

## Supplementary Material

Cartesian Coordinates and Frequencies of Optimized Stationary Structures of The Reaction of Hydroxyl Radical (OH) with Propene (C<sub>3</sub>H<sub>6</sub>) at The B3LYP/cc-pVTZ Level of Theory

Cartesian Coordinates, Å				Frequencies, cm <sup>-1</sup>		
<b>R (OH)</b>						
O	0.00000000	0.00000000	0.10829200	3698		
H	0.00000000	0.00000000	-0.86633400			
<b>R (CH<sub>3</sub>CH=CH<sub>2</sub>)</b>						
C	1.27786800	0.21987300	0.00000400	206	425	593
C	0.13407900	-0.45226600	0.00000300	924	948	950
H	1.29878900	1.30342900	-0.00001600	1030	1075	1193
H	2.23356700	-0.28672700	-0.00001100	1331	1410	1452
H	0.16671100	-1.53813400	-0.00001200	1479	1495	1712
C	-1.23058900	0.16195500	-0.00000300	3014	3055	3091
H	-1.80381700	-0.15348000	-0.87590700	3123	3130	3211
H	-1.80373000	-0.15330000	0.87602600			
H	-1.17966500	1.25083900	-0.00010800			
<b>Complex C</b>						
C	-0.61880100	1.33440400	-0.21215800	53	77	118
C	-0.82827700	0.20339400	0.45527500	212	287	385
H	-0.40518200	2.26356200	0.29925400	424	609	923
H	-0.67421400	1.37294700	-1.29406000	952	958	1038
C	-1.13806300	-1.12435400	-0.16095200	1081	1195	1332
H	-2.08567700	-1.51537500	0.21754200	1413	1452	1481
H	-1.20326800	-1.05861900	-1.24700200	1495	1701	3020
H	-0.36868900	-1.85730300	0.09389300	3066	3095	3124
H	-0.77224300	0.22197900	1.54008400	3129	3210	3600
O	2.43052800	-0.26483000	-0.00532100			
H	1.57589700	0.21078700	-0.06013200			
<b>I1</b>						
C	1.09482200	-0.95012600	-0.11144700	158	241	326
C	0.04833900	-0.00756500	0.36170400	337	410	476
H	1.42811500	-1.77512400	0.50181800	566	833	921
H	1.43546700	-0.89057700	-1.13657600	958	1020	1126
C	-1.35605000	-0.38372700	-0.11500900	1153	1275	1367
H	-2.07418600	0.35563800	0.24139200	1373	1395	1451
H	-1.38804300	-0.40388000	-1.20429100	1484	1495	2958
H	-1.64270000	-1.36448900	0.26359700	3033	3102	3110
H	0.04353500	0.00177500	1.45998300	3135	3242	3805
O	0.28492500	1.32136700	-0.12704800			
H	1.19575100	1.55423300	0.07896800			
<b>I2</b>						
				192	235	356
C	-1.28490600	-0.62688400	0.07763200	394	450	802
H	-1.31489100	-1.60736300	-0.39889400	887	913	977
H	-2.15897000	-0.05598200	-0.23137500	1040	1066	1155
H	-1.33165500	-0.77143700	1.15793300	1199	1245	1386
C	0.00000000	0.12541600	-0.29221500	1408	1480	1485
H	0.00000000	0.26523600	-1.39582800	1495	1504	2821

	C	1.28490600	-0.62688400	0.07763200	3030	3036	3095
	H	1.31489000	-1.60736300	-0.39889300	3101	3114	3115
	H	2.15897000	-0.05598200	-0.23137500			
	H	1.33165500	-0.77143700	1.15793300			
	O	0.00000000	1.42180500	0.14527500			
<b>I3</b>							
	C	-1.36252700	-0.53764100	0.02570800	167		325
	H	-1.44983700	-1.53697400	-0.40049800	359	183	431
	H	-2.13055900	0.09720200	-0.41806400	791	374	979
	H	-1.58888300	-0.61526000	1.10120000	1009	955	1139
