

Supplementary Information

OH-initiated Oxidation of Vinyl Butyrate in the Atmosphere: *Ab initio* Insights

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Contents

Table S1. Optimized geometries, electronic energies at 0 K (E_{elec0} K), zero-point energy (ZPE) corrections and harmonic wavenumbers of the species involved with the lowest-energy conformer of a given species, calculated at M06-2X/aug-cc-pVTZ level of theory for the VB + OH/O ₂ /NO reactions.....	3
Table S2. Calculated total rate constants, $k_{total}(T, P)$, of the “VB + OH → products” reaction at different pressures for the temperature range of 200 - 2000 K. Units: cm ³ molecule ⁻¹ s ⁻¹	37
Table S3. Calculated Eckart tunneling factors via transition state channels at $P = 760$ Torr for the temperature range of 200 - 400 K.	38
Table S4. Individual rate constants $k(T, P)$ for “VB + OH → products” reaction at $P = 760$ Torr for the temperature range of 200 - 2000 K. Units: cm ³ molecule ⁻¹ s ⁻¹	39
Table S5. Individual rate constants $k(T, P)$ for “P5 + O ₂ → Products” at $P = 760$ Torr for the temperature range of 200 - 400 K. Units: cm ³ molecule ⁻¹ s ⁻¹	39
Table S6. Individual rate constants $k(T, P)$ for “P5 → Products” decomposition at $P = 760$ Torr for the temperature range of 200 - 400 K. Unit: s ⁻¹	40
Table S7. Individual rate constants $k(T, P)$ for “IM7 + NO → Products” at $P = 760$ Torr for the temperature range of 200 - 400 K. Units: cm ³ molecule ⁻¹ s ⁻¹	40
Table S8. Estimated branching ratios for “VB + OH → products” reactions at $P = 760$ Torr for the temperature range of 200 - 2000 K.....	41
Table S9. Estimated branching ratios for “P5 + O ₂ → products” reactions at $P = 760$ Torr for the temperature range of 200 - 400 K.....	41
Table S10. Estimated branching ratios for each species of “IM7 + NO → products” reactions at $P = 760$ Torr for the temperature range of 200 - 400 K.....	42
Figure S1. Estimated total rate constants for “P5 + O ₂ → products” reactions at $P = 760$ Torr for the temperature range of 200 - 400 K.....	43
Figure S2: Branching ratios (Γ) for the products formation of “P5 + O ₂ → products” reactions at $P = 760$ Torr for the temperature range of 200 - 400 K.....	43
Figure S3. Estimated total rate constants for the “IM7 + NO → products” reactions at $P = 760$ Torr for the temperature range of 200 - 400 K.....	44
Figure S4: Branching ratios (Γ) for the products formation of “IM7 + NO → products” reactions at $P = 760$ Torr for the temperature range of 200 - 400 K.....	44
Figure S5. Geometries for the species involved in the VB + OH/O ₂ /NO/ reaction were optimized at M06-2X/aug-cc-pVTZ level. All structures were obtained for the lowest-energy conformer. Bond lengths and bond angles are in Å and degree (°), respectively.....	58
Figure S6: Hindrance potentials for the species involved in the VB + OH/O ₂ /NO reaction, obtained at M06-2X/cc-pVDZ level.	87

Table S1. Optimized geometries, electronic energies at 0 K (E_{elec}^{0K}), zero-point energy (ZPE) corrections and harmonic wavenumbers of the species involved with the lowest-energy conformer of a given species, calculated at M06-2X/aug-cc-pVTZ level of theory for the VB + OH/O₂/NO reactions.

VB + OH channels									
Species	Cartesian coordinate (Å)				E_{elec}^{0K} (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm ⁻¹)		
OH (C _{∞v})	O	0	0	0.108021	-75.7338101	0.008331	3766.188		
	H	0	0	-0.86417	-75.733167				
VB (C _i)	C	-2.85273	0.399159	0.882604	-385.0801224	0.148724	36.2886	76.3784	109.5438
	H	-3.85462	0.815889	0.791148			150.8887	161.1449	228.2719
	H	-2.16497	1.220734	1.07898			301.1221	354.0097	430.8772
	H	-2.84536	-0.26804	1.74605			485.8096	577.4686	675.7778
	C	-2.4527	-0.34935	-0.38291			736.9696	801.8686	890.0218
	H	-3.16578	-1.15003	-0.58149			899.6319	912.2005	925.389
	H	-2.48183	0.326837	-1.23745			1005.05	1015.227	1073.653
	C	-1.06173	-0.95751	-0.28334			1107.042	1131.319	1186.861
	H	-0.94844	-1.56312	0.617644			1225.378	1256.381	1304.413
	H	-0.85358	-1.62417	-1.12392			1332.539	1377.418	1407.154
	C	0.030665	0.077269	-0.28819			1416.483	1430.026	1460.017
	C	2.341612	0.313151	0.051603			1489.006	1503.554	1512.334
	H	2.161328	1.343339	-0.21658			1742.995	1860.283	3062.113
	C	3.516225	-0.19649	0.367271			3068.553	3078.172	3105.751
	H	4.387342	0.439186	0.36709			3115.89	3134.265	3146.169
	H	3.626711	-1.23929	0.627138			3192.674	3245.568	3290.369
	O	1.220767	-0.48679	0.04811					
O	-0.09438	1.234445	-0.56697						
RC (C _i)	C	-1.986	1.125518	-1.07263	-460.8257283	0.159519	29.232	60.5821	73.9924
	H	-2.31994	1.915738	-1.74321			90.5782	110.6253	129.4668
	H	-2.86385	0.565183	-0.74624			151.6967	213.5721	240.3276
	H	-1.35659	0.445451	-1.64873			291.4179	392.8146	435.7274
	C	-1.23814	1.706025	0.120565			468.854	484.0895	579.6702
	H	-1.88596	2.390577	0.66783			634.6388	723.1549	742.6561
	C	-0.76576	0.62498	1.105685			821.0054	873.2831	890.3657
	H	-0.28057	1.086364	1.964388			924.962	933.3617	1007.214
	H	-1.61237	0.027359	1.440013			1012.217	1072.602	1104.839
	C	0.211873	-0.29671	0.441778			1116.066	1186.492	1231.019
	C	2.439983	-0.43364	-0.28566			1284.097	1312.077	1332.141
	H	2.142884	-1.39328	-0.68004			1361.676	1387.517	1423.303
	C	3.64556	0.090994	-0.37433			1426.983	1486.75	1496.175
	H	4.42591	-0.45658	-0.87843			1505.235	1509.483	1743.56
	H	3.871077	1.059682	0.047467			1821.214	3056.842	3075.252
	O	1.435678	0.26302	0.35727			3092.877	3107.436	3128.848
	O	-0.03897	-1.38695	-0.0076			3138.399	3152.666	3193.628
H	-0.37549	2.284461	-0.21317	3250.177	3292.081	3585.838			
O	-2.86037	-1.75336	-0.06659						
H	-1.88091	-1.80964	-0.08706						
IM1 (C _i)	C	2.812068	-1.06813	0.768458	-460.8688901	0.162404	39.3653	53.0892	126.5498
	H	3.598134	-1.80227	0.599189			140.9157	156.4947	192.3911
	H	1.868748	-1.60521	0.861798			237.4464	268.7202	310.2757

	H	3.018145	-0.57002	1.717172			323.5811	390.7999	477.5769
	C	2.750372	-0.05848	-0.37112			526.8667	553.5868	591.8229
	H	3.710402	0.448782	-0.46988			681.6187	797.1952	868.5819
	H	2.56062	-0.57332	-1.31295			891.1548	904.2976	931.1396
	C	1.671946	0.993451	-0.15771			1067.458	1069.878	1092.012
	H	1.763217	1.474085	0.817675			1104.772	1122.908	1171.342
	H	1.742339	1.794264	-0.89826			1239.209	1252.152	1276.259
	C	0.279806	0.436544	-0.2767			1303.624	1353.483	1378.504
	C	-1.97359	0.992633	0.189434			1399.586	1414.353	1420.554
	H	-2.59504	1.868028	0.104895			1440.824	1459.733	1489.179
	C	-2.46541	-0.33697	0.6403			1493.166	1504.723	1512.327
	H	-1.75241	-0.76598	1.353494			1831.872	3028.694	3062.548
	H	-3.41213	-0.19157	1.159474			3068.734	3080.017	3107.207
	O	-0.63581	1.317439	0.182321			3115.531	3117.231	3135.576
	O	-0.00946	-0.63098	-0.74708			3144.453	3257.115	3817.532
	O	-2.73589	-1.24517	-0.41075					
	H	-1.90386	-1.36144	-0.88458					
IM2	C	3.028381	0.977831	-0.12701	-460.8756449	0.161772	37.3001	68.2132	126.8013
(C _i)	H	3.918571	1.337312	0.387008			133.6951	145.0452	166.8226
	H	2.212162	1.663498	0.09747			237.3735	302.7773	312.9913
	H	3.222055	1.017349	-1.20007			398.0705	423.4654	444.1464
	C	2.677925	-0.43982	0.308046			502.5049	558.6421	595.6921
	H	3.513792	-1.10868	0.100346			623.2526	715.8372	810.1825
	H	2.505337	-0.46467	1.384056			869.9113	893.4093	910.3352
	C	1.443473	-0.97592	-0.40153			938.2991	979.8296	1070.211
	H	1.525301	-0.87869	-1.48519			1097.99	1107.294	1134.533
	H	1.298941	-2.04074	-0.20176			1178.09	1229.231	1255.707
	C	0.171369	-0.29422	0.032209			1303.539	1307.13	1370.827
	C	-2.13912	-0.01581	-0.45125			1382.359	1413.38	1426.06
	H	-2.73961	-0.26093	-1.32953			1440.425	1458.373	1460.798
	C	-2.65983	-0.67752	0.771951			1488.043	1503.19	1511.413
	H	-3.35625	-0.14386	1.397619			1816.554	3062.24	3067.915
	H	-2.48406	-1.72939	0.930466			3076.036	3077.806	3106.649
	O	-0.84149	-0.56433	-0.80145			3116.825	3134.256	3143.925
	O	0.058108	0.395805	1.015112			3188.933	3304.647	3806.781
	O	-2.11055	1.364431	-0.37443					
	H	-1.59796	1.594243	0.411274					
IM3	C	3.414413	0.434565	0.67523	-460.8785877	0.163228	39.1165	59.9726	66.4065
(C _i)	H	4.250092	1.119569	0.540646			113.7135	152.7559	205.2615
	H	3.795503	-0.49414	1.09857			246.3689	315.0837	336.5108
	H	2.714766	0.876906	1.382524			364.8673	456.1023	507.2791
	C	2.712113	0.17928	-0.66974			563.0461	582.0094	678.8482
	H	2.341865	1.129889	-1.05497			769.0045	792.7644	838.2637
	H	3.425648	-0.22847	-1.38503			905.521	959.0077	977.343
	C	1.573229	-0.75318	-0.50902			1040.092	1072.854	1092.933
	H	1.683493	-1.81833	-0.64867			1110.448	1152.915	1163.209
	C	0.28949	-0.26001	-0.06242			1242.346	1253.045	1299.527
	C	-1.90973	-0.87385	0.595987			1315.085	1331.841	1388.838
	H	-2.3876	-1.83457	0.769			1399.185	1407.335	1459.475
	C	-2.75393	-0.01816	-0.34244			1466.352	1483.576	1495.509

	H	-2.47393	-0.25824	-1.37538			1501.76	1505.586	1510.765
	H	-3.79942	-0.29862	-0.2127			1736.132	3022.139	3067.283
	O	-0.62206	-1.23409	0.068773			3076.176	3086.333	3105.855
	O	0.057321	0.913102	0.17072			3120.501	3143.157	3150.51
	O	-2.68248	1.360903	-0.08681			3155.557	3226.262	3782.216
	H	-1.74743	1.589167	-0.00743					
	H	-1.77878	-0.35445	1.546411					
IM4 (C _i)	C	-2.34075	1.38206	0.045752	-460.8689577	0.164254	25.7781	56.5588	69.7808
	H	-2.82573	1.122041	0.988572			126.9546	149.5895	157.4137
	H	-2.94295	2.132831	-0.46401			215.37	274.7315	357.9449
	H	-1.38181	1.851924	0.300617			363.3583	404.1716	419.8842
	C	-2.1401	0.179598	-0.80206			459.4521	551.2772	643.8233
	H	-2.00563	0.296726	-1.86752			784.7148	850.5614	898.1362
	C	-1.69966	-1.10706	-0.17747			908.4153	925.4946	937.2554
	H	-2.33653	-1.36577	0.669173			1002.445	1076.107	1107.684
	H	-1.69335	-1.91673	-0.90355			1115.766	1152.226	1157.983
	C	-0.30512	-0.90428	0.368398			1219.028	1258.911	1283.426
	C	1.971101	-0.72307	-0.23673			1307.054	1322.051	1372.697
	H	2.151503	-1.0075	0.799655			1383.002	1414.627	1423.258
	C	2.241836	0.751054	-0.45467			1452.442	1467.492	1476.119
	H	3.289565	0.941417	-0.1952			1489.15	1497.784	1513.638
	H	2.10499	0.997036	-1.50821			1814.039	3005.404	3029.152
	O	0.623486	-1.05226	-0.58772			3078.951	3082.165	3092.047
	O	-0.0555	-0.58239	1.502694			3105.598	3132.52	3149.449
	O	1.372736	1.589032	0.273003			3151.502	3208.529	3823.751
	H	1.146517	1.163101	1.107406					
	H	2.603752	-1.31999	-0.89016					
IM5 (C _i)	C	-2.31817	1.245445	0.506848	-460.8785299	0.162311	40.2014	69.3242	119.3023
	H	-2.50631	2.28599	0.292849			143.3697	155.6159	201.5985
	H	-2.22622	0.948124	1.541906			235.0965	259.3243	350.7174
	C	-2.43523	0.216862	-0.56056			391.6846	460.6847	479.0282
	H	-3.48707	-0.03174	-0.74868			491.2743	518.6942	557.323
	H	-2.04377	0.607348	-1.50104			677.4673	710.9544	837.9143
	C	-1.69538	-1.07638	-0.19921			881.9514	901.9372	916.2512
	H	-2.15017	-1.56018	0.662506			934.8395	979.5083	1090.118
	H	-1.71011	-1.7681	-1.04166			1095.569	1100.316	1117.078
	C	-0.26486	-0.77856	0.162164			1185.609	1198.744	1231.748
	C	1.707035	0.344585	-0.58262			1301.88	1348.255	1363.482
	H	2.051547	0.635889	-1.5715			1376.42	1407.533	1424.312
	C	1.602465	1.548847	0.331488			1462.383	1468.805	1471.536
	H	1.256536	1.253647	1.320178			1483.418	1493.238	1500.471
	H	2.585054	2.008255	0.42012			1815.172	3008.464	3077.79
	O	0.381732	-0.18451	-0.84417			3089.675	3093.577	3135.494
	O	0.233235	-1.0205	1.235212			3150.634	3154.638	3166.748
	O	2.571576	-0.63635	-0.13683			3168.608	3271.91	3800.129
	H	2.258373	-0.92664	0.729462					
	H	0.904633	2.273484	-0.08649					
IM6 (C _i)	C	-3.45876	-0.18	0.783317	-460.8957507	0.163687	42.6206	60.5172	108.4645
	H	-4.4446	0.282519	0.790263			145.1497	152.5578	226.0217
	H	-2.84577	0.29987	1.544511			234.888	301.0748	320.9513

	H	-3.57101	-1.23262	1.041094			368.2025	430.6084	482.7908
	C	-2.80232	-0.01833	-0.59854			547.3417	561.0117	633.3259
	H	-3.43802	-0.46575	-1.36193			695.259	774.7266	812.0934
	H	-2.70183	1.046022	-0.81354			875.3116	915.4547	947.6272
	C	-1.46092	-0.64504	-0.63032			988.1021	1047.258	1082.022
	H	-1.31388	-1.66338	-0.95856			1102.606	1128.446	1153.734
	C	-0.31295	0.073876	-0.12621			1190.866	1241.855	1300.069
	C	1.993184	0.018797	0.341456			1307.855	1331.238	1394.284
	H	1.750335	0.303603	1.368049			1400.121	1407.368	1468.203
	C	3.120078	-0.97356	0.271654			1479.606	1484.976	1491.556
	H	4.016986	-0.52884	0.696467			1496.405	1501.638	1510.528
	H	2.864674	-1.875	0.823892			1729.898	3067.051	3073.207
	O	0.824693	-0.64158	-0.18675			3077.023	3084.66	3120.997
	O	-0.35729	1.211085	0.309725			3142.502	3150.856	3166.481
	O	2.317161	1.132539	-0.41596			3170.326	3226.969	3820.473
	H	1.628235	1.790861	-0.26478					
	H	3.308434	-1.2281	-0.76976					
TS1 (C _i)	C	3.467968	-0.67459	0.874976	-460.8015086	0.153658	-1519.06	34.1033	45.2401
	H	4.406751	-1.21788	0.779519			65.1751	82.6411	126.5229
	H	2.679195	-1.40106	1.066385			156.1024	163.559	207.7433
	H	3.547771	-0.01846	1.743138			227.9451	294.2847	357.5063
	C	3.169926	0.1288	-0.38501			379.7361	476.9208	547.2274
	H	3.981242	0.831118	-0.57814			583.7206	673.3612	767.9159
	H	3.110999	-0.53866	-1.24484			799.7191	833.301	881.4366
	C	1.870882	0.914032	-0.28007			888.442	912.5154	976.5109
	H	1.837907	1.524059	0.624379			988.868	1072.58	1103.709
	H	1.750082	1.606578	-1.11685			1118.813	1161.283	1178.401
	C	0.653707	0.031008	-0.28857			1206.957	1254.005	1303.083
	C	-1.66451	0.093237	0.067277			1304.034	1327.685	1377.598
	H	-1.62289	-0.95711	-0.18472			1405.507	1417.971	1458.143
	C	-2.76663	0.734505	0.384869			1489.921	1503.905	1512.777
	H	-2.89269	1.779097	0.627397			1727.395	1867.851	3062.31
	O	-0.45559	0.749087	0.054793			3068.418	3078.885	3106.245
	O	0.618714	-1.129	-0.57312			3116.241	3134.648	3145.475
	H	-3.78566	0.044749	0.411899			3232.672	3244.919	3809.034
	O	-4.74339	-0.68233	0.081316					
	H	-4.75869	-0.51648	-0.87297					
TS2 (C _i)	C	2.308006	1.066491	-0.78832		0.154364	-1581.65	35.5162	50.2599
	H	2.818648	1.403541	-1.68868			89.4018	111.8311	157.77
	H	2.803984	1.51712	0.072366			172.716	208.0859	268.1523
	H	1.287312	1.453324	-0.82232			309.1435	369.898	383.0899
	C	2.321972	-0.45388	-0.69014			409.8056	444.8572	578.4935
	H	1.795879	-0.88878	-1.53982			622.8632	695.3393	723.074
	H	3.345859	-0.82622	-0.7234			798.3679	821.6381	872.6749
	C	1.677688	-0.95801	0.607637			892.9338	915.5427	924.4084
	H	1.629847	-2.04734	0.608172			996.3988	1043.364	1067.829
							1104.202	1114.011	1181.891
							1219.546	1283.201	1287.482
	C	-1.76754	-0.34682	-0.35978			1362.891	1375.363	1383.313
	C	-2.86207	-1.02654	-0.61048			1408.201	1427.582	1477.751

	H	-3.79376	-0.5044	-0.76111			1495.446	1505.82	1511.112
	H	-2.84146	-2.10731	-0.67192			1746.459	1858.563	3055.707
	O	-0.52166	-0.88655	-0.24062			3080.731	3091.045	3108.842
	O	-0.09846	0.34539	1.591911			3130.043	3141.064	3153.303
	H	-1.78793	0.875254	-0.31075			3173.741	3280.562	3758.875
	O	-1.63758	2.11034	-0.09016					
	H	-1.23103	2.018183	0.788311					
TS3 (C _i)	C	3.287137	0.195895	0.966211	-460.8031554	0.153328	-1557.92	28.9266	50.5155
	H	4.358178	0.000577	0.979682			73.9065	100.2622	133.5923
	H	2.780119	-0.69494	1.334784			158.7077	187.8886	227.5924
	H	3.087807	1.015276	1.658602			262.2721	299.2798	350.4163
	C	3.120078	-0.97356	0.271654			1479.606	1484.976	1491.556
	H	4.016986	-0.52884	0.696467			1496.405	1501.638	1510.528
	H	2.864674	-1.875	0.823892			1729.898	3067.051	3073.207
	O	0.824693	-0.64158	-0.18675			3077.023	3084.66	3120.997
	O	-0.35729	1.211085	0.309725			3142.502	3150.856	3166.481
	O	2.317161	1.132539	-0.41596			3170.326	3226.969	3820.473
	H	1.628235	1.790861	-0.26478					
	H	3.308434	-1.2281	-0.76976					
TS1 (C _i)	C	3.467968	-0.67459	0.874976	-460.8015086	0.153658	-1519.06	34.1033	45.2401
	H	4.406751	-1.21788	0.779519			65.1751	82.6411	126.5229
	H	2.679195	-1.40106	1.066385			156.1024	163.559	207.7433
	H	3.547771	-0.01846	1.743138			227.9451	294.2847	357.5063
	C	3.169926	0.1288	-0.38501			379.7361	476.9208	547.2274
	H	3.981242	0.831118	-0.57814			583.7206	673.3612	767.9159
	H	3.110999	-0.53866	-1.24484			799.7191	833.301	881.4366
	C	1.870882	0.914032	-0.28007			888.442	912.5154	976.5109
	H	1.837907	1.524059	0.624379			988.868	1072.58	1103.709
	H	1.750082	1.606578	-1.11685			1118.813	1161.283	1178.401
	C	0.653707	0.031008	-0.28857			1206.957	1254.005	1303.083
	C	-1.66451	0.093237	0.067277			1304.034	1327.685	1377.598
	H	-1.62289	-0.95711	-0.18472			1405.507	1417.971	1458.143
	C	-2.76663	0.734505	0.384869			1489.921	1503.905	1512.777
	H	-2.89269	1.779097	0.627397			1727.395	1867.851	3062.31
	O	-0.45559	0.749087	0.054793			3068.418	3078.885	3106.245
	O	0.618714	-1.129	-0.57312			3116.241	3134.648	3145.475
	H	-3.78566	0.044749	0.411899			3232.672	3244.919	3809.034
	O	-4.74339	-0.68233	0.081316					
	H	-4.75869	-0.51648	-0.87297					
TS2 (C _i)	C	2.308006	1.066491	-0.78832	-460.8056653	0.154364	-1581.65	35.5162	50.2599
	H	2.818648	1.403541	-1.68868			89.4018	111.8311	157.77
	H	2.803984	1.51712	0.072366			172.716	208.0859	268.1523
	H	1.287312	1.453324	-0.82232			309.1435	369.898	383.0899
	C	2.321972	-0.45388	-0.69014			409.8056	444.8572	578.4935
	H	1.795879	-0.88878	-1.53982			622.8632	695.3393	723.074
	H	3.345859	-0.82622	-0.7234			798.3679	821.6381	872.6749
	C	1.677688	-0.95801	0.607637			892.9338	915.5427	924.4084
	H	1.629847	-2.04734	0.608172			996.3988	1043.364	1067.829
	H	2.240505	-0.62654	1.477557			1104.202	1114.011	1181.891
	C	0.287571	-0.41794	0.754839			1219.546	1283.201	1287.482

	C	-1.76754	-0.34682	-0.35978			1362.891	1375.363	1383.313
	C	-2.86207	-1.02654	-0.61048			1408.201	1427.582	1477.751
	H	-3.79376	-0.5044	-0.76111			1495.446	1505.82	1511.112
	H	-2.84146	-2.10731	-0.67192			1746.459	1858.563	3055.707
	O	-0.52166	-0.88655	-0.24062			3080.731	3091.045	3108.842
	O	-0.09846	0.34539	1.591911			3130.043	3141.064	3153.303
	H	-1.78793	0.875254	-0.31075			3173.741	3280.562	3758.875
	O	-1.63758	2.11034	-0.09016					
	H	-1.23103	2.018183	0.788311					
TS3 (C _i)	C	3.287137	0.195895	0.966211	-460.8031554	0.153328	-1557.92	28.9266	50.5155
	H	4.358178	0.000577	0.979682			73.9065	100.2622	133.5923
	H	2.780119	-0.69494	1.334784			158.7077	187.8886	227.5924
	H	3.087807	1.015276	1.658602			262.2721	299.2798	350.4163
	C	2.813135	0.546871	-0.43871			421.6132	475.9012	574.3497
	H	3.348913	1.42353	-0.80337			653.5492	656.7383	702.0356
	H	3.036032	-0.27322	-1.12135			801.4351	842.7931	844.256
	C	1.32106	0.840624	-0.49272			889.337	912.6698	933.9554
	H	1.029747	1.583944	0.252013			947.2303	1004.24	1073.727
	H	1.026311	1.249258	-1.46262			1107.284	1128.883	1177.492
	C	0.477582	-0.38585	-0.28061			1210.191	1254.92	1302.535
	C	-1.74924	-1.05383	0.066174			1310.838	1378.094	1407.331
	H	-1.33348	-2.05271	0.052307			1418.937	1459.209	1464.017
	C	-3.02049	-0.77203	0.227993			1488.58	1504.139	1512.488
	H	-3.81612	-1.48668	0.367497			1745.451	1869.921	3063.119
	O	-0.83129	-0.0398	-0.1022			3066.471	3079.475	3104.058
	O	0.85546	-1.5192	-0.28426			3116.103	3135.571	3146.159
	H	-3.36022	0.412697	0.223019			3211.902	3261.34	3786.741
	O	-3.34208	1.660787	0.162319					
	H	-2.38915	1.777848	0.022511					
TS4 (C _i)	C	-1.49545	1.652188	1.025704	-460.8116142	0.154208	-1207.57	21.8869	67.4146
	H	-0.59462	1.362533	1.569789			77.0118	92.6813	128.6654
	H	-2.31035	1.008803	1.356916			139.4488	192.7094	227.946
	H	-1.73082	2.67917	1.298633			280.7252	367.5105	410.2383
	C	-1.29297	1.5221	-0.47851			432.6711	462.9978	619.3915
	H	-2.17568	1.873166	-1.01266			679.2402	732.1306	739.9109
	H	-0.45492	2.143489	-0.80441			817.907	870.7376	890.1788
	C	-1.02136	0.089428	-0.90233			922.8891	931.2291	938.8634
	H	-0.8922	-0.02669	-1.97831			1010.321	1011.642	1080.578
	C	0.120293	-0.55421	-0.17031			1112.585	1129.302	1181.385
	C	2.426051	-0.33252	0.211216			1217.753	1267.44	1288.12
	H	2.295937	-1.20472	0.833556			1323.473	1333.663	1381.65
	C	3.563394	0.301456	0.008333			1420.806	1425.752	1472.849
	H	4.460902	-0.05331	0.489545			1479.589	1505.164	1506.061
	H	3.61824	1.170535	-0.63106			1742.571	1839.012	3058.141
	O	1.272012	0.115459	-0.40141			3061.697	3105.841	3116.482
	O	0.046722	-1.51981	0.538573			3131.284	3146.847	3194.397
	H	-1.98324	-0.57029	-0.62442			3249.724	3292.808	3734.71
	O	-2.80854	-1.41571	-0.02757					
	H	-2.11458	-1.89283	0.461103					
TS5	C	2.301906	-1.17695	1.03885	-460.8154394	0.155176	-871.755	31.2325	71.8664

(C _i)	H	3.342718	-1.05054	1.329816			75.4661	119.0543	134.9233
	H	2.049794	-2.23621	1.133735			157.1941	178.0615	221.7406
	H	1.684604	-0.61577	1.739151			271.5192	357.8893	434.6936
	C	2.078867	-0.70416	-0.38123			437.4966	486.7224	577.8151
	H	2.75309	-1.19145	-1.08523			634.7811	734.6338	766.0214
	C	0.651188	-0.81417	-0.87344			881.7799	898.8237	906.4254
	H	0.571546	-0.49929	-1.91699			932.1997	932.4404	1005.649
	H	0.299654	-1.84779	-0.83762			1011.437	1058.716	1100.415
	C	-0.33098	0.031519	-0.10684			1110.541	1156.574	1185.095
	C	-2.63367	0.311378	0.249604			1215.309	1243.78	1270.87
	H	-2.33087	1.165515	0.835732			1331.91	1363.288	1397.13
	C	-3.87637	-0.08369	0.058938			1416.575	1428.064	1440.797
	H	-4.68373	0.47048	0.510553			1449.678	1491.719	1504.6
	H	-4.10601	-0.95178	-0.54171			1744.358	1840.018	3053.131
	O	-1.59462	-0.39139	-0.32711			3065.714	3103.326	3105.195
	O	-0.065	0.972515	0.590591			3125.319	3152.428	3194.627
	H	2.407794	0.422394	-0.44824			3250.532	3293.116	3729.387
	O	2.552208	1.797527	-0.36009					
H	1.725011	1.921614	0.138363						
TS6 (C _i)	C	-1.86851	0.776332	1.136631	-460.8133187	0.156092	-1105.6	31.6551	73.1819
	H	-2.5373	1.349084	1.774665			93.6391	121.2584	141.906
	H	-1.0813	0.314219	1.730462			159.4169	209.9431	254.3435
	C	-1.35159	1.550285	-0.05729			370.0646	399.8902	428.2553
	H	-2.15758	2.124395	-0.5122			468.285	480.7479	632.52
	H	-0.59405	2.265207	0.273098			722.7826	741.0015	801.1733
	C	-0.75108	0.643577	-1.14537			834.4838	876.1607	895.265
	H	-1.53871	0.041834	-1.59232			929.9318	944.5395	974.7753
	H	-0.2653	1.247351	-1.90942			1008.858	1013.424	1077.255
	C	0.249214	-0.29934	-0.54635			1098.526	1119.257	1181.964
	C	2.449247	-0.40753	0.266275			1210.805	1273.126	1308.034
	H	2.190667	-1.42443	0.519638			1319.221	1333.018	1349.704
	C	3.616222	0.163147	0.488997			1391.023	1426.959	1471.167
	H	4.401437	-0.4038	0.963265			1477.543	1485.608	1494.276
	H	3.805735	1.188437	0.206114			1744.28	1834.539	3060.647
	O	1.438597	0.310234	-0.34097			3097.113	3104.342	3118.526
	O	0.031233	-1.43926	-0.23125			3165.768	3168.66	3194.73
	H	-2.52867	-0.13952	0.750426			3246.414	3292.974	3700.317
O	-2.93368	-1.30079	0.18233						
H	-2.04518	-1.68309	0.05806						
TS7 (C _i)	C	-1.84885	1.640291	0.20115	-460.8183228	0.160206	-399.055	23.5206	47.8643
	H	-2.14957	2.59474	-0.22778			55.5116	104.9579	143.7351
	H	-0.7693	1.675903	0.363573			187.3794	230.9024	274.5921
	H	-2.33142	1.540075	1.174448			301.3294	338.3533	385.9365
	C	-2.23087	0.485345	-0.71644			427.095	498.9119	611.376
	H	-3.29932	0.507667	-0.93174			696.3479	758.8436	783.1535
	H	-1.71052	0.578496	-1.66933			820.1754	880.9189	893.0501
	C	-1.9019	-0.87807	-0.09747			923.457	950.4401	983.6882
	H	-2.49677	-1.05699	0.79572			1002.254	1061.31	1102.075
	H	-2.09516	-1.67739	-0.81445			1112.955	1196.761	1219.824
	C	-0.46318	-0.95522	0.318385			1279.621	1288.538	1323.283

	C	1.710373	-0.75429	-0.46753			1365.52	1381.349	1426.891
	H	2.044679	-1.58289	0.140566			1431.699	1475.32	1496.088
	C	2.495758	0.24834	-0.87982			1506.391	1513.419	1645.033
	H	3.56028	0.188468	-0.72286			1856.726	3052.717	3079.205
	H	2.105517	1.026554	-1.51644			3086.634	3107.792	3128.38
	O	0.366874	-0.72467	-0.74			3139.364	3150.151	3205.342
	O	-0.04471	-1.15078	1.42304			3225.325	3307.225	3752.646
	O	2.027832	1.462303	0.793138					
	H	1.773624	0.792124	1.449235					
TS8 (C _i)	C	-2.13444	1.418836	0.329322	-460.8183695	0.159663	-356.709	27.9521	56.568
	H	-2.45252	2.414439	0.023437			70.5362	108.9899	133.7443
	H	-1.14773	1.507579	0.787269			166.4759	214.1519	233.905
	H	-2.82751	1.061419	1.092066			281.2075	290.7848	388.96
	C	-2.0999	0.468515	-0.86099			432.0712	470.1298	626.0858
	H	-3.07267	0.438104	-1.35239			666.6536	683.97	704.5309
	H	-1.37974	0.82087	-1.59985			814.351	865.298	885.6439
	C	-1.73218	-0.96223	-0.44998			892.7244	920.531	1006.749
	H	-2.47634	-1.376	0.227281			1015.702	1065.308	1100.538
	H	-1.65855	-1.60119	-1.33083			1113.959	1210.978	1216.719
	C	-0.41735	-0.99569	0.270533			1275.393	1285.09	1309.661
	C	1.81871	-0.38428	-0.01586			1362.55	1378.734	1424.654
	H	1.923306	-0.67908	1.016401			1427.366	1476.815	1494.446
	C	2.836814	0.004895	-0.80046			1504.608	1512.642	1631.57
	H	3.814111	0.1439	-0.36832			1883.151	3057.454	3076.256
	H	2.683654	0.203284	-1.85164			3086.93	3108.033	3130.675
	O	0.595705	-0.6049	-0.57027			3138.238	3150.052	3190.791
	O	-0.23196	-1.29588	1.409787			3253.6	3300.464	3786.454
	O	1.545608	1.605131	0.734072					
	H	1.689264	2.131553	-0.06754					
TS9 (C _i)	C	1.727131	1.646003	-0.40435	-460.8234558	0.158462	-1709.87	55.9749	81.597
	H	2.547479	2.341936	-0.57183			85.7677	128.7342	184.5068
	H	0.839936	2.212969	-0.12527			199.8507	274.9579	291.1453
	H	1.520366	1.141837	-1.34909			359.1422	426.3414	476.1802
	C	2.091078	0.632919	0.674447			551.5047	570.2371	619.657
	H	2.983211	0.075839	0.36836			730.9913	758.5814	858.8356
	H	2.346333	1.141134	1.604786			885.3355	914.8748	941.1167
	C	0.997534	-0.3634	0.949			949.3159	1035.52	1081.994
	H	1.169868	-1.01142	1.807813			1107.749	1121.002	1122.659
	H	-0.253	0.073277	1.232169			1167.49	1176.896	1234.14
	C	0.495619	-1.15465	-0.22007			1291.432	1313.929	1361.229
	C	-1.44449	-0.46782	0.817931			1373.391	1375.29	1390.829
	H	-1.86199	-1.04346	1.640776			1415.122	1423.527	1472.922
	C	-2.33796	0.575884	0.217475			1493.232	1500.381	1511.718
	H	-3.21199	0.091809	-0.23783			1728.821	1901.638	3006.376
	H	-2.69658	1.242728	1.000523			3034.76	3067.373	3095.905
	O	-0.86804	-1.28615	-0.1696			3117.818	3119.67	3135.762
	O	1.128316	-1.61795	-1.11657			3137.145	3147.279	3857.58
	O	-1.65668	1.368521	-0.72855					
	H	-1.38589	0.804274	-1.4593					
TS10	C	3.661585	0.650844	0.922895	-460.8198129	0.158083	-405.66	43.4453	53.6987

(C _i)	H	4.422583	1.246083	0.441673			71.6825	103.9772	111.968
	H	3.954592	-0.29798	1.342738			169.7736	216.4459	277.4538
	H	2.822402	1.163766	1.365244			333.7584	362.5265	444.9398
	C	2.524367	-0.07121	-0.98164			480.2846	494.7846	519.571
	H	2.326765	0.978528	-1.14996			561.2992	635.2159	688.4863
	H	3.433611	-0.48688	-1.39091			811.1814	823.0077	844.5514
	C	1.526867	-0.87265	-0.55988			911.2834	975.9025	982.5608
	H	1.627885	-1.94568	-0.49171			1000.091	1076.998	1092.578
	C	0.264862	-0.28142	-0.10671			1103.179	1154.325	1249.283
	C	-1.89724	-0.76766	0.748739			1254.5	1316.262	1319.758
	H	-2.37107	-1.69044	1.072989			1394.689	1409.299	1422.632
	C	-2.78404	-0.03345	-0.25076			1429.894	1442.132	1461.337
	H	-2.56418	-0.41614	-1.25478			1493.129	1505.791	1608.08
	H	-3.82324	-0.27599	-0.0276			1772.399	3023.201	3088.146
	O	-0.64097	-1.21204	0.207812			3106.816	3125.131	3155.64
	O	0.05698	0.910949	-0.0134			3176.017	3231.534	3272.675
	O	-2.68499	1.366136	-0.18982			3290.355	3298.734	3777.408
	H	-1.74442	1.585891	-0.19309					
	H	-1.71145	-0.12831	1.612773					
TS11 (C _i)	C	0.623535	2.069685	-0.68761	-460.8286728	0.158387	-1599.28	67.9075	82.8138
	H	-0.17367	2.810227	-0.6757			99.9094	150.9158	179.8725
	H	0.377598	1.33209	-1.45412			212.7005	256.163	332.4058
	H	1.548208	2.565575	-0.9975			380.7204	462.1904	476.2457
	C	0.789767	1.415517	0.65716			536.2388	557.0686	608.3045
	H	0.905452	2.100248	1.492541			690.7266	797.2591	850.391
	H	-0.32498	0.73592	0.922592			897.2886	916.3978	945.0109
	C	1.726276	0.231442	0.700044			959.4721	1044.805	1087.603
	H	2.721865	0.452956	0.315681			1103.726	1122.964	1143.669
	H	1.836246	-0.1293	1.72583			1171.192	1218.408	1230.1
	C	1.19873	-0.92119	-0.1333			1267.091	1310.772	1346.54
	C	-0.92654	-0.48323	0.903888			1362.119	1375.442	1402.665
	H	-0.8443	-0.88831	1.912571			1416.42	1425.435	1462.836
	C	-2.32183	-0.35896	0.372992			1483.221	1491.24	1493.761
	H	-2.76652	-1.35591	0.259097			1585.482	1877.27	3008.581
	H	-2.92814	0.199905	1.084501			3037.925	3066.687	3097.062
	O	-0.13197	-1.18582	-0.02043			3102.77	3120.308	3123.071
	O	1.859111	-1.58153	-0.87576			3138.086	3148.42	3860.467
	O	-2.35769	0.344029	-0.85018					
H	-1.84698	-0.15637	-1.49356						
TS12 (C _i)	C	-4.03878	-0.13922	0.168582	-460.8051883	0.15595	-795.956	55.4975	79.0365
	H	-4.21276	0.900583	0.437494			110.2923	130.8682	185.6926
	H	-4.41918	-0.77528	0.9713			192.7181	196.7661	282.2385
	H	-4.62418	-0.37716	-0.72109			337.442	383.004	410.8069
	C	-2.59712	-0.41524	-0.06363			420.8458	449.6081	510.291
	H	-2.31054	-1.41722	-0.36451			560.8253	740.2776	747.6671
	C	-1.61288	0.478606	0.121648			836.2192	872.4145	922.7546
	H	-1.81584	1.519424	0.335722			986.207	991.1422	1020.047
	H	-1.05511	0.364717	1.957663			1070.126	1085.338	1091.978
	C	-0.21324	0.123101	-0.21659			1138.861	1152.543	1238.021
	C	1.984911	0.977546	-0.42354			1252.475	1311.852	1317.416

	H	2.093758	0.558679	-1.42431			1350.437	1398.362	1409.477
	C	2.68651	0.076929	0.590202			1418.015	1458.928	1478.939
	H	3.686299	0.470364	0.771968			1486.281	1494.755	1504.758
	H	2.132999	0.128362	1.536493			1681.644	1805.238	3016.655
	O	0.588338	1.183246	-0.14187			3053.613	3092.153	3106.36
	O	0.160998	-0.9855	-0.51821			3111.787	3148.602	3161.206
	O	2.860403	-1.24719	0.155625			3185.224	3210.637	3799.293
	H	1.99478	-1.5704	-0.12328					
	H	2.395445	1.983186	-0.40185					
TS13	C	-2.44814	1.195022	0.317749	-460.8171116	0.161026	-332.713	45.8236	67.5375
(C _i)	H	-2.84564	0.63777	1.164478			93.705	101.4533	145.2925
	H	-3.22225	1.868785	-0.055			155.6461	181.2515	237.3969
	H	-1.62244	1.820905	0.664265			296.2095	345.2059	383.4139
	C	-1.97275	0.279587	-0.7555			433.2951	476.289	543.18
	H	-1.53264	0.739573	-1.63353			684.503	738.6296	861.3232
	C	-1.95876	-1.0638	-0.64911			911.3343	932.8735	944.1844
	H	-2.46127	-1.55417	0.175085			949.3041	1010.93	1032.08
	H	-1.65079	-1.68558	-1.4783			1056.118	1104.422	1117.082
	C	0.007247	-1.2251	0.399788			1158.472	1199.128	1256.004
	C	2.150046	-0.44593	-0.2013			1301.684	1306.88	1366.194
	H	2.383173	-0.64919	0.844053			1397.475	1403.452	1440.078
	C	2.013731	1.037302	-0.45869			1450.353	1473.069	1493.064
	H	2.970503	1.5107	-0.20991			1494.503	1512.882	1632.748
	H	1.817107	1.210076	-1.51738			1821.367	3029.929	3049.839
	O	0.928752	-1.139	-0.54751			3090.975	3103.008	3105.935
	O	0.078725	-0.84789	1.528098			3140.133	3157.099	3159.674
	O	0.949953	1.628861	0.252996			3174.295	3251.244	3823.859
	H	0.834443	1.176608	1.096202					
	H	2.922112	-0.87375	-0.8363					
TS14	C	-1.6943	1.343312	0.4813	-460.8386858	0.159146	-1652.78	77.9339	142.1633
(C _i)	H	-2.03313	2.357175	0.287437			179.0666	231.8206	247.9626
	H	-0.34741	1.469641	0.353215			331.9973	359.8975	367.9036
	H	-1.7969	1.072426	1.530483			469.6662	478.6501	525.2053
	C	-2.21231	0.30954	-0.49259			542.9672	551.2502	676.9327
	H	-3.30581	0.298317	-0.48024			723.4765	745.2081	832.3093
	H	-1.91186	0.577191	-1.50547			858.7438	897.8763	930.9835
	C	-1.69991	-1.10753	-0.17755			940.9309	985.6656	1048.441
	H	-2.18203	-1.52361	0.703965			1078.058	1095.336	1107.529
	H	-1.86552	-1.76946	-1.02673			1126.459	1169.124	1216.932
	C	-0.23252	-0.9856	0.114015			1240.739	1288.079	1339.427
	C	1.527724	0.42233	-0.57737			1350.234	1367.981	1390.254
	H	1.834758	0.821723	-1.53931			1406.576	1433.13	1450.512
	C	1.015211	1.520671	0.33548			1459.223	1471.542	1474.182
	H	1.261255	1.372427	1.381927			1487.611	1825.586	3049.714
	H	1.24924	2.52263	-0.00777			3096.912	3098.41	3108.149
	O	0.431172	-0.46318	-0.92859			3130.61	3146.978	3157.178
	O	0.280547	-1.19693	1.184035			3180.957	3212.033	3802.613
	O	2.607346	-0.28045	-0.07416					
	H	2.321495	-0.69034	0.752495					
TS15	C	2.250142	1.428319	-0.22437	-460.8357384	0.160271	-561.71	54.3794	61.1863

(C _i)	H	1.446152	1.952719	0.274333			77.5814	145.9614	158.0415
	H	2.576155	1.815669	-1.17978			223.5957	247.2438	253.5349
	C	2.75797	0.278281	0.278235			352.8881	384.3952	439.3185
	H	3.632039	-0.17523	-0.17037			476.8988	523.0335	570.3652
	H	2.521396	-0.02472	1.289897			659.6978	724.1112	744.7041
	C	1.475441	-1.38115	-0.47264			789.2601	827.8754	835.009
	H	1.673852	-1.30909	-1.52978			924.8213	934.756	984.7614
	H	1.955727	-2.1563	0.103374			1007.64	1028.714	1044.798
	C	0.221104	-0.87384	0.03923			1100.973	1122.295	1186.522
	C	-1.60906	0.588367	-0.4261			1246.438	1301.643	1308.474
	H	-1.79512	1.28281	-1.24172			1346.747	1401.573	1421.153
	C	-2.77056	-0.37007	-0.26065			1460.555	1469.399	1472.618
	H	-2.58402	-1.06159	0.557791			1492.334	1505.611	1586.952
	H	-3.66966	0.204731	-0.04618			1745.965	3080.665	3132.237
	O	-0.42393	-0.11372	-0.86304			3153.303	3156.999	3164.534
	O	-0.17344	-1.04305	1.17901			3172.235	3190.079	3235.224
	O	-1.35288	1.360963	0.695664			3263.376	3304.717	3788.515
	H	-1.18281	0.752091	1.426717					
H	-2.92194	-0.93401	-1.17949						
TS16 (C _i)	C	2.697702	-0.75265	-0.56374	-460.8387519	0.158217	-1570.29	77.1237	78.8618
	H	3.773495	-0.90313	-0.49112			132.6783	152.3557	199.0392
	H	2.520095	0.082629	-1.24026			283.2991	337.418	362.3299
	H	2.260945	-1.65122	-1.00211			410.5715	430.5057	479.7192
	C	2.091925	-0.47035	0.807599			518.0927	537.2128	610.6975
	H	2.289179	-1.30036	1.485826			699.4471	751.5487	774.1703
	H	2.565331	0.416793	1.237709			859.4477	911.6448	915.1392
	C	0.606359	-0.2285	0.74952			954.0972	972.2451	1067.189
	H	-0.02944	-1.14648	0.061573			1089.082	1104.498	1110.315
	H	0.066893	-0.30835	1.690444			1128.388	1144.012	1203.244
	C	0.18465	0.985609	-0.00942			1263.021	1293.949	1340.621
	C	-1.89607	-0.19122	-0.40276			1359.896	1370.106	1412.664
	H	-2.69547	0.000168	-1.12219			1415.731	1424.531	1462.978
	C	-1.12659	-1.43783	-0.72085			1475.604	1502.492	1512.402
	H	-1.56576	-2.35198	-0.34223			1551.571	1852.551	3051.368
	H	-0.74495	-1.48706	-1.73452			3063.51	3067.574	3103.677
	O	-1.08085	0.97808	-0.51601			3132.684	3143.98	3144.44
	O	0.885332	1.932644	-0.2231			3146.391	3241.638	3866.394
O	-2.41027	-0.31601	0.890045						
H	-2.94185	0.460866	1.087283						
TS17 (C _i)	C	-3.69348	-0.22284	1.122584	-460.8367147	0.15806	-411.145	46.4752	56.098
	H	-4.61508	0.284036	0.880126			106.2551	123.6035	138.0164
	H	-2.95579	0.315451	1.696221			171.9879	236.4328	275.539
	H	-3.71718	-1.29732	1.208305			319.5079	338.603	426.832
	C	-2.61206	0.008749	-0.9295			467.2132	487.5969	496.9447
	H	-3.43642	-0.46606	-1.44139			558.383	591.7204	663.6271
	H	-2.67738	1.071586	-0.74105			703.614	809.2359	845.8663
	C	-1.42098	-0.61019	-0.81368			878.9007	930.6983	961.9264
	H	-1.26462	-1.63792	-1.10662			985.0477	1000.747	1082.478
	C	-0.29101	0.099409	-0.20723			1091.877	1131.029	1191.813
	C	1.983718	-0.00078	0.387783			1252.198	1308.403	1318.063

