          17
4496      C          0.14099700  -0.97869900  -0.32239800
4497      C          1.21099700  -0.18524500  -0.03819900
4498      C          1.01290600  1.21583700  0.15518800
4499      C          -0.28100600  1.78068600  0.06851000
4500      C          -1.37041600  1.01057500  -0.21359600
4501      C          -1.26403800  -0.46815400  -0.42165900
4502      H          1.86322500  1.84760900  0.38399600
4503      H          -0.40260700  2.84570600  0.23380800
4504      H          -2.36371900  1.44077000  -0.26934000
4505      C          2.60530400  -0.74771900  0.08222800
4506      H          2.61160600  -1.82600200  -0.08195000
4507      H          3.27417400  -0.28656500  -0.64966000
4508      H          3.01997100  -0.54980900  1.07447700
4509      O          -2.13809300  -1.18196200  0.49153600
4510      H          -1.81337900  -0.99991100  1.38073800
4511      H          -1.68362200  -0.73293100  -1.40072400
4512      H          0.27063700  -2.04685600  -0.46407300
4513      Core  RigidRotor
4514      SymmetryFactor          0.5

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4515           End
4516 Rotor Hindered           !freq=122
4517           Group           11 12 13
4518           Axis           2 10
4519           Symmetry       3
4520 Potential[kcal/mol]      12
4521     0.000 0.047 0.171 0.353 0.552 0.702 0.756 0.700 0.546 0.356 0.174 0.050
4522           End
4523 Rotor Hindered           !freq=290
4524           Group           15
4525           Axis           6 14
4526           Symmetry       1
4527 Potential[kcal/mol]      36
4528     0.000 0.100 0.406 0.870 1.428 1.986 2.449 2.752 2.871 2.841 2.712 2.557
4529     2.440 2.397 2.430 2.520 2.632 2.724 2.762 2.731 2.647 2.535 2.440 2.397
4530     2.431 2.536 2.676 2.789 2.812 2.688 2.400 1.968 1.443 0.904 0.434 0.118
4531           End
4532           Frequencies[1/cm]      43
4533     91.89  175.96  330.34  371.13  435.12  466.20  495.93  535.98  619.64
4534     699.25  762.67  786.67  847.46  897.67  950.54  961.86  986.66
4535     989.91 1024.75 1040.74 1084.71 1133.73 1161.11 1175.99 1272.16
4536     1282.10 1324.70 1344.54 1369.46 1389.61 1437.26 1449.26 1515.76
4537     1577.37 2898.68 2929.59 2986.09 3014.93 3058.36 3060.12 3075.37
4538     3084.80 3670.76
4539           ZeroEnergy[kcal/mol]      -16.64
4540           ElectronicLevels[1/cm]      1
4541           0 2
4542 End
4543 End
4544 !*****
4545 Barrier      B4m3      W4m2      P4m           # TS4m3
4546 RRHO
4547           Geometry[angstrom]      17
4548 C           -0.05072100  -0.97334300  -0.01973500
4549 C           -1.22376700  -0.22700800  -0.01481400
4550 C           -1.13291700  1.17672500  -0.00966100
4551 C           0.11461100   1.81011600  -0.03017800
4552 C           1.28954600   1.07397300  -0.02420500
4553 C           1.22096500  -0.34003500  0.08041800
4554 H           -2.04231800  1.77201500  -0.01640800
4555 H           0.16514000   2.89520600  -0.06675600
4556 H           2.26645400   1.54472200  -0.05273600
4557 C           -2.57297900  -0.90803600  -0.01993900
4558 H           -3.04075900  -0.86432200  0.97231300
4559 H           -3.26148700  -0.42565600  -0.72290500

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4560 H -2.49022500 -1.96356100 -0.29816800
4561 O 2.38642900 -1.02527200 -0.17468600
4562 H 2.24484800 -1.96376100 0.02515200
4563 H 1.29299000 -0.40571800 1.82435600
4564 H -0.09450600 -2.06110000 -0.03868200
4565 Core RigidRotor
4566 SymmetryFactor 0.5
4567 End
4568 Tunneling Eckart
4569 ImaginaryFrequency[1/cm] 1207.49
4570 WellDepth[kcal/mol] 26.61
4571 WellDepth[kcal/mol] 8.95
4572 End
4573 Frequencies[1/cm] 44
4574 59.26 202.24 207.01 274.54 296.67 416.91 453.07 504.34
4575 518.52 525.68 583.48 677.41 693.96 752.96 802.40 858.55
4576 913.03 950.31 983.14 975.51 990.57 1025.98 1069.44 1130.44
4577 1144.81 1161.71 1238.16 1287.10 1302.23 1370.47 1405.74 1442.05
4578 1453.30 1475.50 1567.40 1585.66 2932.14 2992.28 3013.28 3051.30
4579 3064.63 3080.30 3101.60 3703.68
4580 ZeroEnergy[kcal/mol] 9.97
4581 ElectronicLevels[1/cm] 1
4582 0 2
4583 End
4584 !*****
4585 Barrier B4m2 W W4m2
4586 Variational
4587 RRHO ! 1
4588 Geometry[angstrom] 17
4589 C -1.25487500 -0.10749200 -0.08864300
4590 C -0.92487200 1.17583000 0.36987000
4591 C 0.34591800 1.71263800 0.15496300
4592 C 1.31251200 0.97161300 -0.52571200
4593 C 0.99973600 -0.31269200 -0.98121800
4594 C -0.27669200 -0.84096900 -0.76677600
4595 H -1.67018500 1.75915400 0.90335100
4596 H 0.57987900 2.70693900 0.51952300
4597 H 2.29977600 1.38247800 -0.69710700
4598 H 1.73601500 -0.89042500 -1.52628700
4599 H -0.51147600 -1.83534300 -1.13050200
4600 C -2.62651800 -0.68526300 0.16034300
4601 H -3.39771000 0.09829500 0.13342000
4602 H -2.87587100 -1.44078800 -0.59097900
4603 H -2.67776800 -1.16889800 1.14838200
4604 O 2.13502100 -1.42370600 1.23441500

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4605 H 1.50457500 -0.80183300 1.61895800
4606 Core RigidRotor
4607 SymmetryFactor 0.412697798
4608 End
4609 Rotor Hindered
4610 Group 13 14 15
4611 Axis 12 1
4612 Symmetry 3
4613 Potential[kcal/mol] 12
4614 0.000 0.004 -0.001 -0.002 0.003 0.016 0.041 0.062 0.066 0.061 0.051 0.021
4615 End
4616 Rotor Hindered
4617 Group 17
4618 Axis 16 5
4619 Symmetry 1
4620 Potential[kcal/mol] 36
4621 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
4622 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
4623 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
4624 End
4625 Frequencies[1/cm] 42
4626 55.88 208.60 222.55 240.66 349.70 403.20 460.94 525.79
4627 632.67 639.46 735.05 799.77 851.50 893.72 951.95 960.42
4628 977.82 981.40 1009.91 1034.23 1071.31 1139.40 1160.28 1190.52
4629 1297.17 1309.81 1380.54 1416.87 1447.56 1457.23 1470.35 1562.22
4630 1582.77 2875.14 2927.28 2977.50 3045.42 3063.48 3068.44 3082.02
4631 3095.05 3697.13
4632 ZeroEnergy[kcal/mol] -3.42
4633 ElectronicLevels[1/cm] 1
4634 0.0000000000000000 2.0000000000000000
4635 End
4636 !*****
4637 RRHO ! 2
4638 Geometry[angstrom] 17
4639 C -1.25857400 -0.10438000 -0.08687800
4640 C -0.93949200 1.18916100 0.35189900
4641 C 0.33231200 1.72513900 0.14845600
4642 C 1.31309700 0.97329600 -0.50381500
4643 C 1.00969900 -0.31811700 -0.94333000
4644 C -0.26852600 -0.84624000 -0.74053300
4645 H -1.69646400 1.78145400 0.85655100
4646 H 0.55463400 2.72935200 0.48950700
4647 H 2.30249400 1.38409000 -0.66479700
4648 H 1.76501500 -0.90983700 -1.44895000
4649 H -0.49108400 -1.84996900 -1.08535100

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4650  C          -2.63164000  -0.67969200   0.15723600
4651  H          -3.41159400   0.04315200  -0.09140300
4652  H          -2.79534600  -1.57568500  -0.44229500
4653  H          -2.76029900  -0.95425300   1.20821600
4654  O           2.14312700  -1.44553800   1.18255300
4655  H           1.60951600  -0.79590400   1.66347100
4656  Core  RigidRotor
4657          SymmetryFactor  0.412697798
4658  End
4659  Rotor                      Hindered
4660  Group  13 14 15
4661  Axis           12           1
4662  Symmetry           3
4663  Potential[kcal/mol]           12
4664  0.000 -0.005 -0.005 0.000 0.016 0.041 0.061 0.062 0.056 0.032 0.014 -0.005
4665  End
4666  Rotor                      Hindered
4667  Group  17
4668  Axis           16           5
4669  Symmetry           1
4670  Potential[kcal/mol]           36
4671  0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
4672  2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
4673  2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
4674  End
4675  Frequencies[1/cm]           42
4676  18.02  86.18  202.73  308.70  340.71  402.56  454.12  525.71
4677  629.17  632.99  733.97  799.69  850.13  889.21  948.95  954.69
4678  965.30  979.24  1008.60 1019.13 1069.51 1139.15 1160.51 1191.02
4679  1294.94 1308.87 1370.26 1416.13 1440.38 1453.96 1469.56 1559.77
4680  1583.22 2932.71 2990.47 3017.47 3052.49 3061.03 3072.29 3077.97
4681  3090.65 3657.74
4682  ZeroEnergy[kcal/mol]  -2.98
4683  ElectronicLevels[1/cm]           1
4684  0.000000000000000000  2.0000000000000000
4685  End
4686  !*****
4687  RRHO          !           3
4688  Geometry[angstrom]           17
4689  C          -1.25367800  -0.10846300  -0.07572700
4690  C          -0.94563900   1.19907100   0.33023000
4691  C           0.32995800   1.73136300   0.14052200
4692  C           1.32564200   0.96328400  -0.46417500
4693  C           1.03507800  -0.34233600  -0.87323800
4694  C          -0.24848400  -0.86810200  -0.67764700

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4740  C          -0.94581600   1.20039400   0.32422400
4741  C           0.33131400   1.73074300   0.14038100
4742  C           1.33020700   0.95888400  -0.45261600
4743  C           1.03988900  -0.34765400  -0.85932000
4744  C          -0.24256800  -0.87476600  -0.66134500
4745  H          -1.71911900   1.81156200   0.77898400
4746  H           0.54421600   2.74527400   0.45713100
4747  H           2.32554100   1.36113400  -0.59529700
4748  H           1.79562200  -0.94240800  -1.35455300
4749  H          -0.45101500  -1.89332000  -0.96946900
4750  C          -2.63408400  -0.67367400   0.14328600
4751  H          -3.39728600   0.00429900  -0.24650300
4752  H          -2.74848100  -1.63631100  -0.35725200
4753  H          -2.83930900  -0.82269100   1.20722300
4754  O           2.09248200  -1.39680800   1.04235700
4755  H           1.52368500  -0.88147100   1.63872500
4756  Core  RigidRotor
4757          SymmetryFactor   0.412697798
4758  End
4759  Rotor          Hindered
4760  Group   13 14 15
4761  Axis           12           1
4762  Symmetry        3
4763  Potential[kcal/mol]           12
4764  0.000 -0.004 0.000 0.008 0.030 0.054 0.065 0.063 0.054 0.026 0.005 0.005
4765  End
4766  Rotor          Hindered
4767  Group   17
4768  Axis           16           5
4769  Symmetry        1
4770  Potential[kcal/mol]           36
4771  0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
4772  2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
4773  2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
4774  End
4775  Frequencies[1/cm]           42
4776  163.24 182.49 205.48 340.68 403.67 455.59 513.69 525.04
4777  624.58 633.55 738.87 801.16 854.59 888.96 945.51 954.64
4778  965.89 981.84 1010.31 1020.28 1069.05 1139.25 1160.10 1192.08
4779  1294.53 1307.97 1370.42 1415.09 1439.58 1453.99 1469.85 1562.98
4780  1584.54 2930.58 2987.96 3012.49 3052.93 3067.33 3073.16 3087.13
4781  3102.49 3611.30
4782  ZeroEnergy[kcal/mol]   -2.19
4783  ElectronicLevels[1/cm]           1
4784  0.000000000000000000 2.0000000000000000

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4785 End
4786 !*****
4787 RRHO ! 5
4788 Geometry[angstrom] 17
4789 C -1.24833100 -0.11357200 -0.06638500
4790 C -0.94560700 1.20152200 0.31770200
4791 C 0.33399000 1.72902800 0.14318100
4792 C 1.33376400 0.95562000 -0.44537400
4793 C 1.04750800 -0.35631600 -0.83950800
4794 C -0.23832200 -0.87993600 -0.64949900
4795 H -1.72117800 1.81565800 0.76471000
4796 H 0.54457400 2.74606200 0.45305300
4797 H 2.33028000 1.35595400 -0.58442200
4798 H 1.80048800 -0.94838800 -1.34127200
4799 H -0.44444500 -1.90086400 -0.95087700
4800 C -2.63374900 -0.67346800 0.14096200
4801 H -3.39355000 0.00640000 -0.25208400
4802 H -2.74772400 -1.63557400 -0.36068000
4803 H -2.84446400 -0.82263800 1.20382900
4804 O 2.07614900 -1.38074800 1.01391200
4805 H 1.51597300 -0.88410600 1.63293400
4806 Core RigidRotor
4807 SymmetryFactor 0.412697798
4808 End
4809 Rotor Hindered
4810 Group 13 14 15
4811 Axis 12 1
4812 Symmetry 3
4813 Potential[kcal/mol] 12
4814 0.000 -0.004 -0.001 0.007 0.028 0.053 0.065 0.063 0.055 0.027 0.006 0.006
4815 End
4816 Rotor Hindered
4817 Group 17
4818 Axis 16 5
4819 Symmetry 1
4820 Potential[kcal/mol] 36
4821 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
4822 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
4823 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
4824 End
4825 Frequencies[1/cm] 42
4826 169.06 173.46 205.83 340.55 404.48 457.20 524.68 539.94
4827 627.10 635.48 742.31 801.58 857.62 890.74 951.53 956.51
4828 965.89 982.76 1010.50 1020.53 1069.01 1139.09 1160.12 1192.47
4829 1293.44 1307.41 1370.44 1414.84 1439.65 1453.84 1469.69 1563.32

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4830      1585.14 2930.57 2988.01 3012.61 3052.72 3068.72 3074.07 3088.60
4831      3105.16 3617.28
4832 ZeroEnergy[kcal/mol]      -1.73
4833      ElectronicLevels[1/cm]                                1
4834      0.000000000000000000      2.0000000000000000
4835      End
4836      !*****
4837      RRHO      !      6
4838      Geometry[angstrom]      17
4839      C      -1.24593900      -0.11597900      -0.06292300
4840      C      -0.94493300      1.20196900      0.31277300
4841      C      0.33586100      1.72816300      0.14330800
4842      C      1.33807300      0.95166100      -0.43524900
4843      C      1.05426600      -0.36404900      -0.82136800
4844      C      -0.23370400      -0.88595800      -0.63537400
4845      H      -1.72316800      1.81952500      0.75035100
4846      H      0.54444800      2.74728000      0.44765900
4847      H      2.33543400      1.35039200      -0.57216900
4848      H      1.80433000      -0.95326100      -1.32987000
4849      H      -0.43777400      -1.90866900      -0.93178800
4850      C      -2.63336600      -0.67305100      0.13818700
4851      H      -3.38985300      0.00869300      -0.25789500
4852      H      -2.74706600      -1.63462000      -0.36452500
4853      H      -2.84915600      -0.82246300      1.20000700
4854      O      2.06009100      -1.36494900      0.98517400
4855      H      1.50751300      -0.88551200      1.62379200
4856      Core      RigidRotor
4857      SymmetryFactor      0.412697798
4858      End
4859      Rotor      Hindered
4860      Group      13 14 15
4861      Axis      12      1
4862      Symmetry      3
4863      Potential[kcal/mol]      12
4864      0.000 -0.005 -0.002 0.005 0.026 0.051 0.065 0.063 0.055 0.028 0.007 0.006
4865      End
4866      Rotor      Hindered
4867      Group      17
4868      Axis      16      5
4869      Symmetry      1
4870      Potential[kcal/mol]      36
4871      0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
4872      2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
4873      2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
4874      End

