

Supporting Information

1 Vibrational Analysis

apfd/pyCCCCC_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	56.7999	0.0648	0.0000
2	B1	79.8991	0.1271	0.0190
3	B1	149.1978	0.2098	0.0006
4	A1	209.9367	0.8712	0.0611
5	B2	219.0971	0.8779	0.4391
6	A1	221.3825	0.8041	0.0567
7	B2	232.6275	1.1065	0.0112
8	B1	285.1958	0.6464	0.6747
9	B2	321.3286	1.7030	0.1095
10	A1	344.1511	1.9917	0.2967
11	A2	369.1605	1.0053	0.0000
12	A1	393.2779	2.9670	0.1476
13	A1	541.7568	3.0003	6.8030
14	B1	581.2350	2.4708	1.2827
15	B2	586.3448	2.6673	0.0333
16	A2	635.5080	2.8804	0.0000
17	B2	689.2321	4.4218	95.6275
18	B1	741.5889	3.9598	0.1184
19	A1	831.3157	5.6141	93.5440
20	B2	880.5866	6.0198	5.4375
21	A1	1096.8954	8.9433	32.7060
22	A1	1228.4865	10.9823	5.0347
23	B2	1290.2152	11.9167	65.6718
24	A1	1370.0203	13.4491	130.7833
25	B2	1374.1431	13.8617	392.0406
26	A1	1551.4860	17.1342	105.1605
27	B2	1589.3677	18.7437	67.1372

apfd/pyCCCCC_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	58.7778	0.0694	0.0000
2	B1	82.0434	0.1336	0.0130
3	B1	149.8644	0.2116	0.0010
4	A1	208.8100	0.8720	0.0323
5	B2	218.9371	0.8725	0.3648
6	A1	221.9449	0.8041	0.0324
7	B2	227.7315	1.0625	0.0009
8	B1	287.5452	0.6580	0.6666
9	B2	323.9624	1.7159	0.1302

10	A1	347.8301	2.0102	0.2504
11	A2	372.7186	1.0249	0.0000
12	A1	396.3198	3.0124	0.1240
13	A1	548.8576	3.0883	5.4075
14	B1	589.1724	2.5386	1.1837
15	B2	593.3254	2.7374	0.0067
16	A2	650.7921	3.0209	0.0000
17	B2	699.1473	4.5456	88.6068
18	B1	765.9439	4.2255	1.2745
19	A1	833.7342	5.6557	87.8793
20	B2	877.8470	6.0113	4.8459
21	A1	1095.6861	8.9320	29.8361
22	A1	1225.5759	10.9256	6.2412
23	B2	1290.7647	11.9368	58.9271
24	A1	1367.7559	13.4018	111.8603
25	B2	1371.2455	13.8040	358.3705
26	A1	1549.2382	17.0781	95.0518
27	B2	1582.8932	18.5601	59.6360

apfd/pyCCCCC_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	58.9766	0.0698	0.0000
2	B1	82.3649	0.1346	0.0153
3	B1	150.5996	0.2138	0.0036
4	A1	210.4590	0.8860	0.0434
5	B2	220.6526	0.8858	0.3254
6	A1	224.0852	0.8202	0.0308
7	B2	228.9412	1.0738	0.0000
8	B1	288.5695	0.6627	0.6079
9	B2	326.5033	1.7408	0.1461
10	A1	350.1383	2.0296	0.2665
11	A2	375.1850	1.0386	0.0000
12	A1	398.9704	3.0499	0.1118
13	A1	553.1984	3.1384	5.2436
14	B1	592.1170	2.5642	1.1585
15	B2	600.0629	2.7981	0.0169
16	A2	654.0739	3.0518	0.0000
17	B2	705.7206	4.6359	89.3835
18	B1	768.1696	4.2498	1.2566
19	A1	837.7382	5.7149	90.9583
20	B2	883.8337	6.0980	4.3405
21	A1	1100.4045	9.0134	30.4725
22	A1	1227.8956	10.9693	5.8685
23	B2	1292.5920	11.9632	64.3120
24	A1	1369.7823	13.4401	114.5500
25	B2	1373.2776	13.8434	353.5460
26	A1	1549.6264	17.0867	98.7696
27	B2	1585.7973	18.6442	59.0862

apfd/pyCCCCC_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	57.3857	0.0662	0.0000
2	B1	80.0672	0.1274	0.0166
3	B1	148.4505	0.2077	0.0151
4	A1	205.5593	0.8296	0.0434
5	B2	214.8604	0.8481	0.3015
6	A1	216.2085	0.7706	0.0086
7	B2	229.5724	1.0749	0.0182
8	B1	284.4518	0.6431	0.3803
9	B2	314.7114	1.6455	0.1452
10	A1	337.5820	1.9356	0.3085
11	A2	369.7067	1.0082	0.0000
12	A1	385.4639	2.8608	0.2222
13	A1	530.9297	2.8774	7.6073
14	B2	572.0929	2.5424	0.1599
15	B1	579.4820	2.4531	0.9704
16	A2	636.7591	2.8919	0.0000
17	B2	671.8077	4.1931	95.8407
18	B1	746.0898	4.0143	1.5525
19	A1	821.2709	5.4676	95.4724
20	B2	868.7472	5.8377	4.6967
21	A1	1087.0909	8.7780	34.2794
22	A1	1222.9560	10.8682	4.6356
23	B2	1287.8319	11.8711	61.3224
24	A1	1364.1304	13.3298	128.7561
25	B2	1367.3657	13.7179	386.0770
26	A1	1548.0065	17.0583	105.3710
27	B2	1583.4164	18.6063	64.3255

apfd/pyFCFCF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	92.0519	0.1066	0.0000
2	B1	110.3501	0.1565	0.0046
3	A1	178.4705	0.4913	0.0039
4	B1	215.5716	0.4132	2.4715
5	B2	219.3510	0.6386	0.0493
6	B2	308.1768	1.2155	0.8477
7	B1	318.0298	0.8260	0.3803
8	A1	321.4933	1.3615	0.1400
9	A2	382.0386	1.0783	0.0000
10	B2	401.7572	1.7114	0.0502
11	A1	407.3167	1.9581	0.8878
12	A1	581.1036	3.1384	2.3944
13	A1	612.2765	3.7049	1.7542
14	B1	655.3322	3.1407	1.2951
15	B2	701.6644	3.8671	1.5205
16	A2	703.2011	3.5491	0.0000
17	B1	764.7114	4.2178	14.9666
18	B2	798.1851	5.3901	113.0029

19	A1	1083.5439	9.5909	184.5752
20	B2	1105.0110	9.9798	26.5168
21	A1	1155.6598	10.0317	4.9190
22	B2	1347.4937	13.1937	15.9157
23	A1	1442.0437	15.4919	49.7148
24	B2	1471.5930	15.9323	451.2270
25	A1	1490.7766	16.2889	93.5761
26	A1	1637.1124	19.1304	216.8316
27	B2	1657.7426	20.1708	75.3649

apfd/pyFCFCF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	93.2285	0.1093	0.0000
2	B1	111.3911	0.1593	0.0000
3	A1	180.1469	0.5027	0.0005
4	B1	213.3122	0.4044	2.2316
5	B2	221.9060	0.6518	0.0347
6	B2	311.4107	1.2382	0.9344
7	B1	319.1749	0.8333	0.5385
8	A1	324.0413	1.3677	0.1509
9	A2	374.2689	1.0345	0.0000
10	B2	405.2752	1.7462	0.1091
11	A1	410.1050	1.9885	0.7220
12	A1	583.9095	3.1832	1.7692
13	A1	616.7804	3.7551	1.2304
14	B1	656.7776	3.1552	1.2470
15	B2	706.7214	3.9194	0.5030
16	A2	710.5587	3.6255	0.0000
17	B1	779.9882	4.3866	11.8375
18	B2	801.4124	5.4468	105.7967
19	A1	1089.6499	9.6707	166.0084
20	B2	1112.1781	10.1068	21.3496
21	A1	1156.2087	10.0605	2.7440
22	B2	1342.4402	13.1083	11.7388
23	A1	1448.6499	15.6143	56.7547
24	B2	1471.7941	15.9390	426.9914
25	A1	1490.8092	16.3316	74.6289
26	A1	1634.0318	19.0585	207.2454
27	B2	1651.3286	19.9959	76.9487

apfd/pyFCFCF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	93.0904	0.1090	0.0000
2	B1	111.2491	0.1589	0.0011
3	A1	183.4302	0.5221	0.0001
4	B1	214.0062	0.4072	1.9637
5	B2	225.6282	0.6735	0.0297
6	B2	313.7432	1.2548	0.9239

7	B1	320.1809	0.8380	0.4915
8	A1	325.7072	1.3732	0.1341
9	A2	377.1401	1.0506	0.0000
10	B2	406.1290	1.7539	0.1294
11	A1	411.7561	2.0037	0.6710
12	A1	586.2555	3.2356	1.4725
13	A1	618.1566	3.7519	1.2936
14	B1	657.5653	3.1630	1.0216
15	B2	710.4276	3.9575	0.4131
16	A2	711.6757	3.6370	0.0000
17	B1	779.8493	4.3850	11.1441
18	B2	806.0524	5.5244	104.3850
19	A1	1091.4870	9.7080	168.0551
20	B2	1114.5519	10.1447	20.1166
21	A1	1159.9241	10.1197	3.2033
22	B2	1345.5965	13.1644	13.0611
23	A1	1453.0919	15.7280	55.1435
24	B2	1475.0132	16.0096	419.0843
25	A1	1492.9696	16.3657	82.8672
26	A1	1635.7640	19.1022	212.2479
27	B2	1654.9592	20.0967	79.3202

apfd/pyFCFCF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	92.0250	0.1065	0.0000
2	B1	110.1822	0.1558	0.0042
3	A1	176.8227	0.4816	0.0088
4	B1	212.5627	0.4012	2.1459
5	B2	218.4191	0.6339	0.0214
6	B2	306.8395	1.2100	0.6809
7	B1	316.6615	0.8206	0.2240
8	A1	319.6737	1.3622	0.0603
9	A2	371.9201	1.0211	0.0000
10	B2	399.8440	1.6930	0.0120
11	A1	404.3164	1.9264	0.9758
12	A1	577.2242	3.0546	2.3500
13	A1	611.2926	3.7204	1.1509
14	B1	652.7549	3.1154	0.6732
15	B2	696.4646	3.8124	1.4634
16	A2	704.1005	3.5612	0.0000
17	B1	767.9398	4.2543	17.7712
18	B2	788.1680	5.2316	108.2729
19	A1	1084.2601	9.5646	180.9993
20	B2	1107.4897	10.0237	22.0778
21	A1	1149.2223	9.9392	2.0634
22	B2	1348.8318	13.2362	11.7547
23	A1	1450.5631	15.6651	55.7437
24	B2	1473.7182	15.9715	442.4508
25	A1	1493.5226	16.3958	82.1317
26	A1	1637.3395	19.1364	221.7564
27	B2	1654.5528	20.1034	73.5516

apfd/pyFCFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	97.6656	0.1190	0.0006
2	A"	141.0798	0.2190	0.0016
3	A'	195.7454	0.5289	0.0400
4	A"	215.5516	0.4122	3.3344
5	A'	273.3386	0.8325	0.2953
6	A'	312.1306	1.1942	0.6421
7	A"	329.6643	0.8781	0.7945
8	A'	337.2553	1.2513	0.5987
9	A'	400.3903	1.7583	0.3172
10	A"	415.4195	1.2900	1.4015
11	A'	469.9705	2.0979	0.4574
12	A'	596.4101	3.5603	0.9974
13	A'	630.6674	3.6787	7.2178
14	A"	645.2325	3.0474	1.8788
15	A"	697.2442	3.4909	0.2989
16	A'	730.5687	4.1855	0.6500
17	A"	750.4004	4.0628	10.2818
18	A'	912.4975	7.0303	148.4631
19	A'	1090.1893	9.7188	183.6101
20	A'	1117.2347	10.1330	51.5353
21	A'	1267.6565	12.3689	21.8272
22	A'	1355.5743	13.3523	20.9384
23	A'	1448.8293	15.6002	41.0747
24	A'	1491.4746	16.3126	302.1203
25	A'	1538.2087	17.5919	438.4100
26	A'	1658.1797	19.6657	181.2696
27	A'	1680.9689	20.6095	13.1989

apfd/pyFCFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	99.0993	0.1224	0.0002
2	A"	142.2297	0.2227	0.0015
3	A'	198.0836	0.5423	0.0289
4	A"	214.0775	0.4061	2.8153
5	A'	274.6151	0.8388	0.3435
6	A'	314.5379	1.2056	0.6699
7	A"	331.3896	0.8884	0.8929
8	A'	338.2918	1.2589	0.5358
9	A'	403.0116	1.7851	0.2343
10	A"	415.3186	1.2899	1.1245
11	A'	470.8529	2.1041	0.5211
12	A'	599.2813	3.5893	0.9431
13	A'	634.1509	3.7372	5.6624
14	A"	650.1437	3.0968	2.0573
15	A"	711.9832	3.6412	0.5644

16	A'	733.5038	4.2163	0.4465
17	A''	777.8789	4.3598	7.6578
18	A'	915.2744	7.0641	135.7934
19	A'	1095.8836	9.8071	161.0088
20	A'	1123.2902	10.2518	53.3660
21	A'	1271.9252	12.4637	20.0779
22	A'	1349.4418	13.2538	16.3485
23	A'	1453.4852	15.6911	44.2179
24	A'	1491.0485	16.3079	288.8581
25	A'	1537.8945	17.6087	414.3539
26	A'	1654.1139	19.5730	176.9933
27	A'	1674.5596	20.4384	11.2215

apfd/pyFCFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	98.8752	0.1218	0.0000
2	A''	141.5692	0.2207	0.0002
3	A'	201.7971	0.5633	0.0298
4	A''	214.3722	0.4072	2.4854
5	A'	275.8629	0.8456	0.3404
6	A'	316.3063	1.2132	0.6697
7	A''	332.0955	0.8922	0.8429
8	A'	339.2677	1.2674	0.4799
9	A'	404.2829	1.7971	0.2220
10	A''	416.3716	1.2960	1.0474
11	A'	471.5325	2.1106	0.5419
12	A'	599.9954	3.6099	0.7233
13	A'	637.0260	3.7697	5.4037
14	A''	649.5390	3.0903	1.7329
15	A''	710.8173	3.6292	0.3674
16	A'	735.3072	4.2345	0.4177
17	A''	772.2481	4.2999	7.1447
18	A'	917.9518	7.1125	134.8279
19	A'	1097.7592	9.8385	164.3015
20	A'	1126.0855	10.2967	50.1533
21	A'	1275.0826	12.5229	20.3675
22	A'	1352.4238	13.3090	17.3551
23	A'	1457.7518	15.7935	45.2017
24	A'	1493.9866	16.3620	273.9791
25	A'	1540.7842	17.6798	423.7612
26	A'	1656.6216	19.6266	179.4969
27	A'	1677.4609	20.5281	12.0834

apfd/pyFCFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	97.7740	0.1191	0.0004
2	A''	140.6399	0.2177	0.0005
3	A'	194.4790	0.5212	0.0664

4	A''	213.4441	0.4036	2.9689
5	A'	275.2639	0.8461	0.2902
6	A'	310.9124	1.1946	0.5598
7	A''	328.3932	0.8726	0.5955
8	A'	336.2566	1.2423	0.5301
9	A'	398.1412	1.7361	0.3378
10	A''	413.9443	1.2811	1.6374
11	A'	469.0634	2.0872	0.5462
12	A'	595.8029	3.5201	1.3831
13	A'	626.0967	3.6376	6.3562
14	A''	645.5349	3.0517	1.5470
15	A''	706.0071	3.5818	1.1136
16	A'	727.1474	4.1467	0.5979
17	A''	766.4575	4.2344	9.6409
18	A'	908.7161	6.9497	138.6781
19	A'	1091.1858	9.7287	174.7134
20	A'	1118.3973	10.1521	48.7891
21	A'	1269.6611	12.4298	19.7829
22	A'	1357.5292	13.4091	18.0017
23	A'	1456.2710	15.7584	44.7619
24	A'	1493.0177	16.3539	286.4453
25	A'	1543.4656	17.7405	435.7554
26	A'	1658.2244	19.6873	181.0908
27	A'	1680.3399	20.5758	11.7143

apfd/pyFFCFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	116.7130	0.1488	0.0000
2	B1	122.6883	0.1852	0.0260
3	B2	204.2669	0.5912	0.0344
4	B1	209.9515	0.3858	3.1060
5	A1	281.0723	0.9002	0.7769
6	B2	310.4745	1.0443	0.2837
7	A1	334.9723	1.3703	0.9103
8	B1	336.8163	0.9302	0.8585
9	A1	433.7904	2.0074	0.0253
10	A2	449.6534	1.5061	0.0000
11	B2	457.5096	1.9774	0.0617
12	A1	546.1237	3.1163	1.6911
13	B1	600.9550	2.6388	8.5153
14	A2	699.5222	3.5131	0.0000
15	A1	704.1003	4.5605	9.5905
16	B2	731.1216	4.1608	0.0010
17	B1	740.7813	3.9586	2.8344
18	A1	939.4147	7.1870	145.2118
19	B2	984.6806	8.3934	174.2201
20	B2	1182.5664	11.2411	0.5819
21	A1	1266.6039	12.2051	65.1616
22	B2	1351.6600	13.2465	33.1822
23	A1	1455.0398	15.8685	6.0340
24	A1	1498.7192	16.2807	89.7800

25	B2	1522.8824	17.2588	760.2220
26	A1	1669.2435	19.9111	129.8003
27	B2	1670.0966	20.4382	4.5749

apfd/pyFFCFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.5918	0.1511	0.0000
2	B1	124.4619	0.1908	0.0412
3	B2	202.8751	0.5829	0.0256
4	B1	209.1605	0.3824	2.5184
5	A1	281.3304	0.9025	0.9104
6	B2	311.5501	1.0512	0.3048
7	A1	335.0082	1.3707	0.7206
8	B1	337.9559	0.9368	0.8482
9	A1	433.8117	2.0069	0.0101
10	A2	448.9728	1.5016	0.0000
11	B2	457.7347	1.9776	0.0472
12	A1	547.8637	3.1320	1.9238
13	B1	603.0269	2.6599	8.0429
14	A1	704.7996	4.5672	7.4449
15	A2	714.8745	3.6695	0.0000
16	B2	732.7753	4.1813	0.0503
17	B1	771.3948	4.2888	2.2737
18	A1	938.9485	7.1760	134.8103
19	B2	989.2353	8.4637	155.7066
20	B2	1189.7853	11.3744	0.4825
21	A1	1269.5191	12.2678	61.9168
22	B2	1343.1653	13.1067	29.5730
23	A1	1457.5439	15.9155	7.8142
24	A1	1498.0074	16.2851	86.0601
25	B2	1522.4595	17.2599	722.3362
26	B2	1663.3666	20.2580	3.8371
27	A1	1663.6467	19.7849	122.0600

apfd/pyFFCFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.2065	0.1500	0.0000
2	B1	124.3328	0.1904	0.0366
3	B2	204.8865	0.5947	0.0183
4	B1	209.4501	0.3836	2.2075
5	A1	282.7241	0.9116	0.9062
6	B2	312.6780	1.0589	0.2683
7	A1	335.8976	1.3756	0.6808
8	B1	338.1453	0.9375	0.7985
9	A1	434.5679	2.0139	0.0028
10	A2	450.3587	1.5110	0.0000
11	B2	458.6117	1.9858	0.0524
12	A1	548.5369	3.1428	1.9067

13	B1	604.7266	2.6748	7.6873
14	A1	705.7491	4.5789	6.9370
15	A2	712.9042	3.6499	0.0000
16	B2	734.0154	4.1956	0.0351
17	B1	766.8865	4.2395	1.6641
18	A1	942.1897	7.2277	135.2265
19	B2	990.7858	8.4867	154.6921
20	B2	1192.7618	11.4265	0.2263
21	A1	1273.1739	12.3352	62.1953
22	B2	1345.7441	13.1569	30.3630
23	A1	1461.1527	16.0058	6.3702
24	A1	1499.8366	16.3178	87.5233
25	B2	1526.2500	17.3396	720.6122
26	B2	1665.3011	20.3215	4.4418
27	A1	1666.3721	19.8519	123.4649

apfd/pyFFCFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	115.8870	0.1467	0.0000
2	B1	123.0695	0.1864	0.0323
3	B2	205.5481	0.5983	0.0045
4	B1	207.9986	0.3781	2.6860
5	A1	282.5917	0.9109	0.7822
6	B2	311.4886	1.0514	0.2767
7	A1	333.8220	1.3645	0.7494
8	B1	335.0066	0.9210	0.6936
9	A1	432.0825	1.9923	0.0376
10	A2	448.4015	1.4975	0.0000
11	B2	456.2668	1.9643	0.0644
12	A1	545.6669	3.1008	1.9280
13	B1	595.5006	2.5927	10.2454
14	A1	702.6330	4.5371	8.0638
15	A2	710.0208	3.6208	0.0000
16	B2	728.9981	4.1361	0.0016
17	B1	761.5317	4.1817	1.3417
18	A1	932.8811	7.0780	139.5261
19	B2	986.7385	8.4203	161.9000
20	B2	1188.5877	11.3586	0.2200
21	A1	1266.1928	12.2021	60.4562
22	B2	1354.1516	13.3091	31.7474
23	A1	1461.3012	16.0048	5.3130
24	A1	1499.9806	16.3251	91.7436
25	B2	1528.3462	17.4023	750.0778
26	B2	1669.8456	20.4214	2.6370
27	A1	1670.2456	19.9440	126.5980

apfd/pyFFFFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	118.7530	0.1541	0.0000
2	B1	157.7948	0.2696	0.0007
3	B1	216.8321	0.4158	4.4979
4	B2	269.9262	0.8061	0.0540
5	A1	272.5174	0.8106	0.7208
6	B2	321.4333	1.1032	0.7642
7	A1	349.8319	1.2632	1.3811
8	B1	353.6194	1.0128	3.2126
9	A2	438.5813	1.4333	0.0000
10	B2	452.3269	1.9355	0.0890
11	A1	477.6167	2.1368	0.2322
12	A1	600.0142	3.6869	0.0128
13	B1	634.8080	2.9527	2.9102
14	A2	692.2419	3.4409	0.0000
15	A1	705.4279	4.5399	6.5759
16	B1	732.5709	3.8765	5.9267
17	B2	751.7567	4.4227	0.0387
18	B2	1003.9934	8.6531	218.3787
19	A1	1103.2982	10.0252	245.6897
20	B2	1183.1760	11.3012	0.0336
21	A1	1312.0177	13.2331	29.4976
22	B2	1363.7833	13.4995	21.8093
23	A1	1461.5237	15.8227	16.7168
24	B2	1533.0085	17.5269	726.4192
25	A1	1565.5984	18.0975	165.8817
26	A1	1680.2088	20.1422	120.2815
27	B2	1694.6705	20.9364	4.5803

apfd/pyFFFFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	119.8405	0.1569	0.0000
2	B1	159.2361	0.2748	0.0000
3	B1	216.1350	0.4127	3.5664
4	B2	271.0851	0.8130	0.0546
5	A1	273.2802	0.8150	0.8361
6	B2	322.4147	1.1095	0.7166
7	A1	350.0441	1.2646	1.1566
8	B1	355.8483	1.0266	2.8466
9	A2	439.3349	1.4384	0.0000
10	B2	453.3929	1.9438	0.0822
11	A1	478.7250	2.1445	0.3033
12	A1	602.8977	3.7208	0.0222
13	B1	644.7796	3.0540	3.4206
14	A1	705.6209	4.5431	5.0538
15	A2	713.8049	3.6584	0.0000
16	B2	754.1319	4.4531	0.0000
17	B1	776.3107	4.3397	4.4191
18	B2	1009.1994	8.7345	200.7659
19	A1	1109.0890	10.1264	229.4695
20	B2	1190.0025	11.4274	0.0001
21	A1	1316.2712	13.3303	27.0255