	C	-0.00930600	0.02538600	-0.21955900	1300	1089	1410
	C	1.22492500	-0.77075800	0.03151800	1421	1377	1476
	H	1.12587900	-1.77942000	-0.36925000	1484	1464	2912
	H	2.10127000	-0.31417900	-0.43900100	2927	1493	3054
	H	1.44832200	-0.86435700	1.10734600	3091	3019	3812
	O	0.05195800	1.37858300	0.05473500		3102	
	H	0.95959100	1.68240700	-0.04562200			
<b>I4</b>							
	C	-0.78408000	0.57845400	0.23454900	91	112	271
	C	0.61660700	0.62449600	-0.26440900	329	399	564
	H	-1.35724400	1.42423700	-0.15984200	868	909	973
	H	-0.81720900	0.65323100	1.32911600	1000	1109	1139
	C	1.60047200	-0.43239700	0.08960500	1206	1355	1380
	H	2.37422900	-0.54192300	-0.67243700	1395	1410	1480
	H	2.12143400	-0.19754500	1.03011700	1482	1493	2944
	H	1.11045700	-1.39628400	0.23065900	2971	3007	3045
	H	0.96638800	1.53513000	-0.73454300	3093	3162	3796
	O	-1.44921400	-0.66190100	-0.04782500			
	H	-1.40234000	-0.80496400	-0.99894000			
<b>I5</b>							
	C	-0.84936600	0.43875700	0.26417600	134	214	300
	C	0.57052400	0.65838100	-0.25786500	456	500	786
	H	-1.49234900	1.32151400	0.10189800	862	972	990
	H	-0.84139000	0.32860300	1.36897500	1080	1101	1210
	C	1.52104000	-0.47879500	0.10651000	1289	1337	1346
	H	2.50734800	-0.32703800	-0.33224800	1382	1418	1484
	H	1.64686000	-0.55675000	1.18875200	1499	1508	2852
	H	1.13323200	-1.43150200	-0.25413500	2909	3020	3026
	H	0.93905400	1.60891800	0.13870400	3051	3087	3102
	O	-1.48319600	-0.67823100	-0.19317000			
	H	0.51961200	0.77203700	-1.34350700			
<b>I6</b>							
	C	-0.73085100	0.52331700	0.30179600	120	161	287
	C	0.68296100	0.61004300	-0.28415500	359	454	549
	H	-1.30319700	1.40914400	0.02658000	826	860	905
	H	-0.67154700	0.49390100	1.39770000	1042	1080	1131
	C	1.55909100	-0.51628700	0.13174500	1193	1243	1356
	H	2.23244800	-0.99988600	-0.56026600	1376	1419	1455
	H	1.63401700	-0.78850100	1.17720700	1470	1513	2928
	H	1.11477300	1.56782300	0.04796500	2971	3056	3077
	O	-1.46776000	-0.58375800	-0.19618400	3131	3235	3791
	H	0.61396100	0.66369200	-1.37233300			
	H	-0.94558400	-1.37854400	-0.04369600			
<b>I7</b>							
	C	-0.75584700	0.53627200	0.27743500	111	223	277
	C	0.61110700	0.62518400	-0.29346100	370	477	589

H	-0.96394800	0.85554500	1.29394200	783	877	986
C	1.55675000	-0.51285800	0.14227200	1050	1088	1204
H	2.53306500	-0.41306400	-0.33553800	1245	1322	1337
H	1.70690300	-0.50442100	1.22310900	1396	1448	1471
H	1.14031500	-1.48173000	-0.13246100	1496	1506	3009
H	1.04122300	1.58751500	-0.00703900	3024	3052	3084
O	-1.51505900	-0.50184100	-0.21040000	3102	3121	3833
H	-2.34689300	-0.54550100	0.26924500			
H	0.53774700	0.62479700	-1.38553200			
<b>TS_C-II/-I4</b>						
C	0.29646300	1.26177300	-0.21154000	-74	144	175
C	-0.43369100	0.35880300	0.46459400	209	234	425
H	0.98130000	1.92866900	0.29380200	598	608	923
