

Supplemental Information to the paper

**Formation of C₅H₆ isomers: A combination of experimental
and computational investigation**

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In this supporting information, we present:

- 1) Figure S1. Schematic diagram of SiC reactor.
- 2) Figure S2. Comparison of matches for experimental PIE of $m/z = 66$ in C_3H_3Br/C_2H_4 system using different isomers.
- 3) Figure S3. Experimental PIE for $m/z = 39, 54, 76$ and 78 in C_3H_3Br/C_2H_4 system.
- 4) Figure S4. Experimental PIE of $m/z = 66$ in C_3H_3Br/C_2H_4 system using 0 K Franck-Condon simulation result in 1,2,4-pentatriene and 3-methylidenecyclobut-1-ene.
- 5) Figure S5. Computed FCFs of 1,2,4-pentatriene and 3-methylidenecyclobut-1-ene at 0 K.
- 6) Figure S6. Computed FCFs of 1,2,4-pentatriene and 3-methylidenecyclobut-1-ene at 1000 K.
- 7) Figure S7. Rate constants for the reaction of propargyl + ethylene \rightarrow products within 300-1600 K at pressures of 760, 7600, and 76000 Torr.
- 8) Table S1. Summary of calculated ionization energies for structures with $m/z = 65$.
- 9) Table S2. Cartesian coordinates and frequencies of optimized structures at M062X/6-311++G(d,p) level for all species in this work.

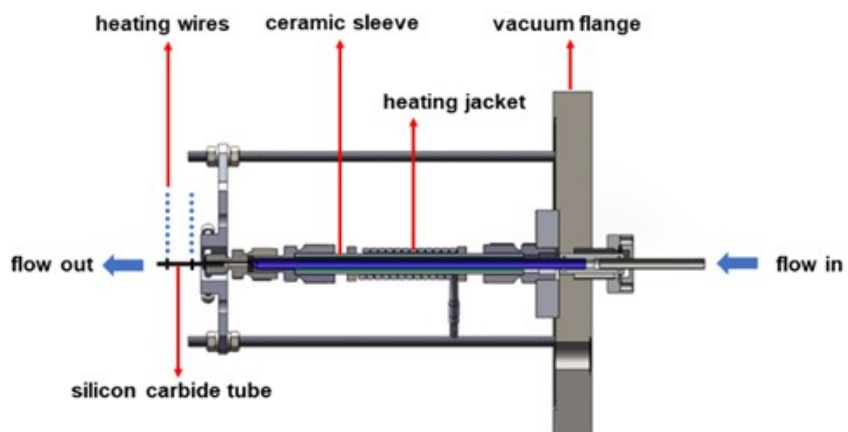


Figure S1. Schematic diagram of silicon carbide micro reactor.

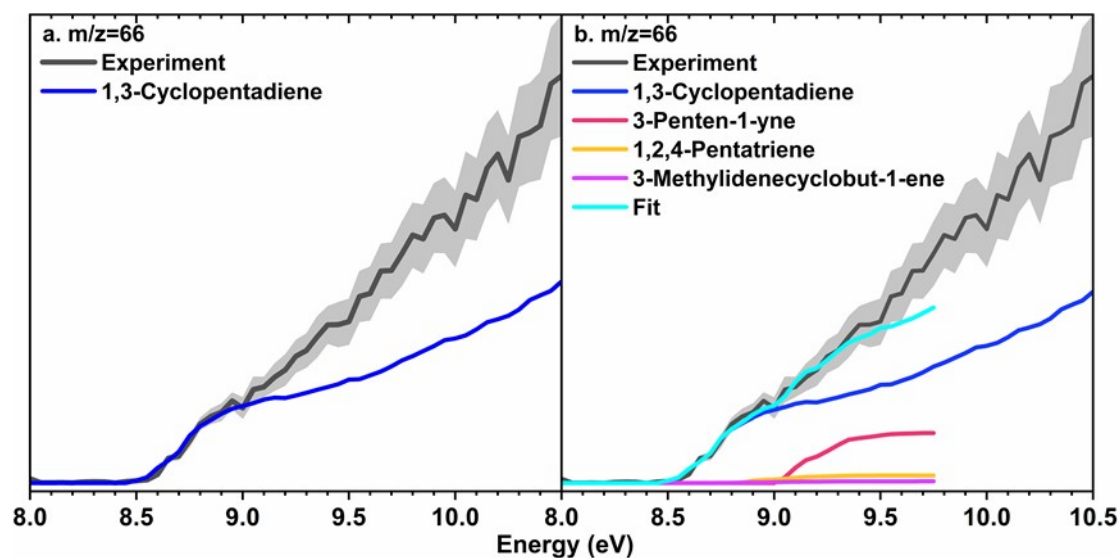


Figure S2. Comparison of matches for experimental PIE of $m/z = 66$ in propargyl bromide (C_3H_3Br)/ethylene (C_2H_4) system using referred /calculated Franck-Condon factor simulation of (a) 1,3-cyclopentadiene with C_5H_5 isotope, (b) 1,3-cyclopentadiene, 3-penten-1-yne, 1,2,4-pentatriene, 3-methylidenecyclobut-1-ene and C_5H_5 isotope. The colored lines refer to reference /calculated PIE curves and the cyan line shows the overall fit via the linear combination of reference curves. The black lines refer to the experimental data and the overall error bars consist of two parts: $\pm 10\%$ based on the accuracy of photodiode and a 1σ error of PIE curve averaged over the individual scans.

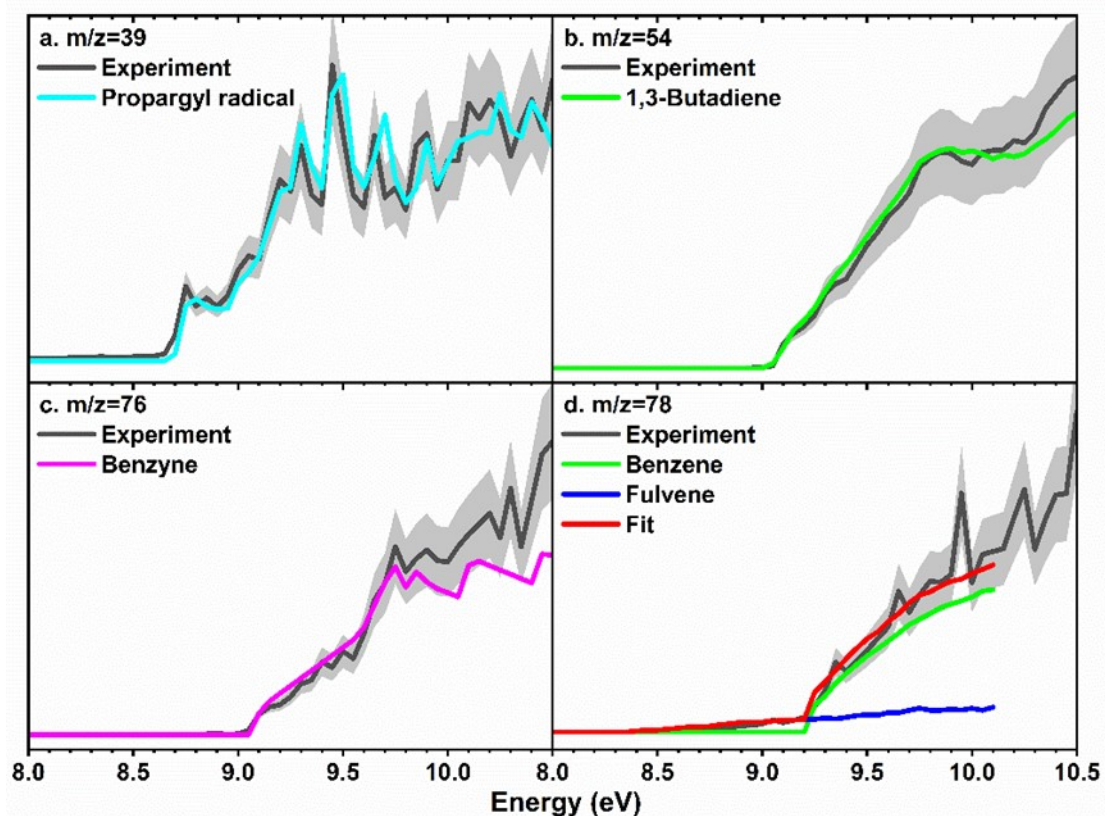


Figure S3. Experimental photoionization efficiency curves (PIE, black lines) for $m/z = 39, 54, 76$ and 78 in propargyl bromide (C_3H_3Br)/ethylene (C_2H_4) system, with 1σ error limits defined in the shaded area. The colored lines refer to the reference PIE curves and the red lines show the overall fit via the linear combination of the reference curves.

Figure S3 shows PIE curves of $m/z = 39, 54, 76$ and 78 in propargyl bromide (C_3H_3Br)/ethylene (C_2H_4) system. Propargyl (C_3H_3) can be determined according to the experimental and referred PIE curves (Fig. S3a) and it is generated from Br-losing atom from C_3H_3Br molecule. Propargyl can also undergo recombination and isomerization, forming fulvene and benzene at $m/z = 78$ as shown in Fig. S3d. Species at $m/z = 78$ could also have H-elimination under the high experimental temperature, which produces a signal at $m/z = 76$. Figure S3b shows the PIE curve of $m/z = 54$ and 1,3-butadiene can be identified. In the high temperature, the side-product of 1,3-butadiene can be generated through the C_2H_4 recombination and H-loss reactions¹.