22	B2	1355.6958	13.3625	18.1563
23	A1	1464.0694	15.8615	20.5903
24	B2	1532.5216	17.5177	700.5993
25	A1	1565.3936	18.1227	157.3623
26	A1	1675.3707	20.0301	114.3002
27	B2	1688.1349	20.7649	3.4886

apfd/pyFFFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	119.1658	0.1551	0.0000
2	B1	158.1921	0.2711	0.0004
3	B1	216.0990	0.4125	3.1581
4	B2	272.0709	0.8189	0.0579
5	A1	274.1865	0.8203	0.8479
6	B2	323.0381	1.1137	0.6906
7	A1	350.5513	1.2684	1.0663
8	B1	355.5751	1.0250	2.6549
9	A2	440.0252	1.4430	0.0000
10	B2	453.8671	1.9481	0.0878
11	A1	478.9216	2.1463	0.3468
12	A1	603.1958	3.7238	0.0281
13	B1	642.9277	3.0344	2.9366
14	A1	706.5111	4.5540	4.7903
15	A2	710.6124	3.6266	0.0000
16	B2	754.5788	4.4580	0.0003
17	B1	765.7312	4.2270	3.9253
18	B2	1010.4743	8.7556	197.9445
19	A1	1110.7998	10.1561	230.0952
20	B2	1192.7890	11.4797	0.0164
21	A1	1318.8923	13.3828	27.7876
22	B2	1358.4181	13.4148	18.9491
23	A1	1468.1211	15.9529	20.9124
24	B2	1536.4851	17.6087	691.2463
25	A1	1567.8529	18.1807	155.2710
26	A1	1677.5960	20.0852	116.3762
27	B2	1690.9235	20.8414	3.9451

apfd/pyFFFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.8632	0.1517	0.0000
2	B1	157.3441	0.2681	0.0000
3	B1	215.7065	0.4113	4.0750
4	B2	272.5498	0.8217	0.0572
5	A1	274.0465	0.8199	0.7490
6	B2	321.1983	1.1017	0.7939
7	A1	348.7833	1.2551	1.3070
8	B1	352.7790	1.0090	2.9976
9	A2	439.0040	1.4360	0.0000

10	B2	451.6829	1.9288	0.0903
11	A1	477.6643	2.1343	0.2692
12	A1	600.5380	3.6909	0.0062
13	B1	639.6958	3.0045	3.2363
14	A1	703.7543	4.5161	5.3260
15	A2	708.4695	3.6051	0.0000
16	B2	749.4484	4.3939	0.0057
17	B1	765.0665	4.2163	4.2492
18	B2	1005.5711	8.6744	202.8155
19	A1	1104.7439	10.0455	233.6439
20	B2	1189.0964	11.4153	0.0005
21	A1	1314.7163	13.3083	27.3803
22	B2	1365.9398	13.5550	19.4222
23	A1	1467.5751	15.9461	19.0480
24	B2	1537.5482	17.6421	710.6775
25	A1	1571.1102	18.2516	162.6971
26	A1	1681.5096	20.1788	117.7793
27	B2	1694.3771	20.9228	2.8677

apfd/pyFFHFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	115.1322	0.1450	0.0000
2	B1	205.0657	0.3325	3.6360
3	A1	281.7027	0.8482	0.6413
4	B1	299.4534	0.4399	1.0078
5	B2	304.1805	0.9703	0.1978
6	A1	364.7184	1.2555	2.6598
7	B2	452.7596	1.7433	0.0744
8	A2	464.1784	1.6044	0.0000
9	B1	488.4663	0.6192	0.4824
10	A1	511.2667	2.2774	1.7902
11	B2	669.9200	1.5924	2.5913
12	A1	695.7065	4.2541	16.9651
13	A2	704.6775	3.5633	0.0000
14	B1	732.7013	2.6944	10.8511
15	A1	760.5820	3.2842	10.4651
16	B1	895.3136	0.6574	31.6909
17	B2	924.7138	2.7536	133.6035
18	B2	1167.3177	3.8753	22.6521
19	B2	1205.6289	1.5622	57.3617
20	A1	1243.2961	10.2652	203.6284
21	B2	1353.7746	12.8899	82.4971
22	A1	1438.7430	14.3599	0.3373
23	A1	1482.9362	14.8231	46.0689
24	B2	1537.4897	10.8659	744.3958
25	A1	1679.4412	19.1167	26.8907
26	B2	1687.4812	15.3582	1.4578
27	A1	3231.3244	6.7305	4.8250

apfd/pyFFHFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	116.3860	0.1481	0.0000
2	B1	205.3608	0.3358	2.8332
3	A1	282.1584	0.8506	0.6989
4	B1	301.8547	0.4451	0.9996
5	B2	305.1686	0.9765	0.1527
6	A1	364.9283	1.2563	2.2275
7	B2	452.8243	1.7417	0.0565
8	A2	464.4240	1.6062	0.0000
9	B1	492.5865	0.6147	0.4289
10	A1	512.8261	2.2857	2.0293
11	B2	672.4492	1.5957	2.5567
12	A1	697.6327	4.3044	14.3041
13	A2	723.0879	3.7520	0.0000
14	B1	757.2489	2.1743	12.8885
15	A1	761.5763	3.2863	10.9938
16	B1	913.5768	0.7286	24.9857
17	B2	927.8706	2.7237	117.7370
18	B2	1173.9558	3.6036	26.2260
19	B2	1209.0023	1.6471	48.7147
20	A1	1248.8539	10.3618	186.2712
21	B2	1345.2286	12.4984	76.7594
22	A1	1442.0021	14.3936	0.5912
23	A1	1482.5491	14.9099	48.4036
24	B2	1537.1855	10.9418	725.3916
25	A1	1674.8887	19.0319	26.3471
26	B2	1681.4441	14.9294	2.4787
27	A1	3224.7190	6.6994	3.9670

apfd/pyFFHFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	115.9709	0.1470	0.0000
2	B1	205.3034	0.3351	2.5250
3	A1	283.0784	0.8560	0.7069
4	B1	301.3117	0.4439	0.9918
5	B2	305.9074	0.9812	0.1458
6	A1	365.2391	1.2590	2.0947
7	B2	453.4912	1.7478	0.0541
8	A2	465.2427	1.6120	0.0000
9	B1	491.5625	0.6168	0.3538
10	A1	513.1389	2.2886	2.0743
11	B2	673.0441	1.6005	2.5148
12	A1	698.5930	4.3129	13.8686
13	A2	721.0540	3.7315	0.0000
14	B1	754.1693	2.3046	10.8007
15	A1	762.3187	3.2926	11.0665
16	B1	906.3486	0.7049	26.4761
17	B2	929.1649	2.7245	115.2663
18	B2	1177.0669	3.5071	27.2687

19	B2	1211.5781	1.6779	44.9486
20	A1	1252.1446	10.4032	187.5577
21	B2	1348.0225	12.5684	79.4150
22	A1	1445.0982	14.4070	0.5030
23	A1	1486.1422	15.0498	48.2478
24	B2	1541.5633	10.9904	714.3673
25	A1	1676.9040	19.0850	27.2966
26	B2	1684.4306	15.0203	2.2195
27	A1	3228.5409	6.7154	3.7109

apfd/pyFFHFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	114.5401	0.1434	0.0000
2	B1	203.9278	0.3310	3.2437
3	A1	283.2378	0.8571	0.6637
4	B1	299.7350	0.4409	1.0307
5	B2	305.7133	0.9811	0.2067
6	A1	363.9018	1.2494	2.3904
7	B2	452.2223	1.7401	0.0704
8	A2	463.5306	1.5998	0.0000
9	B1	487.5731	0.6070	0.3806
10	A1	511.7291	2.2768	1.7956
11	B2	669.8683	1.6092	2.3934
12	A1	695.4805	4.2710	14.3644
13	A2	717.2323	3.6925	0.0000
14	B1	749.1337	2.1930	12.3220
15	A1	760.1061	3.2727	10.9913
16	B1	904.5506	0.7069	28.7793
17	B2	926.4247	2.7369	123.7387
18	B2	1173.4323	3.5884	23.4745
19	B2	1209.8371	1.6228	47.9115
20	A1	1244.8466	10.2966	195.4937
21	B2	1357.3362	12.8881	75.0599
22	A1	1445.4968	14.4190	0.3204
23	A1	1485.2383	14.9427	46.5689
24	B2	1541.1729	11.1506	735.6311
25	A1	1682.0211	19.1977	26.6475
26	B2	1686.3131	15.3100	2.5358
27	A1	3235.6768	6.7485	6.0300

apfd/pyFHFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	128.7659	0.1629	0.1289
2	A''	211.6969	0.3573	3.9939
3	A''	261.1863	0.2898	1.1696
4	A'	272.5494	0.8097	0.2174
5	A'	323.1163	1.0569	1.0466
6	A'	357.2501	1.2376	1.4887

7	A''	389.5848	0.9302	0.8279
8	A'	464.4945	1.8125	0.4654
9	A'	522.6719	1.7569	2.2967
10	A'	602.0815	3.6990	0.0051
11	A''	634.6828	1.2884	6.0298
12	A'	677.4154	1.6943	2.5127
13	A''	689.0113	1.9674	0.0013
14	A''	744.1545	2.2285	1.4985
15	A'	806.0961	3.8497	39.3434
16	A''	849.1766	0.6672	39.3069
17	A'	1039.3850	2.6693	91.4548
18	A'	1092.6579	7.8647	184.1383
19	A'	1174.1756	1.5629	97.2887
20	A'	1264.5017	6.1868	41.2956
21	A'	1368.4975	12.7832	10.7830
22	A'	1436.1236	12.0795	50.7022
23	A'	1483.8398	13.9967	178.5303
24	A'	1551.1872	10.4678	433.6344
25	A'	1672.3109	16.6146	272.2857
26	A'	1691.3634	19.1978	48.9483
27	A'	3245.6223	6.7914	5.3129

apfd/pyFHFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	129.5684	0.1649	0.1026
2	A''	211.6786	0.3615	3.1476
3	A''	263.4090	0.2920	1.2556
4	A'	273.7879	0.8169	0.2615
5	A'	324.3969	1.0631	0.9219
6	A'	358.5302	1.2477	1.1552
7	A''	389.9204	0.9399	0.7617
8	A'	464.8825	1.8176	0.4199
9	A'	523.2345	1.7662	1.9823
10	A'	605.7080	3.7372	0.0085
11	A''	641.3980	1.2721	6.3262
12	A'	680.6217	1.7022	2.6455
13	A''	699.5562	1.8062	0.0001
14	A''	767.4215	1.9797	0.2482
15	A'	807.7000	3.8501	34.5265
16	A''	863.7017	0.7519	35.8538
17	A'	1042.0455	2.5619	79.9189
18	A'	1100.7008	7.9225	166.7718
19	A'	1179.7784	1.6094	99.2265
20	A'	1268.6587	6.4587	37.3124
21	A'	1361.0723	12.3897	10.8814
22	A'	1441.1994	12.3103	54.2903
23	A'	1482.9717	13.9196	164.7815
24	A'	1551.3337	10.5115	423.5974
25	A'	1667.8047	16.3483	259.8058
26	A'	1685.3818	18.8928	46.4238
27	A'	3239.5772	6.7629	4.2165

apfd/pyFHFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	129.0840	0.1637	0.0927
2	A"	211.4519	0.3591	2.8652
3	A"	262.7177	0.2917	1.2438
4	A'	274.7983	0.8231	0.2667
5	A'	325.1821	1.0681	0.9071
6	A'	359.1208	1.2519	1.0964
7	A"	389.8996	0.9402	0.6545
8	A'	465.4757	1.8225	0.4136
9	A'	523.9079	1.7717	1.8415
10	A'	606.1993	3.7420	0.0076
11	A"	640.8531	1.2919	5.6963
12	A'	681.2680	1.7049	2.5519
13	A"	699.1073	1.8433	0.0036
14	A"	762.2804	2.1154	0.4197
15	A'	808.7339	3.8597	34.0876
16	A"	855.9834	0.7136	34.8230
17	A'	1043.7625	2.5424	78.4251
18	A'	1103.2911	7.9949	164.8398
19	A'	1182.5564	1.6161	96.8318
20	A'	1271.3052	6.5649	37.7381
21	A'	1364.1946	12.4003	11.5817
22	A'	1445.3958	12.5466	53.9341
23	A'	1486.8107	13.9318	155.2969
24	A'	1554.6747	10.5859	422.2866
25	A'	1670.2861	16.3698	263.7289
26	A'	1688.0897	18.9836	47.4673
27	A'	3243.4538	6.7789	3.9847

apfd/pyFHFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	128.1960	0.1614	0.1193
2	A"	211.0210	0.3585	3.6368
3	A"	261.1690	0.2894	1.2759
4	A'	274.3164	0.8200	0.2285
5	A'	322.5821	1.0554	1.0253
6	A'	356.1139	1.2299	1.3527
7	A"	388.4580	0.9257	0.7142
8	A'	463.6089	1.8037	0.4674
9	A'	521.7984	1.7557	1.9081
10	A'	602.5803	3.7028	0.0047
11	A"	637.5147	1.2905	6.2238
12	A'	675.9277	1.7070	2.4619
13	A"	695.0807	1.8180	0.0010
14	A"	760.9464	2.0730	0.3233
15	A'	805.5278	3.8346	35.5511

16	A''	857.9114	0.7184	39.7853
17	A'	1039.6966	2.6471	87.6292
18	A'	1094.4512	7.9174	170.8132
19	A'	1178.6958	1.5606	89.8306
20	A'	1268.1174	6.2702	37.3952
21	A'	1370.1254	12.8693	10.7141
22	A'	1443.1521	12.3090	56.4277
23	A'	1486.8845	13.9801	164.1442
24	A'	1554.9246	10.7237	435.8872
25	A'	1672.6373	16.6605	268.8653
26	A'	1691.3631	19.1857	44.5234
27	A'	3250.6358	6.8123	6.5666

apfd/pyHHHHH_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	377.7321	0.2146	0.0000
2	B1	414.3057	0.3785	3.8479
3	A1	604.3736	1.5182	3.4706
4	B2	634.3011	1.5158	0.3766
5	B1	716.3084	0.4153	69.7219
6	B1	761.2343	0.7991	12.3156
7	A2	897.0563	0.5918	0.0000
8	B1	958.5822	0.7225	0.0260
9	A2	1001.2253	0.8687	0.0000
10	A1	1008.8798	4.4156	4.2903
11	B1	1009.4736	0.7736	0.0069
12	A1	1044.0929	3.1969	5.2384
13	B2	1086.4671	1.2018	0.0179
14	A1	1101.1894	1.1529	7.0857
15	B2	1178.1433	0.9137	2.3894
16	A1	1250.4649	1.1539	4.5184
17	B2	1318.3290	7.8374	0.0021
18	B2	1379.8913	1.3467	0.0108
19	B2	1476.4596	2.6995	27.6504
20	A1	1516.7855	2.8024	3.0048
21	B2	1639.1964	9.7618	11.4544
22	A1	1645.0516	8.6580	24.7414
23	B2	3162.6487	6.4061	25.4050
24	A1	3164.9214	6.4327	3.3017
25	A1	3184.4320	6.5064	4.6609
26	B2	3201.4030	6.6046	22.0888
27	A1	3209.1080	6.6685	5.3742

apfd/pyHHHHH_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	379.7957	0.2143	0.0000
2	B1	416.3653	0.3785	3.6306
3	A1	606.7363	1.5313	4.2441

4	B2	643.4130	1.5534	0.2156
5	B1	721.0873	0.4058	64.8269
6	B1	769.1955	0.8228	8.4487
7	A2	902.8441	0.5997	0.0000
8	B1	967.8088	0.7395	0.0190
9	A1	1011.7119	4.3942	5.2376
10	A2	1015.8589	0.9005	0.0000
11	B1	1025.2949	0.8226	0.0150
12	A1	1049.5054	3.1262	5.4692
13	B2	1086.5353	1.2029	0.0142
14	A1	1101.5261	1.1690	4.7818
15	B2	1175.2348	0.9154	2.6016
16	A1	1248.7993	1.1592	3.6519
17	B2	1312.9735	7.4978	0.0181
18	B2	1382.9649	1.3538	0.0535
19	B2	1478.4874	2.7167	26.8660
20	A1	1520.1062	2.7968	2.8507
21	B2	1638.0906	9.5694	10.9525
22	A1	1643.2177	8.5235	24.1791
23	B2	3156.8499	6.3829	24.9262
24	A1	3159.2449	6.4112	3.6018
25	A1	3180.7666	6.4894	4.2173
26	B2	3197.4015	6.5858	21.3849
27	A1	3205.3585	6.6508	5.3899

apfd/pyHHHHH_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	380.6595	0.2150	0.0000
2	B1	417.3256	0.3818	3.5789
3	A1	607.6757	1.5382	4.4383
4	B2	645.3749	1.5646	0.2778
5	B1	721.1406	0.3989	65.8793
6	B1	770.9706	0.8507	7.2877
7	A2	903.2405	0.6001	0.0000
8	B1	967.1289	0.7408	0.0143
9	A1	1013.4609	4.4164	5.8016
10	A2	1015.4041	0.9006	0.0000
11	B1	1027.4618	0.8235	0.0039
12	A1	1050.7437	3.1279	5.8864
13	B2	1088.0291	1.2069	0.0075
14	A1	1103.0882	1.1716	4.7743
15	B2	1178.0880	0.9200	2.4717
16	A1	1250.9703	1.1629	3.4419
17	B2	1315.7986	7.5198	0.0043
18	B2	1384.8870	1.3571	0.0419
19	B2	1481.3949	2.7243	27.7542
20	A1	1522.4781	2.8087	3.3903
21	B2	1640.8691	9.6243	10.6388
22	A1	1645.4442	8.5452	24.7229
23	B2	3159.5367	6.3936	26.0974
24	A1	3162.0462	6.4231	4.6431

25	A1	3184.1278	6.5028	4.6239
26	B2	3200.9559	6.6001	21.7382
27	A1	3208.8376	6.6656	5.3341

apfd/pyHHHHH_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	379.0988	0.2143	0.0000
2	B1	414.7266	0.3778	3.7787
3	A1	604.6862	1.5217	3.6045
4	B2	634.9006	1.5176	0.4391
5	B1	715.7902	0.3964	75.9594
6	B1	766.2507	0.8345	9.6475
7	A2	897.1848	0.5919	0.0000
8	B1	959.9770	0.7280	0.0446
9	A1	1007.7149	4.4026	4.9640
10	A2	1007.9203	0.8850	0.0000
11	B1	1019.7672	0.8087	0.0328
12	A1	1045.7047	3.1801	5.1321
13	B2	1086.8160	1.1975	0.0705
14	A1	1100.8933	1.1516	7.2482
15	B2	1177.9817	0.9064	2.3165
16	A1	1249.8767	1.1494	3.8953
17	B2	1319.3337	8.1420	0.0247
18	B2	1377.7305	1.3433	0.0149
19	B2	1474.6828	2.7095	29.2580
20	A1	1514.8632	2.8027	4.0186
21	B2	1638.0755	9.8292	10.0774
22	A1	1645.1956	8.7954	24.2128
23	B2	3168.6014	6.4307	19.8605
24	A1	3170.7445	6.4570	3.1823
25	A1	3190.7404	6.5318	3.9686
26	B2	3207.1193	6.6282	16.4432
27	A1	3214.7813	6.6932	3.5228

b3lyp/pyCCCCC_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	56.7015	0.0647	0.0000
2	A''	79.2614	0.1252	0.0166
3	A''	146.4796	0.2020	0.0033
4	A'	205.1486	0.8136	0.0876
5	A'	217.4586	0.8564	0.3503
6	A'	220.2012	0.8266	0.0719
7	A'	227.7510	1.0652	0.0012
8	A''	281.4758	0.6294	0.7436
9	A'	332.0591	1.8958	0.4134
10	A'	349.2984	2.0775	0.1051
11	A''	362.5813	0.9695	0.0000
12	A'	384.0279	2.8634	0.2116

