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Calculation of IR Spectra Using Density Functional Theory for Nerve-Agent-Sorbent Binding

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14. ABSTRACT

Calculations of vibrational absorption spectra are presented using density function theory (DFT) for the custom sorbent polymer SiFA4H, nerve agent simulant DMMP, and the molecular structure SiFA4H-DMMP. The DFT calculated absorption spectra corresponding to vibrational excitation states of these molecular structures provide quantitative estimates of IR spectra that can be correlated with additional information obtained from laboratory measurements or spectra associated with detection in the field. Specifically, these DFT calculated IR spectra can provide general understanding of the process of nerve agent detection based on spectral analysis. The DFT software GAUSSIAN was used for the calculations of excitation states presented here. This case study provides proof of concept for using DFT calculated spectra to construct templates, which are for spectral-feature comparison, and thus detection of spectral-signature features associated with target materials.

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Introduction

Detection methodologies based on infrared (IR) spectroscopy are based on identification of unknown materials by comparison of measured spectra with reference spectra associated with known materials. In particular, that a pattern of frequencies, which is within an existing database of spectra corresponding to known molecular structures, can be compared to a measured spectrum for identification of the unknown molecules (see [1] and references therein). Comparison of spectra for the purpose of identifying an unknown material is accomplished in principle using signal processing algorithms [2], where signature structure within a measured signal is filtered using signal templates having patterns associated with known materials. These algorithms are typically based on least-squares [3], Kalman-filter [4,5] and cross-correlation methods [6,7], are statistical in nature, and can be used in principle together. In addition, for detection in practice, different types of databases can be referenced together, providing complimentary information, as well as utilization of other types of information concerning interpretation of spectral features, e.g., knowledge of other measured chemical properties of the unknown material.

Typically, spectral databases are constructed using different types of spectroscopic measurements, which include different types of spectroscopies based on transmission and reflection [8,9], e.g., attenuated total reflection (ATR) spectroscopy. The present study demonstrates calculation of IR absorption spectra for a prototype molecular structure characterizing molecular interactions associated with detection of nerve agents, e.g., Sarin nerve agent, which provides complementary information to that obtained from laboratory measurement. This complementary information should be in terms of the physical interpretation of spectral features with respect to molecular structure. In addition, this study provides proof of concept for constructing templates for spectral-feature comparison using DFT calculated spectra, which can be used in filter algorithms for detection of spectral features associated with target materials.

The present study presents calculation of IR spectra, using DFT, for the custom sorbent polymer SiFA4H, nerve agent simulant DMMP and molecular structure SiFA4H-DMMP. The properties of these molecular structures are of major importance for monitoring and detection of nerve-agent based weapons. A range of hazardous chemicals, including phosphate esters (typically nerve agents) and pesticides, are characterized by strong hydrogen-bond (HB) basicity. Accordingly, developed of HB acidic sorbent materials based on sorbent polymers has been considered, which can be adopted as coatings for concentrating analytes of interest for detection purposes. This process establishes a general foundation for infrared molecular binding spectroscopy in sorbent-coated devices. References [10, 11, 12] examine a prototype process for nerve-agent detection that is based on infrared molecular binding spectroscopy and analyte-sorbent interaction, which entails interaction of a nerve agent simulant DMMP and a sorbent polymer SiFA4H (See Figure 1). References [10, 11] describe a detection procedure using infrared molecular binding spectroscopy that applies attenuated total reflection (ATR). In particular, these studies examined the molecular binding that occurs between analyte and sorbent functional groups, and its effect on infrared absorption spectra, for a nerve-agent-detection process based on the SiFAH4-DMMP interaction. Reference [12] describes experimental measurements of absorbance for SiFAH4, both with and without DMMP present, estimated permittivity functions for bulk systems of SiFAH4 and SiFAH4-DMMP using inverse spectral analysis based on the Kramers-Kronig relations [13], and estimated molecular polarizabilities for SiFAH4 and SiFAH4-DMMP molecular structures based on the Claussious-Mossotti relation [14].

Reference [15] describes the formalism underlying DFT calculations of absorption spectra corresponding to vibrational states of molecules, which the present study considers. The DFT software GAUSSIAN09 (G09) can be used to compute an approximation of the IR absorption spectrum for a molecule or molecules [16,17]. This program calculates vibrational frequencies by determining second derivatives of the energy with respect to the Cartesian nuclear coordinates, and then transforming to mass-weighted coordinates at a stationary point of the geometry. The IR absorption spectrum is obtained using density functional theory to compute the ground state electronic structure in the Born-Oppenheimer approximation using Kohn-Sham density functional

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theory [18-24]. GAUSSIAN uses specified orbital basis functions to describe the electronic wavefunctions and density. For a given set of nuclear positions, the calculation directly gives the electronic charge density of the molecule, the potential energy *V,* and the displacements in Cartesian coordinates of each atom. The procedure for vibrational analysis used in GAUSSIAN is described in reference [17], and is reviewed in reference [23].

DFT Calculation of IR Spectra

Results of a computational investigation using DFT concerning sorbent polymer SiFA4H, nerve agent simulant DMMP and the molecular structure SiFA4H-DMMP are presented. These results include the energy-minimized configuration of these molecules, and their ground-state oscillation frequencies and IR intensities. For these calculations geometry energy optimization and vibrational analysis was effected using the DFT model B3LYP [24,25] and basis functions 6-311+G(d) [26,27]. These basis functions designate the 6-311G basis set supplemented by diffuse functions, indicated by the sign +, and polarization functions (d), having one set of d functions on heavy atoms [28]. Graphical representations of molecular geometries for stable molecules of DMMP. SiFA4H and the molecular structure SiFA4H-DMMP, their ground-state energies and IR spectra, are shown in Figs. (2) through (5). Values of the IR intensities as a function of frequency for these molecules are given in Tables 1, 2, 3 and 4.

Discussion

A wide range of detection methodologies are based on measuring differences between spectral signatures associated with reference sorbent molecules and signatures for molecular structures formed by sorbent and target molecules. Accordingly, DFT provides an approach for estimating IR absorption spectra for target molecules using such methods. As discussed, identification of unknown molecules by comparison of spectra is accomplished using signal templates having patterns associated with known materials, which are adopted by different types of filter algorithms [3-7]. In practice, because spectral features of target molecules are within complex spectral-signature backgrounds, filter algorithms associated with detection require reasonable estimates of target spectral features for construction of comparison templates, e.g., cross-correlation. In addition, one would expect small shifts of measured-spectra maxima relative to those of template spectra due to different types of detector designs and ambient environments, which would result in different levels of coupling between molecular vibrational modes and intermolecular interactions. This coupling of molecular and intermolecular modes, depending on the detection scenario, implies the need for “lag” parameters in application of spectrum-comparison algorithms, e.g., cross-correlation [2]. In particular, the DFT calculated spectra in Tables 1, 2, 3 and 4 were calculated for isolated molecules within a weakly interacting background, and are therefore quite similar spectra of isolated molecules in space, where there are no shifts due to intermolecular couplings.