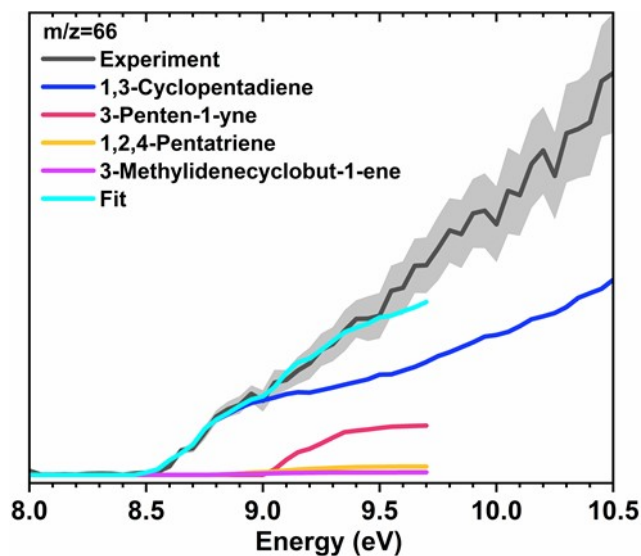


Figure S4. Experimental PIE of $m/z = 66$ in propargyl bromide (C_3H_3Br)/ethylene (C_2H_4) system with 0 K Franck-Condon simulation result including 1,2,4-pentatriene and 3-methylidenecyclobut-1-ene. The colored lines refer to reference /calculated PIE curves and the cyan line shows the overall fit via the linear combination of reference curves. The black lines refer to the experimental data and the overall error bars consist of two parts: $\pm 10\%$ based on the accuracy of photodiode and a 1σ error of PIE curve averaged over the individual scans.

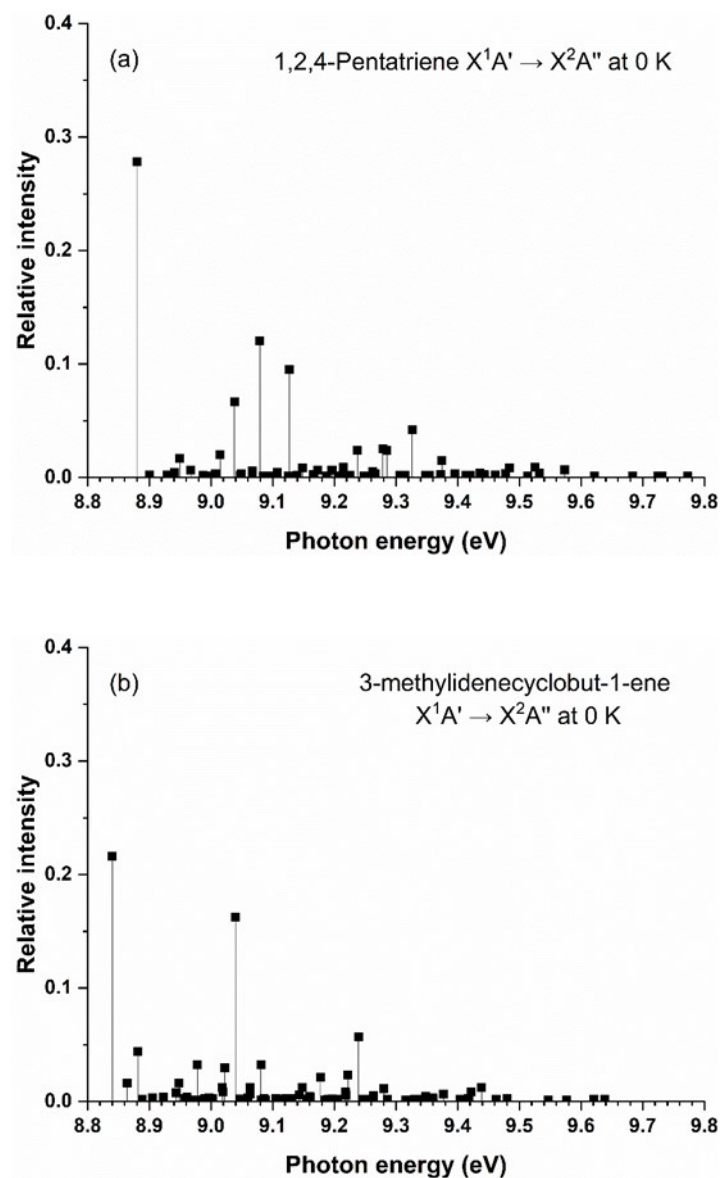


Figure S5. The computed FCFs of (a) 1,2,4-pentatriene and (b) 3-methylidenecyclobut-1-ene ionization to X^2A'' states at 0 K.

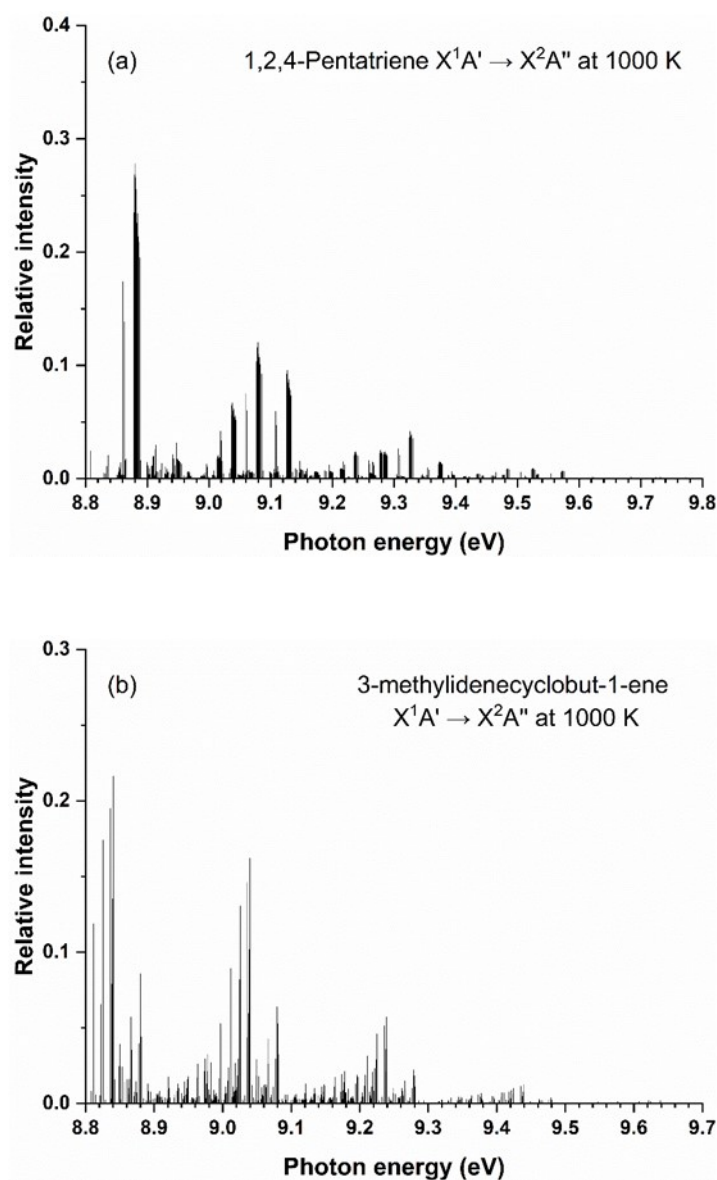


Figure S6. The computed FCFs of (a) 1,2,4-pentatriene and (b) 3-methylenecyclobut-1-ene ionization to X^2A'' states at 1000 K.

