

DFT-Calculated IR Absorption Spectra for PFAS Molecules

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14. ABSTRACT Density function theory (DFT) is used for calculation of vibration absorption spectra for PFAS molecules within the IR range of frequencies. The DFT software GAUSSIAN was used for the calculations of IR absorption spectra presented here. This study continues presentation of the concept of using DFT to calculate template spectra for practical detection of target substances, by comparison with spectra within databases. Specifically, PFAS molecules, which include toxic and carcinogenic environmental contaminants, and whose detection based on IR spectroscopy is thus of great importance.						
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Introduction

Identification of unknown materials using infrared (IR) spectroscopy is by comparison of measured spectra with reference (or template spectra) of known materials, which are within a database of known molecular structures [1] using signal processing algorithms [2]. Algorithms for signal processing of measured spectra for correlation with template spectra within a database are described in references [3-7]. For detection in practice, measured spectra can be correlated with different databases, providing complementary information, which includes different types of information concerning interpretation of spectral features. Typically, databases of spectra consist of spectroscopic measurements, which are obtained using different types of spectroscopies, based on transmission and reflection [8,9]. Presented in this report are calculations of IR absorption spectra of molecular structures using density functional theory (DFT) and associated software technology (e.g., see reference [10] for DFT-calculated spectra of water), which provides complementary information to that obtained from laboratory measurement.

This report presents DFT calculated IR spectra for PFAS molecules within a water background. The group of chemicals called PFASs, which are highly fluorinated aliphatic molecules, are among toxic and carcinogenic contaminants commonly found in the environment [11-16]. IR spectral signatures can be correlated with the presence of target molecules (see references [17-19]). A previous study [17] introduced and demonstrated the concept of using DFT calculated IR spectra. The concept of database enhancement using DFT calculated spectra is independent of specific types of detection technology. Methodologies for comparison of detected spectral features with database spectra represent a separate problem. This study continues presentation of the concept of using DFT to calculate template spectra for practical detection of target substances, by comparison with spectra within databases. Specifically, PFAS molecules, which include toxic and carcinogenic environmental contaminants, and whose detection based on IR spectroscopy is thus of great importance.

Given in reference [17] is a description of the formalism underlying DFT calculation of IR spectra, and implementation of this formalism in terms of the DFT software GAUSSIAN16. The commercial computer program GAUSSIAN16 (G16) is designed to compute the IR spectrum of a molecule, including the effect of a continuous solvent background [20-22]. Second derivatives of the energy with respect to the Cartesian nuclear coordinates are calculated and subsequently changed to mass-weighted coordinates at the equilibrium geometry of the molecule. The IR spectrum is obtained from the ground state energy surface calculated in the Born-Oppenheimer approximation by solving the DFT Kohn-Sham equations [23-29]. The electronic density, the potential energy V , and the equilibrium geometry are calculated. The details followed by GAUSSIAN for IR analysis are given in references [22] and [28].

DFT Calculation of IR Spectra

DFT-calculated IR spectra for a collection of PFAS molecules are presented, i.e., ground-state energies for energy-minimized configuration of these molecules within a water solvent background, and their ground-state oscillation frequencies and IR intensities. For these calculations, geometry-energy optimization and vibration analysis was effected using the computer program Gaussian 16. All but three of the calculations in this study employed the DFT chemical model B3LYP/6-311++g(3df,3pd) (see [29-32]), which is a reasonably large basis set, including a set of diffuse functions, and polarization functions on heavy atom. Two calculations (CAS 375-16-6, CAS 51851-37-7) employed B3LYP/6-311++g(3d2f,3p2d) to correct for a flattened potential energy surface encountered with B3LYP/6-311++g(3df,3pd). All of these basis functions designate the 6-311G basis set supplemented by diffuse functions, indicated by the sign ++, and polarization functions (df), having a set of d and f functions on heavy atoms [33]. The calculation of CAS 354-64-3, was carried out with the B3LYP /LANL2MB for representation of the relativistic effects present in the heavy iodine atom. DFT-calculated IR spectra of these molecules (with water background) are shown in Figs. (1) through (29). Values of the IR intensities ($\text{M}^{-1}\text{cm}^{-1}$) as a function of frequency (cm^{-1}) for these molecules within a water background are given in Tables 1 through 29.

Conclusion

The DFT calculated IR spectra given here are to be adopted as database information concerning spectral features of PFAS molecules, which is complementary to that obtained from laboratory measurement. These DFT calculated absorption spectra provide information concerning molecular level dielectric response structure, and serve as reasonable estimates of molecular level response characteristics, providing interpretation of dielectric response features for comparison with experimental measurements. Specifically, the DFT calculated IR spectra calculated here should provide reasonable templates for filtering of IR spectral measurements associated with different types of detector schemes.