	H	1.687434	0.244359	1.410447			1398.02	1407.792	1422.926
	C	3.101552	-1.00436	0.337496			1430.605	1442.503	1480.268
	H	3.979602	-0.58863	0.826307			1490.804	1496.72	1606.711
	H	2.807219	-1.92336	0.839141			1771.232	3074.081	3084.298
	O	0.837108	-0.62498	-0.22938			3123.484	3166.461	3169.843
	O	-0.34902	1.212548	0.273529			3175.979	3230.37	3272.344
	O	2.359245	1.137872	-0.30466			3288.394	3297.283	3819.711
	H	1.665436	1.794829	-0.17026					
	H	3.341733	-1.22038	-0.70192					
P1 (C _i)	C	-2.6551	0.694142	0.753487	-384.3898473	0.13514	42.7485	70.3725	128.7419
	H	-3.5634	1.269015	0.57939			164.7704	184.0309	240.4472
	H	-1.85006	1.39654	0.96616			310.9822	341.3503	425.3568
	H	-2.81422	0.077145	1.639323			520.5141	583.642	680.819
	C	-2.31328	-0.1704	-0.45375			724.2459	780.9902	839.9085
	H	-3.13934	-0.8484	-0.6705			891.9359	898.7731	912.5343
	H	-2.17471	0.459304	-1.33272			920.0493	1048.61	1078.449
	C	-1.05544	-0.99862	-0.23793			1107.832	1137.83	1203.219
	H	-1.105	-1.5741	0.6879			1255.031	1303.421	1349.384
	H	-0.91249	-1.72599	-1.04083			1378.5	1407.153	1417.114
	C	0.196233	-0.15959	-0.2027			1459.938	1489.047	1503.097
	C	2.513143	-0.32902	0.325234			1512.755	1676.809	1852.982
	H	3.195515	-1.07704	0.707672			3062.448	3069.035	3078.314
	C	2.912195	0.870949	0.012227			3106.452	3116.358	3134.438
	H	2.570912	1.813423	-0.36393			3145.259	3198.87	3346.079
	O	1.241081	-0.88803	0.253061					
	O	0.284702	0.983693	-0.54705					
P2 (C _i)	C	2.882358	-0.54567	0.679852	-384.3936333	0.135	37.7199	61.5022	94.7899
	H	3.867196	-0.94758	0.447218			139.4692	175.357	230.6735
	H	2.198919	-1.38488	0.802644			298.4527	337.9756	412.8628
	H	2.952653	-0.01826	1.632475			468.7013	565.0609	629.0043
	C	2.399128	0.389469	-0.42185			683.7571	798.1904	872.1647
	H	3.10678	1.208779	-0.55081			887.0555	889.584	912.0288
	H	2.352225	-0.14716	-1.36962			992.4667	1073.018	1102.225
	C	1.029646	0.981413	-0.12279			1118.85	1159.082	1173.827
	H	0.993206	1.439156	0.86758			1253.92	1303.638	1377.216
	H	0.767915	1.771366	-0.83109			1399.099	1408.343	1418.515
	C	-0.07073	-0.03773	-0.20269			1458.425	1489.619	1504.414
	C	-2.32984	-0.29528	0.28484			1513.258	1747.458	1886.294
	C	-3.5842	0.010975	0.079502			3062.9	3069.132	3078.843
	H	-4.35201	-0.73881	0.190752			3105.774	3116.088	3135.088
	H	-3.86908	1.017304	-0.21028			3142.601	3146.724	3259.563
	O	-1.24397	0.49062	0.293926					
	O	-0.00304	-1.14299	-0.63893					
P3 (C _i)	C	-2.78815	0.483915	0.847517	-384.3909558	0.135411	38.6572	90.3634	113.5448
	H	-3.78077	0.914896	0.726231			156.9504	161.5876	230.2841
	H	-2.08452	1.301541	0.999176			300.6696	352.6285	438.9521
	H	-2.79809	-0.13136	1.748609			483.1921	579.3578	673.7905
	C	-2.39842	-0.34557	-0.36979			688.557	770.7682	815.4987
	H	-3.12684	-1.142	-0.52473			875.6548	889.4953	912.3443
	H	-2.41021	0.27946	-1.26283			972.463	1072.744	1096.146

	C	-1.02096	-0.97562	-0.22714			1112.139	1153.041	1221.963
	H	-0.92432	-1.53234	0.706549			1256.579	1293.815	1304.897
	H	-0.82152	-1.69163	-1.0283			1377.735	1408.44	1418.316
	C	0.092133	0.034948	-0.28311			1459.387	1488.858	1503.696
	C	2.398707	0.25628	0.062812			1512.901	1715.222	1859.041
	H	2.233409	1.271371	-0.28187			3062.972	3069.28	3078.838
	C	3.559061	-0.21861	0.419388			3106.542	3116.682	3134.976
	H	4.557045	0.173399	0.477143			3145.98	3176.197	3314.269
	O	1.266484	-0.53162	0.102932					
	O	-0.00379	1.174691	-0.63519					
P4 (C _i)	C	3.057841	0.100977	0.835502	-384.4241103	0.1355	49.4635	59.2468	97.6047
	H	3.092146	-0.75241	1.511858			154.1771	163.0441	239.1068
	H	2.468782	0.889202	1.301448			305.8566	347.1732	428.9434
	H	4.07333	0.466597	0.691158			484.1852	574.3254	693.425
	C	2.435287	-0.29167	-0.51558			729.134	760.44	811.3872
	H	2.414764	0.588898	-1.15852			904.3894	918.7979	920.8197
	H	3.047613	-1.05484	-0.99474			1011.181	1018.929	1052.674
	C	1.052991	-0.79268	-0.34031			1107.37	1145.119	1192.992
	H	0.836629	-1.8435	-0.21729			1226.654	1297.022	1329.587
	C	-0.04101	0.141355	-0.23153			1332.899	1398.578	1424.682
	C	-2.36094	0.266265	0.092155			1461.448	1485.71	1502.371
	H	-2.19565	1.330261	0.010386			1511.069	1739.384	1763.97
	C	-3.53361	-0.30596	0.291564			3067.526	3076.845	3121.253
	H	-4.41447	0.309096	0.384019			3143.417	3151.543	3194.599
	H	-3.63218	-1.37932	0.364333			3228.351	3244.112	3292.566
	O	-1.22953	-0.50128	-0.02863					
O	0.060233	1.343324	-0.30682						
P5 (C _i)	C	3.662812	-0.44609	-0.02122	-384.4138163	0.133056	35.8639	61.1642	83.2738
	H	3.837589	-0.96972	0.92725			110.5803	125.7683	140.2168
	H	4.494561	0.237152	-0.17661			260.8614	299.7883	343.0207
	H	3.701654	-1.21195	-0.8024			412.4441	472.3048	567.4644
	C	2.359746	0.263579	-0.02283			734.3549	735.6015	903.9821
	H	2.300676	1.337444	0.055175			910.4407	925.6689	928.9054
	C	1.102265	-0.51874	0.032349			995.5143	1017.472	1021.669
	H	1.028103	-1.23529	-0.79475			1112.953	1164.403	1187.659
	H	1.043107	-1.14331	0.935024			1198.763	1220.525	1321.169
	C	-0.14128	0.328419	0.008609			1334.189	1409.921	1425.94
	C	-2.48066	0.142499	-0.00754			1439.241	1446.781	1478.986
	H	-2.45285	1.2218	-0.01128			1489.239	1743.664	1867.109
	C	-3.57655	-0.59087	-0.01268			2998.195	3003.059	3030.753
	H	-4.5393	-0.10516	-0.02112			3049.465	3143.315	3193.977
	H	-3.53268	-1.67032	-0.00869			3239.813	3245.505	3291.894
	O	-1.24456	-0.46461	0.003341					
O	-0.18531	1.522934	0.00132						
P6 (C _i)	C	2.858105	0.48492	0.860857	-384.4095008	0.13382	37.8712	76.1702	107.7465
	H	2.473801	1.488333	0.952125			110.4393	153.0594	175.4237
	H	3.400368	0.060553	1.691865			269.9395	347.3011	415.773
	C	2.511671	-0.3434	-0.32508			464.2218	521.8999	581.7868
	H	2.53854	0.267489	-1.22902			675.2013	736.618	794.5697
	H	3.233978	-1.15026	-0.44959			897.5206	901.2883	925.9165


	C	1.116102	-0.96961	-0.21904			968.7333	1015.184	1031.857
	H	0.926785	-1.65846	-1.04644			1087.746	1115.111	1183.616
	H	1.004523	-1.54798	0.698661			1214.006	1227.608	1294.529
	C	0.026235	0.066262	-0.25644			1332.829	1348.752	1399.18
	C	-2.28872	0.313286	0.038901			1428.739	1457.374	1463.703
	H	-2.09799	1.34287	-0.22423			1487.49	1743.592	1860.235
	C	-3.47147	-0.19247	0.328757			3066.799	3070.627	3111.366
	H	-4.34012	0.446343	0.311167			3121.147	3179.112	3193.01
	H	-3.59103	-1.23519	0.584886			3245.869	3285.944	3290.623
	O	-1.17087	-0.49157	0.05909					
	O	0.16332	1.220617	-0.54124					
P7 (C ₁)	C	3.133688	-0.49968	0.180606	-420.9973142	0.126202	64.3723	71.2674	135.4227
	H	2.877544	-1.51514	-0.09294			160.6259	219.5907	331.0409
	H	4.162892	-0.27628	0.42323			357.4281	456.6033	507.5118
	C	2.197875	0.435629	0.211711			542.3987	552.9166	683.7288
	H	2.401291	1.462972	0.47791			822.2014	849.3392	909.2239
	C	0.795349	0.097228	-0.12949			978.1369	1030.968	1038.438
	C	-1.37856	1.005022	-0.41584			1073.738	1087.802	1096.988
	H	-1.75855	2.022868	-0.40427			1154.158	1251.576	1257.586
	C	-2.18476	0.116844	0.526034			1315.285	1343.152	1395.106
	H	-1.73884	0.176259	1.526218			1413.316	1447.014	1459.064
	H	-3.1952	0.519938	0.593539			1493.257	1504.617	1725.914
	O	0.002602	1.163632	-0.03894			1806.767	3023.658	3091.658
	O	0.4106	-1.00224	-0.45077			3109.35	3161.048	3173.196
	O	-2.32113	-1.21075	0.089909			3227.05	3268.85	3790.768
	H	-1.43873	-1.53205	-0.13386					
	H	-1.42851	0.606056	-1.42954					
P8 (C ₁)	C	-4.04894	-0.14051	0.248407	-460.3118825	0.154138	55.6352	65.9022	120.7958
	H	-4.22789	0.897156	0.522012			125.3131	197.6149	211.7831
	H	2.468934	-1.78928	0.786869			1490.712	1495.328	1726.113
	O	0.297877	-0.64536	-0.03962			1805.795	3078.874	3085.328
	O	-0.8274	1.231483	0.44201			3167.61	3171.293	3173.441
	O	1.730083	1.096106	-0.62912			3226.541	3269.207	3823.876
	H	1.067003	1.771644	-0.44307					
	H	2.686781	-1.28827	-0.90351					
H (D _{∞h})	H	0	0	0	-0.4982065	0			
H₂O (C _{2v})	O	0	0	0.116392	-76.4301067	0.02093	1619.5383	3869.626	3972.571
	H	0	0.762467	-0.46557					
	H	0	-0.76247	-0.46557					
CH₃ (D _{3h})	C	-3E-06	0.000018	0.000046	-39.8253538	0.028859	432.1876	1411.548	1411.95
	H	0.880838	0.617978	-9.3E-05			3145.682	3322.149	3322.566
	H	-0.97567	0.453717	-9.3E-05					
	H	0.09485	-1.07181	-9.3E-05					
C₂H₄ (D _{2h})	C	-0.66105	-4E-06	-7.6E-05	-78.5728476	0.049824	825.6164	989.1604	1002.481
	H	-1.22751	0.921938	-0.00003			1059.512	1241.551	1386.222
	H	-1.22755	-0.92192	-4.4E-05			1473.304	1714.294	3159.595
	C	0.66105	-4E-06	0.000033			3175.56	3234.758	3261.209
	H	1.22756	-0.92191	0.000173					
	H	1.227515	0.921934	0.000158					

C₃H₆ (C _s)	C	-1.22714	0.162147	-4.2E-05	-117.8852525	0.07783	206.8079	430.3893	595.9599
	H	-1.1646	1.249309	-0.00011			938.2638	946.3078	965.7324
	H	-1.79703	-0.15079	0.876426			1033.365	1079.366	1194.823
	H	-1.79704	-0.15091	-0.87646			1328.857	1406.705	1453.474
	C	0.134514	-0.4558	-0.00001			1484.627	1497.022	1737.882
	H	0.171068	-1.54083	0.000026			3056.802	3110.993	3137.603
	C	1.272229	0.221631	0.000043			3158.457	3167.008	3247.972
	H	1.279843	1.305225	0.000059					
	H	2.230131	-0.27988	0.000119					
PC1 (C _i)	C	-3.38701	0.651619	0.937786	-460.8254289	0.157938879	21.6393	48.644	54.6351
	H	-4.31535	1.21407	0.851008			65.7861	79.6755	107.0861
	H	-2.57693	1.364291	1.088046			134.2047	172.7706	177.2235
	H	-3.45875	0.022409	1.82634			244.9021	256.561	291.2837
	C	-3.14028	-0.19393	-0.30556			312.0437	345.0721	427.6181
	H	-3.97153	-0.88315	-0.45664			525.2307	583.6806	684.328
	H	-3.09027	0.447216	-1.18574			719.3499	785.5626	846.1926
	C	-1.85581	-1.00409	-0.21212			890.8765	915.4044	921.3492
	H	-1.81299	-1.58933	0.707908			931.4152	1055.22	1081.196
	H	-1.77379	-1.7214	-1.03242			1108.226	1138.965	1202.217
	C	-0.61939	-0.14606	-0.27901			1254.325	1302.812	1352.452
	C	1.735939	-0.28757	0.039241			1377.609	1406.129	1417.668
	H	2.47129	-1.02062	0.346604			1459.522	1489.858	1503.971
	C	2.081397	0.92705	-0.29241			1512.469	1621.492	1668.356
	H	1.688024	1.866728	-0.6232			1854.668	3062.591	3069.579
	O	0.474531	-0.86365	0.071894			3078.778	3107.021	3116.707
	O	-0.57625	1.002191	-0.61454			3134.663	3145.047	3199.018
	H	4.679395	0.10501	-0.50834			3340.37	3851.261	3942.973
O	4.945961	-0.13875	0.382215						
H	4.517833	0.514321	0.942249						
PC2	C	2.368234	0.823284	-0.72627	-460.832675	0.158586148	34.3203	52.9963	62.6965
	H	2.468934	-1.78928	0.786869			1490.712	1495.328	1726.113
	O	0.297877	-0.64536	-0.03962			1805.795	3078.874	3085.328
	O	-0.8274	1.231483	0.44201			3167.61	3171.293	3173.441
	O	1.730083	1.096106	-0.62912			3226.541	3269.207	3823.876
	H	1.067003	1.771644	-0.44307					
	H	2.686781	-1.28827	-0.90351					
H (D _{∞h})	H	0	0	0	-0.4982065	0			
H₂O (C _{2v})	O	0	0	0.116392	-76.4301067	0.02093	1619.5383	3869.626	3972.571
	H	0	0.762467	-0.46557					
	H	0	-0.76247	-0.46557					
CH₃ (D _{3h})	C	-3E-06	0.000018	0.000046	-39.8253538	0.028859	432.1876	1411.548	1411.95
	H	0.880838	0.617978	-9.3E-05			3145.682	3322.149	3322.566
	H	-0.97567	0.453717	-9.3E-05					
	H	0.09485	-1.07181	-9.3E-05					
C₂H₄ (D _{2h})	C	-0.66105	-4E-06	-7.6E-05	-78.5728476	0.049824	825.6164	989.1604	1002.481
	H	-1.22751	0.921938	-0.00003			1059.512	1241.551	1386.222
	H	-1.22755	-0.92192	-4.4E-05			1473.304	1714.294	3159.595
	C	0.66105	-4E-06	0.000033			3175.56	3234.758	3261.209
	H	1.22756	-0.92191	0.000173					

	H	1.227515	0.921934	0.000158					
C₃H₆ (C _s)	C	-1.22714	0.162147	-4.2E-05	-117.8852525	0.07783	206.8079	430.3893	595.9599
	H	-1.1646	1.249309	-0.00011			938.2638	946.3078	965.7324
	H	-1.79703	-0.15079	0.876426			1033.365	1079.366	1194.823
	H	-1.79704	-0.15091	-0.87646			1328.857	1406.705	1453.474
	C	0.134514	-0.4558	-0.00001			1484.627	1497.022	1737.882
	H	0.171068	-1.54083	0.000026			3056.802	3110.993	3137.603
	C	1.272229	0.221631	0.000043			3158.457	3167.008	3247.972
	H	1.279843	1.305225	0.000059					
	H	2.230131	-0.27988	0.000119					
PC1 (C _i)	C	-3.38701	0.651619	0.937786	-460.8254289	0.157938879	21.6393	48.644	54.6351
	H	-4.31535	1.21407	0.851008			65.7861	79.6755	107.0861
	H	-2.57693	1.364291	1.088046			134.2047	172.7706	177.2235
	H	-3.45875	0.022409	1.82634			244.9021	256.561	291.2837
	C	-3.14028	-0.19393	-0.30556			312.0437	345.0721	427.6181
	H	-3.97153	-0.88315	-0.45664			525.2307	583.6806	684.328
	H	-3.09027	0.447216	-1.18574			719.3499	785.5626	846.1926
	C	-1.85581	-1.00409	-0.21212			890.8765	915.4044	921.3492
	H	-1.81299	-1.58933	0.707908			931.4152	1055.22	1081.196
	H	-1.77379	-1.7214	-1.03242			1108.226	1138.965	1202.217
	C	-0.61939	-0.14606	-0.27901			1254.325	1302.812	1352.452
	C	1.735939	-0.28757	0.039241			1377.609	1406.129	1417.668
	H	2.47129	-1.02062	0.346604			1459.522	1489.858	1503.971
	C	2.081397	0.92705	-0.29241			1512.469	1621.492	1668.356
	H	1.688024	1.866728	-0.6232			1854.668	3062.591	3069.579
	O	0.474531	-0.86365	0.071894			3078.778	3107.021	3116.707
	O	-0.57625	1.002191	-0.61454			3134.663	3145.047	3199.018
H	4.679395	0.10501	-0.50834	3340.37	3851.261	3942.973			
O	4.945961	-0.13875	0.382215						
H	4.517833	0.514321	0.942249						
PC2 (C _i)	C	2.368234	0.823284	-0.72627	-460.832675	0.158586148	34.3203	52.9963	62.6965
	H	2.905112	1.138707	-1.61943			87.0121	94.099	133.6984
	H	2.944183	1.142561	0.143517			141.6519	178.8699	183.451
	H	1.4146	1.354244	-0.70644			221.4845	253.1799	286.4403
	C	2.17023	-0.68713	-0.71899			382.2613	421.6183	439.4148
	H	1.578455	-0.99451	-1.58128			471.822	611.8872	645.2601
	H	3.130609	-1.1975	-0.79369			706.6852	815.9706	854.0183
	C	1.480254	-1.177	0.560629			875.1355	890.9349	919.9414
	H	1.324539	-2.25563	0.517399			997.2357	1056.15	1096.444
	H	2.075749	-0.93915	1.4394			1111.385	1161.806	1211.277
	C	0.148992	-0.51821	0.747548			1274.823	1285.547	1363.549
	C	-1.93051	-0.31848	-0.2795			1380.524	1405.754	1429.773
	C	-3.07709	-0.82704	-0.64825			1477.605	1497.218	1507.62
	H	-3.96541	-0.21481	-0.66717			1513.989	1627.14	1747.804
	H	-3.15347	-1.87175	-0.93213			1868.037	3056.685	3079.063
	O	-0.70868	-0.8661	-0.27098			3088.7	3109.871	3131.292
	O	-0.17403	0.227502	1.622838			3139.488	3142.873	3152.156
	H	-1.59351	2.459791	-0.45744			3260.901	3817.411	3933.329
	O	-0.72815	2.585563	-0.06185					
H	-0.73467	2.029753	0.726168						

PC3 (C _i)	C	2.248385	1.166686	-0.43345	-460.8281392	0.158509244	36.3306	38.4352	75.6103
	H	2.845986	1.629613	-1.21727			96.0284	110.6761	151.1311
	H	2.621858	1.521957	0.5281			162.9958	172.2415	206.7851
	H	1.222898	1.524789	-0.54051			218.6871	243.8504	278.4515
	C	2.327752	-0.35226	-0.51518			378.662	425.9031	459.9168
	H	1.951573	-0.70011	-1.47747			482.1106	640.2314	694.5768
	H	3.364628	-0.68147	-0.44214			719.1371	794.2355	857.0398
	C	1.538802	-1.03666	0.606387			873.6285	875.4845	895.2416
	H	1.619058	-2.12079	0.516696			927.2262	1047.896	1100.723
	H	1.912192	-0.73468	1.582711			1110.662	1156.649	1220.834
	C	0.081183	-0.67616	0.56751			1275.831	1285.562	1340.636
	C	-1.83859	-0.93247	-0.80723			1365.321	1383.251	1429.238
	H	-2.10571	-1.37581	-1.76047			1477.272	1497.128	1507.888
	C	-2.70729	-0.34168	-0.03103			1513.724	1632.374	1685.82
	H	-3.76586	-0.17284	-0.11398			1844.348	3056.957	3076.128
	O	-0.49077	-1.11385	-0.58225			3086.521	3107.576	3130.044
	O	-0.52249	-0.07899	1.414286			3138.147	3149.19	3167.897
	H	-1.76357	2.114394	-0.59675			3296.15	3827.29	3929.832
O	-1.08264	2.467984	-0.01975						
H	-1.03732	1.829082	0.700789						
PC4 (C _i)	C	-2.54041	-1.0533	0.880468	-460.8656893	0.159033196	37.3207	59.1989	64.7547
	H	-3.61403	-0.90202	0.788935			91.8462	93.5058	109.1409
	H	-2.13159	-0.20787	1.430595			146.7354	158.468	190.8812
	H	-2.35748	-1.96693	1.445388			237.3618	310.2623	345.0848
	C	-1.90546	-1.13467	-0.52006			357.4302	435.5938	491.392
	H	-2.33375	-1.9723	-1.06899			547.8956	587.8012	701.4053
	H	-2.14556	-0.21517	-1.05547			728.7481	766.2424	817.6862
	C	-0.43764	-1.29832	-0.4322			908.724	921.8674	924.6838
	H	0.033175	-2.2693	-0.47738			1010.143	1011.084	1048.91
	C	0.414793	-0.16422	-0.18926			1115.322	1144.794	1193.657
	C	2.655313	0.4565	0.131681			1238.065	1291.966	1324.275
	H	2.250837	1.452908	0.224929			1329.541	1401.834	1424.372
	C	3.933873	0.143311	0.222533			1468.917	1488.901	1496.144
	H	4.658148	0.921279	0.403975			1512.795	1640.572	1740.152
	H	4.273022	-0.87714	0.119154			1744.054	3070.444	3080.214
	O	1.722033	-0.52571	-0.09891			3124.621	3148.963	3158.882
	O	0.043645	0.987257	-0.07505			3194.644	3226.874	3249.322
	H	-2.67208	2.949003	-0.13999			3293.244	3744.996	3940.656
O	-2.63879	1.992192	-0.09554						
H	-1.69871	1.761851	-0.07415						
PC5 (C _i)	C	-2.17475	1.393455	-0.91421	-460.8552332	0.157792258	34.4863	50.6864	72.6735
	H	-1.73875	0.761366	-1.69977			81.5426	93.6996	119.2807
	H	-2.56007	2.291217	-1.39384			126.7413	144.8609	150.3049
	H	-3.00478	0.818401	-0.49927			211.2968	245.8552	352.6527
	C	-1.17887	1.722418	0.135566			382.4163	420.2405	447.7823
	H	-0.59703	2.630455	0.069167			471.6054	545.1468	646.9896
	C	-0.70445	0.654078	1.071789			733.2393	785.8412	872.1926
	H	-0.19431	1.077933	1.933828			904.8779	929.9442	934.1977
	H	-1.53883	0.027068	1.38869			998.1422	1012.536	1021.148
	C	0.255592	-0.22531	0.311367			1100.858	1150.454	1184.285

	C	2.50563	-0.41394	-0.32474			1228.293	1289.043	1314.796
	H	2.155752	-1.23806	-0.92752			1334.762	1386.656	1423.657
	C	3.755529	-0.00381	-0.24205			1426.727	1470.619	1479.506
	H	4.518258	-0.51002	-0.81208			1485.254	1638.829	1743.886
	H	4.034534	0.830394	0.385126			1815.045	2997.63	3081.564
	O	1.523181	0.229682	0.399469			3082.985	3141.994	3149.835
	O	-0.05471	-1.17907	-0.35688			3193.847	3207.295	3247.44
	H	-3.10646	-2.60845	0.073562			3291.866	3736.1	3937.813
	O	-2.82108	-1.69536	0.134737					
	H	-1.89953	-1.68368	-0.16277					
PC6 (C _i)	C	-1.58801	1.474821	1.152437	-460.8508071	0.157771576	32.9379	68.5971	76.9467
	H	-1.40493	2.082896	2.024445			88.246	100.1468	135.1902
	H	-2.31867	0.680363	1.213365			142.5413	151.4874	182.2302
	C	-1.02673	1.859451	-0.1692			207.162	275.3022	369.3977
	H	-1.70843	2.535236	-0.70056			405.3752	435.3616	472.8456
	H	-0.08964	2.404275	-0.04791			512.3899	548.0175	632.917
	C	-0.79902	0.637979	-1.07429			702.4288	738.2513	870.2051
	H	-1.73696	0.114161	-1.24612			887.0871	909.9617	928.0905
	H	-0.37482	0.951617	-2.02805			929.7637	1013.589	1031.337
	C	0.150468	-0.32534	-0.42492			1094.015	1106.984	1186.507
	C	2.379591	-0.53808	0.279478			1199.131	1229.669	1310.322
	H	2.044293	-1.47041	0.707479			1330.836	1366.912	1379.326
	C	3.613832	-0.07743	0.323119			1426.987	1470.502	1475.678
	H	4.376877	-0.65254	0.823015			1489.208	1636.918	1744.603
	H	3.879623	0.866222	-0.13075			1830.933	3004.223	3091.085
	O	1.395257	0.194238	-0.35048			3095.355	3155.975	3164.582
O	-0.12711	-1.4162	0.001963			3194.266	3249.846	3274.927	
H	-3.41487	-2.3096	0.365834			3292.327	3734.255	3938.866	
O	-2.96966	-1.49113	0.140816						
H	-2.02117	-1.68591	0.161086						

P5 + O ₂ channels									
Species	Cartesian coordinate (Å)				 (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm ⁻¹)		
P5 (C _i)	C	3.662812	-0.446087	-0.021218	-384.413816	0.133056	35.8639	61.1642	83.2738
	H	3.837589	-0.969723	0.92725			110.5803	125.7683	140.2168
	H	4.494561	0.237152	-0.176611			260.8614	299.7883	343.0207
	H	3.701654	-1.211951	-0.802397			412.4441	472.3048	567.4644
	C	2.359746	0.263579	-0.022834			734.3549	735.6015	903.9821
	H	2.300676	1.337444	0.055175			910.4407	925.6689	928.9054
	C	1.102265	-0.518737	0.032349			995.5143	1017.472	1021.669
	H	1.028103	-1.23529	-0.794747			1112.953	1164.403	1187.659
	H	1.043107	-1.143313	0.935024			1198.763	1220.525	1321.169
	C	-0.141276	0.328419	0.008609			1334.189	1409.921	1425.94
	C	-2.480661	0.142499	-0.007542			1439.241	1446.781	1478.986
	H	-2.452846	1.2218	-0.01128			1489.239	1743.664	1867.109
	C	-3.576547	-0.590872	-0.012678			2998.195	3003.059	3030.753
	H	-4.539301	-0.105158	-0.021124			3049.465	3143.315	3193.977
	H	-3.53268	-1.670317	-0.008694			3239.813	3245.505	3291.894
	O	-1.244556	-0.464614	0.003341					
O	-0.185307	1.522934	0.00132						
O₂ (D _{∞h})	O	0	0	0.594893	-150.324815	0.00389	1758.343		
	O	0	0	-0.594893					
IM7 (C _i)	C	3.035313	-0.949939	-0.548382	-534.798878	0.144343	28.5235	56.6011	81.2232
	H	2.945785	-2.016205	-0.751345			116.3817	130.4796	158.7725
	H	3.942357	-0.780715	0.028575			225.6783	243.3031	300.3351
	H	3.113725	-0.415778	-1.493692			327.9461	390.2289	438.0228
	C	1.824618	-0.475237	0.224241			486.0032	557.5284	640.8856
	H	1.732887	-0.976926	1.18551			735.1964	744.6401	835.3032
	C	0.533688	-0.596377	-0.557005			907.174	920.7876	930.1354
	H	0.53479	0.090866	-1.401908			946.1844	1014.661	1022.506
	H	0.444966	-1.605264	-0.965751			1069.78	1131.558	1156.149
	C	-0.68124	-0.350898	0.299363			1186.1	1225.793	1245.534
	C	-2.979422	0.083095	0.148338			1272.58	1328.765	1338.788
	H	-2.938736	0.070319	1.226963			1400.54	1415.309	1422.473
	C	-4.063903	0.279849	-0.574199			1431.853	1449.569	1489.568
	H	-5.007457	0.445501	-0.079073			1506.61	1744.83	1864.118
	H	-4.029387	0.281676	-1.653964			3077.295	3086.488	3130.945
	O	-1.766185	-0.125396	-0.475914			3143.49	3155.443	3162.23
	O	-0.704597	-0.37846	1.494896			3194.795	3248.057	3293.153
	O	2.014759	0.916722	0.623548					
O	2.111866	1.70758	-0.398712						
IM8 (C _i)	C	-2.227801	-0.954967	-0.675486	-534.786984	0.144786	87.7288	100.8959	113.5972
	H	-3.251986	-0.683634	-0.422449			132.3436	212.385	240.3897
	H	-2.211942	-1.987023	-1.020572			290.4662	355.8236	368.4426
	H	-1.889856	-0.308167	-1.482839			418.3255	440.5098	480.4973
	C	-1.346311	-0.80633	0.550633			517.7416	609.3366	660.5732
	H	-1.761304	-1.380463	1.37988			733.0088	760.0961	838.028

	C	-1.201235	0.659773	0.999953			880.1049	911.5786	933.0748
	H	-2.165319	1.159298	0.939831			945.157	971.1189	1011.132
	H	-0.826823	0.690224	2.021926			1046.032	1120.211	1132.737
	C	-0.2117	1.381051	0.125185			1158.505	1161.039	1198.046
	C	1.569909	-0.022691	-0.434446			1256.891	1305.058	1349.566
	H	1.845901	0.393303	-1.409644			1369.187	1373.641	1389.475
	C	2.693288	-0.704129	0.238458			1419.839	1458.276	1476.195
	H	2.835356	-0.58531	1.299071			1493.198	1502.541	1897.402
	H	3.287372	-1.406287	-0.323026			3051.861	3076.593	3094.149
	O	1.082357	0.989835	0.417333			3104.491	3150.768	3161.886
	O	-0.455596	2.187203	-0.713713			3164.38	3196.482	3315.228
	O	-0.075225	-1.435092	0.376493					
	O	0.508676	-0.892967	-0.806108					
IM9 (C _i)	C	2.881237	0.143977	0.358195	-534.794962	0.146933	88.9935	125.6242	158.2156
	H	3.307229	1.145156	0.329556			215.8003	246.6757	247.8533
	H	3.518119	-0.526603	-0.214407			322.009	326.4656	435.9672
	H	2.855867	-0.196081	1.39347			452.5931	469.6038	485.8641
	C	1.48233	0.160788	-0.224129			543.0035	593.9686	680.657
	H	1.499665	0.489729	-1.266154			778.5644	869.9375	877.7061
	C	0.551394	1.068634	0.58115			922.875	930.6687	957.0054
	H	0.458324	0.672548	1.592288			976.0253	1045.33	1075.506
	H	1.001058	2.059516	0.619973			1124.202	1138.369	1156.325
	C	-0.808066	1.274404	-0.048301			1199.988	1246.706	1276.428
	C	-1.5831	-0.751496	0.902814			1298.342	1315.225	1378.804
	H	-2.175085	-1.03234	1.761119			1383.178	1393.742	1409.033
	C	-1.164678	-1.757982	-0.108865			1415.662	1460.442	1467.871
	H	-0.858021	-2.687536	0.373666			1490.39	1504.031	1889.199
	H	-1.980161	-1.973339	-0.809608			3029.566	3069.016	3074.792
	O	-1.838297	0.506561	0.440296			3091.177	3102.447	3146.52
	O	-1.043484	2.109433	-0.863015			3152.515	3162.14	3222.855
	O	1.052831	-1.192044	-0.188688					
	O	-0.143763	-1.271574	-0.956729					
TS18 (C _i)	C	-2.803335	-1.544123	-0.192491	-534.749924	0.139164	-964.5533	43.8862	83.6045
	H	-2.871548	-1.490514	-1.2779			91.8087	124.0163	148.2411
	H	-3.765349	-1.278622	0.24114			165.5853	212.6794	241.6301
	H	-2.58115	-2.576086	0.086188			277.5604	375.9208	414.2284
	C	-1.716362	-0.662509	0.323042			463.2506	502.6302	620.1721
	H	-1.658508	-0.527397	1.397047			648.8989	722.3156	743.4533
	C	-0.543155	-0.424265	-0.39981			774.9444	910.6741	922.7077
	H	-0.400878	-0.905465	-1.359084			934.6859	938.5458	1012.739
	H	-0.988567	0.883251	-0.760697			1017.381	1061.692	1118.106
	C	0.671339	-0.09329	0.36143			1149.623	1185.556	1214.585
	C	3.000791	0.059976	0.1457			1230.265	1281.142	1326.176
	H	2.955213	0.409052	1.166348			1367.361	1398.408	1415.142
	C	4.104762	-0.084684	-0.561332			1426.94	1478.295	1490.232
	H	5.055758	0.157794	-0.114499			1556.89	1725.974	1743.83
	H	4.078851	-0.44065	-1.581015			1833.615	3064.769	3131.315
	O	1.779795	-0.24279	-0.412551			3155.694	3190.227	3194.649
	O	0.705622	0.283726	1.501581			3197.905	3246.408	3292.339

	O	-1.858801	1.704116	-0.651376					
	O	-2.640124	1.0377	0.08025					
TS19 (C _i)	C	2.980997	-0.834192	-0.498831	-534.741053	0.138941	-1097.961	23.154	69.4138
	H	3.869175	-1.12695	0.046133			81.1482	115.2823	138.4413
	H	3.080007	0.523199	-0.499231			159.0483	217.4298	304.2794
	H	2.980478	-1.06381	-1.558737			352.8278	425.3144	455.7016
	C	1.770783	-0.808252	0.173179			482.0355	549.0908	571.5962
	H	1.7344	-0.941652	1.246298			639.905	679.8452	736.4611
	C	0.465514	-0.961613	-0.53622			756.4661	907.8917	917.67
	H	0.464459	-0.43559	-1.489727			930.4428	938.3998	1004.527
	H	0.297754	-2.021084	-0.759624			1014.114	1025.533	1067.323
	C	-0.703368	-0.513313	0.303891			1146.481	1183.535	1218.186
	C	-2.921215	0.220303	0.131959			1237.905	1281.513	1302.17
	H	-2.873989	0.256042	1.209768			1330.472	1367.832	1405.529
	C	-3.976251	0.520612	-0.598509			1427.149	1444.947	1457.889
	H	-4.886248	0.832943	-0.111441			1591.613	1654.38	1745.035
	H	-3.950164	0.463808	-1.677015			1867.834	3050.248	3130.018
	O	-1.749923	-0.174569	-0.482314			3140.475	3194.253	3209.698
	O	-0.72611	-0.496167	1.498883			3231.148	3248.453	3292.074
O	1.570875	1.241834	0.395473						
O	2.603328	1.650379	-0.194445						
TS20 (C _i)	C	-2.273926	-0.704262	-0.784871	-534.75804	0.143814	-765.2694	86.5894	121.3711
	H	-3.266691	-0.275382	-0.653871			160.7353	199.1706	233.087
	H	-2.375858	-1.742225	-1.095618			257.635	317.9285	354.6793
	H	-1.757877	-0.15334	-1.568401			393.2596	434.0209	442.9593
	C	-1.516166	-0.633117	0.526145			486.2074	562.9397	616.4428
	H	-2.093849	-1.108788	1.318796			673.947	782.7692	808.2529
	C	-1.220862	0.817238	0.964552			823.5224	870.1765	909.7557
	H	-2.107935	1.431256	0.826991			933.6263	958.1963	998.5668
	H	-0.907063	0.826852	2.006072			1040.767	1072.747	1114.251
	C	-0.106215	1.33831	0.114734			1142.854	1204.973	1207.59
	C	1.761528	0.082216	-0.344862			1248.549	1273.609	1293.826
	H	1.68074	0.412585	-1.371497			1370.51	1384.187	1419.97
	C	2.801546	-0.690021	0.098852			1421.589	1476.545	1491.514
	H	3.405351	-1.225933	-0.614462			1502.519	1529.795	1900.482
	H	2.946493	-0.854533	1.155261			3077.224	3096.593	3108.712
	O	1.101768	0.84311	0.575021			3151.989	3162.684	3169.015
	O	-0.186809	2.015329	-0.858989			3195.952	3212.851	3307.155
O	-0.327231	-1.43848	0.502646						
O	0.387428	-1.241544	-0.649999						
TS21 (C _i)	C	-1.693106	-1.492731	-0.608629	-534.756347	0.144292	-225.9631	51.0166	133.6073
	H	-2.725984	-1.329623	-0.304621			155.2755	189.0546	221.2772
	H	-1.576672	-2.521809	-0.942856			262.0002	282.898	315.6385
	H	-1.483164	-0.820738	-1.437993			391.3197	445.1871	495.627
	C	-0.776091	-1.219649	0.566023			549.0424	611.4682	640.695
	H	-1.004537	-1.9071	1.383273			659.5089	745.3609	832.9903
	C	-0.883884	0.203542	1.118135			869.8294	882.9551	928.4743
	H	-1.877936	0.305172	1.551195			938.7997	973.8311	994.1242
	H	-0.146247	0.347653	1.904525			1010.387	1049.965	1107.635

	C	-0.781641	1.313881	0.081069			1172.646	1216.631	1227.238
	C	1.798315	0.102713	-0.584539			1281.64	1318.064	1326.174
	H	2.098671	0.591759	-1.500135			1365.048	1392.156	1423.058
	C	2.318738	0.429804	0.625817			1439.601	1472.729	1487.083
	H	2.081758	-0.125753	1.516524			1503.416	1592.016	1753.807
	H	2.965768	1.289031	0.681397			3081.096	3083.33	3103.594
	O	0.405575	1.718797	-0.305852			3154.829	3157.282	3164.878
	O	-1.776177	1.840937	-0.365678			3217.824	3238.167	3327.409
	O	0.580287	-1.608609	0.294034					
	O	1.012108	-0.932868	-0.877324					
TS22 (C _i)	C	2.900294	0.177612	0.31447	-534.758071	0.144267	-717.5839	49.3997	108.9468
	H	3.286479	1.188364	0.19786			135.6094	194.2772	219.1262
	H	3.540524	-0.51046	-0.232811			263.2694	312.6143	359.4264
	H	2.927517	-0.087639	1.371616			425.2479	447.8274	475.0577
	C	1.481076	0.09868	-0.212737			489.7014	527.951	592.8817
	H	1.438774	0.368062	-1.269254			697.6636	766.1689	869.4214
	C	0.547071	1.010124	0.595041			872.4366	909.4081	926.2414
	H	0.406285	0.578465	1.585609			952.0521	961.6704	1023.106
	H	1.045665	1.971914	0.704318			1069.173	1112.372	1137.24
	C	-0.773489	1.337731	-0.069641			1146.787	1196.9	1202.715
	C	-1.664735	-0.648245	0.829286			1278.554	1291.907	1313.891
	H	-1.469161	-0.697332	1.891644			1373.438	1383.921	1415.23
	C	-1.614237	-1.719127	-0.007645			1420.069	1471.119	1490.897
	H	-1.514379	-2.704426	0.421363			1504.168	1556.872	1891.119
	H	-2.069972	-1.63927	-0.98454			3074.002	3087.749	3097.557
	O	-1.869754	0.600893	0.303258			3146.311	3152.262	3164.375
	O	-0.911745	2.228413	-0.845728			3180.089	3208.799	3281.408
	O	1.113703	-1.276245	-0.095202					
	O	0.061845	-1.554102	-0.909634					
TS23 (C _i)	C	2.8881	-0.265361	0.402077	-534.743806	0.14345	-539.4672	77.4425	128.2925
	H	3.48497	0.644636	0.41942			142.9414	189.2639	217.8174
	H	3.4053	-1.015203	-0.19272			233.5683	247.7026	305.5934
	H	2.786215	-0.637416	1.421618			360.3173	384.8195	456.5464
	C	1.523273	0.021023	-0.192586			466.7549	486.9235	599.1653
	H	1.611204	0.406262	-1.211372			610.3072	829.0263	852.982
	C	0.734912	1.014745	0.669586			901.601	907.0171	926.3997
	H	0.45575	0.531646	1.606788			941.0419	988.77	1064.898
	H	1.358274	1.883674	0.887374			1085.001	1119.617	1125.146
	C	-0.483144	1.582113	0.003737			1179.527	1225.454	1290.624
	C	-1.769504	-0.689111	0.864029			1295.22	1339.814	1366.945
	H	-1.75749	-1.073343	1.890526			1383.941	1389.618	1412.86
	C	-1.380752	-1.605482	-0.272194			1442.151	1464.429	1488.745
	H	-1.127668	-2.607366	0.076637			1504.509	1532.764	1999.968
	H	-2.199085	-1.66227	-0.993528			3045.178	3067.786	3070.248
	O	-2.073045	0.487031	0.631776			3073.175	3080.006	3123.347
	O	-0.623693	2.214376	-0.964332			3131.678	3149.499	3160.956
	O	0.867848	-1.233152	-0.233933					
	O	-0.307958	-1.070526	-1.027589					
P12	C	3.63255	-0.516271	-0.000031	-383.856787	0.125083	61.9483	91.2013	127.2518