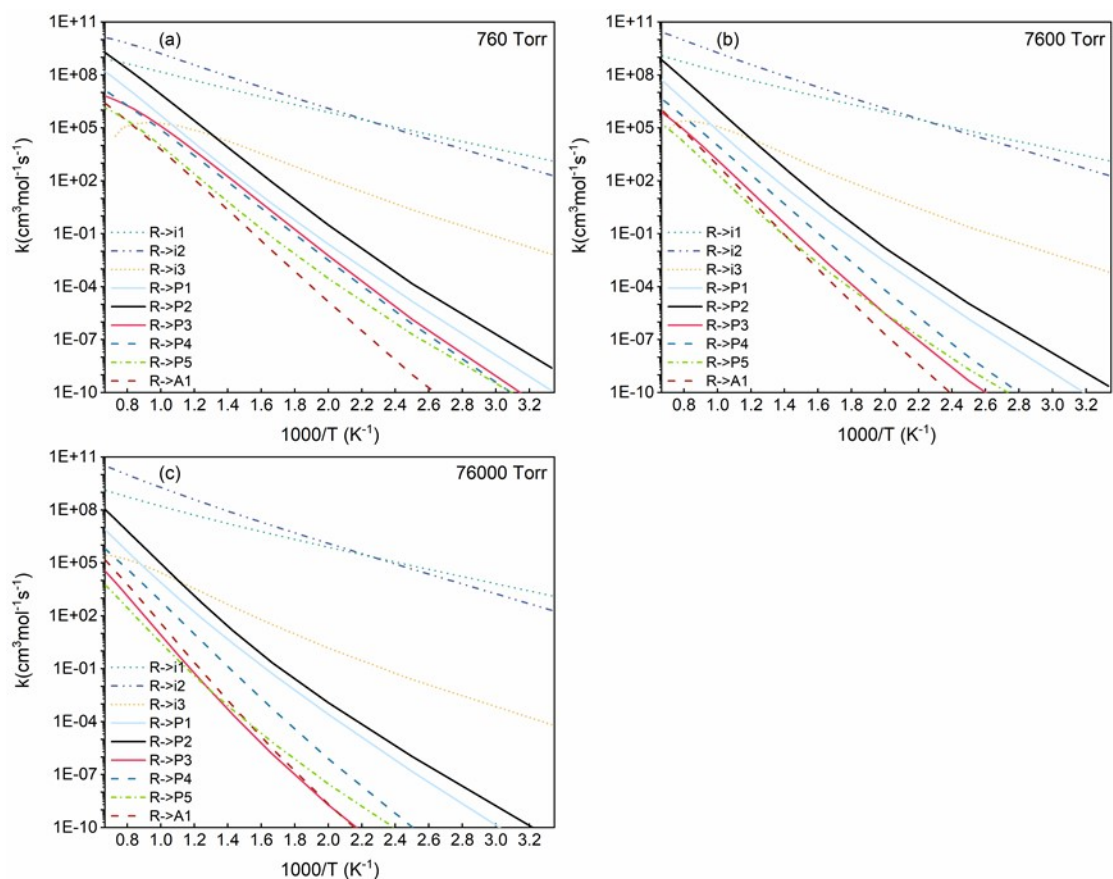
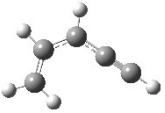
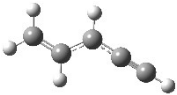
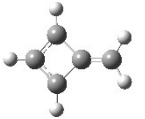
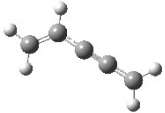


Figure S7. Rate constants for the reactions of propargyl (C_3H_3) + ethylene (C_2H_4) \rightarrow products (P1: 4-penten-1-yne + H, P2: 1,2,4-pentatriene + H, P3: 1,3-cyclopentadiene + H, P4: 3-penten-1-yne + H, P5: 3-methylidenecyclobut-1-ene + H and A1: 1,2,3-butatriene + methyl) within 300-1600 K at pressures of (a) 760 Torr, (b) 7600 Torr, and (c) 76000 Torr.

Table S1: Summary of calculated ionization energy results for structures with $m/z = 65$.

Structure	Structure diagram	Ionization energy (eV)	Calculation method
cis-pent-1-en-4-yn-3-yl radical		7.98	CBS-QB3
trans-pent-1-en-4-yn-3-yl radical		7.91	
3-methylenecyclobut-1-ene radical		7.71	
1,2,4-pentatriene radical		7.86	

The ionization energies of these four $\cdot\text{C}_5\text{H}_5$ isomers were calculated, and the results are provided in the table. The results show that the ionization energies of the four possible linear isomers at $m/z = 65$ are all below 8.0 eV. As clearly shown in Fig. 4a, the PIE curve begins to rise at 8.40 ± 0.05 eV, which aligns well with the ionization energy of cyclopentadienyl at 8.41 eV. This indicates that the four linear isomers have no or negligible contribution to experimental ions collected at $m/z = 65$.

Table S2: Cartesian coordinates and frequencies (cm^{-1}) of reactants, intermediates, transition states, and products.

C_3H_3				
Atom	X	Y	Z	Å
C	1.337175	0.000171	-0.00002	
C	0.120443	-0.000112	0.000064	
H	2.400845	-0.000501	-0.000096	
C	-1.256052	0.000006	0.000015	
H	-1.805202	-0.931069	-0.000128	
H	-1.805045	0.931175	-0.000128	
Frequencies (cm^{-1})				
359.3012	411.3266	577.8062	669.5679	
696.8377	1033.6678	1069.7291	1457.5041	
2028.2515	3184.838	3286.2399	3485.5889	

C_2H_4				
Atom	X	Y	Z	Å
C	0	0	-0.66289	
H	0	-0.923572	-1.230818	
H	0	0.923572	-1.230818	
C	0	0	0.66289	
H	0	0.923572	1.230818	
H	0	-0.923572	1.230818	
Frequencies (cm^{-1})				
829.9146	986.9828	998.7481	1063.6198	
1238.705	1385.3261	1470.2164	1712.1449	
3159.2687	3175.6359	3238.6169	3264.2018	

il				
Atom	X	Y	Z	Å
C	-0.014644	0.971727	-0.272787	
C	1.238953	0.353222	0.374043	
C	-1.208367	0.152657	-0.062708	
C	1.582762	-0.979430	-0.191731	
H	1.059955	0.277972	1.456892	
H	2.075944	1.046416	0.249967	
H	-0.192374	1.968010	0.140289	
H	0.149959	1.090258	-1.347621	
C	-2.173861	-0.535814	0.125223	
H	0.794202	-1.666387	-0.470860	
H	2.597254	-1.350578	-0.149730	
H	-3.034000	-1.139866	0.288821	
Frequencies (cm^{-1})				
122.2483	144.6466	197.2104	356.3808	
364.4951	474.2708	555.7449	713.677	
718.3343	764.3573	875.8599	944.991	
1003.6356	1074.9502	1122.2117	1188.0684	
1278.3034	1346.8449	1371.2887	1465.6872	

1474.5212 1477.6776 2251.9414 2999.9791
 3067.682 3086.9098 3109.9069 3173.7078
 3281.1567 3495.3548

i2				
Atom	X	Y	Z	Å
C	0.022148	0.971727	-0.272787	
C	1.425344	0.353222	0.374043	
C	-1.072090	0.152657	-0.062708	
C	1.505891	-0.979430	-0.191731	
H	1.943803	0.277972	1.456892	
H	1.970560	1.046416	0.249967	
H	-0.070333	1.968010	0.140289	
C	-2.166126	1.090258	-1.347621	
H	2.426679	-0.535814	0.125223	
H	0.711367	-1.666387	-0.470860	
H	-2.641117	-1.350578	-0.149730	
H	-2.631963	-1.139866	0.288821	
Frequencies (cm-1)				
63.8257	89.3001	197.2104	356.3808	
349.9124	466.2696	555.7449	713.677	
780.4137	894.0638	875.8599	944.991	
1020.31	1036.419	1122.2117	1188.0684	
1210.366	1325.218	1371.2887	1465.6872	
1466.499	1483.541	2251.9414	2999.9791	
3072.72	3156.398	3109.9069	3173.7078	
3238.326	3281.509			

i3				
Atom	X	Y	Z	Å
C	1.248028	-0.404391	0.106639	
C	0.610620	0.991407	-0.143599	
C	0.048236	-1.279031	-0.067001	
C	-0.906507	0.820165	0.120778	
H	0.759331	1.257446	-1.191817	
H	1.062298	1.772206	0.468943	
H	2.057645	-0.626613	-0.589680	
H	1.646375	-0.501047	1.121589	
C	-1.123561	-0.676909	-0.061378	
H	-1.175532	1.112955	1.141395	
H	-1.513045	1.421159	-0.560013	
H	-2.097969	-1.143549	-0.123051	
Frequencies (cm-1)				
161.7857	382.8148	602.5444	756.3731	
771.3196	824.4859	894.1067	902.235	
941.3828	987.2208	1033.713	1055.203	
1143.523	1196.307	1220.713	1234.526	
1303.059	1311.172	1339.914	1482.268	
1489.602	1507.941	1696.354	3053.119	
3065.104	3087.105	3107.937	3120.878	

3143.376 3232.408

i4

Atom	X	Y	Z	Å
C	0.000063	-0.272515	-0.000190	
C	1.245542	0.396009	-0.000061	
C	-1.245649	0.395912	-0.000036	
C	2.450225	-0.229609	0.000089	
H	1.221042	1.483558	0.000071	
H	2.516974	-1.311824	-0.000055	
H	0.000308	-1.359748	0.000011	
C	-2.450204	-0.229616	0.000100	
H	3.377391	0.327608	0.000333	
H	-1.221123	1.483474	-0.000018	
H	-3.377342	0.327667	0.000154	
H	-2.517115	-1.311821	0.000089	

Frequencies (cm-1)

152.821	205.038	251.069	456.570
493.026	594.492	632.402	841.883
891.614	901.488	922.420	992.323
1007.905	1033.834	1125.048	1253.365
1299.203	1302.072	1310.049	1440.251
1466.720	1530.651	1607.015	3161.848
3162.928	3170.667	3172.907	3174.861
3270.995	3271.101		

i5

Atom	X	Y	Z	Å
C	-0.042884	-0.485254	-0.000022	
C	1.018126	0.423336	-0.000132	
C	-1.347420	-0.155467	-0.000135	
C	2.450533	0.007519	0.000085	
H	0.787910	1.483058	-0.000220	
H	2.978759	0.394815	-0.877724	
H	0.192787	-1.548499	-0.000019	
C	-2.606338	0.166501	0.000108	
H	2.547314	-1.079694	-0.000013	
H	2.978431	0.394574	0.878210	
H	-3.158509	0.308091	0.927032	
H	-3.158798	0.307844	-0.926693	

Frequencies (cm-1)