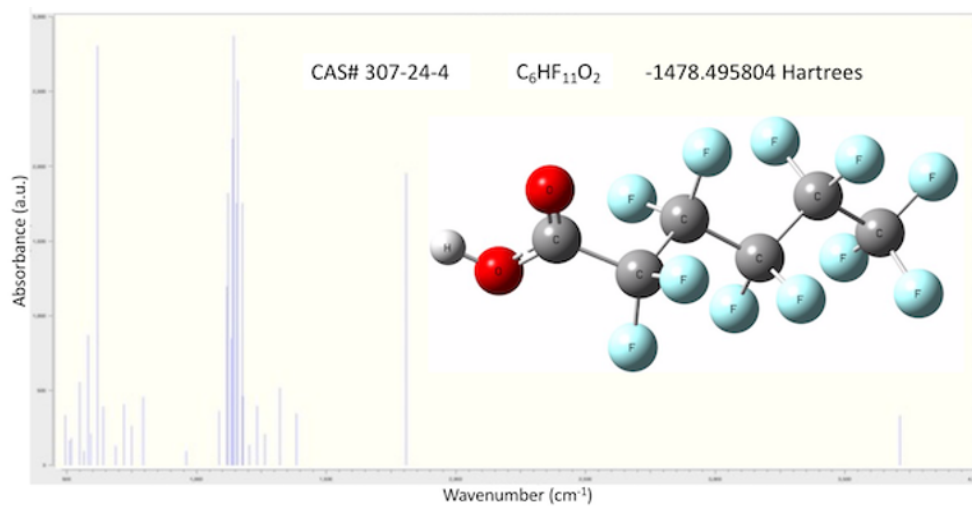


Figure 1. DFT-calculated IR spectra and molecular geometry for CAS# 307-24-4

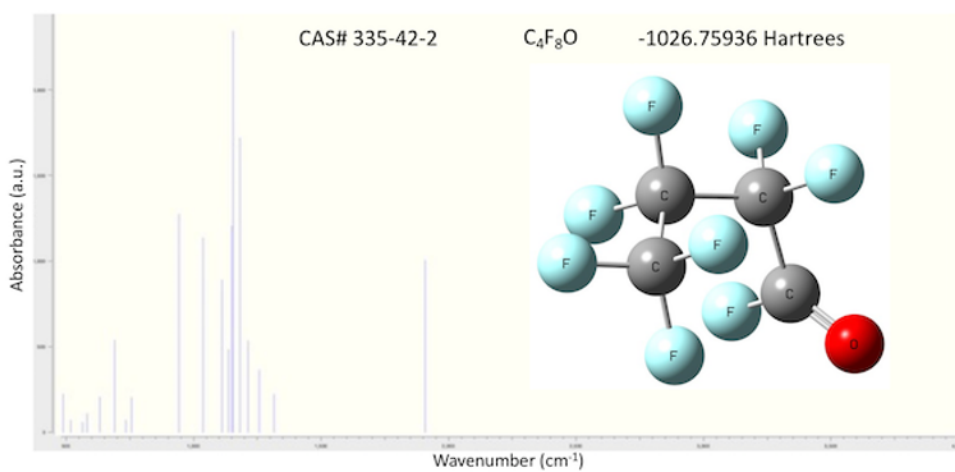


Figure 2. DFT-calculated IR spectra and molecular geometry for CAS# 335-42-2

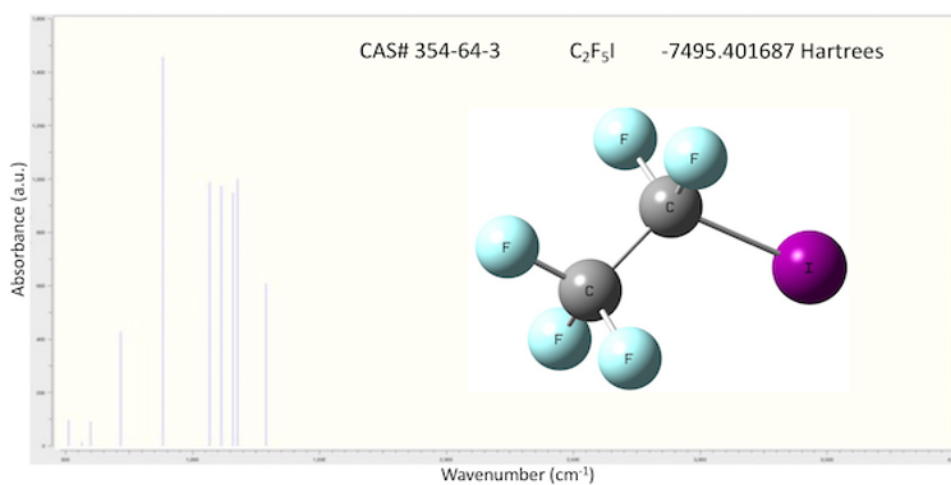


Figure 3. DFT-calculated IR spectra and molecular geometry for CAS# 354-64-3

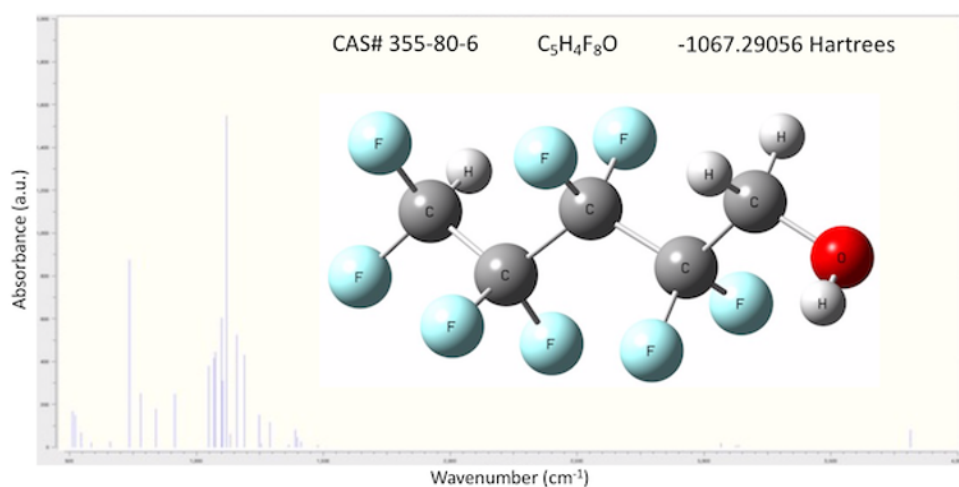


Figure 4. DFT-calculated IR spectra and molecular geometry for CAS# 355-80-6

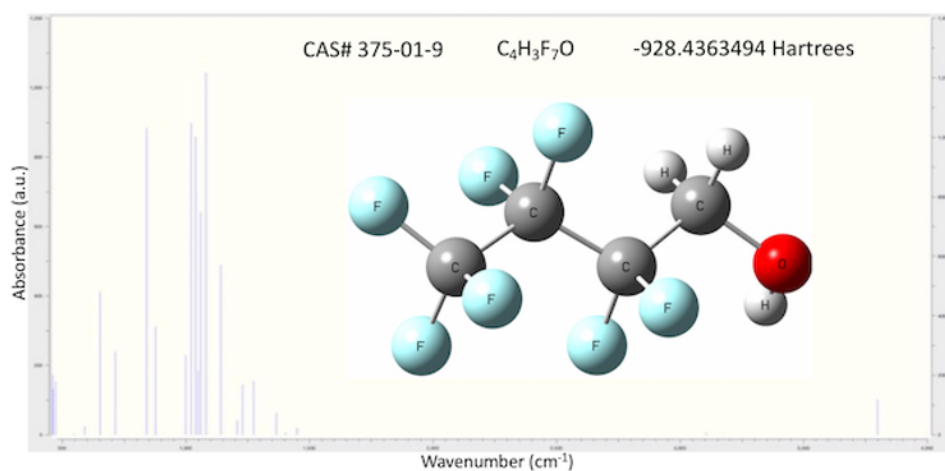


Figure 5. DFT-calculated IR spectra and molecular geometry for CAS# 375-01-9

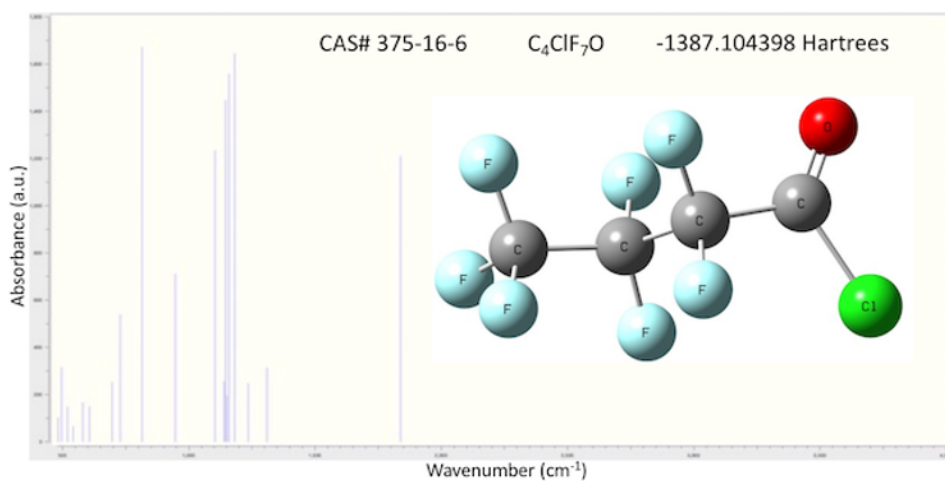


Figure 6. DFT-calculated IR spectra and molecular geometry for CAS# 375-16-6

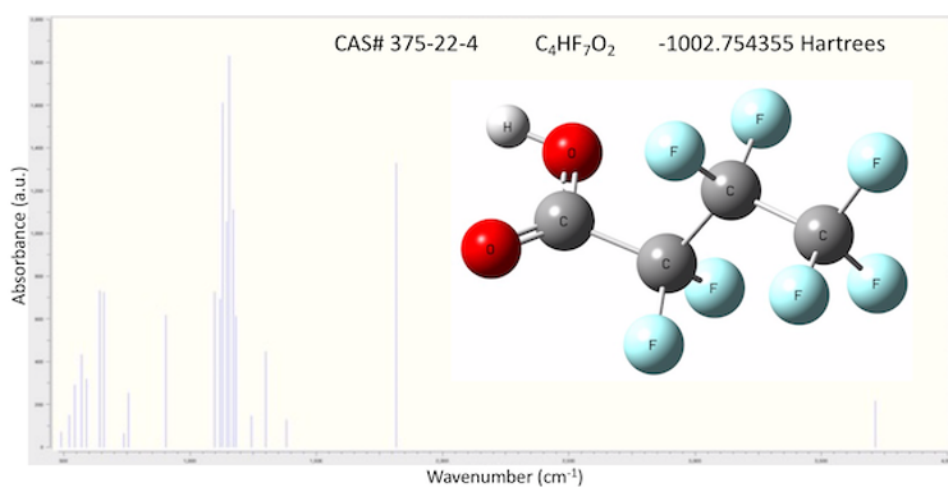


Figure 7. DFT-calculated IR spectra and molecular geometry for CAS# 375-22-4

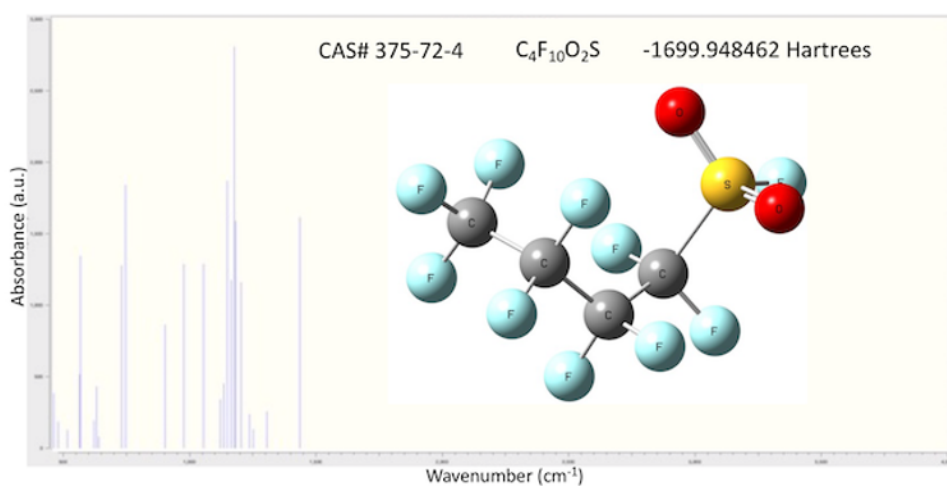


Figure 8. DFT-calculated IR spectra and molecular geometry for CAS# 375-72-4

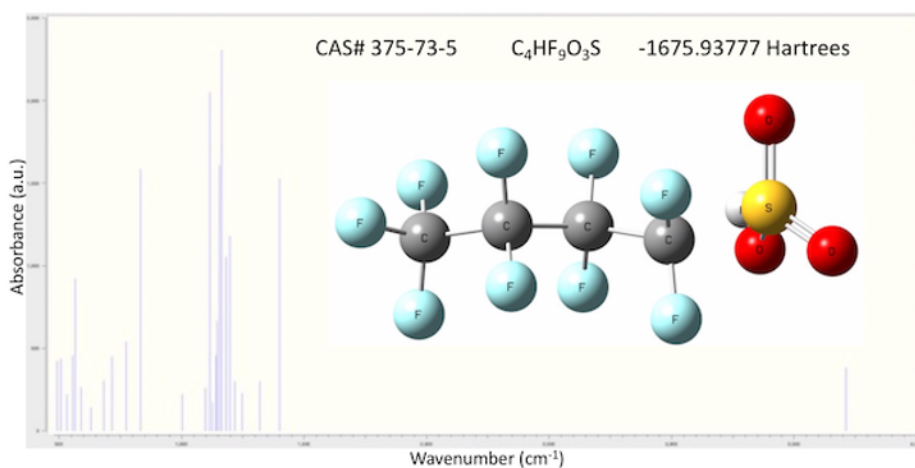


Figure 9. DFT-calculated IR spectra and molecular geometry for CAS# 375-73-5

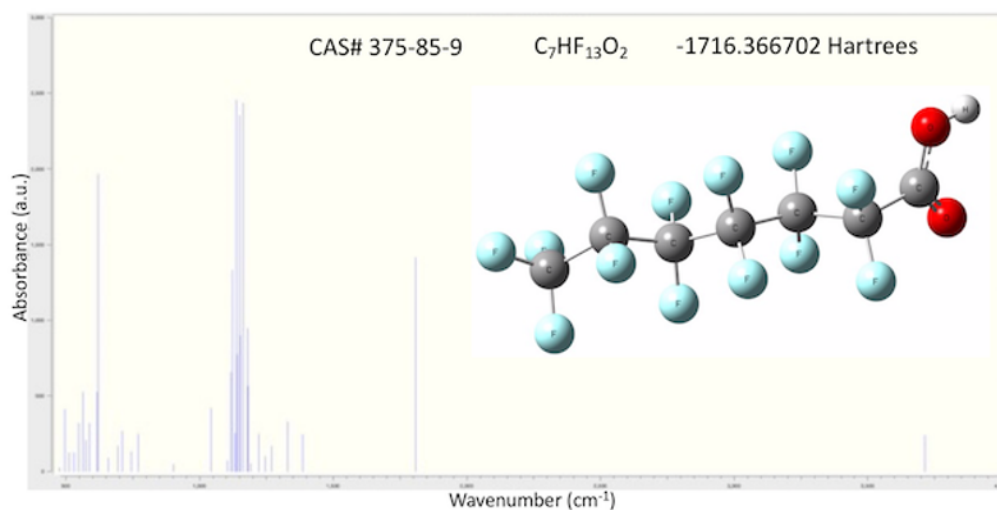


Figure 10. DFT-calculated IR spectra and molecular geometry for CAS# 375-85-9

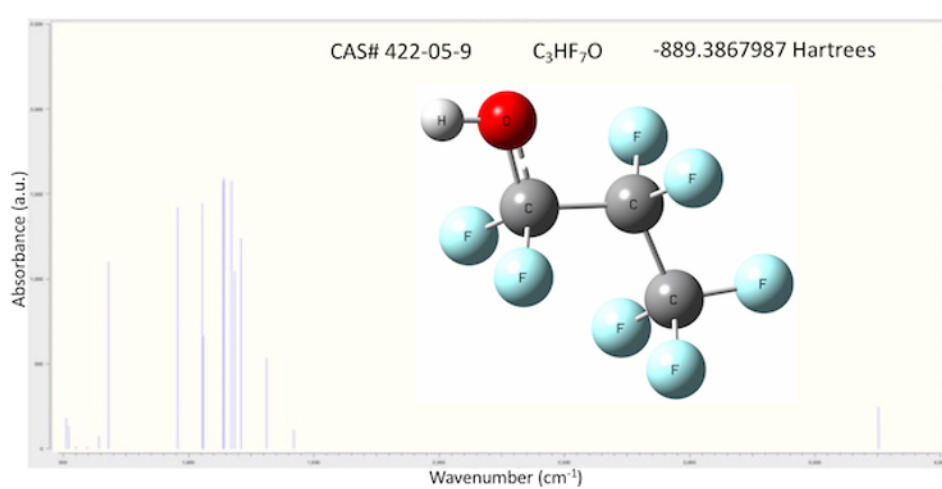


Figure 11. DFT-calculated IR spectra and molecular geometry for CAS# 422-05-9

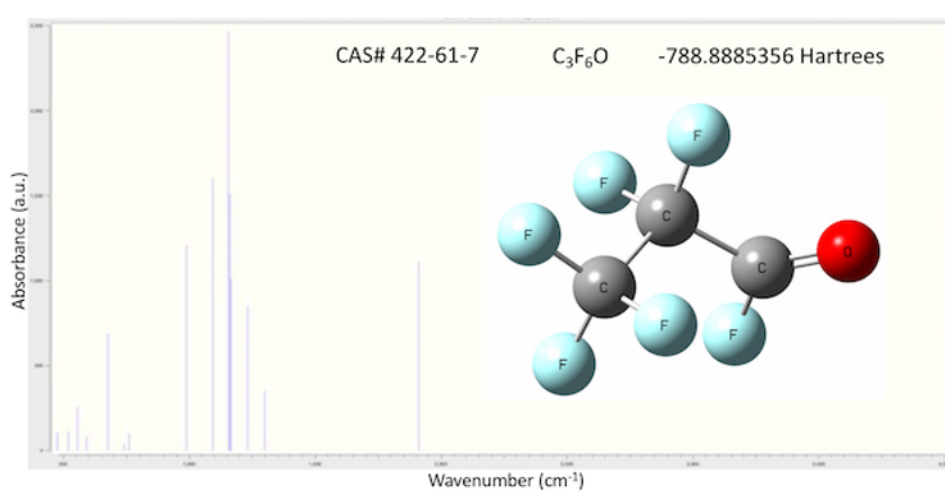


Figure 12. DFT-calculated IR spectra and molecular geometry for CAS# 422-61-7

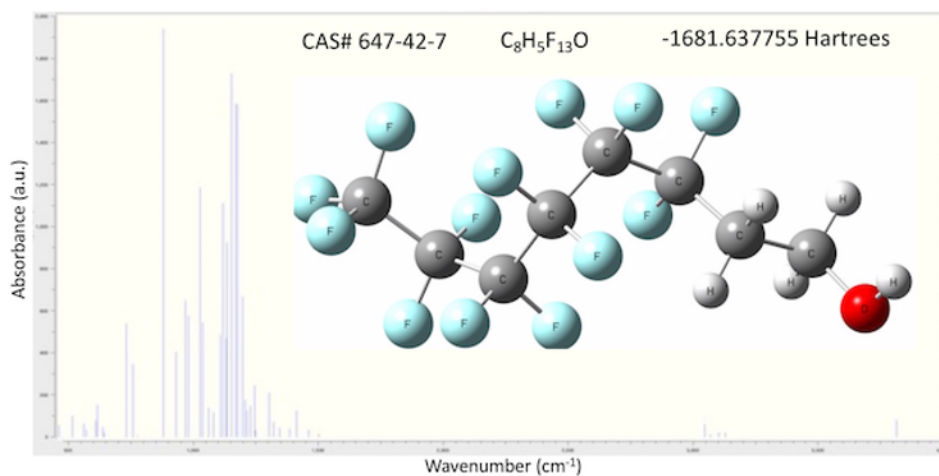


Figure 13. DFT-calculated IR spectra and molecular geometry for CAS# 647-42-7

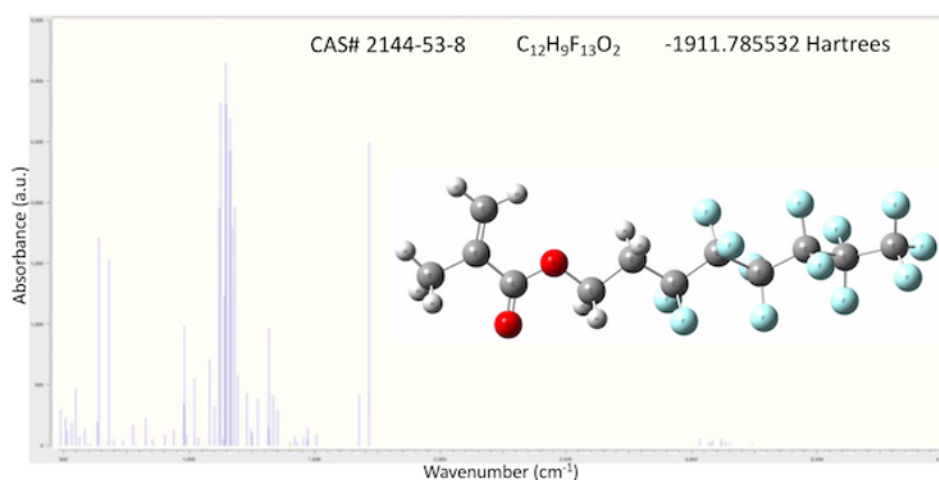


Figure 14. DFT-calculated IR spectra and molecular geometry for CAS# 2144-53-8

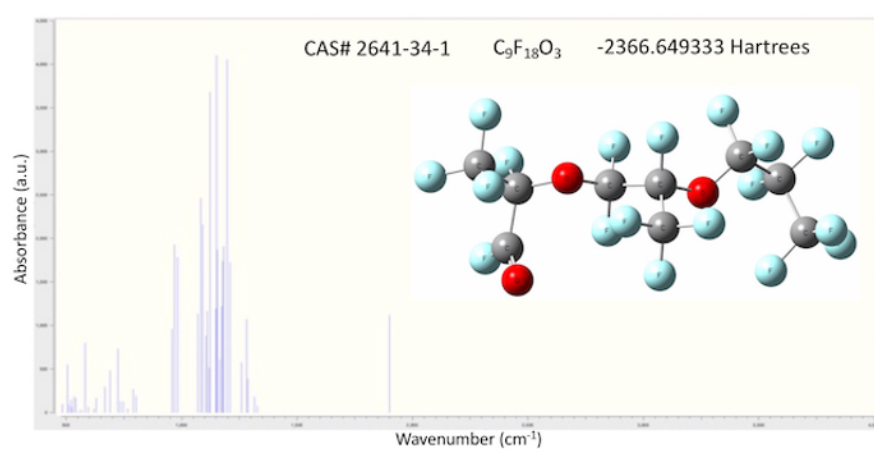


Figure 15. DFT-calculated IR spectra and molecular geometry for CAS# 2641-34-1

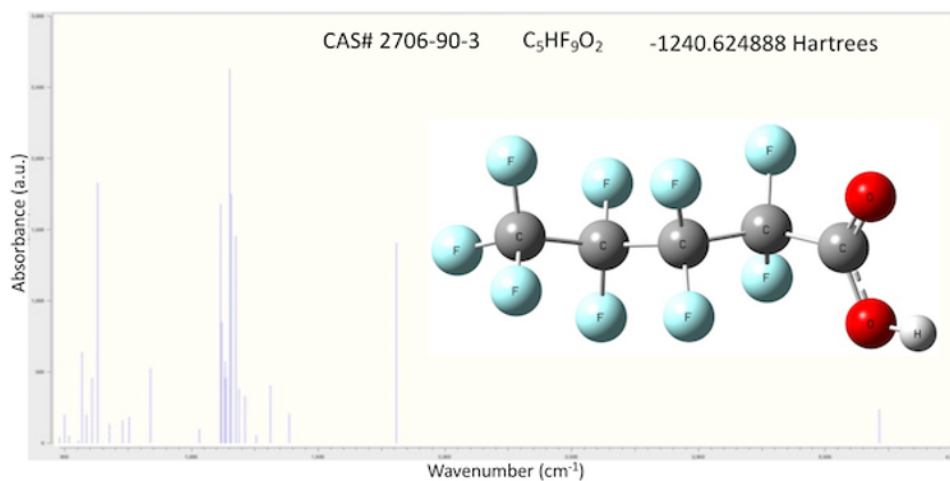


Figure 16. DFT-calculated IR spectra and molecular geometry for CAS# 2706-90-3

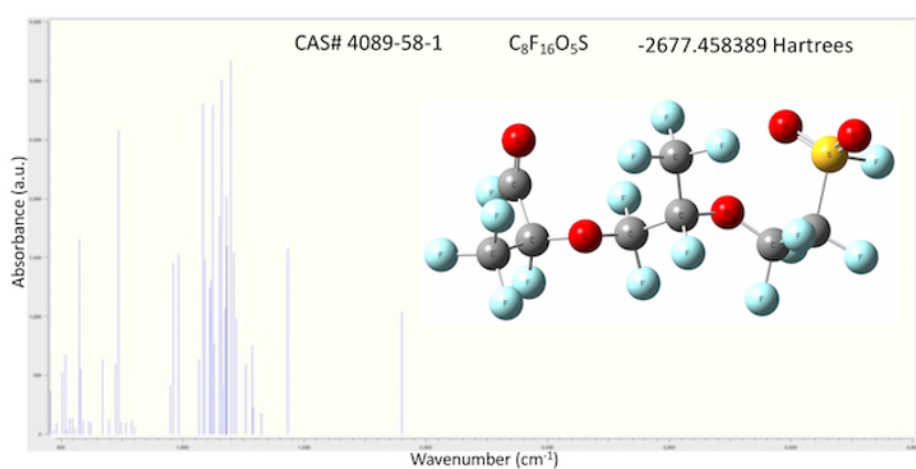


Figure 17. DFT-calculated IR spectra and molecular geometry for CAS# 4089-58-1

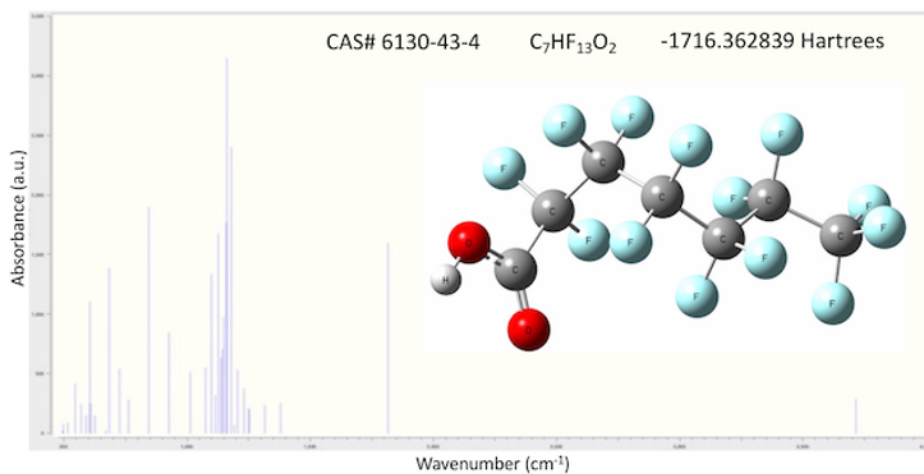


Figure 18. DFT-calculated IR spectra and molecular geometry for CAS# 6130-43-4

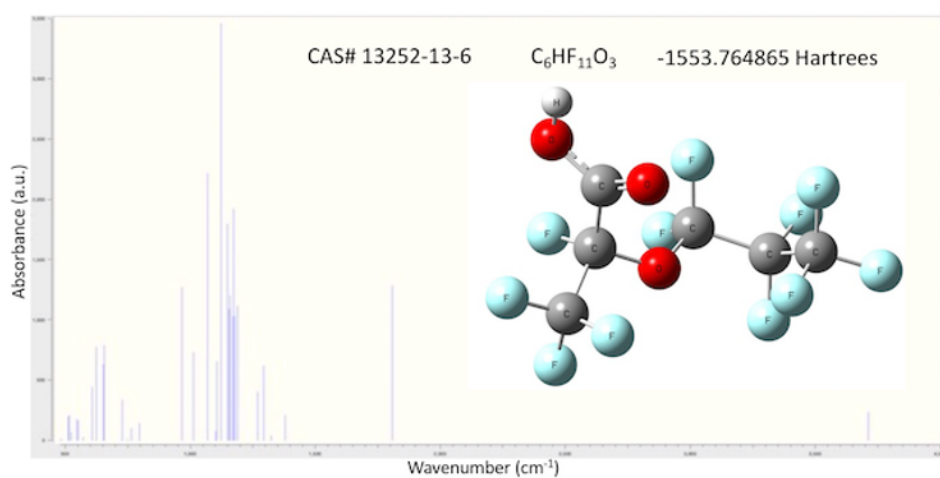


Figure 19. DFT-calculated IR spectra and molecular geometry for CAS# 13252-13-6

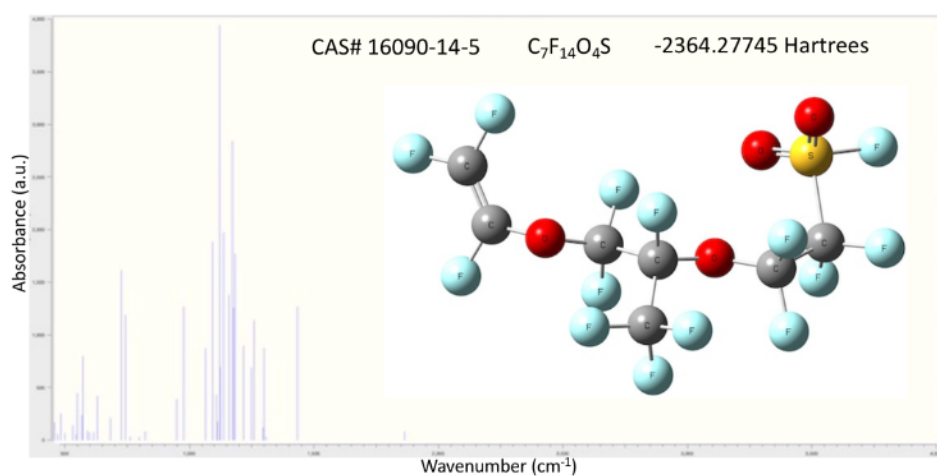


Figure 20. DFT-calculated IR spectra and molecular geometry for CAS# 16090-14-5

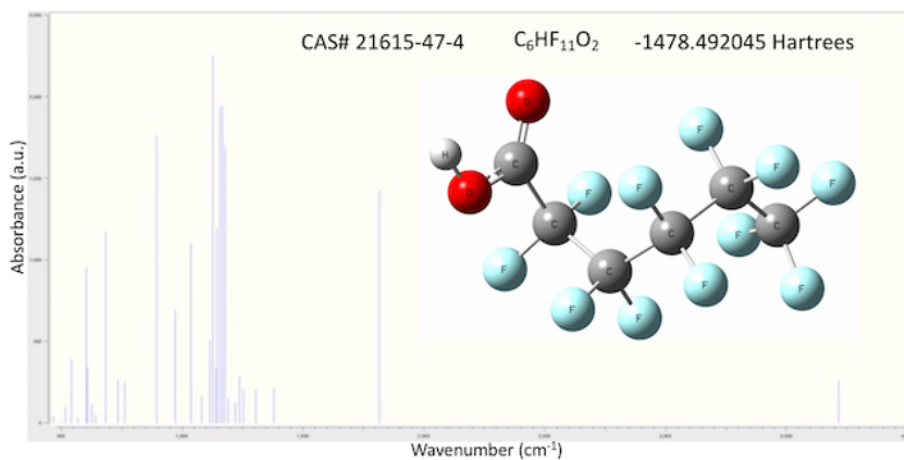


Figure 21. DFT-calculated IR spectra and molecular geometry for CAS# 21615-47-4

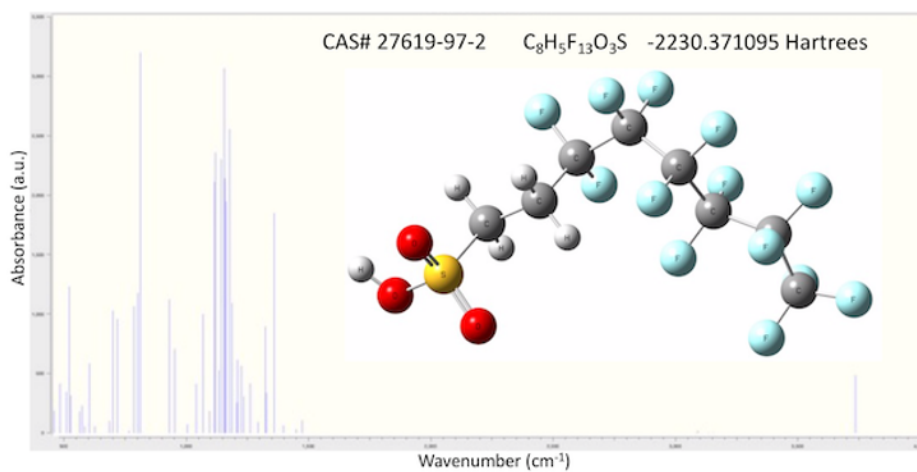


Figure 22. DFT-calculated IR spectra and molecular geometry for CAS# 27619-97-2

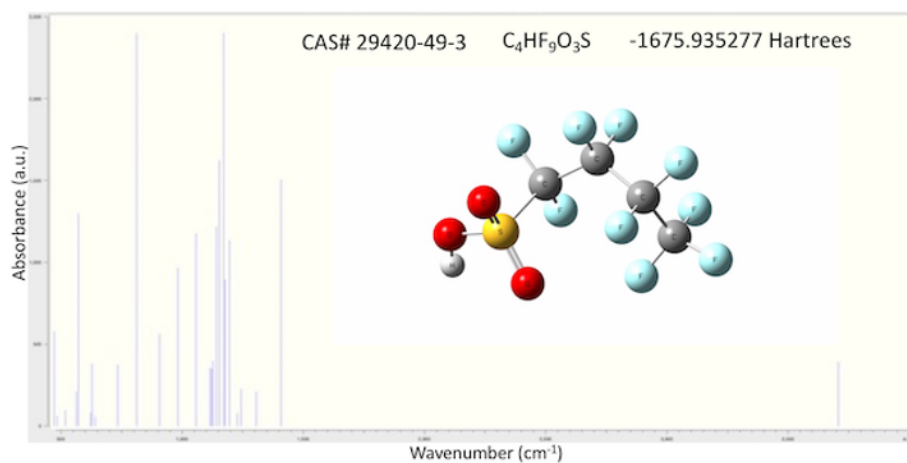


Figure 23. DFT-calculated IR spectra and molecular geometry for CAS# 29420-49-3

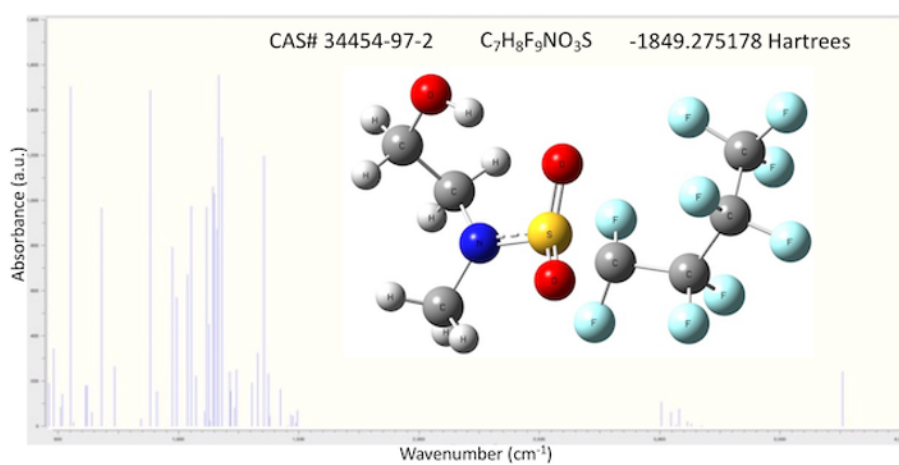


Figure 24. DFT-calculated IR spectra and molecular geometry for CAS# 34454-97-2

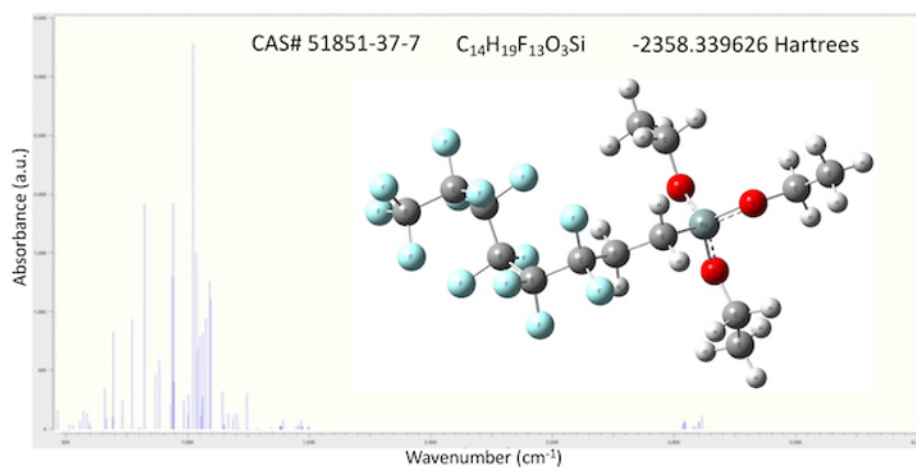


Figure 25. DFT-calculated IR spectra and molecular geometry for CAS# 51851-37-7