(C _s)	H	4.214549	-0.223961	0.875331			147.889	209.3722	229.1366
	H	4.214752	-0.223537	-0.875114			268.0607	378.1391	425.33
	H	3.518043	-1.598007	-0.000297			477.9267	704.3967	740.5381
	C	2.315226	0.177196	-0.000001			769.6954	875.1122	915.405
	H	2.316126	1.26273	0.000046			924.6057	938.0326	1013.344
	C	1.135649	-0.432034	-0.000014			1018.699	1056.788	1088.703
	H	1.036562	-1.508954	-0.000065			1131.696	1186.536	1222.975
	C	-0.10817	0.360397	0.000029			1327.329	1329.941	1355.684
	C	-2.439537	0.109791	0.000004			1411.475	1427.313	1482.681
	H	-2.439642	1.189226	0.000077			1488.319	1738.417	1753.251
	C	-3.516587	-0.651619	-0.000056			1841.463	3061.998	3116.496
	H	-4.491469	-0.191195	-0.000032			3151.482	3181.356	3195.535
	H	-3.444568	-1.729336	-0.000129			3217.532	3248.814	3293.179
	O	-1.190042	-0.464762	-0.000025					
	O	-0.189851	1.557046	0.000099					
	P13 (C _i)	C	2.007793	-1.792334	-0.269167	-534.758071	0.143512	56.923	65.7835
H		1.776977	-2.82686	-0.520513			125.1402	163.5529	212.0155
H		2.814411	-1.781488	0.461158			227.3281	263.5617	316.5892
H		2.344538	-1.281236	-1.169314			321.4073	372.307	452.9445
C		0.782194	-1.113543	0.313039			543.1833	593.5523	617.7579
H		0.425542	-1.646686	1.195131			636.9099	730.2411	843.1688
C		-0.352477	-1.016399	-0.70079			888.0573	910.3917	919.2663
H		-0.099557	-0.320199	-1.500664			940.8184	966.1206	1001.83
H		-0.526389	-1.992534	-1.157629			1010.582	1080.011	1110.096
C		-1.648064	-0.604821	-0.034419			1154.417	1188.146	1209.204
C		0.791164	2.070303	-0.352013			1249.853	1309.226	1330.749
H		1.222716	2.68214	-1.134095			1378.335	1395.049	1414.748
C		-0.31867	2.375751	0.297352			1433.542	1450.587	1490.927
H		-0.832943	3.283984	0.026386			1505.555	1730.278	1779.456
H		-0.713869	1.763982	1.092749			3075.826	3085.188	3106.984
O		-2.475632	-0.036037	-0.893827			3134.458	3151.353	3160.486
O	-1.953966	-0.77966	1.113122			3199.761	3216.03	3297.88	
O	1.090379	0.162851	0.8634						
O	1.591336	0.978491	-0.184847						
P14 (C _i)	C	-1.608724	2.206993	-0.48701	-534.769341	0.143131	43.4675	54.5462	100.7913
	H	-2.411037	2.212417	-1.222698			117.4267	140.8102	156.4705
	H	-0.804285	2.847075	-0.844664			177.3618	229.902	240.5982
	H	-1.985089	2.61097	0.452327			320.4082	356.2434	412.6976
	C	-1.104664	0.792668	-0.285973			481.4758	515.1394	606.7742
	H	-0.77532	0.364216	-1.236991			639.0597	742.1689	808.0454
	C	-2.155515	-0.120185	0.339443			878.2285	895.3999	936.9676
	H	-2.267018	0.095362	1.400376			994.973	1062.664	1070.421
	H	-3.126341	0.038621	-0.137109			1107.328	1136.185	1137.743
	C	-1.86945	-1.595829	0.142822			1182.358	1210.791	1275.961
	C	2.659241	0.173667	0.164075			1284.195	1342.184	1375.894
	H	2.697607	0.8163	1.062498			1390.191	1414.107	1417.527
	C	1.467905	-0.756576	0.096576			1435.789	1458.763	1488.809
	H	1.105628	-0.842398	-0.929902			1503.866	1874.232	1968.011
	H	1.769089	-1.75054	0.435262			2977.139	3058.746	3072.788

	O	3.509451	0.201273	-0.678546			3074.656	3078.303	3122.595
	O	-1.29529	-2.102435	-0.748691			3144.439	3150.692	3156.313
	O	0.014506	0.933737	0.586618					
	O	0.454334	-0.357131	0.990782					
P15 (C _i)	C	3.47213	-0.379263	-0.468465	-383.84867	0.125275	38.6808	74.5985	77.5618
	H	4.403529	0.161408	-0.561617			142.59	155.5148	278.6377
	H	3.404939	-1.338556	-0.96768			372.6988	426.3845	474.7839
	C	2.457925	0.111124	0.224049			555.9477	619.2635	734.1659
	H	2.54065	1.079662	0.702509			760.2552	906.7055	925.661
	C	1.154063	-0.59926	0.401573			932.3562	959.6759	982.6923
	H	1.088624	-1.48994	-0.222919			1015.402	1024.938	1044.156
	H	1.032268	-0.93938	1.435216			1143.447	1180.909	1214.795
	C	-0.03326	0.283254	0.114345			1247.439	1325.066	1333.243
	C	-2.36467	0.193275	-0.131025			1375.224	1427.742	1445.858
	H	-2.2767	1.260124	-0.271483			1468.98	1742.886	1745.105
	C	-3.49258	-0.48893	-0.157346			1865.737	3053.553	3121.018
	H	-4.42189	0.03001	-0.330496			3161.736	3193.537	3194.251
	H	-3.50791	-1.55894	-0.009116			3246.161	3250.627	3292.415
		O	-1.17009	-0.45809			0.088568		
	O	-0.00806	1.467391	-0.047717					
HO₂ (C _s)	H	-0.880783	-0.865155	0	-150.908108	0.014185	1255.572	1461.847	3695.095
	O	0.055049	-0.600018	0					
	O	0.055049	0.708163	0					

P5 decomposition channels									
Species	Cartesian coordinate (Å)			E_{elec}^{0K} (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm ⁻¹)			
P5 (C _i)	C	3.662812	-0.44609	-0.02122	-384.413816	0.133056	35.8639	61.1642	83.2738
	H	3.837589	-0.96972	0.92725			110.5803	125.7683	140.2168
	H	4.494561	0.237152	-0.17661			260.8614	299.7883	343.0207
	H	3.701654	-1.21195	-0.8024			412.4441	472.3048	567.4644
	C	2.359746	0.263579	-0.02283			734.3549	735.6015	903.9821
	H	2.300676	1.337444	0.055175			910.4407	925.6689	928.9054
	C	1.102265	-0.51874	0.032349			995.5143	1017.472	1021.669
	H	1.028103	-1.23529	-0.79475			1112.953	1164.403	1187.659
	H	1.043107	-1.14331	0.935024			1198.763	1220.525	1321.169
	C	-0.14128	0.328419	0.008609			1334.189	1409.921	1425.94
	C	-2.48066	0.142499	-0.00754			1439.241	1446.781	1478.986
	H	-2.45285	1.2218	-0.01128			1489.239	1743.664	1867.109
	C	-3.57655	-0.59087	-0.01268			2998.195	3003.059	3030.753
	H	-4.5393	-0.10516	-0.02112			3049.465	3143.315	3193.977
	H	-3.53268	-1.67032	-0.00869			3239.813	3245.505	3291.894
	O	-1.24456	-0.46461	0.003341					
O	-0.18531	1.522934	0.00132						
IM10 (C _i)	C	2.882358	-0.54567	0.679852	-384.393633	0.135	37.7199	61.5022	94.7899
	H	3.867196	-0.94758	0.447218			139.4692	175.357	230.6735
	H	2.198919	-1.38488	0.802644			298.4527	337.9756	412.8628
	H	2.952653	-0.01826	1.632475			468.7013	565.0609	629.0043
	C	2.399128	0.389469	-0.42185			683.7571	798.1904	872.1647
	H	3.10678	1.208779	-0.55081			887.0555	889.584	912.0288
	H	2.352225	-0.14716	-1.36962			992.4667	1073.018	1102.225
	C	1.029646	0.981413	-0.12279			1118.85	1159.082	1173.827
	H	0.993206	1.439156	0.86758			1253.92	1303.638	1377.216
	H	0.767915	1.771366	-0.83109			1399.099	1408.343	1418.515
	C	-0.07073	-0.03773	-0.20269			1458.425	1489.619	1504.414
	C	-2.32984	-0.29528	0.28484			1513.258	1747.458	1886.294
	C	-3.5842	0.010975	0.079502			3062.9	3069.132	3078.843
	H	-4.35201	-0.73881	0.190752			3105.774	3116.088	3135.088
	H	-3.86908	1.017304	-0.21028			3142.601	3146.724	3259.563
	O	-1.24397	0.49062	0.293926					
O	-0.00304	-1.14299	-0.63893						
TS24 (C _i)	C	-3.44022	-0.2911	-0.4881	-384.343102	0.126316	-622.45	41.8605	61.5167
	H	-4.34347	0.290954	-0.6039			78.5436	130.3119	144.2997
	H	-4.43738	-1.35844	0.905753			220.6701	277.3712	347.4845
	H	-3.39077	-1.23347	-1.01966			384.9342	427.1949	476.9593
	C	-2.37704	0.201441	0.149588			561.9851	656.2322	736.0212
	H	-2.42397	1.177032	0.617087			764.3173	907.3055	927.906
	C	-1.09919	-0.55123	0.317184			930.4223	961.2549	991.8411
	H	-1.01424	-0.9438	1.337196			1014.156	1025.951	1027.987
	H	-1.04391	-1.41531	-0.3445			1144.293	1180.222	1215.404
	C	0.11982	0.308498	0.101901			1241.247	1316.261	1329.787
	C	2.452347	0.161073	-0.09635			1372.268	1427.726	1442.896

	H	2.399398	1.236153	-0.17922			1465.252	1685.974	1743.944
	C	3.559143	-0.55395	-0.13639			1865.168	3040.375	3119.167
	H	4.507444	-0.05575	-0.26057			3162.693	3194.202	3199.129
	H	3.538681	-1.63041	-0.0473			3246.151	3254.041	3292.154
	O	1.233648	-0.4642	0.061652					
	O	0.131234	1.499774	0.001861					
TS25 (C _i)	C	3.619726	-0.49931	-0.12104	-384.349747	0.126413	-785.983	64.523	92.6142
	H	4.178496	-0.19388	-1.00723			126.3775	145.1005	182.364
	H	3.500565	-1.58075	-0.1347			213.8307	266.3817	348.76
	H	4.23111	-0.22709	0.742534			378.7916	405.5081	430.8068
	C	2.309152	0.198806	-0.06114			480.4763	722.1316	744.6421
	H	2.306296	1.283512	-0.07017			770.1992	868.1475	915.524
	C	1.123962	-0.42029	0.054794			926.3796	937.6872	1016.343
	H	1.027566	-1.4953	-0.01749			1018.782	1053.796	1070.708
	H	0.796173	-0.7072	1.935366			1131.633	1185.423	1222.612
	C	-0.12801	0.371928	0.024929			1319.865	1329.467	1348.216
	C	-2.45587	0.117592	-0.03529			1410.104	1427.472	1479.728
	H	-2.45907	1.196759	-0.00394			1486.424	1681.232	1744.148
	C	-3.52909	-0.64719	-0.08576			1847.393	3053.363	3106.243
	H	-4.50571	-0.1901	-0.09671			3148.407	3186.119	3194.12
	H	-3.45246	-1.72438	-0.11517			3211.947	3246.886	3291.677
		O	-1.20393	-0.45393			-0.01826		
	O	-0.20385	1.567582	0.03183					
TS26 (C _i)	C	1.757135	-1.74356	-0.26679	-384.360732	0.131474	-339.273	37.6711	44.545
	H	1.466691	-1.9936	0.752283			85.4248	104.828	143.4824
	H	2.571124	-2.40229	-0.57443			170.7799	232.6741	268.8059
	H	0.909068	-1.95918	-0.92269			428.5756	441.9167	444.6751
	C	2.152351	-0.31081	-0.37744			686.3016	721.8062	767.7774
	H	2.499356	0.032245	-1.34607			885.9105	927.1403	933.5834
	C	2.009454	0.590059	0.614356			943.5512	963.7286	1010.097
	H	1.758469	0.265201	1.616801			1019.415	1057.429	1113.395
	H	2.359769	1.606056	0.500233			1154.985	1196.868	1306.487
	C	-0.1206	1.188003	0.237693			1329.057	1404.126	1420.045
	C	-2.00485	-0.13578	-0.16826			1441.561	1476.166	1492.383
	H	-2.25739	0.644829	-0.87104			1631.916	1737.337	1862.54
	C	-2.71793	-1.21718	0.069502			3043.844	3097.166	3138.976
	H	-3.64075	-1.3732	-0.46689			3158.267	3172.984	3189.952
	H	-2.39971	-1.95298	0.793938			3238.144	3252.929	3287.67
		O	-0.81363	0.072939			0.515874		
	O	-0.40137	2.040621	-0.53294					
TS27 (C _i)	C	-2.76879	0.387412	0.086706	-384.366888	0.129761	-1617.06	90.6669	103.3486
	H	-3.45656	-0.45977	0.158146			115.0179	200.3076	237.8806
	H	-3.23432	1.140761	-0.54584			271.6625	338.2671	395.8394
	H	-2.65532	0.802707	1.089096			463.3997	556.6099	577.9893
	C	-1.43678	-0.04941	-0.46433			670.7743	701.4906	808.8386
	H	-1.45006	-0.30086	-1.52345			834.4529	884.2847	907.8264
	C	-0.68089	-1.05894	0.370401			941.7262	1014.84	1079.365

	H	-0.75299	-0.7739	1.424921			1118.051	1140.041	1180.132
	H	-1.06261	-2.07369	0.271993			1216.338	1278.747	1296.845
	C	0.79441	-1.11822	0.038976			1330.866	1379.456	1407.712
	C	0.733372	1.248767	-0.06861			1413.283	1462.05	1491.713
	H	-0.60354	0.909961	-0.37821			1496.362	1614.484	1723.311
	C	1.251705	2.440802	0.128462			1897.419	3043.202	3054.52
	H	0.620389	3.315147	0.098337			3102.685	3118.32	3133.867
	H	2.312407	2.564288	0.317189			3144.965	3153.894	3265.248
	O	1.433341	0.087756	-0.11063					
	O	1.432211	-2.11614	-0.0721					
TS28 (C _i)	C	2.398914	-0.69942	1.049181	-384.354841	0.130253	-678.993	25.5373	36.9951
	H	2.948903	-1.61254	1.269046			90.1081	108.283	159.0464
	H	1.466327	-0.72916	1.615512			183.4931	242.5299	291.893
	H	2.986406	0.145084	1.412375			341.4104	375.5854	521.3813
	C	2.12044	-0.57224	-0.44208			531.9741	576.2195	726.2338
	H	3.053372	-0.5831	-1.00523			771.2711	828.0225	899.7378
	H	1.521452	-1.41372	-0.78639			923.5091	944.296	1055.023
	C	1.384479	0.724518	-0.77735			1071.28	1088.274	1130.919
	H	1.963875	1.608379	-0.49765			1227.517	1277.591	1344.796
	H	1.157751	0.778521	-1.84407			1377.907	1417.833	1419.425
	C	0.066865	0.807741	-0.087			1444.373	1491.56	1503.45
	C	-2.09926	-0.73073	-0.22084			1507.466	1898.429	2010.094
	C	-3.20695	-0.33676	0.35425			3052.984	3056.891	3087.824
	H	-3.20781	0.543611	0.987611			3111.991	3116.194	3139.155
	H	-4.12562	-0.88398	0.207774			3140.403	3144.238	3244.472
	O	-0.93503	-0.7516	-0.55953					
	O	-0.53392	1.625125	0.482538					
P16 (C _i)	C	3.472129	-0.37926	-0.46847	-383.84867	0.125284	38.6818	74.5989	77.5604
	H	4.403528	0.16141	-0.56162			142.59	155.5151	278.6377
	H	3.404937	-1.33855	-0.96769			372.6988	426.3847	474.7838
	C	2.457925	0.111123	0.224051			555.9482	619.2636	734.1667
	H	2.540651	1.079658	0.702516			760.2552	906.7054	925.6612
	C	1.154063	-0.59927	0.401572			932.356	959.6758	982.6926
	H	1.088624	-1.48994	-0.22292			1015.402	1024.938	1044.157
	H	1.032266	-0.93938	1.435214			1143.447	1180.909	1214.796
	C	-0.03326	0.283253	0.114345			1247.439	1325.066	1333.243
	C	-2.36467	0.193276	-0.13103			1375.224	1427.742	1445.858
	H	-2.2767	1.260124	-0.27149			1468.98	1742.886	1745.105
	C	-3.49258	-0.48893	-0.15735			1865.737	3053.555	3121.019
	H	-4.42189	0.030012	-0.3305			3161.735	3193.538	3194.251
	H	-3.50791	-1.55894	-0.00911			3246.161	3250.627	3292.415
	O	-1.17009	-0.45809	0.088568					
	O	-0.00806	1.46739	-0.04772					
P17 (C _s)	C	3.632549	-0.51627	-2.6E-05	-383.856787	0.125065	61.9425	91.2017	127.2515
	H	4.214611	-0.22392	0.875279			147.8886	209.3697	229.1361
	H	4.214686	-0.22357	-0.87517			268.0611	378.1395	425.3303
	H	3.518045	-1.598	-0.00024			477.9268	704.397	740.5383

	C	2.315223	0.177195	0.000055			769.6952	875.1123	915.4051
	H	2.316119	1.262728	0.000245			924.6061	938.0331	1013.344
	C	1.135649	-0.43204	-8.9E-05			1018.699	1056.788	1088.703
	H	1.036563	-1.50896	-0.00028			1131.695	1186.536	1222.975
	C	-0.10817	0.360394	0.000013			1327.33	1329.941	1355.685
	C	-2.43954	0.109792	0.00001			1411.475	1427.314	1482.681
	H	-2.43964	1.189228	0.000105			1488.319	1738.419	1753.255
	C	-3.51659	-0.65162	-4.2E-05			1841.463	3061.999	3116.498
	H	-4.49147	-0.19119	0.000011			3151.481	3181.357	3195.535
	H	-3.44457	-1.72933	-0.00014			3217.531	3248.814	3293.179
	O	-1.19004	-0.46476	-0.00006					
	O	-0.18985	1.557044	0.000142					
C₃H₆ (C _s)	C	1.227147	0.162153	0.00002	-117.885253	0.07783	206.829	430.3826	595.9591
	H	1.796852	-0.15041	0.876745			938.2616	946.3016	965.8084
	H	1.164595	1.249316	-0.00051			1033.377	1079.371	1194.811
	H	1.797215	-0.15127	-0.87615			1328.858	1406.707	1453.505
	C	-0.13451	-0.4558	0.000067			1484.63	1497.028	1737.92
	H	-0.17107	-1.54082	0.000254			3056.795	3110.99	3137.595
	C	-1.27222	0.221615	0.00			3158.417	3166.981	3247.865
	H	-2.23016	-0.27985	-1.3E-05					
	H	-1.27995	1.305215	-0.00031					
P18 (C _s)	C	1.229748	0.320985	0.000037	-266.478525	0.053269	95.5912	232.1194	241.4289
	C	-1.08696	0.406783	-2.8E-05			496.9458	615.3055	724.8141
	H	-0.9265	1.475347	-6.3E-05			933.6616	946.3311	994.0768
	C	-2.25752	-0.19209	0.000048			1175.476	1195.568	1339.464
	H	-3.15555	0.404215	0.000079			1421.364	1745.377	1950.393
	H	-2.33796	-1.26891	0.000075			3199.317	3230.139	3298.657
	O	0.077944	-0.34689	-8.7E-05					
	O	2.310605	-0.1312	0.000033					
H	H	0	0	0	-0.4982065	0			
P19 (C _i)	C	-1.59397	-0.7335	-0.27835	-231.787025	0.098412	112.2572	165.7691	211.49
	H	-2.43674	-1.17246	0.25358			287.6716	355.1808	634.0802
	H	-0.86163	-1.52083	-0.45337			771.8512	795.3603	848.1928
	H	-1.955	-0.38217	-1.24614			913.8678	1055.693	1069.38
	C	-0.98005	0.411436	0.516817			1121.222	1231.294	1280.168
	H	-1.73088	1.180996	0.70382			1339.093	1375.703	1417.896
	H	-0.63971	0.051326	1.488387			1444.404	1490.819	1505.03
	C	0.197187	1.058618	-0.20875			1513.26	1975.378	3058.352
	H	-0.06012	1.350179	-1.22874			3065.438	3070.988	3103.733
	H	0.541239	1.968722	0.287927			3113.728	3129.72	3141.661
	C	1.423103	0.171044	-0.2967					
O	1.608153	-0.86517	0.224562						
P20 (C _{2v})	C	0.103236	-0.00019	0.00001	-152.598692	0.030938	448.6755	574.9146	608.5927
	C	-1.20406	0.000047	-3.3E-05			990.8089	1184.534	1417.437
	H	-1.72864	0.940547	0.00007			2256.528	3201.27	3303.092
	H	-1.72889	-0.94026	0.00007					
	O	1.257811	0.000072	0					

IM7 + NO channels									
Species	Cartesian coordinate (Å)			E_{elec}^{0K} (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm ⁻¹)			
IM7 (C ₁)	C	3.035313	-0.94994	-0.54838	-534.798878	0.144343	28.5235	56.6011	81.2232
	H	2.945785	-2.01621	-0.75135			116.3817	130.4796	158.7725
	H	3.942357	-0.78072	0.028575			225.6783	243.3031	300.3351
	H	3.113725	-0.41578	-1.49369			327.9461	390.2289	438.0228
	C	1.824618	-0.47524	0.224241			486.0032	557.5284	640.8856
	H	1.732887	-0.97693	1.18551			735.1964	744.6401	835.3032
	C	0.533688	-0.59638	-0.55701			907.174	920.7876	930.1354
	H	0.53479	0.090866	-1.40191			946.1844	1014.661	1022.506
	H	0.444966	-1.60526	-0.96575			1069.78	1131.558	1156.149
	C	-0.68124	-0.3509	0.299363			1186.1	1225.793	1245.534
	C	-2.97942	0.083095	0.148338			1272.58	1328.765	1338.788
	H	-2.93874	0.070319	1.226963			1400.54	1415.309	1422.473
	C	-4.0639	0.279849	-0.5742			1431.853	1449.569	1489.568
	H	-5.00746	0.445501	-0.07907			1506.61	1744.83	1864.118
	H	-4.02939	0.281676	-1.65396			3077.295	3086.488	3130.945
	O	-1.76619	-0.1254	-0.47591			3143.49	3155.443	3162.23
	O	-0.7046	-0.37846	1.494896			3194.795	3248.057	3293.153
O	2.014759	0.916722	0.623548						
O	2.111866	1.70758	-0.39871						
NO (C _{ov})	N	0	0	-0.60637	-129.893355	0.004577	2069.264		
	O	0	0	0.53057					
IM11 (C ₁)	C	2.578182	-2.01849	0.092414	-664.731238	0.152391	20.9654	42.6776	72.5966
	H	2.434406	-2.7228	0.910027			84.9555	119.482	129.2606
	H	3.581184	-1.60296	0.162279			160.1661	220.1621	226.0368
	H	2.483521	-2.55066	-0.85382			256.5093	293.4625	331.0674
	C	1.5465	-0.91474	0.183934			390.858	417.9918	464.0083
	H	1.609735	-0.39953	1.143097			501.1388	539.9627	595.7504
	C	0.127882	-1.41644	-0.03095			626.4345	734.1324	753.5239
	H	-0.04639	-1.64141	-1.08183			859.2944	898.2313	905.3756
	H	-0.01081	-2.34186	0.533481			927.421	929.8555	949.7142
	C	-0.91437	-0.45423	0.477046			1014.608	1024.376	1040.236
	C	-3.12742	0.229828	0.13105			1099.128	1137.168	1178.685
	H	-2.93058	0.901479	0.95279			1185.217	1224.777	1260.301
	C	-4.27078	0.126378	-0.51625			1332.046	1346.603	1383.711
	H	-5.10119	0.751123	-0.22813			1414.079	1423.459	1432.147
	H	-4.39515	-0.56972	-1.33298			1450.436	1490.068	1505.513
	O	-2.05723	-0.56128	-0.23485			1746.257	1837.54	1855.564
	O	-0.77396	0.280719	1.412468			3073.726	3077.682	3102.535
	O	1.928858	-0.00455	-0.86184			3142.479	3151.743	3160.552
	O	0.971464	1.013006	-0.98195			3194.934	3247.594	3293.037
N	1.250242	2.132048	-0.15365						
O	2.178813	2.014374	0.52206						

IM12 (C _i)	C	2.427878	0.961521	0.890917	-459.631417	0.139183	37.3625	80.3333	83.5751
	H	1.631427	1.702317	0.930634			124.3438	150.3873	219.3347
	C	1.082182	1.49312	0.41928			1392.216	1402.014	1421.294
	H	1.631762	2.271972	0.921716			1426.875	1462.49	1478.881
	C	-0.11359	1.770471	-0.41807			1490.572	1504.546	1881.385
	H	-0.35384	2.828821	-0.34681			2981.945	3001.494	3070.93
	H	0.114767	1.534081	-1.46882			3077.204	3139.611	3145.887
	O	1.843904	0.386953	0.182986			3154.766	3159.317	3246.763
	O	1.891382	-1.7102	-0.49426					
	O	-1.28819	1.078191	-0.03154					
IM15 (C _i)	C	-3.24751	-0.84577	-0.02086	-459.625757	0.139812	32.3146	58.7313	89.2273
	H	-3.22955	-1.7071	-0.68797			134.7736	154.9192	231.5358
	H	-4.15516	-0.27526	-0.20591			253.5055	308.0445	358.7197
	H	-3.26874	-1.1986	1.010637			423.2807	461.1523	481.523
	C	-2.03469	0.03374	-0.2378			505.714	588.8944	633.3172
	H	-2.02248	0.395437	-1.27175			747.814	868.9148	876.3263
	C	-0.74563	-0.74032	0.016801			899.9279	925.4205	964.7654
	H	-0.72193	-1.09538	1.050355			1009.187	1080.183	1113.041
	H	-0.67044	-1.62046	-0.62436			1131.784	1179.92	1194.114
	C	0.471864	0.10575	-0.20539			1240.81	1301.26	1353.901
	C	2.790275	-0.0115	-0.24486			1399.821	1400.498	1411.23
	C	3.929369	-0.18293	0.372024			1440.067	1451.695	1488.225
	H	4.809274	0.349765	0.046265			1504.515	1748.506	1864.932
	H	4.004265	-0.85527	1.220568			3033.284	3068.162	3072.004
	O	1.614687	-0.63657	-0.06295			3116.467	3141.128	3144.372
	O	0.492795	1.270864	-0.46908			3156.283	3261.939	3845.245
	O	-2.14366	1.128685	0.650008					
H	-1.43791	1.749169	0.438821						
TS29 (C _i)	C	2.800677	-0.3515	0.044611	-459.605777	0.139449	-481.942	65.8167	100.435
	H	3.093304	-1.24802	0.591779			151.6631	207.1732	241.5374
	H	3.429022	0.478575	0.359216			276.1096	324.1657	379.9971
	H	2.949647	-0.5213	-1.02129			454.6551	484.5345	542.2026
	C	1.333075	-0.0315	0.320212			594.949	626.5413	708.5215
	H	1.223421	0.164147	1.392704			850.0222	864.8855	886.6259
	C	0.451031	-1.22368	-0.07023			922.6873	940.4872	993.2801
	H	0.650636	-2.07934	0.570852			1000.843	1060.158	1113.787
	H	0.694987	-1.49629	-1.10167			1148.332	1192.795	1226.488
	C	-1.03698	-0.99676	-0.06058			1267.366	1311.121	1312.104
	C	-1.01944	1.345176	-0.40593			1357.442	1383.959	1395.296
	H	-0.92886	2.017172	-1.24438			1431.721	1453.847	1482.388
	C	-1.02635	1.769735	0.876577			1502.101	1589.499	1894.682
	H	-0.73371	2.782363	1.101351			3020.022	3060.113	3065.887
	H	-1.2606	1.095438	1.689003			3140.521	3149.186	3159.136
	O	-1.45764	0.111158	-0.77572			3182.443	3248.073	3294.64
	O	-1.84582	-1.74636	0.382988					
O	1.037212	1.102505	-0.42796						
TS30	C	2.472123	-1.13982	0.10196	-459.620002	0.140436	-221.717	55.4901	87.9451

(C _i)	H	2.512785	-2.00641	0.759962			207.3824	242.4559	254.8136
	H	3.319707	-0.49283	0.319724			282.0078	326.9545	375.2874
	H	2.547127	-1.48104	-0.92994			444.6658	490.3731	579.4386
	C	1.169945	-0.39912	0.305809			608.7532	630.7402	676.4396
	H	1.130537	-0.01251	1.32413			839.8601	867.6073	878.0274
	C	-0.03685	-1.27523	0.007455			922.1875	966.3446	983.7741
	H	-0.0821	-2.08736	0.731373			1011.007	1070.577	1143.309
	H	0.112462	-1.73256	-0.97434			1166.218	1249.327	1269.209
	C	-1.43734	-0.66823	-0.04364			1286.602	1311.829	1370.22
	C	0.314847	1.683486	-0.41011			1382.737	1399.865	1423.765
	H	0.119697	2.248675	-1.31155			1450.094	1469.838	1490.629
	C	-0.19685	2.101635	0.783331			1504.879	1598.776	1750.478
	H	-0.00188	1.615355	1.72437			3068.854	3073.665	3098.004
	H	-0.88838	2.927706	0.772925			3137.489	3153.191	3155.681
	O	-1.59463	0.592413	-0.35213			3213.929	3222.032	3314.615
	O	-2.39371	-1.39524	0.109109					
	O	1.177676	0.703399	-0.61767					
TS31 (C _i)	C	2.796049	-0.44863	-0.08363	-459.608444	0.139906	-445.616	35.9153	94.2486
	H	3.00127	-1.48387	0.187188			136.4952	192.6445	237.0995
	H	3.484951	0.201363	0.451361			282.5387	315.8433	405.3652
	H	2.950847	-0.31885	-1.15425			456.2298	473.8107	545.885
	C	1.353718	-0.09517	0.27922			596.8568	695.9182	781.7011
	H	1.197149	-0.30623	1.345922			876.7364	887.2386	922.1975
	C	0.3789	-0.95002	-0.54839			935.1388	967.4979	971.7831
	H	0.376787	-0.56091	-1.56765			1009.971	1057.012	1106.233
	H	0.724217	-1.98174	-0.55162			1130.742	1188.609	1217.902
	C	-1.03483	-1.01794	-0.01921			1274.408	1307.869	1320.209
	C	-1.43441	1.290209	-0.4172			1358.505	1382.634	1394.334
	H	-1.72054	1.81754	-1.31638			1433.435	1464.483	1483.548
	C	-0.71775	1.843226	0.573742			1501.891	1612.653	1886.548
	H	-0.44727	2.884101	0.516847			2995.028	3068.182	3085.843
	H	-0.59571	1.332701	1.518747			3145.849	3154.316	3157.928
	O	-1.88557	0.005813	-0.37937			3190.39	3220.065	3298.726
	O	-1.47358	-1.93099	0.604882					
O	1.231418	1.260903	0.007313						
TS32 (C _i)	C	2.704317	0.402727	0.160471	-459.604897	0.140275	-625.241	69.0939	143.5615
	H	2.977676	1.452579	0.067684			204.4941	239.9972	283.9335
	H	3.358092	-0.19017	-0.47593			306.248	332.6421	360.5993
	H	2.851121	0.088861	1.194152			390.0912	478.1163	506.4182
	C	1.260124	0.191211	-0.24468			508.5266	631.0468	789.7465
	H	1.092351	0.556828	-1.26539			846.408	899.3924	920.2354
	C	0.315104	0.957275	0.706882			937.853	976.4172	1065.774
	H	0.232744	0.406158	1.644353			1107.488	1113.084	1137.178
	H	0.732304	1.944805	0.905847			1167.122	1228.983	1283.6
	C	-1.05335	1.243556	0.1478			1301.647	1344.634	1369.557
	C	-1.2817	-1.34625	0.453028			1381.969	1399.148	1418.963
	H	-1.2466	-1.9699	1.353766			1445.489	1486.893	1488.686

	C	-0.26041	-1.60824	-0.62107			1504.503	1551.718	1962.739
	H	-0.1873	-2.6763	-0.82413			3022.489	3044.07	3051.135
	H	-0.55787	-1.08284	-1.53496			3070.048	3081.14	3122.629
	O	-2.0739	-0.39255	0.384114			3138.109	3146.051	3156.085
	O	-1.38144	1.898155	-0.76356					
	O	1.035698	-1.20207	-0.20555					
TS33 (C ₁)	C	-1.93727	-0.66392	-1.02609	-459.596715	0.13417	-1786.58	53.6405	104.3852
	H	-2.75493	0.05143	-0.93411			133.5107	202.108	245.3995
	H	-2.31488	-1.58167	-1.47137			313.5616	350.0797	370.3366
	H	-1.18855	-0.24228	-1.69943			408.2926	472.609	547.9201
	C	-1.32101	-0.96416	0.330497			551.7136	609.2504	690.4337
	H	-2.06363	-1.44158	0.978751			749.7755	824.231	852.8153
	C	-0.8635	0.313304	1.066834			869.3493	912.4103	931.6009
	H	-1.72711	0.850543	1.448616			974.8776	1007.895	1055.405
	H	-0.22116	0.022898	1.899229			1102.75	1149.69	1178.267
	C	-0.14683	1.291096	0.170258			1217.231	1267.46	1294.682
	C	1.576134	-0.32818	-0.1292			1353.07	1367.713	1406.661
	H	0.721308	-1.25545	0.019254			1418.396	1468.59	1478.248
	C	2.857036	-0.61881	-0.09262			1491.291	1504.415	1732.274
	H	3.174556	-1.64021	0.045728			1899.114	3035.58	3062.286
	H	3.600998	0.160949	-0.20221			3091.249	3132.324	3157.199
	O	1.047704	0.888284	-0.38609			3165.99	3166.741	3278.274
O	-0.545	2.376161	-0.10848						
O	-0.27945	-1.90202	0.244242						
TS34 (C ₁)	C	3.242451	-0.16071	-0.39394	-459.586238	0.127871	-669.362	43.9486	50.1539
	H	3.485917	0.456984	-1.25787			96.2417	129.4356	163.3212
	H	3.707589	-1.1363	-0.51579			172.916	239.6814	255.9393
	H	3.654246	0.30612	0.50133			318.137	357.7787	414.0082
	C	1.744223	-0.32342	-0.2458			452.1334	486.6269	519.5427
	H	1.333934	-0.80969	-1.13479			545.3959	573.7448	742.4311
	C	1.07665	1.04222	-0.08397			805.3561	876.4774	922.7215
	H	1.4795	1.54852	0.797999			953.1038	986.425	1053.51
	H	1.249054	1.684981	-0.95185			1072.389	1084.256	1191.497
	C	-0.40019	0.984821	0.113864			1213.299	1285.784	1306.003
	C	-2.28601	-0.85753	-0.23838			1396.231	1402.844	1414.222
	C	-3.53783	-0.49853	-0.12312			1418.069	1446.309	1487.812
	H	-3.79238	0.499397	0.216897			1505.597	1891.023	2019.714
	H	-4.32933	-1.19379	-0.35915			3048.479	3059.037	3069.218
	O	-1.0705	-0.77742	-0.22291			3105.252	3139.951	3141.38
	O	-1.24362	1.764908	0.28482			3159.048	3242.867	3835.078
O	1.511649	-1.12002	0.895493						
H	0.595544	-1.41705	0.872151						

TS35 (C _i)	C	1.287116	1.47634	-0.657396	-459.6067698	0.136439	-612.9903	46.1044	50.45
	H	0.402253	1.220868	-1.237717			88.5837	106.0099	177.4556
	H	1.906394	2.146373	-1.255865			206.4973	228.7932	250.7569
	H	1.00015	1.99658	0.254401			349.475	412.6061	460.2239
	C	2.126845	0.262092	-0.336614			491.8107	661.9268	730.0677
	H	2.135648	-0.52746	-1.106859			749.5223	754.1497	871.1599
	C	0.951057	-0.894312	0.844707			876.7006	877.1945	932.4683
	H	1.553799	-1.78839	0.816734			970.5477	1013.8996	1031.6098
	H	0.947073	-0.321711	1.759805			1054.4902	1084.5527	1128.9294
	C	-0.286741	-0.934932	0.059708			1191.5418	1285.5947	1329.2552
	C	-2.386296	0.086637	-0.140132			1365.6753	1399.2401	1427.1703
	H	-2.503544	-0.581559	-0.980083			1465.0168	1473.5714	1477.3358
	C	-3.274093	0.976347	0.259139			1555.6071	1741.5238	1812.7374
	H	-4.205822	1.071872	-0.275291			2966.0475	3067.3276	3139.0529
	H	-3.090264	1.612181	1.113005			3164.7347	3186.588	3192.0308
	O	-1.193383	-0.0439	0.537254			3244.8254	3290.575	3297.0332
	O	-0.468862	-1.626204	-0.906376					
	O	3.080618	0.33738	0.461047					
P21 (C _i)	C	0.055993	2.064117	0.525185	-459.626227	0.140417	30.3657	43.3604	131.9765
	H	1.066172	2.04793	0.934922			159.8478	197.6921	234.6381
	H	-0.6017	2.549424	1.242907			264.5711	309.8621	366.8198
	H	0.057417	2.645374	-0.39669			413.0568	466.3684	521.4011
	C	-0.41731	0.654275	0.250492			622.6233	664.6683	731.5998
	H	-0.46087	0.08678	1.181424			873.4371	878.7607	893.0402
	C	0.505839	-0.07281	-0.73495			911.2574	937.2974	1011.577
	H	0.724394	0.566453	-1.59061			1026.306	1043.633	1120.135
	H	0.031139	-0.98523	-1.09897			1164.437	1191.119	1255.315
	C	1.773306	-0.50028	-0.03121			1262.902	1311.977	1364.125
	C	-2.49938	-0.35955	-0.27766			1388.743	1400.103	1428.315
	H	-3.45107	-0.15107	-0.74789			1454.105	1466.174	1488.215
	C	-2.22263	-1.55236	0.236006			1507.295	1710.371	1781.407
	H	-2.98238	-2.31615	0.18474			3069.184	3079.499	3093.867
	H	-1.28663	-1.80565	0.711507			3132.381	3143.856	3158.029
	O	1.845172	-1.02118	1.048194			3195.66	3217.385	3284.246
	O	2.837717	-0.22868	-0.76502					
	O	-1.71681	0.745067	-0.31174					
P22 (C _i)	C	-0.95495	2.161408	-0.54899	-459.630015	0.140071	45.6947	69.0893	84.9648
	H	-1.56086	2.284358	-1.44618			140.0013	160.7297	175.7579
	H	-0.00823	2.67382	-0.71304			224.4851	273.8754	318.6169
	H	-1.46355	2.638008	0.289093			351.7434	433.048	453.142
	C	-0.73975	0.686695	-0.24971			589.5406	668.6878	730.9602
	H	-0.25996	0.19403	-1.10467			805.3817	855.4304	891.631
	C	-2.0598	-0.011	0.041423			952.5807	1053.289	1059.331
	H	-2.47749	0.350559	0.9816			1123.136	1131.074	1150.054
	H	-2.79987	0.190849	-0.7354			1196.686	1231.748	1289.186
	C	-1.94155	-1.51824	0.126208			1299.215	1351.473	1375.033
	C	2.020571	-0.54615	-0.06088			1404.538	1414.839	1419.263

	H	1.388716	-1.45336	-0.06366			1431.604	1471.265	1495.172
	C	1.439299	0.640797	0.684044			1500.972	1864.303	1977.78
	H	1.921047	0.682194	1.662734			2984.587	3022.346	3058.169
	H	1.698099	1.558463	0.148282			3069.102	3084.399	3110.689
	O	3.096836	-0.5138	-0.58856			3128.597	3144.303	3146.531
	O	-1.03464	-2.19229	-0.19219					
	O	0.060197	0.506082	0.909337					
P23 (C _i)	C	-2.15032	-0.31816	-0.13182	-307.018297	0.103216	92.0651	182.035	199.121
	H	-2.35473	-1.26677	-0.62716			236.0242	331.4581	409.2874
	H	-2.80054	0.446754	-0.55195			461.1165	478.6162	651.4259
	H	-2.37802	-0.41737	0.929884			843.325	849.8883	906.4279
	C	-0.70076	0.082846	-0.30959			962.7051	1071.107	1081.441
	H	-0.47635	0.19315	-1.37639			1176.162	1214.487	1290.254
	C	0.231779	-0.98266	0.272331			1301.462	1384.634	1401.23
	H	0.060741	-1.09223	1.346716			1426.236	1446.514	1486.861
	H	0.069069	-1.96189	-0.17942			1503.124	1964.143	3038.38
	C	1.693365	-0.63655	0.108078			3056.016	3072.491	3126.993
	O	2.15462	0.379423	-0.26742			3134.295	3142.919	3852.713
	O	-0.52066	1.318276	0.351075					
	H	0.363748	1.643911	0.155069					
P24 (C _{2v})	C	0.103236	-0.00019	0.00001	-152.598692	0.030938	448.6755	574.9146	608.5927
	C	-1.20406	0.000047	-3.3E-05			990.8089	1184.534	1417.437
	H	-1.72864	0.940547	0.00007			2256.528	3201.27	3303.092
	H	-1.72889	-0.94026	0.00007					
	O	1.257811	0.000072	0					
P25 (C _i)	C	-2.0641	-0.86013	0.000015	-459.6067698	0.139496	83.9378	147.5195	224.3893
	H	-3.07536	-0.49157	0.000002			373.1647	414.3953	458.9535
	H	-1.85227	-1.91588	0.000047			626.2036	669.1002	732.3538
	C	-0.99339	0.104832	-3E-06			766.4527	866.1816	923.4856
	C	1.344216	0.288726	-6E-06			1015.62	1020.891	1064.138
	H	1.142512	1.349216	-0.00003			1199.883	1296.267	1332.696
	C	2.54546	-0.2569	0.000008			1428.222	1464.601	1742.073
	H	3.415966	0.379057	-5E-06			1768.077	3195.58	3206.023
	H	2.67783	-1.32884	0.000032			3244.853	3293.412	3327.709
	O	0.22504	-0.50881	0.000009					
	O	-1.13777	1.302424	-2.6E-05					
CH₃CHO (C _i)	C	1.162433	-0.14769	0.000052	-305.8001503	0.079384	151.822	510.1776	776.4245
	H	1.695372	0.223264	0.877167			900.4127	1137.312	1144.032
	H	1.695608	0.223763	-0.87671			1377.939	1430.32	1463.83
	H	1.147115	-1.23369	-0.00025			1472.177	1867.09	2967.654
	C	-0.23316	0.398227	0.000037			3050.086	3116.41	3166.298
	H	-0.31482	1.501853	0.00019					
	O	-1.22487	-0.2773	-0.00012					

Table S2. Calculated total rate constants, $k_{\text{total}}(T, P)$, of the “ $VB + OH \rightarrow \text{products}$ ” reaction at different pressures for the temperature range of 200 - 2000 K. Units: $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$.

T (K)	0.76 Torr	7.6 Torr	76 Torr	760 Torr	7600 Torr
200	1.33E-10	1.35E-10	1.48E-10	2.03E-10	3.16E-10
298	1.88E-11	1.89E-11	1.93E-11	2.16E-11	2.79E-11
300	1.81E-11	1.82E-11	1.86E-11	2.07E-11	2.67E-11
400	3.69E-12	3.69E-12	3.70E-12	3.82E-12	4.55E-12
500	1.33E-12	1.34E-12	1.34E-12	1.37E-12	1.52E-12
600	9.80E-13	9.82E-13	9.96E-13	9.92E-13	1.02E-12
700	1.16E-12	1.17E-12	1.17E-12	1.17E-12	1.19E-12
800	1.70E-12	1.70E-12	1.69E-12	1.69E-12	1.70E-12
900	2.54E-12	2.53E-12	2.53E-12	2.52E-12	2.53E-12
1000	3.69E-12	3.69E-12	3.69E-12	3.69E-12	3.68E-12
1100	5.18E-12	5.19E-12	5.17E-12	5.18E-12	5.21E-12
1200	7.09E-12	7.05E-12	7.10E-12	7.07E-12	7.04E-12
1300	9.38E-12	9.34E-12	9.37E-12	9.37E-12	9.36E-12
1400	1.21E-11	1.21E-11	1.21E-11	1.21E-11	1.21E-11
1500	1.53E-11	1.53E-11	1.53E-11	1.53E-11	1.53E-11
1600	1.90E-11	1.91E-11	1.91E-11	1.90E-11	1.90E-11
1700	2.33E-11	2.33E-11	2.33E-11	2.32E-11	2.33E-11
1800	2.80E-11	2.80E-11	2.81E-11	2.81E-11	2.81E-11
1900	3.34E-11	3.34E-11	3.35E-11	3.35E-11	3.34E-11
2000	3.94E-11	3.94E-11	3.94E-11	3.94E-11	3.94E-11

Table S3. Calculated Eckart tunneling factors via transition state channels at $P = 760$ Torr for the temperature range of 200 – 400 K.

T(K)	200	250	300	350	400
via TS1	184.0	27.9	9.9	5.4	3.6
via TS2	52.8	15.1	7.2	4.5	3.3
via TS3	98.0	21.1	8.8	5.1	3.6
via TS4	36.6	9.0	4.4	2.9	2.3
via TS5	5.6	2.9	2.1	1.7	1.5
via TS6	23.2	6.6	3.6	2.5	2.0
via TS7	1.5	1.3	1.2	1.1	1.1
via TS8	1.3	1.2	1.1	1.1	1.1
via TS9	3.6×10^8	3.1×10^4	264.0	27.2	9.0
via TS10	1.5	1.3	1.2	1.1	1.1
via TS11	1.5×10^6	1.6×10^3	59.4	12.9	5.9
via TS12	4.3	2.5	1.9	1.6	1.4
via TS13	1.2	1.2	1.1	1.1	1.1
via TS14	3.8×10^6	3.0×10^3	87.9	16.3	6.9
via TS15	2.2	1.6	1.4	1.3	1.2
via TS16	2.2×10^6	1.7×10^3	56.8	12.1	5.6
via TS17	1.5	1.3	1.2	1.1	1.1
via TS18	17.3	4.9	2.8	2.1	1.7
via TS19	51.7	8.5	3.9	2.6	2.0
via TS20	5.6	2.6	1.9	1.6	1.4
via TS21	1.1	1.1	1.1	1.0	1.0
via TS22	4.3	2.3	1.7	1.5	1.4
via TS23	2.1	1.6	1.4	1.3	1.2
via TS24	2.3	1.7	1.4	1.3	1.2
via TS25	4.1	2.4	1.8	1.6	1.4
via TS26	1.3	1.2	1.1	1.1	1.1
via TS27	5.4×10^4	4.4×10^2	39.1	11.2	5.6
via TS28	3.5	2.1	1.6	1.4	1.3

Table S4. Individual rate constants $k(T, P)$ for “ $VB + OH \rightarrow products$ ” reaction at $P = 760$ Torr for the temperature range of 200 - 2000 K. Units: $\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$.