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4875      Frequencies[1/cm]          42
4876      162.20 176.25 205.85 340.44 403.22 458.44 524.49 565.08
4877      611.14 634.61 746.63 802.32 861.61 893.31 954.30 960.71
4878      966.02 983.70 1010.71 1020.81 1068.93 1138.97 1160.13 1192.97
4879      1292.15 1306.79 1370.46 1414.54 1439.89 1453.72 1469.66 1563.77
4880      1585.92 2930.67 2988.19 3012.76 3052.81 3069.82 3074.41 3089.77
4881      3108.30 3619.77
4882      ZeroEnergy[kcal/mol]    -1.27
4883      ElectronicLevels[1/cm]          1
4884      0.000000000000000000      2.0000000000000000
4885      End
4886      !*****
4887      RRHO          !          7
4888      Geometry[angstrom]          17
4889      C              -1.24361500   -0.11841400   -0.05975500
4890      C              -0.94399700    1.20199300    0.30841600
4891      C              0.33756700    1.72744300    0.14288100
4892      C              1.34228700    0.94790100   -0.42517000
4893      C              1.06141800   -0.37216600   -0.80190900
4894      C              -0.22947500   -0.89163000   -0.62213200
4895      H              -1.72474900    1.82272200    0.73680100
4896      H              0.54380200    2.74900900    0.44044000
4897      H              2.34046100    1.34512700   -0.55987000
4898      H              1.80789000   -0.95763300   -1.31968000
4899      H              -0.43161900   -1.91596400   -0.91393000
4900      C              -2.63297200   -0.67258800    0.13553700
4901      H              -3.38621400    0.01111800   -0.26322800
4902      H              -2.74668600   -1.63360200   -0.36821500
4903      H              -2.85328000   -0.82218200    1.19638100
4904      O              2.04410000   -1.34923100    0.95650600
4905      H              1.49937800   -0.88598000    1.61324300
4906      Core      RigidRotor
4907              SymmetryFactor      0.412697798
4908      End
4909      Rotor              Hindered
4910      Group      13 14 15
4911      Axis              12          1
4912      Symmetry              3
4913      Potential[kcal/mol]          12
4914      0.000 -0.005 -0.002 0.004 0.025 0.050 0.064 0.063 0.055 0.028 0.008 0.006
4915      End
4916      Rotor              Hindered
4917      Group      17
4918      Axis              16          5
4919      Symmetry              1

```

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4920 Potential[kcal/mol]          36
4921 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
4922 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
4923 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
4924 End
4925   Frequencies[1/cm]          42
4926 164.02 170.33 206.89 340.32 403.01 460.70 524.24 596.97
4927 625.31 644.24 752.37 803.12 866.17 896.99 961.06 972.91
4928 966.09 984.44 1010.85 1021.79 1068.86 1138.99 1160.18 1193.36
4929 1290.38 1306.33 1370.48 1414.30 1440.04 1453.51 1469.70 1563.99
4930 1586.67 2930.88 2988.55 3012.94 3053.47 3070.89 3075.09 3090.76
4931 3108.87 3620.72
4932 ZeroEnergy[kcal/mol]   -0.63
4933   ElectronicLevels[1/cm]          1
4934   0.000000000000000000    2.0000000000000000
4935 End
4936 !*****
4937 RRHO          !          8
4938 Geometry[angstrom]      17
4939 C              -1.24150900   -0.12073400   -0.05747700
4940 C              -0.94269900    1.20151300    0.30514700
4941 C              0.33907300    1.72702900    0.14162500
4942 C              1.34626400    0.94463300   -0.41549600
4943 C              1.06954600   -0.38131300   -0.78011200
4944 C              -0.22597100   -0.89684600   -0.61031100
4945 H              -1.72555000    1.82476700    0.72584900
4946 H              0.54272500    2.75121600    0.43182100
4947 H              2.34484800    1.34093700   -0.54924100
4948 H              1.81052700   -0.96082700   -1.31194700
4949 H              -0.42679600   -1.92209000   -0.89951700
4950 C              -2.63260300   -0.67209100    0.13308200
4951 H              -3.38322600    0.01327500   -0.26764200
4952 H              -2.74660900   -1.63279100   -0.37118300
4953 H              -2.85606000   -0.82157900    1.19327100
4954 O              2.02822200   -1.33364200    0.92809500
4955 H              1.49241100   -0.88541700    1.60197500
4956   Core   RigidRotor
4957           SymmetryFactor   0.412697798
4958 End
4959   Rotor          Hindered
4960   Group   13 14 15
4961   Axis           12          1
4962   Symmetry       3
4963   Potential[kcal/mol]          12
4964 0.000 -0.005 -0.002 0.004 0.024 0.049 0.064 0.063 0.055 0.029 0.009 0.006

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4965 End
4966 Rotor Hindered
4967 Group 17
4968 Axis 16 5
4969 Symmetry 1
4970 Potential[kcal/mol] 36
4971 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
4972 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
4973 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
4974 End
4975 Frequencies[1/cm] 42
4976 126.24 172.22 208.33 340.21 401.73 462.42 523.80 626.15
4977 629.16 670.66 759.84 804.11 871.70 901.49 967.28 991.34
4978 966.32 984.75 1010.65 1023.09 1068.70 1138.87 1159.87 1193.47
4979 1287.64 1305.91 1370.49 1413.76 1440.20 1453.20 1469.43 1563.21
4980 1586.82 2931.06 2988.90 3013.16 3054.11 3071.96 3075.67 3091.76
4981 3109.49 3622.01
4982 ZeroEnergy[kcal/mol] -0.02
4983 ElectronicLevels[1/cm] 1
4984 0.000000000000000000 2.0000000000000000
4985 End
4986 !*****
4987 RRHO ! 9
4988 Geometry[angstrom] 17
4989 C -1.23974700 -0.12282100 -0.05637800
4990 C -0.94119100 1.20059800 0.30326800
4991 C 0.34033900 1.72683600 0.13959300
4992 C 1.34983200 0.94211800 -0.40671200
4993 C 1.07905300 -0.39176200 -0.75558300
4994 C -0.22329200 -0.90132100 -0.60040000
4995 H -1.72563400 1.82568400 0.71811900
4996 H 0.54125900 2.75381300 0.42140000
4997 H 2.34821700 1.33855600 -0.54108000
4998 H 1.81295800 -0.96322300 -1.30692400
4999 H -0.42363300 -1.92679000 -0.88894700
5000 C -2.63233500 -0.67161600 0.13094200
5001 H -3.38111900 0.01500800 -0.27096600
5002 H -2.74702000 -1.63233800 -0.37310500
5003 H -2.85719300 -0.82046400 1.19089900
5004 O 2.01268400 -1.31843400 0.90026800
5005 H 1.48625200 -0.88407800 1.58991100
5006 Core RigidRotor
5007 SymmetryFactor 0.412697798
5008 End
5009 Rotor Hindered

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5010 Group    13 14 15
5011 Axis          12          1
5012 Symmetry      3
5013 Potential[kcal/mol]          12
5014 0.000 0.000 0.000 0.000 0.001 0.002 0.003 0.003 0.002 0.001 0.000 0.000
5015 End
5016 Rotor                      Hindered
5017 Group    17
5018 Axis          16          5
5019 Symmetry      1
5020 Potential[kcal/mol]          36
5021 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
5022 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
5023 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
5024 End
5025 Frequencies[1/cm]          42
5026 102.16 176.13 210.46 340.14 398.85 463.75 523.09 627.72
5027 649.36 707.78 768.73 805.74 878.52 906.59 974.07 964.78
5028 975.77 983.66 1011.20 1024.72 1068.62 1138.91 1159.21 1193.04
5029 1283.97 1305.69 1370.41 1412.86 1440.36 1452.71 1468.76 1560.74
5030 1585.66 2931.30 2989.33 3013.43 3054.89 3072.46 3076.54 3091.48
5031 3104.21 3624.13
5032 ZeroEnergy[kcal/mol] 0.55
5033 ElectronicLevels[1/cm]          1
5034 0.000000000000000000 2.0000000000000000
5035 End
5036 !*****
5037 RRHO          !          10
5038 Geometry[angstrom]          17
5039 C          -1.23848100  -0.12495100  -0.05663400
5040 C          -0.94007900   1.19985900   0.30265600
5041 C           0.34179800   1.72691900   0.13720200
5042 C           1.35272500   0.94164500  -0.39971700
5043 C           1.09127900  -0.40477200  -0.72789400
5044 C          -0.22258200  -0.90504500  -0.59294500
5045 H          -1.72545300   1.82592300   0.71404300
5046 H           0.54018300   2.75625900   0.41191900
5047 H           2.35044200   1.33885800  -0.53617600
5048 H           1.81296900  -0.96272900  -1.30811800
5049 H          -0.42309800  -1.93006000  -0.88276200
5050 C          -2.63222100  -0.67123900   0.12924400
5051 H          -3.38006600   0.01617200  -0.27301400
5052 H          -2.74781400  -1.63231800  -0.37386100
5053 H          -2.85699300  -0.81898600   1.18937800
5054 O           1.99799000  -1.30401800   0.87364800

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5055 H 1.48159600 -0.88221000 1.57767000
5056 Core RigidRotor
5057 SymmetryFactor 0.412697798
5058 End
5059 Rotor Hindered
5060 Group 13 14 15
5061 Axis 12 1
5062 Symmetry 3
5063 Potential[kcal/mol] 12
5064 0.000 -0.005 -0.003 0.003 0.023 0.048 0.064 0.063 0.055 0.029 0.009 0.007
5065 End
5066 Rotor Hindered
5067 Group 17
5068 Axis 16 5
5069 Symmetry 1
5070 Potential[kcal/mol] 36
5071 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
5072 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
5073 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
5074 End
5075 Frequencies[1/cm] 42
5076 125.93 175.13 214.19 340.32 395.86 463.88 521.66 626.01
5077 658.97 750.90 776.81 810.94 884.53 910.69 980.97 963.82
5078 977.14 987.01 1014.89 1026.71 1067.69 1138.17 1156.07 1191.52
5079 1277.87 1304.83 1370.41 1409.72 1440.47 1451.89 1465.61 1554.14
5080 1581.11 2931.44 2989.56 3013.79 3056.10 3073.42 3077.25 3092.43
5081 3104.36 3628.74
5082 ZeroEnergy[kcal/mol] 0.81
5083 ElectronicLevels[1/cm] 1
5084 0.0000000000000000 2.0000000000000000
5085 End
5086 !*****
5087 RRHO ! 11
5088 Geometry[angstrom] 17
5089 C -1.23755777 -0.12736542 -0.05754242
5090 C -0.93946377 1.19957058 0.30283958
5091 C 0.34360223 1.72739458 0.13493258
5092 C 1.35528823 0.94297158 -0.39422542
5093 C 1.10556723 -0.41965942 -0.69864742
5094 C -0.22344377 -0.90855742 -0.58737942
5095 H -1.72537477 1.82604058 0.71215558
5096 H 0.53954923 2.75877558 0.40353358
5097 H 2.35231223 1.34098258 -0.53268742
5098 H 1.81085923 -0.95977842 -1.31419342
5099 H -0.42426977 -1.93299342 -0.87868642

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5100  C          -2.63230377  -0.67101242   0.12786958
5101  H          -3.37949577   0.01704058  -0.27449742
5102  H          -2.74890577  -1.63256242  -0.37400542
5103  H          -2.85623677  -0.81733742   1.18839058
5104  O           1.98397723  -1.29029842   0.84822658
5105  H           1.47652523  -0.87987042   1.56464358
5106  Core      RigidRotor
5107          SymmetryFactor    0.412697798
5108  End
5109  Rotor                      Hindered
5110  Group      13 14 15
5111  Axis           12           1
5112  Symmetry           3
5113  Potential[kcal/mol]           12
5114  0.000 -0.068 -0.034 0.084 0.264 0.454 0.611 0.683 0.659 0.535 0.351 0.154
5115  End
5116  Rotor                      Hindered
5117  Group      17
5118  Axis           16           5
5119  Symmetry           1
5120  Potential[kcal/mol]           36
5121  0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
5122  2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
5123  2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
5124  End
5125  Frequencies[1/cm]           42
5126  133.14 183.20 219.98 340.72 393.10 462.63 519.32 622.61
5127  655.11 773.07 786.70 836.66 885.74 911.87 984.66 997.21
5128  966.56 991.57 1019.32 1028.18 1065.74 1137.02 1150.06 1189.03
5129  1270.46 1303.25 1370.36 1404.04 1440.45 1450.80 1458.79 1543.18
5130  1573.43 2931.54 2989.71 3014.26 3057.97 3074.65 3078.03 3093.76
5131  3105.19 3631.89
5132  ZeroEnergy[kcal/mol]    0.35
5133  ElectronicLevels[1/cm]           1
5134  0.000000000000000000    2.0000000000000000
5135  End
5136  !*****
5137  RRHO          !           12
5138  Geometry[angstrom]       17
5139  C          -1.23663500  -0.12978000  -0.05845000
5140  C          -0.93884900   1.19928200   0.30302400
5141  C           0.34540600   1.72787000   0.13266300
5142  C           1.35785200   0.94429800  -0.38873400
5143  C           1.11985600  -0.43454700  -0.66940100
5144  C          -0.22430600  -0.91206900  -0.58181400

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5145 H -1.72529700 1.82615800 0.71026800
5146 H 0.53891500 2.76129200 0.39514800
5147 H 2.35418300 1.34310700 -0.52919800
5148 H 1.80875000 -0.95682800 -1.32026900
5149 H -0.42544200 -1.93592700 -0.87461100
5150 C -2.63238700 -0.67078600 0.12649500
5151 H -3.37892600 0.01790900 -0.27598100
5152 H -2.74999800 -1.63280700 -0.37415000
5153 H -2.85548000 -0.81568900 1.18740300
5154 O 1.96996500 -1.27657900 0.82280500
5155 H 1.47145400 -0.87753100 1.55161700
5156 Core RigidRotor
5157 SymmetryFactor 0.412697798
5158 End
5159 Rotor Hindered
5160 Group 13 14 15
5161 Axis 12 1
5162 Symmetry 3
5163 Potential[kcal/mol] 12
5164 0.000 -0.068 -0.034 0.084 0.264 0.454 0.611 0.683 0.659 0.536 0.351 0.154
5165 End
5166 Rotor Hindered
5167 Group 17
5168 Axis 16 5
5169 Symmetry 1
5170 Potential[kcal/mol] 36
5171 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
5172 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
5173 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
5174 End
5175 Frequencies[1/cm] 42
5176 151.22 207.97 228.36 341.12 391.04 461.57 516.59 617.49
5177 646.72 769.89 792.41 870.58 888.71 913.56 984.99 990.43
5178 961.58 998.47 1028.57 1033.24 1065.62 1137.22 1142.88 1186.66
5179 1266.18 1301.87 1370.18 1398.15 1440.29 1449.56 1450.53 1532.54
5180 1565.88 2931.59 2989.81 3014.71 3059.49 3073.65 3078.43 3086.56
5181 3099.89 3630.11
5182 ZeroEnergy[kcal/mol] -0.54
5183 ElectronicLevels[1/cm] 1
5184 0.0000000000000000 2.0000000000000000
5185 End
5186 !*****
5187 RRHO ! 13
5188 Geometry[angstrom] 17
5189 C -1.23590500 -0.13251300 -0.05971000

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5235 End
5236 !*****
5237 RRHO ! 14
5238 Geometry[angstrom] 17
5239 C -1.23517100 -0.13545500 -0.06120800
5240 C -0.93900500 1.19985300 0.30481100
5241 C 0.34998700 1.72924300 0.12834700
5242 C 1.36218200 0.95047600 -0.38055900
5243 C 1.15190100 -0.46730300 -0.60910300
5244 C -0.22912100 -0.91856500 -0.57402000
5245 H -1.72581300 1.82659500 0.71001800
5246 H 0.53853500 2.76638800 0.37986400
5247 H 2.35754100 1.35055400 -0.52342700
5248 H 1.79922500 -0.94565300 -1.33807300
5249 H -0.43075500 -1.94168000 -0.86862400
5250 C -2.63275600 -0.67055900 0.12421400
5251 H -3.37827300 0.01935400 -0.27825000
5252 H -2.75261300 -1.63365400 -0.37363300
5253 H -2.85356200 -0.81194900 1.18617700
5254 O 1.94370600 -1.25101000 0.77470500
5255 H 1.45910600 -0.87055400 1.52156100
5256 Core RigidRotor
5257 SymmetryFactor 0.412697798
5258 End
5259 Rotor Hindered
5260 Group 13 14 15
5261 Axis 12 1
5262 Symmetry 3
5263 Potential[kcal/mol] 12
5264 0.000 -0.068 -0.033 0.086 0.266 0.456 0.613 0.684 0.659 0.535 0.350 0.154
5265 End
5266 Rotor Hindered
5267 Group 17
5268 Axis 16 5
5269 Symmetry 1
5270 Potential[kcal/mol] 36
5271 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
5272 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
5273 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
5274 End
5275 Frequencies[1/cm] 42
5276 173.55 240.90 264.51 344.01 395.85 462.42 510.52 602.90
5277 631.86 753.90 791.78 848.18 875.26 940.78 979.73 989.97
5278 967.82 1011.88 1028.50 1052.43 1114.39 1131.65 1143.12 1180.25
5279 1262.71 1296.73 1368.72 1380.68 1423.92 1439.66 1448.85 1517.30

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5280      1558.82 2931.03 2989.08 3015.25 3043.34 3063.52 3077.86 3079.00
5281      3098.60 3634.44
5282 ZeroEnergy[kcal/mol]   -4.80
5283   ElectronicLevels[1/cm]                               1
5284      0.000000000000000000      2.0000000000000000
5285 End
5286 !*****
5287 RRHO      !      15
5288 Geometry[angstrom]      17
5289 C      -1.23451700   -0.13816200   -0.06261200
5290 C      -0.93930400    1.20021800    0.30600300
5291 C      0.35221100    1.73001200    0.12609400
5292 C      1.36443700    0.95310000   -0.37657000
5293 C      1.16789000   -0.48349400   -0.57889100
5294 C      -0.23095300   -0.92185900   -0.57010000
5295 H      -1.72624700    1.82682800    0.71045500
5296 H      0.53811800    2.76932700    0.37123000
5297 H      2.35901300    1.35505600   -0.52095000
5298 H      1.79361100   -0.93975300   -1.34193400
5299 H      -0.43398600   -1.94456100   -0.86581700
5300 C      -2.63301700   -0.67042800    0.12299300
5301 H      -3.37817400    0.01998800   -0.27941900
5302 H      -2.75413600   -1.63418900   -0.37326700
5303 H      -2.85276900   -0.80985600    1.18552900
5304 O      1.93062800   -1.23835200    0.75042100
5305 H      1.45249400   -0.86639300    1.50520400
5306   Core   RigidRotor
5307           SymmetryFactor   0.412697798
5308 End
5309 Rotor      Hindered
5310 Group   13 14 15
5311 Axis      12      1
5312 Symmetry      3
5313 Potential[kcal/mol]      12
5314 0.000 -0.067 -0.032 0.087 0.267 0.457 0.614 0.684 0.659 0.535 0.350 0.154
5315 End
5316 Rotor      Hindered
5317 Group   17
5318 Axis      16      5
5319 Symmetry      1
5320 Potential[kcal/mol]      36
5321 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
5322 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
5323 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
5324 End

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5325      Frequencies[1/cm]          42
5326      179.20 260.00 283.83 346.89 404.53 465.73 508.89 596.86
5327      628.75 747.75 790.51 835.08 863.79 934.13 977.65 986.77
5328      979.09 1027.62 1034.53 1049.97 1109.40 1136.77 1174.88 1187.08
5329      1262.47 1293.63 1364.50 1373.24 1411.70 1439.32 1448.69 1514.90
5330      1561.62 2930.37 2988.21 3015.03 3028.54 3064.03 3075.55 3078.36
5331      3096.46 3636.98
5332      ZeroEnergy[kcal/mol]    -7.90
5333      ElectronicLevels[1/cm]          1
5334      0.000000000000000000      2.0000000000000000
5335      End
5336      !*****
5337      RRHO          !          16
5338      Geometry[angstrom]      17
5339      C              -1.23388400   -0.14049400   -0.06371200
5340      C              -0.93939400    1.20034700    0.30718800
5341      C              0.35406100    1.73087800    0.12369300
5342      C              1.36713500    0.95443400   -0.37189700
5343      C              1.18302000   -0.49872300   -0.54929300
5344      C              -0.23137400   -0.92553000   -0.56521800
5345      H              -1.72661800    1.82697600    0.71070200
5346      H              0.53721900    2.77272800    0.36092600
5347      H              2.36052700    1.35936600   -0.51856700
5348      H              1.78846300   -0.93451700   -1.34178900
5349      H              -0.43673800   -1.94765900   -0.86250700
5350      C              -2.63339400   -0.67024100    0.12152000
5351      H              -3.37814500    0.02060100   -0.28101300
5352      H              -2.75585100   -1.63475100   -0.37302100
5353      H              -2.85230400   -0.80764500    1.18457600
5354      O              1.91699500   -1.22530100    0.72532500
5355      H              1.44649000   -0.86294200    1.48892100
5356      Core      RigidRotor
5357              SymmetryFactor      0.412697798
5358      End
5359      Rotor              Hindered
5360      Group      13 14 15
5361      Axis              12          1
5362      Symmetry              3
5363      Potential[kcal/mol]          12
5364      0.000 -0.067 -0.031 0.088 0.268 0.458 0.614 0.685 0.659 0.535 0.349 0.153
5365      End
5366      Rotor              Hindered
5367      Group      17
5368      Axis              16          5
5369      Symmetry              1

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5370 Potential[kcal/mol] 36
5371 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
5372 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
5373 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
5374 End
5375 Frequencies[1/cm] 42
5376 273.13 294.03 304.02 351.30 418.63 473.30 508.32 594.13
5377 627.57 744.17 788.96 824.35 856.47 924.46 975.92 984.15
5378 981.27 1027.64 1042.54 1071.41 1104.14 1137.21 1172.87 1233.93
5379 1261.49 1290.91 1355.52 1371.13 1402.51 1439.06 1448.61 1513.38
5380 1563.85 2929.73 2987.43 3013.40 3014.69 3063.08 3071.85 3077.59
5381 3093.22 3640.41
5382 ZeroEnergy[kcal/mol] -10.72
5383 ElectronicLevels[1/cm] 1
5384 0.0000000000000000 2.0000000000000000
5385 End
5386 !*****
5387 RRHO ! 17
5388 Geometry[angstrom] 17
5389 C -1.23306200 -0.14265200 -0.06442000
5390 C -0.93916200 1.20016500 0.30824000
5391 C 0.35565300 1.73173000 0.12096900
5392 C 1.37026200 0.95472000 -0.36614600
5393 C 1.19712300 -0.51277300 -0.52082000
5394 C -0.23061800 -0.92963600 -0.55887500
5395 H -1.72683700 1.82699900 0.71039700
5396 H 0.53575500 2.77643600 0.34875600
5397 H 2.36233600 1.36274800 -0.51575200
5398 H 1.78345700 -0.92944600 -1.33954900
5399 H -0.43820800 -1.95122100 -0.85778800
5400 C -2.63387200 -0.66995700 0.11968900
5401 H -3.37797800 0.02130600 -0.28338400
5402 H -2.75762200 -1.63525000 -0.37307100
5403 H -2.85246500 -0.80528200 1.18313800
5404 O 1.90266000 -1.21179200 0.69941100
5405 H 1.44214800 -0.86142100 1.47389400
5406 Core RigidRotor
5407 SymmetryFactor 0.412697798
5408 End
5409 Rotor Hindered
5410 Group 13 14 15
5411 Axis 12 1
5412 Symmetry 3
5413 Potential[kcal/mol] 12
5414 0.000 -0.067 -0.031 0.088 0.269 0.459 0.615 0.685 0.659 0.535 0.349 0.153

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5415 End
5416 Rotor Hindered
5417 Group 17
5418 Axis 16 5
5419 Symmetry 1
5420 Potential[kcal/mol] 36
5421 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
5422 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
5423 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
5424 End
5425 Frequencies[1/cm] 42
5426 289.64 315.49 356.61 406.74 451.74 508.01 526.07 608.28
5427 629.55 746.02 786.98 815.77 852.82 914.27 974.34 982.11
5428 980.26 1027.26 1039.33 1088.52 1117.86 1137.13 1170.66 1258.49
5429 1278.44 1290.96 1346.70 1370.34 1395.91 1438.87 1448.58 1512.29
5430 1565.02 2929.21 2986.79 2995.60 3014.28 3061.41 3067.93 3076.67
5431 3089.96 3644.68
5432 ZeroEnergy[kcal/mol] -13.34
5433 ElectronicLevels[1/cm] 1
5434 0.0000000000000000 2.0000000000000000
5435 End
5436 !*****
5437 RRHO ! 18
5438 Geometry[angstrom] 17
5439 C -1.23188000 -0.14505000 -0.06443300
5440 C -0.93845400 1.19956400 0.30896600
5441 C 0.35717600 1.73268100 0.11749900
5442 C 1.37412700 0.95423800 -0.35837500
5443 C 1.20942600 -0.52477600 -0.49445500
5444 C -0.22877500 -0.93469300 -0.54981600
5445 H -1.72689000 1.82694800 0.70874400
5446 H 0.53343600 2.78079600 0.33357400
5447 H 2.36505200 1.36484600 -0.51109600
5448 H 1.77778600 -0.92361900 -1.33619800
5449 H -0.43765000 -1.95620200 -0.84940000
5450 C -2.63447700 -0.66947900 0.11713100
5451 H -3.37715400 0.02239600 -0.28759400
5452 H -2.75945600 -1.63561600 -0.37374800
5453 H -2.85413800 -0.80235000 1.18071800
5454 O 1.88774900 -1.19812400 0.67245600
5455 H 1.43835500 -0.86170100 1.45837900
5456 Core RigidRotor
5457 SymmetryFactor 0.412697798
5458 End