It follows that the DFT calculated IR spectra calculated here, given in Tables 2 and 3, should provide a reasonable template for filtering of IR spectral measurements associated with different types of detector schemes. In principle, this template can be a linear combination of the spectra given in Tables 2 and 3, having adjustable weight coefficients of the component spectra, as well as correlation-lag parameters for adjustment of absorption-maxima frequencies. A qualitative analysis of prototypical spectral features as would occur in a realistic detection environment, using DFT calculated spectra (i.e., Table 1), may be applied to the measurements of reference [12]. A qualitative comparison of the measured spectral features described in [12] and those given in Tables 2 and 3 show good correlation within a small correlation lag, i.e., frequency shift of absorption maxima. Ground state and interaction energies of the molecular structures are as follows. SiFA4H-DMMP (-4606.2219 kcal/mol), SiFA4H (-3919.2520 kcal/mol), DMMP (-686.9540 kcal/mol) and interaction energy of SiFA4H and DMMP I_E = -0.0158 a.u. = -9.94 kcal/mol, where I_E = E(SiFA4H-DMMP) - E(SiFA4H) - E(DMMP). For another calculation, SiFA4H (-3919.1324 kcal/mol), SiFA4H- SiFA4H (-7838.2928 kcal/mol) and interaction energy

of SiFA4H and SiFA4H I_E = -0.0281 a.u. = -17.65 kcal/mol, where I_E = E(SiFA4H-SiFA4H) - E(SiFA4H) - E(SiFA4H).

Conclusion

The DFT calculated absorption spectra given here provide information concerning molecular level dielectric response structure. The calculations of IR spectra associated with sorbent polymer SiFA4H, nerve agent simulant DMMP and the molecular structure SiFA4H-DMMP using DFT are meant to 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 a reasonable template for filtering of IR spectral measurements associated with different types of detector schemes.

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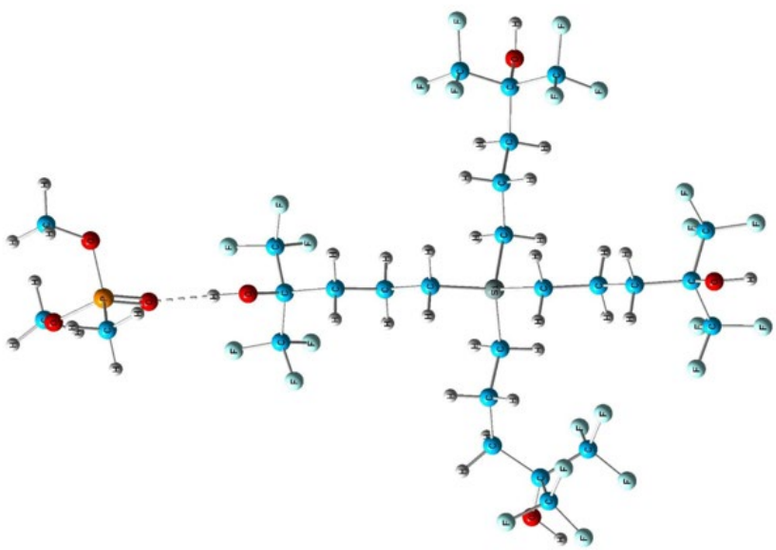

Figure 1. Molecular complex consisting of nerve-agent simulant DMMP and a sorbant polymer SiFA4H.

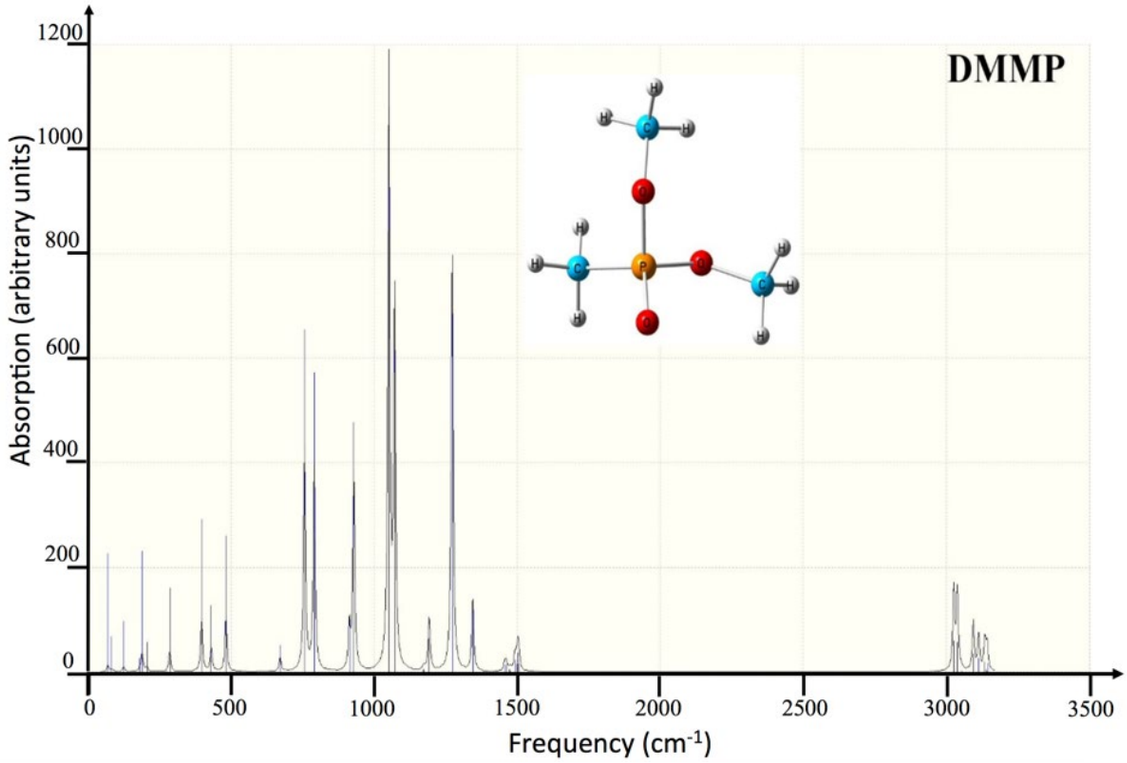

Figure 2. DFT calculated equilibrium geometry, minimal energy and IR spectra of isolated DMMP molecule.