13	A'	541.9047	3.0030	8.8417
14	A''	576.4213	2.4307	1.3346
15	A'	583.9117	2.7159	2.4088
16	A''	628.8659	2.8195	0.0000
17	A'	676.0940	4.1547	99.1205
18	A''	738.0753	3.9229	0.1583
19	A'	822.2252	5.4420	94.6512
20	A'	888.5784	6.0162	3.5653
21	A'	1089.2991	8.7864	35.0710
22	A'	1226.9165	10.9028	4.1730
23	A'	1261.1909	11.4131	38.8859
24	A'	1345.7534	13.2811	415.0801
25	A'	1349.5469	13.0313	126.1703
26	A'	1529.7908	16.6516	102.1232
27	A'	1559.5674	17.9522	61.9366

b3lyp/pyCCCCC_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	58.7062	0.0693	0.0000
2	B1	81.3194	0.1315	0.0114
3	B1	147.9021	0.2059	0.0090
4	A1	202.5745	0.8055	0.0420
5	B2	215.0600	0.8385	0.3331
6	A1	217.7330	0.7982	0.0441
7	B2	222.8139	1.0193	0.0017
8	B1	285.3321	0.6474	0.7116
9	B2	332.2461	1.8981	0.4187
10	A1	349.9459	2.0875	0.0885
11	A2	367.4945	0.9961	0.0000
12	A1	384.5259	2.8711	0.2392
13	A1	542.4026	3.0090	7.6725
14	B2	582.2521	2.7032	1.6990
15	B1	586.4687	2.5164	1.2560
16	A2	646.0427	2.9759	0.0000
17	B2	676.5523	4.1541	91.4375
18	B1	763.0183	4.1927	1.3107
19	A1	822.8597	5.4502	88.3635
20	B2	887.6638	6.0041	3.4324
21	A1	1089.4061	8.7901	32.1269
22	A1	1226.6273	10.8881	5.1375
23	B2	1257.7281	11.3675	33.8140
24	B2	1343.0018	13.2160	379.9753
25	A1	1345.9832	12.9616	108.7758
26	A1	1525.1187	16.5464	93.6683
27	B2	1552.7227	17.7817	57.2206

b3lyp/pyCCCCC_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	58.8746	0.0697	0.0000
2	B1	81.6400	0.1324	0.0138
3	B1	148.5804	0.2079	0.0000
4	A1	203.5512	0.8148	0.0540
5	B2	216.1859	0.8473	0.2993
6	A1	218.9408	0.8062	0.0396
7	B2	223.5503	1.0260	0.0011
8	B1	286.2030	0.6515	0.6756
9	B2	333.4905	1.9091	0.4235
10	A1	351.3043	2.0986	0.1062
11	A2	369.7378	1.0085	0.0000
12	A1	386.4783	2.8972	0.2254
13	A1	545.1417	3.0379	7.3917
14	B2	585.7851	2.7378	1.9385
15	B1	589.0220	2.5383	1.2272
16	A2	649.0340	3.0039	0.0000
17	B2	681.4785	4.2123	91.0071
18	B1	764.4146	4.2079	1.2381
19	A1	826.6258	5.5059	91.0676
20	B2	892.8249	6.0792	2.9465
21	A1	1093.9302	8.8678	32.6696
22	A1	1228.8194	10.9294	4.6786
23	B2	1259.4676	11.3935	36.9697
24	B2	1344.7662	13.2507	376.2785
25	A1	1348.1887	13.0040	110.7285
26	A1	1525.4696	16.5545	97.5716
27	B2	1554.8947	17.8408	55.8008

b31yp/pyCCCCC_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	57.4452	0.0664	0.0000
2	A"	79.5689	0.1260	0.0153
3	A"	145.8455	0.2002	0.0041
4	A'	203.8186	0.8019	0.0618
5	A'	216.2017	0.8469	0.2191
6	A'	218.5095	0.8156	0.0246
7	A'	226.2421	1.0512	0.0015
8	A"	281.1678	0.6281	0.4374
9	A'	329.7000	1.8780	0.4942
10	A'	346.7675	2.0571	0.1009
11	A"	363.3856	0.9738	0.0000
12	A'	380.3747	2.8177	0.2235
13	A'	536.4794	2.9440	9.5293
14	A"	575.4257	2.4198	1.0424
15	A'	579.7576	2.6843	3.4564
16	A"	630.6205	2.8354	0.0000
17	A'	668.7550	4.0533	100.0734
18	A"	742.0367	3.9702	1.5482
19	A'	815.3515	5.3427	97.6141
20	A'	881.1942	5.9039	3.0109
21	A'	1081.0400	8.6482	36.9010

22	A'	1223.0410	10.8221	3.7085
23	A'	1264.8059	11.4754	36.9155
24	A'	1342.8381	13.2201	402.2314
25	A'	1346.1946	12.9628	120.8897
26	A'	1530.3861	16.6620	102.4967
27	A'	1558.3483	17.9271	59.6880

b3lyp/pyFCFCF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	91.2009	0.1046	0.0000
2	A"	108.5680	0.1515	0.0024
3	A'	185.7971	0.5392	0.0231
4	A"	213.5337	0.4057	2.9778
5	A'	227.6146	0.6859	0.0398
6	A'	314.1666	1.2490	0.8662
7	A"	316.2652	0.8163	0.4416
8	A'	323.6517	1.3424	0.2583
9	A"	376.9884	1.0500	0.0000
10	A'	408.2866	2.0237	0.7261
11	A'	411.4243	1.8543	0.0560
12	A'	582.0770	3.2165	1.7965
13	A'	616.1547	3.6973	2.9977
14	A"	646.6910	3.0589	1.4726
15	A"	693.6697	3.4514	0.0000
16	A'	703.4846	3.8747	0.8997
17	A"	758.6591	4.1494	14.3610
18	A'	789.5955	5.2774	125.2251
19	A'	1066.7176	9.3027	186.2908
20	A'	1092.6192	9.6450	22.8237
21	A'	1143.8370	9.7649	8.1919
22	A'	1317.7611	12.6357	10.3452
23	A'	1430.7150	15.1612	50.5871
24	A'	1445.6163	15.3499	445.6084
25	A'	1464.9234	15.6995	90.8444
26	A'	1614.0802	18.5931	206.5382
27	A'	1631.3517	19.4994	68.9023

b3lyp/pyFCFCF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	92.5631	0.1078	0.0000
2	B1	109.8917	0.1551	0.0002
3	A1	184.3300	0.5307	0.0076
4	B1	212.0382	0.3998	2.6347
5	B2	226.4848	0.6787	0.0325
6	B2	314.5498	1.2548	0.8384
7	B1	318.4398	0.8285	0.5839
8	A1	324.0085	1.3478	0.2160
9	A2	372.2781	1.0237	0.0000

10	A1	409.0188	2.0299	0.6923
11	B2	411.8496	1.8532	0.0746
12	A1	583.2316	3.2032	1.6333
13	A1	618.6355	3.7507	2.1234
14	B1	649.7052	3.0878	1.3874
15	A2	702.7724	3.5438	0.0000
16	B2	705.0688	3.8937	0.4111
17	B1	775.4567	4.3341	11.7404
18	B2	788.8082	5.2584	116.4786
19	A1	1073.0888	9.3927	169.2103
20	B2	1097.9849	9.7503	19.2824
21	A1	1143.4051	9.7693	5.3597
22	B2	1312.8254	12.5583	8.2635
23	A1	1436.6590	15.2616	60.0737
24	B2	1447.7771	15.3968	420.2391
25	A1	1465.5652	15.7653	67.9590
26	A1	1610.5970	18.5150	200.3703
27	B2	1626.0673	19.3654	72.2275

b31yp/pyFCFCF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	92.4223	0.1075	0.0000
2	B1	109.7406	0.1547	0.0008
3	A1	186.2252	0.5416	0.0036
4	B1	212.5600	0.4020	2.3305
5	B2	228.6036	0.6919	0.0258
6	B2	315.9180	1.2648	0.8051
7	B1	319.3972	0.8329	0.5429
8	A1	325.3092	1.3561	0.1846
9	A2	375.0314	1.0391	0.0000
10	A1	410.2239	2.0420	0.6744
11	B2	412.7712	1.8611	0.0754
12	A1	584.3293	3.2267	1.4399
13	A1	619.6505	3.7524	2.0768
14	B1	649.8778	3.0899	1.1468
15	A2	703.5212	3.5515	0.0000
16	B2	707.2486	3.9181	0.4409
17	B1	774.5749	4.3240	10.6921
18	B2	793.1563	5.3211	114.3540
19	A1	1075.0398	9.4277	170.9810
20	B2	1101.4493	9.8028	17.6963
21	A1	1147.6119	9.8386	5.6709
22	B2	1315.8973	12.6151	9.3527
23	A1	1441.8330	15.3876	58.1344
24	B2	1451.1998	15.4714	411.1548
25	A1	1467.7028	15.8023	74.6437
26	A1	1612.1206	18.5534	205.8929
27	B2	1629.7029	19.4634	74.4116

b31yp/pyFCFCF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	91.4244	0.1051	0.0000
2	B1	108.6467	0.1515	0.0037
3	A1	185.8654	0.5397	0.0005
4	B1	210.7675	0.3948	2.5812
5	B2	228.5524	0.6916	0.0171
6	B2	314.0208	1.2505	0.7564
7	B1	315.1387	0.8120	0.2607
8	A1	323.1153	1.3426	0.1633
9	A2	368.7906	1.0042	0.0000
10	A1	406.4084	2.0061	0.7787
11	B2	410.0873	1.8412	0.0193
12	A1	580.9472	3.1733	1.7756
13	A1	615.4849	3.7112	2.2319
14	B1	644.3740	3.0361	0.7782
15	A2	694.9215	3.4664	0.0000
16	B2	700.6515	3.8447	0.8208
17	B1	761.8245	4.1852	17.4663
18	B2	782.9017	5.1713	119.4346
19	A1	1068.8670	9.3145	184.6004
20	B2	1095.2407	9.7021	19.7934
21	A1	1138.0202	9.6780	4.7524
22	B2	1322.4059	12.7359	6.9138
23	A1	1438.3998	15.3099	58.2998
24	B2	1449.5030	15.4271	435.5524
25	A1	1469.1363	15.8367	77.6335
26	A1	1616.8210	18.6545	209.7958
27	B2	1630.4588	19.4784	65.9831

b3lyp/pyFCFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	96.7454	0.1169	0.0003
2	A''	140.1519	0.2160	0.0052
3	A'	204.5861	0.5801	0.0257
4	A''	213.1845	0.4032	3.9332
5	A'	277.6973	0.8558	0.2619
6	A'	313.7351	1.1766	0.7311
7	A''	327.1525	0.8646	0.8775
8	A'	334.7152	1.2445	0.6787
9	A'	407.8489	1.8993	0.2848
10	A''	409.4976	1.2533	1.3960
11	A'	473.3136	2.1311	0.4835
12	A'	592.6822	3.5447	0.7562
13	A'	635.1474	3.7301	8.5922
14	A''	637.8136	2.9787	2.1297
15	A''	689.3472	3.4102	0.3931
16	A'	724.3828	4.1040	0.6408
17	A''	746.2168	4.0147	9.8194
18	A'	899.1068	6.8479	162.0500

19	A'	1072.3274	9.4033	193.7048
20	A'	1105.1238	9.7899	37.0565
21	A'	1249.4774	11.9537	23.8776
22	A'	1325.9709	12.8022	13.7831
23	A'	1432.7355	15.1900	51.4071
24	A'	1465.8472	15.7222	298.8739
25	A'	1512.3821	16.9712	418.9844
26	A'	1636.3054	19.1319	174.3116
27	A'	1652.8073	19.9057	10.5106

b3l1p/pyFCFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	98.3719	0.1208	0.0003
2	A"	141.6264	0.2207	0.0046
3	A'	203.3424	0.5729	0.0197
4	A"	212.2306	0.3992	3.3226
5	A'	278.1007	0.8582	0.3024
6	A'	314.2278	1.1835	0.6773
7	A"	329.8152	0.8797	0.9675
8	A'	335.1771	1.2468	0.5941
9	A'	408.4026	1.9004	0.2479
10	A"	410.0061	1.2565	1.1175
11	A'	474.4017	2.1397	0.5470
12	A'	595.4487	3.5609	0.8649
13	A'	636.0254	3.7521	7.1948
14	A"	643.3022	3.0321	2.2074
15	A"	704.0324	3.5576	0.5254
16	A'	726.8746	4.1332	0.4830
17	A"	772.9123	4.3031	7.7115
18	A'	901.7253	6.8729	148.7814
19	A'	1078.4780	9.4996	173.5119
20	A'	1110.0057	9.8917	38.8343
21	A'	1254.5692	12.0589	22.1682
22	A'	1321.3420	12.7381	11.2610
23	A'	1438.0439	15.2944	52.9413
24	A'	1467.0472	15.7512	278.7545
25	A'	1513.6970	17.0245	401.5337
26	A'	1633.5096	19.0746	173.0048
27	A'	1648.8660	19.7986	9.0968

b3l1p/pyFCFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	98.1599	0.1203	0.0000
2	A"	140.9369	0.2186	0.0014
3	A'	205.3056	0.5842	0.0218
4	A"	212.3176	0.3995	2.9305
5	A'	279.0061	0.8636	0.3014
6	A'	315.1758	1.1884	0.6620

7	A''	330.4127	0.8830	0.9192
8	A'	336.0826	1.2543	0.5354
9	A'	409.3848	1.9094	0.2463
10	A''	410.7842	1.2608	1.0118
11	A'	474.9821	2.1450	0.5529
12	A'	595.9886	3.5723	0.7349
13	A'	637.5312	3.7678	6.8081
14	A''	642.0646	3.0197	1.8508
15	A''	702.0996	3.5381	0.2990
16	A'	728.1164	4.1472	0.4653
17	A''	765.9687	4.2292	7.0212
18	A'	904.4506	6.9176	146.7536
19	A'	1080.5447	9.5357	176.5090
20	A'	1113.5976	9.9465	35.1063
21	A'	1257.9596	12.1233	22.2453
22	A'	1324.4367	12.7965	12.2025
23	A'	1442.7093	15.4044	54.8940
24	A'	1470.0294	15.8065	261.0862
25	A'	1516.8269	17.1019	409.3698
26	A'	1635.9429	19.1286	174.8783
27	A'	1652.0864	19.8902	10.5740

b3lyp/pyFCFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	97.0681	0.1176	0.0005
2	A''	139.9621	0.2155	0.0026
3	A'	205.1262	0.5828	0.0303
4	A''	211.1210	0.3949	3.5080
5	A'	278.5825	0.8614	0.2713
6	A'	313.4517	1.1779	0.7062
7	A''	326.0719	0.8601	0.6651
8	A'	334.0765	1.2399	0.5841
9	A'	406.3709	1.8856	0.3032
10	A''	407.9002	1.2435	1.6353
11	A'	472.9750	2.1254	0.5523
12	A'	593.2925	3.5346	0.9337
13	A'	632.6170	3.7052	7.6306
14	A''	637.4057	2.9753	1.6679
15	A''	696.6862	3.4852	1.0287
16	A'	722.0475	4.0772	0.5666
17	A''	759.7418	4.1594	9.6616
18	A'	897.0347	6.7969	151.7594
19	A'	1074.6350	9.4341	184.9508
20	A'	1107.2518	9.8393	37.4010
21	A'	1251.9019	12.0222	21.7283
22	A'	1330.9271	12.9123	10.6707
23	A'	1439.7426	15.3362	53.5496
24	A'	1468.7975	15.7910	284.8732
25	A'	1518.4442	17.1310	412.8381
26	A'	1639.1729	19.2120	174.3875
27	A'	1653.7089	19.9090	7.8106

b3lyp/pyFFCFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	116.4298	0.1483	0.0000
2	A"	121.0936	0.1804	0.0258
3	A'	204.4396	0.5922	0.0395
4	A"	207.5116	0.3767	3.6888
5	A'	282.2335	0.9118	0.7388
6	A'	308.9156	1.0346	0.3152
7	A'	329.7402	1.3298	0.8531
8	A"	332.9872	0.9088	0.9073
9	A'	430.5426	2.0060	0.1177
10	A"	441.7989	1.4536	0.0000
11	A'	462.3851	2.0328	0.0830
12	A'	542.7502	3.0632	1.7071
13	A"	596.0140	2.5968	8.6589
14	A"	691.4124	3.4299	0.0000
15	A'	698.9369	4.5096	11.1729
16	A'	721.5970	4.0537	0.0095
17	A"	736.0876	3.9067	2.8186
18	A'	917.9888	6.8300	146.2680
19	A'	965.5891	8.0817	183.5216
20	A'	1161.6228	10.7713	0.5120
21	A'	1250.9546	11.8633	63.6907
22	A'	1319.4288	12.6534	20.1019
23	A'	1433.3544	15.3469	4.6057
24	A'	1472.0020	15.6778	85.1279
25	A'	1494.5873	16.5870	751.9947
26	A'	1637.1843	19.6159	3.5798
27	A'	1645.1404	19.3379	129.7750

b3lyp/pyFFCFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	117.7140	0.1516	0.0000
2	A"	123.0430	0.1865	0.0394
3	A'	203.4687	0.5864	0.0319
4	A"	207.1525	0.3749	3.0158
5	A'	282.5173	0.9134	0.8290
6	A'	309.7327	1.0399	0.3218
7	A'	330.0072	1.3341	0.6801
8	A"	334.7245	0.9186	0.8855
9	A'	431.3901	2.0131	0.0887
10	A"	441.7490	1.4534	0.0000
11	A'	462.7942	2.0341	0.0669
12	A'	544.8868	3.0825	1.9354
13	A"	599.9347	2.6333	8.2746
14	A'	701.2988	4.5389	9.0563
15	A"	706.5344	3.5819	0.0000

16	A'	724.4182	4.0865	0.0252
17	A''	766.3561	4.2318	2.2895
18	A'	918.3231	6.8306	136.8839
19	A'	971.5397	8.1763	166.4690
20	A'	1169.2042	10.9107	0.4068
21	A'	1255.7441	11.9588	60.8378
22	A'	1314.0700	12.5746	18.2597
23	A'	1436.8273	15.4206	5.3383
24	A'	1473.3045	15.7181	82.0417
25	A'	1496.6424	16.6383	714.5687
26	A'	1633.2209	19.5105	3.3331
27	A'	1642.5787	19.2840	122.9019

b3lyp/pyFFCFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	117.2991	0.1504	0.0000
2	A''	122.9315	0.1861	0.0340
3	A'	205.4215	0.5980	0.0228
4	A''	207.2303	0.3753	2.6393
5	A'	283.6985	0.9210	0.8222
6	A'	310.6984	1.0463	0.2872
7	A'	330.9139	1.3388	0.6550
8	A''	334.6953	0.9182	0.8372
9	A'	432.2086	2.0204	0.0589
10	A''	442.7677	1.4601	0.0000
11	A'	463.6319	2.0420	0.0699
12	A'	545.6434	3.0944	1.9120
13	A''	601.4190	2.6463	7.7288
14	A'	702.2543	4.5500	8.3911
15	A''	703.5096	3.5519	0.0000
16	A'	725.6690	4.1007	0.0174
17	A''	760.4453	4.1674	1.6560
18	A'	921.8012	6.8853	136.7689
19	A'	973.4284	8.2044	164.4065
20	A'	1172.7965	10.9739	0.1676
21	A'	1259.5468	12.0292	60.8889
22	A'	1317.1977	12.6346	18.8033
23	A'	1440.6547	15.5146	3.9542
24	A'	1475.6254	15.7622	83.4168
25	A'	1500.7655	16.7257	709.9921
26	A'	1635.4209	19.5770	3.8474
27	A'	1645.6800	19.3590	123.9126

b3lyp/pyFFCFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	115.9455	0.1470	0.0000
2	A''	121.6835	0.1822	0.0294
3	A'	205.2002	0.5964	0.0079

4	A"	205.5368	0.3690	3.2017
5	A'	283.0417	0.9180	0.7515
6	A'	309.5072	1.0387	0.3161
7	A'	328.8293	1.3250	0.6958
8	A"	331.1889	0.8998	0.7370
9	A'	429.1272	1.9941	0.1428
10	A"	440.5835	1.4454	0.0000
11	A'	461.7316	2.0243	0.0815
12	A'	542.5486	3.0513	1.9682
13	A"	591.1709	2.5556	10.4268
14	A'	698.2027	4.4958	9.4181
15	A"	700.2541	3.5194	0.0000
16	A'	719.7807	4.0337	0.0022
17	A"	754.6579	4.1054	1.3521
18	A'	913.2763	6.7521	140.8307
19	A'	968.4952	8.1233	172.0310
20	A'	1168.3313	10.9032	0.2365
21	A'	1251.0896	11.8729	60.1068
22	A'	1324.5370	12.7630	18.2291
23	A'	1439.4351	15.4747	4.3737
24	A'	1474.4945	15.7492	84.5779
25	A'	1500.9131	16.7426	739.3329
26	A'	1638.3190	19.6293	1.8858
27	A'	1648.4374	19.4206	126.6287

b3lvp/pyFFFFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	118.5024	0.1536	0.0000
2	A"	156.9604	0.2672	0.0036
3	A"	214.0851	0.4051	5.2125
4	A'	273.4641	0.8298	0.0435
5	A'	274.0072	0.8222	0.6872
6	A'	318.1217	1.0809	0.7803
7	A'	344.7225	1.2281	1.4631
8	A"	349.7088	0.9902	3.3395
9	A"	431.6367	1.3881	0.0000
10	A'	461.4464	2.0292	0.1440
11	A'	481.8454	2.1798	0.1746
12	A'	595.6645	3.6550	0.0014
13	A"	629.3220	2.9043	3.3479
14	A"	685.4967	3.3717	0.0000
15	A'	699.5623	4.4767	7.7873
16	A"	730.8697	3.8539	5.6595
17	A'	740.7139	4.2957	0.1038
18	A'	984.3624	8.3241	226.6089
19	A'	1084.2561	9.6716	247.1970
20	A'	1166.5571	10.8892	0.0001
21	A'	1294.5103	12.8259	30.1983
22	A'	1333.1862	12.9384	13.5188
23	A'	1442.1335	15.3335	18.5904
24	A'	1505.3640	16.8700	716.9716