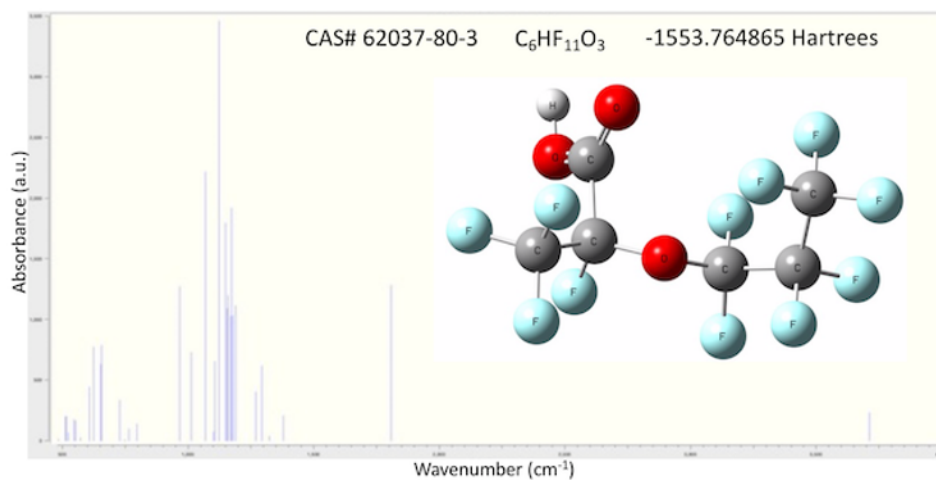


Figure 26. DFT-calculated IR spectra and molecular geometry for CAS# 62037-80-3

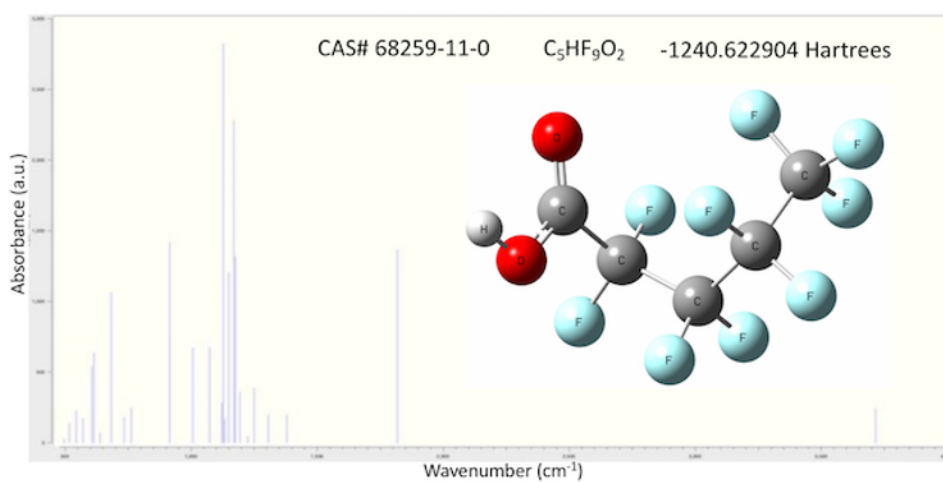


Figure 27. DFT-calculated IR spectra and molecular geometry for CAS# 68259-11-0

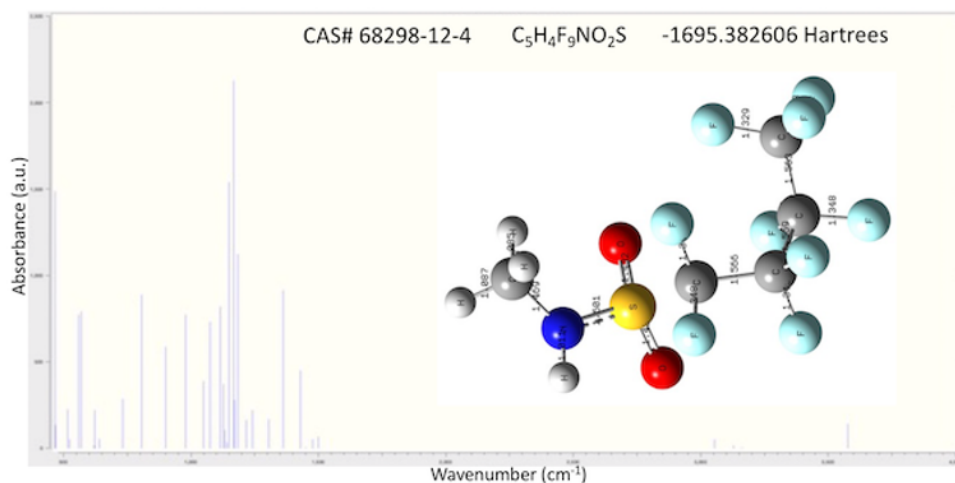


Figure 28. DFT-calculated IR spectra and molecular geometry for CAS# 68298-12-4

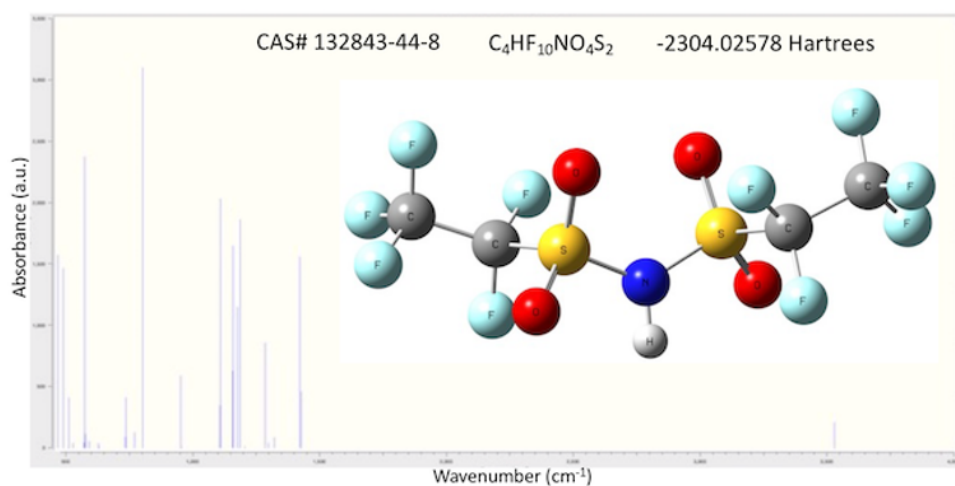


Figure 29. DFT-calculated IR spectra and molecular geometry for CAS# 132843-44-8

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Table 1

CAS# 307-24-4		CAS# 355-80-6		CAS# 335-42-2		CAS# 354-64-3	
Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)
24.3236	75.0690	28.9118	481.2920	37.5581	11.4186	60.2947	8.0126
35.3008	305.8092	54.7605	93.3814	51.3682	63.0156	127.7283	41.4499
43.6672	44.7386	63.3251	96.0604	81.1019	13.4780	212.1812	78.2551
47.7329	133.0721	91.9816	315.7763	120.2497	40.8993	252.0304	21.5797
60.0129	5.1319	110.4251	25.5206	162.6937	79.0015	260.5024	0.1914
89.0031	21.9768	172.3029	16.5385	213.6408	97.3929	294.4728	67.5876
138.4448	24.4012	203.5443	49.6479	242.2608	52.6165	356.2448	0.3528
168.5781	3.6397	223.1947	138.2523	260.7450	92.9215	423.8375	14.0501
192.4973	13.3818	240.8973	15.3699	286.5953	8.7640	528.1179	121.3292
201.8643	175.0764	255.4825	44.0082	309.3756	18.5301	579.8274	16.0174
222.3692	5.5454	275.6909	2151.5080	332.7680	4.6084	613.4251	109.9959
243.2640	1.4678	293.5935	91.9620	360.6069	29.6964	730.8821	533.2813
247.1698	0.6989	308.5964	170.3968	375.8362	14.2301	896.7564	1820.9099
261.7570	39.7009	329.1293	32.3548	432.6953	50.8817	1080.5028	1234.8019
286.5816	76.6345	341.8540	188.0719	503.2789	178.8725	1126.1283	1216.5992
310.5340	1.0278	371.1505	18.2707	533.9931	56.6009	1172.5507	1185.6497
319.0808	4.8386	393.2957	121.0891	579.3293	46.1929	1190.9071	1247.4007
346.2108	7.6087	451.6881	45.0345	598.0239	87.0568	1302.4695	758.0835
363.0984	9.8126	528.8332	210.6440	647.1808	165.4552		
372.2072	38.8868	538.2095	186.2509	704.8842	430.0037		
377.5577	7.5264	562.2912	84.4406	748.7903	56.0904		
387.8257	20.4528	601.9276	26.3431	771.0102	162.8662		
459.1465	12.2198	675.2747	32.4723	955.6567	1019.5912		
509.9444	200.2129	751.2290	1092.7845	1049.8932	910.5764		
525.0198	100.1415	794.3236	313.8281	1123.2139	712.7159		
533.0181	107.1824	854.5918	221.2148	1150.0202	387.7141		
565.6356	332.6332	927.9403	309.3779	1162.3116	964.2380		
580.9707	55.8276	1062.1165	471.8124	1167.7591	1875.8081		
598.6270	521.4959	1082.2122	520.7919	1193.0740	1376.7847		
608.2843	125.3745	1087.5367	555.1333	1225.7953	427.1412		
634.5563	1682.8809	1111.3208	752.5576	1269.2963	290.5304		
655.2121	232.6460	1116.5299	387.9645	1328.5241	178.3131		
703.5340	76.5649	1132.9402	1936.2469	1918.5405	802.6284		
734.4965	244.6938	1146.0783	76.7444				
764.8344	158.0488	1171.7557	656.3457				

Table 1 continued

CAS# 307-24-4		CAS# 355-80-6	
Frequency (cm^{-1})	Intensity ($\text{M}^{-1}\text{cm}^{-1}$)	Frequency (cm^{-1})	Intensity ($\text{M}^{-1}\text{cm}^{-1}$)