5459 Rotor Hindered

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5460 Group    13 14 15
5461 Axis          12          1
5462 Symmetry      3
5463 Potential[kcal/mol]          12
5464 0.000 -0.067 -0.031 0.088 0.268 0.458 0.614 0.685 0.659 0.535 0.349 0.153
5465 End
5466 Rotor                      Hindered
5467 Group    17
5468 Axis          16          5
5469 Symmetry      1
5470 Potential[kcal/mol]          36
5471 0.000 0.025 0.263 0.684 1.220 1.775 2.261 2.606 2.779 2.788 2.690 2.548
5472 2.433 2.381 2.408 2.494 2.606 2.699 2.744 2.721 2.640 2.529 2.429 2.381
5473 2.407 2.510 2.660 2.801 2.859 2.786 2.546 2.142 1.624 1.069 0.567 0.191
5474 End
5475     Frequencies[1/cm]          42
5476     295.45  324.39  362.86  424.26  462.16  507.64  563.04  624.35
5477     698.00  781.65  788.53  809.84  856.38  905.60  973.06  980.61
5478     978.41 1026.80 1036.33 1086.24 1136.79 1145.81 1172.59 1257.55
5479     1284.03 1322.78 1339.83 1369.78 1391.46 1438.76 1448.62 1511.97
5480     1566.06 2928.74 2978.51 2986.22 3013.89 3059.04 3064.13 3075.51
5481     3086.81 3653.26
5482 ZeroEnergy[kcal/mol]   -15.22
5483 ElectronicLevels[1/cm]          1
5484 0.000000000000000000    2.0000000000000000
5485 End
5486 !*****
5487 RRHO          !          19
5488 Geometry[angstrom]      17
5489 C             -1.23066700   -0.15223200   -0.04775600
5490 C             -0.94284200    1.20459600    0.29288000
5491 C             0.35326800    1.74283600    0.10588900
5492 C             1.38097900    0.95897700   -0.32694200
5493 C             1.21188100   -0.52239100   -0.47404900
5494 C             -0.22304500   -0.95103300   -0.49800000
5495 H             -1.74156100    1.84134600    0.65629200
5496 H             0.51884800    2.79156300    0.30917800
5497 H             2.37895500    1.35940700   -0.45852200
5498 H             1.74686700   -0.88890500   -1.35878400
5499 H             -0.41207500   -1.98989900   -0.74670000
5500 C             -2.64194700   -0.66293500    0.10140800
5501 H             -3.35460800    0.01283700   -0.38291400
5502 H             -2.74827600   -1.65227600   -0.34854400
5503 H             -2.92450100   -0.73625700    1.15799500
5504 O             1.89083600   -1.19871700    0.61687300

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5505 H 1.44095800 -0.97640000 1.46174600
5506 Core RigidRotor
5507 SymmetryFactor 0.412697798
5508 End
5509 Rotor Hindered
5510 Group 13 14 15
5511 Axis 12 1
5512 Symmetry 3
5513 Potential[kcal/mol] 12
5514 0.000 -0.050 0.002 0.134 0.321 0.508 0.652 0.706 0.661 0.524 0.332 0.141
5515 End
5516 Rotor Hindered
5517 Group 17
5518 Axis 16 5
5519 Symmetry 1
5520 Potential[kcal/mol] 36
5521 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
5522 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
5523 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
5524 End
5525 Frequencies[1/cm] 42
5526 302.82 350.52 434.28 467.52 501.56 561.06 586.96 625.70
5527 711.47 784.71 798.81 842.83 897.76 949.09 961.26 984.05
5528 983.70 1030.92 1037.71 1086.60 1134.25 1161.13 1209.29 1268.11
5529 1282.40 1340.56 1363.02 1373.07 1387.09 1439.68 1450.73 1516.45
5530 1575.47 2912.50 2920.49 2967.35 3001.69 3064.21 3069.14 3078.76
5531 3103.43 3437.38
5532 ZeroEnergy[kcal/mol] -15.80
5533 ElectronicLevels[1/cm] 1
5534 0.0000000000000000 2.0000000000000000
5535 End
5536 !*****
5537 Tunneling Eckart
5538 ImaginaryFrequency[1/cm] 449.63
5539 WellDepth[kcal/mol] 4.20
5540 WellDepth[kcal/mol] 17.38
5541 End
5542 End
5543 !*****
5544 Well W4o2 # oHOC6CH5CH3
5545 Species
5546 RRHO
5547 Geometry[angstrom] 17
5548 C 0.72707500 -0.56931700 0.11837200
5549 C -0.23304100 -1.49219200 -0.18886700

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5550  C          -1.60934300  -1.16231400  -0.22480300
5551  C          -2.02716900   0.15946600   0.07390800
5552  C          -1.11888800   1.12448100   0.38666100
5553  C           0.35577700   0.86978400   0.37224100
5554  H           0.06630600  -2.51384400  -0.40152900
5555  H          -2.34081200  -1.91973100  -0.47590700
5556  H          -3.08484700   0.39817000   0.05694200
5557  H          -1.43232400   2.13779500   0.61109000
5558  C           2.18409800  -0.90674900   0.19889500
5559  H           2.56334100  -0.72514800   1.21144700
5560  H           2.36617300  -1.95252200  -0.05359700
5561  H           2.76721900  -0.27131000  -0.47271800
5562  O           1.00495600   1.74222300  -0.59603100
5563  H           0.57819900   1.57286500  -1.44396200
5564  H           0.80604800   1.19698700   1.31803800
5565          Core      RigidRotor
5566          SymmetryFactor      0.5
5567          End
5568      Rotor Hindered      !freq=150
5569          Group      12 13 14
5570          Axis      1 11
5571          Symmetry      3
5572      Potential[kcal/mol]      12
5573          0.000 0.065 0.274 0.583 0.931 1.219 1.338 1.237 0.966 0.627 0.312 0.094
5574          End
5575      Rotor Hindered      !freq=323
5576          Group      16
5577          Axis      6 15
5578          Symmetry      1
5579      Potential[kcal/mol]      36
5580          0.000 0.089 0.377 0.810 1.301 1.754 2.099 2.306 2.380 2.352 2.283 2.224
5581          2.208 2.245 2.328 2.431 2.524 2.579 2.589 2.563 2.537 2.547 2.632 2.809
5582          3.072 3.383 3.670 3.856 3.847 3.596 3.099 2.447 1.735 1.057 0.501 0.137
5583          End
5584          Frequencies[1/cm]      43
5585          77.96  220.62  267.37  377.09  401.02  485.87  507.54  567.10
5586          632.51  697.17  766.85  795.22  876.05  910.95  962.75  972.28
5587          997.92  984.75  1010.78 1025.34 1085.97 1138.84 1162.89 1175.05
5588          1263.16 1294.47 1342.65 1364.06 1374.74 1383.84 1426.23 1444.83
5589          1504.05 1569.86 2902.16 2914.34 2972.35 3012.16 3051.22 3060.36
5590          3078.5  3093.82 3667.04
5591          ZeroEnergy[kcal/mol]      -17.79
5592          ElectronicLevels[1/cm]      1
5593          0  2
5594      End

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5595 End
5596 !*****
5597 Barrier B4o3 W4o2 P4o # TS4o3
5598 RRHO
5599 Geometry[angstrom] 17
5600 C 0.57534600 -0.66804400 -0.02000100
5601 C -0.57107100 -1.45073500 -0.01224800
5602 C -1.84920600 -0.88642800 -0.00578300
5603 C -1.99427800 0.50136700 -0.03766100
5604 C -0.87381400 1.31428600 -0.05503100
5605 C 0.41333500 0.74135900 0.08055000
5606 H -0.46295400 -2.52986600 -0.03341900
5607 H -2.72330900 -1.52576600 -0.00002100
5608 H -2.98130500 0.94627900 -0.07947800
5609 H -0.97040700 2.39450500 -0.08857200
5610 C 1.95781800 -1.24791000 -0.02879400
5611 H 2.53690000 -0.86961700 -0.87442800
5612 H 2.49775400 -0.96016600 0.87872200
5613 H 1.91960800 -2.33642500 -0.08480100
5614 O 1.55225300 1.48958600 -0.13565200
5615 H 1.36508400 2.41059200 0.06877600
5616 H 0.45181400 0.73040100 1.77224700
5617 Core RigidRotor
5618 SymmetryFactor 0.5
5619 End
5620 Tunneling Eckart
5621 ImaginaryFrequency[1/cm] 1156.69
5622 WellDepth[kcal/mol] 26.36
5623 WellDepth[kcal/mol] 7.87
5624 End
5625 Frequencies[1/cm] 44
5626 152.38 163.32
5627 249.66 274.75 290.19 408.53 445.67 495.21 536.66 565.02
5628 582.06 673.28 717.45 756.64 806.77 848.00 880.92 950.43
5629 981.69 973.56 1027.50 1033.31 1079.50 1136.20 1147.73 1194.93
5630 1215.66 1280.65 1300.48 1368.76 1411.86 1429.87 1454.07 1474.94
5631 1565.42 1588.92 2928.12 2985.80 3018.19 3057.53 3062.49 3077.57
5632 3092.48 3706.17
5633 ZeroEnergy[kcal/mol] 8.58
5634 ElectronicLevels[1/cm] 1
5635 0 2
5636 End
5637 !*****
5638 Barrier B4o2 W W4o2
5639 Variational

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5640 RRHO ! 1
5641 Geometry[angstrom] 17
5642 C -0.13262800 -1.44097100 0.35089000
5643 C 0.75568900 -0.55899100 -0.27630100
5644 C 0.23879200 0.62098600 -0.83791300
5645 C -1.12864200 0.90785600 -0.76922400
5646 C -2.00067500 0.02270800 -0.13598000
5647 C -1.49692700 -1.15504700 0.42366000
5648 H 0.24820600 -2.35756100 0.79183600
5649 H 0.90580600 1.30473200 -1.34676800
5650 H -1.50514600 1.82383600 -1.21121500
5651 H -3.06018500 0.24325500 -0.08232400
5652 H -2.16680400 -1.85107400 0.91789300
5653 C 2.23419700 -0.84036200 -0.31771400
5654 H 2.74445900 -0.29063000 0.47627700
5655 H 2.43995600 -1.90375200 -0.18659900
5656 H 2.66706300 -0.52319400 -1.26697600
5657 O 0.98934700 1.96220800 1.18870500
5658 H 0.24476200 1.51086900 1.64766800
5659 Core RigidRotor
5660 SymmetryFactor 0.423178412
5661 End
5662 Rotor Hindered
5663 Group 13 14 15
5664 Axis 12 2
5665 Symmetry 3
5666 Potential[kcal/mol] 12
5667 0.000 0.089 0.183 0.251 0.287 0.278 0.217 0.128 0.030 -0.042 -0.076 -0.064
5668 End
5669 Rotor Hindered
5670 Group 17
5671 Axis 16 3
5672 Symmetry 1
5673 Potential[kcal/mol] 36
5674 0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
5675 3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
5676 2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
5677 End
5678 Frequencies[1/cm] 42
5679 70.51 208.67 341.57 405.43 446.33 460.62 526.88 609.17
5680 632.18 640.15 733.98 799.87 853.32 890.79 951.97 962.79
5681 965.93 977.85 1010.07 1018.29 1069.37 1138.55 1159.73 1192.33
5682 1295.00 1308.61 1365.13 1414.68 1439.37 1453.41 1469.73 1559.12
5683 1580.88 2942.49 3006.64 3019.43 3047.68 3062.07 3068.37 3083.85
5684 3092.58 3461.52

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5685 ZeroEnergy[kcal/mol] -3.74
5686 ElectronicLevels[1/cm] 1
5687 0.0000000000000000 2.0000000000000000
5688 End
5689 !*****
5690 RRHO ! 2
5691 Geometry[angstrom] 17
5692 C -0.13466400 -1.45077700 0.33866200
5693 C 0.75770100 -0.56265800 -0.26693500
5694 C 0.24687300 0.63237000 -0.80592600
5695 C -1.12254700 0.91783400 -0.74674800
5696 C -1.99839200 0.02472900 -0.13297200
5697 C -1.50015200 -1.16362100 0.40657300
5698 H 0.24184100 -2.37267600 0.77113000
5699 H 0.91286000 1.31143800 -1.32032700
5700 H -1.49538300 1.83817700 -1.18235500
5701 H -3.05896800 0.24253100 -0.08691100
5702 H -2.17432100 -1.86735500 0.88331200
5703 C 2.23521800 -0.84336100 -0.31840800
5704 H 2.76926200 -0.17939700 0.37102700
5705 H 2.45151500 -1.88075200 -0.04453700
5706 H 2.62970400 -0.66494000 -1.32532100
5707 O 0.98021600 1.95636400 1.16252800
5708 H 0.21706000 1.64201700 1.65071800
5709 Core RigidRotor
5710 SymmetryFactor 0.423178412
5711 End
5712 Rotor Hindered
5713 Group 13 14 15
5714 Axis 12 2
5715 Symmetry 3
5716 Potential[kcal/mol] 12
5717 0.000 0.063 0.153 0.246 0.313 0.349 0.340 0.278 0.190 0.091 0.020 -0.014
5718 End
5719 Rotor Hindered
5720 Group 17
5721 Axis 16 3
5722 Symmetry 1
5723 Potential[kcal/mol] 36
5724 0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
5725 3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
5726 2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
5727 End
5728 Frequencies[1/cm] 42
5729 73.57 173.29 200.10 248.89 347.55 406.96 459.19 526.45

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5730      631.98  640.44  734.60  800.58  853.81  890.87  953.53  959.69
5731      972.25  983.00 1011.88 1027.32 1069.92 1138.86 1159.17 1192.53
5732      1296.98 1308.58 1371.05 1415.30 1440.75 1458.34 1470.96 1561.16
5733      1581.34 2906.64 2967.51 2984.26 3050.60 3063.21 3070.43 3084.28
5734      3099.94 3777.83
5735      ZeroEnergy[kcal/mol]   -3.64
5736      ElectronicLevels[1/cm]                               1
5737      0.000000000000000000      2.0000000000000000
5738      End
5739      !*****
5740      RRHO      !      3
5741      Geometry[angstrom]      17
5742      C      -0.13630300      -1.45877600      0.32311000
5743      C      0.75965000      -0.56227800      -0.26429200
5744      C      0.25239200      0.64224900      -0.78766600
5745      C      -1.11614900      0.93153400      -0.72261300
5746      C      -1.99453600      0.03281400      -0.12013100
5747      C      -1.50077600      -1.16781700      0.39542900
5748      H      0.23644100      -2.38992800      0.73719600
5749      H      0.92084200      1.32649500      -1.29274500
5750      H      -1.48424000      1.86313500      -1.13674100
5751      H      -3.05253400      0.25904600      -0.05851300
5752      H      -2.17708100      -1.87602900      0.86203800
5753      C      2.23843300      -0.83639500      -0.29996900
5754      H      2.76119900      -0.12017100      0.33945800
5755      H      2.46315900      -1.84456300      0.05201700
5756      H      2.63636600      -0.73024500      -1.31261500
5757      O      0.96529800      1.93355300      1.11855900
5758      H      0.20382600      1.62404800      1.63359000
5759      Core      RigidRotor
5760      SymmetryFactor      0.423178412
5761      End
5762      Rotor      Hindered
5763      Group      13 14 15
5764      Axis      12      2
5765      Symmetry      3
5766      Potential[kcal/mol]      12
5767      0.000 0.043 0.123 0.218 0.300 0.350 0.365 0.325 0.248 0.148 0.062 0.011
5768      End
5769      Rotor      Hindered
5770      Group      17
5771      Axis      16      3
5772      Symmetry      1
5773      Potential[kcal/mol]      36
5774      0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358

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5775 3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
5776 2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
5777 End
5778 Frequencies[1/cm] 42
5779 78.37 140.78 214.33 343.34 406.25 458.74 494.04 526.53
5780 631.70 643.67 736.02 800.78 856.29 893.79 955.16 960.55
5781 966.68 981.65 1011.83 1020.72 1069.01 1138.46 1159.08 1192.85
5782 1295.44 1308.00 1365.43 1414.82 1436.77 1457.07 1470.42 1561.00
5783 1581.32 2931.09 2992.44 3011.87 3054.18 3065.92 3073.39 3085.23
5784 3097.56 3635.75
5785 ZeroEnergy[kcal/mol] -3.32
5786 ElectronicLevels[1/cm] 1
5787 0.0000000000000000 2.0000000000000000
5788 End
5789 !*****
5790 RRHO ! 4
5791 Geometry[angstrom] 17
5792 C -0.13631900 -1.46183100 0.31706800
5793 C 0.76374900 -0.55762600 -0.25028500
5794 C 0.26042900 0.65583000 -0.75908300
5795 C -1.10780700 0.94850500 -0.69185400
5796 C -1.99062200 0.03996100 -0.11262800
5797 C -1.50118800 -1.17112800 0.38140000
5798 H 0.23196600 -2.40078700 0.71624900
5799 H 0.92991600 1.33891700 -1.26506400
5800 H -1.47015200 1.89050800 -1.08602300
5801 H -3.04855800 0.26612700 -0.05343900
5802 H -2.18231100 -1.88918300 0.82440200
5803 C 2.24192700 -0.83136500 -0.28687500
5804 H 2.76532300 -0.10203000 0.33649000
5805 H 2.46998900 -1.83263800 0.08171700
5806 H 2.63435900 -0.74259700 -1.30322600
5807 O 0.94249600 1.90234500 1.06021700
5808 H 0.21239800 1.59039300 1.61892400
5809 Core RigidRotor
5810 SymmetryFactor 0.423178412
5811 End
5812 Rotor Hindered
5813 Group 13 14 15
5814 Axis 12 2
5815 Symmetry 3
5816 Potential[kcal/mol] 12
5817 0.000 0.031 0.106 0.199 0.287 0.343 0.368 0.341 0.270 0.172 0.080 0.021
5818 End
5819 Rotor Hindered

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5820 Group 17
5821 Axis 16 3
5822 Symmetry 1
5823 Potential[kcal/mol] 36
5824 0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
5825 3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
5826 2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
5827 End
5828 Frequencies[1/cm] 42
5829 80.87 187.12 218.33 343.00 406.89 461.12 526.12 570.81
5830 631.28 644.34 738.82 801.38 859.94 900.48 956.92 961.79
5831 965.72 982.58 1012.88 1020.02 1069.12 1138.18 1159.24 1193.64
5832 1294.02 1307.50 1364.24 1414.43 1435.84 1456.76 1470.70 1562.15
5833 1582.37 2932.58 2994.21 3013.99 3057.60 3068.88 3076.77 3086.80
5834 3095.98 3622.96
5835 ZeroEnergy[kcal/mol] -2.56
5836 ElectronicLevels[1/cm] 1
5837 0.0000000000000000 2.0000000000000000
5838 End
5839 !*****
5840 RRHO ! 5
5841 Geometry[angstrom] 17
5842 C -0.13572400 -1.46177000 0.31656200
5843 C 0.76598600 -0.55437600 -0.24130800
5844 C 0.26494500 0.66489700 -0.74026400
5845 C -1.10462200 0.95592200 -0.67840200
5846 C -1.98902500 0.04246800 -0.11163500
5847 C -1.50084700 -1.17185900 0.37531600
5848 H 0.23025800 -2.40498600 0.70751500
5849 H 0.93341700 1.34392000 -1.25324700
5850 H -1.46436800 1.90212900 -1.06447500
5851 H -3.04780200 0.26593400 -0.05894600
5852 H -2.18413600 -1.89443200 0.80708000
5853 C 2.24328200 -0.82973200 -0.28330300
5854 H 2.77017300 -0.09819400 0.33438800
5855 H 2.47255300 -1.83004600 0.08706300
5856 H 2.62983000 -0.74448100 -1.30223400
5857 O 0.93123300 1.88527900 1.03094800
5858 H 0.21714800 1.57344300 1.61036700
5859 Core RigidRotor
5860 SymmetryFactor 0.423178412
5861 End
5862 Rotor Hindered
5863 Group 13 14 15
5864 Axis 12 2

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```

5865 Symmetry 3
5866 Potential[kcal/mol] 12
5867 0.000 0.027 0.098 0.190 0.280 0.339 0.368 0.346 0.277 0.182 0.088 0.025
5868 End
5869 Rotor Hindered
5870 Group 17
5871 Axis 16 3
5872 Symmetry 1
5873 Potential[kcal/mol] 36
5874 0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
5875 3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
5876 2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
5877 End
5878 Frequencies[1/cm] 42
5879 82.94 205.13 219.46 342.94 405.77 462.60 525.93 608.30
5880 631.61 648.91 741.21 801.76 862.61 906.88 959.99 964.49
5881 965.45 983.28 1013.86 1020.03 1069.26 1138.24 1159.41 1194.10
5882 1293.10 1307.26 1363.71 1414.10 1435.44 1456.49 1471.27 1563.01
5883 1583.18 2932.70 2994.37 3014.55 3058.64 3069.78 3077.86 3087.02
5884 3095.59 3618.88
5885 ZeroEnergy[kcal/mol] -1.92
5886 ElectronicLevels[1/cm] 1
5887 0.000000000000000000 2.0000000000000000
5888 End
5889 !*****
5890 RRHO ! 6
5891 Geometry[angstrom] 17
5892 C -0.13456000 -1.46086000 0.31760800
5893 C 0.76823100 -0.55195200 -0.23360600
5894 C 0.27046800 0.67704500 -0.71662200
5895 C -1.10269000 0.96158300 -0.66916200
5896 C -1.98751200 0.04528900 -0.11036900
5897 C -1.50032300 -1.17258100 0.36922500
5898 H 0.22923600 -2.40798300 0.70101600
5899 H 0.93596000 1.34795300 -1.24332800
5900 H -1.46082600 1.90988700 -1.05117300
5901 H -3.04736700 0.26529500 -0.06440900
5902 H -2.18500700 -1.89778400 0.79437000
5903 C 2.24443000 -0.82901300 -0.28156600
5904 H 2.77393100 -0.09647200 0.33279400
5905 H 2.47455700 -1.82930900 0.08816000
5906 H 2.62597900 -0.74416000 -1.30255100
5907 O 0.92006000 1.86741100 1.00262400
5908 H 0.22063300 1.56415400 1.60324900
5909 Core RigidRotor

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5955 H 2.47613100 -1.82929500 0.08766400
5956 H 2.62061600 -0.74357900 -1.30372800
5957 O 0.90930800 1.84982000 0.97484100
5958 H 0.22364400 1.55255200 1.59338000
5959 Core RigidRotor
5960 SymmetryFactor 0.423178412
5961 End
5962 Rotor Hindered
5963 Group 13 14 15
5964 Axis 12 2
5965 Symmetry 3
5966 Potential[kcal/mol] 12
5967 0.000 0.019 0.086 0.176 0.269 0.332 0.366 0.352 0.287 0.196 0.099 0.031
5968 End
5969 Rotor Hindered
5970 Group 17
5971 Axis 16 3
5972 Symmetry 1
5973 Potential[kcal/mol] 36
5974 0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
5975 3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
5976 2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
5977 End
5978 Frequencies[1/cm] 42
5979 87.49 196.02 208.13 343.04 400.67 468.80 525.28 628.65
5980 663.08 709.50 750.59 801.75 871.91 930.26 974.42 990.80
5981 972.14 985.22 1015.46 1022.97 1068.50 1137.86 1158.88 1193.50
5982 1288.10 1305.91 1362.34 1411.62 1434.84 1455.40 1471.90 1560.91
5983 1581.80 2931.67 2992.81 3015.81 3059.55 3070.86 3078.80 3085.99
5984 3095.23 3626.04
5985 ZeroEnergy[kcal/mol] -1.29
5986 ElectronicLevels[1/cm] 1
5987 0.000000000000000000 2.0000000000000000
5988 End
5989 !*****
5990 RRHO ! 8
5991 Geometry[angstrom] 17
5992 C -0.13220900 -1.46056200 0.31576500
5993 C 0.77247800 -0.54787500 -0.21748700
5994 C 0.28358800 0.70603100 -0.66451400
5995 C -1.10108500 0.97164100 -0.65249200
5996 C -1.98516900 0.04828500 -0.11383400
5997 C -1.49841700 -1.17146600 0.36490700
5998 H 0.22785400 -2.41496200 0.68397500
5999 H 0.93952500 1.35148200 -1.23393700

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6000	H		-1.45851500	1.91970800	-1.03533500
6001	H		-3.04698800	0.26085600	-0.08279100
6002	H		-2.18550100	-1.90125200	0.77781500
6003	C		2.24572600	-0.82875400	-0.27978000
6004	H		2.78147200	-0.09567000	0.32866500
6005	H		2.47778100	-1.82977700	0.08644100
6006	H		2.61648500	-0.74266400	-1.30493700
6007	O		0.89926400	1.83280700	0.94833000
6008	H		0.22512000	1.54402900	1.58243200
6009	Core	RigidRotor			
6010		SymmetryFactor	0.423178412		
6011	End				
6012	Rotor			Hindered	
6013	Group	13 14 15			
6014	Axis	12	2		
6015	Symmetry	3			
6016	Potential[kcal/mol]		12		
6017	-0.011				
6018	0.076				
6019	0.173				
6020	0.246				
6021	0.287				
6022	0.277				
6023	0.214				
6024	0.122				
6025	0.024				
6026	-0.045				
6027	-0.077				
6028	-0.063				
6029	End				
6030	Rotor			Hindered	
6031	Group	17			
6032	Axis	16	3		
6033	Symmetry	1			
6034	Potential[kcal/mol]		36		
6035	0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358				
6036	3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238				
6037	2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073				
6038	End				
6039	Frequencies[1/cm]		42		
6040	88.99 194.94 206.11 343.37 398.00 472.89 524.41 627.73				
6041	679.75 746.32 760.67 801.00 875.20 941.24 978.62 992.37				
6042	981.98 988.98 1015.21 1024.60 1066.34 1137.03 1157.08 1191.12				
6043	1283.44 1304.26 1361.75 1408.42 1434.40 1454.35 1471.38 1554.86				
6044	1578.25 2930.70 2991.35 3016.26 3060.35 3071.54 3079.73 3086.45				


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6045      3095.73 3630.62
6046 ZeroEnergy[kcal/mol] -0.80
6047 ElectronicLevels[1/cm] 1
6048      0.000000000000000000 2.0000000000000000
6049 End
6050 !*****
6051 RRHO ! 9
6052 Geometry[angstrom] 17
6053 C -0.13058910 -1.46087721 0.31433670
6054 C 0.77454390 -0.54827021 -0.21138930
6055 C 0.29227690 0.72434779 -0.63550730
6056 C -1.10260910 0.97554079 -0.64719030
6057 C -1.98441610 0.04994079 -0.11617230
6058 C -1.49792110 -1.17121221 0.36465870
6059 H 0.22780290 -2.41824421 0.67631570
6060 H 0.93939990 1.34884479 -1.23688530
6061 H -1.46027910 1.92247979 -1.03226830
6062 H -3.04711810 0.25889679 -0.09151630
6063 H -2.18569810 -1.90191721 0.77440470
6064 C 2.24635590 -0.82912721 -0.27937330
6065 H 2.78366690 -0.09547921 0.32719770
6066 H 2.47991590 -1.83039721 0.08505470
6067 H 2.61345490 -0.74151321 -1.30600130
6068 O 0.88971790 1.81639179 0.92295470
6069 H 0.22603090 1.53522779 1.57058570
6070 Core RigidRotor
6071 SymmetryFactor 0.423178412
6072 End
6073 Rotor Hindered
6074 Group 13 14 15
6075 Axis 12 2
6076 Symmetry 3
6077 Potential[kcal/mol] 12
6078 0.000 0.152 0.407 0.727 1.040 1.258 1.292 1.116 0.793 0.441 0.152 -0.012
6079 End
6080 Rotor Hindered
6081 Group 17
6082 Axis 16 3
6083 Symmetry 1
6084 Potential[kcal/mol] 36
6085 0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
6086 3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
6087 2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
6088 End
6089 Frequencies[1/cm] 42