25	A'	1541.3302	17.5174	159.0227
26	A'	1656.4789	19.5764	115.4299
27	A'	1666.8910	20.2128	3.0516

b3lyp/pyFFFFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	119.9205	0.1573	0.0000
2	A"	158.6122	0.2730	0.0010
3	A"	213.6010	0.4027	4.2064
4	A'	274.1040	0.8335	0.0441
5	A'	274.3455	0.8242	0.7713
6	A'	318.8426	1.0855	0.7154
7	A'	345.1347	1.2306	1.2567
8	A"	352.1225	1.0049	2.9501
9	A"	432.4275	1.3933	0.0000
10	A'	461.9781	2.0322	0.1334
11	A'	483.5254	2.1930	0.2372
12	A'	599.0166	3.6943	0.0036
13	A"	638.2039	2.9920	3.5986
14	A'	701.4080	4.5013	6.2583
15	A"	705.6235	3.5725	0.0000
16	A'	744.1652	4.3372	0.0134
17	A"	770.9581	4.2791	4.4963
18	A'	990.5872	8.4236	210.6055
19	A'	1090.8381	9.7865	232.5298
20	A'	1173.3864	11.0185	0.0382
21	A'	1300.3646	12.9517	27.9657
22	A'	1328.2572	12.8636	11.3870
23	A'	1445.8561	15.4017	21.5842
24	A'	1507.5498	16.9184	690.9297
25	A'	1542.8408	17.5745	150.4683
26	A'	1654.4950	19.5331	110.8469
27	A'	1663.3702	20.1196	2.4285

b3lyp/pyFFFFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	119.2503	0.1555	0.0000
2	A"	157.5524	0.2692	0.0001
3	A"	213.3161	0.4016	3.7037
4	A'	274.7564	0.8375	0.0471
5	A'	274.9920	0.8279	0.7831
6	A'	319.3550	1.0888	0.6958
7	A'	345.6424	1.2344	1.1726
8	A"	351.5960	1.0019	2.7237
9	A"	432.6905	1.3950	0.0000
10	A'	462.5948	2.0378	0.1355
11	A'	483.6793	2.1942	0.2786
12	A'	599.4020	3.6981	0.0063

13	A''	635.5846	2.9651	3.0354
14	A''	701.4611	3.5313	0.0000
15	A'	702.3063	4.5120	5.8934
16	A'	744.6065	4.3419	0.0140
17	A''	758.3452	4.1455	3.9411
18	A'	992.1915	8.4500	206.2624
19	A'	1092.8209	9.8206	232.2497
20	A'	1176.8779	11.0832	0.1156
21	A'	1303.2668	13.0107	28.5128
22	A'	1331.5115	12.9254	11.9819
23	A'	1450.3136	15.5010	21.9087
24	A'	1511.7738	17.0150	679.1248
25	A'	1545.5484	17.6385	147.5834
26	A'	1657.1283	19.5974	112.7542
27	A'	1666.4490	20.2002	2.7968

b3lyp/pyFFFFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.8997	0.1520	0.0000
2	B1	156.6950	0.2662	0.0016
3	B1	212.7580	0.3998	4.7499
4	B2	274.2974	0.8347	0.0469
5	A1	274.5435	0.8254	0.7425
6	B2	317.8686	1.0790	0.8399
7	A1	343.8596	1.2216	1.3687
8	B1	348.5969	0.9850	3.1309
9	A2	431.4254	1.3866	0.0000
10	B2	460.8644	2.0218	0.1339
11	A1	481.8711	2.1772	0.2117
12	A1	596.9139	3.6672	0.0011
13	B1	631.8534	2.9312	3.3932
14	A1	698.6016	4.4622	6.3818
15	A2	698.8614	3.5054	0.0000
16	B2	738.6551	4.2713	0.0495
17	B1	757.8097	4.1358	4.3159
18	B2	986.9688	8.3637	211.9806
19	A1	1087.1965	9.7211	236.9313
20	B2	1172.8422	11.0159	0.0150
21	A1	1297.3909	12.9024	27.9966
22	B2	1337.9650	13.0424	11.0411
23	A1	1447.4589	15.4421	20.5784
24	B2	1510.8485	16.9991	698.4032
25	A1	1547.6739	17.6845	153.2706
26	A1	1659.9660	19.6611	113.7013
27	B2	1668.1469	20.2343	1.7449

b3lyp/pyFFHFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A"	115.1905	0.1453	0.0000
2	A"	202.7183	0.3270	4.2035
3	A'	281.8534	0.8519	0.6788
4	A"	296.7651	0.4351	0.9940
5	A'	302.8154	0.9633	0.2188
6	A'	358.9835	1.2168	2.7442
7	A'	455.2865	1.7736	0.0639
8	A"	456.3349	1.5505	0.0000
9	A"	487.1549	0.6124	0.5602
10	A'	512.0968	2.3120	1.6685
11	A'	661.4986	1.5772	2.4225
12	A'	691.1429	4.2528	18.9342
13	A"	696.7653	3.4814	0.0000
14	A"	726.5803	2.5577	11.3111
15	A'	755.6765	3.2207	11.9547
16	A"	894.4271	0.6598	30.3078
17	A'	908.6436	2.8430	143.5722
18	A'	1148.9908	5.4714	13.9882
19	A'	1198.7452	1.3836	74.2888
20	A'	1231.5782	10.0425	201.9691
21	A'	1324.5859	11.9645	63.4902
22	A'	1416.3281	13.8406	0.9178
23	A'	1459.7219	14.3487	43.3440
24	A'	1511.1557	9.9570	728.5182
25	A'	1657.2144	18.5912	26.8264
26	A'	1657.9893	13.9618	3.1682
27	A'	3218.2238	6.6742	4.1731

b31yp/pyFFHFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	116.7475	0.1492	0.0000
2	A"	203.2334	0.3306	3.3369
3	A'	282.4416	0.8554	0.7196
4	A"	299.3842	0.4416	0.9823
5	A'	303.9022	0.9702	0.1669
6	A'	359.9017	1.2221	2.3160
7	A'	455.8331	1.7761	0.0493
8	A"	457.0796	1.5556	0.0000
9	A"	492.2461	0.6118	0.5019
10	A'	514.4125	2.3288	1.8824
11	A'	665.3573	1.5876	2.4107
12	A'	694.6140	4.3190	16.3037
13	A"	714.3163	3.6590	0.0000
14	A"	751.2126	2.1353	13.0016
15	A'	758.4198	3.2382	12.5256
16	A"	912.8486	0.7268	24.2831
17	A'	913.5427	2.8284	128.6822
18	A'	1156.9636	5.4341	15.7424
19	A'	1203.6198	1.4212	67.9143
20	A'	1238.9682	10.1688	186.0755
21	A'	1319.4838	11.5311	61.4982

22	A'	1420.5049	13.8883	1.3332
23	A'	1461.6721	14.4803	45.0325
24	A'	1513.6164	10.0527	707.4643
25	A'	1655.5488	13.5647	4.4242
26	A'	1655.6417	18.5675	26.4281
27	A'	3216.7329	6.6647	3.4738

b3lyp/pyFFHFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	116.3236	0.1481	0.0000
2	A"	203.0455	0.3296	2.9476
3	A'	283.2137	0.8598	0.7274
4	A"	298.6824	0.4397	0.9765
5	A'	304.5166	0.9739	0.1635
6	A'	360.2545	1.2251	2.1866
7	A'	456.5773	1.7817	0.0489
8	A"	457.5802	1.5591	0.0000
9	A"	490.6391	0.6137	0.4047
10	A'	514.7135	2.3304	1.9298
11	A'	665.8938	1.5904	2.3769
12	A'	695.6112	4.3270	15.6683
13	A"	711.5826	3.6316	0.0000
14	A"	746.9521	2.2805	10.6538
15	A'	759.1710	3.2449	12.5620
16	A"	904.7252	0.6998	26.1105
17	A'	915.0953	2.8214	124.8394
18	A'	1160.9107	5.2638	16.8819
19	A'	1206.0052	1.4408	63.0355
20	A'	1242.5136	10.2139	186.3428
21	A'	1322.7096	11.6370	63.5762
22	A'	1424.1296	13.9128	1.1904
23	A'	1465.5605	14.6282	44.8912
24	A'	1518.2052	10.1286	694.9068
25	A'	1658.0016	18.6278	27.3576
26	A'	1658.7657	13.6581	4.1203
27	A'	3221.2067	6.6835	3.2020

b3lyp/pyFFHFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	114.8556	0.1444	0.0000
2	B1	201.5317	0.3252	3.7848
3	A1	282.3375	0.8547	0.7015
4	B1	296.9069	0.4364	1.0279
5	B2	303.3076	0.9668	0.2327
6	A1	358.0532	1.2097	2.5072
7	B2	454.7525	1.7670	0.0614
8	A2	455.5549	1.5450	0.0000
9	B1	486.3226	0.6032	0.4764

10	A1	512.4095	2.3113	1.6837
11	B2	660.8965	1.5876	2.2405
12	A1	691.3430	4.2703	16.2035
13	A2	707.2759	3.5882	0.0000
14	B1	741.7144	2.1561	12.2062
15	A1	756.0913	3.2191	12.5458
16	B1	902.9464	0.7025	27.3648
17	B2	910.5217	2.8110	133.3881
18	B2	1155.3858	5.1319	14.9157
19	B2	1202.1482	1.4127	64.9023
20	A1	1233.4183	10.0770	193.9719
21	B2	1330.2248	12.0099	55.8138
22	A1	1422.9957	13.9237	1.0970
23	A1	1462.4367	14.4470	43.0641
24	B2	1515.5791	10.2953	717.3697
25	B2	1658.0461	13.9592	4.6359
26	A1	1661.7641	18.7066	26.5894
27	A1	3225.0173	6.7024	5.2081

b3lyp/pyFHFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	128.6762	0.1633	0.1456
2	A"	209.7773	0.3555	4.5348
3	A"	260.9409	0.2875	1.1833
4	A'	274.9148	0.8300	0.1911
5	A'	319.2331	1.0366	1.0389
6	A'	350.9026	1.1960	1.5829
7	A"	384.6889	0.9127	0.9125
8	A'	465.8571	1.8222	0.5087
9	A'	535.0391	1.8830	3.4399
10	A'	598.6456	3.6367	0.1175
11	A"	627.3253	1.2699	6.1095
12	A'	668.1592	1.6886	2.6268
13	A"	681.0068	1.9613	0.0123
14	A"	739.4237	2.1816	1.4096
15	A'	801.9523	3.7720	49.7115
16	A"	848.4511	0.6615	37.9871
17	A'	1028.5341	2.9341	100.3643
18	A'	1077.0288	8.0793	176.4432
19	A'	1165.0325	1.5523	86.6597
20	A'	1247.9438	5.2447	52.5849
21	A'	1337.3851	11.8159	9.6170
22	A'	1418.6709	11.6975	58.6609
23	A'	1461.1974	13.5062	169.0144
24	A'	1528.5183	9.4195	413.4826
25	A'	1648.9960	15.7183	267.7990
26	A'	1663.4737	18.4129	43.8120
27	A'	3231.8293	6.7356	4.5383

b3lyp/pyFHFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	129.8281	0.1663	0.1178
2	A''	210.0072	0.3599	3.6265
3	A''	263.6461	0.2909	1.2610
4	A'	275.4418	0.8328	0.2210
5	A'	320.0542	1.0413	0.8952
6	A'	351.8662	1.2025	1.2472
7	A''	385.1716	0.9231	0.8323
8	A'	466.7197	1.8299	0.4825
9	A'	535.6041	1.8875	2.9680
10	A'	602.1827	3.6805	0.0614
11	A''	634.2595	1.2666	6.2717
12	A'	671.4974	1.6977	2.8548
13	A''	691.8123	1.8272	0.0072
14	A''	761.7333	1.9477	0.3214
15	A'	804.8097	3.7947	44.1533
16	A''	863.8106	0.7400	34.9379
17	A'	1032.0186	2.8552	89.6290
18	A'	1084.2926	8.1565	161.6025
19	A'	1171.9793	1.5932	88.5892
20	A'	1253.3207	5.4710	48.7188
21	A'	1332.9361	11.4040	11.0363
22	A'	1424.9934	11.9865	61.0341
23	A'	1462.6976	13.4397	154.0923
24	A'	1530.8927	9.4455	404.6254
25	A'	1647.0853	15.5073	256.5433
26	A'	1660.4618	18.1030	43.2101
27	A'	3230.7330	6.7277	3.6221

b31yp/pyFHFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	129.3070	0.1649	0.1050
2	A''	209.6144	0.3572	3.2696
3	A''	262.8204	0.2904	1.2497
4	A'	276.1315	0.8370	0.2261
5	A'	320.6511	1.0448	0.8871
6	A'	352.4549	1.2065	1.1951
7	A''	384.8259	0.9223	0.7043
8	A'	467.1706	1.8322	0.4655
9	A'	536.1919	1.8927	2.7471
10	A'	602.7062	3.6850	0.0522
11	A''	633.2641	1.2889	5.5790
12	A'	672.0008	1.6989	2.7562
13	A''	690.7420	1.8684	0.0000
14	A''	755.1043	2.0906	0.5192
15	A'	805.9373	3.8032	43.1469
16	A''	854.6507	0.6975	33.9551
17	A'	1033.8257	2.8169	87.5120
18	A'	1087.1891	8.2192	158.1650

19	A'	1174.8683	1.5979	86.2776
20	A'	1256.1382	5.5991	48.2562
21	A'	1336.5366	11.4346	11.4419
22	A'	1429.5006	12.2585	60.8850
23	A'	1466.8543	13.4564	143.6964
24	A'	1534.4379	9.5408	402.6247
25	A'	1649.8701	15.5345	259.9705
26	A'	1663.4116	18.2014	44.2741
27	A'	3235.1060	6.7458	3.3738

b3lyp/pyFHFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	128.3411	0.1624	0.1348
2	A"	209.0536	0.3564	4.1589
3	A"	261.0425	0.2873	1.3030
4	A'	275.6125	0.8340	0.2123
5	A'	318.9485	1.0349	1.0532
6	A'	350.1598	1.1914	1.4504
7	A"	383.1411	0.9064	0.7913
8	A'	465.6674	1.8201	0.4812
9	A'	534.2693	1.8778	2.8956
10	A'	600.0208	3.6536	0.1025
11	A"	629.3687	1.2843	6.0411
12	A'	667.0644	1.6974	2.5013
13	A"	686.1552	1.8325	0.0028
14	A"	753.4237	2.0308	0.4236
15	A'	802.0324	3.7563	45.2465
16	A"	856.8606	0.7050	38.0930
17	A'	1029.3482	2.8692	95.4033
18	A'	1081.0167	8.1065	165.6440
19	A'	1169.2959	1.5553	81.8434
20	A'	1251.7711	5.3346	47.5295
21	A'	1341.3301	12.0431	9.2060
22	A'	1425.7803	11.9081	62.6494
23	A'	1464.7524	13.4753	152.6971
24	A'	1532.9132	9.7206	415.6528
25	A'	1651.4523	15.8574	263.5165
26	A'	1665.0223	18.4110	40.2988
27	A'	3238.9422	6.7653	5.6120

b3lyp/pyHHHHH_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	380.6088	0.2185	0.0000
2	A"	416.7311	0.3845	3.9976
3	A'	617.8750	1.6074	3.6425
4	A'	670.4838	1.6838	0.3024
5	A"	713.7367	0.4093	67.8981
6	A"	757.3539	0.8024	11.0351

7	A''	892.2817	0.5851	0.0000
8	A''	953.3993	0.7137	0.0247
9	A''	995.9973	0.8584	0.0000
10	A''	1005.4730	0.7664	0.0070
11	A'	1012.4632	4.2676	5.1271
12	A'	1050.3737	2.8735	6.2889
13	A'	1077.2724	1.2146	0.0016
14	A'	1094.4153	1.2296	4.9631
15	A'	1171.1359	0.9248	2.4318
16	A'	1242.5368	1.1688	4.6341
17	A'	1285.8216	6.8020	0.0315
18	A'	1383.7816	1.3515	0.0476
19	A'	1470.5844	2.6400	26.8371
20	A'	1511.0977	2.6452	2.3990
21	A'	1618.7531	8.6933	10.2287
22	A'	1624.4580	7.9219	23.8853
23	A'	3148.7481	6.3529	27.7747
24	A'	3151.0547	6.3788	4.0516
25	A'	3171.5514	6.4538	4.8984
26	A'	3186.9793	6.5429	25.3968
27	A'	3195.0106	6.6098	6.9970

b3lyp/pyHHHHH_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	384.1081	0.2195	0.0000
2	B1	420.4782	0.3869	3.8211
3	A1	618.5595	1.6096	4.3980
4	B2	671.1014	1.6840	0.1699
5	B1	720.5492	0.4035	63.8009
6	B1	767.3914	0.8269	7.7929
7	A2	900.8792	0.5966	0.0000
8	B1	964.8589	0.7336	0.0132
9	A2	1012.8824	0.8944	0.0000
10	A1	1014.1312	4.2360	5.3691
11	B1	1025.0003	0.8215	0.0150
12	A1	1054.6648	2.7676	7.1628
13	B2	1079.2051	1.2216	0.0626
14	A1	1097.0195	1.2686	2.9892
15	B2	1170.9089	0.9339	2.6576
16	A1	1242.7018	1.1764	3.8720
17	B2	1283.6293	6.4484	0.0088
18	B2	1389.4316	1.3649	0.1427
19	B2	1475.3720	2.6639	25.6576
20	A1	1517.0247	2.6471	2.0312
21	B2	1619.8981	8.4845	9.8442
22	A1	1625.1412	7.7925	23.3816
23	B2	3148.0951	6.3498	26.7892
24	A1	3150.5815	6.3785	4.2066
25	A1	3173.0433	6.4577	4.3020
26	B2	3188.1428	6.5453	23.9436
27	A1	3196.1724	6.6109	6.8312

b3lyp/pyHHHHH_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	384.5733	0.2198	0.0000
2	A"	420.9663	0.3892	3.7304
3	A'	619.1303	1.6144	4.6266
4	A'	672.4453	1.6925	0.2329
5	A"	719.9926	0.3966	65.3891
6	A"	768.5000	0.8519	6.8357
7	A"	900.4891	0.5960	0.0000
8	A"	963.5273	0.7339	0.0122
9	A"	1011.5866	0.8930	0.0000
10	A'	1015.7325	4.2611	5.9464
11	A"	1024.8650	0.8187	0.0023
12	A'	1055.7170	2.7788	7.6369
13	A'	1080.6281	1.2245	0.0550
14	A'	1098.4362	1.2671	2.8711
15	A'	1173.5502	0.9379	2.4996
16	A'	1244.8532	1.1800	3.5794
17	A'	1286.7397	6.4835	0.0309
18	A'	1391.0821	1.3677	0.1156
19	A'	1478.2252	2.6734	26.8164
20	A'	1519.3375	2.6609	2.6557
21	A'	1622.8238	8.5443	9.4174
22	A'	1627.6824	7.8241	24.0285
23	A'	3151.0202	6.3613	28.2722
24	A'	3153.6314	6.3912	5.5267
25	A'	3176.6740	6.4723	4.7886
26	A'	3191.9599	6.5608	24.6808
27	A'	3199.9149	6.6270	6.8670

b3lyp/pyHHHHH_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	382.3078	0.2181	0.0000
2	A"	417.7902	0.3840	3.9908
3	A'	617.6378	1.6055	3.8279
4	A'	669.4935	1.6770	0.3750
5	A"	714.0053	0.3923	73.3314
6	A"	762.9654	0.8383	8.4189
7	A"	894.1975	0.5876	0.0000
8	A"	955.8958	0.7199	0.0290
9	A"	1004.0360	0.8776	0.0000
10	A'	1011.2161	4.2365	5.8022
11	A"	1017.7348	0.8054	0.0369
12	A'	1052.0421	2.8556	6.3293
13	A'	1078.2986	1.2093	0.0064
14	A'	1094.6479	1.2313	4.9168
15	A'	1171.5130	0.9135	2.3326

16	A'	1242.1562	1.1629	3.9396
17	A'	1288.4611	7.3047	0.0020
18	A'	1381.7131	1.3474	0.0595
19	A'	1469.5927	2.6555	28.2881
20	A'	1509.2994	2.6484	3.2055
21	A'	1618.8445	8.8064	9.0040
22	A'	1625.8323	8.0921	23.5390
23	A'	3156.8289	6.3859	21.7362
24	A'	3158.9464	6.4114	3.9339
25	A'	3180.1018	6.4881	4.2301
26	A'	3194.8925	6.5754	19.0962
27	A'	3202.7307	6.6426	4.8006

b3p86/pyCCCCC_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	57.4650	0.0664	0.0000
2	B1	80.7869	0.1299	0.0187
3	B1	148.5583	0.2078	0.0004
4	A1	204.2855	0.8190	0.0819
5	B2	216.5782	0.8490	0.3526
6	A1	219.2722	0.8074	0.0825
7	B2	225.1482	1.0406	0.0004
8	B1	284.2192	0.6423	0.6901
9	B2	334.4469	1.8947	0.3283
10	A1	351.1218	2.0622	0.1600
11	A2	366.4528	0.9906	0.0000
12	A1	389.0358	2.9116	0.1665
13	A1	548.7896	3.0772	6.8084
14	B1	576.5410	2.4300	1.2683
15	B2	585.8137	2.7147	1.2908
16	A2	630.0998	2.8315	0.0000
17	B2	691.3359	4.3810	95.5050
18	B1	734.9998	3.8923	0.1016
19	A1	833.3007	5.6305	95.9405
20	B2	903.6462	6.2662	3.7864
21	A1	1096.0965	8.9110	34.3593
22	A1	1241.4916	11.2019	3.9776
23	B2	1295.8327	12.0139	60.1140
24	B2	1366.6032	13.7243	406.1858
25	A1	1367.7660	13.3969	130.4148
26	A1	1552.2483	17.1461	103.9459
27	B2	1584.4500	18.5452	60.8944

b3p86/pyCCCCC_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	59.5806	0.0713	0.0000
2	B1	82.9459	0.1366	0.0128
3	B1	149.6274	0.2108	0.0009