H	0.22420400	1.35178900	-1.28664600	938	954	991
C	-1.45066500	-0.54762600	-0.14153800	1064	1201	1324
H	-2.45033900	-0.30006300	0.22643600	1407	1449	1478
H	-1.45331200	-0.47465100	-1.22813000	1493	1653	3023
H	-1.24751600	-1.58226300	0.13535300	3080	3110	3141
H	-0.33457200	0.31355200	1.54380800	3148	3231	3746
O	1.46670200	-0.89543500	-0.11164900			
H	2.07397800	-0.51126000	0.53947400			
<b>TS_I1-I2</b>						
C	1.01554100	-0.87521800	-0.08524100	-1971	233	334
C	-0.07989500	0.01089200	0.43184100	355	456	691
H	1.75771600	-1.24304800	0.61155000	843	884	926
H	0.80505900	-1.48802500	-0.95391200	979	1070	1083
C	-1.47272400	-0.18345100	-0.12649800	1142	1190	1283
H	-2.10439500	0.66982800	0.12119100	1388	1413	1433
H	-1.43945300	-0.27893600	-1.21216200	1484	1496	1927
H	-1.93450400	-1.08015000	0.29112600	3030	3036	3094
H	-0.09879900	0.09320200	1.52044000	3103	3111	3219
O	0.59852200	1.16149300	-0.14501800			
H	1.44866500	0.32185400	-0.53869600			
<b>TS_I1-I3</b>						
C	-1.06611200	-0.99722700	0.06458800	-1878	216	245
C	-0.01887300	0.02073900	-0.17984100	352	397	429
H	-0.79830000	-1.97286800	0.44273400	461	673	809
H	-2.09680500	-0.67677500	0.09505300	933	1008	1054
C	1.41833300	-0.31153600	0.05774700	1166	1271	1312
H	2.06903300	0.41059400	-0.43448700	1373	1422	1425
H	1.64301300	-0.28980300	1.13321800	1477	1490	2117
H	1.65852800	-1.30679500	-0.31587100	2961	3068	3108
H	-0.58931400	-0.68210300	-1.12449000	3135	3252	3695
O	-0.35118800	1.35383800	-0.00975400			
H	-1.07674500	1.41519800	0.62691600			
<b>TS_I2-I3</b>						
C	1.29158900	-0.65916100	0.02869900	-1947	162	196
H	1.30826900	-1.60108700	-0.52032600	363	421	437
H	1.41554600	-0.89112400	1.09385700	710	788	941
H	2.13933700	-0.04864200	-0.27696600	972	1004	1112
C	0.00000000	0.07686300	-0.17611700	1236	1247	1399
H	0.00000000	1.04405300	-1.00452300	1410	1467	1473
C	-1.29159000	-0.65916100	0.02869900	1484	1491	2355
H	-1.41554600	-0.89112400	1.09385700	2987	2992	3070
H	-2.13933700	-0.04864200	-0.27696700	3074	3115	3117
H	-1.30826900	-1.60108700	-0.52032500			

O	0.00000000	1.43580000	0.14046300			
<b>TS_I4-I5</b>						
C	0.80532300	0.67003100	-0.14159600	-1939	165	209
C	-0.39614400	0.07528100	0.53655000	371	652	746
H	1.35493900	1.41616100	0.43348500	878	937	966
H	0.62991900	1.03170700	-1.15669400	1058	1115	1136
C	-1.67346700	-0.12549100	-0.22791200	1150	1192	1304
H	-2.33769200	-0.83020100	0.27092300	1360	1411	1484
H	-2.21281800	0.82242500	-0.33015400	1489	1527	1920
H	-1.47364400	-0.49595400	-1.23396800	3002	3027	3068
H	-0.47469500	0.27248900	1.60145700	3072	3101	3129
O	1.46237300	-0.61593000	-0.13043100			
H	0.40073900	-1.00811100	0.45614600			
<b>TS_I4-I6</b>						
C	-0.72616100	0.50950400	0.32932800	-1876	122	263
C	0.61733300	0.53238700	-0.31645700	301	379	511