P [Torr]	T [K]	RC	IM1	IM2	IM3	IM4	IM5	IM6	P1 + H ₂ O	P2 + H ₂ O	P3 + H ₂ O	P4 + H ₂ O	P5 + H ₂ O	P6 + H ₂ O	P7 + CH ₃	P8 + H	P9 + C ₃ H ₆	P10 + C ₂ H ₄	P11 + CH ₃
760	200	1.04E-11	1.20E-12	3.30E-12	3.20E-17	3.20E-17	3.20E-17	9.61E-17	1.60E-16	1.76E-15	4.90E-15	3.63E-11	1.53E-10	1.96E-12	3.20E-17	3.20E-17	3.20E-17	3.20E-17	3.20E-17
760	298	8.61E-15	3.21E-13	8.08E-13	3.20E-17	3.20E-17	3.20E-17	9.60E-17	1.15E-15	2.62E-15	2.34E-14	4.74E-12	1.55E-11	2.36E-13	3.20E-17	3.20E-17	3.20E-17	3.20E-17	3.20E-17
760	300	7.10E-15	3.16E-13	7.89E-13	3.20E-17	3.20E-17	3.20E-17	6.40E-17	7.68E-16	3.65E-15	2.40E-14	4.56E-12	1.48E-11	2.28E-13	3.20E-17	3.20E-17	3.20E-17	3.20E-17	3.20E-17
760	400	3.20E-17	9.85E-14	2.29E-13	3.20E-17	3.20E-17	3.20E-17	2.24E-16	4.87E-15	6.69E-15	8.08E-14	1.01E-12	2.34E-12	4.47E-14	3.20E-17	3.20E-17	3.20E-17	3.20E-17	3.20E-17
760	500	3.20E-17	3.89E-14	9.60E-14	3.20E-17	3.20E-17	3.20E-17	6.40E-17	1.87E-14	1.50E-14	2.07E-13	3.60E-13	6.15E-13	1.50E-14	3.20E-17	3.20E-17	3.20E-17	3.20E-17	3.20E-17
760	600	3.21E-17	1.92E-14	4.69E-14	3.21E-17	3.21E-17	3.21E-17	6.41E-17	4.86E-14	2.95E-14	4.31E-13	1.81E-13	2.33E-13	6.70E-15	3.21E-17	3.21E-17	3.21E-17	3.21E-17	3.21E-17
760	700	3.21E-17	1.07E-14	2.31E-14	3.21E-17	3.21E-17	3.21E-17	4.49E-16	1.10E-13	4.67E-14	7.83E-13	9.70E-14	1.01E-13	3.01E-15	3.21E-17	3.21E-17	3.21E-17	3.21E-17	3.21E-17
760	800	3.21E-17	6.14E-15	1.39E-14	3.21E-17	6.43E-17	3.21E-17	3.21E-16	2.13E-13	7.93E-14	1.29E-12	5.65E-14	4.83E-14	1.61E-15	3.21E-17	3.21E-17	3.21E-17	3.21E-17	1.29E-16
760	900	3.22E-17	4.28E-15	6.79E-15	3.22E-17	9.66E-17	3.22E-17	7.08E-16	3.65E-13	1.25E-13	1.97E-12	3.31E-14	2.50E-14	9.01E-16	3.22E-17	3.22E-17	3.22E-17	3.22E-17	9.66E-17
760	1000	3.23E-17	1.91E-15	5.00E-15	3.23E-17	3.23E-17	3.23E-17	5.81E-16	5.99E-13	1.86E-13	2.86E-12	2.06E-14	1.47E-14	7.43E-16	3.23E-17	3.23E-17	3.23E-17	3.23E-17	4.84E-16
760	1100	3.24E-17	1.23E-15	2.59E-15	1.30E-16	3.24E-17	3.24E-17	3.89E-16	8.94E-13	2.71E-13	4.00E-12	1.47E-14	8.95E-15	3.89E-16	3.24E-17	3.24E-17	3.24E-17	3.24E-17	6.49E-16
760	1200	3.26E-17	7.49E-16	1.21E-15	6.51E-17	3.26E-17	3.26E-17	3.26E-17	1.30E-12	3.77E-13	5.36E-12	9.64E-15	5.47E-15	2.93E-16	3.26E-17	3.26E-17	3.26E-17	3.26E-17	7.81E-16
760	1300	3.27E-17	5.89E-16	6.22E-16	9.82E-17	3.27E-17	3.27E-17	1.31E-16	1.80E-12	5.12E-13	7.02E-12	7.04E-15	3.27E-15	1.64E-16	9.82E-17	3.27E-17	3.27E-17	3.27E-17	7.53E-16
760	1400	3.30E-17	2.64E-16	1.32E-16	3.30E-17	3.30E-17	3.30E-17	3.30E-17	2.44E-12	6.85E-13	8.96E-12	6.03E-15	2.31E-15	1.65E-16	1.32E-16	3.30E-17	3.30E-17	3.30E-17	7.91E-16
760	1500	3.32E-17	2.99E-16	3.32E-17	3.32E-17	3.32E-17	3.32E-17	3.32E-17	3.20E-12	8.83E-13	1.12E-11	4.75E-15	1.93E-15	2.33E-16	2.33E-16	3.32E-17	3.32E-17	3.32E-17	7.31E-16
760	1600	3.35E-17	1.34E-16	3.35E-17	3.35E-17	3.35E-17	3.35E-17	3.35E-17	4.08E-12	1.14E-12	1.38E-11	4.16E-15	1.85E-15	1.34E-16	1.68E-16	3.35E-17	3.35E-17	3.35E-17	7.71E-16
760	1700	3.39E-17	3.39E-17	3.39E-17	3.39E-17	3.39E-17	3.39E-17	3.39E-17	5.13E-12	1.43E-12	1.67E-11	4.30E-15	1.76E-15	2.37E-16	1.69E-16	3.39E-17	6.77E-17	3.39E-17	6.43E-16
760	1800	3.42E-17	3.42E-17	3.42E-17	3.42E-17	3.42E-17	3.42E-17	3.42E-17	6.29E-12	1.78E-12	2.00E-11	3.53E-15	1.88E-15	1.37E-16	6.85E-17	3.42E-17	3.42E-17	3.42E-17	4.11E-16
760	1900	3.47E-17	3.47E-17	3.47E-17	3.47E-17	3.47E-17	3.47E-17	3.47E-17	7.65E-12	2.17E-12	2.36E-11	2.63E-15	1.35E-15	1.39E-16	3.47E-17	3.47E-17	3.47E-17	3.47E-17	3.47E-16
760	2000	3.52E-17	3.52E-17	3.52E-17	3.52E-17	3.52E-17	3.52E-17	3.52E-17	9.19E-12	2.64E-12	2.76E-11	2.81E-15	1.48E-15	1.06E-16	2.46E-16	3.52E-17	3.52E-17	3.52E-17	1.76E-16

Table S5. Individual rate constants $k(T, P)$ for “ $P5 + O_2 \rightarrow Products$ ” at $P = 760$ Torr for the temperature range of 200 - 400 K. Units: $\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$.

P [Torr]	T [K]	IM7	IM8	IM9	P12+HO ₂	P13	P14	P15+HO ₂
760	200	1.14E-11	4.56E-19	4.56E-19	4.56E-19	4.56E-19	4.56E-19	4.56E-19
760	250	8.39E-12	3.36E-19	3.36E-19	3.36E-19	3.36E-19	3.36E-19	3.36E-19
760	300	6.84E-12	2.74E-19	2.74E-19	2.74E-19	2.74E-19	2.74E-19	2.74E-19
760	350	5.91E-12	2.36E-19	2.36E-19	2.36E-19	2.36E-19	2.36E-19	2.36E-19
760	400	5.3E-12	2.12E-19	2.12E-19	4.24E-19	2.12E-19	2.12E-19	2.12E-19

Table S6. Individual rate constants $k(T, P)$ for “ $P5 \rightarrow Products$ ” decomposition at $P = 760$ Torr for the temperature range of 200 - 400 K. Unit: s^{-1} .

P [Torr]	T [K]	IM10	P16+H	P17+H	P18+C₃H₆	P19+P20
760	200	3.07E-14	6.15E-22	6.15E-22	6.15E-22	6.15E-22
760	250	2.16E-10	4.32E-18	4.32E-18	8.04E-16	4.32E-18
760	300	1.68E-07	3.36E-15	1.68E-14	4.93E-11	1.21E-13
760	350	3.13E-05	6.33E-13	1.56E-10	1.38E-07	1.39E-09
760	400	1.97E-03	6.67E-10	9.22E-08	5.36E-05	1.54E-06

Table S7. Individual rate constants $k(T, P)$ for “ $IM7 + NO \rightarrow Products$ ” at $P = 760$ Torr for the temperature range of 200 - 400 K. Units: cm^3 molecule⁻¹ s⁻¹.

P [Torr]	T [K]	IM11	IM12+NO₂
760	200	7.83E-11	7.24E-13
760	250	6.15E-11	6.34E-12
760	300	2.57E-11	3.50E-11
760	350	9.36E-13	5.48E-11
760	400	9.77E-14	5.20E-11

Table S8. Estimated branching ratios for “ $VB + OH \rightarrow products$ ” reactions at $P = 760$ Torr for the temperature range of 200 - 2000 K

T [K]	RC	IM1	IM2	IM3	IM4	IM5	IM6	P1 + H ₂ O	P2 + H ₂ O	P3 + H ₂ O	P4 + H ₂ O	P5 + H ₂ O	P6 + H ₂ O	P7 + CH ₃	P8 + H	P9 + C ₃ H ₆	P10 + C ₂ H ₄	P11 + CH ₃
200	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.7	0.0	0.0	0.0	0.0	0.0	0.0
298	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.7	0.0	0.0	0.0	0.0	0.0	0.0
300	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.7	0.0	0.0	0.0	0.0	0.0	0.0
400	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.3	0.6	0.0	0.0	0.0	0.0	0.0	0.0
500	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.3	0.5	0.0	0.0	0.0	0.0	0.0	0.0
600	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.4	0.2	0.2	0.0	0.0	0.0	0.0	0.0	0.0
700	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.7	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.0
800	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
900	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.1	0.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1100	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.1	0.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1200	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.1	0.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1300	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.1	0.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1400	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.1	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1500	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.1	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1600	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.1	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1700	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.1	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1800	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.1	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1900	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.1	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.1	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table S9. Estimated branching ratios for “ $P5 + O_2 \rightarrow products$ ” reactions at $P = 760$ Torr for the temperature range of 200 - 400 K.

P [Torr]	T [K]	IM7	IM8	IM9	P12+HO ₂	P13	P14	P15+HO ₂
760	200	1.0	0.0	0.0	0.0	0.0	0.0	0.0
760	250	1.0	0.0	0.0	0.0	0.0	0.0	0.0
760	300	1.0	0.0	0.0	0.0	0.0	0.0	0.0
760	350	1.0	0.0	0.0	0.0	0.0	0.0	0.0
760	400	1.0	0.0	0.0	0.0	0.0	0.0	0.0

Table S10. Estimated branching ratios for each species of “ $IM7 + NO \rightarrow products$ ” reactions at $P = 760$ Torr for the temperature range of 200 - 400 K.

P [Torr]	T [K]	IM11	IM12+NO₂
760	200	1.0	0.0
760	250	0.9	0.1
760	300	0.4	0.6
760	350	0.0	0.9
760	400	0.0	0.9

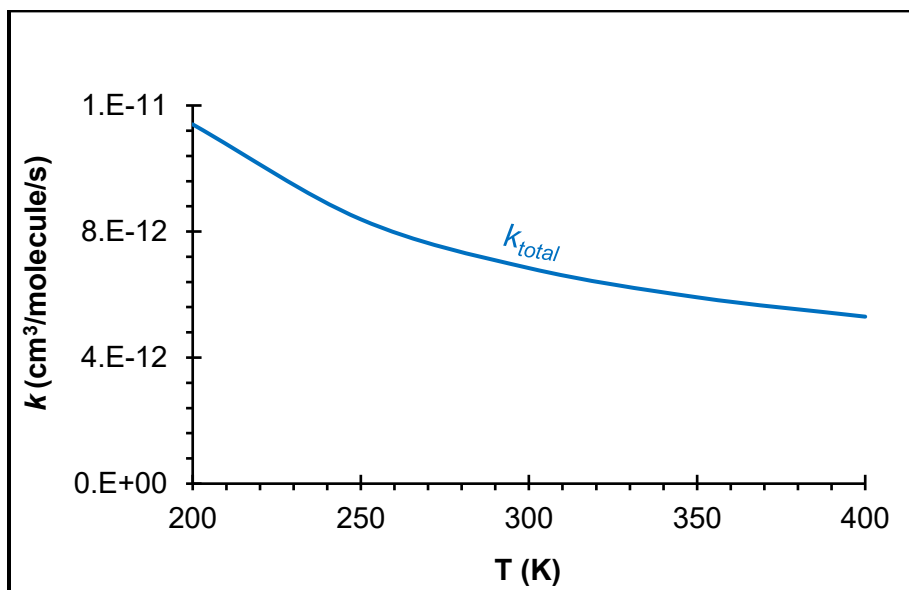


Figure S1. Estimated total rate constants for “ $P5 + O_2 \rightarrow products$ ” reactions at $P = 760$ Torr for the temperature range of 200 - 400 K.

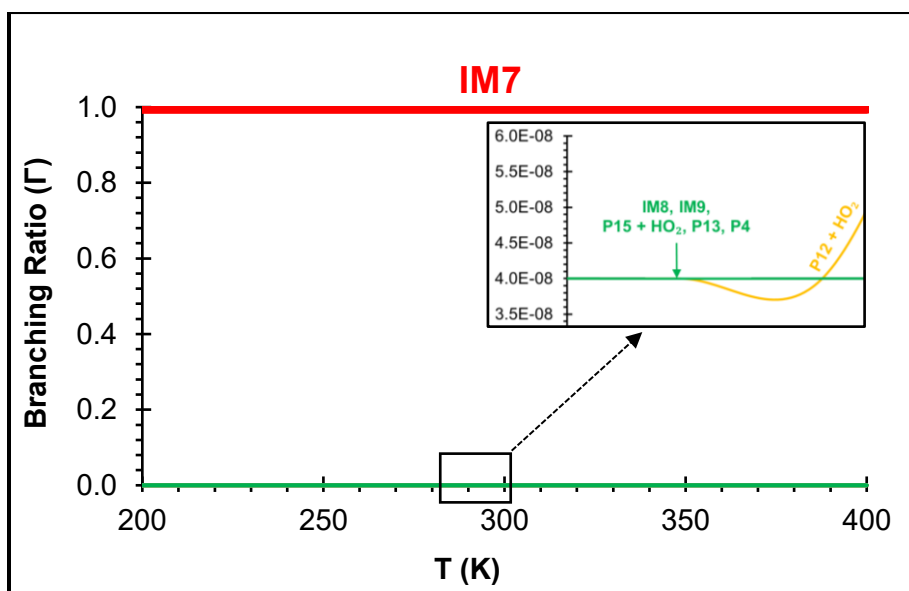


Figure S2: Branching ratios (Γ) for the products formation of “ $P5 + O_2 \rightarrow products$ ” reactions at $P = 760$ Torr for the temperature range of 200 - 400 K.

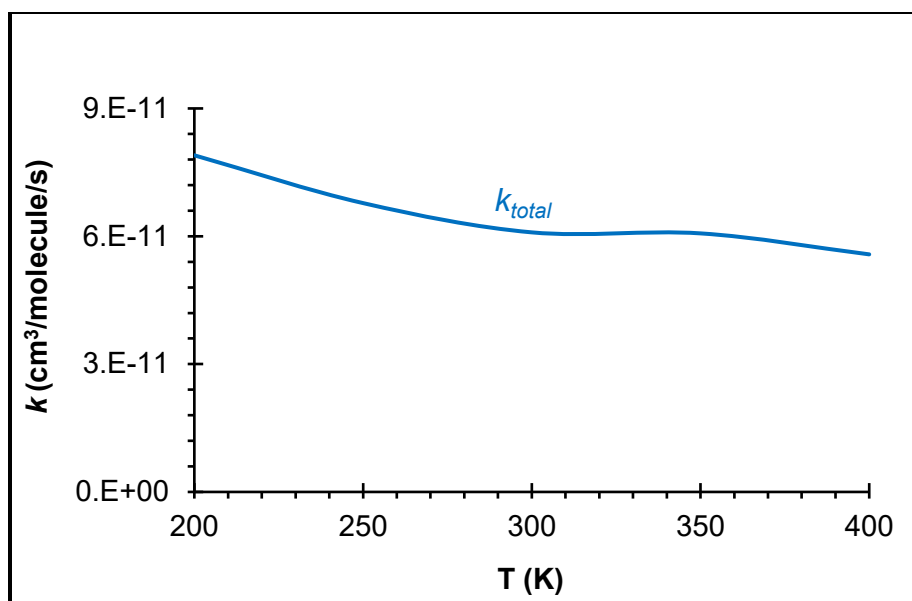


Figure S3. Estimated total rate constants for the “ $IM7 + NO \rightarrow products$ ” reactions at $P = 760$ Torr for the temperature range of 200 - 400 K.

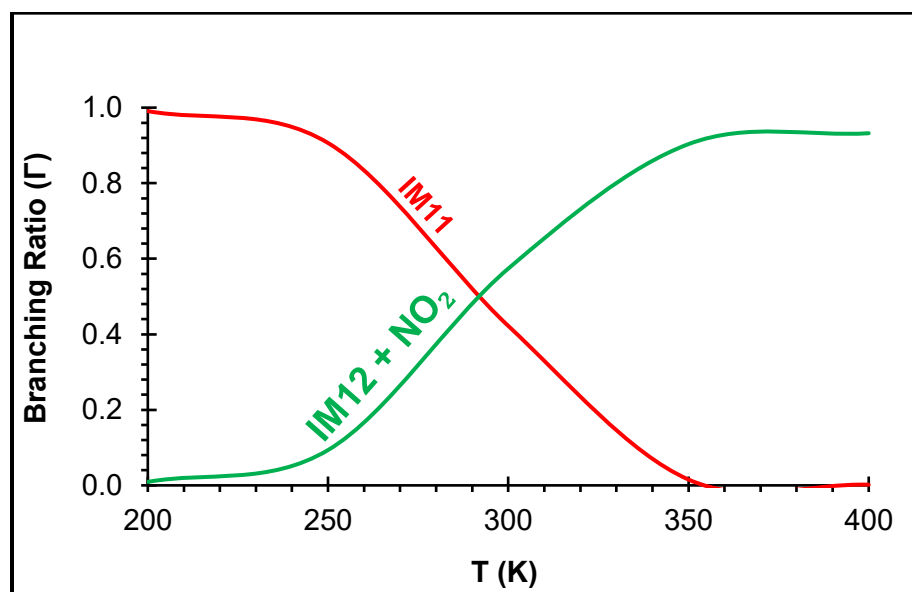
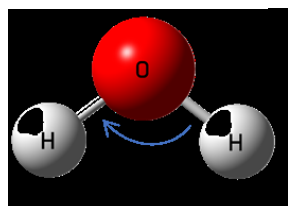
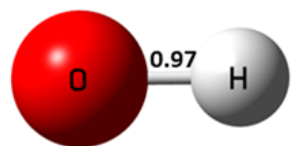
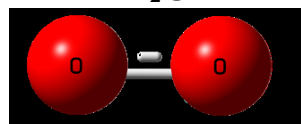


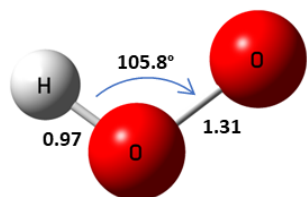
Figure S4: Branching ratios (Γ) for the products formation of “ $IM7 + NO \rightarrow products$ ” reactions at $P = 760$ Torr for the temperature range of 200 - 400 K.



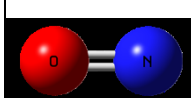
H₂O



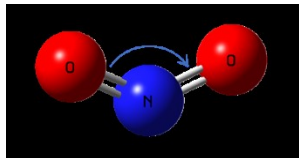
O₂



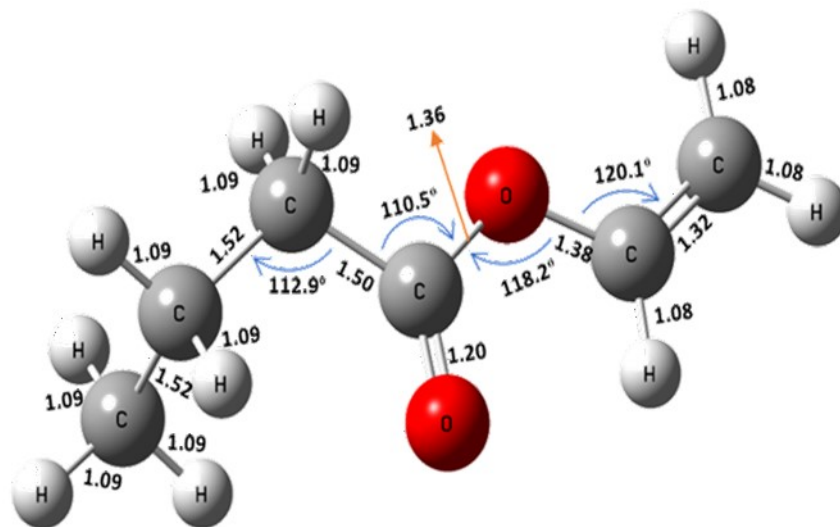
HO₂



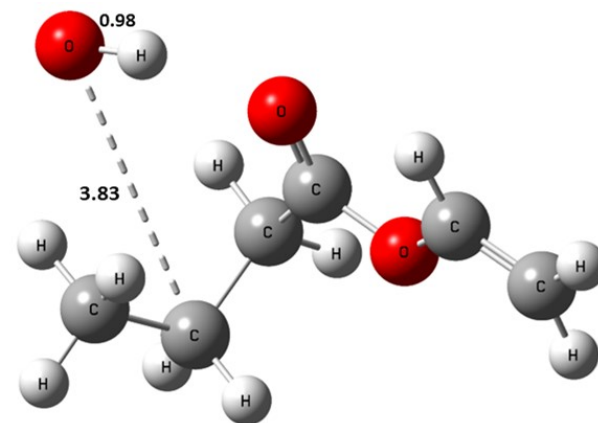
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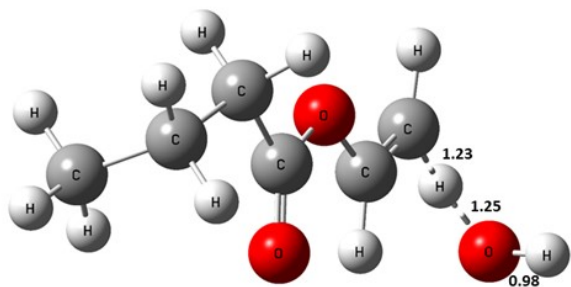
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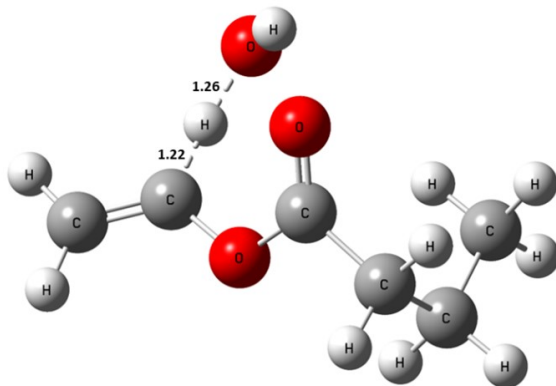
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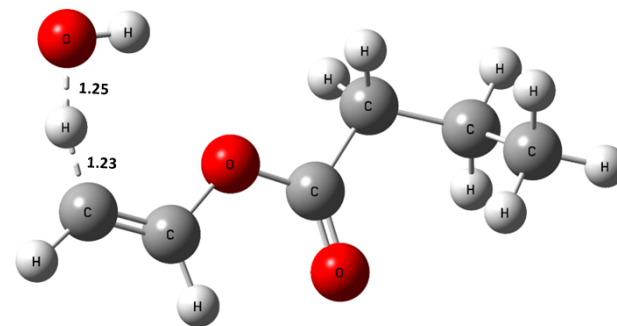
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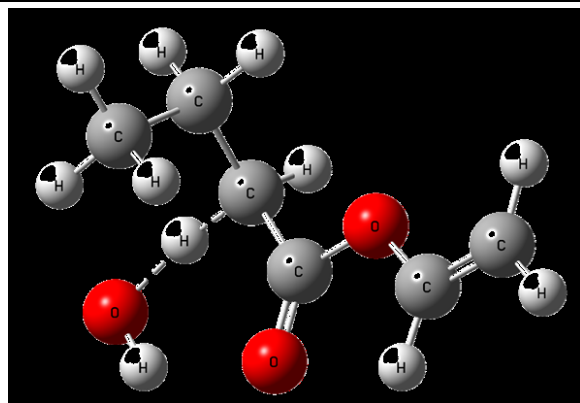
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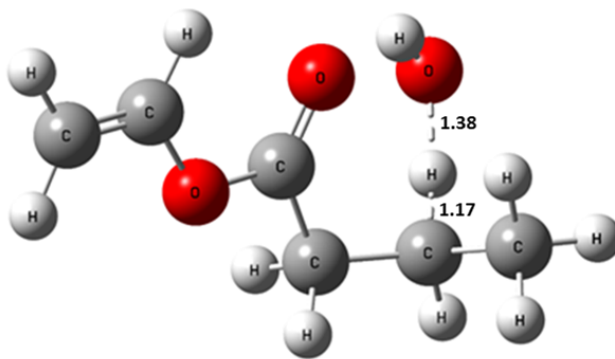
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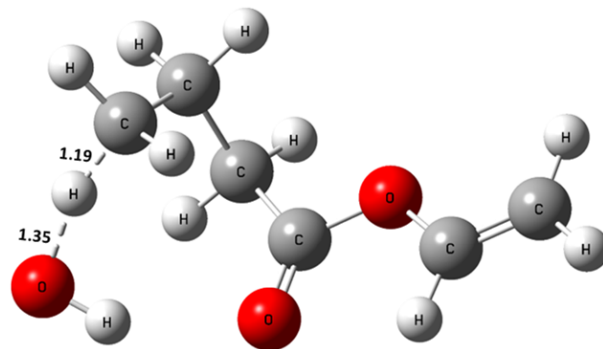
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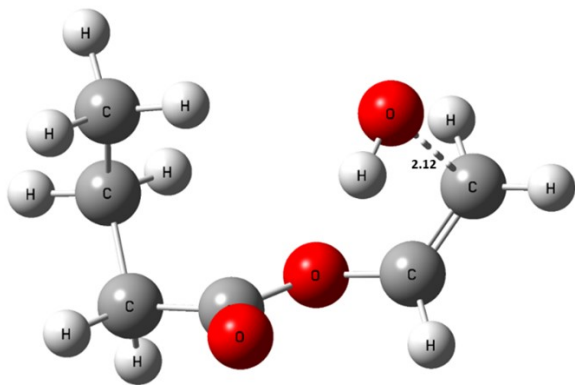
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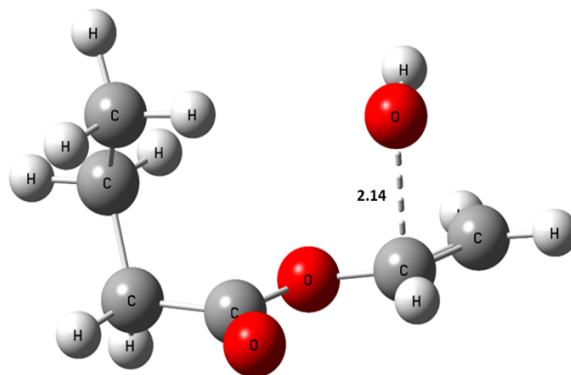
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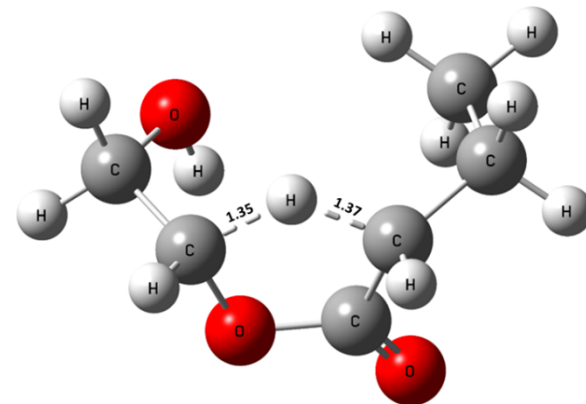
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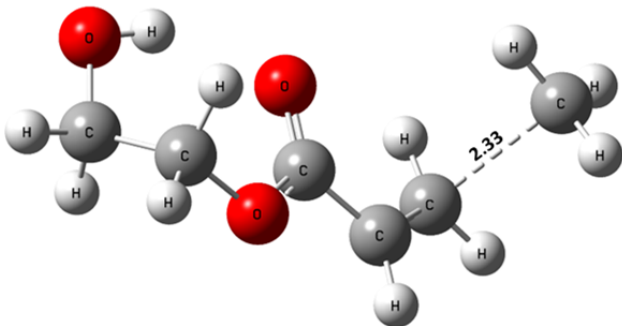
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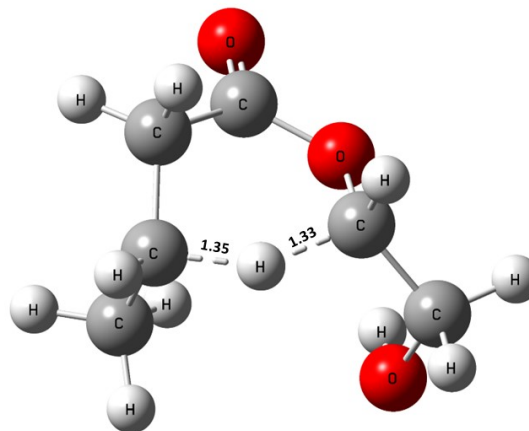
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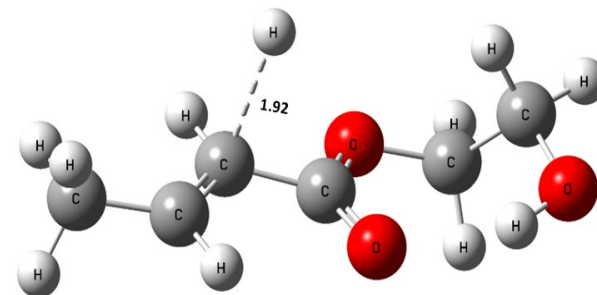
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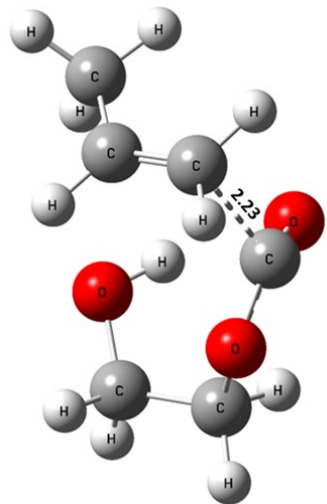
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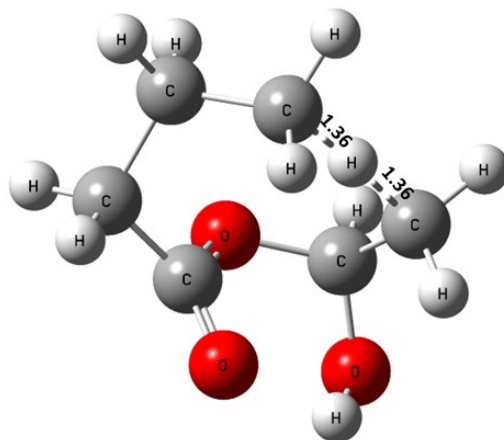
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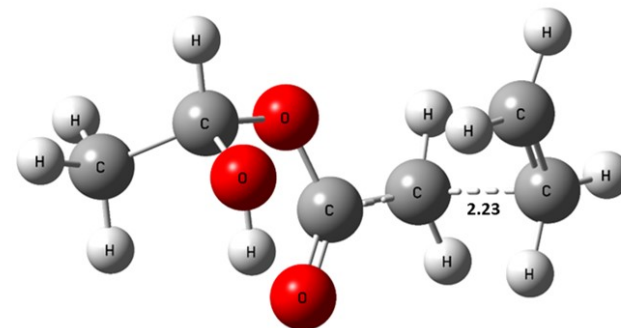
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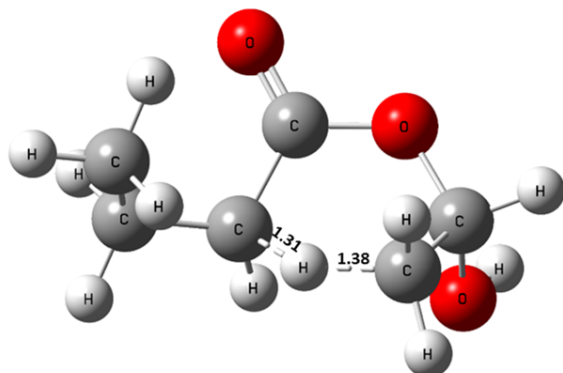
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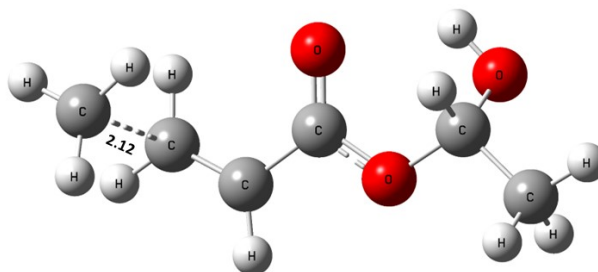
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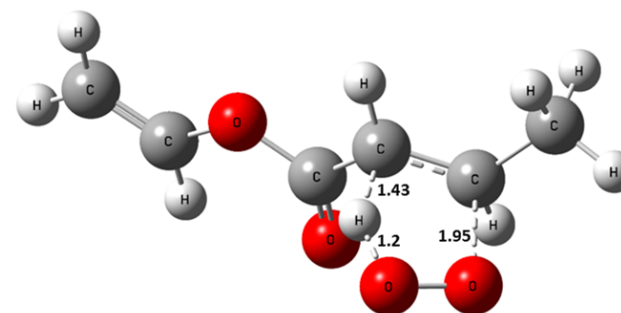
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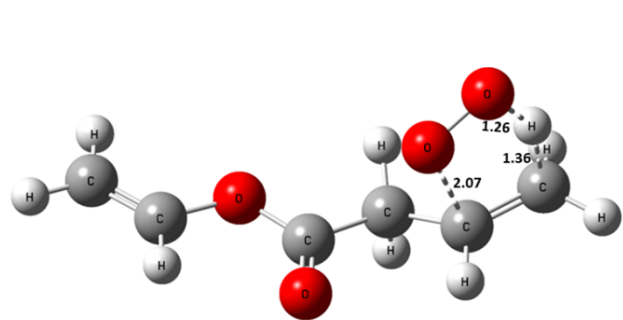
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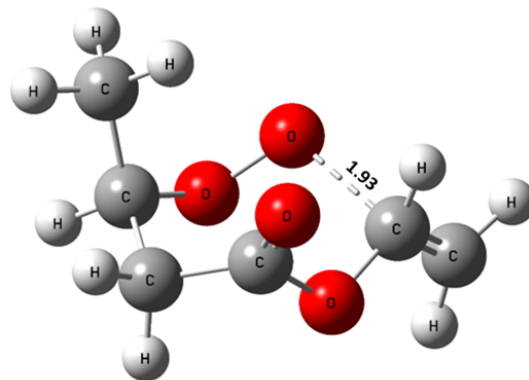
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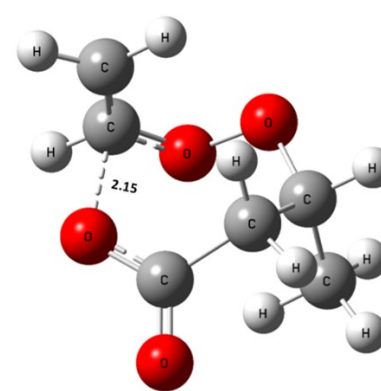
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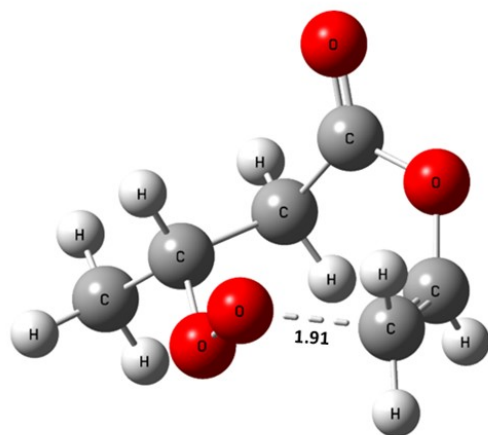
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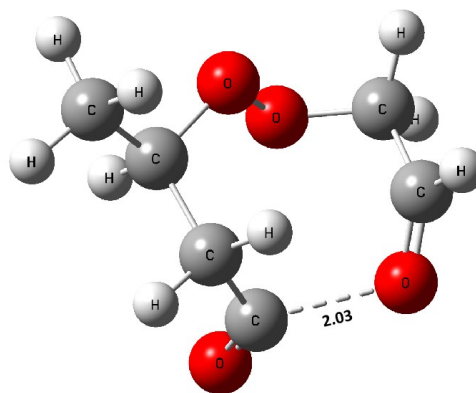
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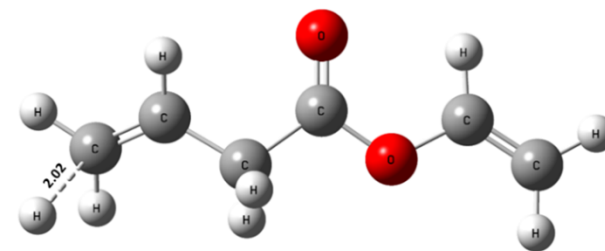
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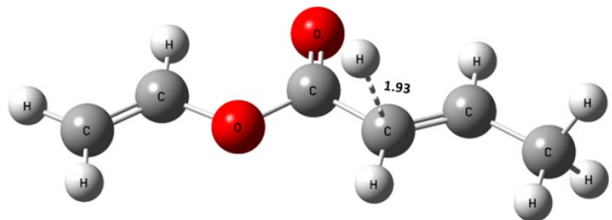
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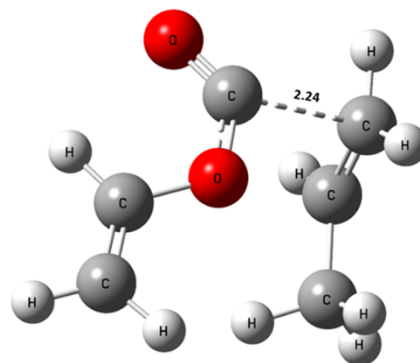
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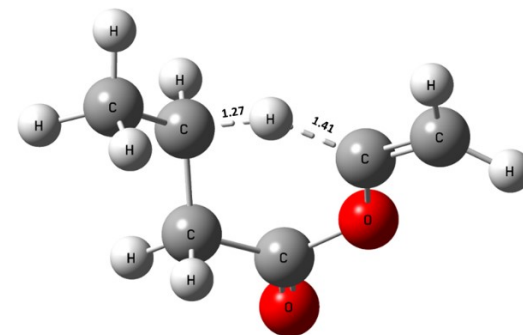
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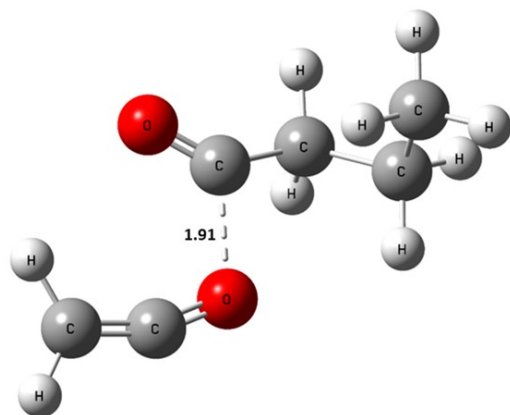
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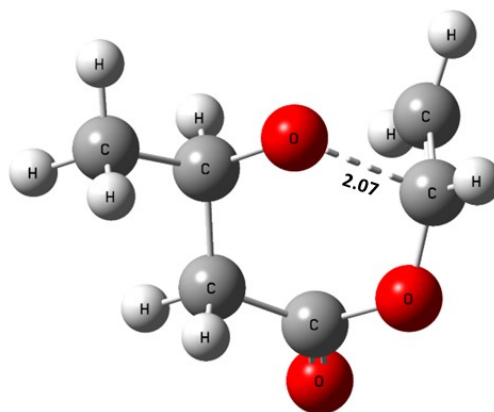
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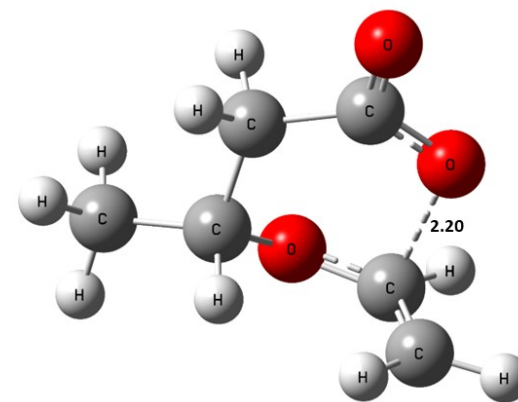
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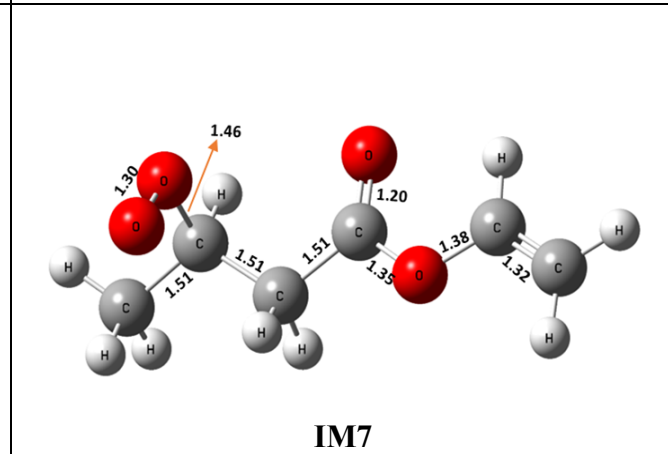
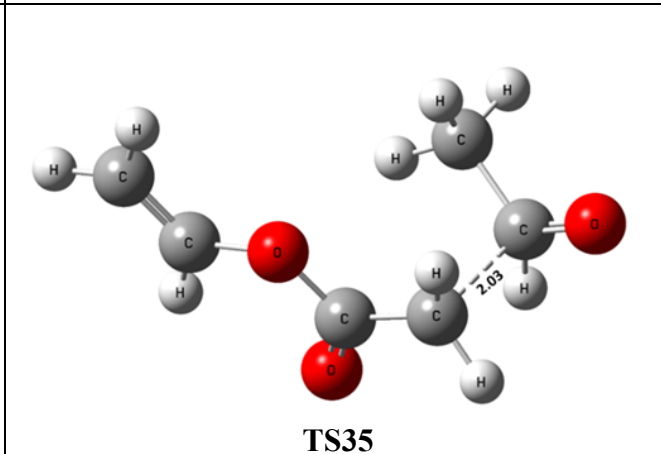
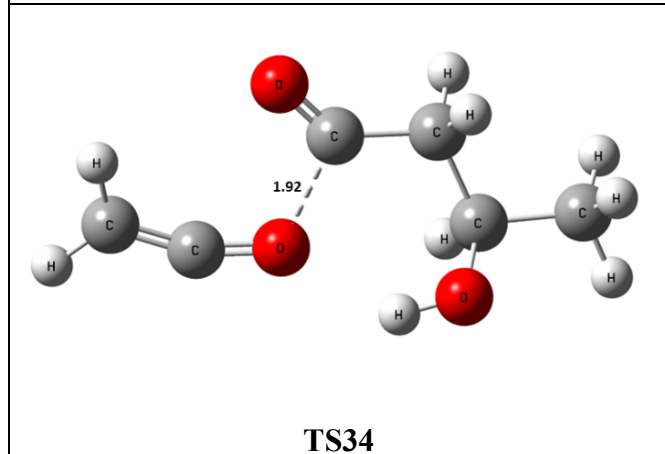
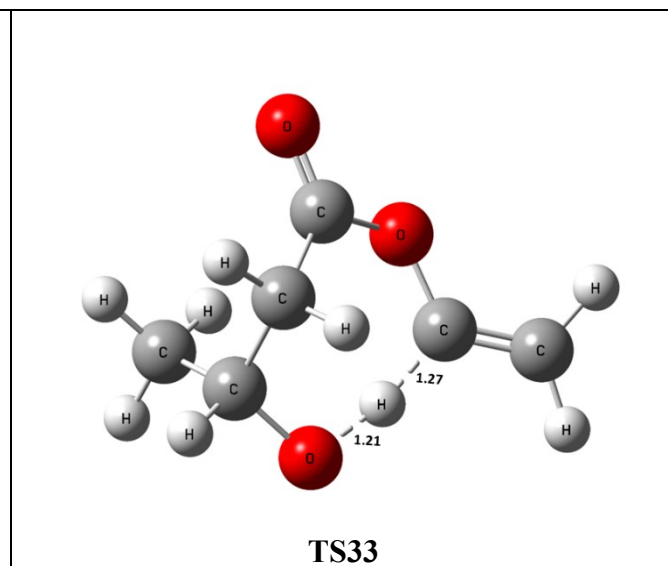
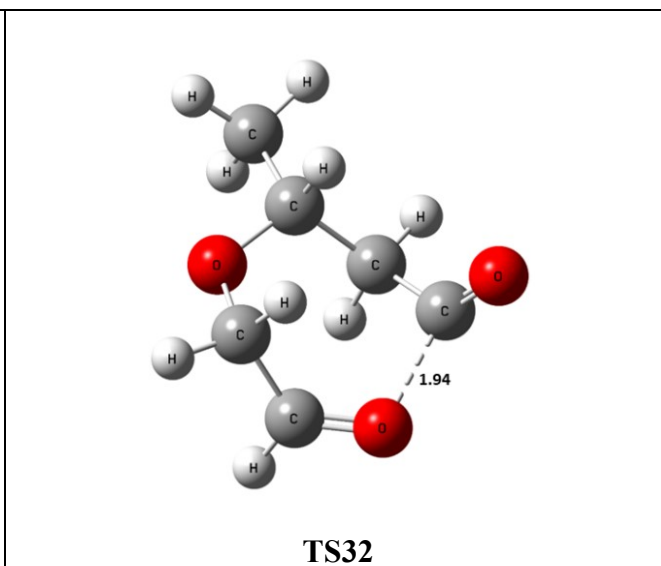
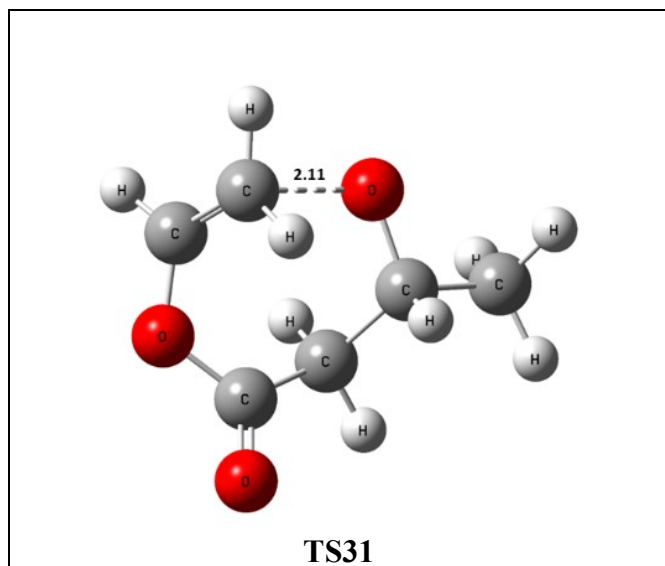
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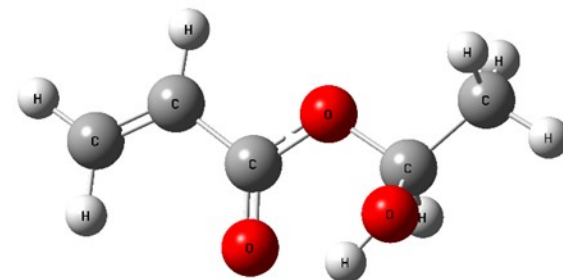
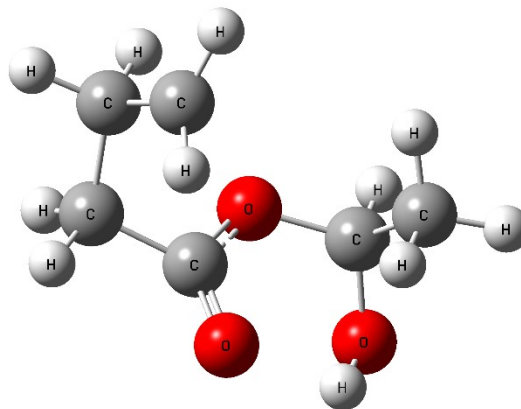
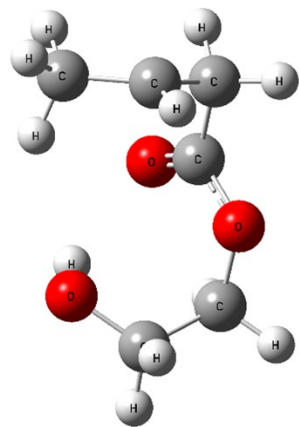
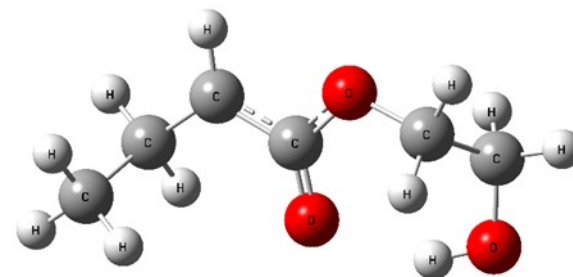
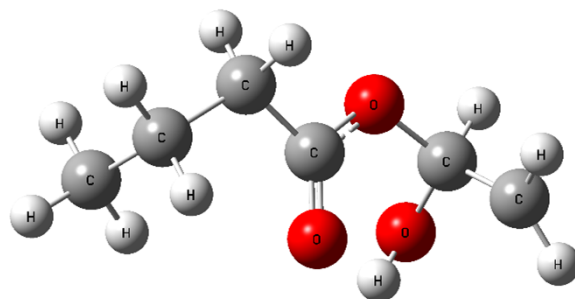
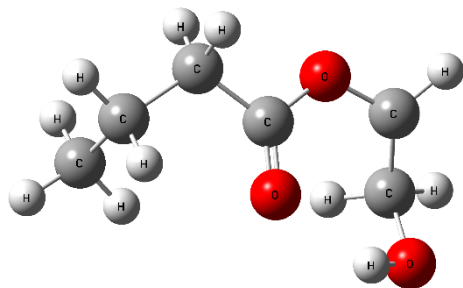