809.2935	273.5670	1202.8837	536.4646
975.5120	55.4284	1258.8305	188.1259
1101.2206	217.0743	1267.2055	21.2565
1129.9117	717.3179	1301.4207	143.4229
1133.8012	1091.1265	1375.1864	15.0666
1145.6364	508.9980	1402.1558	99.9973
1151.9578	1309.6463	1408.8619	59.6764
1156.9222	1723.4914	1424.1402	31.0633
1165.1968	1052.6146	1489.3827	10.6690
1171.3988	1544.6446	3070.9485	23.0638
1190.1738	1052.1089	3128.6375	9.0234
1192.7212	277.7531	3139.2015	10.9998
1216.5216	79.8151	3813.7679	101.0692
1244.8543	237.6687		
1275.1249	124.1235		
1334.4857	309.5889		
1396.7924	207.2196		
1819.0209	1172.4772		
3713.7382	198.3040		

Table 2

CAS# 375-72-4		CAS# 375-01-9		CAS# 375-22-4		CAS# 375-16-6	
Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)
31.6030	14.1888	31.5712	303.7488	19.6554	462.6227	13.5048	122.2685
47.2989	22.3428	72.1514	42.7242	46.8290	160.6357	44.0069	57.6106
51.6950	13.5514	96.2536	398.5145	62.2379	19.4797	63.3427	5.6368
100.1431	11.0946	121.5786	87.6181	119.2838	38.4312	112.7379	58.2709
107.8670	9.0353	204.8010	94.0211	177.5057	31.2197	165.2568	1.5522
137.7545	68.7023	208.2771	99.4490	208.4486	84.2133	198.7991	110.3691
162.6375	65.8614	218.8954	0.1203	230.3102	2.9274	222.9241	19.7712
186.0467	153.6197	271.4063	1036.5299	253.6470	35.2358	230.3936	4.8241
213.3648	145.0630	281.7661	1017.4159	285.7282	47.8150	283.1177	74.3495
223.0546	37.5484	303.1074	108.1099	328.8522	1.4655	311.8780	48.5618
244.4306	75.4839	316.4908	1.3021	344.2451	1.4521	330.0472	0.8522
262.1324	22.7631	328.2105	906.0808	367.2307	8.2106	357.0258	39.7525
283.8454	22.8714	347.7278	32.2258	371.9874	22.3596	367.3432	7.9018
302.1086	14.1956	386.7697	244.4234	448.0303	44.8127	423.7439	104.3114
315.7512	12.2960	475.2282	201.1336	506.0895	62.7699	498.1972	89.9333
325.2387	7.6773	478.1435	154.7230	537.6383	133.1456	511.4155	279.4795
331.5608	8.8918	487.7128	176.2912	558.8119	262.2309	536.6392	130.1225
360.4740	16.4025	561.5421	3.5202	584.7209	388.4553	558.2728	58.4161
379.7505	52.3963	604.6641	27.4630	605.9023	288.0467	595.0011	147.9802
434.9651	151.2800	667.0650	479.3233	657.2616	659.0174	622.5779	131.6753
468.8923	20.3846	730.0548	277.5909	672.8105	650.2326	710.7296	222.2350
477.3619	254.2855	855.9066	1028.9979	752.3187	56.5549	742.7179	478.4068
496.1620	122.5431	891.1248	362.7609	771.5464	227.7367	829.9028	1485.7910
532.8192	84.2887	1013.2464	266.5734	918.9749	556.2058	961.3761	632.4087
580.6937	341.7124	1034.1486	1047.8113	1110.8071	653.2948	1115.2326	1097.4132
584.4538	896.0567	1052.3662	1000.5297	1131.6792	622.3962	1152.2765	227.3529
637.1628	128.1684	1062.5896	214.6693	1141.8537	1448.4814	1157.8915	1286.2888
647.2717	286.1558	1072.2206	747.3316	1157.3694	950.8377	1164.3883	174.1877
655.9108	51.2707	1094.0355	1215.5106	1167.3452	1646.5410	1172.6660	1384.6427
745.9813	851.1010	1154.9615	571.7045	1184.1000	1000.9149	1194.2092	1462.1894
761.4515	1228.0195	1220.5273	47.5200	1193.4863	550.9593	1248.4442	219.6248
916.4172	575.1446	1240.9510	169.0485	1254.8138	132.0324	1322.2990	278.6869