H	-1.25932600	1.44324000	0.15779200	712	766	885
H	-0.62094800	0.38102600	1.41429800	897	979	1111
C	1.66709200	-0.44102100	0.10731400	1168	1229	1250
H	2.48137600	-0.68014200	-0.55790400	1340	1379	1415
H	1.48608900	-1.07642700	0.96177300	1434	1504	2202
H	1.63483900	0.81453200	0.42924800	2974	3088	3145
O	-1.58540900	-0.51202100	-0.20589700	3172	3258	3806
H	0.71803400	0.95488200	-1.30675900			
H	-1.10637300	-1.34616700	-0.17238300			
<b>TS_I4-I7</b>						
C	-0.83990900	0.58201700	0.06932600	-1958	113	184
C	0.63395100	0.71018900	-0.08765800	197	262	544
H	-1.44681800	1.42816000	-0.22917400	651	807	868
H	-0.02862100	0.95899700	1.02337300	997	1059	1102
C	1.53120400	-0.48521400	0.03292200	1205	1273	1296
H	1.58587700	-1.07496200	-0.89202000	1350	1408	1422
H	2.55232400	-0.18629100	0.27160500	1481	1508	2129
H	1.19472100	-1.16243100	0.82252800	2956	3032	3080
H	0.99239700	1.58482400	-0.61664000	3131	3147	3751
O	-1.48408200	-0.64028400	0.00116600			
H	-0.92869700	-1.26797800	-0.47654000			
<b>TS_I5-I6</b>						
C	-0.86527800	0.53776400	0.19201200	-1874	213	424
C	0.59474700	0.81479500	-0.17915800	586	613	846
H	-1.58338000	1.14968400	-0.35929300	891	911	977
H	-1.03184200	0.69230600	1.26534700	1025	1086	1158
C	1.24460700	-0.53553300	0.11557600	1176	1221	1240
H	2.00334100	-0.90319900	-0.56781500	1327	1364	1459
H	1.47926100	-0.73516900	1.15853000	1491	1519	1742
H	0.14037200	-1.18203600	-0.08867500	2974	3037	3044
H	1.04116500	1.64599100	0.37011200	3079	3087	3166
O	-1.07069600	-0.82558600	-0.16309000			
H	0.67219600	1.03495700	-1.24406700			
<b>TS_I5-I7</b>					110	217
C	-0.75669200	0.41573000	0.34574500	-1978	471	643
C	0.58576000	0.63940500	-0.27773100	305	884	911
H	-0.86860700	0.61336000	1.41455100	786	1063	1142
C	1.57233700	-0.47990600	0.09571600	982	1285	1332
H	2.53699300	-0.32109600	-0.38706100	1170	1409	1476
H	1.73768400	-0.51753000	1.17356300	1379	1506	2388

H	1.18680600	-1.44845600	-0.22214700	1498	3031	3040
H	0.97553900	1.60626400	0.04986000	3028	3093	3104
O	-1.57590400	-0.58130800	-0.16957900	3067		
H	-1.84363800	0.58791900	-0.29149200			
H	0.47401800	0.67862300	-1.36302700			
<b>TS_I6-I7</b>						
C	-0.51322700	-0.21407700	0.39715800	-2083	114	365
C	0.62960900	0.72956300	0.06343000	406	408	592
H	-0.64855100	-0.42946100	1.45998200	760	881	917
C	1.62528600	-0.40106100	-0.18511200	968	1010	1072
H	2.01677300	-0.52538700	-1.18790300	1164	1223	1257
H	2.31335000	-0.65797800	0.61247500	1270	1340	1410
H	0.41548300	-1.17380500	-0.02302300	1440	1487	1740
H	0.89667000	1.43728400	0.84726600	3028	3058	3100
O	-1.68915100	0.00618100	-0.30576600	3104	3197	3815
H	-2.32879900	-0.67366800	-0.07219100			
H	0.39827300	1.28701400	-0.84333000			
<b>TS_I1-P3</b>						
C	0.86451300	1.18555100	0.11404800	-539	111	202