121.5724	138.2699	163.2057	269.2259
387.9138	512.9463	566.5188	717.5857
907.5422	912.6003	922.4477	984.8174
1018.621	1028.706	1130.357	1207.317
1300.307	1412.983	1431.424	1467.513
1478.031	1508.589	1925.283	3036.751
3082.195	3108.223	3133.093	3146.647
3178.326	3196.456		

i6

Atom	X	Y	Z	Å
C	0.000000	-1.142621	0.489879	
C	-0.000013	-0.776472	-0.970236	
C	0.000000	0.000000	1.272765	
C	0.000013	0.776472	-0.970236	
H	-0.875983	-1.183685	-1.485407	
H	0.875941	-1.183714	-1.485421	
H	-0.000005	-2.159346	0.856944	
H	0.000000	0.000000	2.355461	
C	0.000000	1.142621	0.489879	
H	0.875983	1.183685	-1.485407	
H	-0.875941	1.183714	-1.485421	
H	0.000005	2.159346	0.856944	
Frequencies (cm-1)				
84.9752	446.9125	607.0636	659.4385	
726.8331	803.9419	815.8718	916.9569	
925.0242	958.9825	991.7698	1044.663	
1053.551	1112.36	1148.175	1227.584	
1288.995	1297.005	1308.636	1383.688	
1469.819	1490.851	1499.529	3045.43	
3055.828	3066.608	3085.673	3221.729	
3239.349	3252.093			

i7

Atom	X	Y	Z	Å
C	0.000001	-0.368865	1.236214	
C	0.000044	-1.216578	0.000000	
C	0.000001	1.031288	0.665245	
C	0.000001	-0.368865	-1.236214	
H	-0.876225	-0.547267	1.875667	
H	-0.000345	-2.296686	0.000000	
H	0.876217	-0.547276	1.875698	
H	0.000039	1.918078	1.287115	
C	0.000001	1.031288	-0.665245	
H	0.876217	-0.547276	-1.875698	
H	-0.876225	-0.547267	-1.875667	
H	0.000039	1.918078	-1.287115	
Frequencies (cm-1)				
188.6073	300.4315	388.2095	688.6943	
743.9409	793.6977	898.8435	926.3996	
939.0128	943.2485	976.766	987.5526	
1043.717	1128.3	1139.146	1139.522	
1292.776	1303.239	1334.896	1394.633	
1464.088	1470.698	1701.634	3003.94	
3006.221	3017.847	3018.132	3210.864	
3234.8	3244.353			

i8

Atom	X	Y	Z	Å
C	0.081956	1.051254	0.169495	
C	-1.213994	0.456845	-0.301479	
C	1.223502	0.141694	0.025726	
C	-1.607130	-0.921498	0.097243	
H	-2.510063	-1.244706	-0.421362	
H	-1.961181	1.141655	-0.681725	
H	0.294982	1.974118	-0.376339	
H	0.010152	1.334861	1.231711	
C	2.149477	-0.612662	-0.093219	
H	-0.806466	-1.635603	-0.117018	
H	-1.804135	-0.987665	1.177807	
H	2.973850	-1.276454	-0.199676	
Frequencies (cm-1)				
167.859	63.544	120.335	327.390	
343.223	381.961	595.822	704.017	
717.051	865.228	882.934	950.838	
996.233	1099.564	1156.167	1235.297	
1336.424	1372.381	1423.630	1458.572	
1479.723	1490.130	2253.334	2983.785	
2998.213	3082.724	3093.313	3142.894	
3212.915	3495.766			

i9

Atom	X	Y	Z	Å
C	0.129026	-0.336324	-0.000023	
C	-1.298597	-0.641663	0.000033	
C	1.317496	-0.059626	-0.000005	
C	-2.170042	0.619966	-0.000017	
H	-1.529583	-1.256807	0.875838	
H	-3.227742	0.351679	0.000004	
H	-1.529633	-1.256886	-0.875706	
C	2.659245	0.246299	0.000004	
H	-1.965253	1.226165	-0.883236	
H	-1.965239	1.226261	0.883133	
H	3.403829	-0.537777	-0.000141	
H	2.990847	1.275463	0.000156	
Frequencies (cm-1)				
61.375	131.389	162.488	269.814	
318.545	434.645	520.690	658.813	
744.919	778.379	991.206	1032.384	
1093.137	1095.906	1234.733	1282.844	
1356.733	1412.603	1464.580	1475.716	
1500.471	1510.295	2161.006	3052.104	
3073.552	3082.018	3151.231	3154.872	
3180.197	3278.286			

i10

Atom	X	Y	Z	Å
C	0.009425	1.006056	-0.008522	

C	0.999928	-0.027614	0.467478
C	-1.355469	0.439927	-0.115558
C	1.993688	-0.502928	-0.272486
H	0.844102	-0.403483	1.475732
H	2.161015	-0.151418	-1.285721
H	-0.009831	1.851967	0.687442
C	-1.923645	-0.738508	-0.059192
H	2.673274	-1.255532	0.109278
H	0.317682	1.402750	-0.980568
H	-1.333970	-1.643625	0.097564
H	-2.995833	-0.862253	-0.174046
Frequencies (cm-1)			
78.3572	165.1749	215.9684	412.2725
442.2757	499.7832	669.4313	903.2704
911.0968	918.9612	943.5835	972.2843
1029.051	1041.713	1122.323	1242.91
1305.748	1326.79	1412.553	1447.292
1466.865	1729.217	1753.092	3052.056
3093.358	3094.66	3159.934	3174.671
3200.178	3251.601		

i11				
Atom	X	Y	Z	Å
C	-0.057923	0.645662	-0.257600	
C	-1.241858	-0.007788	0.420980	
C	1.100165	-0.310109	-0.358171	
C	-2.399424	-0.227612	-0.147220	
H	-1.078961	-0.330856	1.453251	
H	0.921662	-1.206974	-0.947140	
H	-0.361872	0.975413	-1.254620	
C	2.276002	-0.131897	0.232116	
H	-3.343334	-0.670387	0.131690	
H	0.247582	1.529106	0.311029	
H	3.074894	-0.857233	0.135084	
H	2.478257	0.751395	0.830078	
Frequencies (cm-1)				
84.3871	99.6296	316.8966	369.549	
443.8558	634.4611	687.3214	802.2613	
865.4719	911.4792	958.8434	971.5437	
1037.215	1061.992	1140.131	1231.082	
1272.694	1310.997	1328.903	1450.543	
1478.819	1693.847	1731.1	3062.573	
3082.508	3113.042	3157.933	3170.673	
3249.884	3271.614			

i13				
Atom	X	Y	Z	Å
C	-0.369529	1.058355	-0.000049	
C	-1.545953	0.117127	0.000086	
C	0.578946	0.037170	-0.000013	

C	-0.499261	-1.043232	-0.000085	Å
H	-2.183986	0.159626	0.887321	
H	-2.184591	0.159762	-0.886664	
H	-0.292580	2.138513	-0.000351	
C	1.949418	-0.011666	0.000083	
H	-0.517059	-1.673164	0.890386	
H	-0.516913	-1.672679	-0.890892	
H	2.476676	-0.956758	-0.000009	
H	2.536730	0.898172	0.000078	
Frequencies (cm-1)				
172.8419	336.5392	415.3359	539.5901	
668.6985	699.4984	797.9414	807.5175	
887.7649	927.0214	953.1469	1012.367	
1026.735	1088.91	1184.506	1207.468	
1217.109	1256.986	1342.942	1360.536	
1463.016	1489.23	1504.808	3057.844	
3089.618	3098.293	3144.974	3172.805	
3217.435	3272.124			

i14					P1
Atom	X	Y	Z	Å	
C	0.002615	0.494697	1.103437		
C	0.002615	1.519506	0.000000		
C	-0.002723	-0.562939	0.000000		
C	0.002615	0.494697	-1.103437		
H	-0.880612	0.485764	1.753014		
H	0.019577	2.598926	0.000000		
H	0.891941	0.480501	1.745368		
C	-0.008702	-1.885420	0.000000		
H	-0.880612	0.485764	-1.753014		
H	0.891941	0.480501	-1.745368		
H	-0.010380	-2.447351	-0.927511		
H	-0.010380	-2.447351	0.927511		
Frequencies (cm-1)					
65.881	161.708	346.788	401.414		
635.018	687.269	833.161	858.885		
902.191	930.252	961.781	976.800		
1024.293	1037.030	1122.313	1194.008		
1222.400	1264.270	1311.661	1433.852		
1442.949	1462.204	1780.540	3022.320		
3027.444	3056.191	3058.639	3161.988		
3248.293	3250.508				

Atom	X	Y	Z	Å
C	-0.027260	1.043996	-0.000020	
C	-1.346808	0.309074	0.000050	
C	1.150185	0.178955	-0.000106	
C	-1.499054	-1.007777	-0.000003	
H	-2.220521	0.955151	0.000221	
H	0.016229	1.702750	-0.874049	

H	0.016289	1.702784	0.873981
C	2.113874	-0.535842	0.000067
H	-0.643776	-1.674516	-0.000239
H	-2.486410	-1.452810	-0.000013
H	2.972564	-1.163792	0.000172

Frequencies (cm-1)			
154.743	171.312	347.388	395.533
577.499	619.318	715.103	729.267
884.129	954.742	975.184	986.003
1038.582	1094.437	1242.741	1327.739
1360.065	1442.228	1466.358	1736.674
2258.615	3054.289	3082.244	3165.433
3179.379	3259.835	3495.305	