```

```

6090    96.47  198.78  208.09  344.00  395.36  476.42  522.79  625.47
6091    680.95  753.77  792.97  812.94  875.74  949.38  980.32  991.33
6092    983.73  998.09  1013.18 1025.21 1062.22 1134.75 1153.82 1186.83
6093    1277.29 1301.81 1361.13 1403.55 1433.74 1452.83 1469.32 1542.77
6094    1572.09 2929.28 2989.29 3016.58 3061.32 3072.21 3081.15 3087.34
6095    3096.51 3633.76
6096  ZeroEnergy[kcal/mol]   -1.45
6097  ElectronicLevels[1/cm]                               1
6098    0.000000000000000000    2.0000000000000000
6099  End
6100  !*****
6101  RRHO                !                10
6102  Geometry[angstrom]          17
6103  C                    -0.12896900   -1.46119200   0.31290900
6104  C                    0.77660900    -0.54866600  -0.20529200
6105  C                    0.30096600    0.74266500  -0.60650000
6106  C                    -1.10413300   0.97944000  -0.64188800
6107  C                    -1.98366300   0.05159700  -0.11851100
6108  C                    -1.49742500  -1.17095800  0.36441000
6109  H                    0.22775200  -2.42152600  0.66865600
6110  H                    0.93927500   1.34620700  -1.23983300
6111  H                    -1.46204300   1.92525100  -1.02920100
6112  H                    -3.04724800   0.25693700  -0.10024100
6113  H                    -2.18589500  -1.90258200  0.77099500
6114  C                    2.24698600  -0.82950100  -0.27896600
6115  H                    2.78586100  -0.09528800  0.32573100
6116  H                    2.48205000  -1.83101700  0.08366800
6117  H                    2.61042500  -0.74036300  -1.30706600
6118  O                    0.88017200   1.79997700  0.89758000
6119  H                    0.22694200   1.52642600  1.55873900
6120  Core  RigidRotor
6121      SymmetryFactor    0.423178412
6122  End
6123  Rotor                Hindered
6124  Group    13 14 15
6125  Axis          12          2
6126  Symmetry      3
6127  Potential[kcal/mol]          12
6128  0.000 0.146 0.397 0.715 1.030 1.256 1.301 1.134 0.815 0.463 0.169 -0.003
6129  End
6130  Rotor                Hindered
6131  Group    17
6132  Axis          16          3
6133  Symmetry      1
6134  Potential[kcal/mol]          36