C	0.38485200	0.02407000	-0.41544100	276	352	469
H	0.63800800	2.12860000	-0.35799300	554	558	579
H	1.36536300	1.20774200	1.07353500	728	867	940
C	-1.77508600	0.04198400	0.12912100	980	1103	1285
H	-2.03345800	-0.90660000	-0.32136000	1329	1421	1425
H	-1.71616700	0.05657100	1.20837600	1441	1555	3081
H	-2.18627800	0.92792900	-0.33524500	3142	3183	3234
H	0.05690000	-0.02255800	-1.44377600	3236	3244	3799
O	0.73291600	-1.22093200	0.03938100			
H	1.16662400	-1.13384700	0.89504800			
<b>TS_I1-P4</b>						
C	0.99325300	-1.02457800	-0.10901600	-836	211	385
C	0.07598600	-0.03465400	0.04112400	411	449	512
H	0.68808900	-2.05777000	-0.07124300	539	563	666
H	2.05297300	-0.81123800	-0.15092000	801	858	978
C	-1.40669200	-0.23453900	-0.07146900	1023	1065	1198
H	-1.93516100	0.42085100	0.61771500	1361	1410	1451
H	-1.72389600	0.01581700	-1.08639300	1475	1491	1605
H	-1.67594600	-1.26643500	0.13874500	3037	3103	3138
H	0.09725800	-0.24188600	1.88316400	3149	3249	3800
O	0.39593200	1.28902900	-0.05591900			
H	1.35394700	1.39105400	-0.04754300			
<b>TS_I2-P1</b>						
C	-1.17148400	-0.87078700	-0.10846000	-419	126	182
H	-2.19551000	-0.68528100	0.22801100	231	331	487
H	-0.85602200	-1.83124200	0.29761200	583	606	846
H	-1.17731100	-0.90635600	-1.19666500	876	950	1067
C	-0.30984900	0.27541200	0.38268600	1117	1369	1394
H	-0.03263300	0.22264100	1.45308800	1416	1432	1471
C	1.65561300	-0.44256500	-0.07892400	1476	1578	2873
H	1.55761300	-0.54556800	-1.14941600	3024	3087	3093
H	2.24127000	0.39193400	0.27505400	3123	3251	3263
H	1.68354700	-1.35149100	0.50590700			
O	-0.28332900	1.36662500	-0.19817600			
<b>TS_I2-P2</b>						
C	-1.29452500	-0.62393600	-0.05030900	-909	146	192
H	-2.14079700	0.01239200	0.19533400	368	445	502

H	-1.28870200	-1.50777400	0.58608200	531	545	778
H	-1.40426200	-0.96263200	-1.08498700	883	927	1079
C	0.00000000	0.17072800	0.04339500	1098	1214	1384
H	-0.00000100	0.25594200	1.82384600	1391	1464	1469
C	1.29452500	-0.62393500	-0.05030900	1470	1490	1653
H	1.40426200	-0.96263300	-1.08498700	3022	3027	3089
H	2.14079700	0.01239300	0.19533200	3095	3138	3140
H	1.28870300	-1.50777200	0.58608300			
O	0.00000000	1.39036800	-0.10917000			
<b>TS_I3-P2</b>						
C	1.42998200	-0.36832400	0.05367100	-1135	53	134
H	2.10713800	0.47980500	-0.00302500	210	375	386
H	1.67889400	-1.09248100	-0.72535000	516	637	790
H	1.56805300	-0.88068900	1.01209700	893	940	1073
C	0.00549300	0.08992800	-0.08419500	1101	1246	1389
C	-1.09440600	-0.92994400	-0.00096700	1390	1458	1463
H	-1.54330700	-0.85294800	0.99690800	1472	1486	1641
H	-1.87934300	-0.70051500	-0.72014000	3001	3008	3064
H	-0.74381900	-1.95049500	-0.14398400	3082	3126	3136
O	-0.27107800	1.29348900	-0.15600100			
H	-1.06540300	1.89945200	1.02044600			
<b>TS_I3-P4</b>						
C	-1.14524000	-0.68996700	-0.32785600	-127	87	95