4	A1	200.4894	0.8013	0.0366
5	B2	213.2676	0.8239	0.3286
6	A1	216.1916	0.7750	0.0477
7	B2	218.6076	0.9809	0.0005
8	B1	287.7456	0.6592	0.6590
9	B2	334.3390	1.8919	0.3284
10	A1	351.4223	2.0657	0.1416
11	A2	371.1978	1.0165	0.0000
12	A1	389.4383	2.9161	0.1880
13	A1	548.9909	3.0809	5.6701
14	B2	583.0065	2.6905	0.7486
15	B1	587.5501	2.5248	1.1794
16	A2	648.3064	2.9978	0.0000
17	B2	691.9586	4.3843	86.9921
18	B1	763.7536	4.2017	1.2540
19	A1	833.8621	5.6405	88.6343
20	B2	902.7612	6.2570	3.6655
21	A1	1095.7303	8.9079	31.1860
22	A1	1240.8655	11.1819	5.0114
23	B2	1291.9616	11.9626	50.0769
24	B2	1362.8947	13.6405	374.6998
25	A1	1363.9179	13.3214	111.6372
26	A1	1547.1243	17.0289	94.8185
27	B2	1576.4396	18.3370	55.1644

b3p86/pyCCCCC_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	59.8478	0.0719	0.0000
2	B1	83.3420	0.1378	0.0150
3	B1	150.3442	0.2129	0.0024
4	A1	201.2800	0.8084	0.0473
5	B2	214.2615	0.8317	0.2948
6	A1	217.3164	0.7827	0.0420
7	B2	219.2670	0.9867	0.0003
8	B1	288.7600	0.6639	0.6044
9	B2	335.4705	1.9023	0.3405
10	A1	352.6396	2.0761	0.1599
11	A2	373.6324	1.0300	0.0000
12	A1	391.1217	2.9383	0.1851
13	A1	551.4320	3.1067	5.5306
14	B2	586.3547	2.7232	0.9474
15	B1	590.6584	2.5520	1.1838
16	A2	651.7878	3.0304	0.0000
17	B2	696.3171	4.4368	86.8932
18	B1	766.4083	4.2302	1.2904
19	A1	837.3966	5.6933	91.6301
20	B2	907.5381	6.3274	3.2101
21	A1	1100.1795	8.9846	31.7667
22	A1	1242.6552	11.2163	4.5804
23	B2	1293.0296	11.9759	54.8169
24	B2	1364.3793	13.6696	371.0946

25	A1	1365.5867	13.3538	113.9096
26	A1	1546.8925	17.0243	99.1072
27	B2	1578.3103	18.3927	54.6381

b3p86/pyCCCCC_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	58.1833	0.0680	0.0000
2	B1	80.9709	0.1303	0.0162
3	B1	148.0595	0.2064	0.0124
4	A1	202.7996	0.8070	0.0569
5	B2	215.1619	0.8382	0.2077
6	A1	217.4398	0.7946	0.0260
7	B2	223.4510	1.0250	0.0009
8	B1	284.2998	0.6427	0.3865
9	B2	331.9945	1.8758	0.4122
10	A1	348.5666	2.0411	0.1466
11	A2	367.9929	0.9988	0.0000
12	A1	385.3797	2.8669	0.1814
13	A1	543.1814	3.0161	7.5106
14	B1	577.5639	2.4373	0.9983
15	B2	581.5543	2.6801	2.0195
16	A2	633.9524	2.8663	0.0000
17	B2	683.5749	4.2749	97.3308
18	B1	743.5360	3.9869	1.6283
19	A1	825.8698	5.5221	99.0142
20	B2	895.5729	6.1416	3.1879
21	A1	1087.2004	8.7608	36.1088
22	A1	1237.0874	11.1089	3.3930
23	B2	1298.0200	12.0463	60.6513
24	B2	1363.1005	13.6521	391.9670
25	A1	1363.8816	13.3159	126.2029
26	A1	1551.9537	17.1378	104.1635
27	B2	1582.9151	18.5175	58.8750

b3p86/pyFCFCF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	91.7058	0.1058	0.0000
2	B1	109.9167	0.1554	0.0057
3	A1	183.8350	0.5271	0.0197
4	B1	215.3158	0.4123	2.4888
5	B2	225.0839	0.6699	0.0428
6	B2	314.5782	1.2506	0.8642
7	B1	318.0531	0.8256	0.3807
8	A1	324.6933	1.3478	0.2358
9	A2	380.9422	1.0722	0.0000
10	A1	411.7237	2.0327	0.6977
11	B2	413.2879	1.8582	0.0904
12	A1	584.6029	3.2430	1.6508

13	A1	618.3891	3.7279	2.1215
14	B1	651.1819	3.1009	1.3247
15	A2	698.2310	3.4983	0.0000
16	B2	707.4193	3.9147	0.5421
17	B1	760.0043	4.1659	14.6985
18	B2	803.8340	5.4930	120.2519
19	A1	1081.9599	9.5605	184.4233
20	B2	1112.5776	10.0339	20.5414
21	A1	1158.6200	10.0613	6.2821
22	B2	1352.7645	13.2919	12.6069
23	A1	1448.9619	15.6106	50.1409
24	B2	1468.7261	15.8611	453.5172
25	A1	1487.7202	16.2240	97.2867
26	A1	1637.1912	19.1326	211.3965
27	B2	1656.5193	20.1328	74.1301

b3p86/pyFCFCF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	93.0563	0.1089	0.0000
2	B1	111.2486	0.1590	0.0001
3	A1	181.8633	0.5158	0.0047
4	B1	213.3743	0.4046	2.2396
5	B2	223.4677	0.6599	0.0329
6	B2	314.5922	1.2534	0.8614
7	B1	319.9090	0.8366	0.5356
8	A1	324.7074	1.3499	0.2021
9	A2	374.6729	1.0369	0.0000
10	A1	412.0978	2.0344	0.6640
11	B2	413.1666	1.8514	0.1199
12	A1	584.9920	3.2233	1.4629
13	A1	620.1960	3.7721	1.3893
14	B1	653.9961	3.1285	1.2865
15	A2	707.4934	3.5934	0.0000
16	B2	707.9957	3.9226	0.1611
17	B1	777.4996	4.3582	11.6490
18	B2	802.7507	5.4719	110.8765
19	A1	1087.3980	9.6292	165.5737
20	B2	1117.2320	10.1282	16.9065
21	A1	1157.8021	10.0648	3.7454
22	B2	1346.1482	13.1817	9.5110
23	A1	1454.0028	15.6960	59.0401
24	B2	1469.8258	15.8875	427.8389
25	A1	1487.5950	16.2758	73.8591
26	A1	1632.5195	19.0258	204.6669
27	B2	1649.4887	19.9510	77.0626

b3p86/pyFCFCF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	92.9256	0.1086	0.0000
2	B1	111.1322	0.1587	0.0015
3	A1	183.7096	0.5263	0.0014
4	B1	213.9943	0.4072	1.9857
5	B2	225.5772	0.6727	0.0264
6	B2	315.9691	1.2637	0.8201
7	B1	320.8198	0.8407	0.4876
8	A1	325.9353	1.3581	0.1682
9	A2	377.4318	1.0524	0.0000
10	A1	413.1847	2.0453	0.6451
11	B2	414.0338	1.8590	0.1197
12	A1	586.0087	3.2450	1.3017
13	A1	621.0963	3.7733	1.3866
14	B1	654.5691	3.1345	1.0625
15	A2	708.4269	3.6029	0.0000
16	B2	710.0403	3.9454	0.1982
17	B1	776.9131	4.3512	11.2908
18	B2	806.6677	5.5294	109.5457
19	A1	1089.0212	9.6610	168.7165
20	B2	1120.1889	10.1721	15.9174
21	A1	1161.7083	10.1273	4.1145
22	B2	1348.6917	13.2290	10.9603
23	A1	1458.4620	15.8072	57.4610
24	B2	1472.7925	15.9525	420.4108
25	A1	1489.2571	16.3025	80.9787
26	A1	1633.5769	19.0538	211.9865
27	B2	1652.9535	20.0484	80.4280

b3p86/pyFCFCF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	91.8851	0.1061	0.0000
2	B1	109.9939	0.1554	0.0045
3	A1	184.2241	0.5295	0.0000
4	B1	212.5077	0.4010	2.2062
5	B2	226.5626	0.6788	0.0161
6	B2	314.5958	1.2534	0.7695
7	B1	317.1017	0.8224	0.2300
8	A1	324.2267	1.3485	0.1482
9	A2	371.9719	1.0216	0.0000
10	A1	409.8351	2.0153	0.7496
11	B2	411.7433	1.8430	0.0410
12	A1	582.9327	3.1945	1.6243
13	A1	617.6377	3.7398	1.5258
14	B1	649.4372	3.0839	0.7154
15	A2	700.7281	3.5263	0.0000
16	B2	704.5504	3.8837	0.4600
17	B1	764.9902	4.2210	17.9956
18	B2	796.4616	5.3762	115.0053
19	A1	1083.5737	9.5561	182.0329
20	B2	1114.8567	10.0831	17.5276
21	A1	1152.5141	9.9718	3.1844

22	B2	1356.1804	13.3704	8.8041
23	A1	1457.2361	15.7792	56.5878
24	B2	1472.2334	15.9317	446.2372
25	A1	1491.7521	16.3577	86.2370
26	A1	1639.1028	19.1770	215.9098
27	B2	1655.1631	20.1057	72.1510

b3p86/pyFCFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	97.3591	0.1183	0.0008
2	A''	140.9551	0.2186	0.0015
3	A'	202.3687	0.5677	0.0259
4	A''	215.0824	0.4103	3.3639
5	A'	274.7392	0.8372	0.2710
6	A'	314.7742	1.1789	0.7178
7	A''	329.3773	0.8765	0.7934
8	A'	336.6044	1.2584	0.6429
9	A'	410.3344	1.9058	0.2634
10	A''	413.1408	1.2757	1.3536
11	A'	472.5430	2.1149	0.4839
12	A'	596.5337	3.5839	0.7293
13	A'	638.5784	3.7765	7.0443
14	A''	640.7970	3.0051	1.8694
15	A''	691.4403	3.4321	0.2250
16	A'	728.6963	4.1519	0.5699
17	A''	744.2977	3.9976	10.2639
18	A'	913.1007	7.0597	155.1588
19	A'	1088.3335	9.6926	192.8050
20	A'	1124.4937	10.1611	33.4603
21	A'	1267.8606	12.3631	22.5995
22	A'	1360.4228	13.4496	17.1431
23	A'	1452.4378	15.6584	49.3796
24	A'	1488.6919	16.2365	297.3051
25	A'	1537.6287	17.5818	442.7704
26	A'	1659.0682	19.6774	178.3960
27	A'	1678.0036	20.5415	11.2103

b3p86/pyFCFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	98.9872	0.1222	0.0001
2	A''	142.3328	0.2231	0.0013
3	A'	200.6773	0.5580	0.0200
4	A''	213.8873	0.4053	2.8456
5	A'	275.3695	0.8411	0.3140
6	A'	315.1291	1.1854	0.6790
7	A''	331.8765	0.8909	0.8958
8	A'	336.8323	1.2579	0.5685
9	A'	410.4428	1.9018	0.2275

10	A''	414.0290	1.2816	1.0997
11	A'	472.9183	2.1170	0.5502
12	A'	598.7573	3.5951	0.8265
13	A'	638.7297	3.7899	5.7289
14	A''	647.4076	3.0708	2.0975
15	A''	708.7892	3.6076	0.5436
16	A'	730.3599	4.1721	0.4559
17	A''	775.3232	4.3309	7.5526
18	A'	915.1069	7.0756	141.2608
19	A'	1093.8037	9.7784	171.6602
20	A'	1128.5010	10.2468	34.3675
21	A'	1272.5079	12.4654	20.7621
22	A'	1353.8841	13.3466	13.5726
23	A'	1456.7302	15.7423	50.9650
24	A'	1488.7977	16.2463	279.6104
25	A'	1537.9882	17.6146	422.3279
26	A'	1654.7499	19.5855	176.7682
27	A'	1672.4181	20.3888	9.2481

b3p86/pyFCFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	98.7661	0.1216	0.0000
2	A''	141.7069	0.2211	0.0001
3	A'	202.6156	0.5689	0.0232
4	A''	214.0854	0.4061	2.5304
5	A'	276.5587	0.8482	0.3144
6	A'	316.0995	1.1913	0.6583
7	A''	332.4497	0.8940	0.8471
8	A'	337.7091	1.2648	0.5080
9	A'	411.3270	1.9101	0.2273
10	A''	414.7205	1.2854	1.0312
11	A'	473.5508	2.1229	0.5619
12	A'	599.1609	3.6043	0.7075
13	A'	640.1158	3.8046	5.4803
14	A''	646.4456	3.0610	1.7801
15	A''	707.2652	3.5920	0.3634
16	A'	731.5422	4.1854	0.4431
17	A''	769.0493	4.2638	7.2277
18	A'	917.4796	7.1160	140.6670
19	A'	1095.4347	9.8067	175.9431
20	A'	1131.5473	10.2931	31.8298
21	A'	1275.3696	12.5187	21.0407
22	A'	1356.4989	13.3963	14.8620
23	A'	1460.7526	15.8385	52.4561
24	A'	1491.2589	16.2912	263.9532
25	A'	1540.7590	17.6836	433.9098
26	A'	1656.7862	19.6308	180.2669
27	A'	1675.3919	20.4774	10.7011

b3p86/pyFCFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	97.6596	0.1189	0.0004
2	A''	140.7117	0.2180	0.0006
3	A'	203.3786	0.5730	0.0336
4	A''	213.1378	0.4024	3.0548
5	A'	276.8762	0.8505	0.2804
6	A'	314.8808	1.1844	0.7039
7	A''	328.6124	0.8737	0.6118
8	A'	336.1675	1.2539	0.5594
9	A'	408.7505	1.8908	0.2693
10	A''	412.2739	1.2705	1.6101
11	A'	471.9592	2.1072	0.5518
12	A'	596.9638	3.5720	0.9162
13	A'	635.7380	3.7479	6.2710
14	A''	642.2195	3.0204	1.6058
15	A''	702.3625	3.5439	1.0800
16	A'	726.4270	4.1256	0.5170
17	A''	763.0694	4.1966	9.8134
18	A'	910.4626	6.9978	145.6168
19	A'	1090.3686	9.7181	183.9013
20	A'	1126.1144	10.1991	33.7665
21	A'	1270.4835	12.4380	20.7803
22	A'	1364.0904	13.5364	13.8649
23	A'	1459.7798	15.8158	52.3607
24	A'	1491.4369	16.3031	285.1296
25	A'	1543.6371	17.7438	440.1977
26	A'	1660.9914	19.7375	179.4645
27	A'	1678.3780	20.5368	8.3762

b3p86/pyFFCFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	116.7098	0.1489	0.0000
2	B1	122.2590	0.1839	0.0247
3	B2	202.3763	0.5805	0.0377
4	B1	209.5860	0.3844	3.1384
5	A1	279.5910	0.8927	0.7702
6	B2	308.6254	1.0318	0.2828
7	A1	332.3094	1.3472	0.8773
8	B1	335.9181	0.9249	0.8502
9	A1	432.4448	2.0037	0.0379
10	A2	446.6337	1.4859	0.0000
11	B2	462.1802	2.0234	0.0672
12	A1	545.9346	3.1058	1.7793
13	B1	598.3483	2.6157	8.4025
14	A2	693.4194	3.4511	0.0000
15	A1	702.5641	4.5425	9.4089
16	B2	725.6932	4.0996	0.0021
17	B1	734.0422	3.8871	2.8426
18	A1	932.5170	7.0734	145.2491

19	B2	980.9138	8.3282	172.0920
20	B2	1184.4681	11.2439	0.5347
21	A1	1264.3919	12.1534	64.0937
22	B2	1353.4053	13.2891	26.1087
23	A1	1455.6923	15.8623	5.6544
24	A1	1493.3257	16.1712	91.7097
25	B2	1520.5502	17.2003	768.0941
26	B2	1663.0832	20.2655	3.8356
27	A1	1667.5824	19.8790	129.1566

b3p86/pyFFCFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.7983	0.1517	0.0000
2	B1	124.2205	0.1901	0.0399
3	B2	200.9764	0.5723	0.0289
4	B1	209.0536	0.3819	2.5512
5	A1	279.8383	0.8943	0.8796
6	B2	309.5696	1.0379	0.3001
7	A1	332.3330	1.3488	0.7062
8	B1	337.6866	0.9350	0.8398
9	A1	432.8163	2.0056	0.0195
10	A2	446.7212	1.4866	0.0000
11	B2	461.8713	2.0182	0.0517
12	A1	547.6278	3.1211	2.0091
13	B1	601.9324	2.6504	8.0522
14	A1	704.0889	4.5605	7.4285
15	A2	711.3013	3.6319	0.0000
16	B2	727.7800	4.1243	0.0494
17	B1	768.8653	4.2603	2.2299
18	A1	932.2008	7.0646	134.6891
19	B2	986.1272	8.4106	154.2105
20	B2	1191.5929	11.3786	0.4363
21	A1	1268.2874	12.2327	60.6831
22	B2	1346.1449	13.1729	23.3574
23	A1	1458.2299	15.9136	6.9065
24	A1	1493.7562	16.1984	88.1146
25	B2	1521.4876	17.2312	729.6709
26	B2	1657.6335	20.1184	3.2808
27	A1	1663.4441	19.7884	121.4842

b3p86/pyFFCFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.4824	0.1508	0.0000
2	B1	124.1191	0.1898	0.0363
3	B2	202.9478	0.5838	0.0203
4	B1	209.1998	0.3826	2.2529
5	A1	281.1819	0.9030	0.8757
6	B2	310.6369	1.0451	0.2642

7	A1	333.1642	1.3533	0.6719
8	B1	337.7319	0.9350	0.7928
9	A1	433.5590	2.0124	0.0089
10	A2	447.7417	1.4934	0.0000
11	B2	462.7360	2.0265	0.0577
12	A1	548.2707	3.1315	1.9715
13	B1	603.2333	2.6618	7.8522
14	A1	704.9417	4.5710	6.9576
15	A2	709.1284	3.6103	0.0000
16	B2	728.9849	4.1380	0.0336
17	B1	763.5875	4.2025	1.6030
18	A1	935.2994	7.1141	135.4102
19	B2	987.5779	8.4322	154.2576
20	B2	1194.3764	11.4270	0.1931
21	A1	1271.6743	12.2949	61.6855
22	B2	1348.7321	13.2228	24.3044
23	A1	1461.5577	15.9985	5.3242
24	A1	1495.4430	16.2272	89.5738
25	B2	1525.1294	17.3076	731.5534
26	B2	1659.5525	20.1813	3.8538
27	A1	1666.1640	19.8553	123.1244

b3p86/pyFFCFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	116.0980	0.1473	0.0000
2	B1	122.8075	0.1856	0.0322
3	B2	203.6637	0.5877	0.0052
4	B1	207.7898	0.3773	2.7710
5	A1	281.1843	0.9043	0.7927
6	B2	310.0130	1.0413	0.2965
7	A1	331.5617	1.3432	0.7154
8	B1	334.6162	0.9185	0.7042
9	A1	430.8677	1.9905	0.0552
10	A2	445.8243	1.4803	0.0000
11	B2	461.2158	2.0121	0.0659
12	A1	545.7564	3.0939	2.0421
13	B1	593.9265	2.5791	10.3748
14	A1	701.4497	4.5234	7.9412
15	A2	705.9910	3.5788	0.0000
16	B2	724.0108	4.0808	0.0000
17	B1	757.9884	4.1423	1.3310
18	A1	926.9946	6.9807	139.8223
19	B2	983.6081	8.3658	161.3686
20	B2	1191.0400	11.3748	0.2482
21	A1	1264.4932	12.1616	60.3309
22	B2	1357.0948	13.3734	24.6158
23	A1	1462.0254	15.9981	5.1775
24	A1	1495.4605	16.2363	92.3116
25	B2	1526.7953	17.3594	761.1584
26	B2	1663.7928	20.2727	2.1419
27	A1	1669.9425	19.9433	126.0482

b3p86/pyFFFFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	118.7336	0.1541	0.0000
2	B1	157.7420	0.2696	0.0008
3	B1	216.0826	0.4128	4.5416
4	B2	270.4884	0.8112	0.0454
5	A1	271.5387	0.8061	0.7066
6	B2	319.3298	1.0888	0.7509
7	A1	347.2991	1.2457	1.4254
8	B1	352.3938	1.0056	3.1434
9	A2	435.6702	1.4144	0.0000
10	B2	461.3840	2.0219	0.1173
11	A1	480.5986	2.1606	0.2323
12	A1	599.9200	3.6920	0.0043
13	B1	629.8392	2.9052	2.8158
14	A2	685.8596	3.3768	0.0000
15	A1	703.6072	4.5215	6.3829
16	B1	724.6061	3.7945	6.0094
17	B2	745.5986	4.3506	0.0432
18	B2	999.9336	8.5825	215.2744
19	A1	1100.6104	9.9692	244.5471
20	B2	1189.0208	11.3559	0.0010
21	A1	1312.3056	13.2281	28.7877
22	B2	1367.4403	13.5867	17.4348
23	A1	1462.9197	15.8181	19.8464
24	B2	1531.2787	17.4857	733.0950
25	A1	1565.9644	18.1201	168.8221
26	A1	1679.2612	20.1275	115.1022
27	B2	1691.9684	20.8510	3.2495

b3p86/pyFFFFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	120.0455	0.1575	0.0000
2	B1	159.3734	0.2755	0.0000
3	B1	215.5878	0.4104	3.6198
4	B2	271.5707	0.8175	0.0457
5	A1	272.0957	0.8092	0.7986
6	B2	320.0862	1.0936	0.6951
7	A1	347.4906	1.2466	1.2256
8	B1	355.2916	1.0233	2.8022
9	A2	437.3441	1.4254	0.0000
10	B2	461.2442	2.0188	0.1075
11	A1	481.5963	2.1674	0.3051
12	A1	602.7679	3.7253	0.0083
13	B1	642.1079	3.0287	3.4666
14	A1	704.6447	4.5356	4.9806
15	A2	710.4636	3.6232	0.0000