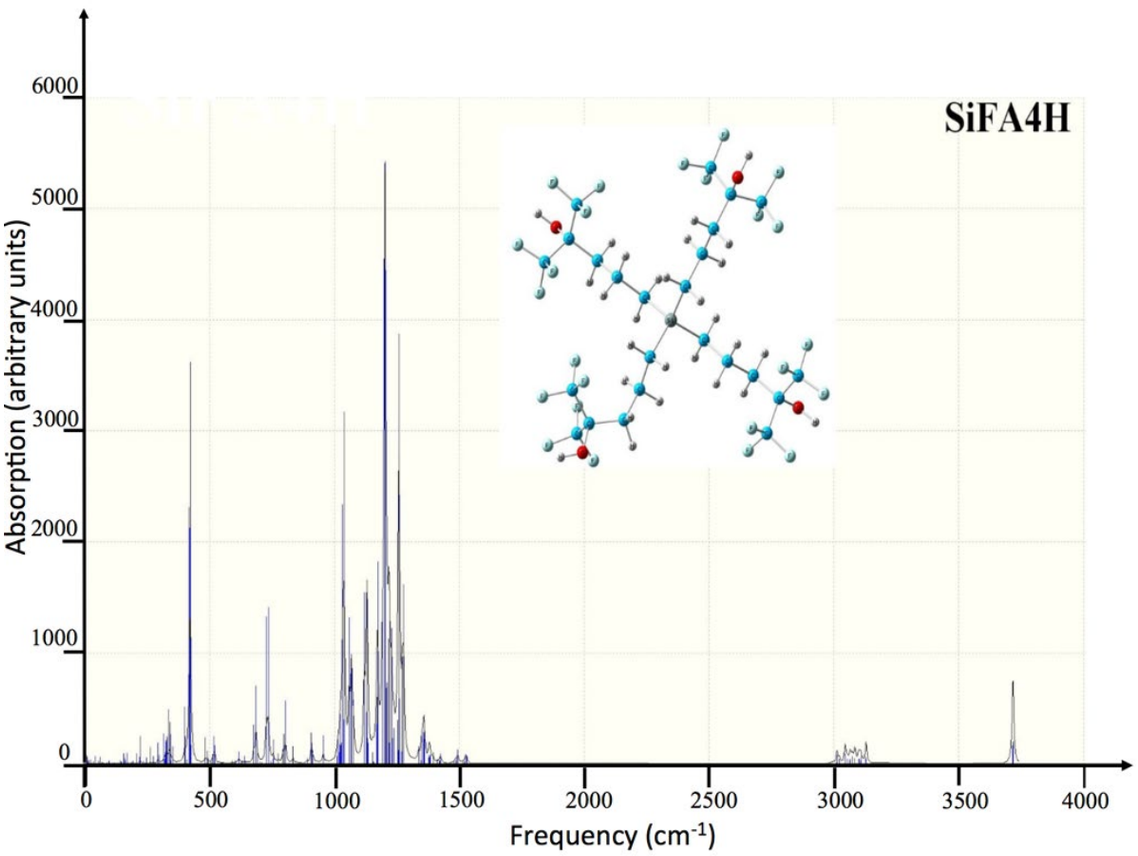

Figure 3. DFT calculated equilibrium geometry, minimal energy and IR spectra of isolated SiFA4H molecule.

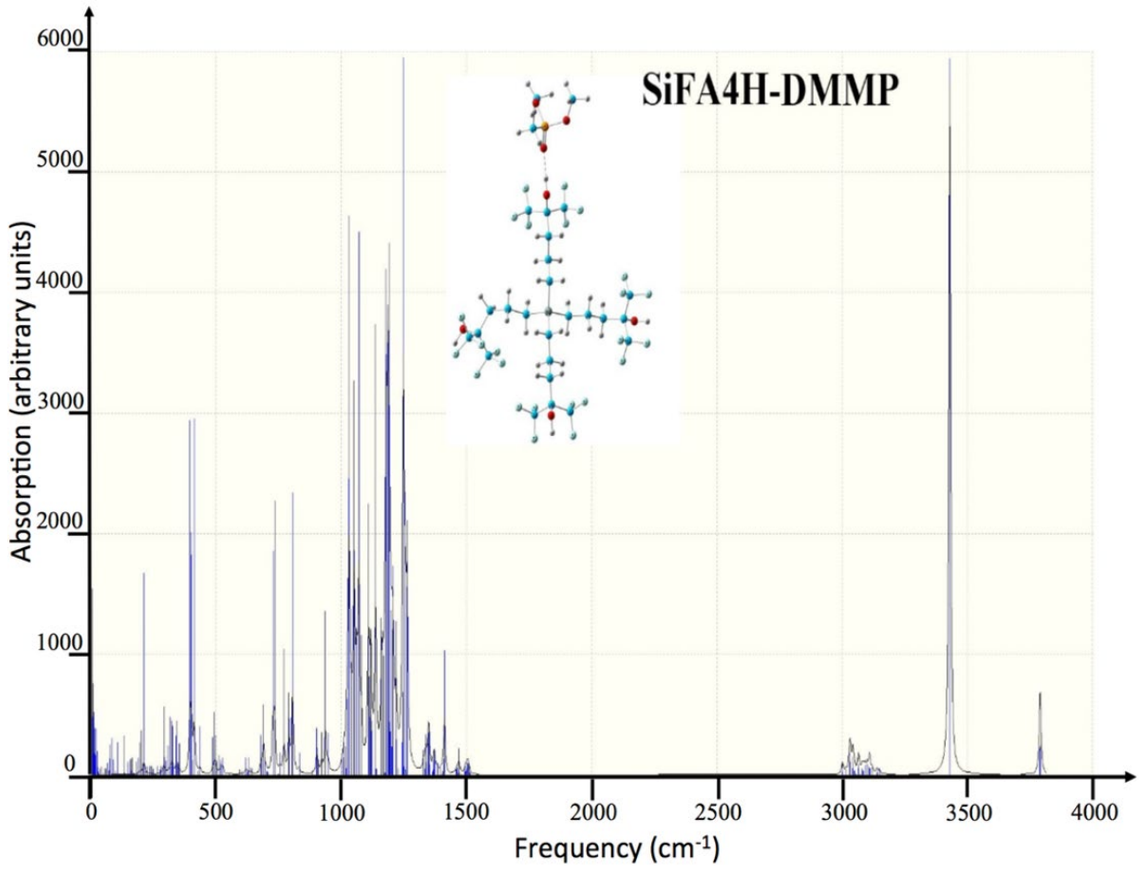

Figure 4. DFT calculated equilibrium geometry, minimal energy and IR spectra of isolated SiFA4H-DMMP molecular structure.