```

```

6135 0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
6136 3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
6137 2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
6138 End
6139 Frequencies[1/cm] 42
6140 112.04 208.01 219.98 344.92 392.68 478.57 520.74 622.18
6141 674.31 752.55 792.56 858.50 876.08 950.37 986.11 990.25
6142 985.35 1009.17 1012.42 1031.70 1058.19 1130.67 1151.08 1182.93
6143 1273.82 1300.37 1360.49 1399.06 1432.78 1451.27 1466.17 1530.16
6144 1564.76 2927.60 2986.95 3016.80 3061.79 3070.72 3075.27 3084.83
6145 3095.61 3632.15
6146 ZeroEnergy[kcal/mol] -2.24
6147 ElectronicLevels[1/cm] 1
6148 0.000000000000000000 2.0000000000000000
6149 End
6150 !*****
6151 RRHO ! 11
6152 Geometry[angstrom] 17
6153 C -0.12705800 -1.46172100 0.31148900
6154 C 0.77866400 -0.55048100 -0.20024500
6155 C 0.31072800 0.76258700 -0.57675700
6156 C -1.10687400 0.98290700 -0.63806500
6157 C -1.98314100 0.05355600 -0.12093100
6158 C -1.49735400 -1.17109700 0.36487500
6159 H 0.22805000 -2.42473000 0.66160700
6160 H 0.93807900 1.34098100 -1.24677500
6161 H -1.46508100 1.92763900 -1.02736200
6162 H -3.04754800 0.25536400 -0.10859200
6163 H -2.18633000 -1.90310700 0.76929300
6164 C 2.24769100 -0.83002200 -0.27865300
6165 H 2.78771400 -0.09516800 0.32446400
6166 H 2.48460700 -1.83167900 0.08225700
6167 H 2.60809100 -0.73914900 -1.30803000
6168 O 0.87110400 1.78430000 0.87336800
6169 H 0.22717200 1.51665200 1.54555200
6170 Core RigidRotor
6171 SymmetryFactor 0.423178412
6172 End
6173 Rotor Hindered
6174 Group 13 14 15
6175 Axis 12 2
6176 Symmetry 3
6177 Potential[kcal/mol] 12
6178 0.000 0.142 0.389 0.705 1.022 1.253 1.307 1.148 0.833 0.480 0.182 0.005
6179 End