P2				
Atom	X	Y	Z	Å
C	0.017657	0.535997	0.000049	
C	1.134020	-0.411614	0.000077	
C	-1.240911	0.171557	0.000039	
C	2.413120	-0.037747	-0.000058	
H	0.870473	-1.464889	0.000099	
H	3.213509	-0.766468	-0.000110	
H	0.255369	1.597314	0.000003	
C	-2.487790	-0.200956	-0.000053	
H	2.693277	1.010412	-0.000132	
H	-3.024530	-0.359917	-0.929520	
H	-3.024677	-0.359877	0.929333	

Frequencies (cm-1)			
121.754	166.221	357.065	403.844
507.504	575.412	734.715	899.258
910.583	924.763	953.508	1010.975
1036.803	1115.005	1194.294	1304.532
1339.771	1441.801	1488.009	1711.984
2068.964	3151.093	3163.114	3169.333
3191.391	3232.287	3263.143	

P3				
Atom	X	Y	Z	Å
C	-0.000224	0.987651	0.734897	
C	-0.000224	-0.280790	1.176055	
C	-0.000224	0.987651	-0.734897	
C	0.000349	-1.214058	0.000000	
H	0.000030	-0.606454	2.206908	
H	0.000282	1.877763	1.349762	
H	0.000282	1.877763	-1.349762	
C	-0.000224	-0.280790	-1.176055	
H	0.879840	-1.869060	0.000000	
H	-0.877193	-1.871543	0.000000	
H	0.000030	-0.606454	-2.206908	

Frequencies (cm-1)

63.544	120.335	167.859	327.390
343.223	381.961	595.822	704.017
717.051	865.228	882.934	950.838
996.233	1099.564	1156.167	1235.297
1336.424	1372.381	1423.630	1458.572
1479.723	1490.130	2253.334	2983.785
2998.213	3082.724	3093.313	

P4

Atom	X	Y	Z	Å
C	-0.084314	0.490694	-0.000073	
C	0.917163	-0.392626	-0.000119	
C	-1.463757	0.118103	0.000040	
C	2.365059	-0.020445	0.000071	
H	0.673845	-1.451863	-0.000165	
H	2.869481	-0.431951	0.878642	
H	0.130222	1.556059	-0.000174	
C	-2.630582	-0.173377	0.000036	
H	2.496450	1.062440	0.000421	
H	2.869598	-0.431514	-0.878579	
H	-3.661007	-0.437266	0.000126	

Frequencies (cm-1)

169.546	170.689	202.131	393.963
460.914	550.477	682.335	727.742
825.057	916.679	993.349	1052.588
1073.232	1136.833	1309.356	1330.810
1415.816	1483.183	1494.404	1732.157
2240.880	3056.490	3113.338	3144.769
3172.386	3183.235	3495.442	

P5

Atom	X	Y	Z	Å
C	0.525845	-1.061768	0.000075	
C	1.492462	0.115057	-0.000091	
C	-0.549401	0.036826	0.000251	
C	0.523622	1.045561	0.000061	
H	0.540684	-1.689423	0.893658	
H	2.573649	0.165339	-0.000555	
H	0.540315	-1.689009	-0.893898	
C	-1.876343	0.034364	-0.000088	
H	0.520508	2.128128	0.000117	
H	-2.439617	0.960321	-0.000314	
H	-2.432649	-0.895595	-0.000256	

Frequencies (cm-1)

207.797	338.662	487.559	709.280
721.003	786.864	882.882	915.260
918.816	968.469	985.038	1015.991
1110.498	1110.510	1195.952	1219.168
1325.944	1439.423	1475.128	1623.440
1772.065	3078.906	3131.084	3169.564

3219.717 3249.476 3258.293

A1-1

Atom	X	Y	Z	Å
C	-0.634313	0.000061	0.000023	
C	-1.946052	-0.000095	-0.000028	
C	0.634309	0.000366	0.000064	
H	-2.505821	0.928735	0.000072	
H	-2.505557	-0.929090	-0.000238	
C	1.946053	-0.000148	0.000126	
H	2.506063	0.928536	-0.000629	
H	2.505331	-0.929282	-0.000319	

Frequencies (cm-1)

226.291	230.883	373.855	580.087
775.091	911.182	912.490	915.913
1022.344	1038.883	1405.034	1464.898
1709.139	2239.646	3156.434	3159.297
3242.765	3242.994		

A1-2

Atom	X	Y	Z	Å
C	0.000000	0.000000	0.000000	
H	0.000000	1.079107	0.000000	
H	0.934534	-0.539553	0.000000	
H	-0.934534	-0.539553	0.000000	

Frequencies (cm-1)

446.315	1413.618	1413.670	3141.674
3322.572	3322.576		

Ts1

Atom	X	Y	Z	Å
C	2.441353	-0.085329	-0.000400	
H	2.939880	0.179914	-0.924842	
H	2.940674	0.181096	0.923273	
C	1.203079	-0.650934	0.000492	
H	0.785400	-1.051597	-0.915971	
H	0.786211	-1.050450	0.917828	
C	-2.507897	-0.454156	-0.000190	
H	-3.402656	-1.029228	-0.000315	
C	-1.511183	0.231104	-0.000053	
C	-0.299096	0.942519	0.000108	
H	-0.003653	1.435533	0.917691	
H	-0.003398	1.435514	-0.917403	

Frequencies (cm-1)

-617.590	62.723	121.116	243.683
361.996	397.021	457.821	614.038
629.199	703.801	807.470	816.561
891.026	1009.796	1036.390	1040.564
1066.548	1236.970	1291.238	1455.523
1465.832	1576.847	2146.366	3158.992

3163.398 3166.826 3240.082 3255.319
 3266.046 3490.248

Ts2

Atom	X	Y	Z	Å
C	-0.264664	0.937512	-0.100512	
C	1.408979	-0.243171	0.625396	
C	-1.347058	0.298068	-0.099911	
C	2.293619	-0.336951	-0.401526	
H	1.571954	0.470398	1.425486	
H	0.752068	-1.072037	0.857702	
H	0.173952	1.886422	-0.335380	
C	-2.425012	-0.484638	-0.052058	
H	3.045356	0.424404	-0.572061	
H	2.226875	-1.137126	-1.128129	
H	-2.723831	-1.069492	-0.913096	
H	-3.041556	-0.527489	0.837139	
Frequencies (cm-1)				
-631.000	47.219	133.698	220.996	
326.673	378.945	425.491	490.994	
699.650	740.219	809.130	818.581	
899.775	995.480	1027.917	1036.556	
1162.411	1237.404	1302.152	1464.296	
1465.684	1581.949	1918.707	3161.479	
3169.053	3171.181	3244.552	3260.319	
3270.357	3366.343			

Ts3

Atom	X	Y	Z	Å
C	0.423443	-1.182576	0.141019	
C	1.207873	0.115214	-0.224086	
C	-0.987213	-0.788408	-0.032685	
C	0.408237	1.323876	0.175407	
H	1.364811	0.127722	-1.304475	
H	2.192751	0.104812	0.253734	
H	0.723109	-2.024523	-0.483744	
H	0.593204	-1.468359	1.183096	
C	-1.577592	0.293884	-0.097654	
H	0.302322	1.540822	1.232861	
H	0.380359	2.180566	-0.486202	
H	-2.405045	0.967030	-0.167277	
Frequencies (cm-1)				
-667.310	172.288	333.309	466.352	
511.713	587.046	694.413	705.369	
806.651	821.938	879.828	913.258	
1002.031	1056.968	1100.744	1196.858	
1228.307	1313.884	1345.131	1465.007	
1478.029	1495.825	1957.397	3062.583	
3076.878	3114.811	3133.579	3152.589	
3253.789	3421.953			

Ts4				
Atom	X	Y	Z	Å
C	-0.005654	1.026418	-0.165127	
C	1.307407	0.291111	0.022045	
C	-1.186181	0.177011	-0.029566	
C	1.463702	-1.034200	-0.118226	
H	1.279316	0.466728	1.927389	
H	2.183800	0.931897	0.058564	
H	-0.073676	1.849076	0.551460	
H	-0.007249	1.481088	-1.162022	
C	-2.150442	-0.528370	0.080852	
H	0.607867	-1.690567	-0.225905	
H	2.447394	-1.483910	-0.073012	
H	-3.010441	-1.146134	0.183656	
Frequencies (cm-1)				
-808.930	111.448	170.075	343.969	
382.648	410.877	493.031	586.143	
630.943	707.271	726.568	883.856	
939.519	957.001	976.197	1048.296	
1093.758	1242.284	1313.248	1360.345	
1436.333	1468.196	1660.395	2259.666	
3058.690	3099.769	3171.479	3180.931	
3269.504	3495.121			

Ts5				
Atom	X	Y	Z	Å
C	0.400876	-1.198819	-0.000064	
C	1.322153	0.034743	0.000172	
C	-0.862859	-0.864292	-0.000174	
C	0.479870	1.286466	-0.000164	
H	1.971302	0.001254	0.880113	
H	1.971971	0.001182	-0.879269	
H	0.807440	-2.202163	-0.000183	
C	-1.582461	0.277585	0.000132	
H	0.386279	1.855288	0.916069	
H	0.386384	1.854736	-0.916755	
H	-2.034268	0.637564	0.920408	
H	-2.034586	0.638041	-0.919794	
Frequencies (cm-1)				
-690.400	98.270	366.161	470.328	
518.464	629.233	680.729	743.142	
828.639	892.990	894.821	919.852	
1026.036	1044.444	1073.466	1107.700	
1241.894	1247.625	1320.836	1461.390	
1481.519	1497.972	1860.135	3058.134	
3095.968	3137.428	3165.203	3215.296	
3222.040	3264.386			