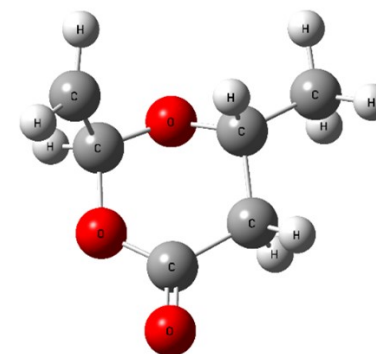
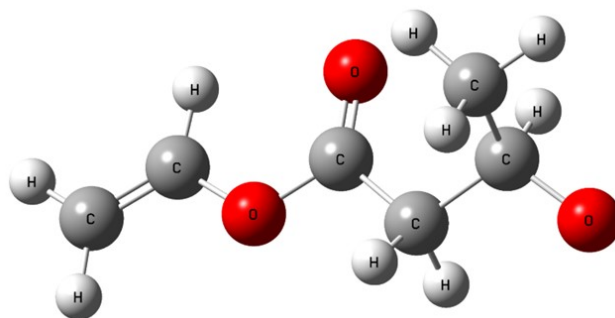
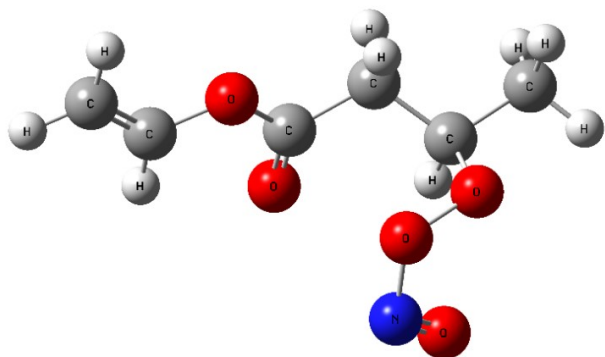
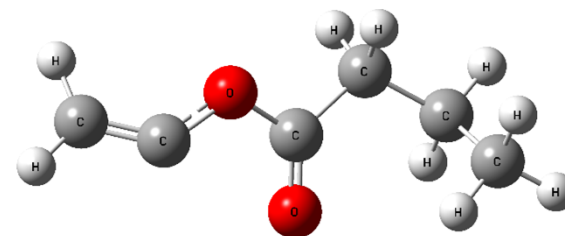
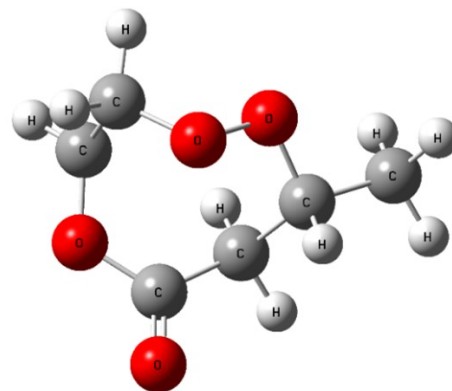
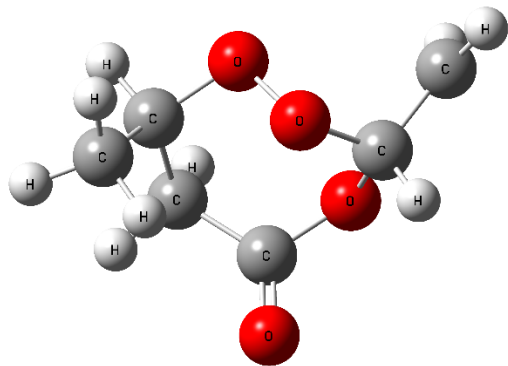
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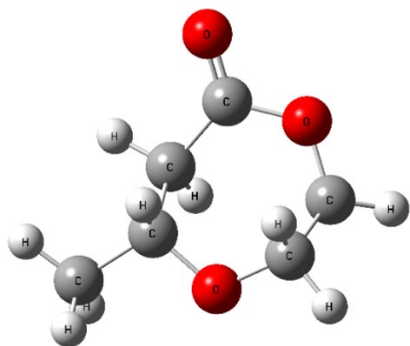


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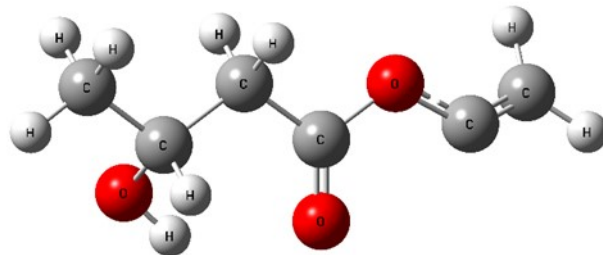




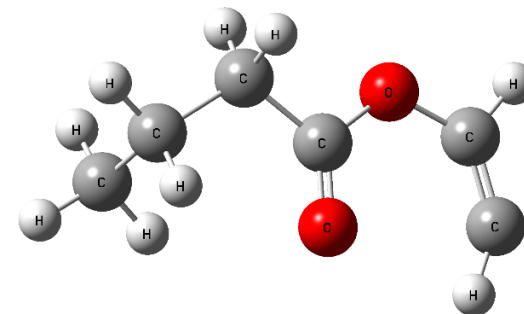




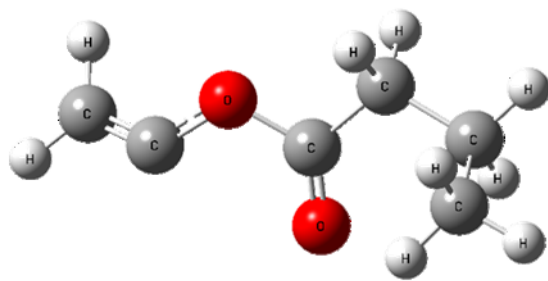
IM14



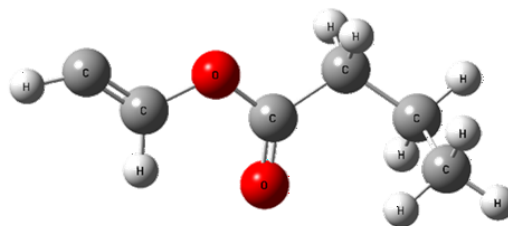
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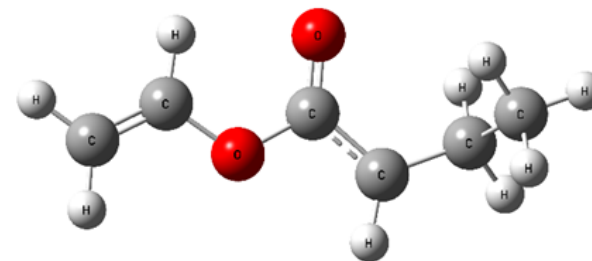
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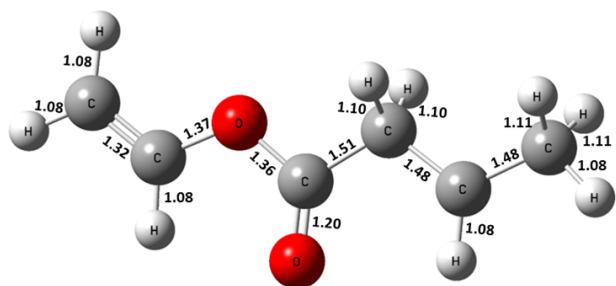
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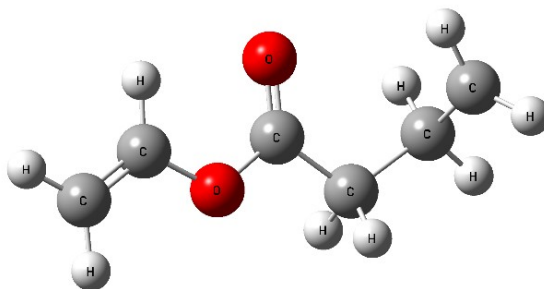
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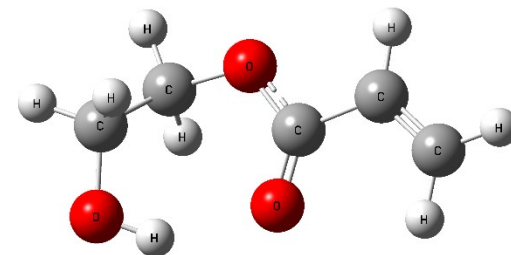
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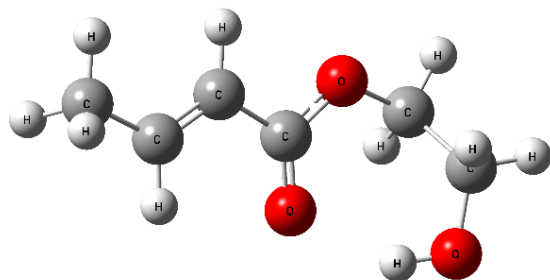
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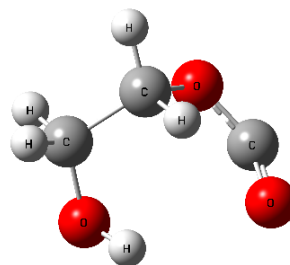
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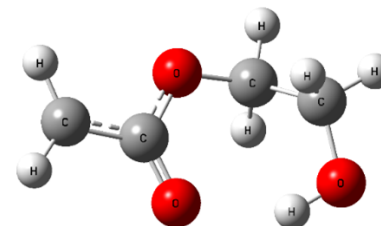
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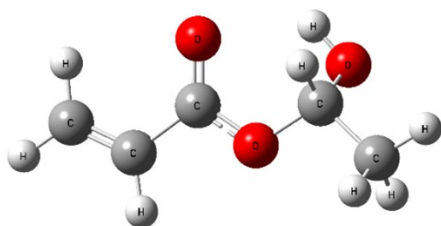
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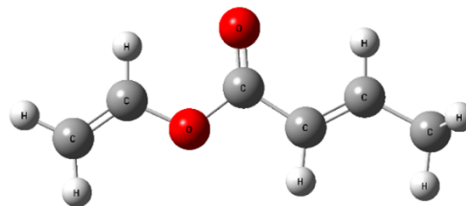
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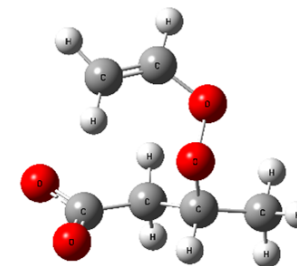
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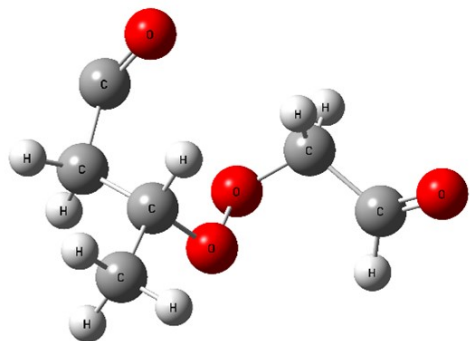
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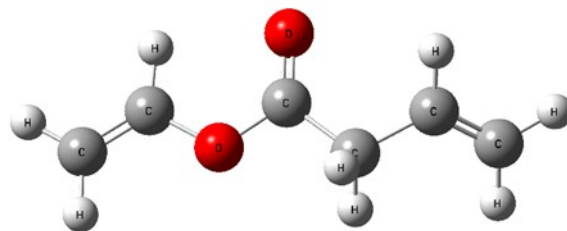
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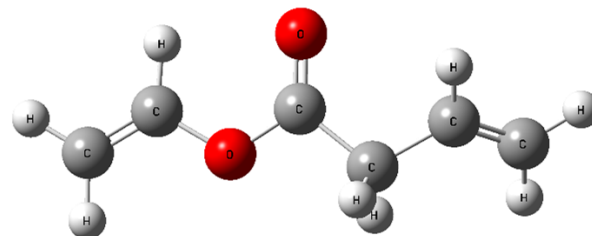
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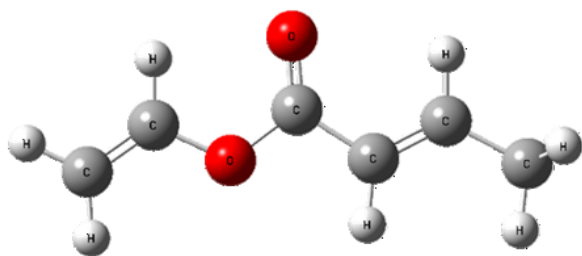
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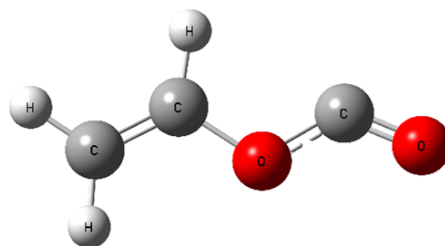
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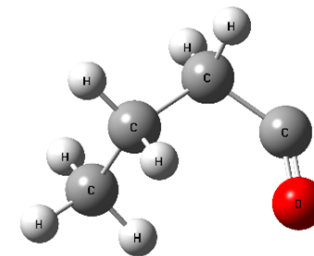
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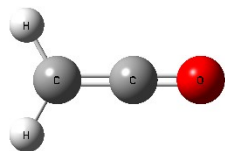
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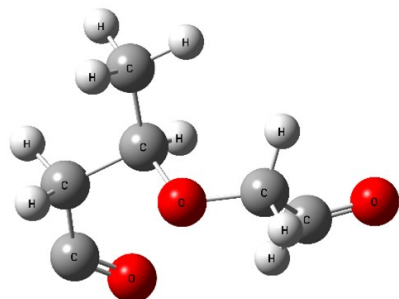
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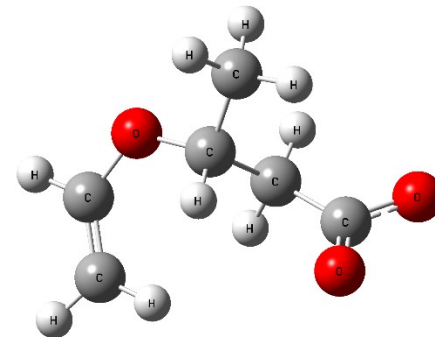
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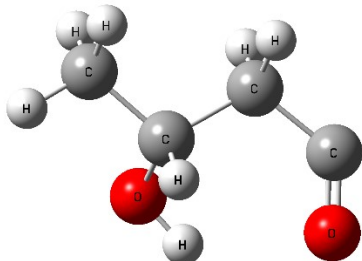
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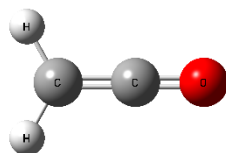
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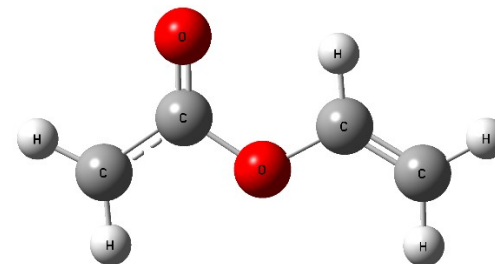
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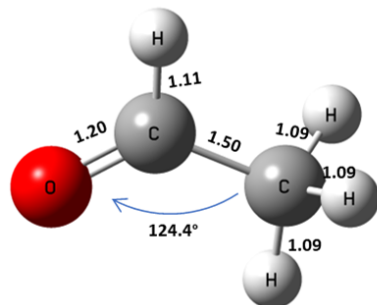
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P24



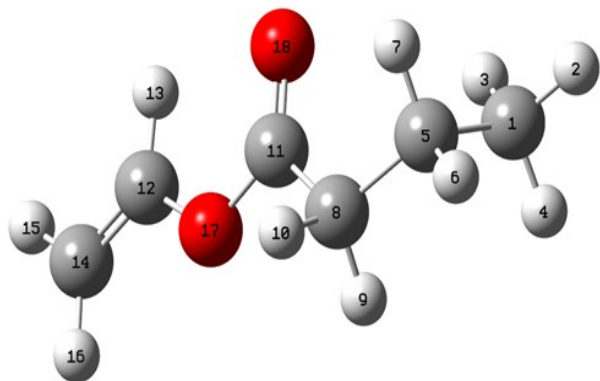
P25



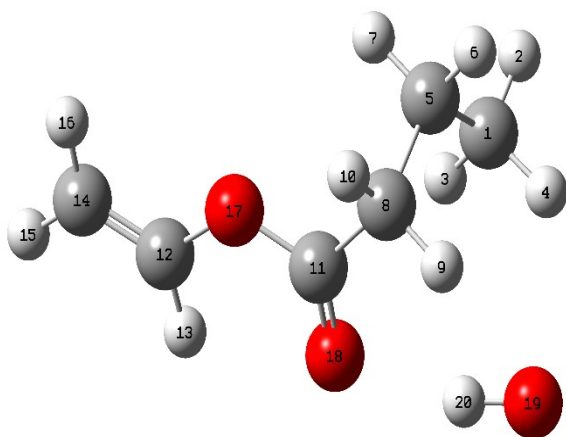
CH₃CHO

Figure S5. Geometries for the species involved in the VB + OH/O₂/NO/ reaction were optimized at M06-2X/aug-cc-pVTZ level. All structures were obtained for the lowest-energy conformer. Bond lengths and bond angles are in Å and degree (°), respectively.

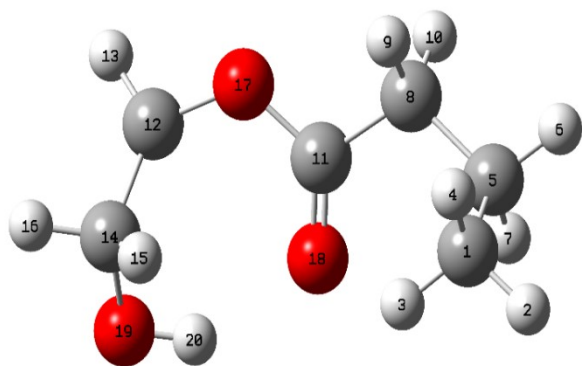
Species



VB

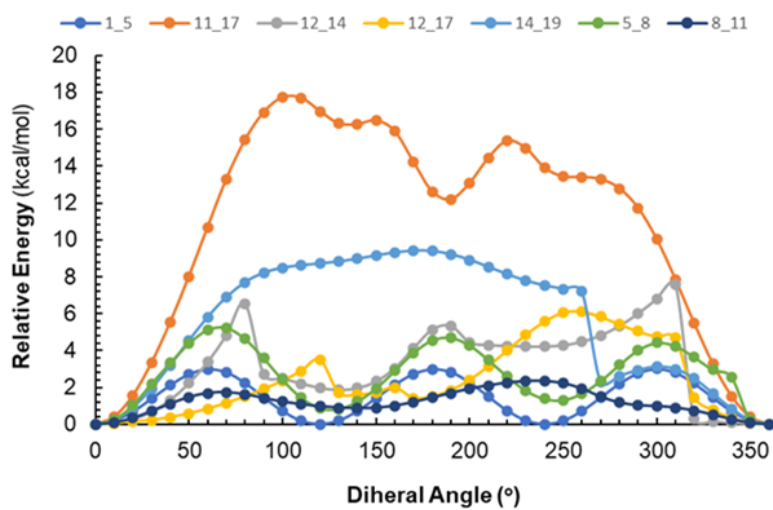
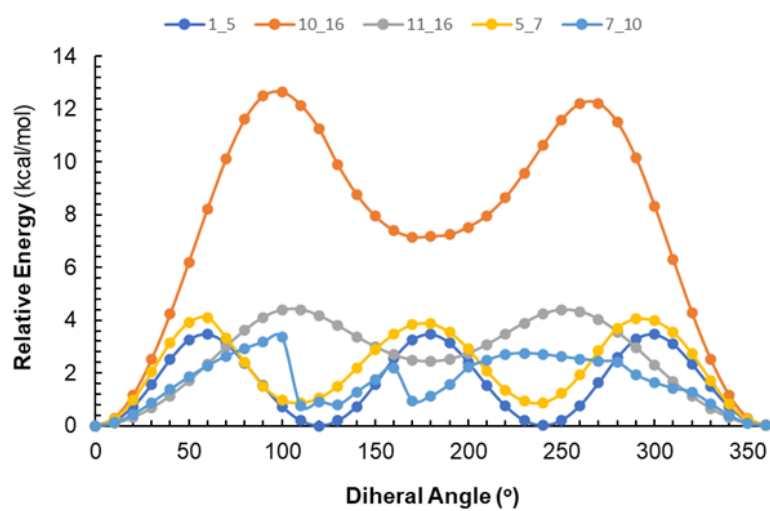
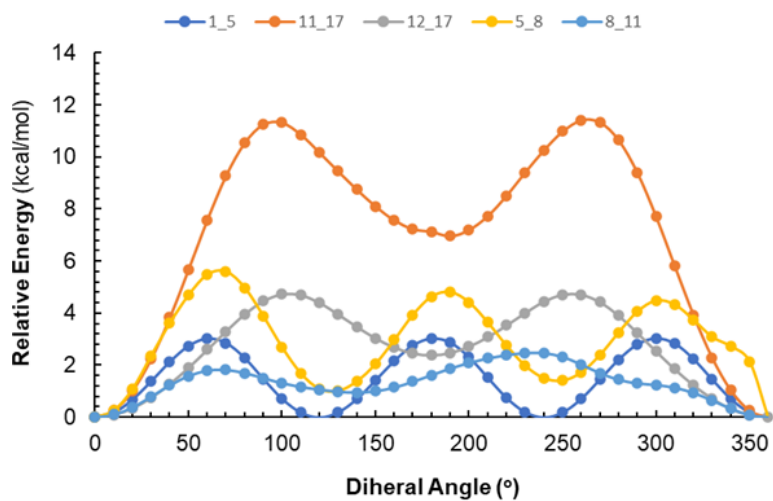


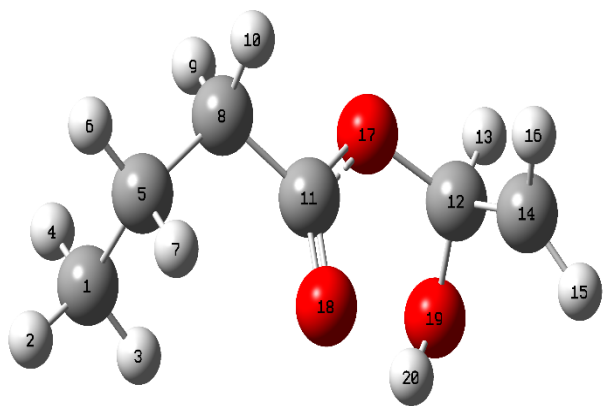
RC



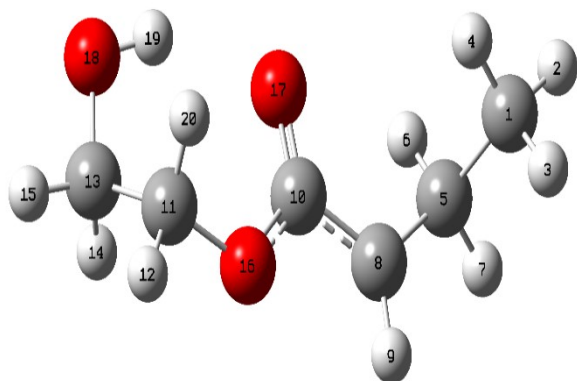
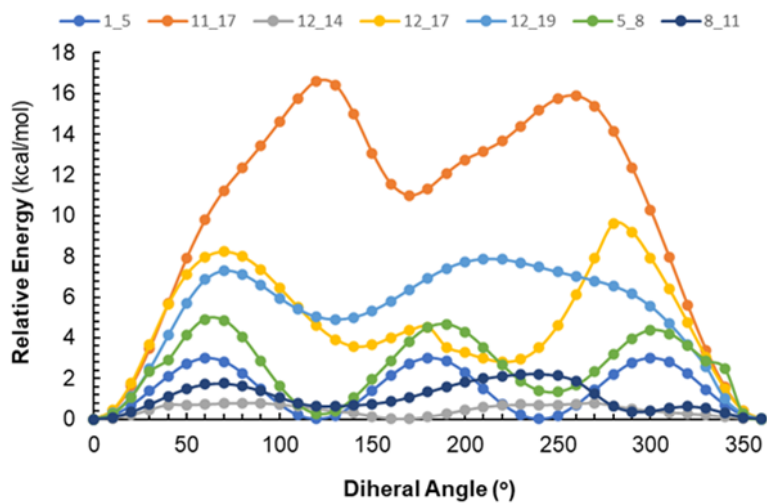
IM1

Hindrance Potentials

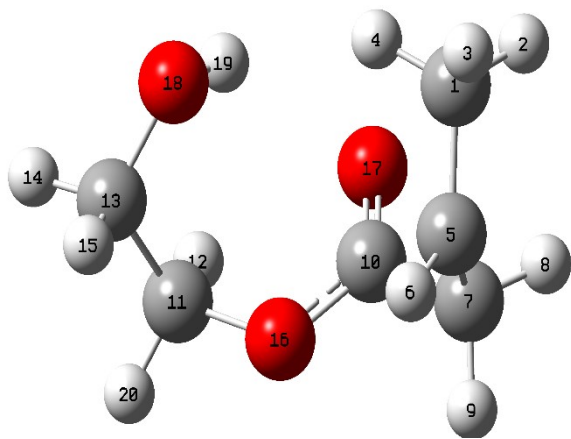
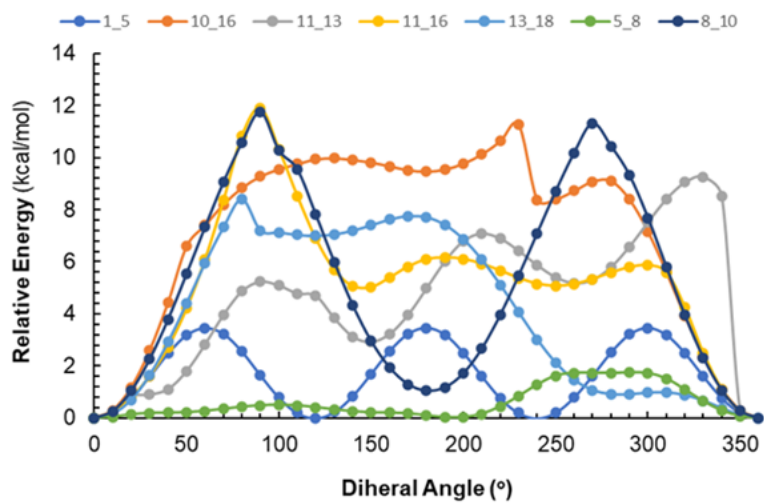




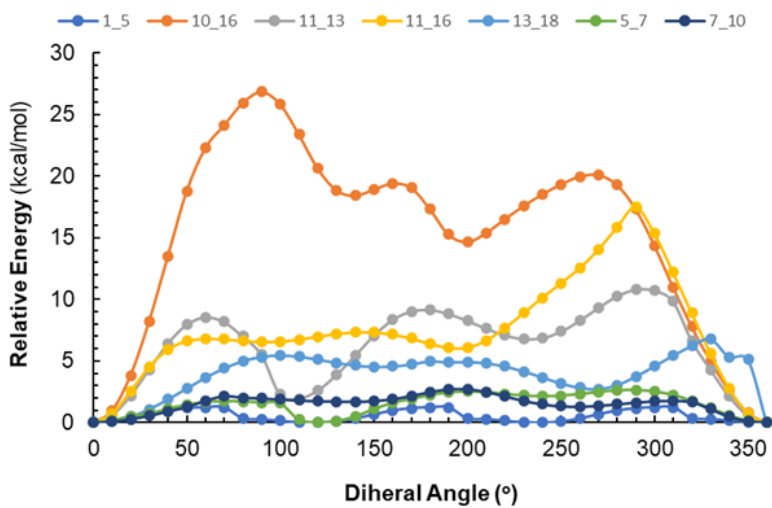
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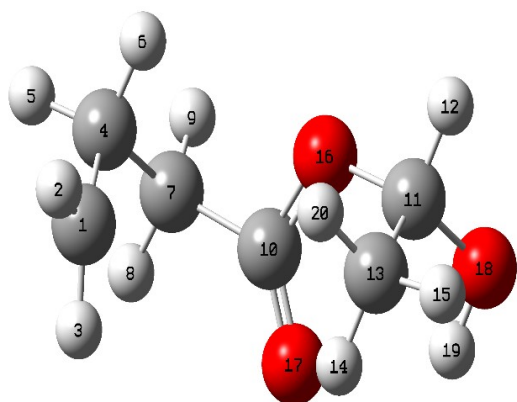


IM3

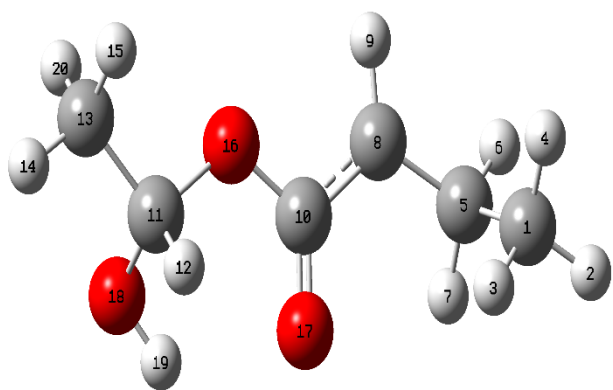
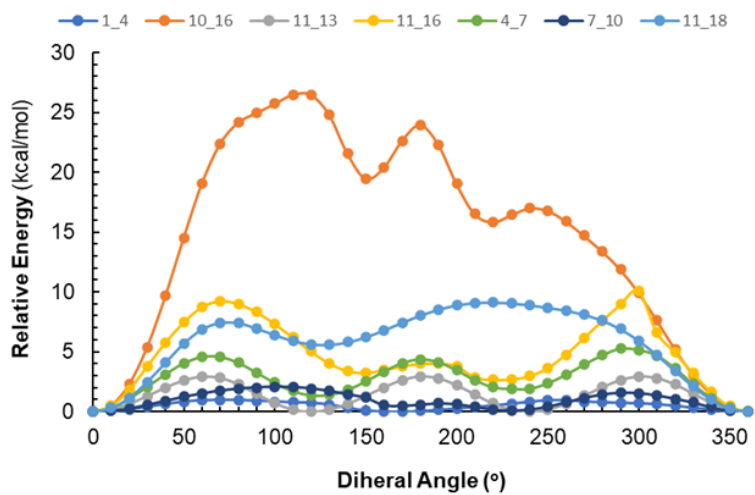


IM4

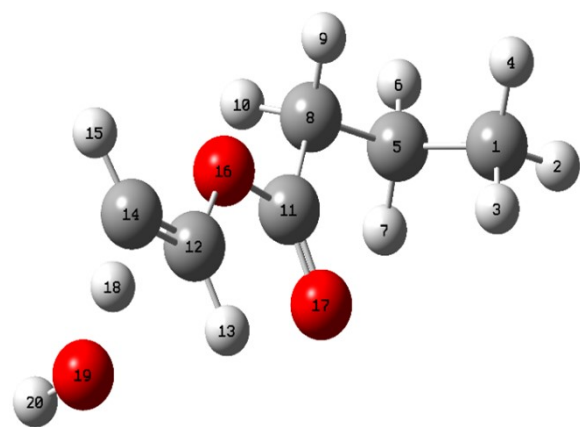
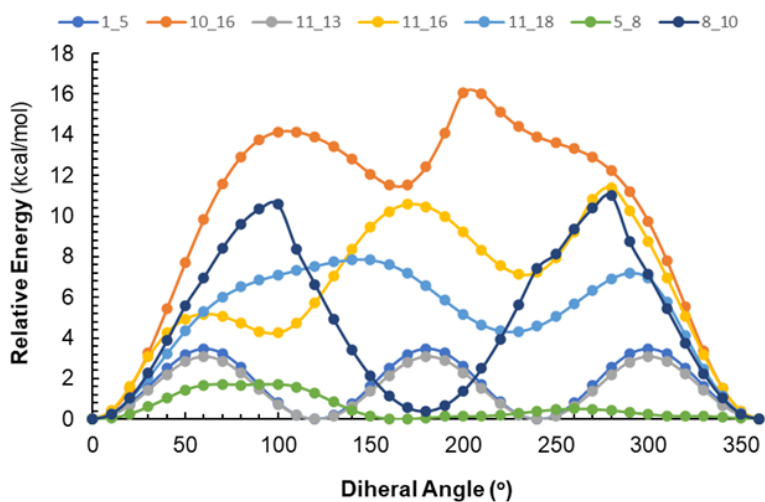




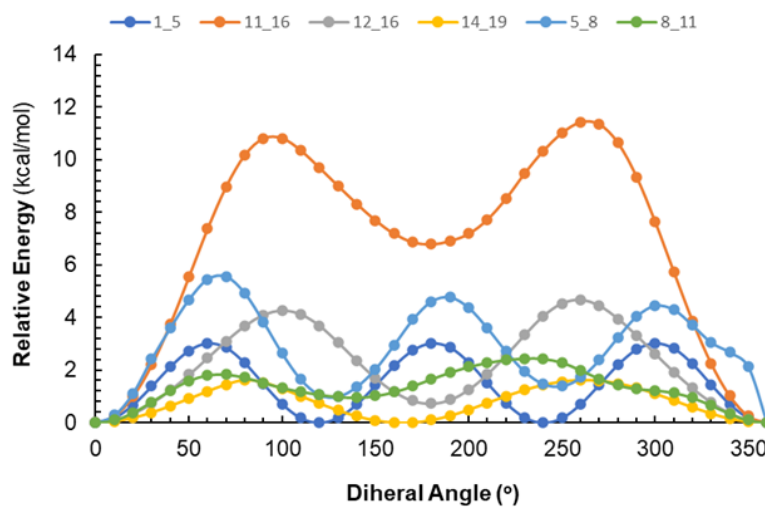
IM5

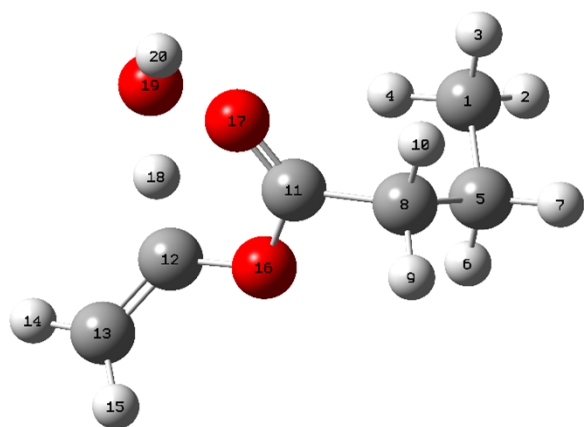


IM6

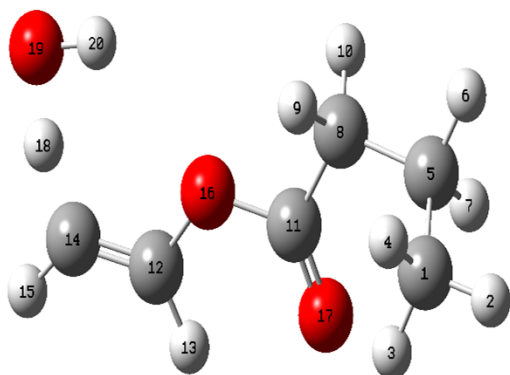
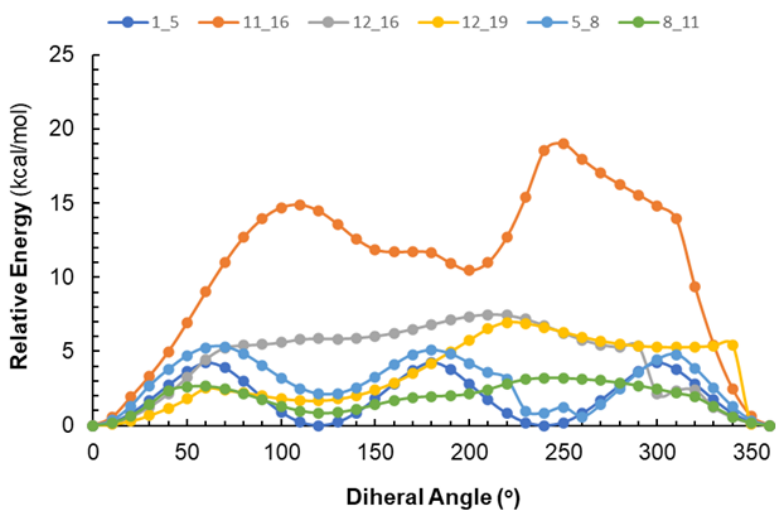


TS1

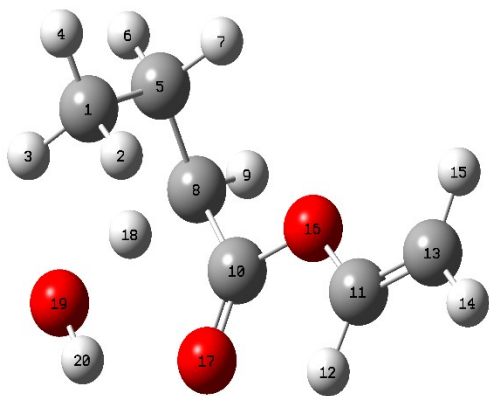
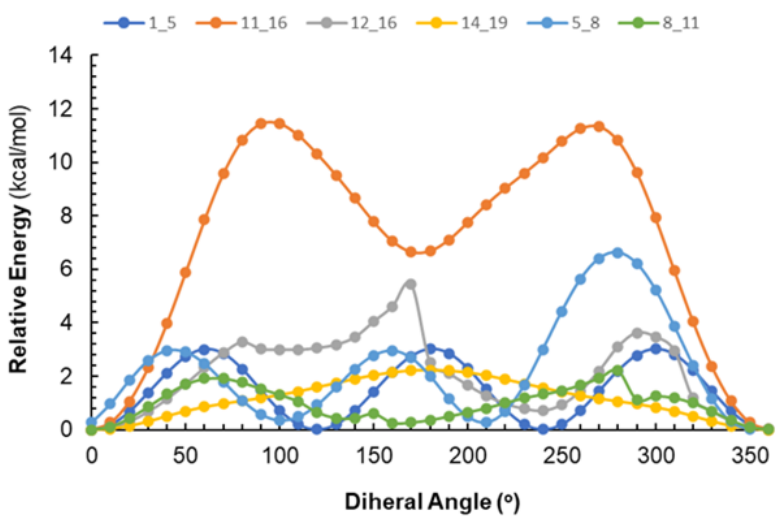




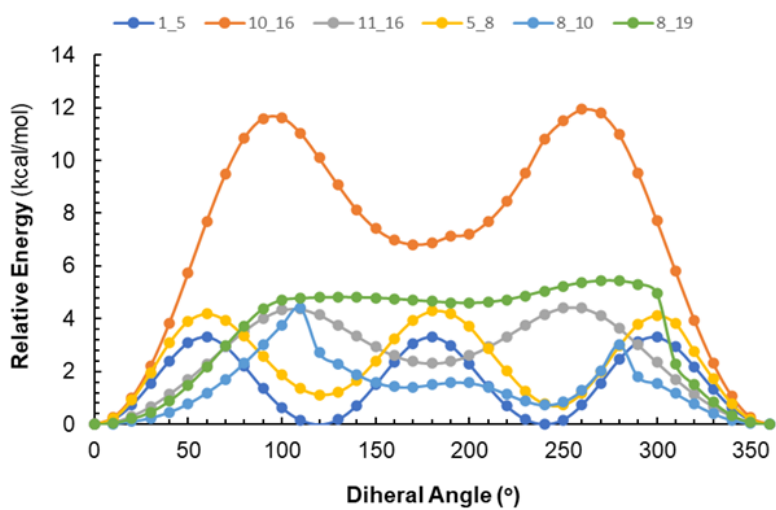
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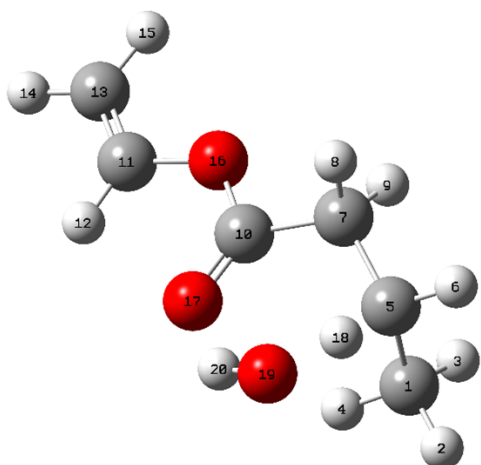


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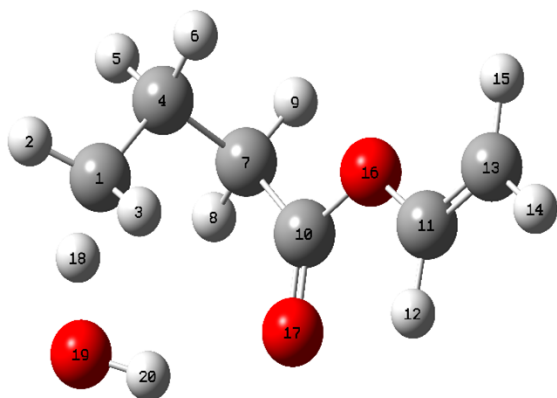
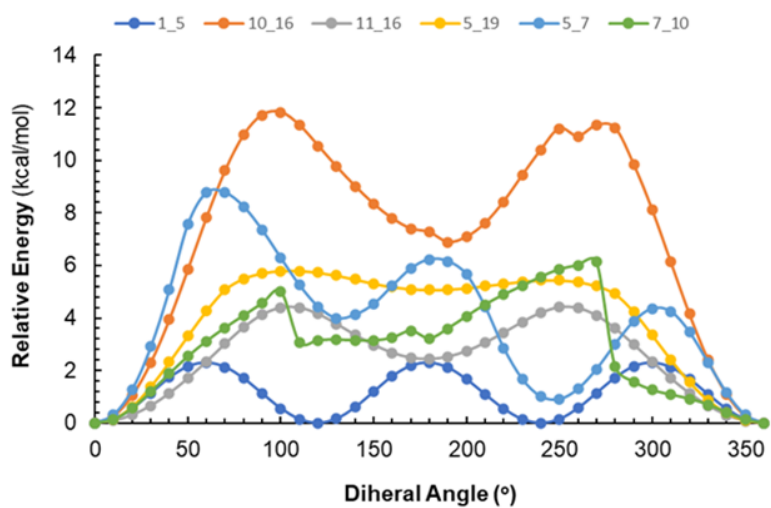