16	B2	748.3942	4.3848	0.0001
17	B1	773.7374	4.3106	4.3521
18	B2	1005.4992	8.6711	198.2300
19	A1	1106.4322	10.0710	228.0785
20	B2	1195.1982	11.4760	0.0243
21	A1	1317.4387	13.3429	26.3889
22	B2	1360.4810	13.4715	14.4367
23	A1	1465.4741	15.8623	23.0927
24	B2	1532.1546	17.5070	706.9929
25	A1	1566.5636	18.1593	160.4337
26	A1	1675.6996	20.0471	109.6520
27	B2	1686.7175	20.7124	2.3958

b3p86/pyFFFFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	119.3921	0.1557	0.0000
2	B1	158.3598	0.2718	0.0003
3	B1	215.4231	0.4097	3.2276
4	B2	272.5917	0.8237	0.0489
5	A1	272.9967	0.8145	0.8157
6	B2	320.6839	1.0976	0.6741
7	A1	347.9839	1.2503	1.1407
8	B1	354.7771	1.0204	2.6224
9	A2	437.5762	1.4270	0.0000
10	B2	461.8710	2.0246	0.1146
11	A1	481.8171	2.1694	0.3458
12	A1	603.0360	3.7279	0.0115
13	B1	639.8044	3.0050	3.0070
14	A1	705.4525	4.5455	4.7501
15	A2	706.8296	3.5870	0.0000
16	B2	748.8289	4.3894	0.0001
17	B1	762.3070	4.1888	3.9374
18	B2	1006.6818	8.6908	196.7944
19	A1	1107.9556	10.0974	230.2462
20	B2	1197.8675	11.5255	0.0877
21	A1	1319.8318	13.3907	27.3195
22	B2	1363.2906	13.5252	15.3149
23	A1	1469.2725	15.9476	23.2779
24	B2	1535.9559	17.5947	700.7075
25	A1	1568.9325	18.2153	159.1913
26	A1	1677.9547	20.1030	112.1251
27	B2	1689.5389	20.7891	2.7521

b3p86/pyFFFFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	118.0348	0.1522	0.0000
2	B1	157.4590	0.2687	0.0001
3	B1	215.0563	0.4086	4.1881

4	B2	272.8883	0.8255	0.0478
5	A1	273.1962	0.8158	0.7677
6	B2	319.6873	1.0911	0.8213
7	A1	346.6592	1.2408	1.3416
8	B1	352.0304	1.0048	2.9812
9	A2	436.6143	1.4204	0.0000
10	B2	460.5188	2.0120	0.1081
11	A1	480.4373	2.1563	0.2665
12	A1	601.0913	3.7032	0.0031
13	B1	636.4016	2.9737	3.3296
14	A1	702.2946	4.5023	5.2117
15	A2	704.5182	3.5640	0.0000
16	B2	743.7216	4.3282	0.0128
17	B1	761.2985	4.1745	4.2998
18	B2	1002.3390	8.6179	201.7964
19	A1	1103.3017	10.0137	234.4557
20	B2	1195.0607	11.4797	0.0080
21	A1	1315.2874	13.3089	26.9458
22	B2	1370.8490	13.6652	14.9875
23	A1	1468.5379	15.9351	21.7875
24	B2	1536.5901	17.6159	720.2235
25	A1	1572.2049	18.2881	165.4686
26	A1	1681.7941	20.1926	113.1454
27	B2	1692.5855	20.8606	1.8862

b3p86/pyFFHFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	115.2078	0.1452	0.0000
2	B1	204.5758	0.3322	3.6560
3	A1	280.3465	0.8402	0.6778
4	B1	298.8079	0.4395	0.9949
5	B2	302.6113	0.9579	0.2117
6	A1	362.1047	1.2382	2.6422
7	B2	454.9203	1.7520	0.0809
8	A2	461.6179	1.5869	0.0000
9	B1	487.7141	0.6188	0.4858
10	A1	511.6161	2.2804	1.7974
11	B2	665.0219	1.5664	2.4497
12	A1	695.0862	4.2657	16.4898
13	A2	698.7209	3.5023	0.0000
14	B1	726.6535	2.6962	10.5317
15	A1	758.7577	3.2594	10.9322
16	B1	890.5999	0.6475	31.9608
17	B2	920.3694	2.6780	131.8228
18	B2	1167.8380	3.3233	27.2091
19	B2	1202.7947	1.6678	52.6487
20	A1	1242.6941	10.2394	203.3341
21	B2	1357.9339	12.9362	71.5967
22	A1	1439.2469	14.3614	0.4154
23	A1	1479.2981	14.7495	47.2890
24	B2	1534.8807	11.0406	754.3535

25	A1	1678.6423	19.1262	26.5468
26	B2	1682.0133	15.1717	2.2510
27	A1	3230.8424	6.7286	4.9896

b3p86/pyFFHFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	116.6736	0.1489	0.0000
2	B1	205.0303	0.3359	2.8591
3	A1	281.0036	0.8438	0.7286
4	B1	301.6557	0.4458	0.9882
5	B2	303.8461	0.9654	0.1642
6	A1	362.7050	1.2416	2.2227
7	B2	454.7672	1.7483	0.0628
8	A2	462.5573	1.5934	0.0000
9	B1	492.8532	0.6154	0.4361
10	A1	513.3132	2.2904	2.0269
11	B2	668.2532	1.5717	2.4269
12	A1	697.8439	4.3249	13.9713
13	A2	719.7894	3.7168	0.0000
14	B1	754.5997	2.1457	12.8666
15	A1	760.6427	3.2699	11.4065
16	B1	910.8494	0.7245	24.8331
17	B2	924.4030	2.6533	116.4570
18	B2	1174.7969	3.1134	30.7672
19	B2	1207.1801	1.7729	44.7361
20	A1	1249.2789	10.3519	185.8941
21	B2	1350.7120	12.5916	66.5288
22	A1	1442.6928	14.4078	0.7365
23	A1	1480.2162	14.8555	49.2640
24	B2	1536.0041	11.1404	734.4875
25	A1	1675.5982	19.0725	26.0196
26	B2	1677.6297	14.7685	3.4763
27	A1	3227.1719	6.7097	4.0407

b3p86/pyFFHFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	116.2696	0.1479	0.0000
2	B1	204.8351	0.3347	2.5565
3	A1	281.9276	0.8492	0.7399
4	B1	301.0453	0.4447	0.9811
5	B2	304.5955	0.9703	0.1578
6	A1	363.0221	1.2443	2.1001
7	B2	455.5521	1.7557	0.0605
8	A2	462.9547	1.5962	0.0000
9	B1	491.4599	0.6173	0.3659
10	A1	513.6375	2.2931	2.0713
11	B2	668.8769	1.5774	2.3922
12	A1	698.7101	4.3321	13.6082

13	A2	717.2127	3.6908	0.0000
14	B1	750.7551	2.2847	10.8398
15	A1	761.3153	3.2756	11.5230
16	B1	903.1701	0.6988	26.7190
17	B2	925.6909	2.6570	114.8620
18	B2	1177.7984	3.0439	31.8157
19	B2	1209.8411	1.8074	41.5848
20	A1	1252.2753	10.3897	188.5717
21	B2	1353.5441	12.6664	69.6791
22	A1	1445.6533	14.4183	0.6147
23	A1	1483.5786	14.9887	48.9752
24	B2	1540.2087	11.1759	726.1429
25	A1	1677.6344	19.1250	27.0221
26	B2	1680.6211	14.8543	3.1547
27	A1	3231.2200	6.7268	3.9022

b3p86/pyFFHFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	114.8282	0.1442	0.0000
2	B1	203.5472	0.3310	3.3197
3	A1	281.6500	0.8478	0.7026
4	B1	299.4692	0.4415	1.0223
5	B2	303.9853	0.9674	0.2298
6	A1	361.2601	1.2319	2.4174
7	B2	454.1484	1.7465	0.0762
8	A2	461.3078	1.5845	0.0000
9	B1	487.4354	0.6076	0.4082
10	A1	511.9951	2.2794	1.8111
11	B2	664.8133	1.5817	2.2510
12	A1	694.9817	4.2814	14.1245
13	A2	713.3144	3.6513	0.0000
14	B1	745.5284	2.1727	12.4026
15	A1	758.7314	3.2537	11.4645
16	B1	902.2556	0.7022	28.4119
17	B2	922.2318	2.6607	122.8600
18	B2	1173.6647	3.0461	28.5152
19	B2	1207.2032	1.7576	43.8052
20	A1	1244.5977	10.2758	195.9757
21	B2	1362.3653	12.9647	64.5044
22	A1	1445.9685	14.4334	0.4461
23	A1	1482.1133	14.8629	47.3528
24	B2	1539.3697	11.3522	748.3618
25	B2	1681.7828	15.1540	3.5009
26	A1	1682.2065	19.2266	26.3698
27	A1	3236.6577	6.7527	5.7976

b3p86/pyFHFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A"	128.9004	0.1634	0.1285
2	A"	211.2594	0.3579	4.0028
3	A"	261.4217	0.2899	1.1830
4	A'	272.3555	0.8131	0.1983
5	A'	320.4016	1.0393	1.0203
6	A'	354.0133	1.2134	1.5341
7	A"	387.6959	0.9256	0.8168
8	A'	465.0466	1.7919	0.4314
9	A'	533.0369	1.8642	2.8398
10	A'	602.7368	3.6856	0.0525
11	A"	630.8702	1.2898	5.9491
12	A'	671.7150	1.6721	2.6110
13	A"	684.4004	1.9824	0.0040
14	A"	738.6400	2.1917	1.6070
15	A'	808.4914	3.7780	43.5519
16	A"	844.9604	0.6546	39.0537
17	A'	1037.7060	2.5357	90.1181
18	A'	1093.6735	8.1158	170.0719
19	A'	1170.9006	1.5575	99.8908
20	A'	1263.4972	6.4063	39.2683
21	A'	1371.1600	12.9238	9.3688
22	A'	1437.6701	12.2295	61.9918
23	A'	1482.1906	13.8281	161.5031
24	A'	1550.1411	10.6315	448.1107
25	A'	1670.5931	16.5495	275.4810
26	A'	1687.8269	19.2025	43.6159
27	A'	3245.1281	6.7939	5.5229

b3p86/pyFHFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	129.8878	0.1659	0.1023
2	A"	211.4110	0.3623	3.1710
3	A"	264.0632	0.2929	1.2661
4	A'	273.1665	0.8175	0.2310
5	A'	321.1129	1.0429	0.8817
6	A'	354.6518	1.2175	1.2041
7	A"	388.6971	0.9382	0.7611
8	A'	465.2025	1.7932	0.4136
9	A'	532.7428	1.8630	2.4267
10	A'	605.7174	3.7220	0.0188
11	A"	638.9939	1.2721	6.3376
12	A'	674.3796	1.6761	2.8319
13	A"	696.8896	1.8065	0.0002
14	A"	764.9257	1.9479	0.2355
15	A'	810.4491	3.7928	38.1686
16	A"	861.0969	0.7454	35.5142
17	A'	1040.0724	2.4663	79.2215
18	A'	1100.1182	8.1541	154.0187
19	A'	1176.9305	1.5981	100.4914
20	A'	1268.5364	6.6638	35.7115
21	A'	1364.4588	12.5803	9.8556

22	A'	1443.1963	12.4855	64.0944
23	A'	1482.3525	13.7686	148.9696
24	A'	1551.3801	10.6658	438.2209
25	A'	1667.0200	16.3088	263.7750
26	A'	1683.1567	18.9400	41.1458
27	A'	3241.9508	6.7770	4.3177

b3p86/pyFHFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	129.4375	0.1648	0.0929
2	A"	211.1147	0.3601	2.8937
3	A"	263.2815	0.2925	1.2609
4	A'	274.1281	0.8233	0.2366
5	A'	321.8011	1.0474	0.8691
6	A'	355.2092	1.2216	1.1484
7	A"	388.3465	0.9371	0.6560
8	A'	465.7109	1.7972	0.4128
9	A'	533.3959	1.8692	2.2879
10	A'	606.0893	3.7251	0.0149
11	A"	638.1175	1.2914	5.7567
12	A'	674.9631	1.6796	2.7468
13	A"	696.0163	1.8405	0.0031
14	A"	759.2276	2.0865	0.4226
15	A'	811.4316	3.8022	37.8854
16	A"	852.6833	0.7053	34.8450
17	A'	1041.6497	2.4542	78.8507
18	A'	1102.4057	8.2266	152.8679
19	A'	1179.6704	1.6039	98.4949
20	A'	1270.9833	6.7540	36.5932
21	A'	1367.6170	12.5996	10.5278
22	A'	1447.0068	12.6991	63.4233
23	A'	1485.9913	13.7773	140.4960
24	A'	1554.5841	10.7307	438.3898
25	A'	1669.4419	16.3260	268.9257
26	A'	1685.8411	19.0313	42.2451
27	A'	3246.0025	6.7939	4.2118

b3p86/pyFHFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	128.4906	0.1624	0.1201
2	A"	210.6938	0.3593	3.7084
3	A"	261.6907	0.2899	1.2945
4	A'	274.3027	0.8245	0.2204
5	A'	320.6173	1.0414	1.0372
6	A'	353.3768	1.2098	1.4058
7	A"	386.9562	0.9228	0.7271
8	A'	464.6704	1.7908	0.4123
9	A'	532.0628	1.8600	2.4104

10	A'	604.0628	3.7000	0.0481
11	A''	634.5766	1.2907	6.2364
12	A'	670.9083	1.6850	2.4937
13	A''	691.8765	1.8165	0.0001
14	A''	757.6091	2.0467	0.3548
15	A'	808.2238	3.7651	39.7035
16	A''	855.4598	0.7108	39.2623
17	A'	1038.5416	2.5088	86.5418
18	A'	1097.3133	8.1398	159.9431
19	A'	1175.5846	1.5596	93.8226
20	A'	1267.5006	6.5205	35.6675
21	A'	1374.0314	13.0539	9.0903
22	A'	1444.8456	12.4425	66.5627
23	A'	1485.7400	13.8283	148.5511
24	A'	1554.7077	10.9136	450.9159
25	A'	1672.2752	16.6352	272.7784
26	A'	1688.8518	19.2011	39.5385
27	A'	3251.5319	6.8206	6.3454

b3p86/pyHHHHH_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	377.6753	0.2149	0.0000
2	B1	414.5707	0.3807	3.8647
3	A1	612.2068	1.5627	3.5456
4	B2	667.2012	1.6584	0.3495
5	B1	715.0142	0.4088	70.1894
6	B1	759.8314	0.8204	11.1475
7	A2	894.4887	0.5883	0.0000
8	B1	955.4435	0.7167	0.0272
9	A2	997.5601	0.8617	0.0000
10	B1	1005.8850	0.7643	0.0060
11	A1	1015.6519	4.3412	6.0936
12	A1	1051.1552	3.1097	3.9914
13	B2	1081.8816	1.1840	0.0158
14	A1	1096.6699	1.1480	6.5446
15	B2	1168.5020	0.8934	2.2262
16	A1	1244.2271	1.1583	4.6425
17	B2	1317.4254	8.2556	0.0017
18	B2	1377.9604	1.3435	0.0086
19	B2	1473.4369	2.7095	27.5124
20	A1	1513.3885	2.7751	2.8878
21	B2	1636.5493	9.6860	11.1341
22	A1	1641.3850	8.6321	24.4235
23	B2	3160.8831	6.4037	26.3471
24	A1	3163.2420	6.4295	3.4667
25	A1	3185.0943	6.5092	4.2387
26	B2	3201.4409	6.6056	20.3647
27	A1	3209.0748	6.6720	5.3472

b3p86/pyHHHHH_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	380.1733	0.2148	0.0000
2	B1	417.1764	0.3805	3.6657
3	A1	611.8588	1.5580	4.2912
4	B2	666.8796	1.6528	0.2023
5	B1	720.5579	0.4012	65.1100
6	B1	768.7040	0.8406	7.6590
7	A2	901.3746	0.5976	0.0000
8	B1	965.8597	0.7355	0.0208
9	A2	1013.5954	0.8965	0.0000
10	A1	1016.5172	4.2877	6.4385
11	B1	1022.3236	0.8161	0.0119
12	A1	1055.0730	3.0438	4.7882
13	B2	1082.8268	1.1865	0.0180
14	A1	1097.8575	1.1691	4.2715
15	B2	1166.5604	0.8959	2.4065
16	A1	1243.1587	1.1636	3.7466
17	B2	1312.9577	7.9320	0.0023
18	B2	1382.1906	1.3530	0.0563
19	B2	1476.6870	2.7322	26.5446
20	A1	1517.8527	2.7731	2.5986
21	B2	1636.0907	9.4941	10.7252
22	A1	1640.4366	8.5087	23.9121
23	B2	3157.9613	6.3910	26.0753
24	A1	3160.5204	6.4198	3.7437
25	A1	3184.4696	6.5041	3.8692
26	B2	3200.4648	6.5989	20.1304
27	A1	3208.1475	6.6645	5.5349

b3p86/pyHHHHH_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	381.1784	0.2156	0.0000
2	B1	418.2154	0.3845	3.6294
3	A1	612.5170	1.5634	4.4809
4	B2	668.2736	1.6618	0.2628
5	B1	720.7019	0.3951	66.9782
6	B1	770.7083	0.8681	6.8278
7	A2	902.2368	0.5986	0.0000
8	B1	965.8451	0.7375	0.0165
9	A2	1013.7930	0.8978	0.0000
10	A1	1017.9833	4.3121	7.1211
11	B1	1026.9675	0.8210	0.0016
12	A1	1055.9781	3.0465	5.1088
13	B2	1084.2322	1.1904	0.0074
14	A1	1099.2866	1.1710	4.3555
15	B2	1169.4435	0.9004	2.3083
16	A1	1245.1932	1.1668	3.5921
17	B2	1315.9345	7.9574	0.0001
18	B2	1383.8790	1.3561	0.0434

19	B2	1479.4653	2.7391	27.3968
20	A1	1519.9753	2.7842	3.0475
21	B2	1638.7059	9.5427	10.4558
22	A1	1642.5632	8.5261	24.5161
23	B2	3161.1063	6.4036	26.8445
24	A1	3163.7530	6.4334	4.6237
25	A1	3188.2148	6.5193	4.1227
26	B2	3204.3338	6.6146	20.0500
27	A1	3211.9111	6.6805	5.3503

b3p86/pyHHHHH_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	379.4461	0.2148	0.0000
2	B1	415.4152	0.3805	3.8455
3	A1	611.8810	1.5613	3.6837
4	B2	665.9004	1.6508	0.4021
5	B1	715.0371	0.3915	75.1921
6	B1	765.5457	0.8553	8.4375
7	A2	895.4961	0.5895	0.0000
8	B1	957.9674	0.7235	0.0409
9	A2	1005.3684	0.8803	0.0000
10	A1	1013.8887	4.3018	6.6281
11	B1	1017.9800	0.8030	0.0300
12	A1	1053.0260	3.1062	4.0310
13	B2	1082.7263	1.1793	0.0459
14	A1	1096.7650	1.1473	6.5665
15	B2	1168.4434	0.8869	2.1756
16	A1	1243.8046	1.1538	4.0504
17	B2	1319.3997	8.5588	0.0022
18	B2	1376.1366	1.3410	0.0107
19	B2	1472.4047	2.7261	28.4320
20	A1	1511.8604	2.7788	3.5344
21	B2	1636.2287	9.7804	10.1527
22	A1	1642.3077	8.7903	23.9374
23	B2	3167.6996	6.4316	21.6746
24	A1	3170.0173	6.4578	3.6160
25	A1	3192.6681	6.5395	3.7524
26	B2	3208.3039	6.6338	16.3304
27	A1	3215.8769	6.7010	3.9323

blyp/pyCCCCC_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	52.2347	0.0549	0.0000
2	B1	74.9516	0.1121	0.0138
3	B1	140.7671	0.1866	0.0000
4	A1	194.9319	0.7377	0.1112
5	B2	206.8088	0.7768	0.4386
6	A1	209.7718	0.7500	0.1032

7	B2	217.4065	0.9699	0.0052
8	B1	270.6043	0.5810	0.5471
9	B2	315.4487	1.7367	0.6233
10	A1	330.1378	1.8831	0.0918
11	A2	348.0563	0.8933	0.0000
12	A1	360.5522	2.5304	0.3959
13	A1	509.2046	2.6495	11.7079
14	B1	548.1007	2.1980	1.0995
15	B2	557.7173	2.5044	6.6025
16	A2	596.6582	2.5376	0.0000
17	B2	632.8916	3.5922	113.0236
18	B1	695.0149	3.4785	0.0798
19	A1	775.7071	4.8270	97.7409
20	B2	830.8623	5.2248	3.3727
21	A1	1024.9463	7.7572	38.0112
22	A1	1155.6791	9.6596	3.5547
23	B2	1233.6879	10.8426	81.3042
24	B2	1276.5851	12.0080	380.3752
25	A1	1277.7504	11.6763	125.1338
26	A1	1449.0394	14.9356	92.7125
27	B2	1478.1011	16.1699	57.2329

blyp/pyCCCCC_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	54.3088	0.0593	0.0000
2	B1	77.0373	0.1181	0.0096
3	B1	142.5807	0.1914	0.0032
4	A1	192.4259	0.7291	0.0557
5	B2	204.4787	0.7606	0.4196
6	A1	207.4436	0.7252	0.0750
7	B2	212.7019	0.9276	0.0086
8	B1	275.1589	0.6014	0.5544
9	B2	315.7744	1.7397	0.6239
10	A1	330.8459	1.8941	0.0717
11	A2	354.1990	0.9253	0.0000
12	A1	361.3037	2.5391	0.4168
13	A1	510.1314	2.6591	10.0900
14	B2	556.3746	2.4946	5.2473
15	B1	559.4905	2.2913	1.0851
16	A2	615.5142	2.7008	0.0000
17	B2	633.8851	3.5982	103.7806
18	B1	720.7571	3.7394	0.9737
19	A1	776.7996	4.8407	90.9260
20	B2	830.5912	5.2227	3.2847
21	A1	1025.7627	7.7718	34.8362
22	A1	1155.5264	9.6492	4.5887
23	B2	1231.4605	10.8251	61.5012
24	B2	1274.1685	11.9491	355.8085
25	A1	1274.8773	11.6233	106.9303
26	A1	1445.1869	14.8530	85.0748
27	B2	1471.9718	16.0213	52.6196

blyp/pyCCCCC_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	54.4521	0.0596	0.0000
2	B1	77.3932	0.1191	0.0122
3	B1	143.2559	0.1933	0.0027
4	A1	193.5314	0.7389	0.0697
5	B2	205.7284	0.7699	0.3680
6	A1	208.7477	0.7335	0.0660
7	B2	213.4569	0.9342	0.0059
8	B1	275.9013	0.6048	0.5338
9	B2	317.2945	1.7524	0.6113
10	A1	332.4771	1.9068	0.0891
11	A2	356.4449	0.9372	0.0000
12	A1	363.5699	2.5675	0.3866
13	A1	513.3579	2.6911	9.5378
14	B2	560.2403	2.5300	5.3871
15	B1	562.0776	2.3124	1.0489
16	A2	618.8474	2.7306	0.0000
17	B2	639.7668	3.6648	102.0580
18	B1	722.3275	3.7557	0.8632
19	A1	781.2719	4.9030	93.0305
20	B2	836.8363	5.3074	2.7724
21	A1	1031.1197	7.8584	34.9432
22	A1	1158.1703	9.6960	4.2027
23	B2	1233.7911	10.8573	70.2469
24	B2	1276.5727	11.9984	342.0913
25	A1	1277.6137	11.6732	107.5690
26	A1	1446.4065	14.8787	88.5546
27	B2	1474.8773	16.0921	50.5702

blyp/pyCCCCC_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	52.9329	0.0564	0.0000
2	B1	75.2151	0.1127	0.0131
3	B1	140.1434	0.1849	0.0178
4	A1	193.7824	0.7272	0.0854
5	B2	205.7997	0.7697	0.3009
6	A1	208.3015	0.7419	0.0445
7	B2	216.1908	0.9591	0.0048
8	B1	270.4742	0.5805	0.2972
9	B2	313.1086	1.7197	0.7118
10	A1	327.6558	1.8632	0.0942
11	A2	349.3510	0.8999	0.0000
12	A1	357.0915	2.4897	0.4146
13	A1	503.9742	2.5959	12.3975
14	B1	547.8028	2.1937	0.8687
15	B2	553.6765	2.4787	8.6653