```

```

6180      Rotor                               Hindered
6181      Group      17
6182      Axis                16                3
6183      Symmetry                1
6184      Potential[kcal/mol]                36
6185      0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
6186      3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
6187      2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
6188      End
6189      Frequencies[1/cm]                42
6190      151.28 216.05 232.76 346.56 391.07 480.59 517.89 617.63
6191      666.91 747.65 788.66 859.96 904.94 944.08 986.36 997.14
6192      989.32 1005.89 1016.33 1052.54 1064.44 1123.28 1148.75 1179.24
6193      1271.20 1298.91 1360.07 1394.25 1431.64 1449.42 1459.77 1516.23
6194      1557.68 2925.48 2984.06 3016.76 3054.08 3062.29 3073.09 3085.60
6195      3095.72 3632.45
6196      ZeroEnergy[kcal/mol]      -3.31
6197      ElectronicLevels[1/cm]                1
6198      0.000000000000000000      2.0000000000000000
6199      End
6200      !*****
6201      RRHO                !                12
6202      Geometry[angstrom]                17
6203      C                -0.12483100      -1.46210800      0.30990000
6204      C                0.78056100      -0.55316700      -0.19574800
6205      C                0.32119100      0.78327200      -0.54664100
6206      C                -1.11032100      0.98593100      -0.63492800
6207      C                -1.98259200      0.05574700      -0.12345700
6208      C                -1.49765000      -1.17155700      0.36575500
6209      H                0.22858100      -2.42773300      0.65473800
6210      H                0.93556600      1.33385800      -1.25374400
6211      H                -1.46879800      1.92975500      -1.02593600
6212      H                -3.04786300      0.25391100      -0.11696900
6213      H                -2.18695800      -1.90361400      0.76867900
6214      C                2.24830700      -0.83055100      -0.27839800
6215      H                2.79023800      -0.09553500      0.32307600
6216      H                2.48719800      -1.83236300      0.08082300
6217      H                2.60616600      -0.73810400      -1.30895600
6218      O                0.86235000      1.76914900      0.84977100
6219      H                0.22656200      1.50706400      1.53119000
6220      Core      RigidRotor
6221      SymmetryFactor      0.423178412
6222      End
6223      Rotor                               Hindered
6224      Group      13 14 15

```

```

6225 Axis 12 2
6226 Symmetry 3
6227 Potential[kcal/mol] 12
6228 0.000 0.138 0.382 0.696 1.014 1.250 1.311 1.158 0.847 0.494 0.193 0.011
6229 End
6230 Rotor Hindered
6231 Group 17
6232 Axis 16 3
6233 Symmetry 1
6234 Potential[kcal/mol] 36
6235 0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
6236 3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
6237 2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
6238 End
6239 Frequencies[1/cm] 42
6240 208.86 230.88 242.26 349.05 391.30 483.02 514.66 612.66
6241 661.61 741.38 784.69 847.81 924.38 936.11 983.83 966.42
6242 1000.19 1001.98 1017.93 1046.63 1111.64 1113.71 1149.05 1176.32
6243 1270.07 1297.49 1360.25 1390.01 1430.54 1446.46 1449.67 1505.95
6244 1555.25 2922.84 2980.55 3015.97 3037.20 3062.01 3072.12 3086.92
6245 3095.76 3635.78
6246 ZeroEnergy[kcal/mol] -5.74
6247 ElectronicLevels[1/cm] 1
6248 0.0000000000000000 2.0000000000000000
6249 End
6250 !*****
6251 RRHO ! 13
6252 Geometry[angstrom] 17
6253 C -0.12266300 -1.46261500 0.30824800
6254 C 0.78237100 -0.55525800 -0.19120200
6255 C 0.33150700 0.80371700 -0.51660900
6256 C -1.11318300 0.98920300 -0.63160100
6257 C -1.98214500 0.05775300 -0.12598500
6258 C -1.49807500 -1.17203000 0.36681500
6259 H 0.22909300 -2.43110500 0.64722800
6260 H 0.93255700 1.32700300 -1.25702500
6261 H -1.47282300 1.93176100 -1.02480000
6262 H -3.04833000 0.25212000 -0.12608700
6263 H -2.18769200 -1.90411700 0.76839400
6264 C 2.24904700 -0.83116700 -0.27817700
6265 H 2.79359300 -0.09650700 0.32163600
6266 H 2.48998900 -1.83319300 0.07923900
6267 H 2.60434800 -0.73716800 -1.30987400
6268 O 0.85347100 1.75396000 0.82590200
6269 H 0.22567800 1.49714100 1.51621400

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6270      Core      RigidRotor
6271          SymmetryFactor      0.423178412
6272      End
6273      Rotor                      Hindered
6274      Group      13 14 15
6275      Axis                12          2
6276      Symmetry                3
6277      Potential[kcal/mol]                12
6278      0.000 0.134 0.374 0.688 1.007 1.247 1.315 1.170 0.862 0.508 0.204 0.017
6279      End
6280      Rotor                      Hindered
6281      Group      17
6282      Axis                16          3
6283      Symmetry                1
6284      Potential[kcal/mol]                36
6285      0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
6286      3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
6287      2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
6288      End
6289          Frequencies[1/cm]                42
6290      215.92  246.33  260.66  352.08  394.65  486.68  511.87  608.45
6291      659.42  736.54  781.29  834.91  926.68  935.09  981.68  967.59
6292      996.73 1011.83 1027.67 1046.33 1104.13 1139.45 1169.24 1176.80
6293      1268.51 1296.43 1360.67 1386.43 1428.82 1433.71 1446.81 1501.32
6294      1556.88 2920.33 2977.21 3014.73 3022.46 3060.62 3070.26 3087.49
6295      3095.12 3638.05
6296      ZeroEnergy[kcal/mol]      -8.69
6297      ElectronicLevels[1/cm]                1
6298      0.000000000000000000      2.0000000000000000
6299      End
6300      !*****
6301      RRHO          !          14
6302      Geometry[angstrom]                17
6303      C              -0.12074500  -1.46330100   0.30654600
6304      C              0.78420700  -0.55610200  -0.18613500
6305      C              0.34123700   0.82331200  -0.48705000
6306      C              -1.11492800   0.99307000  -0.62745000
6307      C              -1.98176300   0.05940500  -0.12850200
6308      C              -1.49846400  -1.17231100   0.36787400
6309      H              0.22944500  -2.43504600   0.63844700
6310      H              0.92946700   1.32086400  -1.25682100
6311      H              -1.47664300   1.93387000  -1.02362200
6312      H              -3.04886600   0.24974200  -0.13654200
6313      H              -2.18848500  -1.90460600   0.76790700
6314      C              2.25001600  -0.83189600  -0.27796700

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6315  H          2.79809900  -0.09824300  0.32010900
6316  H          2.49288600  -1.83430600  0.07730000
6317  H          2.60228700  -0.73632800  -1.31085700
6318  O          0.84411100  1.73845600  0.80138700
6319  H          0.22555700  1.48723500  1.50148000
6320  Core  RigidRotor
6321          SymmetryFactor  0.423178412
6322  End
6323  Rotor          Hindered
6324  Group  13 14 15
6325  Axis          12          2
6326  Symmetry          3
6327  Potential[kcal/mol]          12
6328  0.000 0.129 0.365 0.677 0.997 1.243 1.320 1.182 0.880 0.526 0.218 0.025
6329  End
6330  Rotor          Hindered
6331  Group  17
6332  Axis          16          3
6333  Symmetry          1
6334  Potential[kcal/mol]          36
6335  0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
6336  3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
6337  2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
6338  End
6339  Frequencies[1/cm]          42
6340  229.05 257.55 285.69 356.13 402.58 491.49 509.78 605.65
6341  659.19 734.32 778.21 823.93 921.91 935.71 979.90 965.88
6342  992.79 1013.39 1028.94 1073.43 1096.41 1141.26 1171.15 1219.53
6343  1266.10 1295.80 1361.05 1383.06 1417.12 1430.05 1445.63 1499.55
6344  1559.02 2918.30 2974.40 3006.12 3013.66 3058.57 3067.79 3086.44
6345  3094.29 3640.81
6346  ZeroEnergy[kcal/mol]  -11.53
6347  ElectronicLevels[1/cm]          1
6348  0.000000000000000000  2.0000000000000000
6349  End
6350  !*****
6351  RRHO          !          15
6352  Geometry[angstrom]          17
6353  C          -0.11907500  -1.46406500  0.30474200
6354  C          0.78615900  -0.55577400  -0.18016200
6355  C          0.35028600  0.84174500  -0.45836500
6356  C          -1.11567900  0.99758800  -0.62206900
6357  C          -1.98127400  0.06080100  -0.13110500
6358  C          -1.49869200  -1.17231000  0.36877100
6359  H          0.22949300  -2.43947900  0.62821300

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6360 H          0.92628400   1.31516700  -1.25418100
6361 H         -1.47957400   1.93640200  -1.02176500
6362 H         -3.04926200   0.24673100  -0.14846400
6363 H         -2.18928000  -1.90505400   0.76677500
6364 C          2.25122200  -0.83270700  -0.27773900
6365 H          2.80392100  -0.10078900   0.31845300
6366 H          2.49561900  -1.83579200   0.07482400
6367 H          2.59966700  -0.73552500  -1.31201600
6368 O          0.83402700   1.72259900   0.77615200
6369 H          0.22750600   1.47816300   1.48840000
6370   Core   RigidRotor
6371           SymmetryFactor   0.423178412
6372 End
6373   Rotor                               Hindered
6374   Group   13 14 15
6375   Axis           12           2
6376   Symmetry           3
6377   Potential[kcal/mol]           12
6378   0.000 0.123 0.354 0.663 0.985 1.237 1.325 1.197 0.901 0.547 0.235 0.034
6379 End
6380   Rotor                               Hindered
6381   Group   17
6382   Axis           16           3
6383   Symmetry           1
6384   Potential[kcal/mol]           36
6385   0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
6386   3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
6387   2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
6388 End
6389   Frequencies[1/cm]           42
6390   263.12 301.79 356.67 384.93 466.01 497.11 509.90 606.67
6391   661.95 737.59 775.01 815.59 918.00 932.82 978.28 963.20
6392   989.13 1013.61 1025.05 1090.52 1110.31 1140.79 1169.39 1259.04
6393   1270.11 1295.50 1361.29 1380.00 1404.32 1429.61 1444.75 1498.79
6394   1560.39 2916.59 2971.98 2988.60 3012.25 3056.28 3065.13 3084.26
6395   3093.67 3644.25
6396   ZeroEnergy[kcal/mol]   -14.16
6397   ElectronicLevels[1/cm]           1
6398   0.000000000000000000   2.0000000000000000
6399 End
6400 !*****
6401 RRHO           !           16
6402   Geometry[angstrom]           17
6403   C          -0.11749200  -1.46491000   0.30271000
6404   C          0.78843600  -0.55450300  -0.17255300

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6405	C		0.35834700	0.85840800	-0.43108000
6406	C		-1.11569200	1.00307700	-0.61475700
6407	C		-1.98055500	0.06216300	-0.13404800
6408	C		-1.49867500	-1.17199800	0.36928700
6409	H		0.22908300	-2.44462800	0.61601100
6410	H		0.92265200	1.30901100	-1.25018900
6411	H		-1.48124300	1.94007400	-1.01803400
6412	H		-3.04941600	0.24301500	-0.16240300
6413	H		-2.19010600	-1.90556100	0.76423600
6414	C		2.25276200	-0.83364200	-0.27743100
6415	H		2.81186300	-0.10452800	0.31649500
6416	H		2.49820400	-1.83788600	0.07139100
6417	H		2.59591700	-0.73461800	-1.31353100
6418	O		0.82308800	1.70675500	0.75010800
6419	H		0.23214200	1.46872300	1.47647000
6420	Core	RigidRotor			
6421		SymmetryFactor	0.423178412		
6422	End				
6423	Rotor			Hindered	
6424	Group	13 14 15			
6425	Axis		12		2
6426	Symmetry			3	
6427	Potential[kcal/mol]				12
6428		0.000 0.115 0.340 0.646 0.969 1.229 1.329 1.215 0.927 0.573 0.256 0.046			
6429	End				
6430	Rotor			Hindered	
6431	Group	17			
6432	Axis		16		3
6433	Symmetry			1	
6434	Potential[kcal/mol]				36
6435		0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358			
6436		3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238			
6437		2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073			
6438	End				
6439	Frequencies[1/cm]				42
6440		265.57 316.50 363.21 398.26 502.53 504.12 574.30 630.84			
6441		680.94 765.81 771.53 813.05 915.29 928.90 976.82 997.74			
6442		985.54 1013.36 1021.56 1086.23 1139.07 1146.66 1168.05 1258.91			
6443		1295.32 1310.28 1361.43 1377.34 1393.92 1429.42 1444.09 1498.61			
6444		1561.59 2914.92 2969.59 2970.49 3010.80 3053.61 3062.22 3081.66			
6445		3093.06 3650.36			
6446	ZeroEnergy[kcal/mol]		-16.24		
6447	ElectronicLevels[1/cm]				1
6448		0.0000000000000000		2.0000000000000000	
6449	End				