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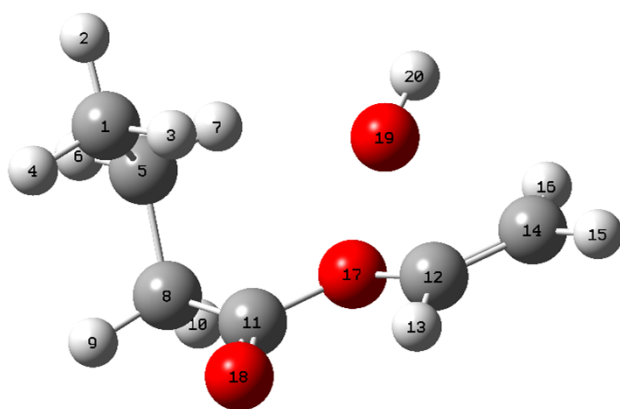
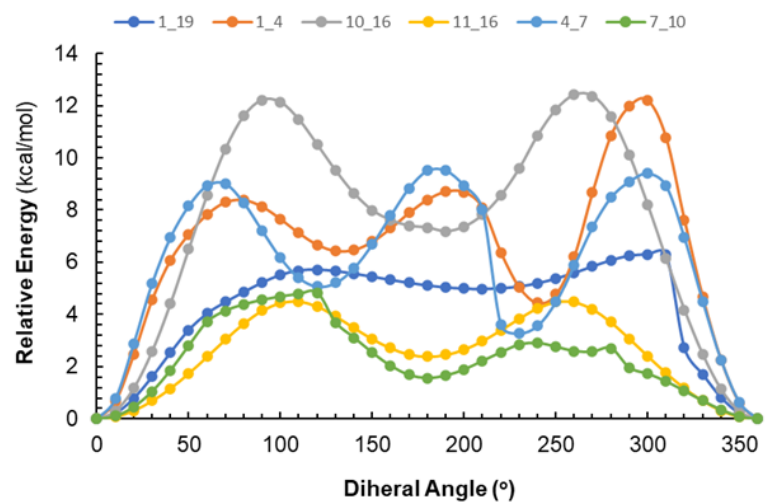




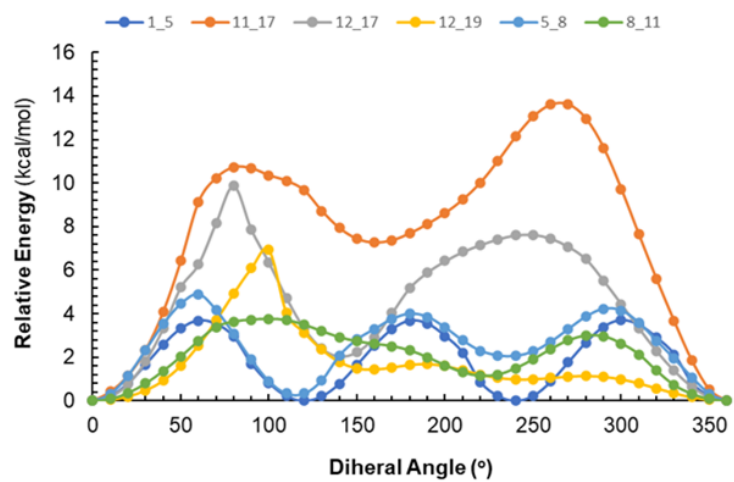
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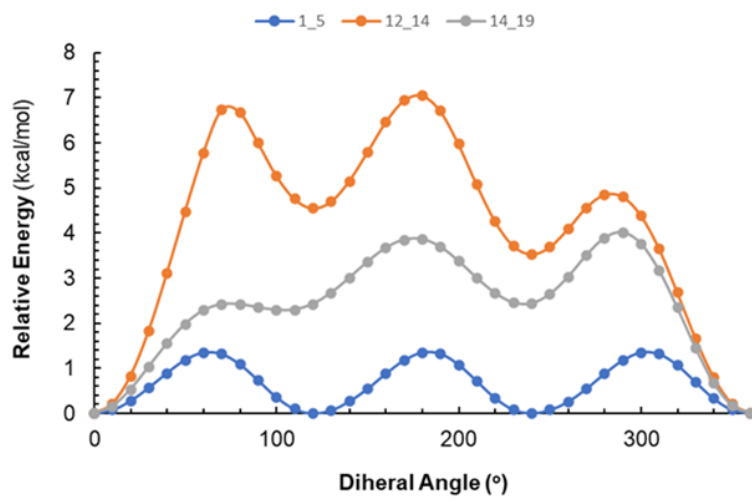
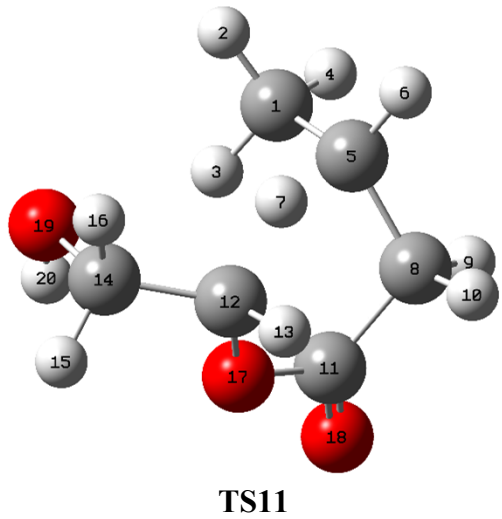
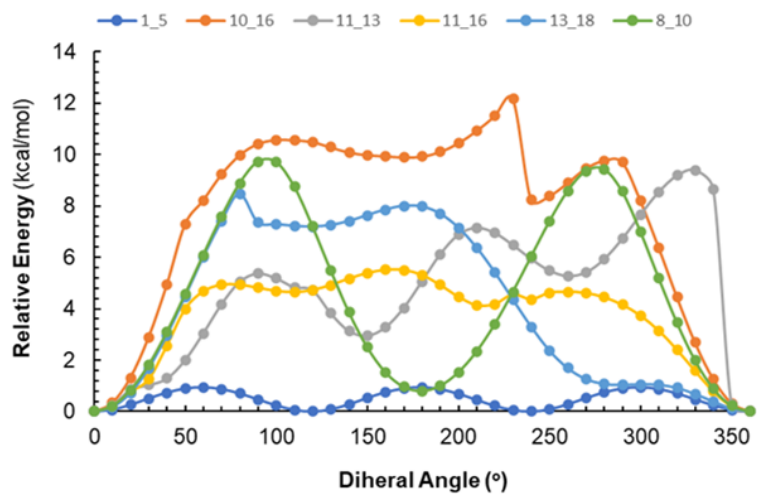
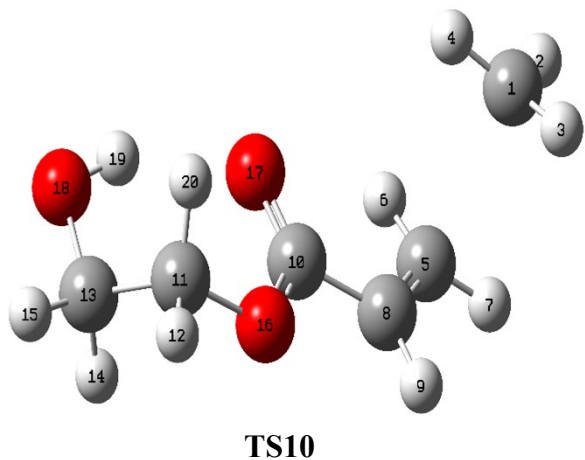
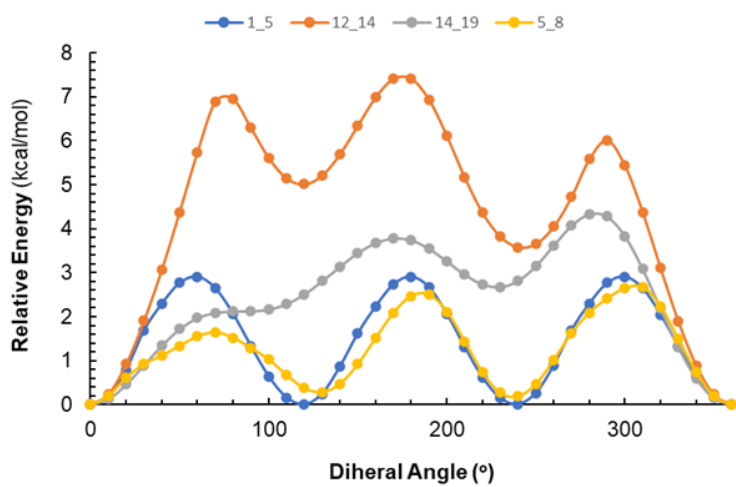
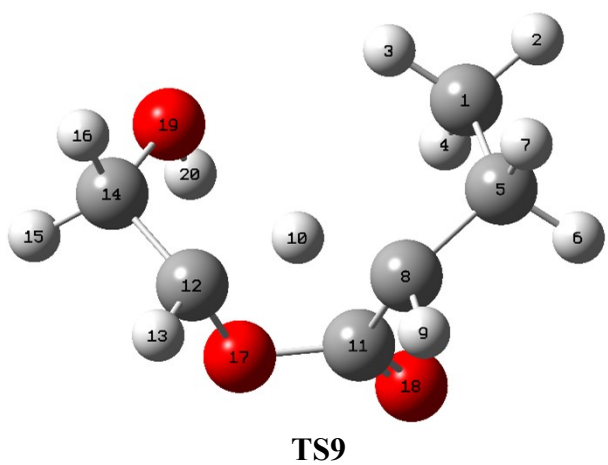


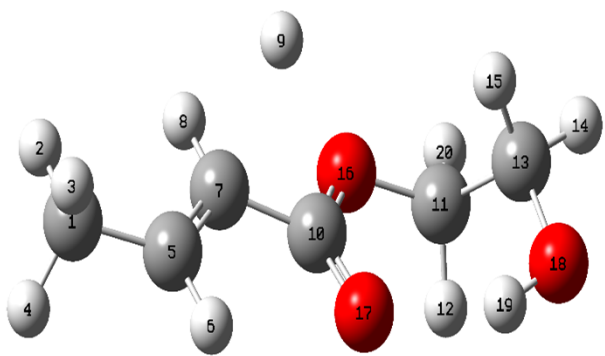
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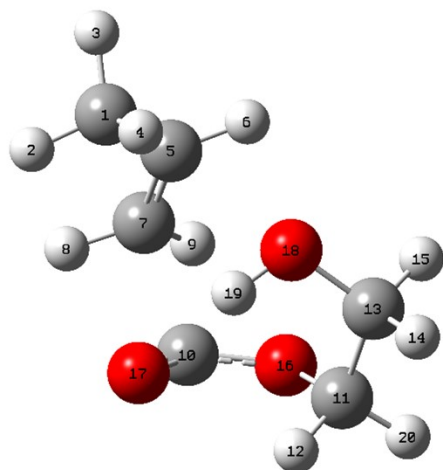
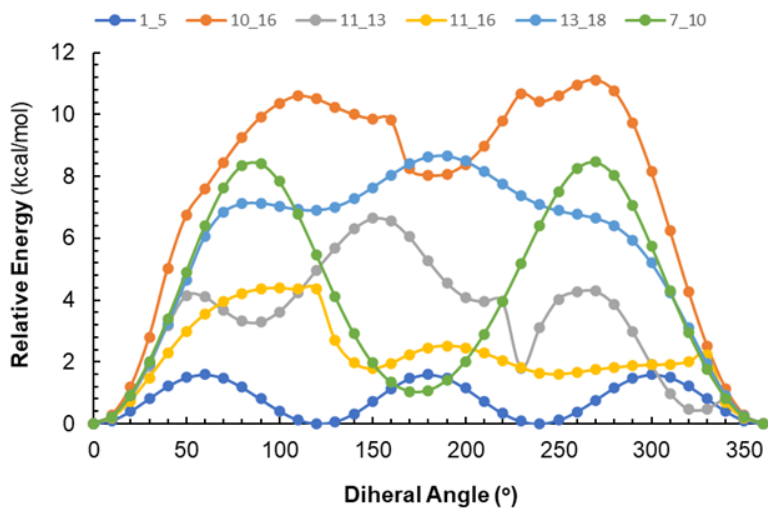
TS8



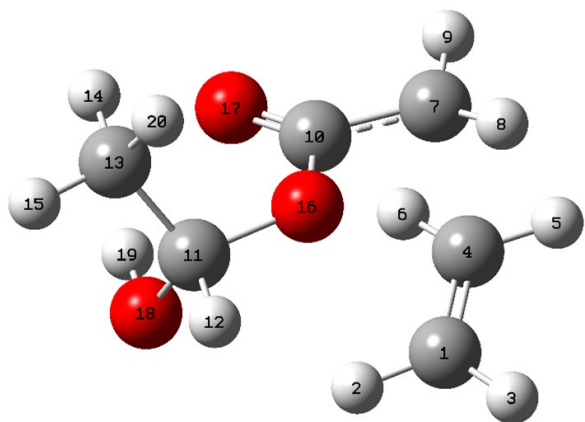
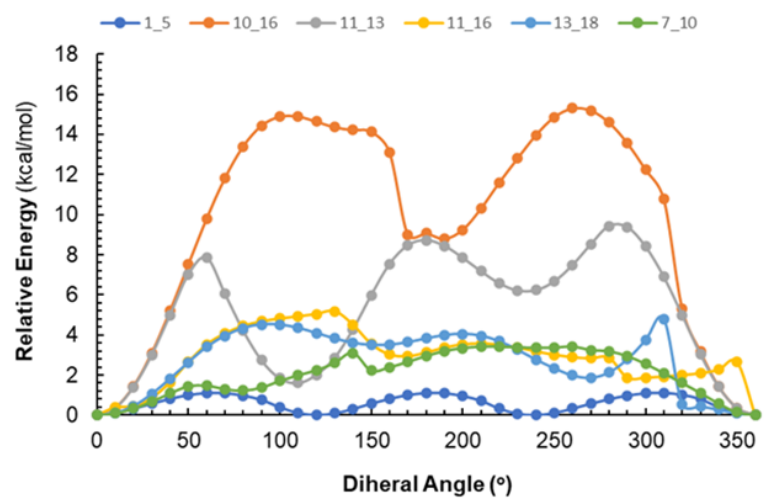




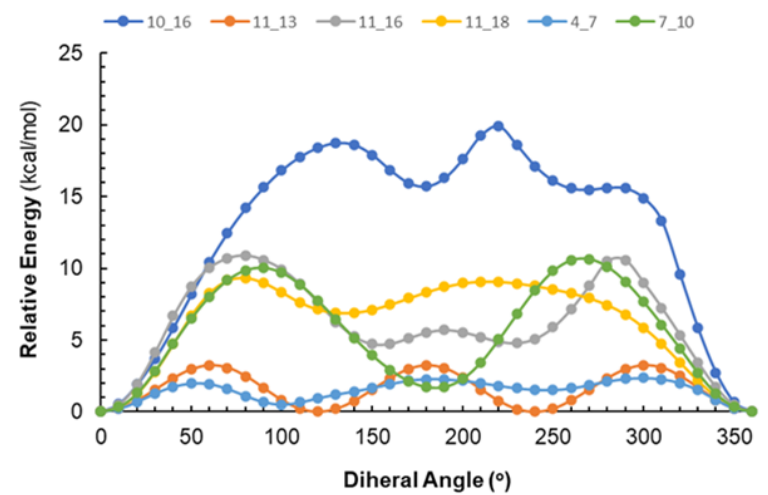
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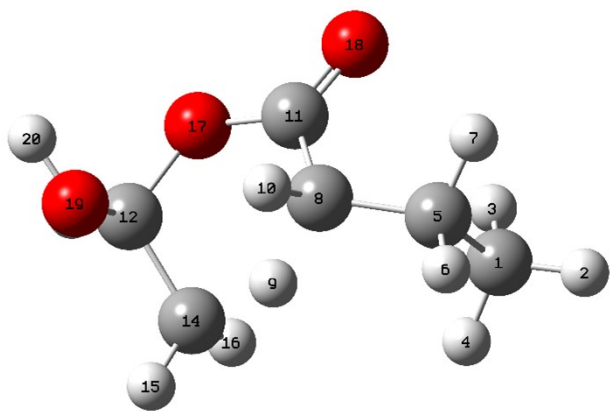


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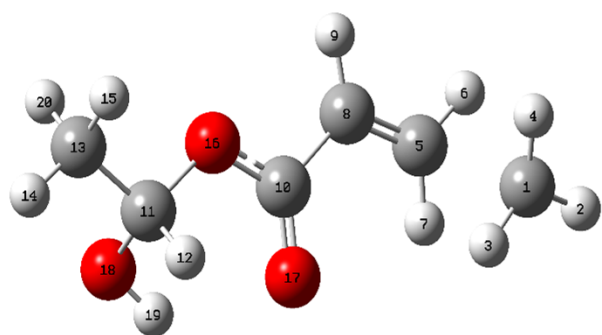
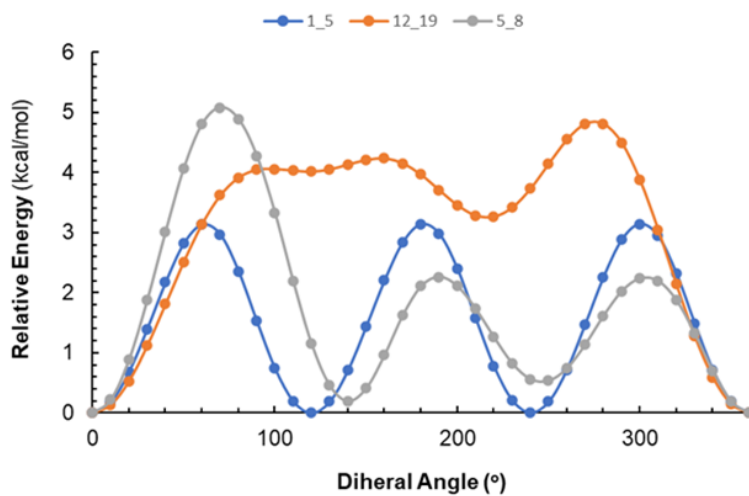


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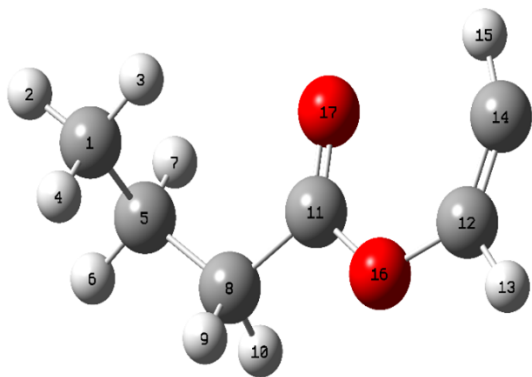
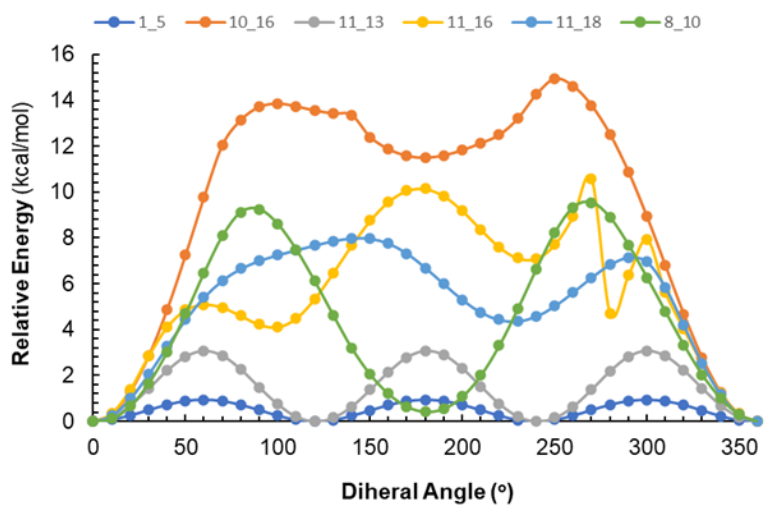




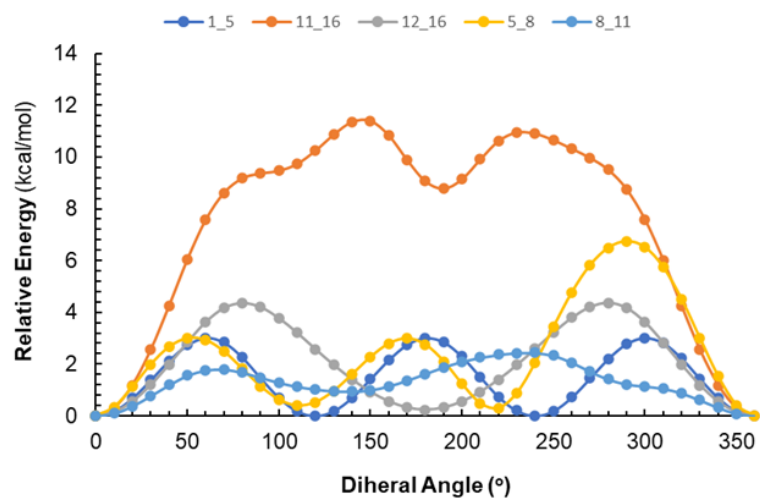
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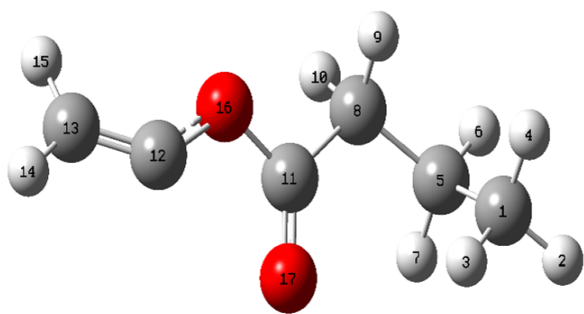


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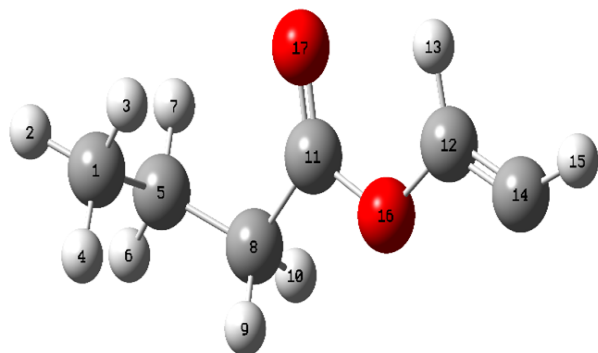
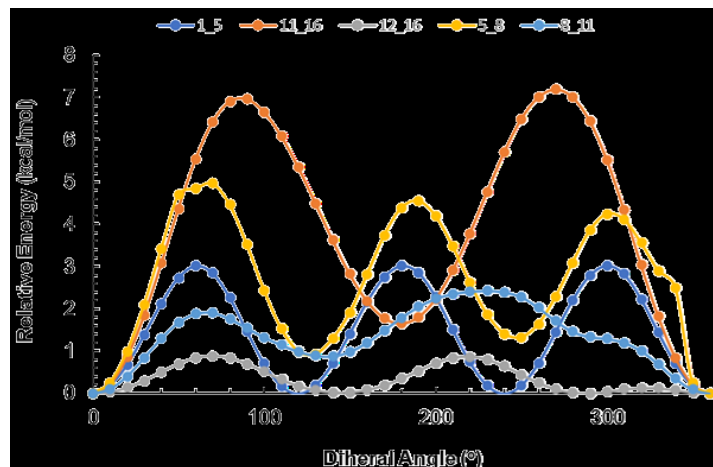


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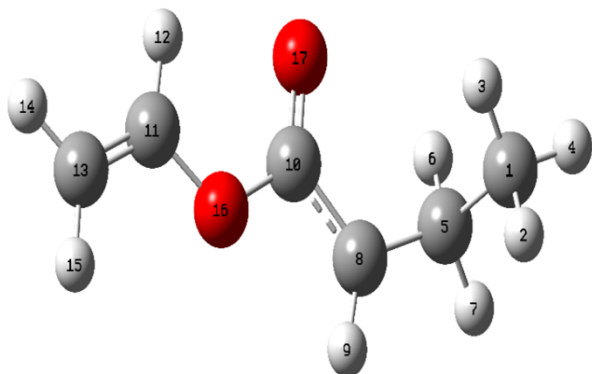
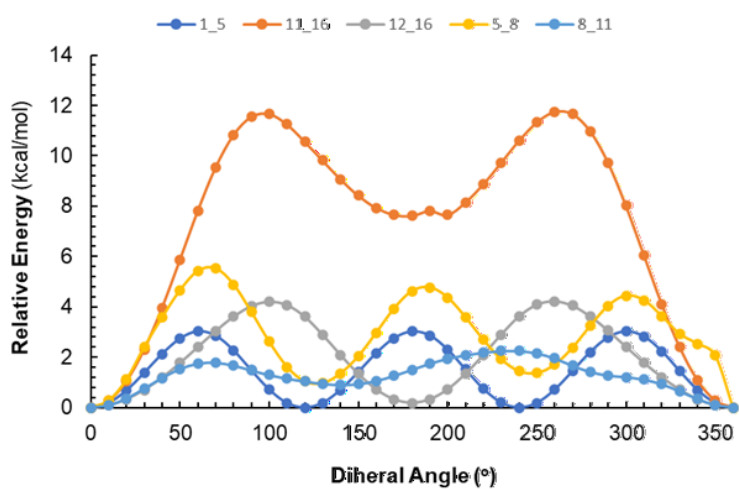




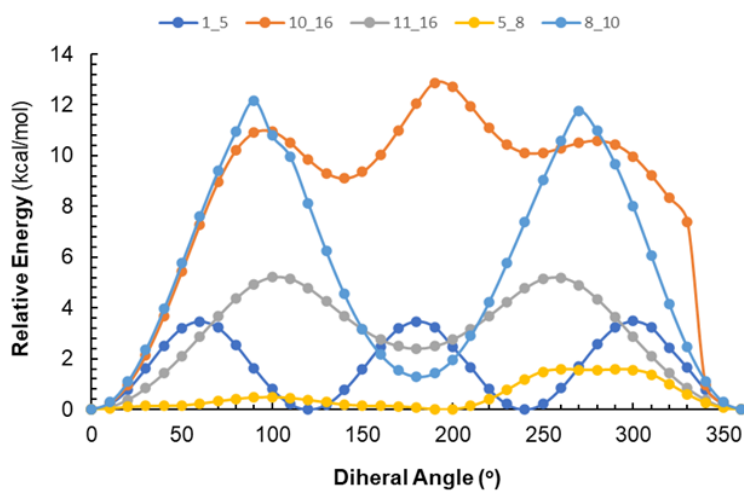
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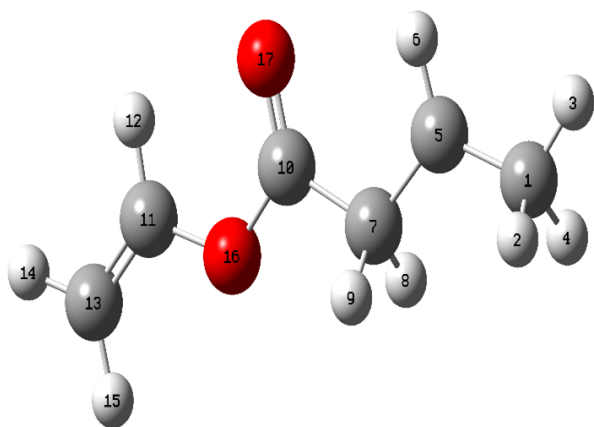


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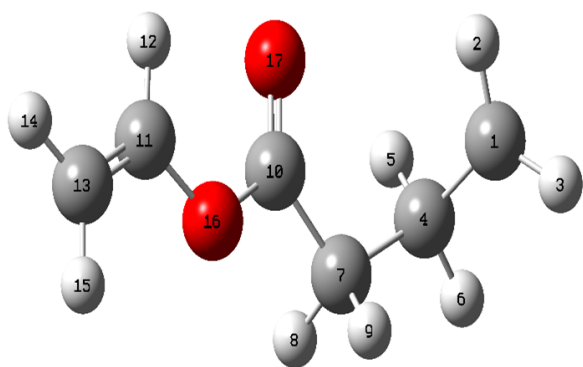
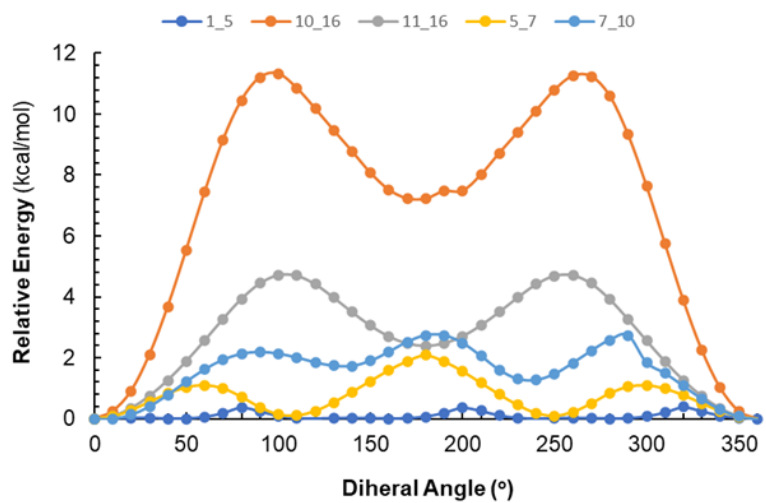


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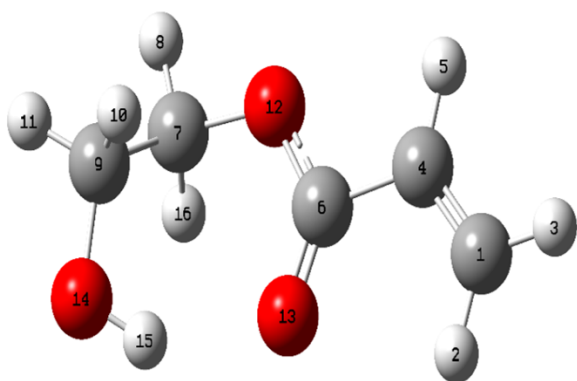
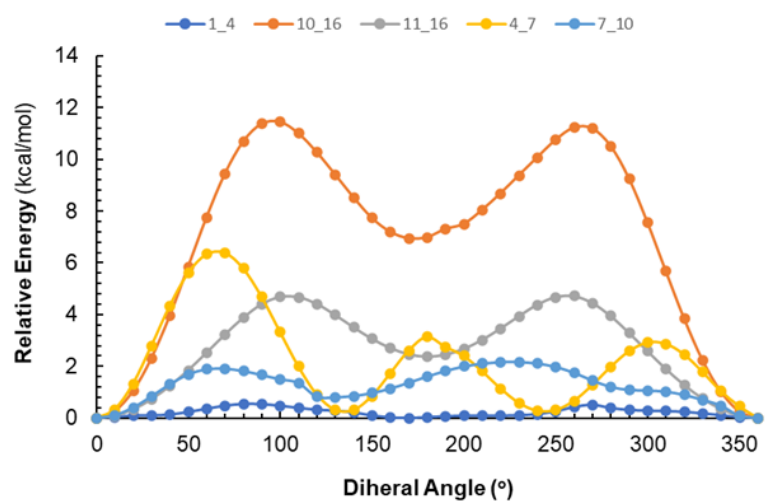




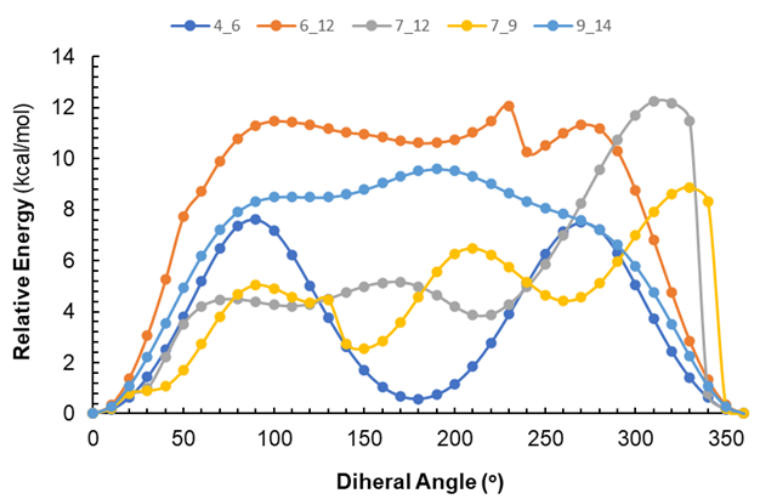
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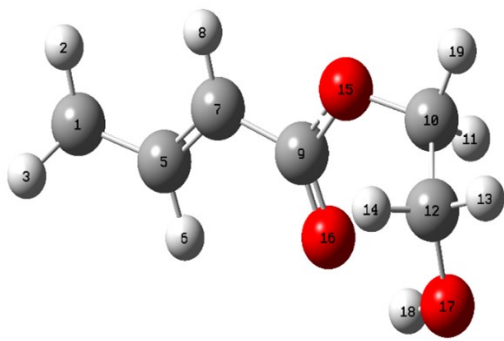


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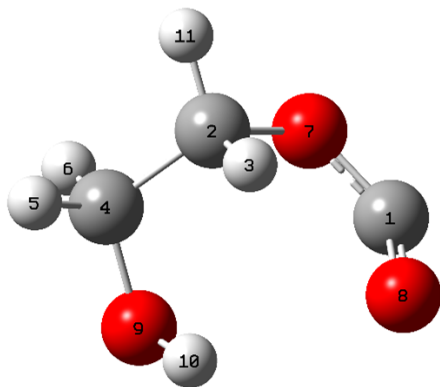
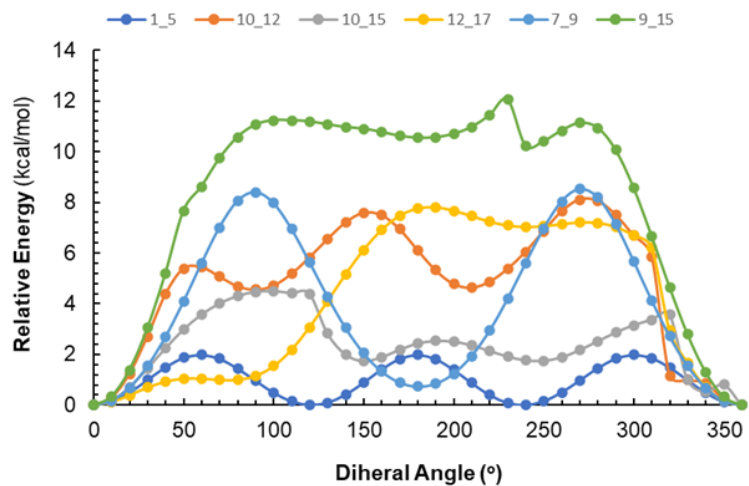


P7

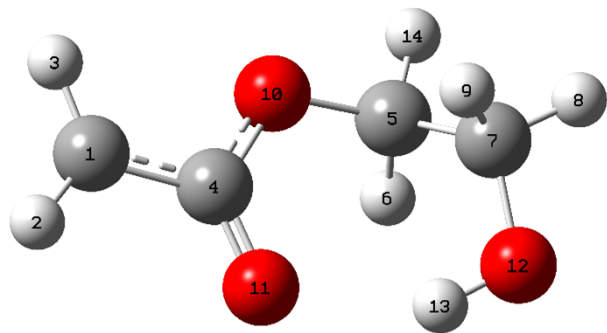
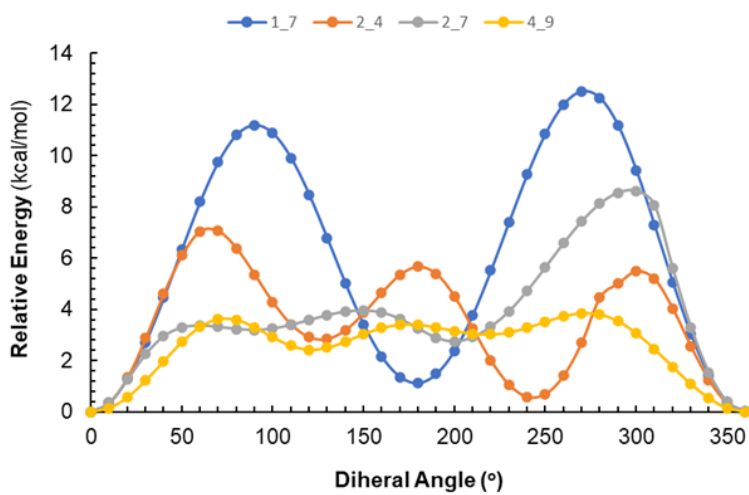




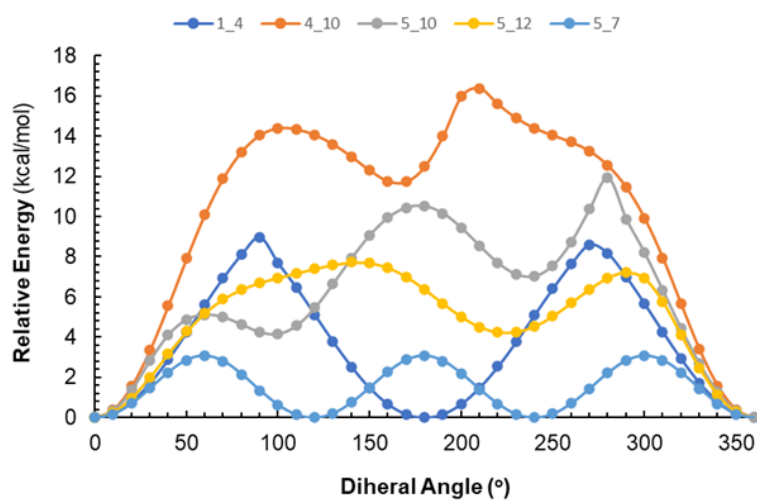
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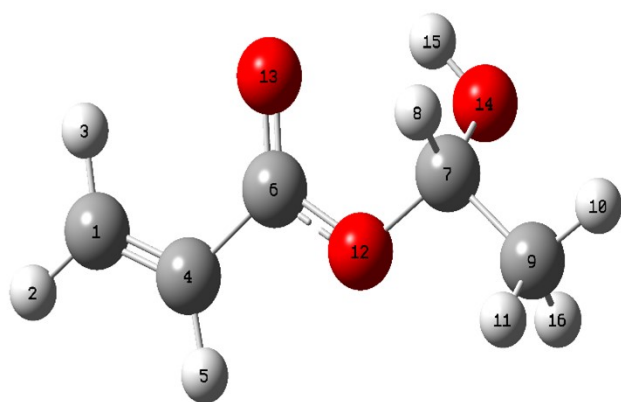


P9

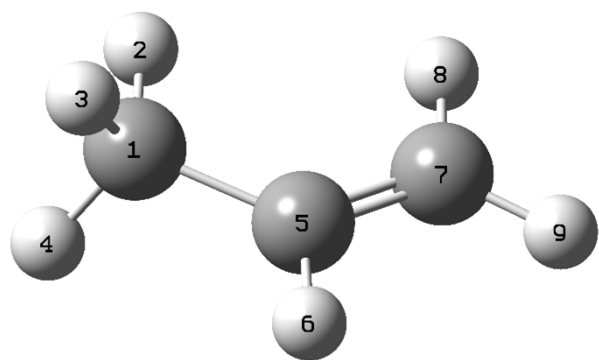
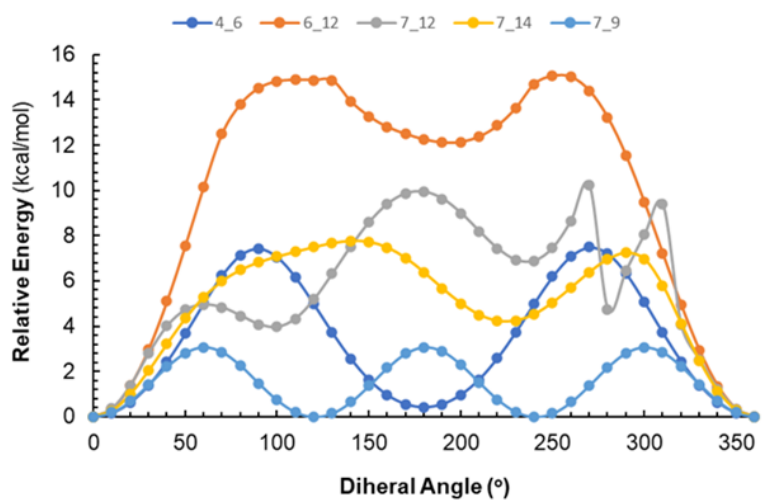


P10

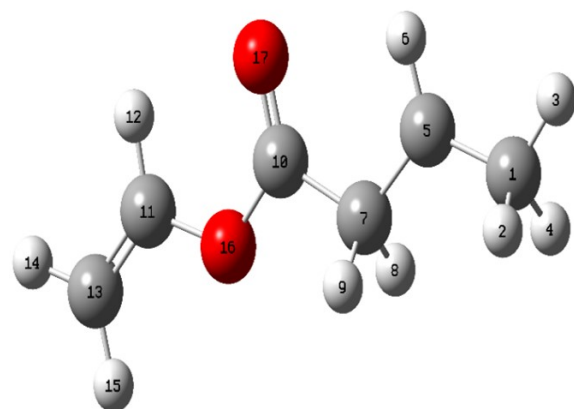
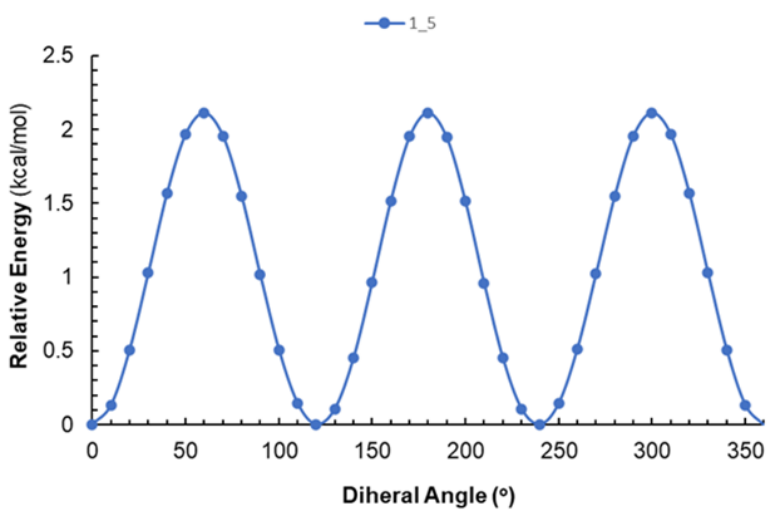




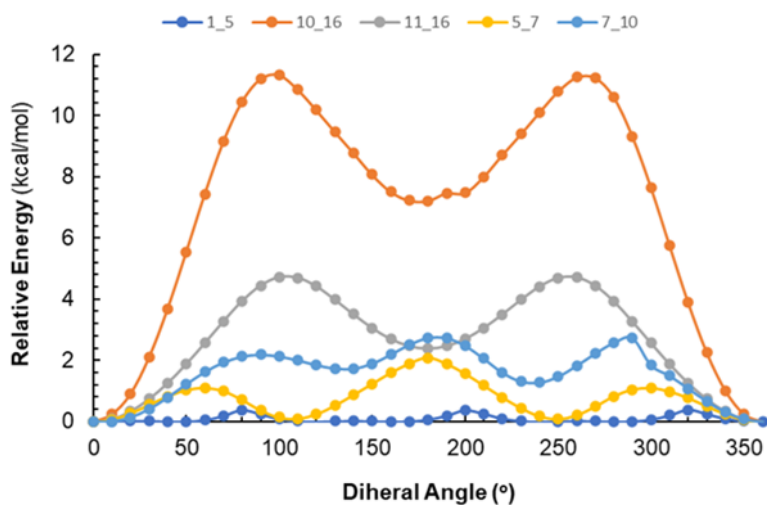
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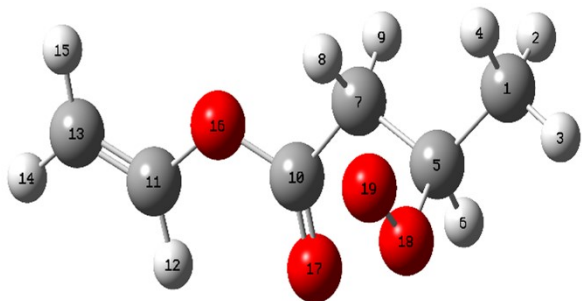