990.2893	859.1735	1286.3620	180.9290	1312.1730	401.0856	1848.1218	1076.6326
1068.7274	857.3931	1376.5972	73.8220	1394.3471	114.9619		
1133.4943	227.8343	1415.1284	4.7634	1826.6351	1194.8372		
1148.0556	301.3131	1460.6011	23.9640	3714.8982	196.4290		

Table 2 continued

CAS# 375-72-4		CAS# 375-01-9	
Frequency (cm^{-1})	Intensity ($\text{M}^{-1}\text{cm}^{-1}$)	Frequency (cm^{-1})	Intensity ($\text{M}^{-1}\text{cm}^{-1}$)
1162.8405	1246.8893	3108.4409	7.4245
1177.5624	781.4804	3179.2081	0.6237
1189.8397	1872.3601	3799.4963	116.9960
1193.7350	1059.6748		
1216.7238	772.6345		
1250.4324	157.9638		
1262.9397	86.3845		
1318.4053	170.5394		
1447.2933	1074.5347		

Table 3

CAS# 375-85-9		CAS# 375-73-5		CAS# 422-05-9		CAS# 422-61-7	
Frequency	Intensity	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
(cm ⁻¹)	(M ⁻¹ cm ⁻¹)	(cm ⁻¹)	(M ⁻¹ cm ⁻¹)	(cm ⁻¹)	(M ⁻¹ cm ⁻¹)	(cm ⁻¹)	(M ⁻¹ cm ⁻¹)
27.7260	236.3624	31.2549	101.0787	24.4583	10.6022	33.8510	55.0603
32.6446	26.6778	47.1844	27.6560	81.0378	23.2262	58.8371	32.1120
41.6318	154.4519	52.4195	201.3668	153.8234	0.5939	134.8057	80.1486
46.8274	62.8474	58.7850	35.4523	212.9775	1407.6324	207.6613	112.2657
54.5012	51.6634	94.7423	80.9903	213.2916	86.1560	237.6722	37.8324
63.1576	38.1521	156.7664	3.5347	241.4267	1810.0029	279.9891	44.6588
79.5330	18.3185	167.1247	12.9618	274.5190	73.1034	348.2536	0.2520
128.9093	25.2159	182.2991	134.5985	315.9436	13.8353	366.1533	24.3502
140.9233	1.7438	211.5482	67.4762	332.2800	3.7603	372.0176	12.2539
181.8150	9.0138	239.4488	4.1885	349.4593	73.5493	491.4394	73.9376
199.9123	180.4318	239.6535	10.8086	376.0214	10.7167	534.9569	78.4819
202.3138	34.8551	252.6529	53.2456	462.7936	178.2108	571.5304	183.7852
220.0894	10.7634	283.3193	191.4794	528.0513	143.4729	608.5475	56.6699
234.9991	2.4802	287.9214	5.2666	536.8747	108.3014	691.1549	493.1608
249.2247	5.8186	299.3218	26.9508	564.8143	10.3497	755.7554	25.2073
251.8125	5.0966	328.4517	22.2297	610.3703	7.4217	775.2153	71.8582
263.7501	30.5130	353.1229	159.8356	658.1590	59.6453	1001.7555	868.8810
286.7253	80.9594	361.7637	122.1101	695.1034	879.3103	1106.5972	1153.1252
305.8140	3.3500	376.3864	19.7961	764.4902	0.8511	1167.7723	1771.6430
313.7455	0.7667	405.7988	995.3183	971.3125	1137.4039	1173.9157	1085.4900
339.3513	4.0817	458.3848	298.4837	1068.9079	1156.7749	1178.8520	728.1118
356.4313	16.0782	464.0852	802.2460	1073.2067	528.9814	1243.3156	609.6164
368.0324	23.4248	506.9837	338.2504	1151.9106	1260.1538	1311.3807	250.0684
368.3292	7.0532	524.8667	350.9494	1153.4565	1274.8236	1918.9889	798.2708
374.3643	33.8396	546.8891	174.7411	1184.0735	1260.3453		
379.3152	1.4493	570.8035	363.4020	1196.2878	834.2778		
431.1766	14.4957	581.9593	734.6907	1222.2347	991.3551		
492.0059	20.9068	606.0633	209.7552	1323.7525	426.6913		
511.7507	343.4065	646.4663	110.3050	1431.0181	88.5964		
528.8076	102.7021	698.3328	244.5998	3755.3822	195.3641		
545.6582	103.8595	730.3057	360.3234				
564.2451	267.0943	789.6928	430.5290				
579.8262	437.3140	846.3813	1267.4663				
590.3395	172.5584	1016.2211	176.2934				