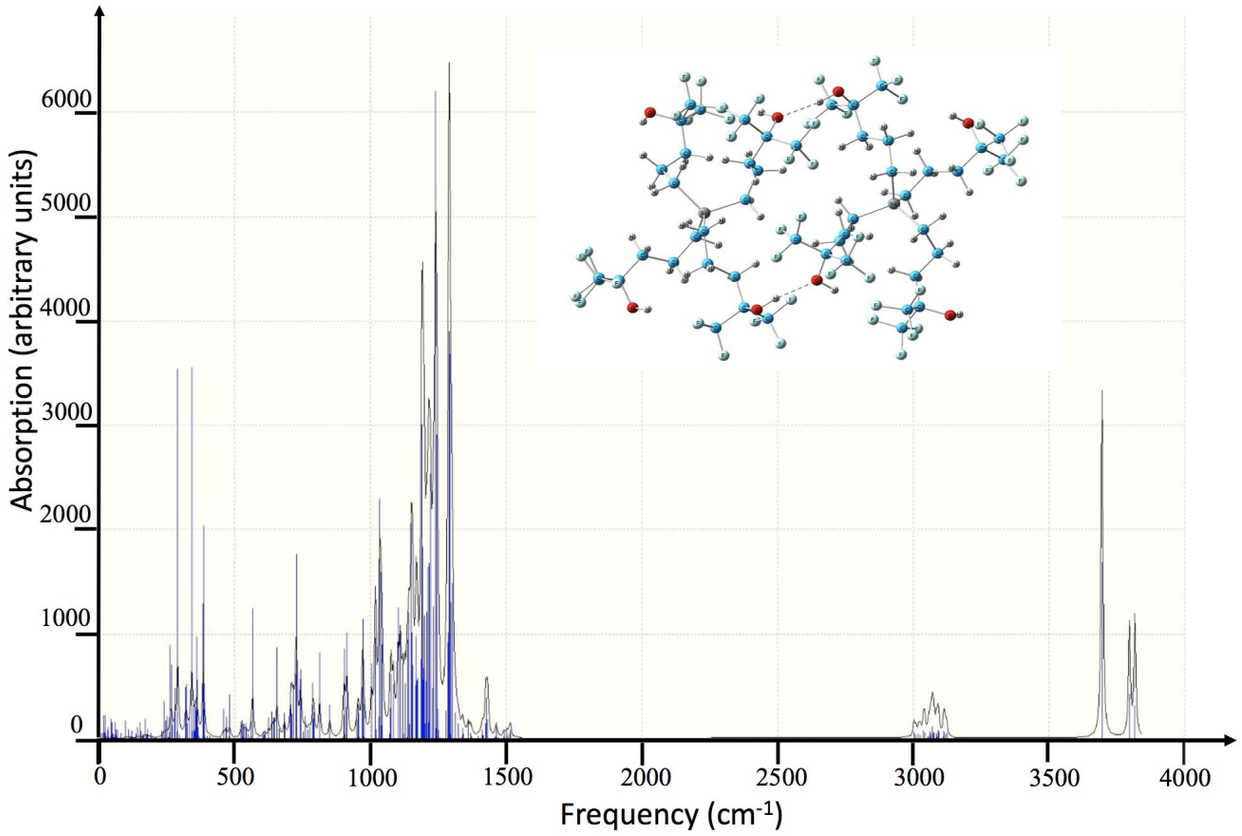

Figure 5. DFT calculated equilibrium geometry, minimal energy and IR spectra of isolated SiFA4H-SiFA4H molecular structure.

Table 1. SiFA4H-DMMP

	Freq (cm^{-1})	IR Intensity (KM/Mol)		Freq (cm^{-1})	IR Intensity (KM/Mol)		Freq (cm^{-1})	IR Intensity (KM/Mol)
1	4.1151	0.5307	96	496.1839	13.6239	191	1194.332	35.6961
2	6.3665	0.2551	97	497.0509	4.5164	192	1199.537	136.5274
3	7.5685	0.1172	98	501.6665	4.7614	193	1203.1027	23.2341
4	9.1656	0.5806	99	510.8986	6.8889	194	1203.9316	121.0693
5	10.5113	0.4061	100	516.395	5.3042	195	1207.1823	174.9415
6	11.2474	0.4899	101	520.6184	4.0711	196	1218.3024	129.5568
7	13.3363	0.1932	102	525.8713	4.5554	197	1221.0306	29.9127
8	13.7253	0.0197	103	526.2942	6.0788	198	1226.1827	5.0034
9	14.9122	0.4851	104	526.6228	3.1807	199	1243.9211	27.8917
10	16.3835	0.2204	105	527.2502	2.1097	200	1246.0571	71.1019
11	19.9252	0.6384	106	527.3184	5.0957	201	1247.421	619.9709
12	23.5969	0.3868	107	552.5959	0.0652	202	1248.468	227.4894
13	27.0856	0.1305	108	553.9899	0.3314	203	1250.4983	7.1435
14	27.7334	0.0566	109	554.0888	0.3979	204	1255.4208	245.7302
15	31.5849	0.0221	110	554.6254	0.2809	205	1256.7372	4.28
16	34.6563	0.1372	111	593.28	2.1178	206	1261.2241	163.9036
17	40.387	0.0744	112	601.9298	1.83	207	1263.1566	222.4197
18	41.0202	0.2287	113	616.9901	4.1109	208	1328.0762	23.1224
19	49.6573	0.0521	114	618.359	7.0633	209	1333.4785	5.1102
20	53.9174	0.2468	115	623.2644	1.1702	210	1337.4424	37.4864
21	58.3041	0.2428	116	626.7655	1.7856	211	1338.35	11.3038
22	58.5588	0.1291	117	629.9178	7.7077	212	1346.5861	28.6565
23	64.6114	0.3462	118	638.6425	3.2232	213	1347.9083	6.3839
24	66.4378	0.5296	119	642.7216	2.9418	214	1348.7291	39.2433
25	71.4776	0.2354	120	677.7233	18.4975	215	1349.9301	48.6302
26	72.3817	0.0958	121	682.0754	7.8843	216	1352.0745	9.4722
27	73.9547	0.8347	122	688.2285	19.7584	217	1364.2621	2.8593
28	77.034	1.582	123	689.0814	33.5523	218	1366.4983	13.5875
29	81.3051	0.0467	124	689.4041	21.7314	219	1368.067	4.5519
30	83.6667	2.1022	125	695.4788	8.3212	220	1371.5988	22.7829
31	87.8368	0.9372	126	702.0908	1.6053	221	1371.9023	10.99
32	97.9891	0.2657	127	703.631	1.4588	222	1373.1848	13.1735
33	102.4623	0.0609	128	706.5977	1.0327	223	1384.4233	11.3821
34	105.3307	0.3521	129	726.2322	112.6796	224	1395.4287	6.8899
35	106.4964	2.3811	130	733.2348	139.119	225	1402.9711	1.0378
36	116.2407	0.0186	131	747.7451	0.3	226	1405.6125	3.2329
37	118.8435	0.0456	132	749.1476	0.2684	227	1407.5194	15.5368
38	131.7218	3.5048	133	754.4113	2.1381	228	1412.0594	121.6678
39	133.6051	0.2306	134	755.7825	11.3618	229	1456.6458	4.8726
40	148.5208	1.2562	135	770.9667	3.8974	230	1460.2145	5.1722
41	157.2638	1.6776	136	771.2672	67.1591	231	1461.9767	3.9379
42	159.9329	0.4499	137	789.0708	10.4186	232	1463.1667	7.2071
43	162.8849	1.9308	138	789.2373	44.9565	233	1467.0309	1.328
44	169.3712	0.2549	139	792.1904	30.7487	234	1469.5675	26.5054
45	172.27	0.0669	140	803.0195	43.2118	235	1474.3304	2.0484
46	181.2848	1.6752	141	805.1559	157.2654	236	1478.2609	1.1011
47	183.4108	0.1045	142	831.1871	12.5105	237	1492.5354	2.8851
48	189.6193	2.1917	143	884.512	2.7681	238	1493.8927	1.0306
49	196.5554	4.3481	144	901.2136	29.0559	239	1494.585	9.1754