Ts6

Atom	X	Y	Z	Å
C	1.163300	0.343472	-0.035829	
C	-0.080488	1.220481	0.024593	
C	0.908187	-1.049161	-0.122503	
C	-1.232428	0.191743	-0.018843	
H	-0.084757	1.895561	-0.834641	
H	-0.103817	1.846309	0.919019	
H	2.147543	0.766556	-0.219861	
H	1.458135	-0.430488	0.932100	
C	-0.524344	-1.139246	0.012728	
H	-1.917975	0.289278	0.829257	
H	-1.847726	0.303480	-0.919114	
H	-1.056762	-2.074429	0.132361	
Frequencies (cm-1)				
-1039.670	72.485	411.573	558.493	
673.698	740.172	788.988	809.739	
909.257	923.739	985.662	1012.455	
1076.781	1126.096	1193.621	1230.341	
1256.049	1291.618	1316.637	1341.362	
1401.880	1459.151	1486.725	2148.853	
3042.870	3074.078	3082.645	3122.621	
3176.308	3215.919			

Ts7				
Atom	X	Y	Z	Å
C	-0.027857	-0.959372	-0.042115	
C	-1.397788	-0.364308	-0.006582	
C	1.111328	-0.240073	-0.149568	
C	-1.672112	0.980716	-0.030971	
H	-2.199324	-1.088280	-0.099774	
H	-0.744210	-0.807018	1.106163	
H	0.015396	-2.035970	-0.167324	
C	2.183627	0.470767	0.049724	
H	-2.694806	1.327746	-0.010137	
H	-0.875692	1.714022	-0.032975	
H	2.535212	0.706797	1.055119	
H	2.780234	0.856325	-0.774001	
Frequencies (cm-1)				
-1921.300	141.252	172.229	295.998	
379.050	483.169	614.458	656.585	
756.852	786.804	899.058	923.322	
996.554	999.568	1017.300	1101.402	
1160.832	1283.597	1354.239	1418.144	
1462.127	1553.213	1630.800	1944.391	
3089.818	3166.357	3185.993	3190.514	
3205.822	3289.337			

Ts8				
Atom	X	Y	Z	Å
C	-0.125609	1.002455	-0.000005	

C	-1.491038	0.343619	0.000033
C	0.823723	-0.163171	-0.000135
C	-1.456373	-0.977561	0.000038
H	-2.401935	0.935482	0.000028
H	-0.091174	-1.144782	-0.000088
H	0.015261	1.636736	-0.881362
C	2.131476	-0.305231	0.000051
H	-2.226358	-1.737554	-0.000063
H	0.015239	1.636691	0.881385
H	2.598179	-1.284518	0.000112
H	2.797711	0.557277	0.000103
Frequencies (cm-1)			
-1775.880	115.201	289.442	339.963
557.089	576.613	646.046	713.238
890.569	912.056	917.468	934.584
973.875	998.440	1072.022	1096.411
1170.075	1252.297	1292.641	1424.069
1465.169	1655.791	1753.786	1758.090
3054.940	3088.934	3112.753	3180.269
3211.830	3248.384		

Ts9				
Atom	X	Y	Z	Å
C	0.261536	-1.178233	0.158032	
C	1.286401	-0.056883	-0.003843	
C	-1.035292	-0.553426	-0.273598	
C	0.839348	1.169610	-0.168157	
H	2.348632	-0.293234	0.033909	
H	-1.507473	-0.895114	-1.187626	
H	0.524811	-2.046731	-0.448354	
C	-1.319143	0.677869	0.230643	
H	1.299793	2.141104	-0.280517	
H	0.242124	-1.509391	1.203471	
H	-2.088019	1.298675	-0.215731	
H	-1.016968	0.951069	1.236387	
Frequencies (cm-1)				
-672.480	242.573	322.261	467.703	
607.888	646.024	708.008	816.060	
883.886	909.988	921.618	935.645	
962.913	995.707	1091.630	1196.985	
1211.727	1273.456	1314.315	1425.713	
1482.126	1582.594	1660.449	3043.712	
3115.053	3146.046	3152.526	3200.766	
3240.589	3255.674			

Ts10				
Atom	X	Y	Z	Å
C	1.180944	-0.135650	-0.117879	

C	0.290378	-1.161707	-0.092087
C	0.431383	1.137248	-0.091024
C	-1.096113	-0.611498	0.052324
H	1.772856	-0.020421	1.672619
H	0.525820	-2.215568	-0.134539
H	2.236078	-0.221977	-0.340277
H	0.891547	2.115427	-0.122776
C	-0.878183	0.875264	0.014473
H	-1.762017	-0.956187	-0.747461
H	-1.559309	-0.925745	0.997544
H	-1.675427	1.602529	0.080046
Frequencies (cm-1)			
-841.400	273.634	356.694	396.585
565.481	702.281	727.631	809.579
816.305	925.285	937.912	976.280
978.581	1006.352	1017.236	1105.851
1126.162	1134.735	1274.382	1321.178
1398.752	1418.467	1545.894	1649.287
3039.460	3075.965	3228.472	3236.873
3254.091	3259.811		

Ts11				
Atom	X	Y	Z	Å
C	0.018961	0.538760	0.140735	
C	-1.108294	-0.389229	-0.056677	
C	1.272402	0.185355	0.016196	
C	-2.385430	0.038521	-0.165155	
H	-0.850149	-1.401315	-0.352593	
H	-1.076183	-1.088114	1.663818	
H	-0.217898	1.569709	0.391714	
C	2.515672	-0.179154	-0.105327	
H	-3.188680	-0.647497	-0.399052	
H	-2.647513	1.072082	0.030339	
H	3.076668	-0.541968	0.749578	
H	3.023888	-0.128416	-1.062437	
Frequencies (cm-1)				
-951.450	101.720	164.682	344.593	
377.674	425.424	467.873	533.529	
575.052	709.546	902.612	904.420	
917.503	921.403	1012.258	1065.434	
1113.961	1183.487	1293.119	1319.917	
1436.099	1485.306	1633.889	2072.122	
3151.963	3166.674	3172.822	3186.245	
3233.850	3270.742			

Ts12				
Atom	X	Y	Z	Å
C	0.043776	0.864731	-0.031338	
C	1.436055	0.425108	-0.054975	

C	-1.039343	-0.026081	0.244932
C	1.815189	-0.858509	-0.037423
H	2.182442	1.212728	-0.074153
H	1.082703	-1.658149	-0.044208
H	-0.406387	0.679486	1.180037
C	-2.255109	-0.381206	-0.126499
H	2.862341	-1.132079	-0.014304
H	-0.195449	1.858217	-0.408059
H	-2.575663	-0.249093	-1.160716
H	-2.953396	-0.855371	0.553220
Frequencies (cm-1)			
-1889.780	130.336	222.668	261.742
327.792	539.929	602.592	681.991
849.797	891.841	911.705	939.118
1009.895	1015.713	1034.371	1099.265
1145.837	1318.243	1336.283	1440.209
1448.373	1669.265	1736.195	2170.301
3099.521	3134.584	3170.827	3193.767
3216.336	3266.112		

Ts13				
Atom	X	Y	Z	Å
C	-1.172938	-0.813236	-0.252426	
C	-1.154103	0.485965	0.184676	
C	0.081904	1.204050	-0.083995	
C	1.178801	0.420773	-0.090668	
C	1.022030	-1.019716	0.209208	
H	-1.885801	-1.528400	0.146501	
H	-0.755580	-1.064048	-1.220462	
H	-1.864081	0.857040	0.915781	
H	0.134013	2.281965	-0.185134	
H	2.165718	0.839711	-0.271955	
H	0.983545	-1.303374	1.258762	
H	1.488017	-1.749912	-0.444269	
Frequencies (cm-1)				
-771.080	212.970	407.834	452.518	
513.999	656.093	720.286	742.893	
781.039	895.464	958.764	977.451	
996.432	1019.701	1052.659	1072.146	
1160.899	1248.638	1369.350	1429.491	
1451.425	1554.568	1625.081	3123.136	
3153.724	3162.619	3195.265	3216.133	
3218.634	3236.891			

Ts14				
Atom	X	Y	Z	Å
C	1.145996	-0.519812	-0.024571	
C	-0.178943	-1.207747	-0.005297	
C	0.866287	0.904617	-0.019047	
C	-1.258483	-0.152463	-0.016534	

H	0.695953	-1.033786	1.022749
H	-0.305964	-2.251289	-0.250497
H	2.063922	-0.991205	-0.345241
H	1.635629	1.664551	0.000502
C	-0.461807	1.134775	-0.000857
H	-1.89319	-0.229818	-0.914938
H	-1.949661	-0.225678	0.834369
H	-0.924984	2.111001	0.050887

Frequencies (cm-1)

-1861.2	255.2705	485.461	548.7807
688.4297	730.2623	801.7217	826.8352
917.535	933.4454	948.8654	954.9515
1017.2649	1057.663	1122.9393	1137.871
1245.2592	1269.9769	1296.4494	1330.2007
1396.0919	1469.7478	1603.9793	2233.7496
2952.3484	3001.7804	3228.4881	3238.2799
3251.3191	3258.7285		