Table 3 continued

CAS# 375-85-9		CAS# 375-73-5	
Frequency	Intensity	Frequency	Intensity
(cm ⁻¹)	(M ⁻¹ cm ⁻¹)	(cm ⁻¹)	(M ⁻¹ cm ⁻¹)
603.0185	265.3563	1109.3518	204.8728
631.1340	437.2406	1129.0822	1640.7476
635.9319	1637.4334	1137.2828	137.7350
672.5623	74.6094	1154.2976	365.0778
708.8488	137.8769	1158.9340	532.0524
724.5944	222.4236	1168.3331	1285.0928
760.1011	110.3541	1175.4113	1843.1433
785.8845	206.0847	1193.2698	842.3050
917.4452	38.6906	1209.2411	942.7109
1055.5454	348.1817	1230.5198	239.2044
1117.7418	59.7245	1258.8913	182.2881
1130.0771	545.0564	1331.2633	239.4061
1135.4259	1107.9274	1412.2521	1222.6775
1146.2392	210.8406	3712.2350	304.4698
1150.0526	2044.8386		
1154.8130	643.2233		
1161.2906	1959.0185		
1166.8060	747.6587		
1175.0638	2028.1162		
1192.7686	789.3723		
1194.6607	468.4355		
1202.9521	45.4889		
1233.6220	207.1119		
1258.7642	82.1840		
1282.4817	139.8994		
1340.8737	275.5026		
1396.4699	203.5025		
1818.5292	1177.4514		
3714.6165	197.814636		

Table 4

CAS# 2144-53-8		CAS# 2641-34-1		CAS# 647-42-7		CAS# 2706-90-3	
Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)
14.8122	1.6699	16.5601	2.0959	29.0381	42.5206	28.0962	190.6082
17.8206	385.6735	17.8231	7.1403	34.7978	55.4768	41.7883	33.4898
24.5382	34.4180	23.1021	7.9263	45.8221	19.7719	47.6304	276.3407
34.7669	32.2783	32.9278	49.1893	64.9612	221.7280	59.9450	5.5903
41.1476	4.7895	34.0562	4.3928	76.8284	179.4098	101.2924	15.9155
49.4671	100.6077	41.4185	2.6680	90.8382	240.0361	167.3934	25.5222
53.4640	10.6704	47.7793	12.4159	98.7822	125.8381	176.8416	2.2559
57.8639	58.6442	52.1717	1.3535	117.8997	31.0896	204.0563	135.7096
65.7070	63.3925	66.6339	2.1913	121.2400	18.9664	233.0170	3.5970
89.0251	19.0227	72.6805	18.1026	143.3708	38.6472	238.5534	2.4366
103.4312	6.0170	88.4982	0.8204	157.0760	22.8632	260.9832	29.7741
119.1574	10.3520	92.8498	11.6180	184.7963	8.5834	285.8045	82.8562
134.0938	15.8155	125.8650	90.7452	214.1788	223.0130	317.0431	5.1792
145.4596	247.6390	148.5550	17.5952	232.0741	196.9033	327.8486	0.5427
171.4777	34.2179	150.8307	45.1334	253.7484	8.6077	354.4006	4.5128
181.8318	33.0658	175.8707	31.9817	263.4223	2.1096	372.4220	26.9729
190.6378	10.7207	188.7620	7.5218	274.2453	274.0505	376.0455	14.4503
202.1948	184.3634	209.8889	14.2839	279.7710	1076.2351	413.4222	34.6627
208.7787	12.8828	216.0827	99.7226	282.2585	1030.5381	496.0624	34.4292
225.6916	18.7634	222.2086	18.5548	300.4857	61.8472	516.7245	164.9665
238.3148	1.8799	230.2328	62.9705	309.3220	22.6256	533.3106	40.9023
254.2098	2.6318	241.7218	22.7921	317.4197	26.5554	570.1734	13.5675
255.7506	1.5427	252.1225	43.9253	325.7918	2.2923	582.7878	530.5483
287.3161	79.5655	266.1255	36.4033	334.8965	9.0522	601.7972	164.3960
296.6343	81.8122	274.1353	43.7642	356.6157	5.2354	623.6967	379.7892
308.7335	1.1875	293.0809	32.8497	358.7713	63.9422	646.2236	1521.3223
313.5293	10.3435	301.6677	59.6569	372.4104	66.9619	691.6139	110.9741
342.2679	0.8217	309.5435	35.5464	379.4048	143.1128	744.0864	132.0471
353.9976	9.7155	324.6949	9.9288	423.6701	42.8413	768.9312	153.1033
360.6221	0.3297	328.7092	5.3061	461.2486	65.6149	852.8775	437.2287
366.9492	84.8913	335.0956	5.3943	478.2476	49.5188	1044.3729	82.4605
374.2643	251.0075	346.6500	0.6007	492.5749	0.8342	1127.2481	1400.5475
384.7370	171.4986	355.7434	22.2614	532.8419	89.8210	1132.5605	705.6756
390.5051	4.6851	370.8146	4.3152	578.2158	55.5168	1146.1923	477.2033

Table 4 continued

CAS# 2144-53-8		CAS# 2641-34-1		CAS# 647-42-7		CAS# 2706-90-3	
Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)
393.0030	204.4637	376.6723	11.0847	586.9921	30.2811	1147.7587	380.2653
403.9852	12.8436	447.0391	106.6316	625.2182	68.1579	1163.5748	2189.4219
465.0899	4.8061	460.8243	59.1530	632.2832	136.7466	1170.9796	1460.0713
503.3810	151.4340	499.0915	63.1424	653.2162	40.7242	1187.1163	1212.8459
523.1200	114.6845	521.9903	364.1875	658.6757	19.3766	1200.5865	317.7880
530.2390	63.3118	528.4255	58.9653	746.8236	482.0443	1223.9849	271.4066
546.9689	95.4884	537.3760	95.1477	772.8858	310.2522	1267.5807	45.5017
564.0615	240.3817	539.7324	43.9776	790.2521	2.2096	1324.5670	336.3008
576.9190	37.0997	549.7345	121.4270	893.9635	1744.5763	1397.4672	172.6047
598.7118	69.3323	557.3631	108.6420	944.7498	360.9507	1819.1882	1171.2791
610.1752	4.0026	572.8871	15.1453	981.7714	583.2805	3714.3359	196.2580
622.2855	9.2432	583.7878	16.9638	994.2571	516.5323		
650.1160	99.2716	596.9208	530.5019	1040.4424	1066.8910		
656.1042	878.4693	611.0616	42.7162	1050.1874	489.3236		
696.0575	785.6830	635.0132	26.7403	1074.9290	124.4663		
714.6020	22.9973	645.6322	108.7508	1093.7155	104.9959		
750.3140	24.2002	683.2447	194.3396	1121.3297	436.1310		
790.2502	86.4900	705.6942	319.4665	1131.5143	999.5121		
800.4740	6.5676	738.8913	484.8684	1143.8860	420.2422		
841.2628	119.2068	749.4498	84.5756	1148.3194	832.2150		
869.7940	28.1957	761.4349	80.0363	1166.7869	1555.2410		
916.5627	44.6403	781.5346	29.0450	1182.1285	1425.5490		
953.0689	68.0179	805.5007	178.6654	1190.9321	1423.7846		
992.5043	174.4800	817.5791	124.5089	1209.1329	600.4653		
994.6616	505.1549	972.7685	637.2412	1219.0134	157.3540		
1002.7808	47.7261	981.6816	1283.0130	1227.9638	111.9472		
1034.3539	282.5548	996.9105	1187.1236	1241.5517	131.1260		
1050.0238	33.5922	1083.5348	750.6468	1257.0214	219.8292		
1075.7422	1.0940	1097.1283	1641.9359	1261.3014	28.5359		
1095.1148	363.7505	1103.5048	1438.4573	1316.3138	187.2451		
1113.8452	164.2094	1117.8994	585.6945	1333.8875	64.1214		
1131.5673	1004.8227	1124.0270	776.2794	1356.6241	37.2572		
1138.8992	1451.3182	1132.3377	339.8605	1398.1861	33.1156		

Table 4 continued

CAS# 2144-53-8		CAS# 2641-34-1		CAS# 647-42-7	
Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)
1148.1947	26.6084	1136.0042	2454.7995	1425.8310	110.7097
1152.8443	632.1125	1162.3503	795.3298	1473.1163	29.5910
1158.3123	1620.2451	1163.7095	2734.8208	1512.4733	10.6786
1160.6088	1443.7560	1167.1308	1241.9058	3050.4738	53.0714
1173.5432	1384.5582	1178.7597	407.3829	3072.4602	7.5735
1175.6565	1247.4300	1186.0030	810.0713	3106.8627	18.7875
1184.1766	928.6474	1189.7436	1156.8258	3132.0045	16.5646
1193.4780	1010.4723	1190.8705	940.9841	3815.4518	71.4083
1206.6257	296.4314	1194.3051	1271.1299		
1241.3476	222.0984	1209.7841	2701.6912		
1257.8760	70.4874	1222.4761	1148.5023		
1263.1049	53.6648	1272.5875	382.2962		
1286.3359	199.6603	1294.4992	713.1518		
1327.8169	76.6878	1299.2071	260.6206		
1329.4569	496.5015	1328.5722	116.1727		
1345.7442	213.3316	1339.3517	51.0428		
1362.7240	148.4883	1910.0801	745.8081		
1412.6333	10.5042				
1431.1167	38.0651				
1440.5926	14.0139				
1466.4816	32.3236				
1480.2783	27.5448				
1483.8835	75.9163				
1516.5085	46.0716				
1686.0085	214.1406				
1726.7567	1282.3302				
3036.2451	28.6726				
3071.8765	14.9514				
3081.4775	11.4718				
3085.6156	23.1922				
3117.7965	6.6273				
3122.1412	26.6267				
3137.5714	15.8147				
3154.3237	11.6919				
3246.9772	3.7201				