50	200.3383	6.2061	145	903.1062	17.0112	240	1495.3738	0.0568
51	207.8314	1.6126	146	906.7795	9.4299	241	1497.1724	3.8008
52	211.4668	29.5125	147	920.861	26.8876	242	1499.6697	6.2659
53	218.9604	1.2283	148	935.9809	105.9392	243	1502.3353	11.9303
54	225.7212	1.2764	149	946.9318	27.5337	244	1505.2969	11.4197
55	235.063	1.4834	150	1001.9159	11.8932	245	1505.5732	8.1408
56	240.5121	1.4528	151	1008.2767	11.9259	246	1509.4713	11.081
57	243.5814	0.1073	152	1011.2643	25.3767	247	1512.3541	2.1915
58	243.9179	0.1163	153	1016.6244	19.6031	248	1515.0104	1.2204
59	247.6614	0.9592	154	1019.1571	4.5135	249	2999.4526	5.384
60	262.9838	1.5894	155	1021.5244	53.567	250	3002.2439	2.5595
61	276.2512	1.0276	156	1022.5731	23.9939	251	3002.4053	23.2095
62	278.2429	1.7035	157	1028.1361	210.9228	252	3016.0559	10.3745
63	285.1496	1.5111	158	1031.1957	399.5638	253	3029.478	1.1565
64	291.3857	13.7746	159	1040.5472	81.3578	254	3030.5122	46.7397
65	291.6919	2.9977	160	1049.7843	286.4338	255	3033.0659	27.2785
66	292.6599	3.047	161	1052.0298	163.4816	256	3033.4441	12.8907
67	293.2803	3.5114	162	1060.2227	93.0657	257	3042.085	13.2011
68	297.6127	2.8579	163	1061.2625	101.1233	258	3043.3386	38.6461
69	308.3318	6.1731	164	1069.5736	402.3417	259	3044.9836	7.938
70	315.8046	12.6688	165	1070.4125	28.9467	260	3049.1985	8.2613
71	321.8823	1.9037	166	1080.3206	104.4461	261	3050.3982	8.897
72	322.505	12.0889	167	1107.4514	207.9689	262	3054.3943	1.1624
73	323.8873	0.0227	168	1109.5356	23.7522	263	3064.884	14.2004
74	324.4233	11.0762	169	1110.5898	75.9067	264	3065.4111	10.034
75	324.6014	0.8631	170	1112.8223	44.2789	265	3066.8372	1.2093
76	326.435	7.3471	171	1117.1903	68.7205	266	3067.0188	23.9948
77	329.1336	2.0774	172	1117.8892	112.539	267	3071.519	2.2039
78	339.1596	9.0222	173	1119.1886	33.8366	268	3079.4998	13.6483
79	341.1041	12.8019	174	1121.4698	41.7902	269	3082.6272	9.4132
80	345.2938	3.0403	175	1135.432	22.9392	270	3085.6355	8.211
81	346.2099	0.2491	176	1136.7534	354.632	271	3091.9504	20.5586
82	346.408	0.8662	177	1138.5941	4.5072	272	3100.2468	22.9077
83	348.0766	2.7285	178	1141.2412	4.6203	273	3108.5476	17.142
84	353.8444	7.7292	179	1159.7659	126.0078	274	3110.0891	14.4438
85	394.0246	96.7504	180	1162.6564	115.9893	275	3111.2798	14.3168
86	397.8458	19.0857	181	1167.9689	96.5296	276	3112.312	5.0954
87	398.9525	67.0412	182	1172.5968	1.084	277	3120.8518	15.2985
88	401.0994	61.2093	183	1174.1827	2.0503	278	3139.093	4.3294
89	404.6184	4.1222	184	1176.9719	412.5089	279	3140.9741	10.4555
90	412.097	12.7932	185	1180.2628	343.7786	280	3142.2285	0.3984
91	412.1302	101.6782	186	1184.9622	385.9546	281	3150.2451	12.0333
92	427.5424	1.0457	187	1187.5404	350.0808	282	3430.2783	1702.8951
93	436.0935	14.4668	188	1191.1451	438.5946	283	3790.7727	69.2484
94	486.0229	12.6359	189	1193.14	2.9738	284	3791.5378	75.2095
95	491.74	21.4888	190	1193.301	43.5789	285	3792.3901	70.4644

Table 2. SiFA4H

	Freq (cm^{-1})	IR Intensity (KM/Mol)		Freq (cm^{-1})	IR Intensity (KM/Mol)		Freq (cm^{-1})	IR Intensity (KM/Mol)
1	6.9114	0.0519	80	497.2398	2.705	159	1186.7758	814.8971
2	8.2782	0.0284	81	500.9306	0.0211	160	1188.2661	315.7454
3	9.3788	0.0101	82	509.4141	1.4823	161	1192.6407	139.4658
4	10.1709	0.06	83	515.4458	4.1921	162	1198.182	129.7221
5	12.7513	0.0063	84	519.1594	13.8278	163	1201.3716	198.6663
6	13.7162	0.0037	85	520.5257	4.3237	164	1202.674	13.5411
7	16.0924	0.0166	86	526.0144	5.5782	165	1203.095	46.9718
8	17.1375	0.0954	87	526.3843	3.4686	166	1206.3959	216.0345
9	23.424	0.1048	88	526.4735	4.9071	167	1217.5991	116.5202
10	27.3675	0.0055	89	526.734	4.3309	168	1223.1215	23.3026
11	30.6753	0.0018	90	553.7786	0.4352	169	1228.089	41.25
12	32.2961	0.004	91	554.4745	0.0878	170	1243.8569	41.2174
13	35.2697	0.0775	92	554.5144	0.6084	171	1245.3555	23.1431
14	41.8313	0.253	93	554.5886	0.27	172	1247.0909	502.1436
15	53.9425	0.1269	94	593.1644	1.9247	173	1248.609	172.7988
16	60.5247	0.1624	95	602.3526	1.7911	174	1251.5748	69.2884
17	62.9637	0.4339	96	616.9695	6.8438	175	1257.9144	19.5223
18	66.4413	0.1056	97	617.7913	6.2142	176	1260.1553	133.4047
19	71.9144	0.0935	98	623.4567	0.4344	177	1265.1599	221.0413
20	72.8523	0.0514	99	626.6499	0.5041	178	1325.183	23.7822
21	76.9761	0.0416	100	629.6785	2.7275	179	1336.4829	3.3887
22	79.5151	0.018	101	637.4609	4.4463	180	1339.3173	27.1079
23	88.4679	0.1258	102	644.1919	2.6605	181	1340.2172	27.0753
24	96.0286	0.3456	103	677.2741	20.1663	182	1346.6683	33.0601
25	98.139	0.2697	104	688.8213	19.8314	183	1348.9851	13.2996
26	113.3899	0.0178	105	689.1957	35.9017	184	1349.5431	32.782
27	120.1588	0.0206	106	690.0895	25.8585	185	1351.3694	34.2898
28	122.4249	0.0664	107	694.6359	9.9046	186	1368.2412	3.4044
29	139.115	0.103	108	701.3294	1.1629	187	1370.6658	17.302
30	147.5275	0.8284	109	704.898	0.7523	188	1370.6953	9.3741
31	155.3645	1.4858	110	708.5819	0.3495	189	1371.9301	10.4956
32	160.8802	0.7322	111	725.1348	115.5633	190	1372.6923	11.8253
33	161.324	0.5169	112	734.3201	124.7015	191	1373.0446	3.026
34	167.5735	1.6816	113	747.5286	0.513	192	1374.9753	16.2468
35	172.8971	0.11	114	749.7743	0.1651	193	1381.8824	16.465
36	185.3617	0.335	115	754.8251	2.2026	194	1395.3961	5.5137
37	190.9458	0.4869	116	756.1088	12.1107	195	1407.6785	3.9588
38	196.8505	0.1048	117	772.1943	6.9251	196	1409.2458	5.8054
39	208.5518	1.6267	118	788.5083	8.7641	197	1411.7653	15.6279
40	219.7492	2.1162	119	791.9249	18.7448	198	1459.1094	4.572
41	222.1589	5.5502	120	801.6444	44.4214	199	1464.4854	3.9512
42	235.3264	0.5997	121	831.26	13.415	200	1466.2616	8.6966
43	242.4411	0.0782	122	885.8553	4.2094	201	1471.894	19.587
44	243.3711	0.0755	123	901.6877	27.7339	202	1492.8719	3.1428
45	244.7575	0.0467	124	903.6368	18.3629	203	1493.6252	1.0242
46	247.0085	1.5885	125	908.7039	11.5211	204	1496.3123	0.2074
47	263.0993	3.3229	126	948.1761	27.3829	205	1498.9376	3.6557
48	274.9643	1.88	127	1004.6007	6.217	206	1506.0142	12.323
49	280.2283	0.0764	128	1008.7847	23.2696	207	1510.1115	9.8241