```

6450 !*****
6451 RRHO ! 17
6452 Geometry[angstrom] 17
6453 C -0.11578400 -1.46638400 0.30037400
6454 C 0.79183700 -0.55221300 -0.16037100
6455 C 0.36374700 0.86989100 -0.40811000
6456 C -1.11496700 1.01128300 -0.60238100
6457 C -1.97965400 0.06384200 -0.13795300
6458 C -1.49821400 -1.17129600 0.36809800
6459 H 0.22736400 -2.45238200 0.59905900
6460 H 0.91738200 1.29909200 -1.24754800
6461 H -1.48018500 1.94818500 -1.00684800
6462 H -3.04956200 0.23776800 -0.18136800
6463 H -2.19139800 -1.90700600 0.75612400
6464 C 2.25537500 -0.83508800 -0.27677400
6465 H 2.82607800 -0.11177900 0.31363900
6466 H 2.50122500 -1.84195500 0.06471800
6467 H 2.58854300 -0.73304900 -1.31618600
6468 O 0.81083700 1.69326900 0.72285500
6469 H 0.24300000 1.45352300 1.46612000
6470 Core RigidRotor
6471 SymmetryFactor 0.423178412
6472 End
6473 Rotor Hindered
6474 Group 13 14 15
6475 Axis 12 2
6476 Symmetry 3
6477 Potential[kcal/mol] 12
6478 0.000 0.103 0.319 0.619 0.943 1.214 1.333 1.238 0.964 0.611 0.287 0.064
6479 End
6480 Rotor Hindered
6481 Group 17
6482 Axis 16 3
6483 Symmetry 1
6484 Potential[kcal/mol] 36
6485 0.000 0.091 0.413 0.936 1.597 2.310 2.980 3.516 3.818 3.872 3.717 3.443
6486 3.131 2.854 2.658 2.557 2.535 2.556 2.585 2.584 2.537 2.451 2.347 2.258
6487 2.211 2.217 2.269 2.339 2.380 2.331 2.151 1.831 1.394 0.904 0.452 0.131
6488 End
6489 Frequencies[1/cm] 42
6490 263.77 327.66 372.56 402.89 501.43 509.55 584.21 646.17
6491 706.23 767.82 798.21 881.23 915.40 939.34 975.78 994.84
6492 983.18 1012.84 1019.98 1083.73 1138.32 1164.68 1179.74 1258.57
6493 1295.87 1344.59 1362.05 1375.71 1387.99 1429.37 1443.82 1499.50
6494 1563.31 2912.53 2953.14 2966.61 3008.60 3049.09 3058.32 3079.22

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6495      3091.68 3653.77
6496 ZeroEnergy[kcal/mol]   -17.26
6497   ElectronicLevels[1/cm]                      1
6498     0.000000000000000000      2.0000000000000000
6499 End
6500 !*****
6501 RRHO      !              18
6502 Geometry[angstrom]      17
6503 C          -0.13228000   -1.50496400   0.24654200
6504 C           0.78404600   -0.55794900  -0.11270800
6505 C           0.34907300    0.85939100  -0.39359300
6506 C          -1.13483900    1.03361400  -0.47926400
6507 C          -1.99969200    0.04645200  -0.11634400
6508 C          -1.52144800   -1.23217100   0.27097700
6509 H           0.21094200   -2.50128500   0.50504000
6510 H           0.83108300    1.21086800  -1.31611200
6511 H          -1.49370500    2.01362200  -0.77375600
6512 H          -3.06796500    0.23214400  -0.12778400
6513 H          -2.21811000   -2.00501700   0.56750200
6514 C           2.25444500   -0.82884800  -0.19336700
6515 H           2.80712900   -0.14195300   0.45437300
6516 H           2.48793000   -1.85497100   0.09499900
6517 H           2.62057800   -0.66378600  -1.21414100
6518 O           0.88694200    1.77376300   0.60742100
6519 H           0.42354600    1.56965000   1.43028800
6520   Core   RigidRotor
6521         SymmetryFactor   0.423178412
6522 End
6523 Rotor                      Hindered
6524 Group   13 14 15
6525 Axis           12           2
6526 Symmetry           3
6527 Potential[kcal/mol]      12
6528 0.000 0.093 0.299 0.594 0.919 1.198 1.333 1.257 0.995 0.644 0.315 0.081
6529 End
6530 Rotor                      Hindered
6531 Group   17
6532 Axis           16           3
6533 Symmetry           1
6534 Potential[kcal/mol]      36
6535 0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
6536 3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
6537 2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
6538 End
6539   Frequencies[1/cm]      42

```