Ts15

Atom	X	Y	Z	Å
C	0.334304	1.17071	-0.099296	
C	1.163387	0.098833	-0.113768	
C	-1.04515	0.708673	0.031544	
C	0.335962	-1.158239	-0.097231	
H	1.55322	0.036466	1.89315	
H	2.231764	0.117394	-0.276681	
H	0.636894	2.207912	-0.14805	
H	-1.906679	1.35879	0.10251	
C	-1.063102	-0.636879	0.051612	
H	0.449276	-1.696003	-1.04785	
H	0.619149	-1.855201	0.696488	
H	-1.936038	-1.267946	0.143267	

Frequencies (cm-1)

-581.33	214.2272	359.2172	426.4787
530.0461	695.319	771.9743	814.9234
818.3977	911.5825	939.3947	967.698
976.9285	983.2187	1031.556	1108.8621
1129.0248	1134.8685	1273.7922	1323.1906
1403.0888	1421.5752	1542.4386	1641.3476
3050.1619	3104.5681	3231.1074	3239.8397
3254.9166	3261.8169		

Ts16

Atom	X	Y	Z	Å
C	0.013028	-0.029695	0.000248	
C	1.285334	0.746373	-0.000162	
C	-1.265558	-0.016228	0.000050	
C	2.117916	-0.543551	-0.000013	
H	1.421404	1.365709	-0.887589	

H	1.421697	1.365923	0.887074
H	0.788679	-1.132377	0.000695
C	-2.580100	-0.101585	-0.000066
H	2.608413	-0.834921	-0.923302
H	2.609320	-0.834162	0.923034
H	-3.136737	-0.130473	0.929256
H	-3.136494	-0.131586	-0.929499
Frequencies (cm-1)			
-	36.792	172.469	271.823
2110.890	506.214	517.820	566.649
390.466	850.598	879.186	935.989
777.778	1019.953	1059.629	1131.225
1014.413	1238.881	1327.715	1425.791
1221.158	1494.417	1825.244	2068.646
1474.947	3134.258	3140.336	3163.540
3091.817	3250.024		
3246.782			

Ts17				
Atom	X	Y	Z	Å
C	0.301839	1.263709	0.22539	
C	-1.663044	0.308643	-0.357882	
C	1.176838	0.428777	0.095906	
C	-1.914657	-0.834246	0.234193	
H	-2.199825	0.871621	-1.11161	
H	-0.15863	2.198022	0.456208	
C	2.036182	-0.721985	-0.147345	
H	-1.230258	-1.247247	0.971376	
H	-2.814886	-1.410095	0.020717	
H	2.874285	-0.452301	-0.792515	
H	2.437535	-1.109877	0.790571	
H	1.468836	-1.519512	-0.636321	
Frequencies (cm-1)				
-538.5	81.1092	87.5207	226.8503	
263.1598	301.4384	386.7679	428.1037	
462.6825	564.726	738.033	792.2052	
858.6633	874.2024	906.3543	1027.693	
1046.5953	1397.5269	1417.3097	1424.5825	
1462.8795	1639.149	2106.4655	3129.3763	
3156.8577	3161.862	3244.2039	3247.8181	
3299.0292	3307.1967			

Ts18				
Atom	X	Y	Z	Å
C	-0.005355	-0.995669	-0.001008	
C	1.345377	-0.464926	0.025955	
C	-1.098214	-0.255927	0.017101	
C	1.623796	0.983908	0.042252	
H	2.150608	-1.130172	0.310083	
H	1.690636	0.131554	-1.017211	

H	-0.116169	-2.074204	-0.060676
C	-2.174703	0.477619	0.006664
H	2.612470	1.335014	0.294403
H	0.806259	1.680294	-0.075845
H	-2.684883	0.747370	0.927105
H	-2.604330	0.840109	-0.923639
Frequencies (cm-1)			
-1830.640	152.944	183.931	320.087
374.736	409.718	591.040	643.365
661.548	806.706	893.026	909.113
916.205	1007.083	1013.784	1100.559
1213.196	1254.889	1363.064	1405.037
1453.013	1481.203	2019.533	2251.713
3126.895	3180.139	3194.480	3201.659
3218.031	3318.213		

Ts19				
Atom	X	Y	Z	Å
C	0.049163	0.967663	-0.094804	
C	-1.218465	0.489729	-0.14066	
C	1.205201	0.116853	-0.047442	
C	-1.608819	-0.933391	0.067373	
H	0.252195	1.528666	1.687057	
H	-2.017523	1.211631	-0.278043	
H	0.235064	2.007951	-0.338904	
C	2.182164	-0.582495	-0.024966	
H	-2.245878	-1.28184	-0.750071	
H	-0.735655	-1.581778	0.13534	
H	3.048178	-1.199857	-0.001361	
H	-2.19184	-1.034924	0.988986	
Frequencies (cm-1)				
-917.07	119.8643	163.1093	251.0531	
312.301	385.2775	442.0139	573.7128	
659.4094	690.3894	732.6548	779.848	
911.6866	972.4844	1017.1391	1056.4802	
1124.546	1249.9692	1391.4741	1429.0716	
1482.0396	1485.9615	1635.3621	2245.028	
3049.4747	3104.3642	3157.3586	3185.0216	
3200.462	3494.5149			

Ts20				
Atom	X	Y	Z	Å
C	-0.001926	0.511217	0.041676	
C	-0.992391	-0.377579	-0.099106	
C	1.372495	0.177049	-0.103342	
C	-2.441995	-0.049023	0.052173	
H	-0.734859	-1.406013	-0.337888	
H	-2.987320	-0.276875	-0.867897	
H	-0.228646	1.546737	0.280635	
C	2.546599	-0.114661	-0.146102	

H	-2.588128	1.005229	0.290649
H	-2.892534	-0.651072	0.846077
H	2.971587	-0.785485	1.707982
H	3.563208	-0.314535	-0.391358
Frequencies (cm-1)			
-663.630	89.743	154.581	174.507
195.945	312.694	395.753	497.482
554.059	711.285	785.958	825.068
917.747	992.413	1056.357	1070.952
1137.426	1312.024	1330.523	1414.180
1482.334	1492.705	1716.194	2174.920
3056.377	3112.919	3146.151	3173.959
3183.275	3475.154		

Ts21				
Atom	X	Y	Z	Å
C	0.312917	-1.048321	-0.000203	
C	1.536392	-0.179892	0.00006	
C	-0.74285	-0.251682	0.000684	
C	0.775943	1.13494	-0.000209	
H	2.163793	-0.314808	0.885213	
H	2.164869	-0.315	-0.884302	
H	0.265617	-2.134369	-0.00034	
C	-2.034552	0.121094	-0.000041	
H	0.705771	1.705923	0.917919	
H	0.704053	1.704244	-0.919243	
H	-2.5452	0.347659	-0.92897	
H	-2.546002	0.349516	0.927981	
Frequencies (cm-1)				
-864.28	134.4468	267.5459	330.4428	
363.6269	572.6385	640.9237	762.2166	
789.412	818.1171	867.0046	974.277	
1020.239	1026.266	1033.039	1079.55	
1215.304	1290.631	1314.683	1451.931	
1456.24	1491.424	1899.784	3063.922	
3105.503	3153.101	3156.567	3169.097	
3245.097	3258.419			

Ts22				
Atom	X	Y	Z	Å
C	0.452493	-1.065101	-0.025699	
C	1.543332	-0.02078	-0.002396	
C	-0.582699	-0.031745	0.010327	
C	0.482406	1.071041	-0.002817	
H	1.118451	-0.812071	1.001863	
H	2.560919	-0.060379	-0.361887	
H	0.459229	-2.107008	-0.315222	
C	-1.9174	-0.0190	-0.0048	
H	0.477185	1.789539	0.818281	
H	0.467096	1.607723	-0.955531	

H	-2.465144	0.915195	0.011463
H	-2.486521	-0.939672	-0.046767
Frequencies (cm-1)			
-1821.24	208.2584	344.4657	451.4342
557.6997	630.272	713.5622	771.0645
865.4329	884.7431	906.6864	935.8858
973.0723	1027.2035	1092.4467	1167.1725
1187.8421	1235.2819	1266.5291	1295.6017
1435.3275	1460.3558	1718.3067	2249.8604
3073.9643	3128.5364	3172.8322	3233.0397
3250.0687	3263.1699		

Ts23

Atom	X	Y	Z	Å
C	-0.102234	1.027478	-0.026557	
C	1.291976	0.495155	-0.002575	
C	-1.232422	0.177686	-0.022779	
C	1.544154	-0.976076	-0.014092	
H	0.574882	0.986101	1.032418	
H	2.068201	1.20011	-0.26788	
H	0.865363	-1.497615	0.665206	
H	-0.236591	2.06265	-0.314117	
C	-2.195006	-0.551564	0.000346	
H	2.56939	-1.204684	0.277106	
H	1.366366	-1.394248	-1.01383	
H	-3.046419	-1.188387	0.015048	
Frequencies (cm-1)				
-1824.33	137	167.6597	227.111	
348.6129	409.0079	581.9816	585.4461	
621.2832	733.5973	805.0219	868.5215	
980.4351	1038.1707	1103.6408	1192.8234	
1250.2045	1359.4467	1373.9395	1424.4779	
1480.6185	1495.2562	2183.7641	2233.828	
3018.3666	3096.4715	3148.3556	3207.6414	
3226.5488	3494.2763			