50	292.7792	5.9145	129	1011.5757	12.4392	208	1512.2231	4.0065
51	293.3349	0.551	130	1016.1131	16.2065	209	1515.8723	0.9929
52	293.7728	3.2815	131	1019.1848	16.8169	210	3000.4792	5.0177
53	298.3449	2.2151	132	1020.6279	50.0269	211	3003.3284	2.2557
54	306.2731	0.0795	133	1023.0829	17.6399	212	3003.5095	21.8909
55	316.5034	9.1825	134	1028.1735	281.7688	213	3015.2671	11.4684
56	320.0129	0.4304	135	1031.9854	89.9368	214	3030.8171	0.783
57	322.5078	6.856	136	1033.3958	322.46	215	3034.1323	25.2417
58	323.2447	1.0405	137	1051.6943	161.7949	216	3034.6836	14.4171
59	323.4594	16.8083	138	1060.9611	124.7352	217	3041.3704	12.7
60	324.6304	12.2414	139	1062.0404	115.0529	218	3046.8479	8.2031
61	328.4222	8.1583	140	1063.3132	61.6131	219	3050.4873	4.8039
62	329.5487	1.8232	141	1069.0232	53.1385	220	3050.7642	13.831
63	337.5044	18.1451	142	1108.3636	198.8048	221	3064.6416	11.6948
64	340.7698	13.2553	143	1110.9395	24.8073	222	3066.4229	8.8086
65	342.6597	9.2087	144	1113.3479	72.021	223	3067.0337	11.4741
66	345.8497	0.2403	145	1115.3171	51.04	224	3067.479	14.0249
67	346.2636	0.1209	146	1117.5767	42.0445	225	3071.4585	2.2818
68	347.0606	0.1113	147	1118.6235	22.0886	226	3080.2014	13.0834
69	353.5083	5.3581	148	1120.0215	239.7088	227	3083.7502	11.7454
70	399.986	26.8105	149	1120.3959	23.8668	228	3089.728	10.3073
71	401.8166	5.4508	150	1133.9813	13.8707	229	3091.0232	14.8916
72	404.122	103.6812	151	1136.9388	7.3772	230	3109.7495	12.7101
73	406.1113	118.1913	152	1137.8372	6.5439	231	3111.0823	15.2897
74	407.3223	80.0408	153	1140.3195	4.4533	232	3112.5088	5.5069
75	408.7697	127.249	154	1160.012	43.4696	233	3112.825	14.801
76	409.9054	1.3765	155	1162.8444	78.6211	234	3790.8057	92.5417
77	426.7621	1.2303	156	1164.2328	246.3475	235	3790.9736	53.2792
78	486.0228	12.7427	157	1179.6455	305.4372	236	3791.8955	88.7477
79	495.449	5.4493	158	1185.6344	317.2749	237	3792.0813	58.6073

Table 3. DMMP

	Freq (cm^{-1})	IR Intensity (KM/Mol)		Freq (cm^{-1})	IR Intensity (KM/Mol)
1	70.4648	3.9912	22	1192.3925	11.0002
2	82.4426	1.3907	23	1192.726	19.1943
3	96.9665	0.007	24	1273.0228	235.9335
4	124.9163	3.0157	25	1344.6284	40.9598
5	181.0658	1.2194	26	1456.313	4.9467
6	189.706	11.0091	27	1462.5096	5.5282
7	206.4944	2.9722	28	1473.6555	1.8135
8	275.6671	0.0964	29	1477.1316	0.9617
9	286.1753	11.5418	30	1491.9661	8.6077
10	397.7291	29.0327	31	1498.283	5.4074
11	431.4144	13.6976	32	1503.1926	13.4705
12	482.49	31.3988	33	1506.941	6.0252
13	671.9982	8.5401	34	3025.3059	45.2995
14	757.159	124.3144	35	3037.6172	43.7284
15	791.1218	113.4632	36	3053.3252	1.6073
16	913.932	24.4669	37	3093.4634	27.3603
17	929.2785	110.921	38	3112.2871	20.6931

18	1051.6599	313.8139	39	3133.3701	15.4015
19	1071.6628	200.9771	40	3136.7119	3.8913
20	1172.4218	1.1593	41	3140.3855	1.1699
21	1174.8158	1.4529	42	3142.3113	12.9762