```

6540      264.31 342.22 395.17 402.36 490.31 509.88 571.74 635.54
6541      698.85 767.50 797.42 880.05 911.25 960.65 970.57 994.64
6542      984.96 1012.12 1024.20 1085.11 1139.31 1164.15 1183.09 1265.23
6543      1295.20 1349.02 1363.95 1374.47 1385.32 1427.31 1444.81 1504.57
6544      1570.70 2896.12 2909.89 2965.91 3010.04 3056.21 3060.58 3078.08
6545      3098.25 3643.05
6546      ZeroEnergy[kcal/mol]   -18.29
6547      ElectronicLevels[1/cm]                               1
6548      0.000000000000000000      2.0000000000000000
6549      End
6550      !*****
6551      Tunneling      Eckart
6552      ImaginaryFrequency[1/cm]      406
6553      WellDepth[kcal/mol]      2.68
6554      WellDepth[kcal/mol]      17.02
6555      End
6556      End
6557      !*****
6558      Well      W4p2      # pHOc6CH5CH3
6559      Species
6560      RRHO
6561      Geometry[angstrom]      17
6562      C      0.70827100      1.24600900      -0.30063200
6563      C      -0.63855300      1.21997800      -0.10413700
6564      C      -1.36430000      0.00032000      -0.00082100
6565      C      -0.63866600      -1.21968600      -0.10425800
6566      C      0.70800700      -1.24599300      -0.30064900
6567      C      1.53505900      -0.00006800      -0.37954300
6568      H      -1.18469100      -2.15502600      -0.02613300
6569      H      1.24027100      -2.18763800      -0.37457500
6570      O      2.56611500      -0.00021400      0.64458400
6571      H      2.10928400      -0.00002200      1.49352900
6572      H      2.12595000      -0.00014600      -1.30348800
6573      H      1.24070600      2.18755300      -0.37455300
6574      H      -1.18433700      2.15543700      -0.02593900
6575      C      -2.84079900      -0.00008900      0.26276900
6576      H      -3.32083100      -0.88095900      -0.16944000
6577      H      -3.05106300      -0.01072200      1.33947900
6578      H      -3.31831500      0.89040200      -0.15192000
6579      Core      RigidRotor
6580      SymmetryFactor      1
6581      End
6582      Rotor      Hindered      !freq=15.76
6583      Group      15 16 17
6584      Axis      3 14

```

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6585          Symmetry                      3
6586  Potential[kcal/mol]          12
6587          0.000 -0.001 0.003 -0.001 0.000 -0.001 -0.002 0.000 -0.001 0.000 0.003 -0.001
6588          End
6589          Rotor Hindered                !freq=268.95
6590          Group                      10
6591          Axis                        6 9
6592          Symmetry                    1
6593  Potential[kcal/mol]          36
6594          0.000 0.106 0.407 0.872 1.424 1.973 2.418 2.711 2.837 2.819 2.704 2.564
6595          2.461 2.424 2.457 2.537 2.635 2.711 2.734 2.702 2.621 2.524 2.448 2.425
6596          2.474 2.586 2.726 2.830 2.831 2.689 2.393 1.954 1.420 0.880 0.416 0.107
6597          End
6598          Frequencies[1/cm]          43
6599          72.37  214.82  330.97  361.72  395.45  453.35  492.38  600.78
6600          626.33  748.09  762.53  766.19  871.29  953.40  960.88  968.20
6601          986.61  971.90  996.28  1019.91 1127.94 1150.12 1177.04 1205.34
6602          1223.74 1295.01 1344.94 1365.69 1366.55 1419.02 1434.20 1437.59
6603          1485.01 1571.82 2905.71 2908.24 2968.89 3005.24 3047.94 3048.96
6604          3076.11 3078.07 3669.76
6605          ZeroEnergy[kcal/mol]      -16.88
6606          ElectronicLevels[1/cm]    1
6607          0  2
6608  End
6609  End
6610  !*****
6611  Barrier      B4p3      W4p2      P4p      # TS4p3
6612  RRHO
6613  Geometry[angstrom]          17
6614  C              0.69740100  -1.22292600  -0.03502200
6615  C              -0.68505400  -1.19954000  -0.03932500
6616  C              -1.40195500   0.00567400  -0.02000200
6617  C              -0.67362900   1.20190200  -0.04259800
6618  C              0.71062700   1.20612300  -0.05191700
6619  C              1.41917400  -0.01294000   0.08290300
6620  H              -1.20475800   2.14685600  -0.08732100
6621  H              1.26080600   2.14042400  -0.08507200
6622  O              2.77762500  -0.08966600  -0.14790800
6623  H              3.19031600   0.73067600   0.13826000
6624  H              1.46461900   0.00862900   1.77073400
6625  H              1.25091600  -2.15301500  -0.05705100
6626  H              -1.22766500  -2.13812000  -0.08112700
6627  C              -2.90808000   0.01209500   0.01956800
6628  H              -3.32062200  -0.84569100  -0.51582700
6629  H              -3.27440100  -0.03614000   1.04992200

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6630 H -3.31110500 0.92138900 -0.43089100
6631 Core RigidRotor
6632 SymmetryFactor 0.5
6633 End
6634 Tunneling Eckart
6635 ImaginaryFrequency[1/cm] 1196.85
6636 WellDepth[kcal/mol] 27.20
6637 WellDepth[kcal/mol] 8.71
6638 End
6639 Frequencies[1/cm] 44
6640 55.86 131.99
6641 250.17 303.19 314.70 393.25 427.27 448.62 510.65 531.54
6642 651.35 656.58 709.66 758.72 823.29 837.48 881.46 965.16
6643 976.72 972.21 988.36 1024.64 1092.88 1142.86 1153.44 1198.79
6644 1217.56 1268.16 1310.57 1370.56 1412.85 1441.40 1451.98 1473.50
6645 1553.42 1597.62 2925.43 2983.17 3008.09 3055.98 3061.47 3072.62
6646 3096.32 3705.05
6647 ZeroEnergy[kcal/mol] 10.31
6648 ElectronicLevels[1/cm] 1
6649 0 2
6650 End
6651 !*****
6652 Barrier B4p2 W W4p2
6653 Variational
6654 RRHO ! 1
6655 Geometry[angstrom] 17
6656 C 1.31381800 0.00001300 -0.84727900
6657 C 0.63772100 1.20709800 -0.63958100
6658 C -0.68966700 1.20375100 -0.21237700
6659 C -1.37128900 -0.00000900 0.01354300
6660 C -0.68967600 -1.20374300 -0.21243800
6661 C 0.63772600 -1.20707100 -0.63966100
6662 H 2.33854000 0.00002800 -1.18817700
6663 H 1.15088900 2.14701800 -0.80592200
6664 H -1.20471000 2.14521700 -0.05060200
6665 H -1.20471700 -2.14521500 -0.05072000
6666 H 1.15088400 -2.14698500 -0.80607700
6667 C -2.79240300 0.00002500 0.51786100
6668 H -2.81515400 0.00151200 1.61213400
6669 H -3.33381000 0.88436200 0.17725400
6670 H -3.33317100 -0.88568400 0.17967300
6671 O 2.56838600 -0.00003800 1.45983500
6672 H 1.65914500 -0.00041300 1.81477500
6673 Core RigidRotor
6674 SymmetryFactor 0.843552272

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6675 End
6676 Rotor Hindered
6677 Group 13 14 15
6678 Axis 12 4
6679 Symmetry 3
6680 Potential[kcal/mol] 12
6681 0.000 0.005 0.006 0.003 0.001 0.001 0.001 -0.001 0.002 0.003 0.006 0.003
6682 End
6683 Rotor Hindered
6684 Group 17
6685 Axis 16 1
6686 Symmetry 1
6687 Potential[kcal/mol] 36
6688 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
6689 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
6690 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
6691 End
6692 Frequencies[1/cm] 42
6693 105.59 208.96 282.85 341.35 401.35 453.14 473.70 526.91
6694 632.26 641.75 732.23 799.86 845.64 891.40 944.45 954.22
6695 966.56 976.99 1008.16 1020.08 1068.71 1138.21 1159.98 1191.80
6696 1293.91 1308.79 1369.45 1416.26 1442.42 1452.52 1467.92 1557.09
6697 1583.13 2928.88 2988.26 3014.16 3055.44 3055.54 3078.99 3080.57
6698 3117.01 3563.62
6699 ZeroEnergy[kcal/mol] -3.44
6700 ElectronicLevels[1/cm] 1
6701 0.0000000000000000 2.0000000000000000
6702 End
6703 !*****
6704 RRHO ! 2
6705 Geometry[angstrom] 17
6706 C 1.31834700 -0.00001200 -0.81844800
6707 C 0.64270200 1.20712300 -0.61222500
6708 C -0.68893700 1.20384700 -0.19927500
6709 C -1.37412000 0.00000800 0.01365600
6710 C -0.68895400 -1.20384200 -0.19927800
6711 C 0.64268400 -1.20713700 -0.61222600
6712 H 2.34510100 -0.00001900 -1.16180900
6713 H 1.15702600 2.14679700 -0.77509200
6714 H -1.20724600 2.14518700 -0.04885500
6715 H -1.20727800 -2.14517500 -0.04885900
6716 H 1.15699400 -2.14681900 -0.77509600
6717 C -2.80633500 0.00001300 0.48642300
6718 H -2.85260100 -0.00015100 1.58016300
6719 H -3.33971200 0.88518000 0.13508200

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6720  H          -3.33980900  -0.88499200   0.13481600
6721  O           2.56995100   0.00000000   1.40287400
6722  H           1.68060100  -0.00000900   1.81062400
6723  Core  RigidRotor
6724          SymmetryFactor   0.843552272
6725  End
6726  Rotor                      Hindered
6727  Group   13 14 15
6728  Axis           12           4
6729  Symmetry           3
6730  Potential[kcal/mol]           12
6731    0.000 0.005 0.006 0.003 0.002 0.001 0.001 -0.001 0.002 0.003 0.006 0.003
6732  End
6733  Rotor                      Hindered
6734  Group   17
6735  Axis           16           1
6736  Symmetry           1
6737  Potential[kcal/mol]           36
6738    0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
6739    2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
6740    2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
6741  End
6742  Frequencies[1/cm]           42
6743    124.67  215.15  338.84  342.50  401.34  458.24  523.81  534.37
6744    632.74  641.01  739.81  799.89  844.64  896.58  947.90  953.92
6745    967.20  977.45 1008.92 1020.49 1069.79 1141.23 1159.91 1191.58
6746    1294.30 1310.30 1369.49 1417.46 1442.53 1453.12 1467.88 1559.48
6747    1583.29 2927.52 2987.26 3013.41 3056.91 3057.20 3076.89 3082.49
6748    3097.22 3534.20
6749  ZeroEnergy[kcal/mol]   -2.76
6750  ElectronicLevels[1/cm]           1
6751    0.000000000000000000    2.0000000000000000
6752  End
6753  !*****
6754  RRHO          !           3
6755  Geometry[angstrom]           17
6756  C           1.32397300  -0.00001100  -0.80113400
6757  C           0.65002100   1.20750200  -0.58920400
6758  C          -0.68272200   1.20404200  -0.18200900
6759  C          -1.37065900   0.00000800   0.02031400
6760  C          -0.68273900  -1.20403800  -0.18200900
6761  C           0.65000300  -1.20751500  -0.58920200
6762  H           2.34934400  -0.00001900  -1.14893400
6763  H           1.16878100   2.14685300  -0.73831600
6764  H          -1.20066300   2.14521600  -0.03049800

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6765 H -1.20069200 -2.14520500 -0.03049700
6766 H 1.16875100 -2.14687300 -0.73831300
6767 C -2.81346100 0.00001300 0.45934400
6768 H -2.89159100 -0.00018800 1.55102400
6769 H -3.33643500 0.88467500 0.09126200
6770 H -3.33653700 -0.88445500 0.09093500
6771 O 2.54763100 -0.00000200 1.34544900
6772 H 1.68073000 0.00001300 1.79321700
6773 Core RigidRotor
6774 SymmetryFactor 0.843552272
6775 End
6776 Rotor Hindered
6777 Group 13 14 15
6778 Axis 12 4
6779 Symmetry 3
6780 Potential[kcal/mol] 12
6781 0.000 0.004 0.006 0.003 0.002 0.001 0.001 -0.001 0.002 0.003 0.005 0.004
6782 End
6783 Rotor Hindered
6784 Group 17
6785 Axis 16 1
6786 Symmetry 1
6787 Potential[kcal/mol] 36
6788 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
6789 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
6790 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
6791 End
6792 Frequencies[1/cm] 42
6793 138.95 219.93 287.85 341.91 400.54 458.75 523.99 540.20
6794 632.57 640.42 744.05 800.25 843.69 898.63 949.49 954.22
6795 967.82 977.97 1008.96 1020.66 1069.99 1141.63 1160.07 1192.27
6796 1294.02 1310.51 1369.78 1417.67 1442.94 1453.03 1467.48 1559.89
6797 1584.05 2928.54 2988.38 3012.50 3058.42 3058.73 3077.74 3084.12
6798 3097.08 3565.66
6799 ZeroEnergy[kcal/mol] -2.45
6800 ElectronicLevels[1/cm] 1
6801 0.000000000000000000 2.0000000000000000
6802 End
6803 !*****
6804 RRHO ! 4
6805 Geometry[angstrom] 17
6806 C 1.33553800 -0.00001100 -0.77186800
6807 C 0.65877200 1.20842400 -0.56520200
6808 C -0.67609800 1.20463800 -0.16929500
6809 C -1.36616400 0.00000800 0.02362500

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6810  C          -0.67611400  -1.20463300  -0.16929500
6811  C           0.65875500  -1.20843700  -0.56520100
6812  H           2.35503000  -0.00001800  -1.13182500
6813  H           1.17975300   2.14699000  -0.71093400
6814  H          -1.19539200   2.14531000  -0.01968600
6815  H          -1.19542000  -2.14529800  -0.01968500
6816  H           1.17972300  -2.14701000  -0.71093100
6817  C          -2.81526100   0.00001200   0.43939700
6818  H          -2.91176400  -0.00019300   1.52953000
6819  H          -3.33194500   0.88468400   0.06268100
6820  H          -3.33204200  -0.88446300   0.06234700
6821  O           2.51235900  -0.00000200   1.28087000
6822  H           1.67758400   0.00001600   1.77860300
6823  Core  RigidRotor
6824          SymmetryFactor   0.843552272
6825  End
6826  Rotor          Hindered
6827  Group   13 14 15
6828  Axis           12           4
6829  Symmetry           3
6830  Potential[kcal/mol]           12
6831  0.000 0.003 0.005 0.003 0.002 -0.001 0.001 -0.001 0.002 0.003 0.005 0.004
6832  End
6833  Rotor          Hindered
6834  Group   17
6835  Axis           16           1
6836  Symmetry           1
6837  Potential[kcal/mol]           36
6838  0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
6839  2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
6840  2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
6841  End
6842  Frequencies[1/cm]           42
6843  153.71 185.72 226.22 341.99 400.19 458.46 523.86 550.53
6844  631.83 640.18 749.37 801.06 843.23 900.72 951.12 955.49
6845  968.04 978.58 1008.26 1020.37 1069.84 1140.44 1160.54 1193.80
6846  1292.18 1309.62 1369.92 1417.91 1442.86 1452.65 1466.35 1558.58
6847  1585.45 2929.17 2988.99 3012.99 3059.30 3059.38 3082.22 3085.27
6848  3107.46 3610.97
6849  ZeroEnergy[kcal/mol]  -1.81
6850  ElectronicLevels[1/cm]           1
6851  0.000000000000000000  2.0000000000000000
6852  End
6853  !*****
6854  RRHO          !           5

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6855 Geometry[angstrom]          17
6856 C          1.34261400 -0.00001100 -0.75386300
6857 C          0.66311500  1.20907800 -0.55307200
6858 C         -0.67330900  1.20507600 -0.16536100
6859 C         -1.36410700  0.00000900  0.02340100
6860 C         -0.67332400 -1.20506900 -0.16536100
6861 C          0.66309800 -1.20909200 -0.55307100
6862 H          2.35822400 -0.00001700 -1.12234700
6863 H          1.18511800  2.14707600 -0.69811300
6864 H         -1.19365000  2.14542800 -0.01679700
6865 H         -1.19367900 -2.14541300 -0.01679600
6866 H          1.18508900 -2.14709700 -0.69811000
6867 C         -2.81479000  0.00001100  0.43228800
6868 H         -2.91573900 -0.00019300  1.52209700
6869 H         -3.32998900  0.88476400  0.05375500
6870 H         -3.33008400 -0.88454400  0.05341900
6871 O          2.49351200 -0.00000300  1.24831600
6872 H          1.67514700  0.00001700  1.77002400
6873   Core   RigidRotor
6874           SymmetryFactor    0.843552272
6875 End
6876   Rotor                               Hindered
6877   Group   13 14 15
6878   Axis           12           4
6879   Symmetry           3
6880   Potential[kcal/mol]           12
6881   0.000 0.003 0.005 0.003 0.002 -0.001 0.001 -0.001 0.002 0.003 0.005 0.004
6882 End
6883   Rotor                               Hindered
6884   Group   17
6885   Axis           16           1
6886   Symmetry           1
6887   Potential[kcal/mol]           36
6888   0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
6889   2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
6890   2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
6891 End
6892   Frequencies[1/cm]           42
6893   135.64 158.11 228.28 342.08 400.36 457.73 524.45 567.44
6894   631.38 640.68 753.93 801.55 843.29 903.54 954.11 956.72
6895   968.12 978.86 1007.54 1020.30 1069.83 1139.67 1160.88 1194.81
6896   1290.42 1309.18 1370.01 1418.19 1442.79 1452.47 1465.51 1557.68
6897   1586.26 2928.91 2988.71 3013.17 3058.94 3058.99 3083.97 3086.28
6898   3113.33 3626.75
6899 ZeroEnergy[kcal/mol]    -1.54

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6900 ElectronicLevels[1/cm] 1
6901 0.0000000000000000 2.0000000000000000
6902 End
6903 !*****
6904 RRHO ! 6
6905 Geometry[angstrom] 17
6906 C 1.34974500 -0.00001100 -0.73374600
6907 C 0.66724300 1.20965300 -0.54103800
6908 C -0.67103800 1.20536400 -0.16326300
6909 C -1.36211000 0.00000900 0.02168200
6910 C -0.67104900 -1.20535500 -0.16326400
6911 C 0.66722900 -1.20966900 -0.54103600
6912 H 2.36193700 -0.00001600 -1.11173800
6913 H 1.19133700 2.14720300 -0.68080600
6914 H -1.19326800 2.14550000 -0.02017100
6915 H -1.19329500 -2.14548300 -0.02017200
6916 H 1.19131000 -2.14722700 -0.68080100
6917 C -2.81320700 0.00001200 0.42753500
6918 H -2.91480700 -0.00019500 1.51725600
6919 H -3.32783000 0.88495900 0.04870600
6920 H -3.32792500 -0.88473700 0.04836700
6921 O 2.47487400 -0.00000300 1.21618000
6922 H 1.66877100 0.00001700 1.75751700
6923 Core RigidRotor
6924 SymmetryFactor 0.843552272
6925 End
6926 Rotor Hindered
6927 Group 13 14 15
6928 Axis 12 4
6929 Symmetry 3
6930 Potential[kcal/mol] 12
6931 0.000 0.004 0.005 0.003 0.002 -0.001 0.001 -0.001 0.002 0.003 0.005 0.004
6932 End
6933 Rotor Hindered
6934 Group 17
6935 Axis 16 1
6936 Symmetry 1
6937 Potential[kcal/mol] 36
6938 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
6939 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
6940 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
6941 End
6942 Frequencies[1/cm] 42
6943 156.09 175.26 227.05 342.19 400.81 456.06 525.46 610.09
6944 631.16 643.69 760.51 802.24 843.57 908.60 958.86 962.02

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6945    968.45  979.40  1006.96 1020.34 1070.25 1139.77 1161.33 1196.07
6946    1289.00 1309.38 1369.90 1418.91 1442.67 1452.50 1464.96 1558.11
6947    1587.17 2929.08 2988.91 3013.42 3059.27 3059.35 3084.74 3087.25
6948    3112.30 3618.85
6949    ZeroEnergy[kcal/mol]   -0.94
6950    ElectronicLevels[1/cm]                               1
6951    0.000000000000000000    2.0000000000000000
6952    End
6953    !*****
6954    RRHO                !                7
6955    Geometry[angstrom]          17
6956    C                    1.35933300   -0.00000800   -0.70780600
6957    C                    0.67022800    1.21043700   -0.53256000
6958    C                   -0.66866200    1.20577600   -0.16102400
6959    C                   -1.36074500    0.00000600    0.01872100
6960    C                   -0.66868600   -1.20577900   -0.16102600
6961    C                    0.67020500   -1.21044000   -0.53255100
6962    H                    2.36491200   -0.00002300   -1.10236300
6963    H                    1.19534300    2.14765500   -0.66995900
6964    H                   -1.19334300    2.14558300   -0.02506700
6965    H                   -1.19337700   -2.14558000   -0.02507000
6966    H                    1.19531000   -2.14766400   -0.66994600
6967    C                   -2.81158000    0.00001100    0.42426400
6968    H                   -2.91131200   -0.00019700    1.51420800
6969    H                   -3.32636100    0.88525400    0.04637000
6970    H                   -3.32645500   -0.88503200    0.04602900
6971    O                    2.45645300   -0.00000300    1.18499100
6972    H                    1.66667100    0.00001800    1.74899700
6973    Core   RigidRotor
6974          SymmetryFactor    0.843552272
6975    End
6976    Rotor                Hindered
6977    Group   13 14 15
6978    Axis           12           4
6979    Symmetry           3
6980    Potential[kcal/mol]          12
6981    0.000 0.004 0.005 0.003 0.002 -0.001 0.001 -0.001 0.002 0.003 0.005 0.003
6982    End
6983    Rotor                Hindered
6984    Group   17
6985    Axis           16           1
6986    Symmetry           1
6987    Potential[kcal/mol]          36
6988    0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
6989    2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421

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6990 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
6991 End
6992 Frequencies[1/cm] 42
6993 124.75 172.38 221.21 342.29 402.09 453.11 525.65 630.71
6994 640.01 661.50 768.51 802.87 844.36 916.09 963.53 979.25
6995 968.58 979.85 1005.23 1020.75 1070.24 1139.24 1161.70 1197.20
6996 1285.77 1309.32 1369.56 1419.51 1442.57 1452.33 1463.63 1556.89
6997 1586.91 2928.86 2988.80 3013.75 3059.71 3059.84 3086.07 3088.46
6998 3113.58 3623.17
6999 ZeroEnergy[kcal/mol] -0.39
7000 ElectronicLevels[1/cm] 1
7001 0.0000000000000000 2.0000000000000000
7002 End
7003 !*****
7004 RRHO ! 8
7005 Geometry[angstrom] 17
7006 C 1.36951000 -0.00000900 -0.68115300
7007 C 0.67326300 1.21128700 -0.52286500
7008 C -0.66703700 1.20617000 -0.16180400
7009 C -1.35908900 0.00001000 0.01758400
7010 C -0.66706200 -1.20616500 -0.16180300
7011 C 0.67323800 -1.21129500 -0.52285800
7012 H 2.36761700 -0.00002000 -1.09583300
7013 H 1.19831000 2.14836400 -0.66106600
7014 H -1.19403200 2.14570200 -0.03359700
7015 H -1.19406800 -2.14569000 -0.03359800
7016 H 1.19827800 -2.14837800 -0.66105500
7017 C -2.80981500 0.00000600 0.42237200
7018 H -2.90822400 -0.00020700 1.51248300
7019 H -3.32462900 0.88554800 0.04526400
7020 H -3.32471400 -0.88534100 0.04491700
7021 O 2.43861000 -0.00000300 1.15441600
7022 H 1.66317700 0.00001700 1.73732800
7023 Core RigidRotor
7024 SymmetryFactor 0.843552272
7025 End
7026 Rotor Hindered
7027 Group 13 14 15
7028 Axis 12 4
7029 Symmetry 3
7030 Potential[kcal/mol] 12
7031 0.000 0.004 0.005 0.003 0.002 -0.001 0.001 -0.001 0.002 0.003 0.005 0.003
7032 End
7033 Rotor Hindered
7034 Group 17

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```

7035 Axis 16 1
7036 Symmetry 1
7037 Potential[kcal/mol] 36
7038 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
7039 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
7040 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
7041 End
7042 Frequencies[1/cm] 42
7043 110.17 167.90 216.06 342.54 401.66 446.98 525.54 630.18
7044 655.26 706.07 781.49 803.20 846.50 928.83 970.57 968.57
7045 968.83 986.33 1002.98 1022.18 1070.08 1139.26 1161.90 1198.42
7046 1281.70 1309.80 1369.14 1420.33 1442.62 1452.22 1461.75 1554.51
7047 1584.52 2928.66 2988.59 3014.12 3060.46 3060.57 3086.03 3089.32
7048 3108.13 3625.80
7049 ZeroEnergy[kcal/mol] -0.08
7050 ElectronicLevels[1/cm] 1
7051 0.0000000000000000 2.0000000000000000
7052 End
7053 !*****
7054 RRHO ! 9
7055 Geometry[angstrom] 17
7056 C 1.38277300 -0.00000400 -0.65103500
7057 C 0.67491900 1.21297000 -0.51525200
7058 C -0.66547600 1.20678200 -0.16341600
7059 C -1.35809900 0.00000500 0.01730300
7060 C -0.66548700 -1.20678000 -0.16341800
7061 C 0.67490600 -1.21297400 -0.51524700
7062 H 2.36761600 -0.00001100 -1.09599000
7063 H 1.19921700 2.14997900 -0.65624000
7064 H -1.19476900 2.14595800 -0.04261800
7065 H -1.19478800 -2.14595300 -0.04262100
7066 H 1.19920000 -2.14998500 -0.65623300
7067 C -2.80847600 0.00000500 0.42132400
7068 H -2.90631800 -0.00020900 1.51163100
7069 H -3.32332500 0.88583900 0.04489500
7070 H -3.32341500 -0.88563100 0.04454600
7071 O 2.42193800 -0.00000400 1.12522500
7072 H 1.66035700 0.00001700 1.72514200
7073 Core RigidRotor
7074 SymmetryFactor 0.843552272
7075 End
7076 Rotor Hindered
7077 Group 13 14 15
7078 Axis 12 4
7079 Symmetry 3

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7080 Potential[kcal/mol]          12
7081 0.000 0.004 0.005 0.003 0.002 -0.001 0.001 -0.001 0.002 0.003 0.006 0.003
7082 End
7083 Rotor                        Hindered
7084 Group      17
7085 Axis              16              1
7086 Symmetry              1
7087 Potential[kcal/mol]          36
7088 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
7089 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
7090 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
7091 End
7092 Frequencies[1/cm]          42
7093 121.14 168.61 220.42 342.58 404.05 446.67 525.91 628.61
7094 678.33 746.47 792.54 802.72 845.74 942.51 977.73 966.01
7095 968.15 993.88 1007.02 1021.80 1068.52 1137.70 1162.42 1199.51
7096 1274.53 1310.02 1368.83 1420.94 1442.30 1451.43 1458.03 1545.63
7097 1582.15 2927.83 2987.80 3014.20 3061.01 3061.21 3086.96 3090.26
7098 3107.83 3630.52
7099 ZeroEnergy[kcal/mol]    0.38
7100 ElectronicLevels[1/cm]          1
7101 0.000000000000000000 2.0000000000000000
7102 End
7103 !*****
7104 RRHO          !          10
7105 Geometry[angstrom]      17
7106 C              1.39846073 -0.00000400 -0.61907474
7107 C              0.67558273  1.21567800 -0.50938874
7108 C             -0.66381827  1.20791700 -0.16517974
7109 C             -1.35773527  0.00000500  0.01751126
7110 C             -0.66382927 -1.20791500 -0.16518174
7111 C              0.67556973 -1.21568100 -0.50938274
7112 H              2.36516573 -0.00001100 -1.10150174
7113 H              1.19902173  2.15259400 -0.65342174
7114 H             -1.19542727  2.14660700 -0.05119674
7115 H             -1.19544527 -2.14660200 -0.05119974
7116 H              1.19900473 -2.15260000 -0.65341374
7117 C             -2.80757227  0.00000500  0.42076326
7118 H             -2.90527027 -0.00020900  1.51130526
7119 H             -3.32245627  0.88608800  0.04486426
7120 H             -3.32254627 -0.88588100  0.04451626
7121 O              2.40602473 -0.00000400  1.09727826
7122 H              1.65709673  0.00001800  1.71209826
7123 Core RigidRotor
7124 SymmetryFactor    0.843552272

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7125 End
7126 Rotor Hindered
7127 Group 13 14 15
7128 Axis 12 4
7129 Symmetry 3
7130 Potential[kcal/mol] 12
7131 0.000 -0.001 0.003 0.000 0.000 0.000 -0.002 0.000 0.000 0.000 0.003 -0.001
7132 End
7133 Rotor Hindered
7134 Group 17
7135 Axis 16 1
7136 Symmetry 1
7137 Potential[kcal/mol] 36
7138 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
7139 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
7140 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
7141 End
7142 Frequencies[1/cm] 42
7143 124.27 178.82 225.52 342.59 406.19 439.05 525.75 625.88
7144 679.88 778.53 800.70 819.49 840.98 956.17 981.43 994.32
7145 966.81 991.04 1014.91 1020.64 1064.60 1135.68 1161.96 1200.61
7146 1264.52 1309.93 1368.41 1421.12 1441.78 1449.50 1452.26 1530.50
7147 1575.76 2926.42 2986.45 3014.07 3061.45 3061.74 3088.31 3091.39
7148 3108.36 3633.75
7149 ZeroEnergy[kcal/mol] -0.06
7150 ElectronicLevels[1/cm] 1
7151 0.0000000000000000 2.0000000000000000
7152 End
7153 !*****
7154 RRHO ! 11
7155 Geometry[angstrom] 17
7156 C 1.41414900 -0.00000400 -0.58711400
7157 C 0.67624700 1.21838600 -0.50352500
7158 C -0.66216100 1.20905200 -0.16694300
7159 C -1.35737100 0.00000500 0.01772000
7160 C -0.66217100 -1.20905000 -0.16694500
7161 C 0.67623400 -1.21838800 -0.50351900
7162 H 2.36271600 -0.00001100 -1.10701300
7163 H 1.19882600 2.15520900 -0.65060300
7164 H -1.19608500 2.14725600 -0.05977500
7165 H -1.19610300 -2.14725100 -0.05977800
7166 H 1.19881000 -2.15521500 -0.65059400
7167 C -2.80666800 0.00000500 0.42020200
7168 H -2.90422200 -0.00020900 1.51097900
7169 H -3.32158800 0.88633700 0.04483400

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7170 H -3.32167700 -0.88613100 0.04448600
7171 O 2.39011200 -0.00000400 1.06933100
7172 H 1.65383600 0.00001900 1.69905400
7173 Core RigidRotor
7174 SymmetryFactor 0.843552272
7175 End
7176 Rotor Hindered
7177 Group 13 14 15
7178 Axis 12 4
7179 Symmetry 3
7180 Potential[kcal/mol] 12
7181 0.000 -0.001 0.003 -0.001 0.000 0.000 -0.002 0.000 -0.001 0.000 0.002 -0.001
7182 End
7183 Rotor Hindered
7184 Group 17
7185 Axis 16 1
7186 Symmetry 1
7187 Potential[kcal/mol] 36
7188 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
7189 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
7190 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
7191 End
7192 Frequencies[1/cm] 42
7193 159.71 206.37 231.78 342.61 408.31 429.10 525.44 622.72
7194 673.39 784.08 798.47 831.70 866.03 965.77 981.29 993.73
7195 965.25 989.40 1016.41 1033.76 1059.42 1135.66 1160.83 1201.52
7196 1256.11 1310.54 1367.77 1421.14 1441.02 1446.79 1446.96 1515.72
7197 1567.74 2924.72 2984.89 3013.84 3061.41 3061.74 3083.75 3092.18
7198 3099.05 3631.79
7199 ZeroEnergy[kcal/mol] -0.74
7200 ElectronicLevels[1/cm] 1
7201 0.0000000000000000 2.0000000000000000
7202 End
7203 !*****
7204 RRHO ! 12
7205 Geometry[angstrom] 17
7206 C 1.43163600 -0.00000500 -0.55414400
7207 C 0.67605600 1.22197700 -0.49907800
7208 C -0.66035600 1.21063900 -0.16871200
7209 C -1.35758900 0.00000600 0.01822900
7210 C -0.66036400 -1.21063400 -0.16871400
7211 C 0.67604600 -1.22198200 -0.49907500
7212 H 2.35806400 -0.00001000 -1.11673200
7213 H 1.19786700 2.15869100 -0.64875900
7214 H -1.19661400 2.14824800 -0.06788800

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7260  C          -0.65834300  -1.21230500  -0.17055700
7261  C           0.67526600  -1.22592300  -0.49535200
7262  H           2.35122700  -0.00000900  -1.12593200
7263  H           1.19643600   2.16258200  -0.64721500
7264  H          -1.19708500   2.14926500  -0.07607600
7265  H          -1.19710000  -2.14925600  -0.07607900
7266  H           1.19642000  -2.16259200  -0.64720800
7267  C          -2.80564500   0.00000500   0.41992900
7268  H          -2.90461200  -0.00020700   1.51127300
7269  H          -3.32082700   0.88665100   0.57600
7270  H          -3.32091700  -0.88644600   0.04483200
7271  O           2.36045800  -0.00000400   1.01665000
7272  H           1.64456200   0.00001600   1.66833000
7273  Core  RigidRotor
7274          SymmetryFactor    0.843552272
7275  End
7276  Rotor                Hindered
7277  Group    13 14 15
7278  Axis           12           4
7279  Symmetry           3
7280  Potential[kcal/mol]           12
7281  0.000 -0.001 0.003 0.000 0.000 0.000 -0.002 0.000 0.000 0.000 0.003 -0.001
7282  End
7283  Rotor                Hindered
7284  Group    17
7285  Axis           16           1
7286  Symmetry           1
7287  Potential[kcal/mol]           36
7288  0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
7289  2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
7290  2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
7291  End
7292  Frequencies[1/cm]           42
7293  222.77 241.16 246.77 342.39 409.38 416.33 525.00 613.69
7294  661.43 778.03 789.52 802.16 912.64 966.78 977.24 997.41
7295  968.66 1004.94 1011.39 1043.99 1117.54 1135.88 1159.87 1205.11
7296  1237.64 1310.85 1366.81 1417.61 1434.89 1434.91 1439.98 1487.63
7297  1558.42 2918.73 2979.59 3012.00 3046.67 3059.85 3060.93 3092.58
7298  3094.55 3635.66
7299  ZeroEnergy[kcal/mol]    -5.01
7300  ElectronicLevels[1/cm]                1
7301  0.000000000000000000    2.0000000000000000
7302  End
7303  !*****
7304  RRHO          !           14

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7305 Geometry[angstrom]          17
7306 C          1.46813400 -0.00000500 -0.48732300
7307 C          0.67509500  1.22949500 -0.49140500
7308 C         -0.65650000  1.21392800 -0.17244200
7309 C         -1.35895700  0.00000700  0.01964900
7310 C         -0.65650900 -1.21392400 -0.17244300
7311 C          0.67508400 -1.22950000 -0.49140100
7312 H          2.34381400 -0.00001000 -1.13105500
7313 H          1.19476400  2.16667700 -0.64605100
7314 H         -1.19785000  2.15029300 -0.08517000
7315 H         -1.19786600 -2.15028500 -0.08517300
7316 H          1.19474800 -2.16668600 -0.64604500
7317 C         -2.80534000  0.00000400  0.42000900
7318 H         -2.90589700 -0.00020700  1.51158300
7319 H         -3.32075800  0.88669700  0.04530400
7320 H         -3.32084700 -0.88649400  0.04496100
7321 O          2.34588200 -0.00000400  0.99027000
7322 H          1.63921900  0.00001600  1.65147100
7323   Core   RigidRotor
7324           SymmetryFactor    0.843552272
7325 End
7326   Rotor                               Hindered
7327   Group   13 14 15
7328   Axis           12           4
7329   Symmetry           3
7330   Potential[kcal/mol]           12
7331   0.000 -0.001 0.003 0.000 0.000 0.000 -0.002 0.000 0.000 0.000 0.003 -0.001
7332 End
7333   Rotor                               Hindered
7334   Group   17
7335   Axis           16           1
7336   Symmetry           1
7337   Potential[kcal/mol]           36
7338   0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
7339   2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
7340   2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
7341 End
7342   Frequencies[1/cm]           42
7343   240.81 241.86 272.22 342.46 405.42 423.20 525.11 609.51
7344   659.64 775.24 786.32 788.51 913.21 966.65 975.31 994.21
7345   968.53 1005.14 1035.68 1037.78 1135.32 1148.39 1179.27 1208.23
7346   1229.91 1309.61 1366.78 1407.27 1429.99 1431.66 1439.16 1482.03
7347   1560.59 2915.28 2976.52 3010.40 3031.53 3057.62 3058.65 3090.66
7348   3092.50 3637.82
7349 ZeroEnergy[kcal/mol] -8.08

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7350 ElectronicLevels[1/cm] 1
7351 0.0000000000000000 2.0000000000000000
7352 End
7353 !*****
7354 RRHO ! 15
7355 Geometry[angstrom] 17
7356 C 1.48513800 -0.00000500 -0.45466000
7357 C 0.67596900 1.23243300 -0.48657400
7358 C -0.65496800 1.21536700 -0.17440900
7359 C -1.35930800 0.00000700 0.02037800
7360 C -0.65497700 -1.21536200 -0.17441000
7361 C 0.67595900 -1.23243900 -0.48657000
7362 H 2.33655400 -0.00001000 -1.13210500
7363 H 1.19332000 2.17061000 -0.64496100
7364 H -1.19899300 2.15120500 -0.09580600
7365 H -1.19901000 -2.15119600 -0.09580900
7366 H 1.19330300 -2.17062000 -0.64495500
7367 C -2.80513600 0.00000500 0.42016000
7368 H -2.90747900 -0.00020700 1.51183700
7369 H -3.32073500 0.88668800 0.04531700
7370 H -3.32082400 -0.88648500 0.04497500
7371 O 2.33079800 -0.00000400 0.96311900
7372 H 1.63454600 0.00001500 1.63464800
7373 Core RigidRotor
7374 SymmetryFactor 0.843552272
7375 End
7376 Rotor Hindered
7377 Group 13 14 15
7378 Axis 12 4
7379 Symmetry 3
7380 Potential[kcal/mol] 12
7381 0.000 -0.001 0.003 0.000 0.000 0.000 -0.002 0.000 0.000 0.000 0.003 -0.001
7382 End
7383 Rotor Hindered
7384 Group 17
7385 Axis 16 1
7386 Symmetry 1
7387 Potential[kcal/mol] 36
7388 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
7389 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
7390 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
7391 End
7392 Frequencies[1/cm] 42
7393 254.29 256.52 296.85 343.09 409.31 431.84 525.40 606.12
7394 660.35 772.36 777.89 786.30 907.32 966.25 973.47 991.29

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7395      966.97  1003.03 1028.05 1074.89 1134.55 1151.30 1203.98 1223.60
7396      1230.96 1307.55 1366.84 1394.01 1425.39 1431.35 1438.52 1479.80
7397      1562.44 2912.61 2974.05 3008.87 3016.51 3054.96 3055.99 3087.37
7398      3089.19 3640.99
7399      ZeroEnergy[kcal/mol]   -10.94
7400      ElectronicLevels[1/cm]                               1
7401      0.000000000000000000      2.0000000000000000
7402      End
7403      !*****
7404      RRHO      !      16
7405      Geometry[angstrom]      17
7406      C      1.50088600  -0.00000500  -0.42315400
7407      C      0.67773300   1.23484800  -0.48047500
7408      C      -0.65355500   1.21658200  -0.17654800
7409      C      -1.35926000   0.00000700   0.02102300
7410      C      -0.65356300  -1.21657700  -0.17654900
7411      C      0.67772300  -1.23485400  -0.48047100
7412      H      2.32929500  -0.00001000  -1.13078200
7413      H      1.19267100   2.17397700  -0.64330300
7414      H      -1.20039500   2.15182800  -0.10805000
7415      H      -1.20041200  -2.15181800  -0.10805200
7416      H      1.19265400  -2.17398600  -0.64329700
7417      C      -2.80494500   0.00000400   0.42030800
7418      H      -2.90900800  -0.00020700   1.51199500
7419      H      -3.32063400   0.88666000   0.04521400
7420      H      -3.32072200  -0.88645700   0.04487200
7421      O      2.31499100  -0.00000500   0.93515000
7422      H      1.63210800   0.00001400   1.61954100
7423      Core      RigidRotor
7424      SymmetryFactor      0.843552272
7425      End
7426      Rotor      Hindered
7427      Group      13 14 15
7428      Axis      12      4
7429      Symmetry      3
7430      Potential[kcal/mol]      12
7431      0.000 -0.001 0.003 0.000 0.000 0.000 -0.002 0.000 0.000 0.000 0.003 -0.001
7432      End
7433      Rotor      Hindered
7434      Group      17
7435      Axis      16      1
7436      Symmetry      1
7437      Potential[kcal/mol]      36
7438      0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
7439      2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421

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7440 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
7441 End
7442 Frequencies[1/cm] 42
7443 260.81 314.54 340.87 380.46 435.91 479.11 523.81 595.57
7444 659.32 759.53 759.88 781.63 887.15 953.48 959.27 976.22
7445 964.82 1001.34 1021.20 1113.37 1133.65 1151.24 1205.85 1218.71
7446 1276.06 1305.11 1366.82 1382.14 1421.42 1431.61 1437.99 1478.78
7447 1563.16 2910.73 2972.16 2999.08 3007.56 3052.25 3053.29 3083.79
7448 3085.64 3644.71
7449 ZeroEnergy[kcal/mol] -13.64
7450 ElectronicLevels[1/cm] 1
7451 0.0000000000000000 2.0000000000000000
7452 End
7453 !*****
7454 RRHO ! 17
7455 Geometry[angstrom] 17
7456 C 1.51465000 -0.00000500 -0.39353600
7457 C 0.68031800 1.23709300 -0.47227700
7458 C -0.65206800 1.21769700 -0.17908500
7459 C -1.35875100 0.00000700 0.02144200
7460 C -0.65207500 -1.21769200 -0.17908700
7461 C 0.68030800 -1.23709800 -0.47227300
7462 H 2.32117800 -0.00001000 -1.12805000
7463 H 1.19332200 2.17685600 -0.63976100
7464 H -1.20209300 2.15216300 -0.12256000
7465 H -1.20210900 -2.15215300 -0.12256300
7466 H 1.19330500 -2.17686600 -0.63975500
7467 C -2.80459000 0.00000400 0.42034500
7468 H -2.91027500 -0.00020600 1.51200100
7469 H -3.32032900 0.88663500 0.04497300
7470 H -3.32041700 -0.88643300 0.04463200
7471 O 2.29863500 -0.00000500 0.90627300
7472 H 1.63138100 0.00001200 1.60465000
7473 Core RigidRotor
7474 SymmetryFactor 0.843552272
7475 End
7476 Rotor Hindered
7477 Group 13 14 15
7478 Axis 12 4
7479 Symmetry 3
7480 Potential[kcal/mol] 12
7481 0.000 -0.002 0.002 0.000 -0.001 0.000 -0.002 0.000 -0.001 -0.001 0.002 -0.001
7482 End
7483 Rotor Hindered
7484 Group 17

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7485 Axis 16 3
7486 Symmetry 1
7487 Potential[kcal/mol] 36
7488 0.000 0.091 0.413 0.936 1.597 2.310 2.980 3.516 3.818 3.872 3.717 3.443
7489 3.131 2.854 2.658 2.557 2.535 2.556 2.585 2.584 2.537 2.451 2.347 2.258
7490 2.211 2.217 2.269 2.339 2.380 2.331 2.151 1.831 1.394 0.904 0.452 0.131
7491 End
7492 Frequencies[1/cm] 42
7493 267.76 329.58 350.49 394.80 451.23 518.12 600.34 613.96
7494 711.80 763.46 766.66 817.52 890.33 965.20 969.58 986.37
7495 962.33 1000.01 1015.09 1132.50 1146.11 1154.04 1205.81 1215.41
7496 1302.40 1317.94 1366.76 1372.61 1418.24 1432.11 1437.52 1478.58
7497 1563.69 2909.31 2970.57 2981.77 3006.34 3049.25 3050.30 3080.20
7498 3082.08 3652.88
7499 ZeroEnergy[kcal/mol] -15.68
7500 ElectronicLevels[1/cm] 1
7501 0.0000000000000000 2.0000000000000000
7502 End
7503 !*****
7504 RRHO ! 18
7505 Geometry[angstrom] 17
7506 C 1.52228100 -0.00000500 -0.37025000
7507 C 0.68431000 1.24013700 -0.45793400
7508 C -0.65060200 1.21924600 -0.18261200
7509 C -1.35731300 0.00000800 0.02028500
7510 C -0.65061000 -1.21924000 -0.18261300
7511 C 0.68430100 -1.24014200 -0.45792900
7512 H 2.30828300 -0.00001000 -1.12915700
7513 H 1.19779200 2.17954000 -0.62754600
7514 H -1.20508800 2.15237600 -0.14197300
7515 H -1.20510400 -2.15236500 -0.14197600
7516 H 1.19777600 -2.17955000 -0.62753900
7517 C -2.80333700 0.00000400 0.41956600
7518 H -2.91004700 -0.00020500 1.51121300
7519 H -3.31935400 0.88662700 0.04425700
7520 H -3.31944100 -0.88642700 0.04391800
7521 O 2.28311100 -0.00000500 0.87613200
7522 H 1.63264900 0.00000900 1.58892000
7523 Core RigidRotor
7524 SymmetryFactor 0.843552272
7525 End
7526 Rotor Hindered
7527 Group 13 14 15
7528 Axis 12 4
7529 Symmetry 3

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7530 Potential[kcal/mol]          12
7531 0.000 -0.001 0.003 0.000 0.000 0.000 -0.002 0.000 0.000 0.000 0.003 -0.001
7532 End
7533 Rotor                        Hindered
7534 Group      17
7535 Axis                16                1
7536 Symmetry                1
7537 Potential[kcal/mol]          36
7538 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
7539 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
7540 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
7541 End
7542   Frequencies[1/cm]          42
7543   266.74  333.14  358.49  397.52  459.99  515.24  597.96  636.48
7544   753.53  760.40  769.25  870.61  936.84  965.37  967.88  985.25
7545   961.14  998.93 1012.17 1131.46 1148.72 1181.49 1205.08 1215.14
7546   1301.06 1351.11 1366.77 1368.14 1416.68 1433.04 1437.07 1479.84
7547   1565.07 2908.21 2961.04 2969.09 3005.10 3045.13 3046.24 3077.59
7548   3079.46 3660.77
7549 ZeroEnergy[kcal/mol]    -16.56
7550 ElectronicLevels[1/cm]                1
7551 0.000000000000000000    2.0000000000000000
7552 End
7553 !*****
7554   Tunneling   Eckart
7555   ImaginaryFrequency[1/cm]    427.07
7556   WellDepth[kcal/mol]        3.80
7557   WellDepth[kcal/mol]        17.23
7558 End
7559 End
7560 End
7561
7562

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