H	-1.10462800	-1.76009100	-0.45165400	186	410	446
H	-2.11221500	-0.21213700	-0.41824000	483	512	728
C	-0.03439800	0.01083200	-0.09079200	818	862	984
C	1.33798500	-0.56171300	0.04130100	1022	1073	1204
H	2.00375100	-0.12072900	-0.70312700	1364	1415	1455
H	1.75045600	-0.32531500	1.02407200	1474	1492	1702
H	1.32585600	-1.64081000	-0.08781700	3033	3080	3133
O	-0.01314400	1.36773800	0.06813000	3147	3244	3797
H	-0.90997300	1.71126600	-0.01060100			
H	-1.79817600	-1.14899700	2.36640900			
<b>TS_I4-P5</b>						
C	-0.81288100	0.60865400	0.11495100	-253	136	170
C	0.66940300	0.65317000	-0.10691100	246	276	300
H	-1.30170200	1.29957800	-0.58565900	604	614	884
H	-1.04085400	0.98229900	1.11771300	954	988	1009
C	1.46294400	-0.41152100	-0.21435800	1034	1131	1210
H	2.52142200	-0.30692600	-0.40436500	1315	1375	1407
H	2.11684300	-0.82174000	1.92810100	1443	1488	1675
H	1.06391300	-1.41559200	-0.17050900	2964	3032	3132
H	1.09454000	1.65090900	-0.16170800	3149	3232	3806
O	-1.38834400	-0.68350200	0.04518200			
H	-1.26420900	-1.02232400	-0.84712500			
<b>TS_I4-P6</b>						
C	-0.76784500	0.51950900	-0.11125500	-613	95	236
C	0.57434800	0.66497800	-0.15055400	277	371	438
H	-1.42892700	1.34149100	-0.34244900	552	656	741
H	-0.91383400	1.16629100	1.73135500	915	984	1038
C	1.57668100	-0.42519100	0.05138000	1050	1122	1244
H	2.44335400	-0.27954000	-0.59484700	1344	1412	1434
H	1.94770200	-0.44804400	1.08180500	1480	1498	1632
H	1.17821300	-1.41764200	-0.17351800	2998	3045	3079
H	0.94107600	1.67801400	-0.24340800	3178	3207	3803
O	-1.45198400	-0.65319200	-0.04696500			

H	-0.85081300	-1.37080900	0.17935600			
<b>TS_I5-P7</b>						
C	-0.78131800	0.15306600	0.33270200	-767	88	228
C	0.52202200	0.59032100	-0.29807700	269	415	426
H	-1.68534900	1.77274500	0.21407000	504	799	874
H	-0.87212100	0.36028700	1.42088000	935	996	1105
C	1.64347400	-0.38147300	0.10193300	1154	1278	1324
H	2.59448700	-0.06002200	-0.32184900	1393	1411	1479
H	1.76124200	-0.42946500	1.18595000	1500	1506	1693
H	1.42962700	-1.38680200	-0.26039700	2841	3032	3038
H	0.77127100	1.59874800	0.03889700	3083	3101	3109
O	-1.58767200	-0.57896400	-0.21454100			
H	0.39714600	0.60473700	-1.38057400			
<b>TS_I5-P8</b>						
C	-1.20667900	0.38336600	0.31747800	-306	90	155
C	0.86401000	0.71300200	-0.27316300	194	315	569
H	-1.49336900	1.37174400	-0.08159700	609	827	837
H	-0.89810700	0.38351200	1.37819100	999	1074	1117
C	1.60532300	-0.51119600	0.13115400	1222	1245	1400
H	2.64073500	-0.46363700	-0.22960600	1472	1473	1478
H	1.64670000	-0.62528700	1.21474300	1490	1625	2881
H	1.15215600	-1.40494100	-0.29654400	2931	2985	3064
H	1.01429400	1.62580300	0.29154900	3106	3117	3212
O	-1.53600100	-0.65638700	-0.25063100			
H	0.64967700	0.85287100	-1.32449800			
<b>TS_I6-P5</b>						