Table 4. SiFA4H- SiFA4H

	Freq	IR Intensity		Freq	IR Intensity		Freq	IR Intensity		Freq	IR Intensity
1	6.4561	0.0019	121	322.2728	12.0917	241	789.956	20.8318	361	1291.693	680.5518
2	8.5018	0.0051	122	322.3671	0.1864	242	790.2517	16.1075	362	1293.549	6.362
3	9.643	0.0672	123	325.5005	0.6823	243	792.2871	1.9045	363	1296.418	241.4353
4	12.6209	0.0867	124	325.6372	2.8857	244	792.2931	27.8602	364	1297.326	203.5047
5	13.6106	0.0046	125	326.334	1.893	245	812.6563	4.8903	365	1297.398	0.8577
6	17.4989	0.1419	126	326.3442	6.465	246	812.6916	95.841	366	1302.358	277.3572
7	17.9345	0.3323	127	332.3879	0.7456	247	850.0844	39.0224	367	1313.304	2.0834
8	17.9943	0.3093	128	332.7376	11.1512	248	850.1194	9.1484	368	1313.403	46.1607
9	18.5961	0.5832	129	341.6999	174.047	249	900.1489	1.0249	369	1323.434	3.0575
10	20.3988	0.1598	130	342.0566	4.054	250	900.6135	28.1002	370	1323.464	26.5476
11	21.4538	0.3926	131	344.7355	3.5608	251	903.5368	110.4931	371	1337.162	1.2618
12	22.5537	0.0328	132	344.7848	0.0983	252	905.0698	4.9434	372	1337.249	3.0695
13	22.6202	0.7116	133	348.4557	10.1864	253	910.88	3.4709	373	1339.286	19.2034
14	24.3274	0.1421	134	349.3119	16.0268	254	911.2646	38.9438	374	1339.425	8.3624
15	26.9379	0.0677	135	350.6602	3.2309	255	913.257	0.2146	375	1341.801	0.3198
16	30.4948	0.3332	136	352.3125	3.896	256	913.9795	132.8971	376	1342.679	7.8162
17	33.1974	0.5121	137	352.572	0.1042	257	949.3629	23.5946	377	1360.157	0.6444
18	35.5969	0.0243	138	352.9198	1.3898	258	949.4062	4.799	378	1360.179	31.0925
19	37.2283	0.0183	139	355.3052	15.1659	259	954.4164	12.6376	379	1368.918	6.097
20	38.3318	0.013	140	355.3584	3.6793	260	954.4437	44.5807	380	1369.44	5.8424
21	42.6683	0.1271	141	356.802	2.5835	261	957.3234	32.8967	381	1369.814	9.9561
22	42.7732	0.0002	142	357.9223	13.4023	262	957.7738	1.7464	382	1369.883	2.1928
23	44.205	0.278	143	359.1761	49.9677	263	970.7496	68.3274	383	1372.372	0.2717
24	44.3289	0.0595	144	360.5773	1.5258	264	971.4715	158.9835	384	1372.544	3.3626
25	45.7997	1.2293	145	363.1119	29.0384	265	975.1419	2.0058	385	1397.587	1.2931
26	46.145	0.2224	146	364.8599	5.7004	266	975.8818	45.5774	386	1397.625	4.0748
27	46.9	0.9892	147	368.3871	1.1687	267	1003.4903	102.7394	387	1410.917	16.8376
28	48.7227	0.0028	148	368.8159	0.2449	268	1004.6923	1.637	388	1410.936	3.7507
29	49.217	0.3153	149	383.3188	70.7997	269	1017.8553	118.5002	389	1411.536	4.4469
30	50.5365	0.0991	150	384.7044	112.194	270	1018.0376	102.639	390	1411.668	3.4562
31	52.6207	0.3047	151	388.1237	15.5335	271	1018.3836	139.9049	391	1414.226	6.3911
32	52.8586	0.1698	152	389.2037	0.8357	272	1020.3127	12.6369	392	1414.848	5.6041
33	54.121	0.0618	153	399.9212	0.0121	273	1031.9869	30.7236	393	1424.192	28.2195
34	55.8793	0.0713	154	400.0045	1.2945	274	1032.205	22.3404	394	1424.2	25.1015
35	58.0177	1.3137	155	409.0413	0.2215	275	1034.1987	340.0095	395	1425.92	79.0988
36	59.9653	0.3255	156	409.1219	1.1466	276	1034.4626	26.9004	396	1426.148	0.1907
37	60.3868	0.1615	157	446.1757	0.3005	277	1039.066	237.2237	397	1431.169	28.2292
38	64.0077	0.3889	158	446.5875	0.012	278	1040.182	17.7086	398	1431.187	32.9405
39	64.1665	0.8123	159	459.1207	18.4954	279	1043.2491	134.7915	399	1432.449	31.8384
40	64.4928	0.359	160	459.1764	1.0803	280	1043.4285	10.5598	400	1432.467	35.8977
41	65.0625	0.0693	161	467.2649	6.8777	281	1071.4294	6.3465	401	1457.752	1.2785
42	66.9747	0.8096	162	468.0654	0.0132	282	1071.9307	15.0647	402	1458.023	1.029
43	68.7132	0.0226	163	468.8439	13.9067	283	1073.0295	18.4142	403	1461.889	0.3208
44	72.7119	0.0006	164	470.2541	2.2271	284	1073.0706	44.1306	404	1462.114	3.6249