Ts24

Atom	X	Y	Z	Å
C	-0.496793	-1.102707	0.087273	
C	-1.482757	0.032726	-0.123652	
C	0.562989	0.002882	-0.019097	
C	-0.528151	0.998953	-0.124576	
H	-0.458488	-1.860126	-0.699156	
H	-2.560525	0.053797	-0.213838	
H	-0.547708	-1.589002	1.065574	
C	1.887604	0.022479	-0.050800	
H	-0.540280	2.056575	-0.355589	
H	-0.443526	1.552933	1.716038	
H	2.432314	0.953459	-0.156014	
H	2.460862	-0.893635	0.028093	

	Frequencies (cm-1)		
-794.670	183.830	308.320	339.880
369.252	531.794	718.310	730.440
773.929	885.255	913.490	925.318
976.449	983.180	1013.156	1100.389
1109.613	1190.705	1220.213	1319.723
1437.935	1465.648	1551.098	1775.714
3068.022	3119.538	3167.608	3219.837
3248.199	3256.743		

Ts25				
Atom	X	Y	Z	Å
C	-0.545965	-1.063202	-0.006505	
C	-1.499981	0.114965	-0.119114	
C	0.534728	0.034916	0.085467	
C	-0.543501	1.046763	0.002939	
H	-0.464752	-1.702611	-0.888132	
H	-2.572489	0.165062	-0.254649	
H	-0.657579	-1.673121	0.892128	
C	1.857222	0.032454	-0.165407	
H	-0.536767	2.128833	0.013213	
H	2.4139	0.9589	-0.2391	
H	2.40618	-0.898916	-0.232686	
H	0.596475	0.026503	1.924951	
	Frequencies (cm-1)			
-942.32	255.0557	322.1479	423.6351	
497.5363	549.3127	652.4594	727.1929	
779.7424	885.299	891.9498	917.6556	
961.9193	982.9434	1008.7906	1103.909	
1114.7567	1194.102	1221.5905	1319.623	
1435.6922	1472.0464	1630.8752	1675.3591	
3081.1225	3135.2789	3167.9517	3223.5247	
3253.1017	3263.0147			

Ts26				
Atom	X	Y	Z	Å
C	0.452493	-1.065101	-0.025699	
C	1.543332	-0.020780	-0.002396	
C	-0.582699	-0.031745	0.010327	
C	0.482406	1.071041	-0.002817	
H	1.118451	-0.812071	1.001863	
H	2.560919	-0.060379	-0.361887	
H	0.459229	-2.107008	-0.315222	
C	-1.917402	-0.018970	-0.004783	
H	0.477185	1.789539	0.818281	
H	0.467096	1.607723	-0.955531	
H	-2.465144	0.915195	0.011463	
H	-2.486521	-0.939672	-0.046767	
	Frequencies (cm-1)			

-1821.240	208.258	344.466	451.434
557.700	630.272	713.562	771.065
865.433	884.743	906.686	935.886
973.072	1027.204	1092.447	1167.173
1187.842	1235.282	1266.529	1295.602
1435.328	1460.356	1718.307	2249.860
3073.964	3128.536	3172.832	3233.040
3250.069	3263.170		

Ts27

Atom	X	Y	Z	Å
C	0.455592	-1.048116	-0.091814	
C	1.441089	-0.120088	-0.120794	
C	-0.600944	-0.034600	-0.018920	
C	0.473070	1.060356	-0.096304	
H	1.980538	0.018662	1.881246	
H	2.511499	-0.179065	-0.267451	
H	0.444037	-2.130350	-0.106817	
C	-1.926730	-0.028854	0.077134	
H	0.536705	1.715207	0.774832	
H	0.444280	1.655186	-1.011436	
H	-2.479717	0.902115	0.116002	
H	-2.489816	-0.953947	0.117812	
Frequencies (cm-1)				
-586.410	167.336	298.356	340.651	
356.804	490.287	702.180	723.416	
821.810	883.722	917.476	920.109	
960.580	984.386	1010.415	1106.233	
1110.880	1198.156	1220.167	1324.307	
1439.804	1473.205	1568.418	1753.912	
3082.601	3136.650	3169.674	3222.736	
3249.272	3259.532			

Ts28

Atom	X	Y	Z	Å
C	0.014602	-0.519298	-0.476225	
C	1.122306	-0.460282	0.586515	
C	-1.301654	-0.093545	-0.137101	
C	1.830963	0.678493	-0.131585	
H	1.702053	-1.379155	0.654974	
H	0.743083	-0.199726	1.57281	
H	0.718677	0.494804	-1.033942	
H	0.090649	-1.328149	-1.198028	
C	-2.394018	0.325253	0.155135	
H	2.754605	0.46906	-0.662032	
H	1.720874	1.679031	0.274114	
H	-3.363132	0.680408	0.411674	
Frequencies (cm-1)				
-1979.86	76.6711	204.7654	312.7916	

463.3247	536.8776	604.8776	645.7776
715.0645	761.3543	868.9298	899.0434
925.702	1025.9426	1093.5578	1103.8777
1223.8268	1258.2833	1302.6362	1338.5881
1426.3311	1495.658	1781.7979	2201.5505
3114.301	3136.88	3163.1329	3175.3052
3248.2988	3494.3452		

Ts29

Atom	X	Y	Z	Å
C	0.073155	-0.952367	0.000121	
C	-1.372822	-0.52583	-0.000103	
C	0.975788	0.098862	-0.000034	
C	-1.411115	0.981174	0.000064	
H	-1.887891	-0.934551	-0.877036	
H	-1.88822	-0.93475	0.876545	
H	0.375003	-1.992517	0.000198	
C	2.294464	0.206778	-0.000027	
H	-1.654709	1.504442	-0.91735	
H	-1.654025	1.50418	0.917808	
H	3.086495	0.932777	-0.000107	
H	0.266522	1.068714	-0.000186	

Frequencies (cm-1)

-1958.15	165.3451	365.0936	404.1107
461.0392	555.2589	615.4279	663.1371
779.3869	821.0829	875.1504	942.4549
975.0232	999.662	1076.3001	1178.3803
1202.2303	1276.0323	1302.7613	1408.9012
1457.1579	1474.0823	1572.9844	1815.9637
3064.2184	3115.753	3133.2249	3225.8598
3230.6291	3269.3153		

Ts30

Atom	X	Y	Z	Å
C	-0.102234	1.027478	-0.026557	
C	1.291976	0.495155	-0.002575	
C	-1.232422	0.177686	-0.022779	
C	1.544154	-0.976076	-0.014092	
H	0.574882	0.986101	1.032418	
H	2.068201	1.20011	-0.26788	
H	0.865363	-1.497615	0.665206	
H	-0.236591	2.06265	-0.314117	
C	-2.195006	-0.551564	0.000346	
H	2.56939	-1.204684	0.277106	
H	1.366366	-1.394248	-1.01383	
H	-3.046419	-1.188387	0.015048	

Frequencies (cm-1)

-1824.3300	137.0000	167.6597	227.1110
348.6129	409.0079	581.9816	585.4461
621.2832	733.5973	805.0219	868.5215

980.4351	1038.1707	1103.6408	1192.8234
1250.2045	1359.4467	1373.9395	1424.4779
1480.6185	1495.2562	2183.7641	2233.8280
3018.3666	3096.4715	3148.3556	3207.6414
3226.5488	3494.2763		

Ts31

Atom	X	Y	Z	Å
C	-0.051547	1.048135	-0.180842	
C	1.24568	0.413892	0.251485	
C	-1.205972	0.158071	-0.028607	
C	1.571993	-0.975244	-0.154733	
H	1.185302	-0.618391	1.031548	
H	2.070345	1.066423	0.50716	
H	-0.233357	1.960652	0.391871	
H	0.011024	1.34059	-1.239737	
C	-2.139643	-0.585337	0.097904	
H	0.812615	-1.570312	-0.642541	
H	2.602775	-1.297719	-0.170679	
H	-2.971768	-1.238343	0.211134	

Frequencies (cm-1)

-1834.44	117.5952	172.198	345.6222
354.8015	371.7035	582.1305	691.4562
705.2767	719.7314	739.079	879.2799
932.8758	950.7333	1078.007	1175.4185
1254.8112	1260.7986	1344.7429	1367.19
1435.8697	1467.6747	2248.8738	2254.9086
2997.4538	3100.2105	3182.6047	3214.7074
3303.2086	3495.5943		

Ts32

Atom	X	Y	Z	Å
C	0.059709	1.083161	0.07247	
C	-1.285268	0.420659	-0.080812	
C	1.197293	0.168434	0.011053	
C	-1.490756	-0.89734	-0.183266	
H	-2.489472	-1.291853	-0.323079	
H	-2.133044	1.098798	-0.054984	
H	0.175422	1.851003	-0.700198	
H	0.08583	1.616903	1.029888	
C	2.12678	-0.588508	-0.038422	
H	-0.65945	-1.588034	-0.270297	
H	-1.581544	-1.551144	1.71209	
H	2.955711	-1.254103	-0.079557	

Frequencies (cm-1)

-644.230	112.228	168.205	226.639
344.452	366.371	400.021	616.888
643.126	712.003	726.987	884.200
954.607	973.580	1000.266	1025.348

1095.213	1237.877	1318.774	1357.290
1435.563	1462.318	1676.052	2259.808
3047.353	3076.084	3168.853	3184.898
3263.656	3495.145		

References

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