C	-0.64333700	0.42434900	0.37832000	-523	116	265
C	0.64970800	0.23089700	-0.36504600	336	362	377
H	-0.98276500	1.45674600	0.30788700	441	665	924
H	-0.50466500	0.18800100	1.43922000	938	949	1027
C	1.69343300	-0.44845000	0.12827100	1039	1141	1231
H	2.57608600	-0.64668600	-0.46436800	1306	1354	1407
H	1.70844300	-0.78497400	1.15809900	1456	1509	1645
H	1.32946800	2.16516000	-0.13427500	2997	3086	3129
O	-1.69194400	-0.35552200	-0.19573200	3146	3217	3805
H	0.63191900	0.50426900	-1.41440000			
H	-1.42175600	-1.27911600	-0.17558000			
<b>TS_I7-P3</b>						
C	0.85526700	0.37129900	0.35180900	-407	90	115
C	-0.22894200	0.87546500	-0.27513100	237	318	462
H	1.10692100	0.62691500	1.37416800	487	497	723
C	-2.07460500	-0.51416300	0.09179500	769	878	907
H	-2.81160500	-0.00980000	-0.51770100	975	1129	1272
H	-1.66876300	-1.43843200	-0.29165700	1323	1420	1424
H	-2.19208800	-0.43813600	1.16288700	1440	1621	3088
H	-0.74069500	1.71358500	0.16924700	3153	3165	3240
O	1.63004200	-0.58649500	-0.24232100	3249	3257	3849
H	2.32049100	-0.86595500	0.36372700			
H	-0.36491600	0.70817800	-1.33293800			

<b>P1</b>						
<b>(CH<sub>3</sub>CHO)</b>						
C	-1.16575700	-0.14832600	-0.00005800	161	509	776
H	-1.70360600	0.22532400	-0.87540100	885	1129	1137
H	-1.70174800	0.22354800	0.87738200	1378	1426	1460
H	-1.15795800	-1.23567600	-0.00105900	1470	1817	2862
C	0.23331000	0.39625800	-0.00015500	3022	3073	3135
H	0.30424500	1.50470600	0.00012300			
O	1.23171900	-0.27568700	0.00003000			
<b>(CH<sub>3</sub>)</b>						
C	0.00000000	0.00000000	0.00000000	526	1407	1407
H	0.00000000	1.07796700	0.00000000	3109	3285	3285
H	0.93354700	-0.53898400	0.00000000			
H	-0.93354700	-0.53898400	0.00000000			
<b>P2 (CH<sub>3</sub>COCH<sub>3</sub>)</b>						
C	1.28812300	-0.61155600	0.00039400	23	133	377
H	1.32288900	-1.27909700	0.86422000	489	535	781
H	2.14081400	0.06170500	0.02143100	884	885	1084
H	1.34098000	-1.24362800	-0.88907900	1120	1233	1386
C	0.00003700	0.18487700	0.00001900	1387	1460	1465
O	-0.00008900	1.39405000	-0.00001000	1470	1488	1794
C	-1.28808700	-0.61168600	-0.00042200	3026	3033	3078
H	-1.32246300	-1.27988100	-0.86374300	3085	3139	3140
H	-1.34125600	-1.24296300	0.88957400			
H	-2.14069000	0.06164500	-0.02226700			
<b>P3</b>						
<b>(CH<sub>2</sub>=CHOH)</b>						
C	1.23506100	-0.06812500	0.00000000	263	484	717
C	0.00000000	0.41212900	0.00000000	858	959	977
H	1.42560200	-1.13189400	0.00000000	1145	1286	1351
H	2.07352900	0.60997400	0.00000000	1442	1729	3139
H	-0.19843800	1.47882400	0.00000000	3163	3254	3852
O	-1.10177100	-0.39541800	0.00000000			
H	-1.89688900	0.14241400	0.00000000			
<b>(CH<sub>3</sub>)</b>						
C	0.00000000	0.00000000	0.00000000	526	1407	1407
H	0.00000000	1.07796700	0.00000000	3109	3285	3285
H	0.93354700	-0.53898400	0.00000000			