16	A2	599.1919	2.5593	0.0000
17	B2	626.2097	3.5002	112.5315
18	B1	698.4284	3.5166	1.1064
19	A1	769.3757	4.7411	100.6970
20	B2	824.1432	5.1292	2.7764
21	A1	1017.3205	7.6376	39.8109
22	A1	1152.5522	9.5969	3.1006
23	B2	1238.2708	10.9144	85.1507
24	B2	1274.7047	11.9771	359.4662
25	A1	1275.1317	11.6254	118.6401
26	A1	1450.3937	14.9608	92.7020
27	B2	1477.6007	16.1614	55.2412

blyp/pyFCFCF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	85.4212	0.0919	0.0000
2	B1	103.3851	0.1375	0.0060
3	A1	178.2593	0.4968	0.0228
4	B1	203.3605	0.3679	2.5759
5	B2	218.8858	0.6347	0.0520
6	B2	300.9179	1.1502	0.4588
7	B1	303.4162	0.7503	0.3347
8	A1	307.9031	1.2247	0.0890
9	A2	361.2001	0.9640	0.0000
10	A1	389.2241	1.8421	0.9052
11	B2	393.6268	1.7050	0.0080
12	A1	554.1789	2.9122	1.7380
13	A1	584.7579	3.3362	3.6822
14	B1	611.0631	2.7324	1.4082
15	A2	654.5007	3.0709	0.0000
16	B2	673.6126	3.5591	2.0621
17	B1	711.9955	3.6528	10.8654
18	B2	743.9252	4.6631	135.2885
19	A1	1010.1792	8.3558	188.3456
20	B2	1026.5897	8.5120	27.3282
21	A1	1079.7070	8.6750	10.6538
22	B2	1291.7756	12.1115	6.0444
23	A1	1342.6876	13.3270	41.1898
24	B2	1364.7216	13.6609	444.8848
25	A1	1385.4779	14.0066	89.0110
26	A1	1532.8201	16.7619	172.4460
27	B2	1546.5620	17.5419	43.8071

blyp/pyFCFCF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	86.9902	0.0953	0.0000
2	B1	104.9837	0.1417	0.0003
3	A1	176.6715	0.4879	0.0096

4	B1	202.4614	0.3646	2.3184
5	B2	217.5114	0.6263	0.0465
6	B2	301.1140	1.1540	0.4599
7	B1	306.1410	0.7646	0.4700
8	A1	308.2369	1.2294	0.0741
9	A2	358.4040	0.9489	0.0000
10	A1	390.0765	1.8493	0.8567
11	B2	394.2022	1.7053	0.0168
12	A1	555.8348	2.9022	1.6343
13	A1	587.6979	3.3949	2.6374
14	B1	614.7232	2.7654	1.3041
15	A2	664.7057	3.1684	0.0000
16	B2	675.0890	3.5757	1.2735
17	B1	730.1416	3.8402	9.0080
18	B2	743.5772	4.6508	125.5845
19	A1	1017.3269	8.4561	173.3928
20	B2	1032.9084	8.6324	24.3706
21	A1	1079.9499	8.6910	6.8782
22	B2	1287.4738	12.0524	3.6028
23	A1	1349.4567	13.4480	47.6301
24	B2	1367.9390	13.7189	419.4369
25	A1	1386.9714	14.0737	70.1477
26	A1	1530.5973	16.7143	167.7753
27	B2	1542.3848	17.4373	46.9564

blyp/pyFCFCF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	86.8235	0.0949	0.0000
2	B1	104.8001	0.1413	0.0038
3	A1	178.7563	0.4994	0.0041
4	B1	202.9321	0.3665	1.9572
5	B2	219.8480	0.6403	0.0352
6	B2	302.7061	1.1652	0.4441
7	B1	307.1601	0.7693	0.4461
8	A1	309.8288	1.2393	0.0582
9	A2	361.3428	0.9648	0.0000
10	A1	391.5350	1.8633	0.8190
11	B2	395.3810	1.7148	0.0183
12	A1	557.0167	2.9272	1.3944
13	A1	589.0798	3.3981	2.5392
14	B1	614.9203	2.7677	1.0714
15	A2	665.8460	3.1795	0.0000
16	B2	677.6859	3.6037	1.2357
17	B1	729.3543	3.8317	7.5853
18	B2	748.8345	4.7221	121.8811
19	A1	1020.0558	8.5009	172.9730
20	B2	1037.7329	8.7053	21.5950
21	A1	1085.0141	8.7715	7.0529
22	B2	1291.6277	12.1230	4.9421
23	A1	1355.7956	13.5899	45.8178
24	B2	1372.0187	13.8065	406.3867

25	A1	1389.9822	14.1302	75.1191
26	A1	1533.0252	16.7711	172.1073
27	B2	1546.9115	17.5518	48.7402

blyp/pyFCFCF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	85.7415	0.0925	0.0000
2	B1	103.6385	0.1380	0.0100
3	A1	178.3584	0.4974	0.0006
4	B1	200.8247	0.3584	2.1606
5	B2	219.7676	0.6398	0.0270
6	B2	300.8467	1.1524	0.3776
7	B1	302.4487	0.7470	0.1803
8	A1	307.4751	1.2264	0.0363
9	A2	354.1383	0.9260	0.0000
10	A1	387.4422	1.8247	0.9682
11	B2	392.4340	1.6931	0.0002
12	A1	553.5059	2.8737	1.7801
13	A1	584.2701	3.3542	2.7546
14	B1	608.9727	2.7125	0.7206
15	A2	656.1659	3.0889	0.0000
16	B2	670.9591	3.5328	1.9913
17	B1	715.1141	3.6861	13.7445
18	B2	737.7680	4.5690	128.7805
19	A1	1013.3072	8.3818	187.7680
20	B2	1030.5816	8.5921	23.7342
21	A1	1074.4846	8.6062	5.8388
22	B2	1297.1234	12.2348	2.0075
23	A1	1351.0604	13.4852	47.0528
24	B2	1369.1444	13.7327	433.8394
25	A1	1389.9837	14.1368	77.5323
26	A1	1536.3867	16.8373	174.9558
27	B2	1546.2417	17.5301	41.2426

blyp/pyFCFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	90.8682	0.1031	0.0014
2	A''	132.9677	0.1948	0.0039
3	A'	196.5026	0.5351	0.0287
4	A''	202.7450	0.3646	3.4156
5	A'	268.6993	0.8018	0.2446
6	A'	300.6045	1.0912	0.4125
7	A''	313.4030	0.7930	0.6917
8	A'	319.6404	1.1301	0.4635
9	A'	389.8074	1.7422	0.3768
10	A''	390.9501	1.1419	1.1485
11	A'	453.9149	1.9663	0.5708
12	A'	563.8574	3.2125	0.6845

13	A''	602.9055	2.6633	2.0180
14	A'	603.3611	3.3666	10.3579
15	A''	651.1762	3.0415	0.3930
16	A'	693.6006	3.7648	0.6936
17	A''	700.8638	3.5390	7.2768
18	A'	850.2728	6.1236	170.7353
19	A'	1014.4869	8.4081	182.5022
20	A'	1039.3496	8.6698	50.1628
21	A'	1178.1028	10.6007	25.4987
22	A'	1300.7184	12.2839	10.0097
23	A'	1346.6294	13.3893	40.0767
24	A'	1385.2180	14.0316	322.7197
25	A'	1428.4430	15.1005	368.4929
26	A'	1553.9618	17.2486	145.8233
27	A'	1566.3622	17.8795	5.9925

blyp/pyFCFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	92.7188	0.1073	0.0000
2	A''	134.7600	0.2002	0.0038
3	A'	195.0479	0.5271	0.0231
4	A''	202.3154	0.3628	2.9386
5	A'	268.8370	0.8026	0.2844
6	A'	300.9088	1.0962	0.3887
7	A''	316.5961	0.8102	0.8016
8	A'	320.1160	1.1324	0.4208
9	A'	390.4994	1.7447	0.3272
10	A''	392.1360	1.1486	0.9306
11	A'	455.1985	1.9759	0.6348
12	A'	567.1229	3.2319	0.8358
13	A'	604.7054	3.3935	8.7851
14	A''	608.2951	2.7123	2.0102
15	A''	665.8294	3.1802	0.4533
16	A'	695.8912	3.7902	0.4179
17	A''	727.4376	3.8097	5.8333
18	A'	853.5269	6.1567	157.1757
19	A'	1021.1181	8.5073	162.5768
20	A'	1045.3917	8.7921	54.2817
21	A'	1184.0015	10.7216	23.4967
22	A'	1296.7493	12.2320	6.7038
23	A'	1352.6950	13.5028	42.1720
24	A'	1387.6981	14.0780	299.4216
25	A'	1430.9537	15.1752	355.6601
26	A'	1552.5483	17.2259	144.5558
27	A'	1563.6811	17.8008	5.2808

blyp/pyFCFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A"	92.4674	0.1067	0.0006
2	A"	133.9534	0.1979	0.0006
3	A'	197.2176	0.5390	0.0241
4	A"	202.2539	0.3625	2.4651
5	A'	269.6818	0.8073	0.2839
6	A'	302.0344	1.1014	0.3871
7	A"	317.1366	0.8132	0.7607
8	A'	321.2093	1.1415	0.3700
9	A'	391.7429	1.7556	0.3146
10	A"	392.8113	1.1521	0.7926
11	A'	455.9061	1.9819	0.6188
12	A'	567.7435	3.2433	0.6949
13	A'	606.6132	3.4131	8.1291
14	A"	606.8377	2.6984	1.6422
15	A"	663.5549	3.1586	0.1985
16	A'	697.4595	3.8074	0.3974
17	A"	719.3112	3.7284	4.9921
18	A'	856.9568	6.2087	152.8988
19	A'	1024.2045	8.5614	165.8093
20	A'	1050.1142	8.8588	46.7590
21	A'	1188.5808	10.8063	23.0718
22	A'	1300.9009	12.3059	8.0354
23	A'	1358.5326	13.6311	43.4933
24	A'	1391.3489	14.1461	277.9944
25	A'	1434.7786	15.2667	360.9588
26	A'	1555.8948	17.2936	146.4842
27	A'	1567.6347	17.9095	5.8202

blyp/pyFCFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	91.2869	0.1039	0.0019
2	A"	132.9632	0.1948	0.0014
3	A'	196.9759	0.5373	0.0341
4	A"	200.8092	0.3573	2.9779
5	A'	269.2457	0.8051	0.2570
6	A'	300.2872	1.0925	0.3961
7	A"	312.3994	0.7892	0.5155
8	A'	319.1309	1.1269	0.4042
9	A'	388.4258	1.7291	0.4213
10	A"	389.1831	1.1313	1.3815
11	A'	453.6556	1.9612	0.6488
12	A'	564.8401	3.2065	0.8918
13	A'	601.0751	3.3456	9.2810
14	A"	601.8138	2.6530	1.4630
15	A"	657.6509	3.1040	0.8920
16	A'	691.4021	3.7406	0.5537
17	A"	712.4700	3.6567	7.3991
18	A'	848.8686	6.0840	159.2717
19	A'	1017.5778	8.4503	172.9922
20	A'	1042.9975	8.7468	51.0338
21	A'	1181.2940	10.6830	22.9162

22	A'	1306.3462	12.4125	5.4850
23	A'	1354.1779	13.5352	42.6266
24	A'	1388.6546	14.0986	305.6576
25	A'	1434.8257	15.2585	363.0893
26	A'	1557.5967	17.3484	143.5043
27	A'	1567.9545	17.8850	6.2138

blyp/pyFFCFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	109.0591	0.1302	0.0000
2	B1	115.2418	0.1637	0.0143
3	B2	196.9715	0.5497	0.0440
4	B1	197.3077	0.3405	3.2026
5	A1	271.8802	0.8474	0.6339
6	B2	297.4978	0.9598	0.2209
7	A1	314.8965	1.2144	0.5555
8	B1	317.7115	0.8263	0.6966
9	A1	412.2571	1.8473	0.1491
10	A2	420.0948	1.3140	0.0000
11	B2	443.8234	1.8805	0.1025
12	A1	515.3945	2.7644	1.5545
13	B1	565.4962	2.3394	7.3743
14	A2	653.1789	3.0594	0.0000
15	A1	665.0163	4.0966	12.2154
16	B1	690.8529	3.4393	2.0533
17	B2	691.0315	3.7185	0.0924
18	A1	868.5712	6.1008	145.8959
19	B2	913.7401	7.2531	195.1990
20	B2	1090.1558	9.4726	1.2673
21	A1	1182.3068	10.5819	62.3454
22	B2	1296.3157	12.1775	10.4680
23	A1	1348.2399	13.5497	4.0736
24	A1	1393.1364	14.0184	74.0763
25	B2	1408.3774	14.6970	717.1297
26	B2	1550.9429	17.6196	2.0498
27	A1	1561.1624	17.4009	119.3030

blyp/pyFFCFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	110.7055	0.1342	0.0000
2	B1	117.3426	0.1699	0.0250
3	B2	195.7504	0.5428	0.0386
4	B1	197.3439	0.3402	2.6694
5	A1	271.9789	0.8478	0.7220
6	B2	298.1252	0.9636	0.2325
7	A1	315.1644	1.2184	0.4426
8	B1	319.7176	0.8370	0.7073
9	A1	413.3190	1.8558	0.1157

10	A2	420.8895	1.3190	0.0000
11	B2	444.3494	1.8822	0.0844
12	A1	517.9080	2.7863	1.7667
13	B1	569.6964	2.3758	7.2163
14	A1	668.0419	4.1328	10.1251
15	A2	668.2786	3.2027	0.0000
16	B2	693.6358	3.7473	0.0039
17	B1	721.2198	3.7463	1.6288
18	A1	869.5815	6.1114	136.7711
19	B2	920.5160	7.3570	178.5587
20	B2	1098.5748	9.6273	1.2227
21	A1	1188.0066	10.6912	60.4153
22	B2	1291.9256	12.1161	8.3591
23	A1	1352.7102	13.6393	5.1196
24	A1	1395.4210	14.0754	69.9751
25	B2	1411.7774	14.7692	682.7400
26	B2	1548.1190	17.5418	1.8470
27	A1	1559.9829	17.3787	112.5453

blyp/pyFFCFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	110.1947	0.1329	0.0000
2	B1	117.2090	0.1695	0.0216
3	B1	197.2973	0.3402	2.2117
4	B2	197.8380	0.5546	0.0259
5	A1	273.2125	0.8554	0.7168
6	B2	299.1891	0.9705	0.2091
7	A1	316.2657	1.2242	0.4235
8	B1	319.5610	0.8361	0.6636
9	A1	414.3492	1.8643	0.0739
10	A2	421.7746	1.3246	0.0000
11	B2	445.4254	1.8918	0.0803
12	A1	518.8268	2.7996	1.7446
13	B1	571.3570	2.3896	6.4151
14	A2	664.6345	3.1687	0.0000
15	A1	669.2662	4.1458	9.1733
16	B2	695.2328	3.7649	0.0052
17	B1	714.3532	3.6759	1.0857
18	A1	873.7533	6.1734	135.4152
19	B2	923.1943	7.3948	172.9423
20	B2	1103.9524	9.7192	0.7567
21	A1	1192.8887	10.7784	59.2260
22	B2	1296.1359	12.1939	8.6932
23	A1	1357.5907	13.7506	3.9811
24	A1	1398.2905	14.1299	70.8560
25	B2	1416.7253	14.8704	671.5319
26	B2	1551.1401	17.6240	2.2295
27	A1	1563.9408	17.4697	112.9926

blyp/pyFFCFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	108.7862	0.1295	0.0000
2	B1	115.9546	0.1657	0.0159
3	B1	195.3824	0.3333	2.7061
4	B2	197.6334	0.5532	0.0102
5	A1	272.5500	0.8525	0.6448
6	B2	298.0004	0.9632	0.2256
7	A1	314.1283	1.2109	0.4336
8	B1	315.7269	0.8169	0.5547
9	A1	411.0240	1.8366	0.1812
10	A2	418.9607	1.3067	0.0000
11	B2	443.3339	1.8734	0.1016
12	A1	515.3814	2.7553	1.8200
13	B1	560.2028	2.2957	9.0370
14	A2	661.1158	3.1354	0.0000
15	A1	664.6828	4.0882	10.2984
16	B2	689.3728	3.7011	0.0612
17	B1	707.9684	3.6120	0.8277
18	A1	864.7113	6.0397	140.2360
19	B2	917.5795	7.3078	182.0916
20	B2	1098.0974	9.6213	0.8144
21	A1	1183.5326	10.6138	58.5906
22	B2	1302.1058	12.3023	7.8122
23	A1	1354.7548	13.6787	4.0888
24	A1	1396.2395	14.0980	73.0382
25	B2	1415.0339	14.8452	701.8586
26	B2	1552.6129	17.6390	0.7538
27	A1	1565.1730	17.4934	116.1610

blyp/pyFFFFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	111.0200	0.1349	0.0000
2	B1	149.1576	0.2414	0.0048
3	B1	203.2559	0.3650	4.5421
4	A1	264.3498	0.7655	0.6415
5	B2	265.3755	0.7815	0.0347
6	B2	305.5934	0.9976	0.5550
7	A1	329.5703	1.1225	1.1399
8	B1	333.9082	0.9022	2.6720
9	A2	411.3403	1.2604	0.0000
10	B2	442.9019	1.8766	0.1636
11	A1	462.2796	2.0128	0.1927
12	A1	566.9711	3.3212	0.0063
13	B1	595.9423	2.6073	3.1988
14	A2	648.1143	3.0122	0.0000
15	A1	665.9178	4.0678	8.2572
16	B1	687.3004	3.4044	4.0260
17	B2	709.1740	3.9413	0.4760
18	B2	931.6652	7.4671	236.4307

19	A1	1026.8758	8.6818	241.0612
20	B2	1095.0294	9.5745	0.0975
21	A1	1220.8962	11.3749	31.4730
22	B2	1309.7798	12.4668	7.4442
23	A1	1357.5334	13.5625	12.8596
24	B2	1419.4937	14.9709	682.6148
25	A1	1457.0432	15.6180	145.8729
26	A1	1573.2042	17.6444	102.3787
27	B2	1579.6589	18.1556	1.5825

blyp/pyFFFFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	112.7516	0.1392	0.0000
2	B1	151.0729	0.2478	0.0021
3	B1	203.1895	0.3643	3.7393
4	A1	264.4917	0.7662	0.7230
5	B2	265.6446	0.7829	0.0360
6	B2	306.1399	1.0008	0.5187
7	A1	330.0253	1.1252	0.9933
8	B1	336.4386	0.9168	2.4209
9	A2	412.5834	1.2681	0.0000
10	B2	443.5910	1.8803	0.1490
11	A1	464.2171	2.0275	0.2526
12	A1	570.8304	3.3645	0.0030
13	B1	603.3227	2.6752	3.2305
14	A2	667.1179	3.1914	0.0000
15	A1	668.4378	4.0997	6.7574
16	B2	712.2909	3.9767	0.2217
17	B1	725.2976	3.7855	3.3088
18	B2	938.5210	7.5734	221.5437
19	A1	1034.0674	8.8028	228.7441
20	B2	1102.7002	9.7170	0.0310
21	A1	1227.4802	11.5079	29.3685
22	B2	1305.7914	12.4125	5.0821
23	A1	1362.2365	13.6468	15.4542
24	B2	1423.0768	15.0399	658.1414
25	A1	1459.9157	15.6998	137.1819
26	A1	1572.7260	17.6354	98.5042
27	B2	1577.5165	18.0958	1.1668

blyp/pyFFFFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	111.9979	0.1372	0.0000
2	B1	149.8225	0.2435	0.0002
3	B1	202.6502	0.3623	3.1220
4	A1	265.0681	0.7694	0.7330
5	B2	266.1644	0.7860	0.0380
6	B2	306.7298	1.0046	0.5065