45	76.191	0.0025	165	479.1477	0.9892	285	1076.1226	94.4837	405	1463.109	12.5734
46	76.4541	0.1842	166	480.9396	28.8845	286	1076.2617	48.0731	406	1464.022	22.2062
47	76.6283	0.0735	167	522.8476	11.9208	287	1084.5879	64.9445	407	1470.503	0.0294
48	79.3879	0.0008	168	522.8975	4.7394	288	1084.9821	79.939	408	1470.57	2.1075
49	80.5587	0.548	169	527.5317	12.657	289	1101.7292	197.4298	409	1490.626	2.6738
50	85.0345	0	170	527.5545	0.4562	290	1102.1794	2.9289	410	1490.666	0.225
51	96.8763	0.2486	171	530.1581	0.0137	291	1109.9427	158.7896	411	1490.965	2.4145
52	97.7041	2.3918	172	530.1833	0.7644	292	1110.2933	57.7281	412	1492.076	14.2543
53	109.3217	0.0072	173	530.6017	8.8275	293	1118.7123	115.7668	413	1501.214	14.3441
54	109.6929	1.3034	174	530.6326	4.1099	294	1123.5778	6.6056	414	1501.436	2.5218
55	116.6129	0.1946	175	530.8244	0.1209	295	1126.816	36.416	415	1503.534	3.4601
56	117.5019	0.2505	176	531.2241	0.1567	296	1126.8759	84.4187	416	1505.6	0.5874
57	121.1427	1.1861	177	533.8186	3.557	297	1134.8604	1.0655	417	1510.663	8.721
58	121.5402	1.1009	178	533.8323	10.1422	298	1136.0569	153.3242	418	1510.671	6.2663
59	137.0412	0.5475	179	540.9278	10.7747	299	1141.6938	197.7184	419	1512.109	2.9873
60	137.0489	0.8997	180	541.1113	0.0002	300	1142.9742	21.5181	420	1512.503	0.2037
61	140.5187	1.384	181	542.5233	4.7877	301	1150.0154	342.6618	421	1515.319	14.3165
62	140.7614	2.152	182	544.0475	6.7089	302	1150.283	2.2845	422	1516.438	2.7122
63	151.1565	0.2593	183	550.6704	3.1188	303	1153.2426	167.7126	423	1516.631	16.7698
64	151.2057	3.2306	184	550.7336	0.1423	304	1153.2844	7.6359	424	1516.705	0.0092
65	154.6891	1.6446	185	557.1804	0.1065	305	1155.6309	116.3167	425	3001.913	18.035
66	155.067	0.1574	186	557.2	0.2752	306	1156.0981	112.1375	426	3001.928	23.6711
67	160.22	0.6976	187	558.2488	0.0279	307	1167.3276	85.6121	427	3009.24	15.0468
68	160.6519	0.2647	188	558.2539	0.2251	308	1168.036	163.6159	428	3009.845	10.5018
69	164.1789	0.0267	189	558.4702	1.1271	309	1169.2823	9.0518	429	3019.727	8.3161
70	164.6285	0.9076	190	559.0931	0.0123	310	1170.5068	5.5647	430	3019.733	18.942
71	170.2965	4.4672	191	560.2559	13.1406	311	1170.8311	92.7841	431	3025.57	13.6064
72	171.0083	2.4355	192	560.356	0.5944	312	1172.9573	96.3338	432	3025.574	12.4637
73	174.7363	0.271	193	566.0267	17.2332	313	1186.7509	128.2454	433	3037.075	7.4631
74	175.5112	0.7453	194	566.1587	101.103	314	1188.1805	1.3201	434	3037.085	32.4424
75	177.9653	0.2647	195	587.052	1.3314	315	1188.8918	512.5512	435	3041.082	14.0929
76	178.6094	0.9903	196	587.0707	0.4614	316	1189.1157	4.3119	436	3041.161	12.4726
77	179.5194	2.1214	197	603.1327	1.0485	317	1190.7836	192.1441	437	3041.805	23.9032
78	179.6156	0.5158	198	603.3273	0.0552	318	1191.8115	62.8718	438	3041.866	2.0167
79	191.4749	1.3414	199	605.9629	0.9491	319	1192.1901	313.5174	439	3052.987	6.4357
80	192.0656	0.0054	200	605.9741	0.1831	320	1192.6211	10.0804	440	3052.993	3.5845
81	195.2304	0.5436	201	607.8784	5.5043	321	1194.2288	28.436	441	3055.904	7.0009
82	195.4474	0.1059	202	609.2886	3.1889	322	1194.7522	95.5521	442	3055.91	6.0387
83	230.2581	0.0595	203	610.2166	0.141	323	1196.1406	114.8653	443	3059.83	29.1989
84	230.4412	2.3876	204	610.8591	6.1366	324	1197.6332	201.6475	444	3059.871	0.8544
85	234.2432	0.0139	205	624.3215	17.5685	325	1198.0195	201.9514	445	3061.699	1.3036
86	234.4154	1.8628	206	624.3734	3.9477	326	1200.8888	24.5393	446	3061.705	7.5707
87	239.9876	12.2347	207	636.2115	23.2358	327	1204.7794	94.4953	447	3064.47	20.1514
88	240.7008	0.2547	208	636.4329	4.1875	328	1205.3092	36.2751	448	3064.51	11.1096
89	246.8294	0.8902	209	644.1686	18.1946	329	1207.752	13.4785	449	3069.565	23.9465
90	247.1917	5.934	210	644.8497	18.1752	330	1208.1113	209.2085	450	3069.581	48.8914
91	250.1897	7.5263	211	655.453	2.1218	331	1213.0865	285.9147	451	3073.948	19.2238
92	250.2596	0.0014	212	655.5722	81.5692	332	1214.9287	0.7467	452	3073.981	7.9304
93	256.3462	0.2383	213	664.4965	8.9489	333	1215.3322	26.3651	453	3074.718	15.3876
94	256.9672	0.1474	214	665.1174	5.2208	334	1215.8711	292.2554	454	3074.723	24.785
95	259.6535	0.231	215	683.3149	23.3212	335	1216.3973	19.3506	455	3083.802	0.3026
96	260.0571	2.1969	216	683.4789	13.4304	336	1216.9692	47.6796	456	3083.857	19.5668

97	261.8906	0.8139	217	705.5158	7.306	337	1220.684	27.4174	457	3086.039	14.6355
98	262.7152	33.537	218	706.0763	28.4216	338	1221.2677	443.0753	458	3086.046	9.6401
99	266.4982	23.9173	219	708.2771	26.7218	339	1227.582	12.8675	459	3087.772	2.884
100	266.5299	27.0561	220	708.3305	33.3201	340	1227.9115	85.0382	460	3087.774	6.3512
101	271.5129	4.9916	221	709.3667	17.2126	341	1231.8969	222.4502	461	3091.601	34.5063
102	272.1368	2.1913	222	710.4423	23.5681	342	1232.0673	114.5695	462	3091.64	7.8939
103	276.9595	10.013	223	715.797	53.3141	343	1239.6857	1100.6508	463	3093.44	29.4107
104	277.9037	0.8167	224	716.0526	25.9722	344	1240.1053	53.4788	464	3093.748	2.6994
105	281.2115	19.2961	225	724.9306	63.886	345	1240.855	16.7519	465	3111.104	6.7267
106	281.2524	0.3784	226	725.4354	29.5963	346	1242.222	6.3087	466	3111.122	5.725
107	286.2267	2.5825	227	726.6488	0.7845	347	1245.0399	38.6412	467	3113.21	28.2371
108	287.4979	1.61	228	727.1819	183.366	348	1245.2524	518.6683	468	3113.216	26.7915
109	289.3035	10.0548	229	741.3924	60.0229	349	1248.4373	50.074	469	3118.513	20.3761
110	289.6203	18.0226	230	743.2417	69.927	350	1249.4003	36.4629	470	3118.53	9.7234
111	289.7111	146.802	231	752.101	5.4088	351	1251.4583	13.9457	471	3123.5	25.0637
112	290.0321	34.7059	232	752.285	6.6702	352	1255.7581	1.684	472	3123.614	0.6283
113	297.3058	1.3884	233	758.7352	0.0429	353	1278.2346	1.3655	473	3694.809	84.62
114	297.318	1.1216	234	758.9894	23.0803	354	1278.2856	48.0886	474	3695.257	890.5644
115	317.8942	0.0112	235	768.0235	9.1112	355	1285.1005	168.4316	475	3795.945	231.8715
116	318.3214	22.2431	236	768.1011	0.2654	356	1285.2769	51.5857	476	3796.185	92.4998
117	319.3927	1.4922	237	774.9147	12.4823	357	1286.6254	0.8306	477	3816.08	30.5052
118	319.8516	1.1434	238	774.9609	9.9238	358	1287.5844	186.1483	478	3816.096	169.261
119	320.3303	23.6771	239	787.3419	60.2272	359	1288.8577	201.0338	479	3816.739	58.5922
120	320.8412	13.9743	240	787.9682	0.0081	360	1289.6588	720.1578	480	3816.768	80.9337