Table 5

CAS# 4089-58-1		CAS# 16090-14-5		CAS# 6130-43-4		CAS# 13252-13-6	
Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)
11.6865	37.6188	10.1224	110.2736	28.1335	49.9003	22.1104	153.5105
16.5354	24.1988	17.9039	36.2533	36.8432	180.5251	31.5317	346.4123
22.8549	1.8852	22.2240	20.0332	40.8214	169.5485	37.5995	104.4048
27.6230	54.0575	31.2451	9.2824	56.5330	144.8188	50.4234	100.3691
30.9424	57.6445	39.5376	5.9835	67.7383	10.1121	64.5682	23.9235
37.7703	5.4818	52.9187	7.6669	92.3997	5.9798	76.4541	27.6503
46.7349	5.2839	62.9571	4.4610	109.0846	9.9146	90.1844	11.7358
50.2125	8.6839	75.5575	4.3454	119.2895	36.9077	135.9514	29.7375
56.7035	2.5187	84.9498	6.6733	139.2283	26.6909	150.4054	37.3940
67.4802	19.3498	110.5849	6.3240	168.8649	12.9629	184.9566	21.2652
80.8119	5.6821	122.1931	7.6887	187.6462	53.5204	201.9105	8.3321
89.2847	10.4287	136.0847	6.7807	218.7206	154.1601	221.3162	45.2537
124.7799	111.3439	165.1506	72.2389	235.6976	42.1980	231.9116	33.2399
138.7794	52.7984	179.2817	59.9272	243.7048	134.8053	259.9433	28.3063
149.2818	37.8598	190.9426	93.8041	255.3692	23.7737	275.7348	74.6995
172.0859	46.1936	194.7733	52.2380	272.5863	7.0586	298.1831	62.9563
186.2013	26.4858	211.9582	6.9847	282.3305	16.8955	307.7784	34.6977
190.4289	41.9494	224.5108	134.0942	288.9722	20.4804	327.5864	15.6721
208.2376	9.4602	229.7235	110.9901	299.2631	60.3789	335.1385	2.6533
211.5377	25.0335	241.0475	21.6510	312.2318	8.8353	352.2636	12.1903
224.7220	147.3571	259.9783	117.1600	322.3683	6.1827	365.5019	0.8699
229.7389	18.3096	267.1147	48.4138	335.6802	1.6365	384.0005	3.9333
239.5160	40.8357	293.7226	4.0679	347.1892	6.7852	451.4510	77.6943
251.7305	47.4739	307.1878	10.0622	368.7885	13.8703	499.7541	9.9169
269.2322	14.1790	311.8705	31.6777	376.8831	4.0817	528.0072	171.1141
274.2701	44.1122	319.4049	9.7310	384.7797	29.6888	532.0353	172.9027
296.0429	80.0904	332.8588	21.1132	427.0018	74.8696	539.2605	58.3983
297.4108	3.0865	345.3803	30.5864	465.2328	19.8101	562.1542	150.0886
309.4217	42.7057	376.1819	0.7222	510.7994	11.2723	568.4007	141.9484
315.2557	26.4947	420.7712	130.0132	514.1290	52.2402	586.8690	21.9187
328.2538	5.6768	428.7396	65.7376	532.1515	65.7448	623.7637	380.8357
334.2279	2.7250	464.7663	176.5239	561.3328	295.6324	639.1820	663.0987
345.4709	35.9792	474.4789	145.0759	586.0229	173.5150	668.1936	537.7785
356.5878	41.3207	488.5901	50.7634	604.9278	107.0005	670.9160	674.6160

Table 5 continued

CAS# 4089-58-1		CAS# 16090-14-5		CAS# 6130-43-4		CAS# 13252-13-6	
Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)
370.5306	3.9299	499.0399	219.8981	622.1023	789.3309	744.0886	286.3360
414.3487	152.6278	515.1836	56.8639	624.4756	176.3165	764.1028	6.1337
453.9172	89.5599	548.2141	118.4716	642.1129	103.9490	778.9023	86.0404
472.2500	263.4362	559.1876	47.5292	686.1228	17.1444	810.7184	119.0946
484.0890	23.5669	565.4217	389.7902	698.7756	990.6057	980.7611	1086.9103
498.5704	68.3511	583.6810	208.8573	741.9064	388.4658	1025.4626	623.5689
521.2613	373.8801	588.1536	694.9106	777.4408	201.3252	1082.3998	1899.6321
534.2205	482.4857	604.9864	80.1399	859.7168	1355.1501	1113.7769	64.1845
538.4181	27.5877	612.7729	61.4204	939.9815	602.7602	1120.1329	559.9548
549.1771	94.6831	632.2217	63.0255	1026.4441	365.7262	1137.0732	2964.1788
560.9740	97.2477	645.5512	365.4851	1088.9994	391.8096	1162.9918	1540.1258
570.9141	31.1478	698.2432	181.1293	1113.1195	952.7121	1167.3977	932.1888
589.7052	1182.4857	740.9467	1412.0656	1127.7235	226.6289	1172.6464	1029.7362
595.3976	392.5076	756.5085	1037.4906	1140.3668	1195.9823	1181.5714	880.9111
605.9745	81.5280	777.0082	26.6799	1149.8898	453.3007	1186.2509	1646.9421
630.5307	74.0043	813.9436	22.3084	1156.1287	503.5515	1191.1245	883.2892
638.3489	61.7931	836.3488	70.8772	1161.9416	698.4478	1202.1318	955.4757
686.2008	448.1119	963.4941	338.2591	1171.8022	1261.9144	1281.4436	343.1799
710.7214	90.0565	990.1600	1106.7737	1174.3744	2246.9762	1305.8698	530.1072
740.2196	429.6357	1078.8774	761.3375	1191.1753	1716.7039	1336.2422	31.8622
751.1450	1840.2857	1105.6579	1650.9023	1203.6747	46.1430	1392.3584	178.2767
760.4619	73.4747	1122.9101	377.9004	1217.2403	378.9392	1818.8088	1100.2285
781.0456	67.2161	1126.8238	151.6116	1243.3346	265.7305	3713.6798	200.0196
804.9560	79.9831	1134.7787	3445.9984	1262.0042	147.3619		
817.8877	43.5816	1138.7987	607.8450	1265.8279	145.9811		
963.4154	293.3995	1150.7907	1723.2156	1328.0008	167.4864		
973.8123	1038.0623	1171.1442	1207.8296	1391.6023	176.6048		
996.8695	1088.6030	1186.0909	2487.8915	1827.0823	1137.7349		
1081.2212	452.8980	1189.6706	1099.8454	3717.3773	202.8860		
1096.7149	2006.8652	1196.4865	1545.5457				
1105.1336	1059.7208	1230.3651	780.1341				
1123.5382	887.7224	1261.6819	601.4790				
1127.4509	937.6172	1271.9313	993.8210				
1136.5970	1994.2515	1306.6558	104.1064				
1141.2964	547.1088	1312.1708	764.8476				

Table 5 continued

CAS# 4089-58-1		CAS# 16090-14-5	
Frequency (cm^{-1})	Intensity ($\text{M}^{-1}\text{cm}^{-1}$)	Frequency (cm^{-1})	Intensity ($\text{M}^{-1}\text{cm}^{-1}$)
1164.4822	1320.4563	1318.9909	25.7619
1172.6926	2147.1632	1444.2976	1107.7915
1180.2577	295.2993	1873.8811	68.5628
1188.2603	762.9800		
1190.9855	1445.0078		
1193.9903	1141.7708		
1210.2546	2265.5330		
1222.2081	1098.6624		
1231.1212	699.2184		
1271.5322	428.1062		
1296.7271	534.4558		
1301.6580	161.5018		
1336.4384	125.8809		
1443.4487	1122.3504		
1909.7429	743.0666		

Table 6

CAS# 27619-97-2		CAS# 34454-97-2		CAS# 21615-47-4		CAS# 29420-49-3	
Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)
18.5300	52.7470	15.3785	636.6278	32.4243	272.8105	21.5750	201.3652
29.9587	49.7365	31.5303	26.7476	42.5326	247.5939	50.7460	296.6773
36.3151	799.2944	36.4260	303.7335	48.5695	16.9943	53.4625	11.3423
49.7254	181.8942	52.3779	235.2224	64.4534	53.4966	102.0653	48.8897
55.7909	13.0928	60.3959	2.2657	101.0138	11.0819	108.4454	15.6051
62.1285	166.8293	90.2695	25.1952	111.0664	3.9080	137.3602	68.8733
69.2920	158.2874	100.6353	79.4745	133.8104	27.1574	165.2715	96.9014
77.8903	137.5412	108.6041	71.7073	154.9541	37.4291	188.1944	97.7113
106.6447	63.5417	117.7098	1002.8280	179.5949	23.8460	214.7318	239.9972
111.1234	38.8911	144.2079	26.7541	215.1175	161.5194	224.7245	44.8496
137.1996	116.4489	159.6409	34.6734	238.0377	134.5622	245.1093	64.6369
169.0525	20.9532	171.8478	17.1162	254.8411	23.4300	265.7886	34.2205
173.8949	62.6232	199.1647	166.0000	266.9508	12.5174	284.9461	73.0702
181.8507	135.5425	201.9548	130.5556	275.8863	5.4313	302.6079	111.1201
197.6627	84.3219	217.9193	73.3497	296.0286	36.5426	315.3279	107.1501
211.7534	140.5508	240.9484	126.0721	300.9069	20.5219	319.8323	512.6793
239.6835	35.6241	264.8406	25.4556	317.9654	6.4189	330.9760	36.6183
248.0128	1.6102	266.0167	34.3801	326.4571	1.6656	353.3185	521.4004
260.2690	135.4687	282.0443	43.0320	351.1185	1.8452	364.5296	129.6881
267.5346	1644.3884	291.2538	1429.6417	365.7400	9.7439	392.1355	191.2489
285.0948	18.5312	304.8847	18.7808	374.1339	6.3903	445.6505	623.5207
288.8892	67.3735	311.8698	570.3446	394.2107	48.7570	470.0747	63.8160
300.9384	33.8638	316.8841	81.9838	450.0937	78.1715	487.4907	460.5972
314.6190	5.3383	326.6418	80.0831	483.7699	32.8655	499.7943	46.4421
324.2879	41.7063	339.3406	27.4040	511.6988	2.3888	533.4015	74.4820
335.6119	134.0074	360.9351	5.0578	533.5473	77.0951	580.3272	165.5656
336.7281	296.7618	382.1919	47.4573	558.5241	310.4217	587.3050	1037.9518
361.4528	22.1371	387.9873	28.4922	583.5708	24.9172	636.7162	63.6126
364.2451	100.3272	448.0710	13.4274	620.2427	762.3212	644.4905	303.4822
376.1146	98.5951	469.8641	155.7317	623.4872	269.7182	655.7092	45.7183
380.0209	5.7833	477.2460	169.2020	642.0396	89.0072	748.5392	298.5347
412.9521	73.3951	497.5737	305.0006	657.6432	37.8719	826.8958	1916.2969
452.6511	404.4630	525.1482	76.3477	698.5033	939.6029	921.5477	448.2002
461.7445	21.9219	533.9642	126.3065	748.4715	212.9934	996.7467	772.7898
476.7723	96.7217	566.8618	1337.4665	777.6565	199.5287	1070.6294	940.2236

Table 6 continued

CAS# 27619-97-2		CAS# 34454-97-2		CAS# 21615-47-4		CAS# 29420-49-3	
Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)
499.3449	212.2875	580.7063	14.2976	909.6233	1410.7167	1127.3874	282.9889
526.6835	177.2266	629.8281	158.4597	983.5905	556.1674	1134.8582	278.8635
537.0419	632.5458	636.4744	161.4596	1050.1949	877.1057	1140.4934	316.5298
543.5381	162.4015	655.2485	55.3007	1093.6672	132.3209	1153.8441	973.9566
579.3909	92.0998	695.7258	858.2993	1128.6147	407.2515	1166.8828	1298.2082
589.3740	117.3919	748.7544	234.6413	1140.8086	1801.9655	1184.7341	1919.3069
600.3076	27.9494	858.5498	28.1570	1152.3606	262.2544	1190.0237	714.5442
620.1317	300.8686	897.7960	1321.7486	1157.6515	951.8177	1206.9862	908.8080
642.4000	26.9259	924.4992	135.8235	1169.1286	1548.3984	1240.7288	62.3051
701.5192	50.7780	989.5003	703.4940	1181.0010	1556.7082	1256.5568	179.7869
715.1965	527.9412	1006.9093	506.1801	1189.5970	1354.3740	1318.3938	165.7874
734.1032	490.7649	1049.9707	594.8665	1203.8770	120.6210	1419.6565	1203.2115
781.6733	7.4508	1065.3993	865.4538	1232.7486	97.4113	3708.1954	313.2092
801.9940	547.4196	1085.4470	195.9333	1249.5589	225.3432		
817.7575	605.2857	1122.3462	59.3906	1265.5506	162.0980		
827.5042	1644.3075	1129.8395	862.9985	1316.8137	166.2442		
945.5039	576.6573	1140.0496	400.3431	1391.4120	169.0310		
966.8779	362.3515	1145.0569	21.3410	1827.0708	1137.1248		
1017.6529	37.2113	1156.8208	941.0832	3717.5933	205.0613		
1054.5034	210.3024	1162.9868	914.6482				
1082.3097	513.3973	1172.0431	776.2095				
1108.8621	92.8120	1180.8676	1382.1430				
1127.1930	1085.5362	1194.5531	1136.6492				
1131.5918	57.9828	1226.3130	212.8841				
1132.1607	1212.0391	1229.7637	138.6164				
1146.1662	270.1864	1246.4360	72.5736				
1156.5371	1182.7768	1253.0337	220.5046				
1168.9362	1576.7884	1317.8614	170.0240				
1170.3292	1100.4432	1341.3697	287.9069				
1175.9765	999.7701	1368.3881	1062.9134				
1190.7757	1313.5506	1385.1898	206.5127				
1200.6552	560.6889	1391.2357	39.3992				
1220.6226	129.1536	1436.1066	144.8285				
1222.1979	314.4762	1462.6355	2.7254				