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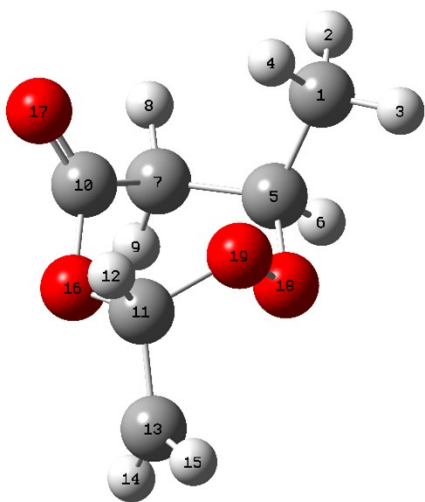
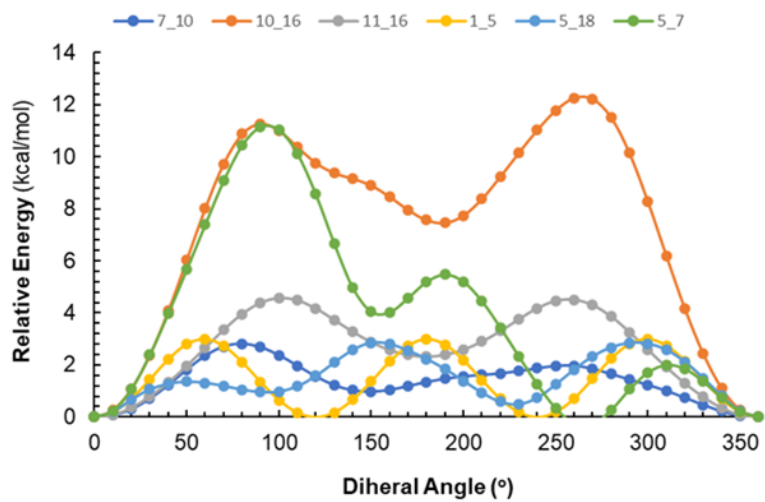


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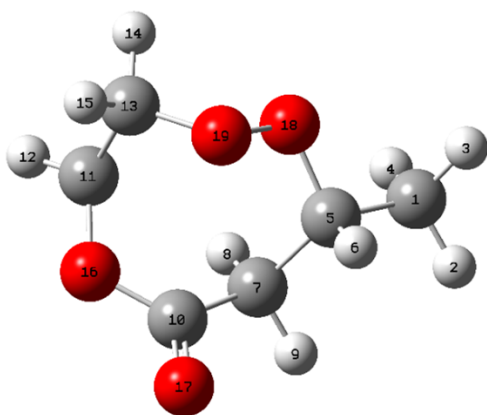
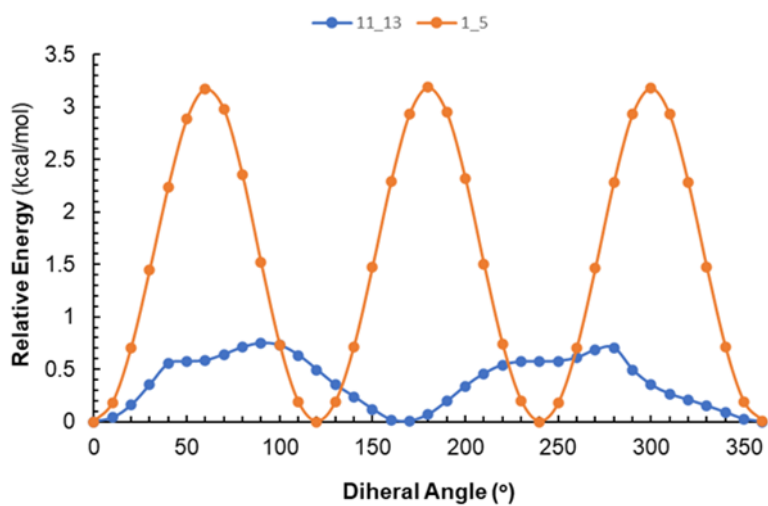




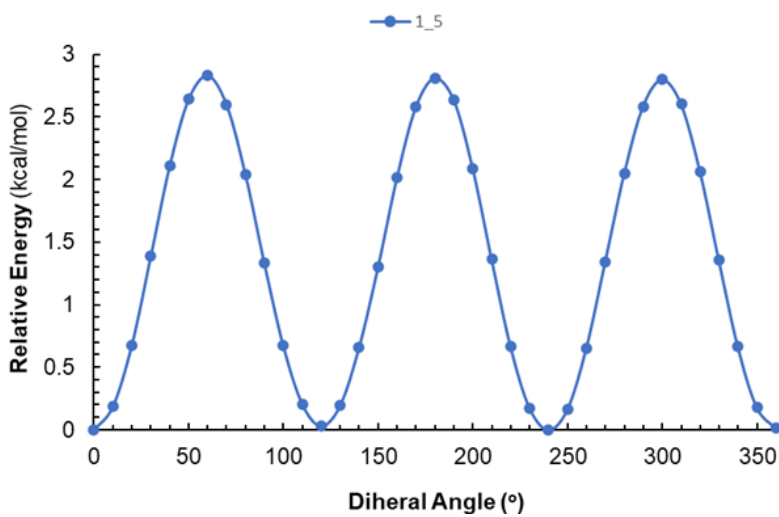
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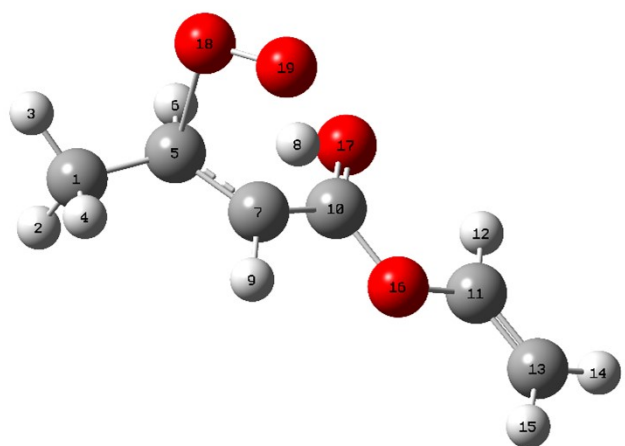


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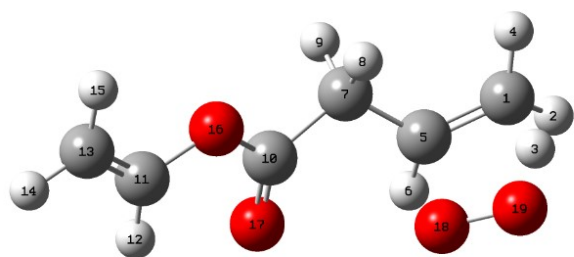
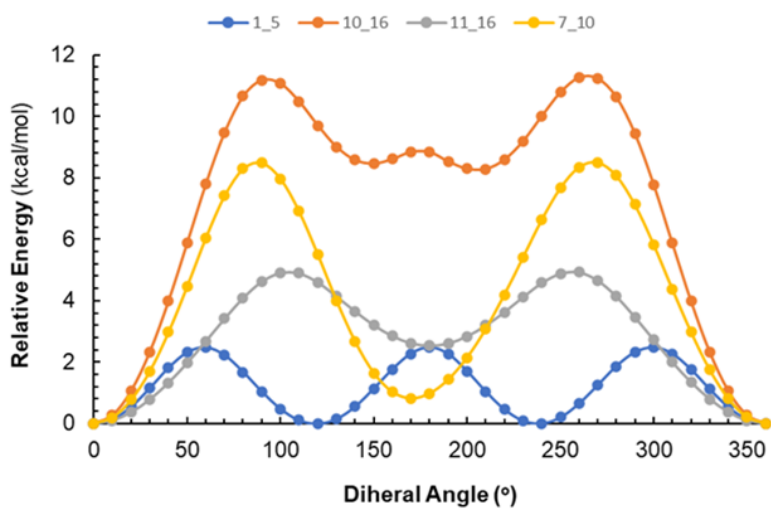


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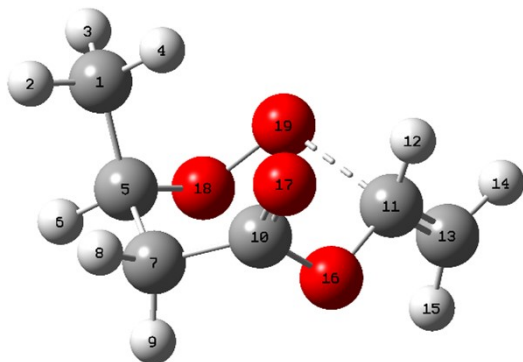
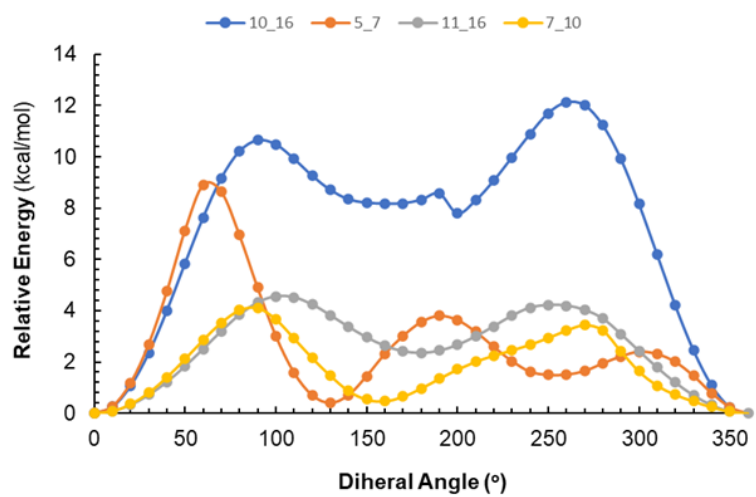




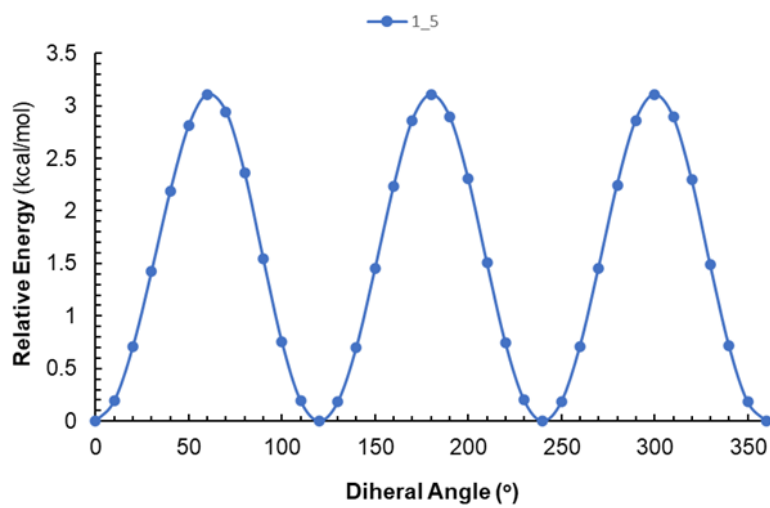
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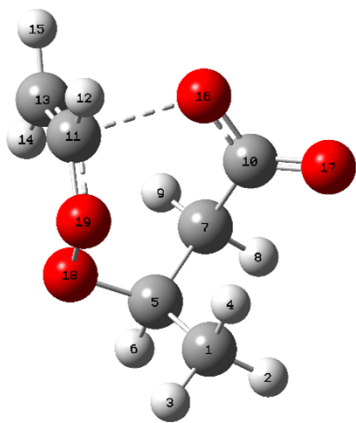


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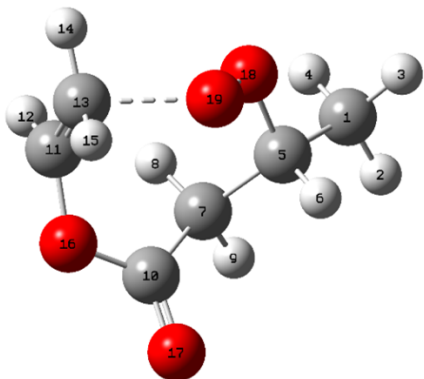
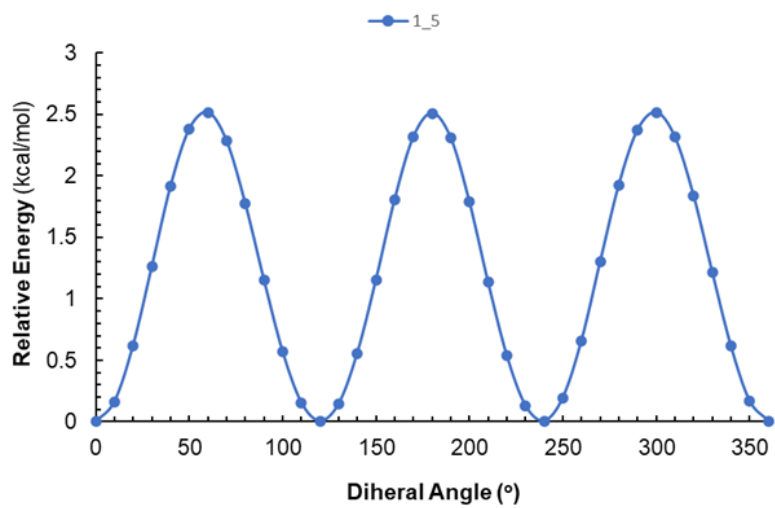


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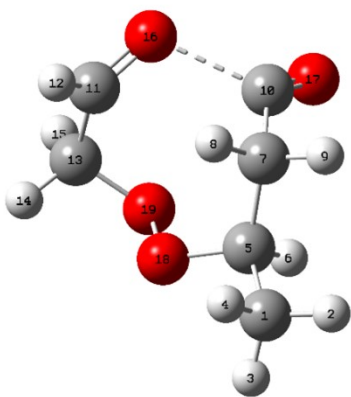
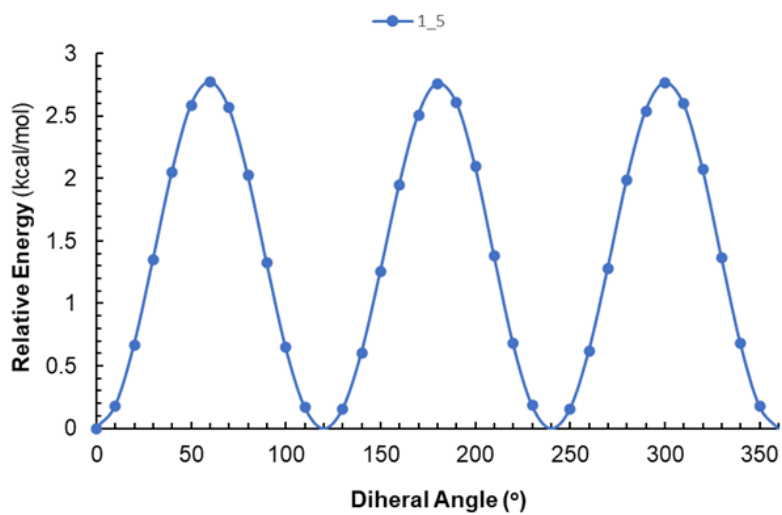




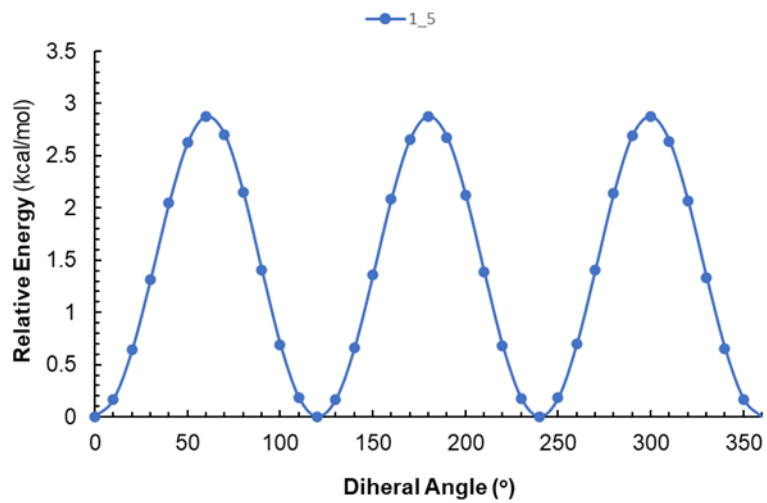
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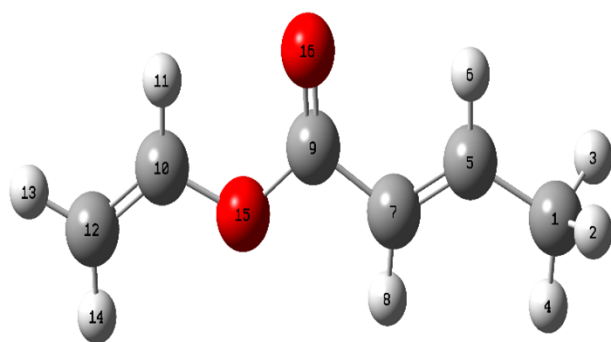


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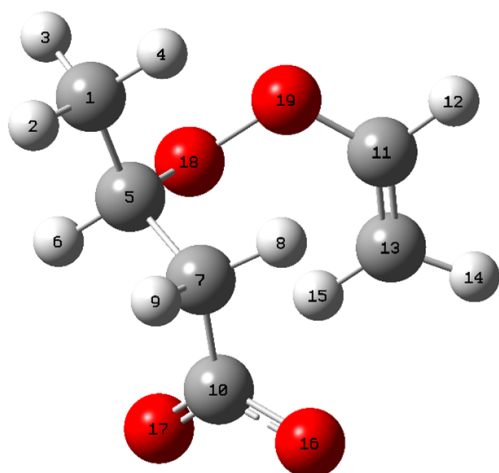
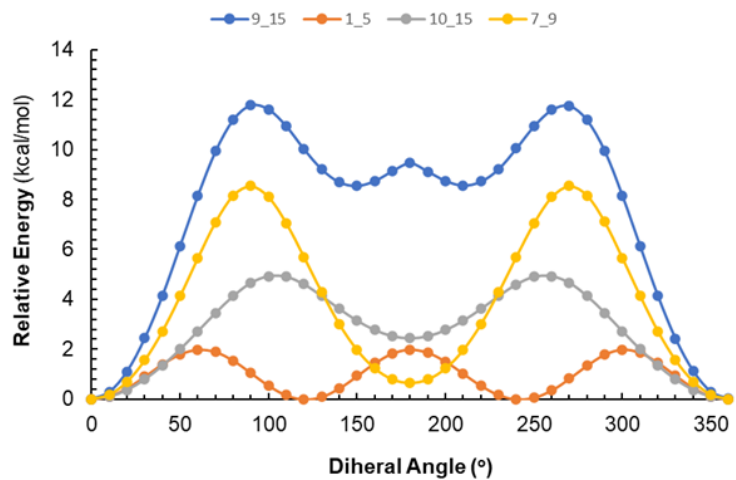


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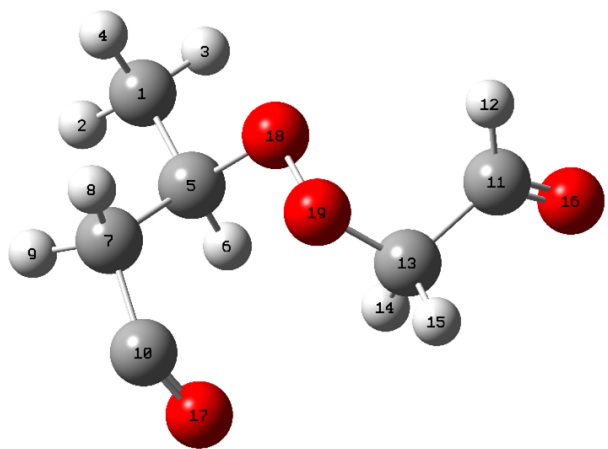
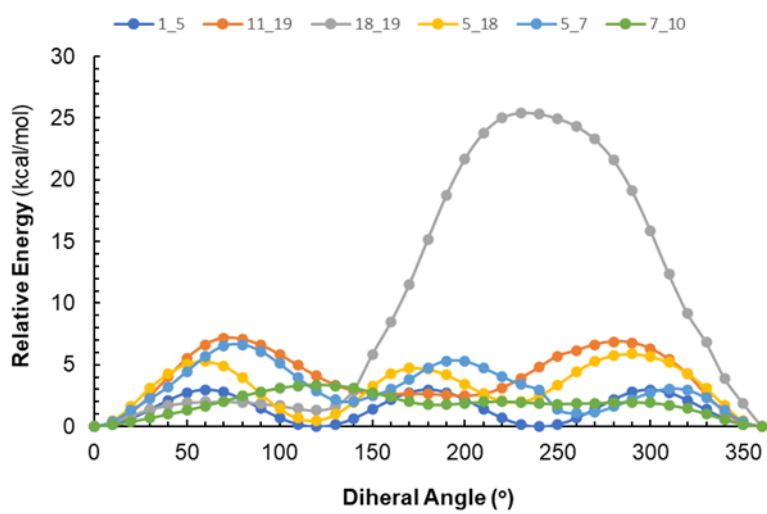




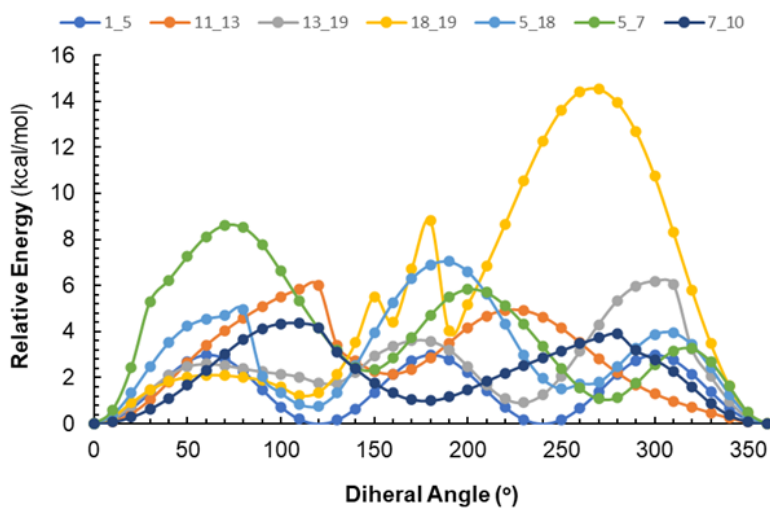
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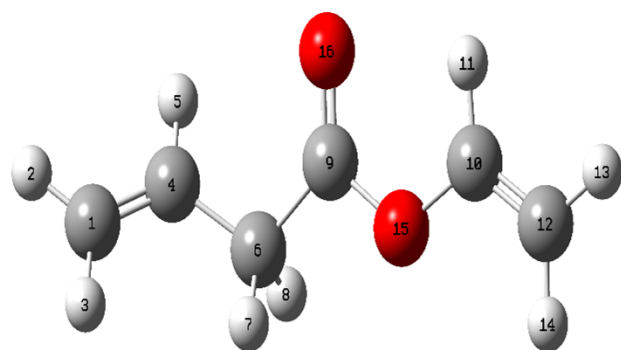


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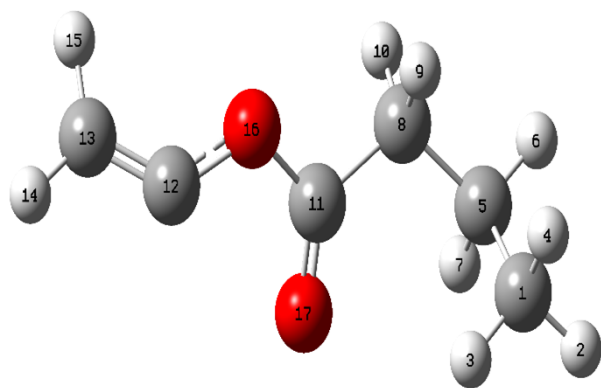
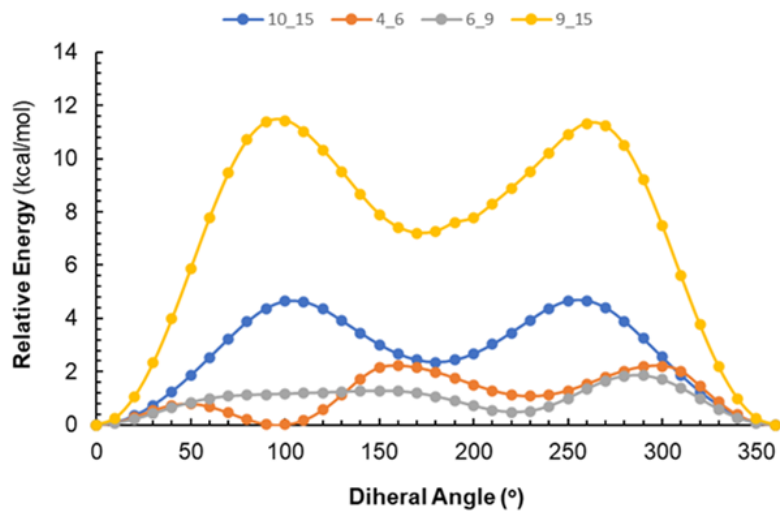


P14

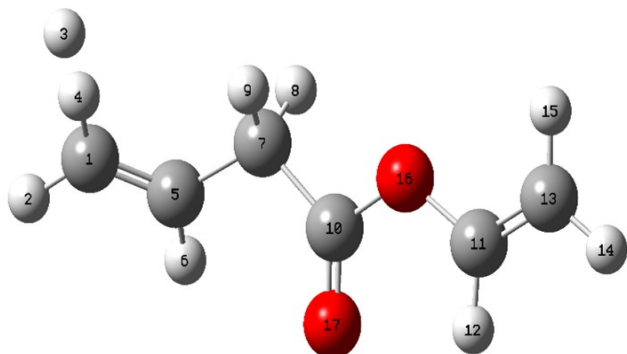
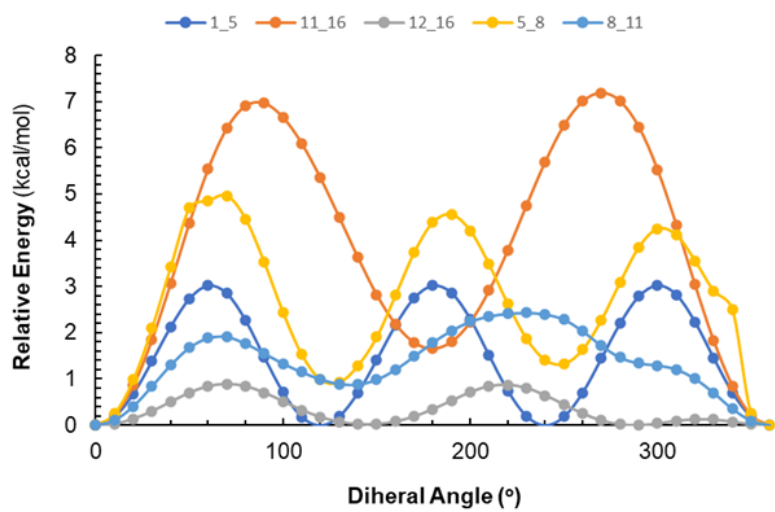




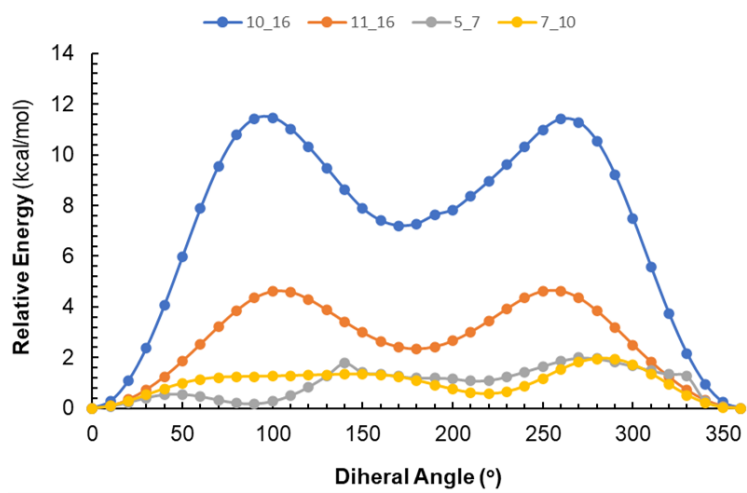
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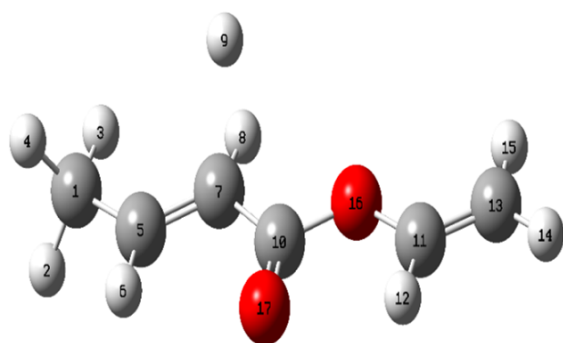


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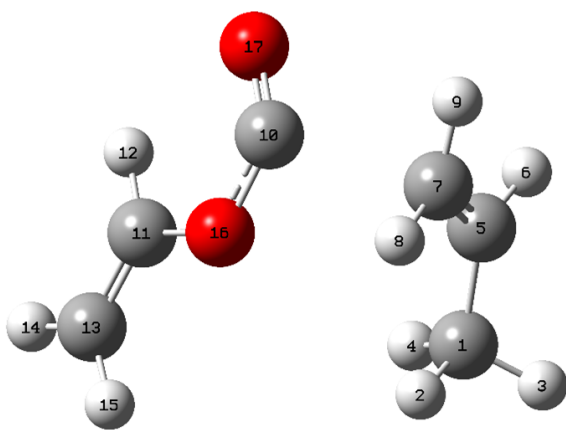
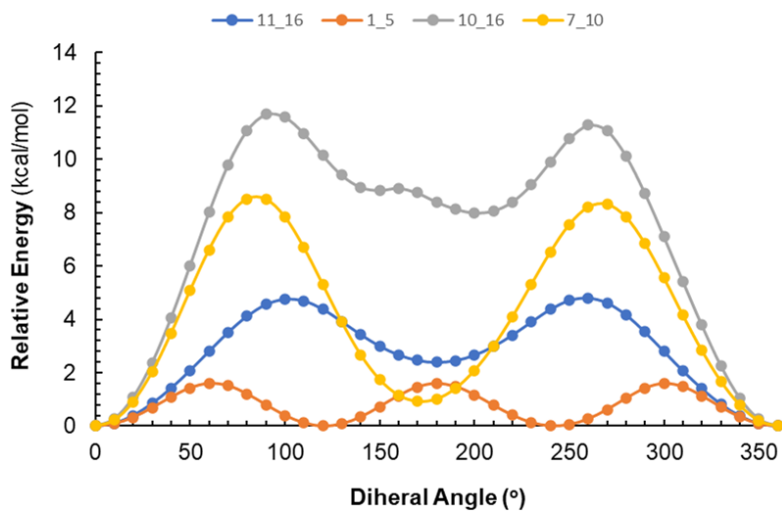


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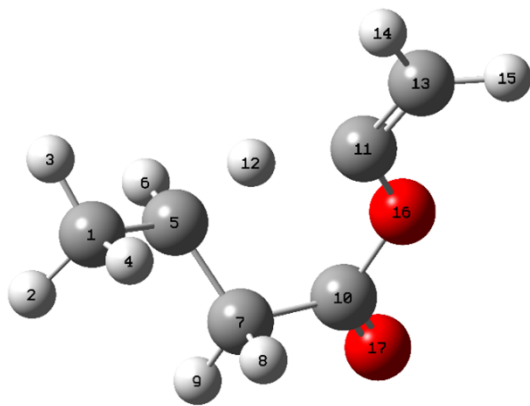
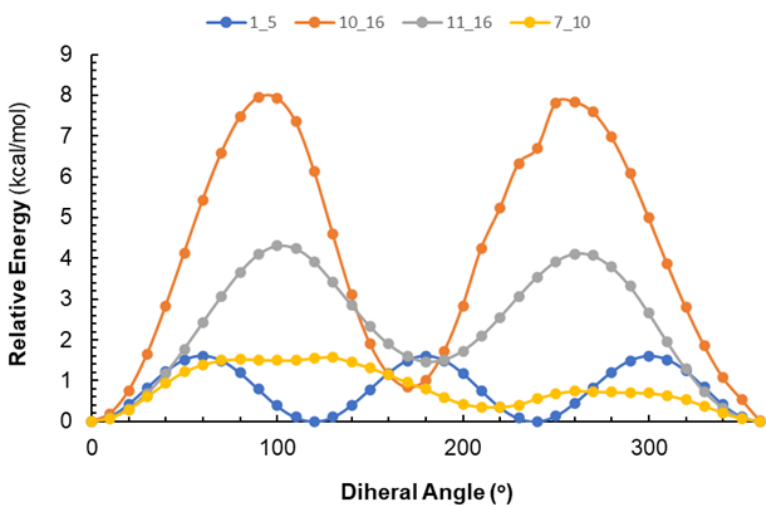




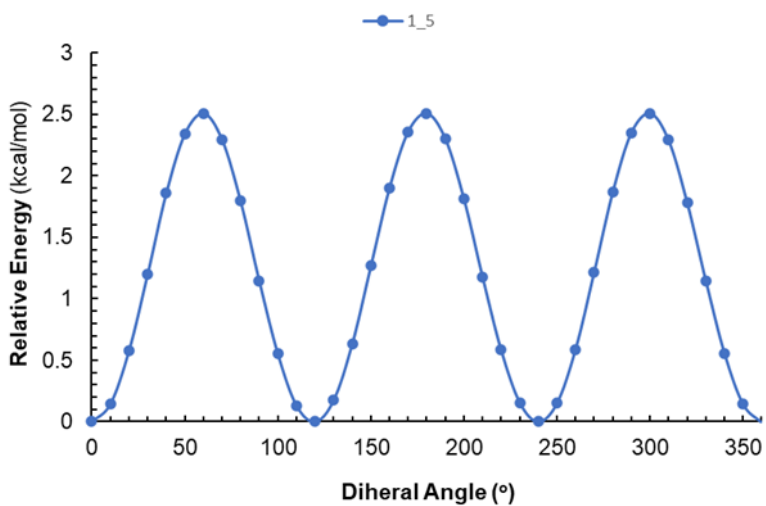
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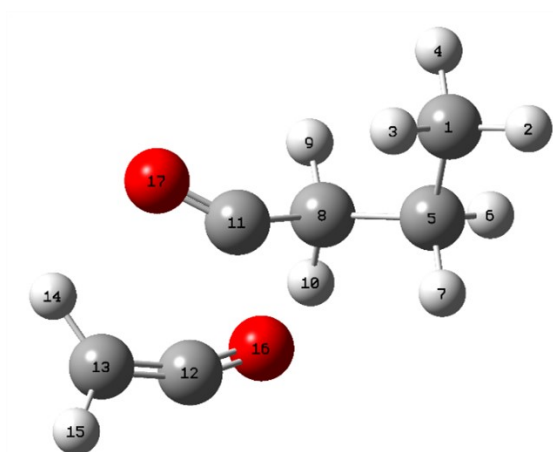


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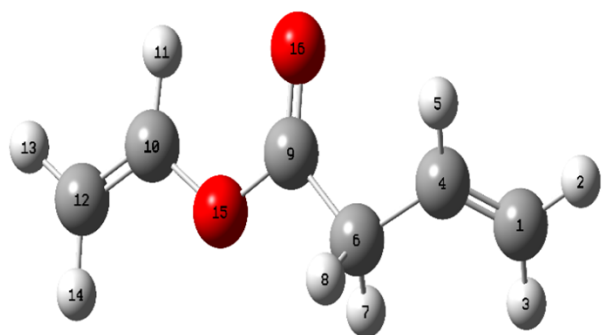
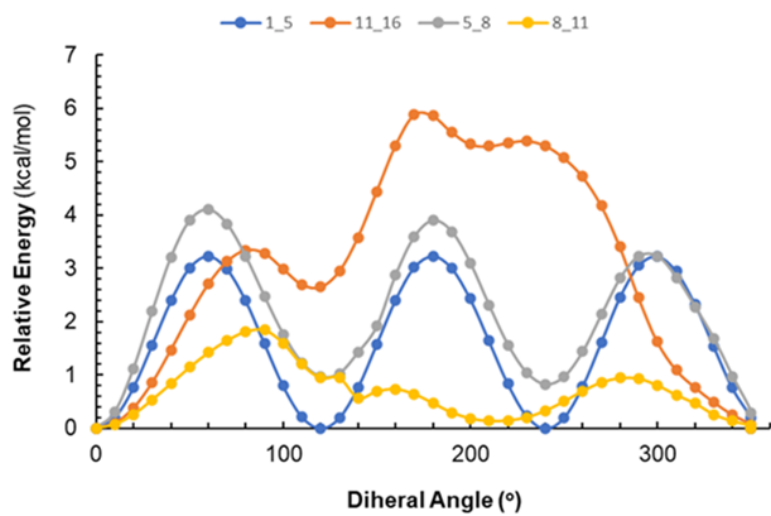


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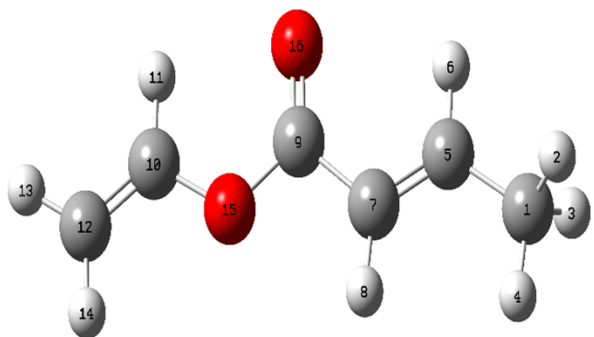
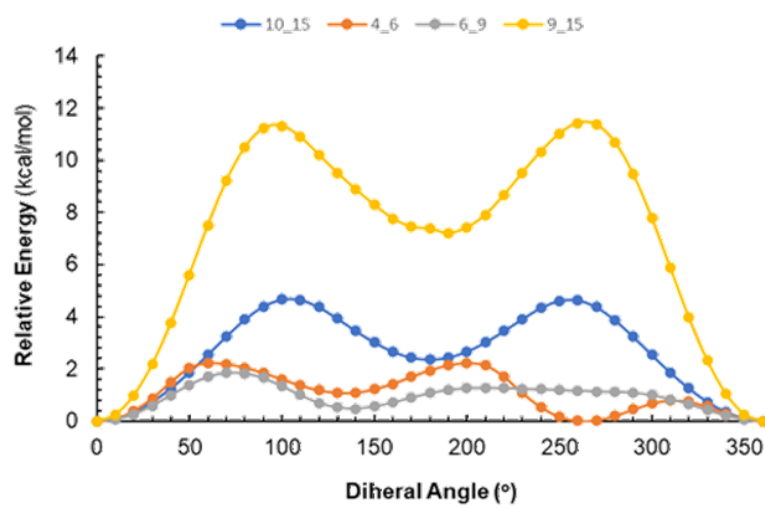




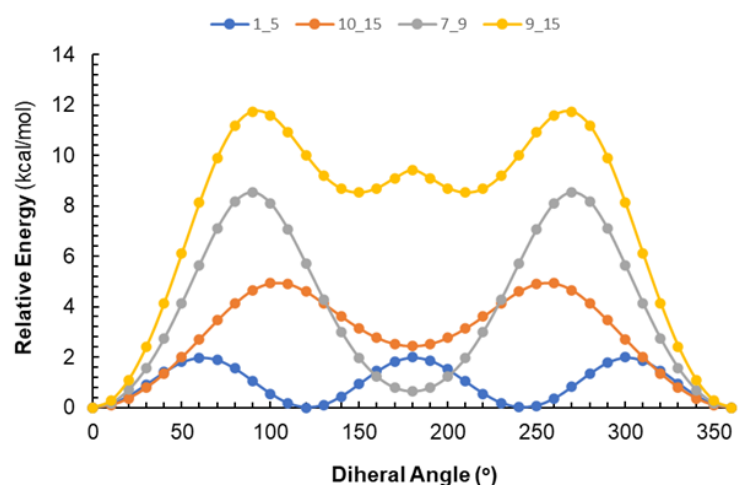
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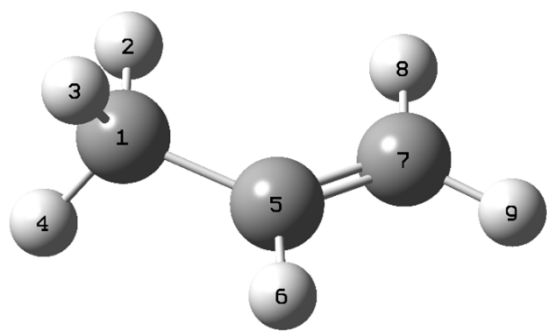


P16

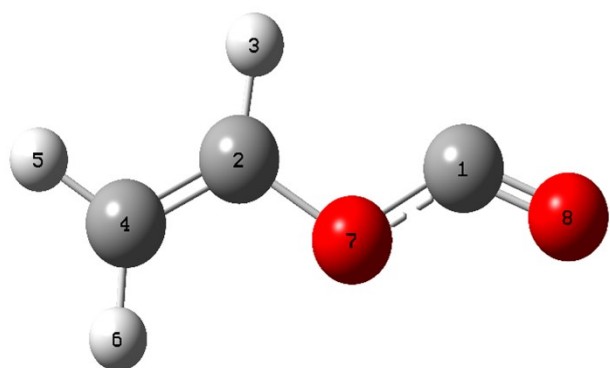
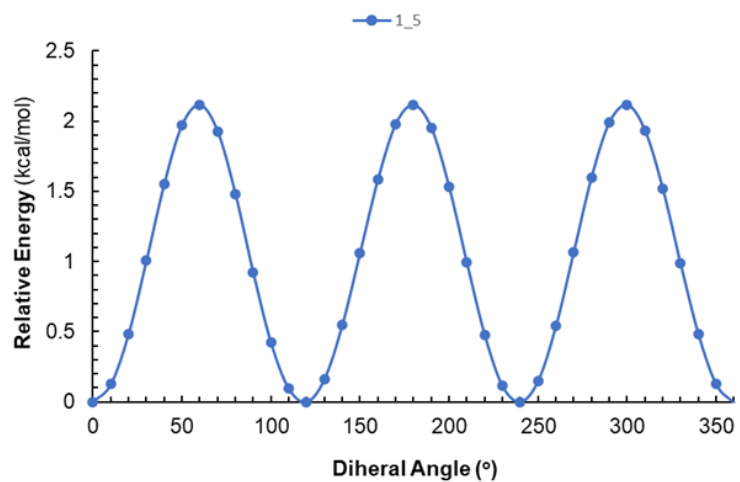


P17

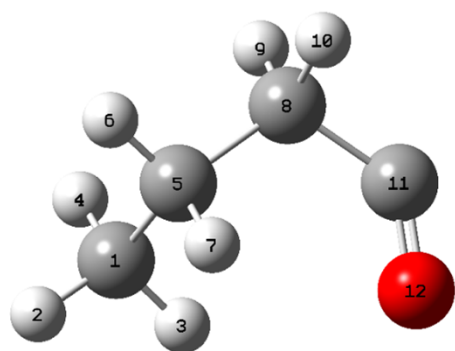
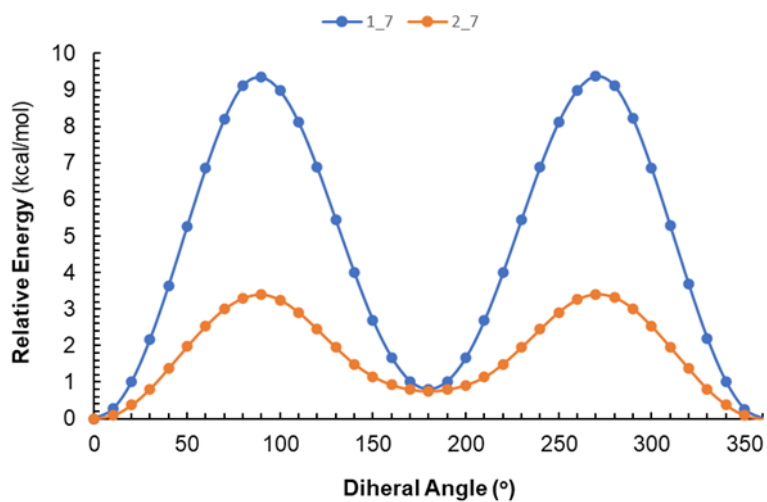




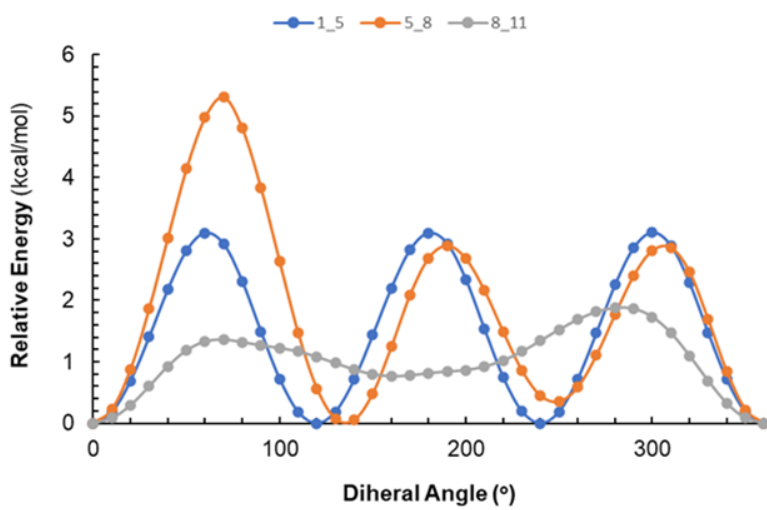
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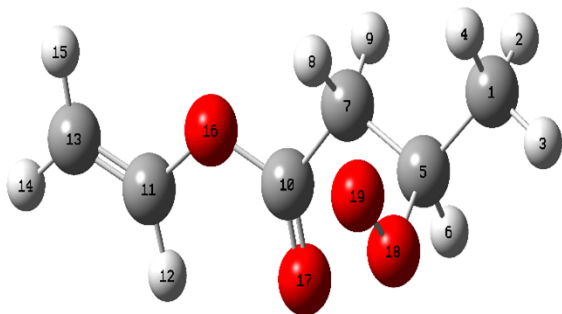