H	-0.93354700	-0.53898400	0.00000000			
<b>P4 (CH<sub>3</sub>COH=CH<sub>2</sub>)</b>						
C	-0.97507100	-1.04050700	0.00000000	185	410	435
H	-0.65375900	-2.06972600	0.00000000	481	509	727
H	-2.04043500	-0.84804900	0.00000200	817	861	982
C	-0.08295100	-0.05119400	0.00000000	1023	1074	1204
C	1.40046300	-0.22367600	-0.00000200	1362	1416	1454
H	1.67174800	-1.27616000	-0.00028000	1474	1492	1716
H	1.83659300	0.25635200	-0.87828300	3033	3079	3132
H	1.83654000	0.25585800	0.87857700	3144	3239	3800
O	-0.41619400	1.27647400	0.00000000			
H	-1.37578000	1.36219700	0.00000100			
<b>P5 (CH<sub>2</sub>=CHCH<sub>2</sub>OH)</b>						
C	0.72704200	0.63237500	-0.02879100	191		311
C	-0.77193900	0.58303500	0.03741500	577	278	884
				954	615	1015



H	1.10262200	1.24319200	0.80382700	1038	992	1213
H	1.03535900	1.14475100	-0.94435900	1321	1131	1410
C	-1.50752400	-0.51772700	-0.03175000	1448	1375	1709
H	-2.58622900	-0.47927700	0.02934500	2963	1491	3127
H	-1.05403000	-1.49070200	-0.16793200	3144	3037	3805
H	-1.25385400	1.54938500	0.15592700		3223	
O	1.36475900	-0.63201400	-0.06150100			
H	1.15259200	-1.09733600	0.75395600			
<b>P6 (CH<sub>3</sub>CH=CHOH)</b>						
C	-0.77004700	0.57548900	-0.00000800	49	273	329
C	0.55616100	0.68745300	0.00000200	500	653	750
H	-1.41429900	1.44368700	-0.00000400	914	964	1039
C	1.54851000	-0.43609700	-0.00000100	1055	1122	1247
H	2.19833400	-0.39377900	-0.87766800	1341	1420	1438
H	2.19790300	-0.39419900	0.87800700	1476	1503	1729
H	1.08265400	-1.42433700	-0.00037000	3012	3055	3064
H	0.95101700	1.69478700	0.00003400	3168	3197	3798
O	-1.51213400	-0.56918500	0.00000000			
H	-0.92627200	-1.33375100	0.00004100			
<b>P7 (CH<sub>3</sub>CH<sub>2</sub>CHO)</b>						
C	0.78382500	-0.23120700	0.29940300	79	209	327
O	1.81246100	-0.04001100	-0.29526800	509	759	875
H	0.70312300	-1.07013600	1.02570400	921	1008	1134
C	-0.47067300	0.58850000	0.14869800	1159	1274	1329
C	-1.68969600	-0.28231400	-0.17729100	1413	1426	1468
H	-0.29946500	1.34923700	-0.61238500	1502	1507	1812
H	-0.63681700	1.09919700	1.10413100	2844	3008	3033
H	-1.57785100	-0.76698700	-1.14755000	3082	3100	3104
H	-1.83299100	-1.06179600	0.57307000			
H	-2.59641800	0.32070200	-0.20569000			
<b>P8(HCHO)</b>						
C	0.00000700	0.52595600	0.00000000	1202	1268	1536
H	-0.93748400	1.11434600	0.00000000	1824	2877	2931
H	0.93738500	1.11454700	0.00000000			
O	0.00000700	-0.67307900	0.00000000			
<b>P8 (C<sub>2</sub>H<sub>3</sub>)</b>						
C	0.00942000	-0.69165500	0.00000000	101	487	813
C	0.00942000	0.79240800	0.00000000	981	1061	1195
H	0.50352400	-1.09898100	0.88445300	1401	1467	1481
H	-1.01138500	-1.10266200	0.00000000	1482	2942	3034
H	0.50352400	-1.09898100	-0.88445300	3077	3143	3241
H	-0.05435100	1.34805300	-0.92436500			
H	-0.05435100	1.34805300	0.92436500			