Table 6 continued

CAS# 27619-97-2		CAS# 34454-97-2	
Frequency (cm^{-1})	Intensity ($\text{M}^{-1}\text{cm}^{-1}$)	Frequency (cm^{-1})	Intensity ($\text{M}^{-1}\text{cm}^{-1}$)
1238.6193	290.0742	1479.0293	43.1105
1248.5164	157.1425	1488.0604	39.1398
1273.9049	211.7595	1498.6927	13.2340
1305.5187	46.0847	1505.0154	61.7982
1334.7579	459.8096	3010.8729	93.9021
1339.6439	172.7475	3051.1998	53.9102
1372.2344	950.3374	3072.1750	5.8726
1409.1452	32.7870	3084.9061	67.8619
1460.2225	14.1916	3117.9172	18.1078
1485.8423	54.1434	3134.2042	8.5237
3086.1822	0.2443	3175.5575	1.4193
3095.3615	8.4302	3761.5047	213.3149
3138.9713	0.2189		
3157.9715	0.2772		
3737.5626	249.1408		

Table 7

CAS# 51851-37-7		CAS# 62037-80-3		CAS# 68259-11-0	
Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)
9.9052	15.2645	22.1111	153.5057	32.1604	35.8992
11.0994	70.3035	31.5297	346.4596	41.1205	232.6182
14.3920	5.0727	37.5995	104.3623	56.2878	179.5760
19.2470	16.0637	50.4216	100.3964	91.7443	8.6229
24.4155	24.7872	64.5675	23.9237	115.0449	25.9973
29.4764	49.5081	76.4539	27.6504	146.1922	22.0766
35.7736	2.9106	90.1840	11.7359	176.0989	18.6060
41.3871	110.7451	135.9512	29.7375	216.6664	129.1443
45.8779	33.2697	150.4050	37.3941	244.1140	94.9965
52.1184	71.9216	184.9565	21.2653	254.8460	23.9055
61.6023	151.4813	201.9105	8.3321	278.5252	11.3512
64.0604	487.0073	221.3163	45.2537	286.1167	9.3141
73.6436	286.8065	231.9115	33.2399	310.9399	10.0165
77.0089	77.9915	259.9433	28.3063	315.3999	17.5665
81.1389	654.6408	275.7348	74.6995	352.5034	4.4058
99.0927	131.1083	298.1830	62.9563	363.8519	3.1062
116.1121	70.1387	307.7785	34.6977	371.0666	14.4377
118.6962	100.9817	327.5864	15.6721	410.8310	57.9837
125.8203	248.7581	335.1384	2.6533	469.5939	61.7099
134.9041	694.8320	352.2635	12.1903	511.3017	21.5113
141.6242	85.3151	365.5017	0.8699	532.4722	114.6714
154.3296	17.2858	384.0005	3.9333	560.1333	189.3644
168.1073	236.7359	451.4510	77.6934	585.5578	145.2842
183.4118	139.6613	499.7541	9.9177	621.1235	451.9384
200.4512	359.5312	528.0072	171.1118	629.1655	532.9581
211.7277	17.6607	532.0349	172.9110	653.6735	60.5166
225.6709	239.0588	539.2603	58.3976	696.4544	887.3585
249.2988	119.3640	562.1541	150.0894	749.6352	151.1637
252.1744	3.1134	568.4004	141.9513	777.4098	204.3727
254.8663	3.7645	586.8690	21.9194	928.3287	1183.2450
260.2215	34.9956	623.7637	380.8382	1020.1022	557.7205
262.1963	2.5896	639.1818	663.0977	1087.1175	562.7007
269.2091	8.9640	668.1934	537.8080	1133.9311	233.2170
274.5249	258.3703	670.9158	674.5800	1139.8698	2351.6173
277.2788	308.4574	744.0887	286.3360	1145.8147	140.0327

Table 7 continued

CAS# 51851-37-7		CAS# 62037-80-3		CAS# 68259-11-0	
Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)
279.1951	58.8432	764.1027	6.1337	1161.6316	1004.8282
287.1794	400.0311	778.9022	86.0410	1181.5434	1899.8210
293.5867	21.8394	810.7184	119.0946	1187.9301	1096.2391
296.5642	23.5478	980.7611	1086.9094	1206.1563	297.7858
308.2735	0.2032	1025.4626	623.5720	1237.8775	39.6685
315.4619	1.0319	1082.3997	1899.6333	1262.2151	320.9894
329.2040	12.0359	1113.7769	64.1849	1317.1215	164.6339
337.9815	6.9004	1120.1330	559.9551	1391.7352	164.2950
341.7315	26.9262	1137.0731	2964.1794	1827.3286	1141.7600
350.6173	90.7685	1162.9918	1540.1217	3716.6066	201.3740
377.8260	492.4846	1167.3976	932.1875		
400.8751	87.7652	1172.6463	1029.7390		
425.5991	136.4197	1181.5713	880.9189		
431.5679	331.1437	1186.2509	1646.9390		
434.7734	426.7604	1191.1244	883.2859		
445.5868	546.0059	1202.1317	955.4745		
465.0810	143.1867	1281.4436	343.1799		
482.3727	153.8742	1305.8698	530.1060		
530.0064	38.2707	1336.2422	31.8622		
545.1829	27.5761	1392.3582	178.2767		
573.0315	62.7345	1818.8087	1100.2288		
586.7032	154.6432	3713.6799	200.0198		
601.2137	132.3837				
611.8999	47.8813				
615.1271	18.1905				
676.2635	346.1690				
682.2967	84.9273				
707.4471	104.7697				
709.6578	825.6273				
746.7471	242.3779				
786.6127	929.2154				
813.6055	5.1245				
816.5261	1.0417				
816.7631	10.7066				

Table 7 continued

CAS# 51851-37-7	
Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)
836.8159	1921.3694
883.8080	458.6967
896.3157	581.3607
945.4985	211.5359
952.2403	1295.4574
954.6445	1925.7256
957.4180	400.4123
998.6196	240.0155
1013.6814	119.8022
1019.3258	294.8025
1037.2546	3281.6966
1047.8747	1495.9208
1053.7366	674.1310
1063.6534	786.7487
1068.5501	112.7873
1073.8732	268.1875
1077.2273	814.4719
1088.6207	937.8109
1103.3149	1258.8286
1107.4930	128.3124
1107.6045	1102.5802
1108.9037	38.5699
1109.0894	52.7925
1156.6781	312.7389
1161.5069	29.0783
1163.0746	3.5882
1164.7050	47.0125
1179.6933	128.7206
1200.6245	98.7105
1203.6551	8.8345
1214.6733	129.8969
1224.0028	18.1504
1255.8214	306.7791
1258.3084	8.9793

Table 7 continued

CAS# 51851-37-7	
Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)
1296.5071	1.3299
1300.8408	0.9872
1303.8115	2.1700
1352.7926	11.0493
1390.8611	22.1690
1393.6440	24.2643
1395.7892	15.7471
1397.1564	15.9815
1402.9349	77.1269
1403.3266	60.5241
1403.9524	69.4275
1456.4391	20.3310
1467.9733	28.6372
1468.4832	31.0174
1469.1010	29.7903
1478.6453	71.6788
1481.8481	10.0211
1482.0073	20.2357
1482.5580	14.6446
1506.1272	29.1511
1508.8115	4.4761
1510.8969	7.4967
3038.8290	27.2706
3038.8514	45.6389
3039.1638	30.9744
3044.8765	72.4820
3045.7599	54.1749
3051.4584	55.0207
3079.4770	4.1445
3083.7264	21.2294
3084.2455	30.2452
3089.6549	16.4818
3090.0748	12.2335
3105.5212	60.6876

Table 7 continued

CAS# 51851-37-7	
Frequency (cm^{-1})	Intensity ($\text{M}^{-1}\text{cm}^{-1}$)
3105.7003	56.4234
3105.7966	51.2159
3118.1713	61.5032
3118.2741	109.9643
3119.1217	90.9536
3124.3326	1.5252
3140.0962	1.9137

Table 8

CAS# 68298-12-4		CAS# 132843-44-8	
Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)	Frequency (cm ⁻¹)	Intensity (M ⁻¹ cm ⁻¹)
19.8694	710.4233	18.2415	4.9426
41.5835	264.9493	21.5039	53.4482
50.9083	19.1052	36.9785	35.5263
86.1712	337.0177	39.1264	8.9828
98.5769	55.0391	61.7505	2.7005
110.6454	58.3345	63.1013	6.4550
120.2991	23.5950	90.4591	2.7123
140.5445	29.3476	119.4333	47.0244
169.3979	52.1148	138.5335	85.9543
191.7919	306.6246	172.3198	158.3005
217.1630	84.7395	192.1265	32.2658
220.1070	48.7503	193.8692	99.8742
241.6423	61.9156	214.1599	19.1758
258.9430	39.2773	214.7333	41.6342
266.0726	8.8882	241.0542	392.8590
285.5881	36.1799	257.8344	336.1137
306.2159	21.6005	260.7033	2.4591
315.7347	12.7869	279.7086	161.1541
330.4479	6.8657	283.3994	12.0133
340.4617	15.9992	312.1210	0.5637
362.7841	5.1475	312.4111	19.1035
385.2694	38.4765	346.2868	103.3043
445.0189	207.4488	350.9372	6.6797
468.6711	233.9300	360.6147	0.2932
481.9895	1487.4552	363.3510	19.6412
483.8481	133.8426	454.8518	0.0991
531.4371	225.9640	462.4304	6.7696
539.6603	49.0805	483.9496	1797.0051
576.3944	771.9476	506.0880	1675.6253
585.6855	788.5709	524.8976	0.2387
635.9160	14.0664	527.3132	468.6967
638.1141	217.3445	544.2517	41.8642
655.0235	53.3914	588.3484	47.7007
748.0168	283.5545	589.4300	2716.0600

Table 8 continued

CAS# 68298-12-4		CAS# 132843-44-8	
Frequency (cm^{-1})	Intensity ($\text{M}^{-1}\text{cm}^{-1}$)	Frequency (cm^{-1})	Intensity ($\text{M}^{-1}\text{cm}^{-1}$)
820.0475	887.7087	590.9981	127.8171
914.9321	585.2832	608.5383	61.6525
992.3790	772.5693	643.0334	43.1186
1061.5602	386.2769	646.2055	8.0040
1089.1229	730.7535	748.7119	100.0973
1127.6164	207.5313	751.4929	469.6874
1129.1328	817.5543	785.7370	142.7327
1139.5484	369.7789	816.3929	3542.8410
1146.8359	103.2657	967.3048	671.3756
1154.0118	31.2349	970.0662	6.3670
1161.9062	1538.5574	1119.7620	392.3558
1179.9663	2124.1632	1121.8323	2319.7539
1183.4906	277.6444	1169.4052	715.1432
1196.3049	1122.8605	1171.7808	1880.9190
1230.1737	163.7475	1172.7546	117.8289
1253.1748	219.6311	1172.8941	479.8951
1317.6235	166.7905	1190.8506	228.8526
1373.6524	912.1606	1190.8601	1308.0335
1440.6037	448.9849	1198.9577	2127.2770
1460.7639	1.6684	1217.2938	8.5419
1489.2304	50.2892	1297.3956	979.7325
1511.9411	64.7622	1308.9535	48.6614
3058.7898	49.8945	1333.2416	95.8802
3132.1314	14.9692	1432.9667	1782.6495
3163.9423	3.2072	1439.0818	526.1824
3580.1140	137.9199	3530.8590	236.7274