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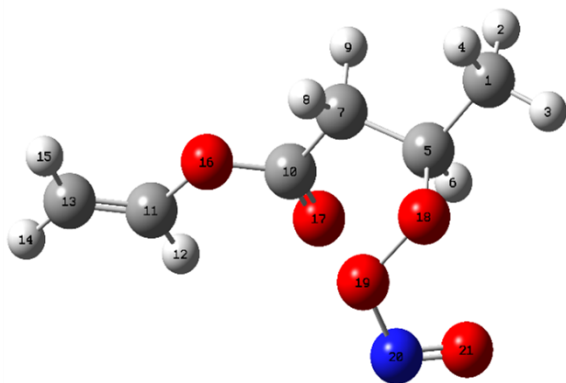
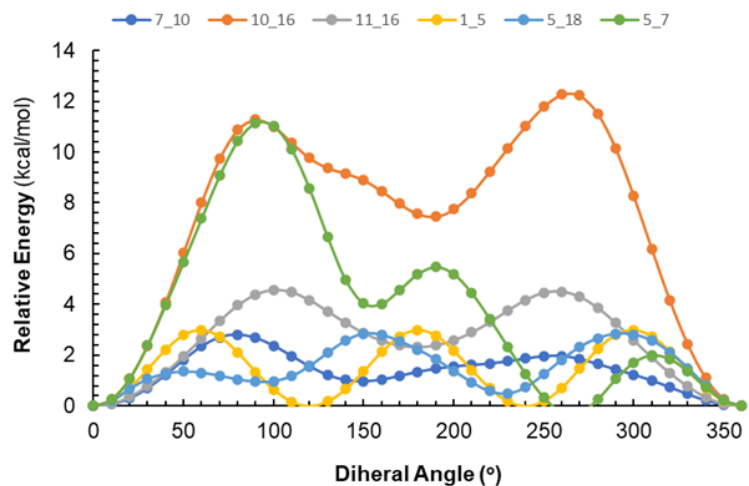


P19

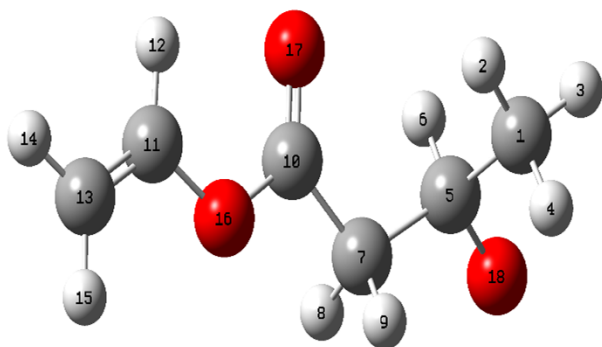
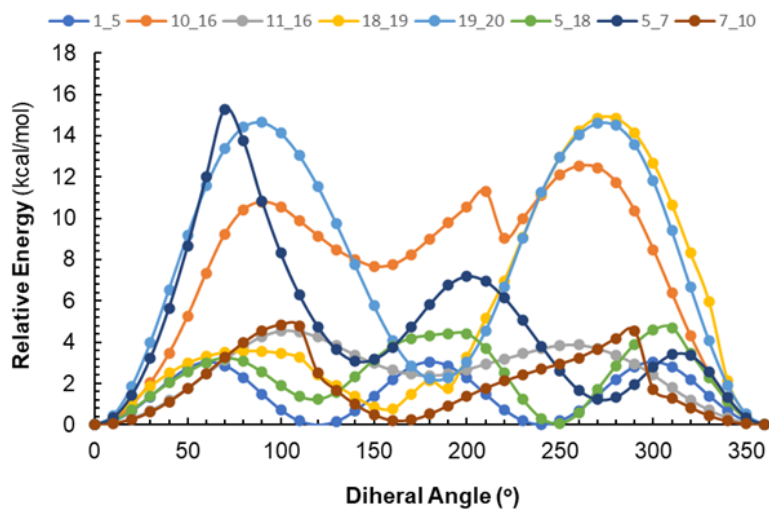




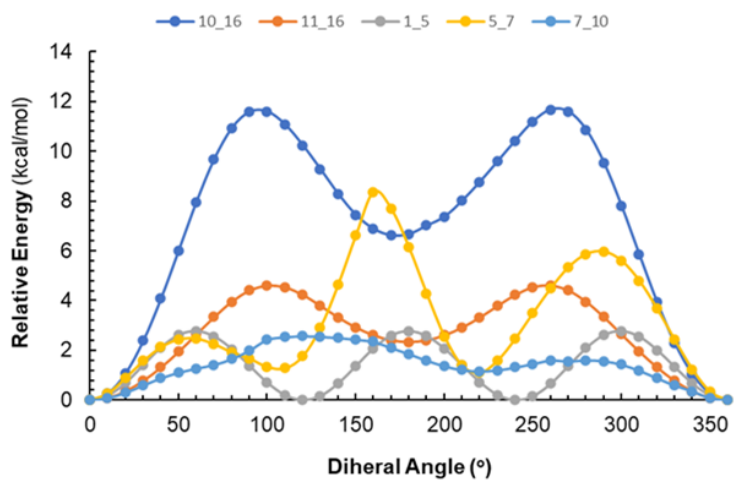
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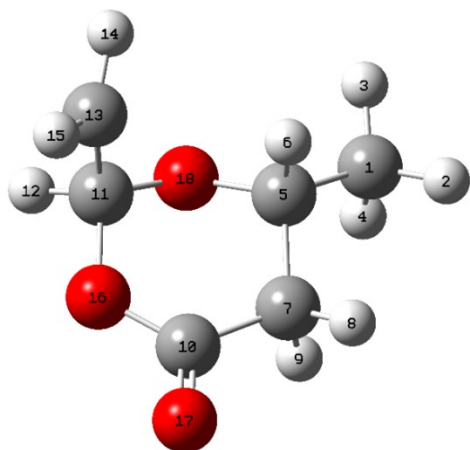


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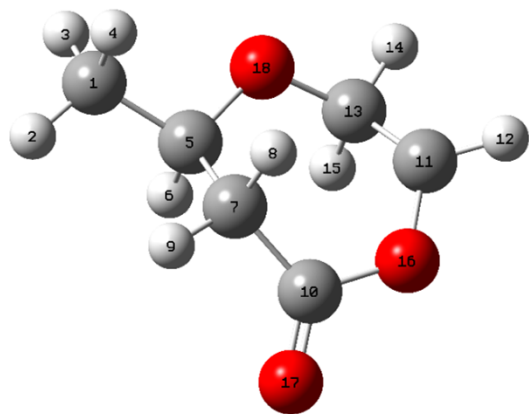
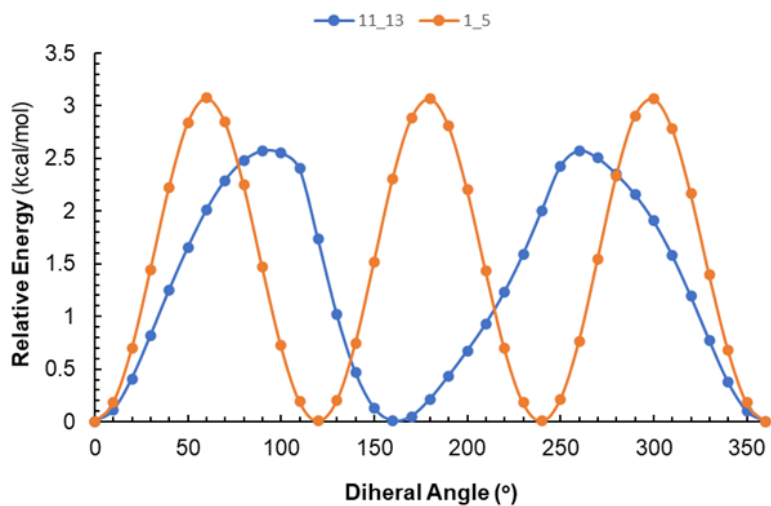


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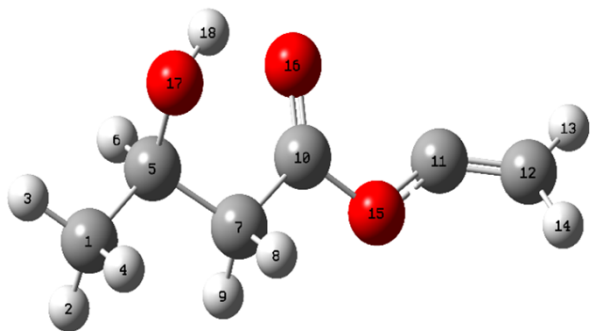
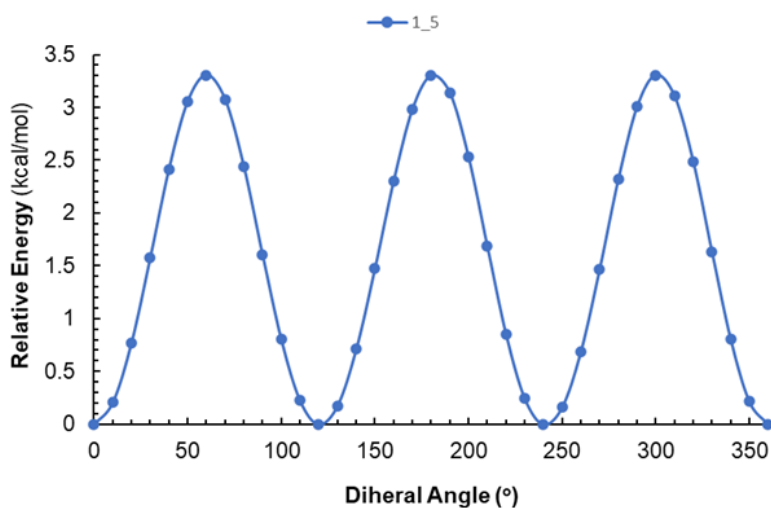




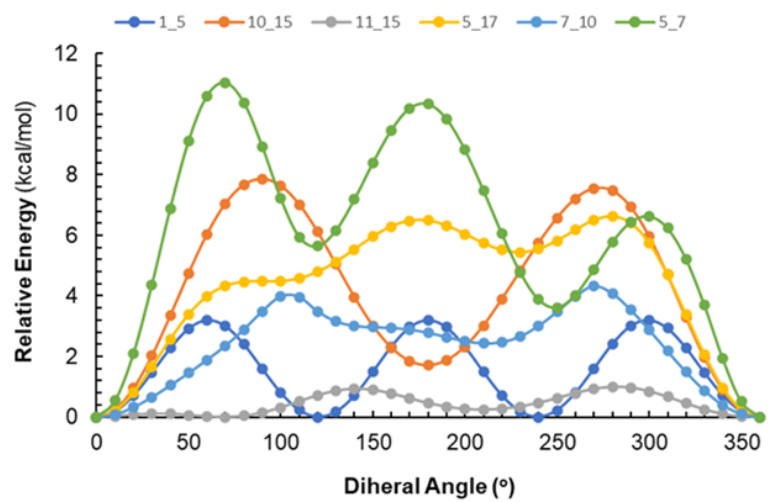
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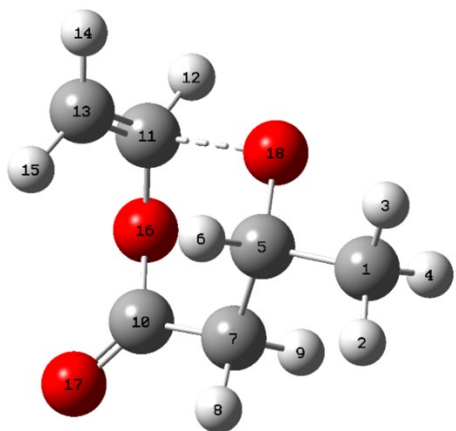


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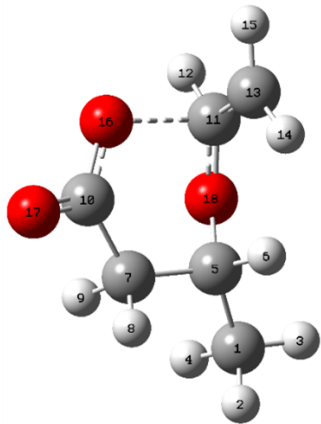
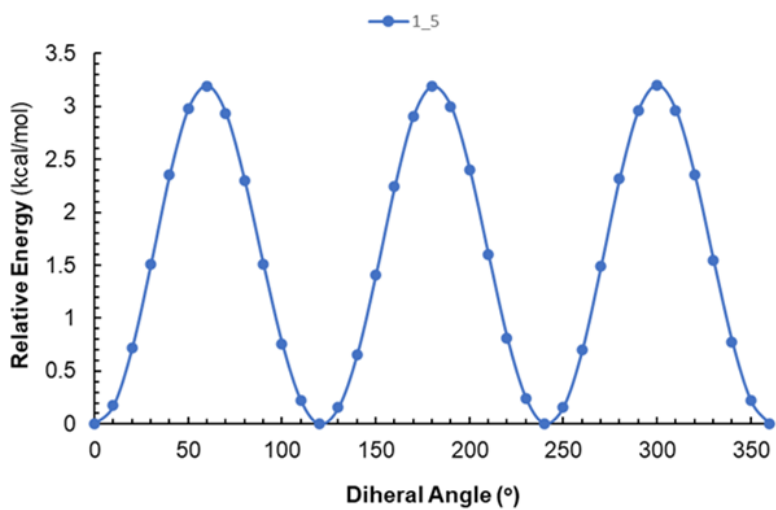


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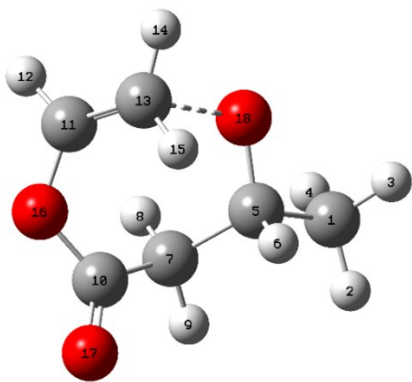
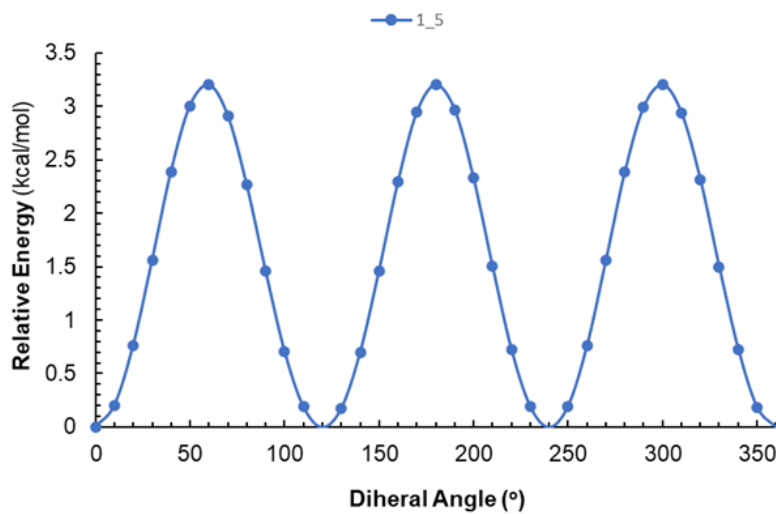




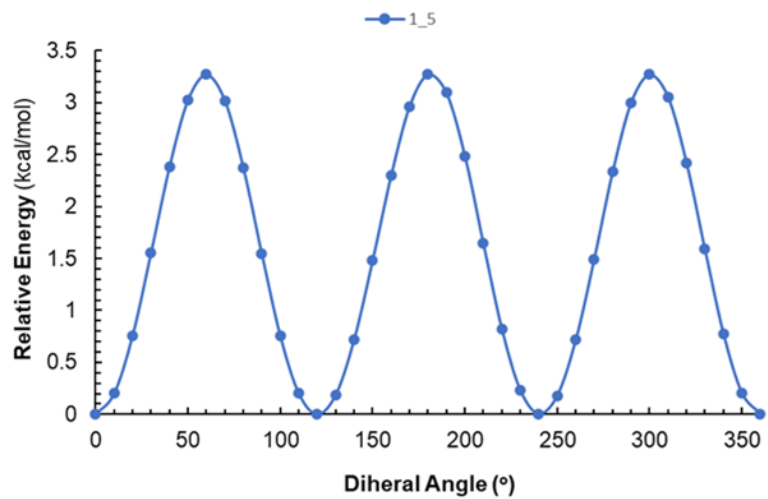
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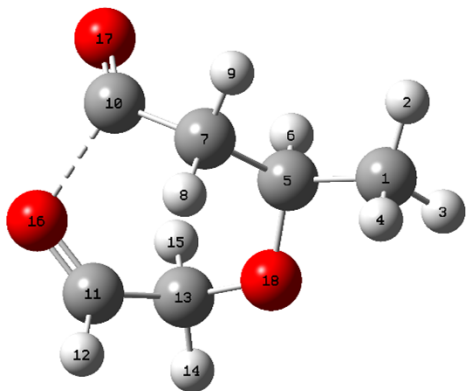


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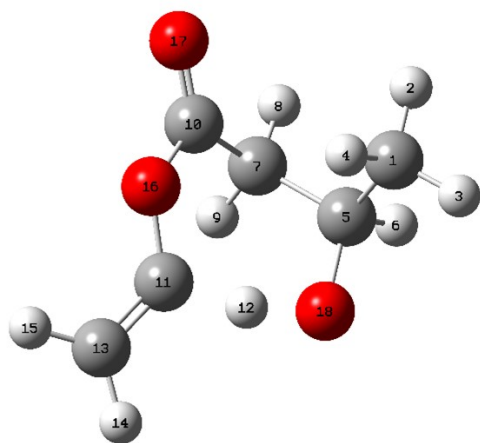
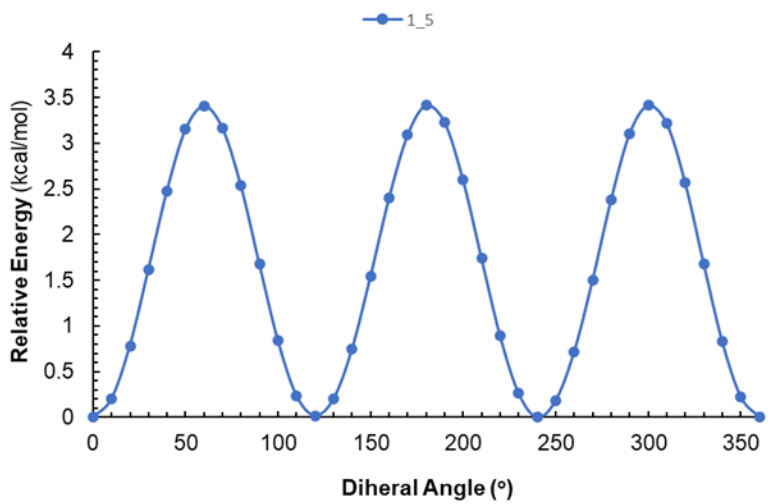


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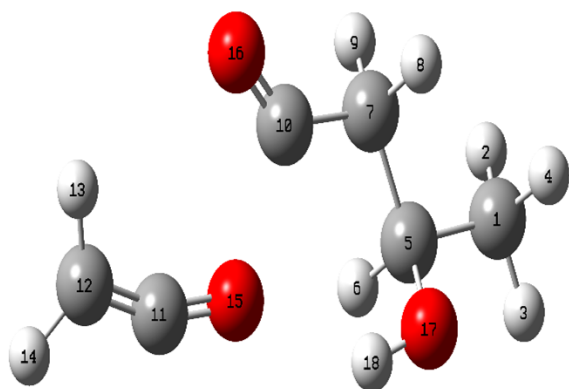
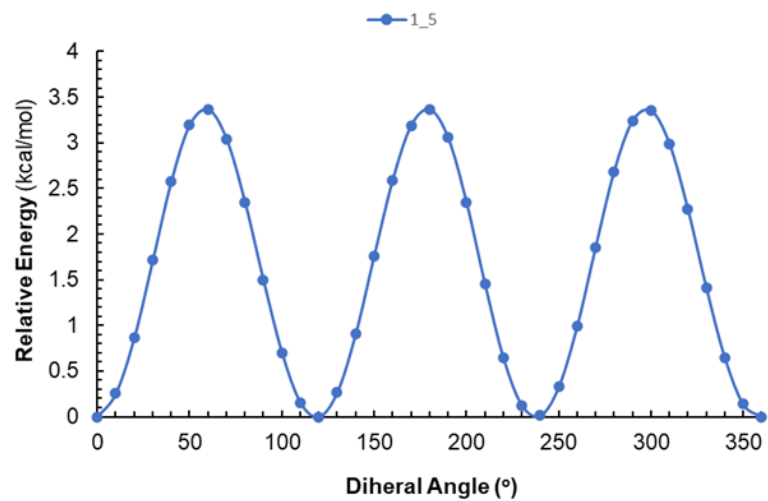




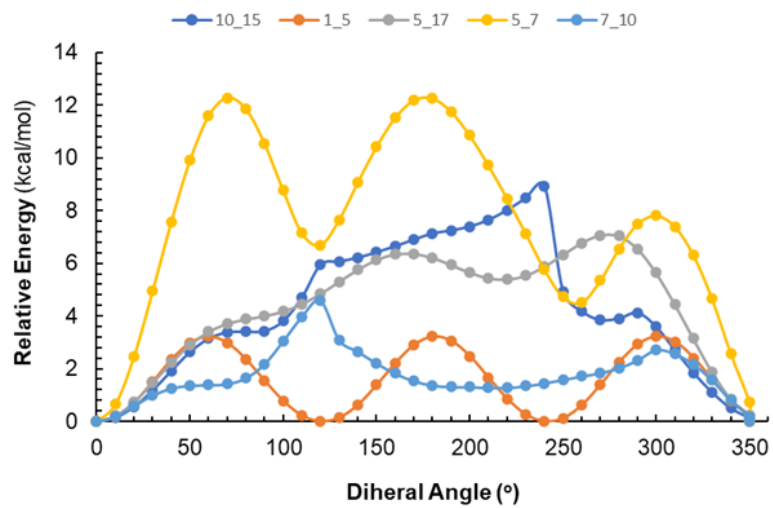
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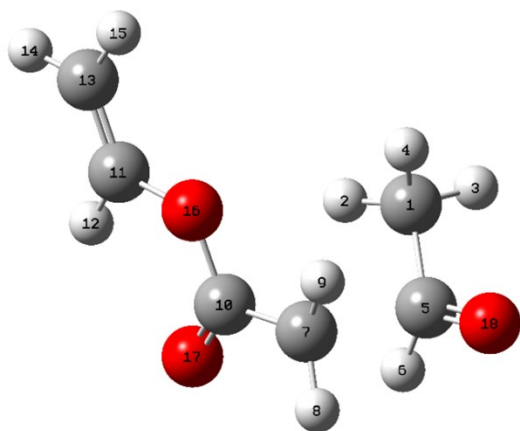


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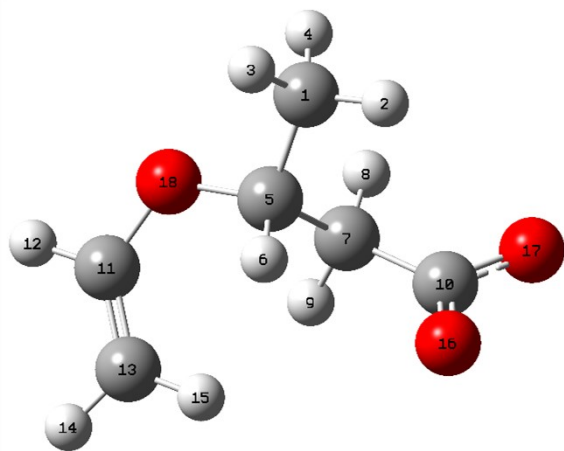
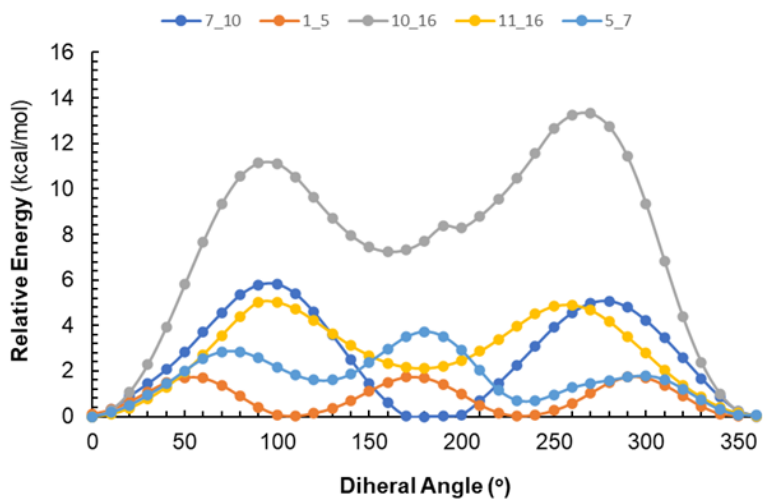


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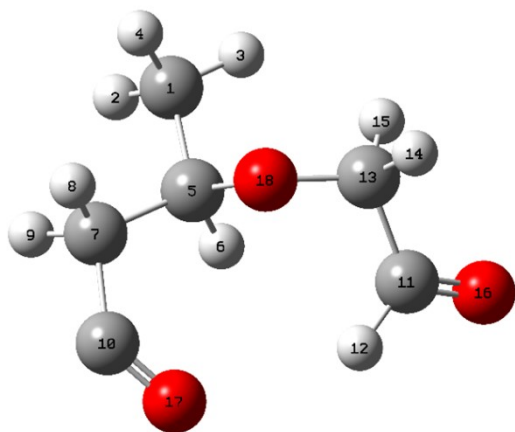
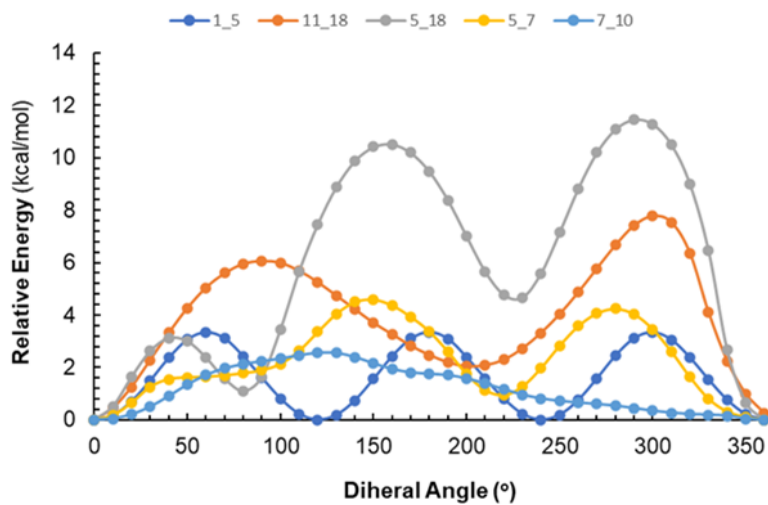




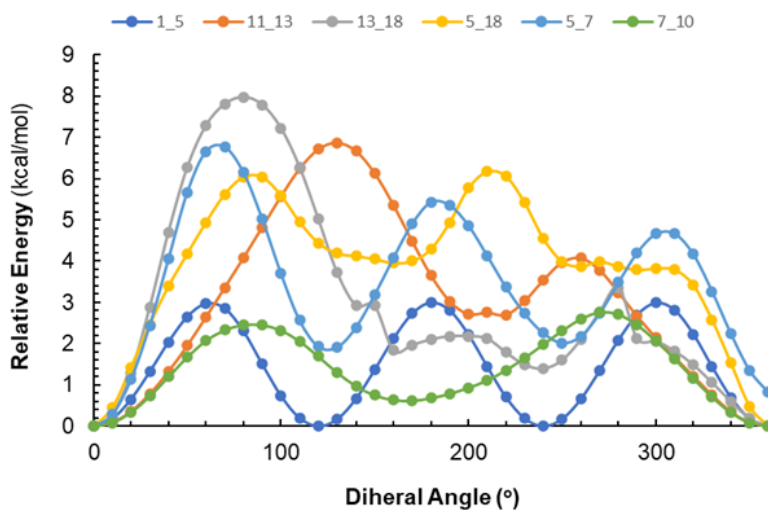
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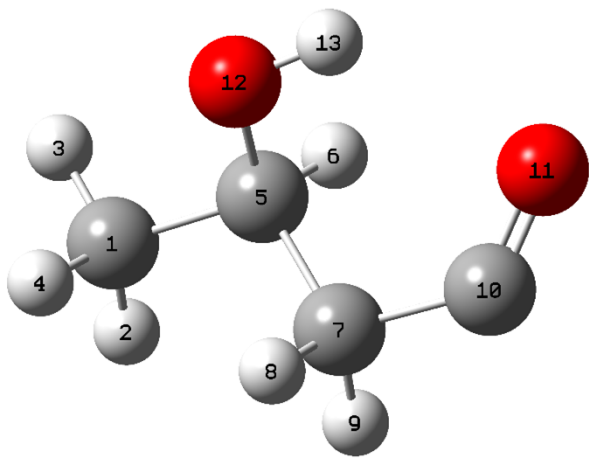


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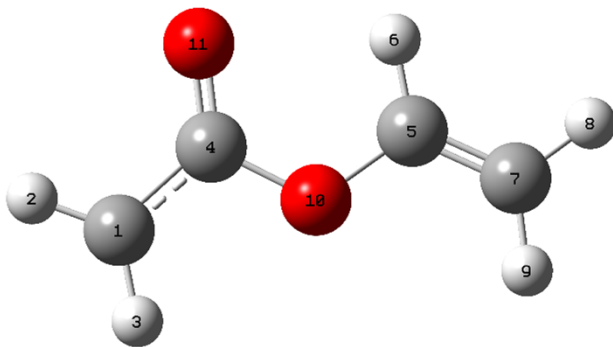
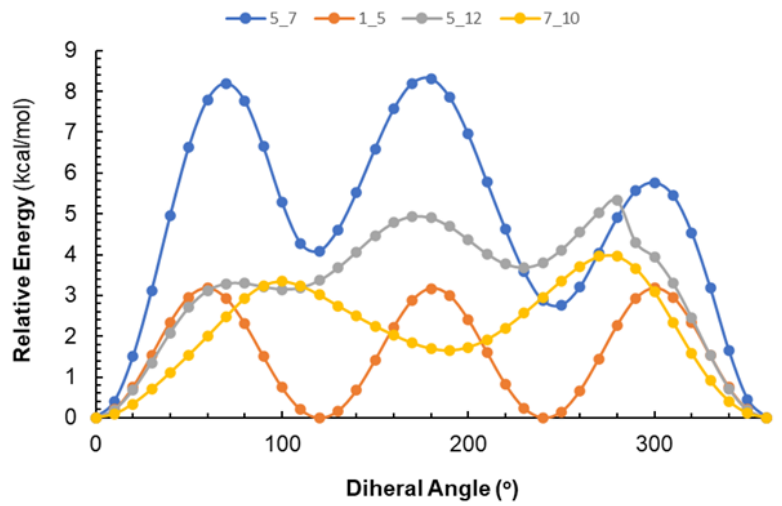


P22

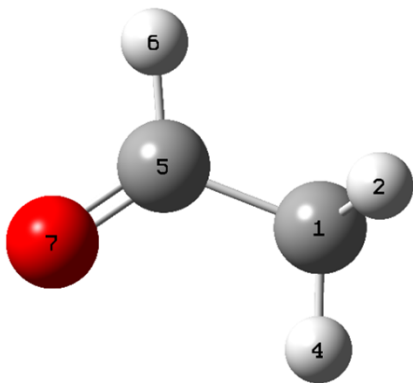
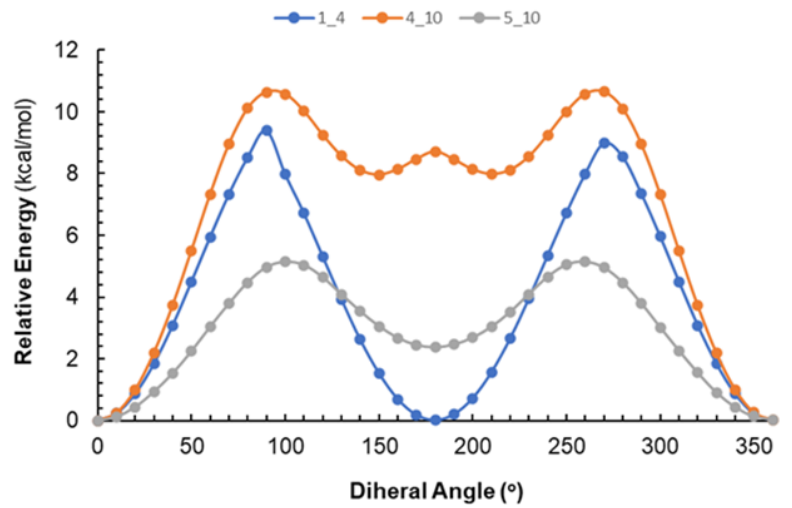




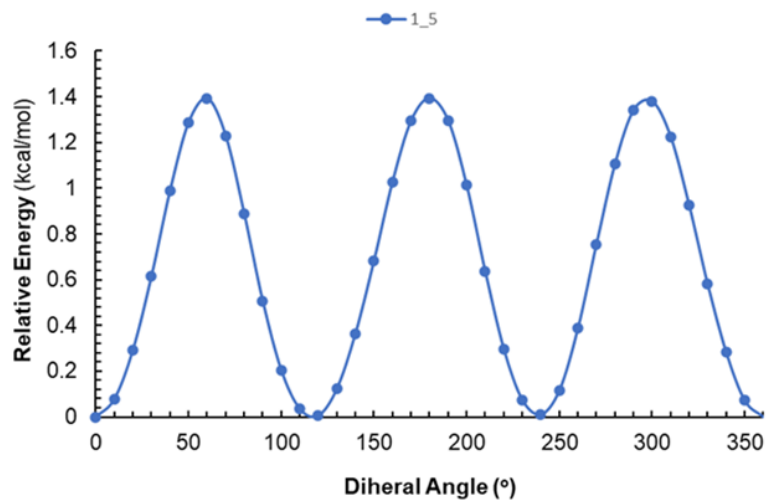
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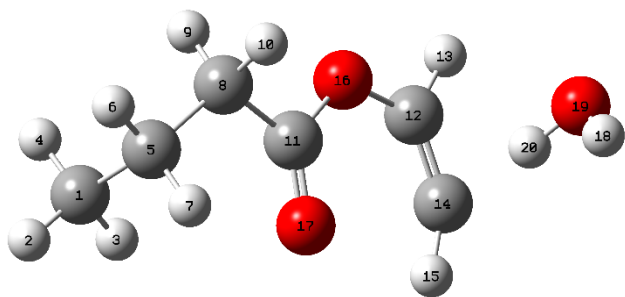


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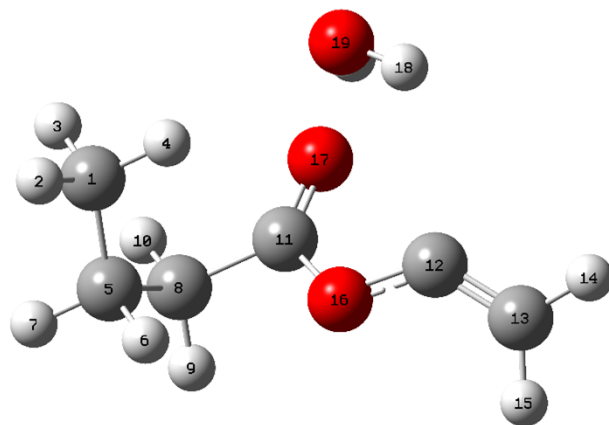
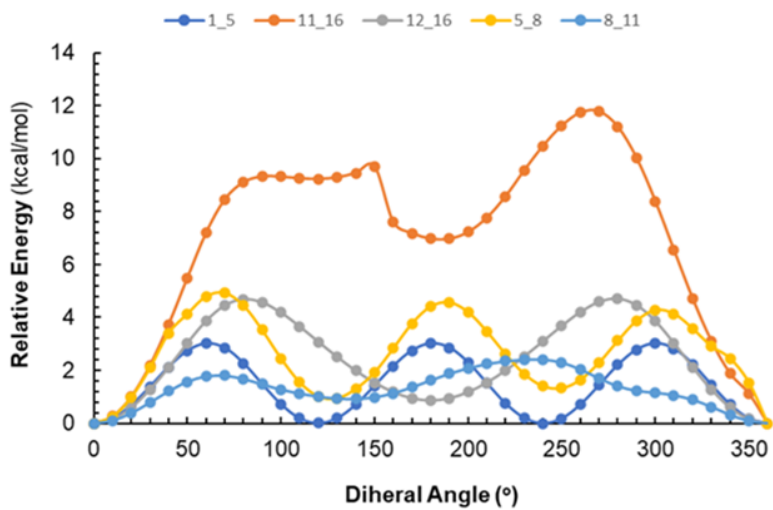


CH₃CHO

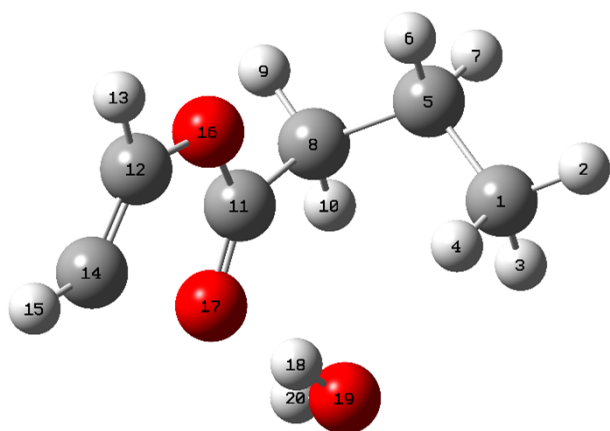
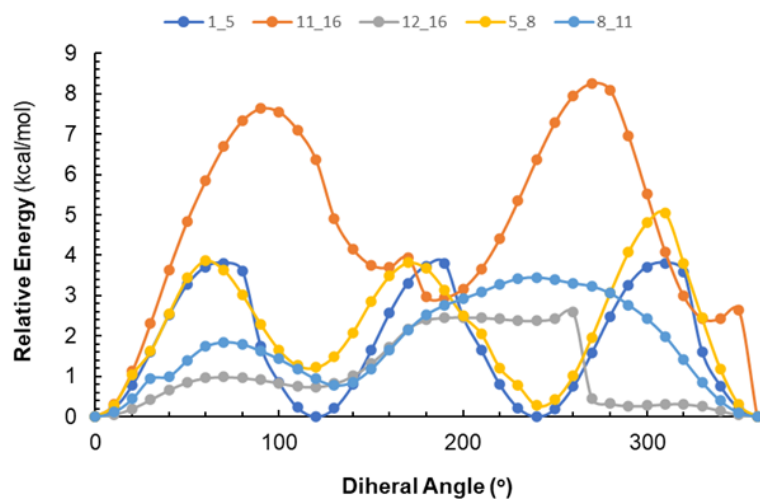




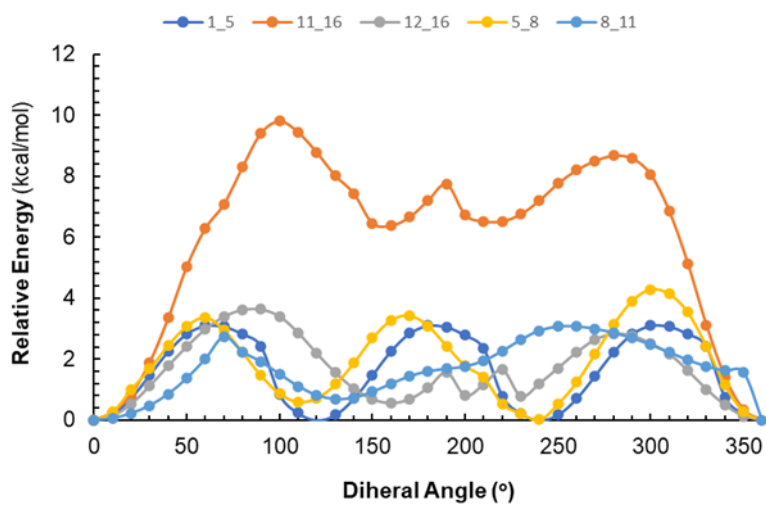
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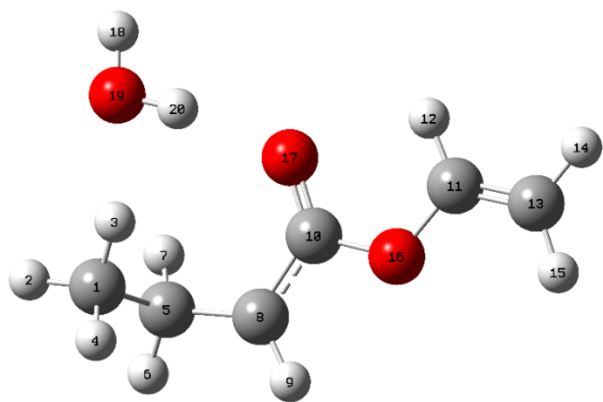


PC2

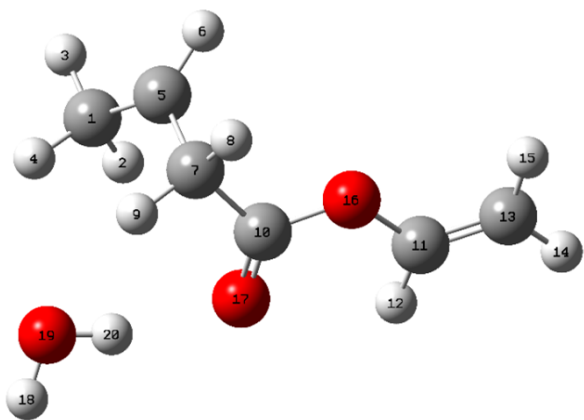
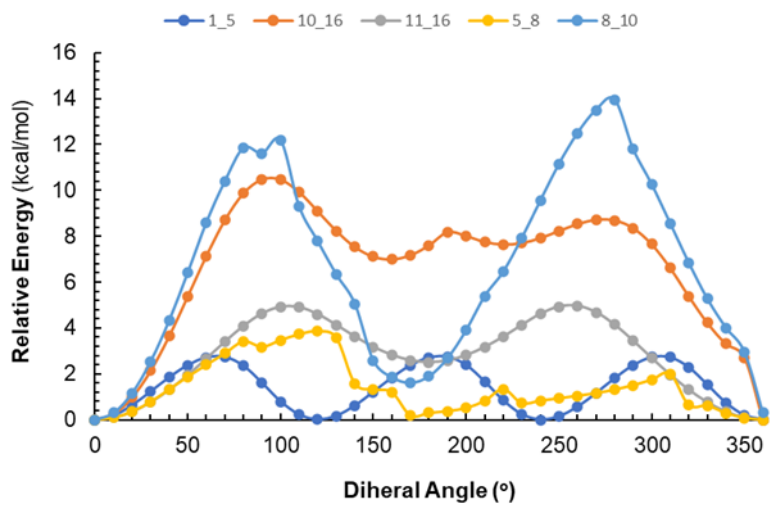


PC3

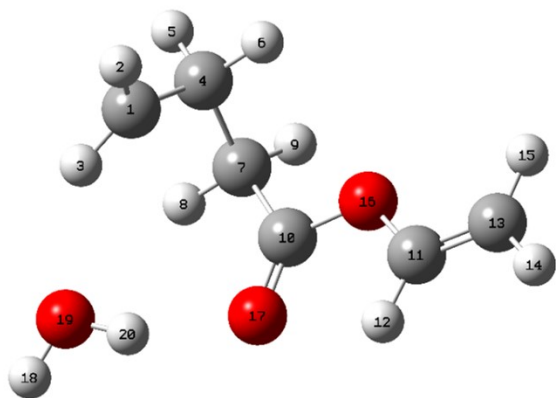
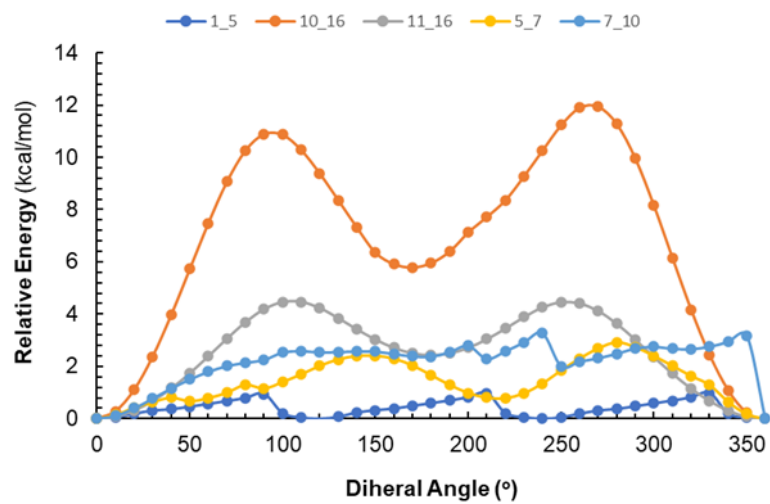




PC4



PC5



PC6

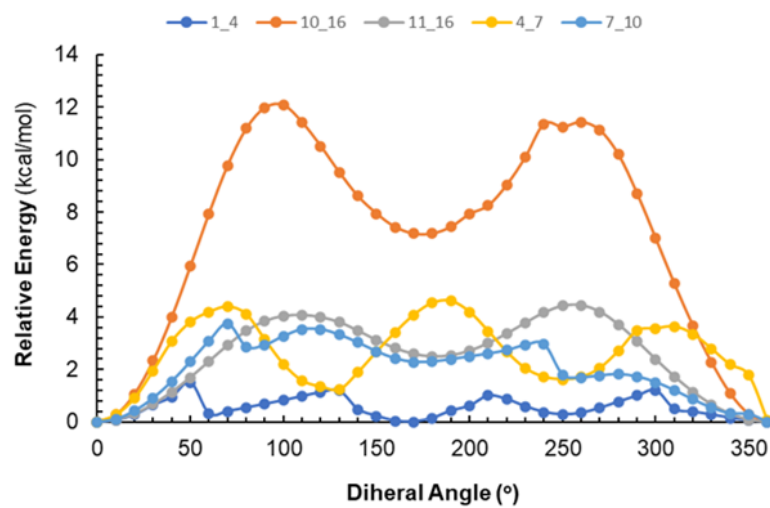


Figure S6: Hindrance potentials for the species involved in the VB + OH/O₂/NO reaction, obtained at M06-2X/cc-pVDZ level.