7	A1	330.6781	1.1298	0.9101
8	B1	335.6278	0.9126	2.1618
9	A2	412.4487	1.2673	0.0000
10	B2	444.3996	1.8872	0.1399
11	A1	464.4087	2.0288	0.2959
12	A1	571.3470	3.3687	0.0008
13	B1	600.0627	2.6436	2.6070
14	A2	662.1231	3.1448	0.0000
15	A1	669.5453	4.1117	6.2184
16	B1	709.9485	3.6330	2.7538
17	B2	712.9969	3.9842	0.2032
18	B2	940.8983	7.6102	212.9338
19	A1	1036.8904	8.8489	225.5980
20	B2	1107.8206	9.8074	0.0008
21	A1	1231.4474	11.5860	29.3656
22	B2	1310.1713	12.4931	5.7228
23	A1	1367.7094	13.7619	15.8837
24	B2	1427.9656	15.1473	640.4747
25	A1	1463.1753	15.7744	132.9600
26	A1	1576.1867	17.7156	99.8793
27	B2	1581.3298	18.1898	1.4746

blyp/pyFFFFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	110.5746	0.1338	0.0000
2	B1	149.0178	0.2409	0.0025
3	B1	201.9303	0.3600	4.0864
4	A1	264.5693	0.7667	0.6968
5	B2	265.7059	0.7833	0.0386
6	B2	305.2470	0.9952	0.6204
7	A1	328.8527	1.1173	1.0691
8	B1	332.3657	0.8951	2.5221
9	A2	410.5973	1.2557	0.0000
10	B2	442.4334	1.8701	0.1526
11	A1	462.3430	2.0106	0.2272
12	A1	568.4899	3.3355	0.0063
13	B1	596.1809	2.6104	2.9563
14	A2	659.3177	3.1184	0.0000
15	A1	665.3319	4.0582	6.7420
16	B2	707.1962	3.9186	0.3173
17	B1	710.0099	3.6296	3.1062
18	B2	935.1454	7.5198	220.0991
19	A1	1030.7614	8.7457	230.6210
20	B2	1102.4888	9.7164	0.0433
21	A1	1224.5823	11.4638	28.7880
22	B2	1315.2405	12.5894	4.4296
23	A1	1363.3310	13.6734	14.8710
24	B2	1425.2977	15.0907	661.7635
25	A1	1463.7798	15.7852	139.0980
26	A1	1577.5288	17.7421	101.1751
27	B2	1581.5865	18.1871	0.6573

blyp/pyFFHFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	107.9175	0.1276	0.0000
2	B1	192.7595	0.2962	3.7879
3	A1	271.6795	0.7927	0.6549
4	B1	282.2472	0.3955	0.9000
5	B2	291.8175	0.8969	0.1338
6	A1	343.4840	1.1136	2.2662
7	A2	435.8303	1.4140	0.0000
8	B2	437.8952	1.6607	0.0416
9	B1	466.7892	0.5740	0.3729
10	A1	490.2570	2.1491	1.4932
11	B2	634.9760	1.4915	1.9291
12	A1	658.0260	3.8897	19.9054
13	A2	659.6448	3.1186	0.0000
14	B1	682.7417	2.2958	9.2350
15	A1	723.1143	2.9429	12.4491
16	B1	851.7190	0.5919	29.0856
17	B2	863.0195	2.8379	157.4540
18	B2	1079.7923	6.5979	6.5807
19	B2	1156.4477	1.2094	108.1637
20	A1	1168.0106	9.0991	199.0628
21	B2	1302.0697	12.1495	52.7956
22	A1	1334.8488	12.4443	2.9616
23	A1	1384.3984	12.6759	31.1709
24	B2	1429.0951	7.8826	665.1926
25	B2	1573.8934	11.8838	5.4638
26	A1	1576.5525	16.7234	20.6456
27	A1	3139.6948	6.3461	3.2319

blyp/pyFFHFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	109.8074	0.1321	0.0000
2	B1	193.5830	0.3005	3.0636
3	A1	272.1154	0.7951	0.6919
4	B1	285.1577	0.4035	0.8903
5	B2	292.7123	0.9023	0.1020
6	A1	344.4395	1.1189	1.9375
7	A2	437.3504	1.4239	0.0000
8	B2	438.5665	1.6624	0.0329
9	B1	472.1605	0.5757	0.3685
10	A1	492.8547	2.1669	1.6835
11	B2	638.5236	1.5004	1.9308
12	A1	662.1109	3.9568	17.3248
13	A2	676.8177	3.2830	0.0000
14	B1	708.8485	1.9435	10.7754
15	A1	726.4638	2.9665	13.0526

16	B2	868.7075	2.8184	142.6650
17	B1	870.7819	0.6519	23.7631
18	B2	1088.5199	6.6322	7.5328
19	B2	1161.4131	1.2352	102.9148
20	A1	1176.0732	9.2339	184.8649
21	B2	1298.0278	11.9384	47.6899
22	A1	1340.1145	12.5232	4.0104
23	A1	1387.0551	12.7930	32.1620
24	B2	1432.5889	8.0240	648.4896
25	B2	1572.9454	11.5054	7.2491
26	A1	1576.4017	16.7282	20.3720
27	A1	3139.3492	6.3416	2.7247

blyp/pyFFHFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	109.3253	0.1309	0.0000
2	B1	193.2532	0.2991	2.5675
3	A1	272.9216	0.7995	0.6964
4	B1	284.2582	0.4010	0.8834
5	B2	293.3896	0.9061	0.1054
6	A1	344.9898	1.1230	1.7923
7	A2	437.6344	1.4258	0.0000
8	B2	439.5124	1.6686	0.0346
9	B1	469.8826	0.5771	0.2650
10	A1	493.2382	2.1685	1.7343
11	B2	639.3523	1.5040	1.8926
12	A1	663.5042	3.9697	16.2938
13	A2	673.8225	3.2547	0.0000
14	B1	703.4160	2.1129	8.2240
15	A1	727.2929	2.9723	13.0039
16	B1	860.6104	0.6214	25.4532
17	B2	870.8873	2.8046	135.1389
18	B2	1094.3538	6.4983	8.3065
19	B2	1164.2926	1.2478	95.3657
20	A1	1180.8945	9.2947	182.1786
21	B2	1302.2239	12.0528	49.6627
22	A1	1345.0226	12.5702	3.8963
23	A1	1391.3693	12.9427	32.0827
24	B2	1437.8955	8.1230	631.0446
25	B2	1576.8977	11.6225	6.7281
26	A1	1579.5107	16.8018	21.1750
27	A1	3144.4709	6.3628	2.3774

blyp/pyFFHFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	107.7356	0.1271	0.0000
2	B1	191.6196	0.2947	3.3540
3	A1	272.0296	0.7945	0.6779

4	B1	282.3553	0.3973	0.9354
5	B2	292.1660	0.8993	0.1522
6	A1	342.7294	1.1080	2.0642
7	A2	435.1733	1.4095	0.0000
8	B2	437.4974	1.6541	0.0383
9	B1	465.4574	0.5652	0.3254
10	A1	490.5434	2.1472	1.4975
11	B2	634.4215	1.5013	1.7660
12	A1	658.6073	3.9077	16.9140
13	A2	668.9841	3.2085	0.0000
14	B1	698.0438	1.9628	9.7173
15	A1	724.0536	2.9468	12.9793
16	B1	858.4957	0.6255	26.7839
17	B2	865.7608	2.7998	145.1102
18	B2	1087.7018	6.4365	7.0152
19	B2	1160.1705	1.2206	96.4315
20	A1	1170.8913	9.1478	190.2015
21	B2	1308.5469	12.2061	42.7077
22	A1	1342.1687	12.5635	3.6742
23	A1	1387.4742	12.7543	30.8478
24	B2	1433.4584	8.1994	655.2831
25	B2	1574.6514	11.8672	7.5776
26	A1	1582.0190	16.8467	20.2427
27	A1	3147.1271	6.3763	4.4757

blyp/pyFHFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	121.3047	0.1444	0.1470
2	A"	199.7412	0.3238	4.0575
3	A"	249.3118	0.2616	1.1396
4	A'	265.8480	0.7762	0.1683
5	A'	306.5811	0.9589	0.7934
6	A'	335.8746	1.0973	1.3261
7	A"	366.7448	0.8356	0.7096
8	A'	447.9497	1.6984	0.5556
9	A'	514.1353	1.7560	3.8930
10	A'	569.1639	3.3128	0.1511
11	A"	596.1728	1.2078	5.7446
12	A'	641.2724	1.5913	1.9716
13	A"	646.7790	1.8256	0.0103
14	A"	698.2917	2.0848	1.0736
15	A'	765.1890	3.4979	54.5722
16	A"	810.0971	0.5815	33.3935
17	A'	980.5750	3.2999	112.2634
18	A'	1017.4484	7.2531	183.8773
19	A'	1113.3110	1.5504	61.2845
20	A'	1187.4586	3.4138	75.0527
21	A'	1307.1313	12.4708	9.3023
22	A'	1339.9794	9.4240	29.0132
23	A'	1383.2847	12.5215	207.0756
24	A'	1449.7586	7.4917	345.9574

25	A'	1569.2682	13.5839	235.5673
26	A'	1580.3506	16.5587	36.3034
27	A'	3149.6929	6.3913	2.7123

blyp/pyFHFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	122.7844	0.1480	0.1210
2	A"	200.4477	0.3296	3.3006
3	A"	252.4005	0.2656	1.2107
4	A'	266.1266	0.7776	0.1971
5	A'	307.2483	0.9624	0.6955
6	A'	336.7996	1.1030	1.0544
7	A"	367.6170	0.8454	0.6730
8	A'	448.9982	1.7060	0.5215
9	A'	514.9197	1.7601	3.3570
10	A'	573.1841	3.3592	0.0929
11	A"	603.0956	1.2170	5.7826
12	A'	644.3305	1.5995	2.1932
13	A"	657.7028	1.6981	0.0007
14	A"	720.5332	1.8654	0.2509
15	A'	768.7199	3.5205	48.8042
16	A"	826.5089	0.6480	30.8963
17	A'	984.9766	3.1780	101.8546
18	A'	1025.3460	7.3441	170.4000
19	A'	1120.1296	1.5874	65.0710
20	A'	1193.5229	3.5350	71.4392
21	A'	1303.4533	12.3022	10.3897
22	A'	1346.5418	9.6885	29.5492
23	A'	1385.9005	12.5004	191.6632
24	A'	1453.2440	7.5680	340.2502
25	A'	1568.9065	13.4250	225.1582
26	A'	1578.5570	16.1953	36.2591
27	A'	3149.3870	6.3869	2.1087

blyp/pyFHFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	122.1545	0.1464	0.1033
2	A"	199.8381	0.3261	2.8402
3	A"	251.3298	0.2649	1.1971
4	A'	266.7434	0.7812	0.2037
5	A'	307.9351	0.9662	0.6901
6	A'	337.5922	1.1083	0.9961
7	A"	366.9831	0.8440	0.5367
8	A'	449.5577	1.7083	0.4774
9	A'	515.6468	1.7661	3.0471
10	A'	573.9444	3.3647	0.0753
11	A"	601.6754	1.2408	4.9735
12	A'	645.0784	1.6019	2.1115

13	A''	656.2184	1.7553	0.0028
14	A''	712.0039	2.0435	0.4537
15	A'	770.1545	3.5299	46.6495
16	A''	815.1499	0.6030	29.6479
17	A'	987.5560	3.1032	97.0525
18	A'	1029.4591	7.4293	163.6069
19	A'	1123.9931	1.5867	63.3704
20	A'	1197.1987	3.6385	68.5631
21	A'	1308.3032	12.3458	10.0185
22	A'	1352.2459	10.0149	30.9593
23	A'	1390.6693	12.5150	177.7280
24	A'	1457.2615	7.6788	337.2700
25	A'	1572.4829	13.4834	226.7815
26	A'	1582.2615	16.2900	37.7025
27	A'	3154.3682	6.4073	1.8209

blyp/pyFHFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	121.1142	0.1439	0.1345
2	A''	199.1894	0.3254	3.6576
3	A''	249.4942	0.2617	1.2573
4	A'	266.2157	0.7782	0.1893
5	A'	306.2664	0.9569	0.8242
6	A'	335.3059	1.0940	1.2160
7	A''	364.8357	0.8274	0.6152
8	A'	447.8538	1.6963	0.5149
9	A'	513.4490	1.7506	3.2530
10	A'	570.8204	3.3314	0.1324
11	A''	597.6184	1.2267	5.4627
12	A'	640.2610	1.6002	1.8697
13	A''	651.6261	1.7029	0.0004
14	A''	710.5298	1.9359	0.3408
15	A'	765.7928	3.4841	49.1297
16	A''	817.1705	0.6150	33.8679
17	A'	982.2337	3.1803	105.2588
18	A'	1022.6689	7.3070	171.8579
19	A'	1118.3188	1.5588	59.0760
20	A'	1191.8029	3.4604	67.7101
21	A'	1311.5781	12.5779	10.7973
22	A'	1347.9337	9.6813	29.9005
23	A'	1387.3089	12.5114	188.8760
24	A'	1454.3468	7.7767	349.3507
25	A'	1572.5998	13.7461	232.1169
26	A'	1582.4740	16.5353	32.7098
27	A'	3157.2755	6.4221	3.9006

blyp/pyHHHHH_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	361.4612	0.1948	0.0000
2	B1	401.0534	0.3584	3.7697
3	A1	600.0847	1.5262	3.4026
4	B2	650.5331	1.5918	0.2690
5	B1	691.3425	0.3736	64.9572
6	B1	730.2195	0.8108	8.7091
7	A2	861.4820	0.5454	0.0000
8	B1	915.4028	0.6546	0.0542
9	A2	952.8727	0.7908	0.0000
10	B1	963.7929	0.6941	0.0005
11	A1	972.5536	3.8511	4.1765
12	A1	1015.8534	2.6838	6.9091
13	B2	1041.2086	1.1761	0.0218
14	A1	1059.1048	1.2276	4.2550
15	B2	1143.7786	0.8663	1.9622
16	A1	1204.2363	1.1167	4.1936
17	B2	1247.4716	7.5163	0.4823
18	B2	1346.1454	1.2797	0.0226
19	B2	1421.8600	2.4469	23.6481
20	A1	1459.7149	2.3305	1.4895
21	B2	1549.5923	7.1356	7.3290
22	A1	1555.0085	6.7831	19.8661
23	B2	3063.0288	6.0063	31.3952
24	A1	3065.3237	6.0319	5.5498
25	A1	3087.2679	6.1099	3.9716
26	B2	3100.3518	6.1861	34.0059
27	A1	3109.6863	6.2562	11.0361

b1yp/pyHHHHH_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	365.5510	0.1966	0.0000
2	B1	405.3904	0.3616	3.6408
3	A1	601.0385	1.5295	4.1127
4	B2	651.1918	1.5921	0.1493
5	B1	699.6059	0.3725	60.8295
6	B1	741.1362	0.8289	6.1983
7	A2	872.1651	0.5592	0.0000
8	B1	928.5095	0.6746	0.0214
9	A2	971.4596	0.8280	0.0000
10	A1	974.4722	3.8331	4.3390
11	B1	987.0214	0.7522	0.0009
12	A1	1020.1704	2.5791	7.7358
13	B2	1043.3276	1.1820	0.1036
14	A1	1062.0544	1.2694	2.5607
15	B2	1143.6891	0.8731	2.1029
16	A1	1204.3616	1.1240	3.5917
17	B2	1245.6946	7.1795	0.3828
18	B2	1351.7391	1.2937	0.0989
19	B2	1426.9082	2.4756	22.4001
20	A1	1465.9643	2.3392	1.1121
21	B2	1551.7863	6.9497	7.0134

22	A1	1556.8626	6.6778	19.4350
23	B2	3063.4875	6.0078	30.1932
24	A1	3065.9090	6.0358	5.5733
25	A1	3089.8489	6.1184	3.3208
26	B2	3102.4589	6.1924	31.6582
27	A1	3111.8441	6.2611	10.5777

blyp/pyHHHHH_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	365.5344	0.1962	0.0000
2	B1	405.4651	0.3628	3.4992
3	A1	601.6024	1.5341	4.3828
4	B2	652.7626	1.6014	0.2101
5	B1	698.0461	0.3637	62.1041
6	B1	741.7541	0.8611	5.0592
7	A2	870.7379	0.5573	0.0000
8	B1	926.0948	0.6736	0.0216
9	A2	969.2102	0.8254	0.0000
10	A1	976.3715	3.8584	4.8047
11	B1	985.0893	0.7470	0.0027
12	A1	1021.4479	2.5974	8.4268
13	B2	1045.1211	1.1856	0.0942
14	A1	1063.7594	1.2656	2.3034
15	B2	1146.7921	0.8765	1.9576
16	A1	1207.0098	1.1276	3.2019
17	B2	1250.0725	7.2886	0.4672
18	B2	1353.7584	1.2968	0.0748
19	B2	1430.2151	2.4845	23.4719
20	A1	1468.6238	2.3542	1.6831
21	B2	1555.3711	7.0306	6.6522
22	A1	1560.0466	6.7285	20.1955
23	B2	3066.8416	6.0209	31.7185
24	A1	3069.4381	6.0502	7.4033
25	A1	3094.0318	6.1349	3.8803
26	B2	3106.9632	6.2106	32.4257
27	A1	3116.2424	6.2801	10.5897

blyp/pyHHHHH_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	362.9144	0.1940	0.0000
2	B1	402.2744	0.3574	3.7351
3	A1	600.0703	1.5254	3.5414
4	B2	649.6809	1.5857	0.3620
5	B1	691.2022	0.3572	71.3371
6	B1	735.6588	0.8530	6.3114
7	A2	863.6767	0.5481	0.0000
8	B1	917.8400	0.6591	0.0558
9	A2	961.5265	0.8109	0.0000

10	A1	971.8361	3.8336	4.7466
11	B1	977.3213	0.7338	0.0061
12	A1	1017.6278	2.6687	6.9696
13	B2	1042.6685	1.1724	0.0005
14	A1	1059.7791	1.2305	4.1974
15	B2	1144.5904	0.8584	1.8140
16	A1	1204.5303	1.1110	3.4200
17	B2	1251.1047	7.9941	0.2845
18	B2	1344.6119	1.2766	0.0341
19	B2	1421.6415	2.4640	25.4554
20	A1	1458.5245	2.3351	2.3144
21	B2	1550.7027	7.2437	6.0284
22	A1	1557.4566	6.9403	19.7452
23	B2	3072.6022	6.0448	23.1248
24	A1	3074.6568	6.0698	4.9747
25	A1	3097.1679	6.1489	3.3616
26	B2	3109.4890	6.2228	23.7478
27	A1	3118.3810	6.2921	7.2143

bmk/pyCCCCC_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	58.6249	0.0692	0.0000
2	B1	80.4494	0.1291	0.0187
3	B1	147.9581	0.2057	0.0252
4	A1	206.0166	0.8012	0.0541
5	B2	215.5694	0.8612	0.1562
6	A1	215.7155	0.8045	0.0082
7	B2	224.2576	1.0025	0.0313
8	B1	282.8370	0.6353	0.8753
9	B2	338.7563	1.9289	0.2034
10	A1	355.1818	2.0885	0.2218
11	A2	363.7496	0.9754	0.0000
12	A1	394.1462	2.9626	0.0444
13	A1	555.8660	3.1592	3.7797
14	B1	575.6491	2.4185	1.4643
15	B2	578.4238	2.6242	0.1233
16	A2	625.4065	2.7881	0.0000
17	B2	705.5312	4.5996	70.4452
18	B1	734.0152	3.8920	0.2560
19	A1	848.7489	5.8611	83.1366
20	B2	934.2284	6.7155	3.3300
21	A1	1118.9157	9.3161	30.5945
22	B2	1235.5345	10.9697	40.0759
23	A1	1262.8981	11.6180	4.7494
24	B2	1370.5752	13.7439	368.4316
25	A1	1372.2754	13.4926	132.4596
26	A1	1539.9167	16.8831	94.4317
27	B2	1590.1078	18.7291	80.7553

bmk/pyCCCCC_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	60.4304	0.0735	0.0000
2	B1	82.6168	0.1358	0.0145
3	B1	149.9165	0.2113	0.0273
4	A1	200.4130	0.7946	0.0196
5	B2	211.3781	0.8216	0.1515
6	A1	212.5068	0.7502	0.0013
7	B2	216.7189	0.9456	0.0196
8	B1	287.8465	0.6586	0.7604
9	B2	337.0034	1.9083	0.2214
10	A1	353.3260	2.0671	0.1893
11	A2	370.3073	1.0111	0.0000
12	A1	392.4887	2.9376	0.0695
13	A1	553.2811	3.1294	3.5059
14	B2	574.5885	2.5912	0.0162
15	B1	589.0074	2.5348	1.2603
16	A2	645.1855	2.9677	0.0000
17	B2	701.8322	4.5446	67.4347
18	B1	765.9777	4.2331	1.4908
19	A1	844.2385	5.8016	78.9394
20	B2	927.1511	6.6145	2.9753
21	A1	1114.9355	9.2470	29.1818
22	B2	1222.4059	10.7381	42.8770
23	A1	1256.5075	11.4932	3.9946
24	B2	1363.7206	13.5946	332.9298
25	A1	1366.0545	13.3675	119.5115
26	A1	1531.2680	16.6996	83.6635
27	B2	1582.6931	18.5758	78.2816

bmk/pyCCCCC_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	60.9207	0.0746	0.0000
2	B1	83.1969	0.1376	0.0150
3	B1	150.5931	0.2133	0.0241
4	A1	200.8395	0.7991	0.0230
5	B2	212.8448	0.8237	0.1411
6	A1	214.3063	0.7624	0.0002
7	B2	217.9407	0.9683	0.0062
8	B1	289.0545	0.6644	0.7534
9	B2	338.0319	1.9201	0.2343
10	A1	354.4186	2.0792	0.2158
11	A2	372.9231	1.0255	0.0000
12	A1	394.0950	2.9648	0.0699
13	A1	555.5560	3.1550	3.3929
14	B2	577.9990	2.6244	0.0774
15	B1	593.0229	2.5709	1.3295
16	A2	650.0496	3.0128	0.0000
17	B2	705.0893	4.5854	67.3212
18	B1	770.5291	4.2807	1.6072

19	A1	847.4855	5.8476	81.8891
20	B2	931.1846	6.6737	2.6792
21	A1	1117.6982	9.2965	29.1187
22	B2	1239.0575	11.0455	36.7215
23	A1	1261.1211	11.5729	4.9354
24	B2	1371.3210	13.7581	344.2832
25	A1	1371.5059	13.4755	113.8740
26	A1	1542.4212	16.9336	92.4020
27	B2	1587.5746	18.6401	69.4582

bmk/pyCCCCC_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	59.8360	0.0720	0.0000
2	B1	81.4807	0.1321	0.0160
3	B1	148.4196	0.2072	0.0166
4	A1	205.8038	0.7970	0.0174
5	B2	216.1475	0.8602	0.0782
6	A1	216.1719	0.8114	0.0011
7	B2	224.8468	1.0153	0.0070
8	B1	284.9785	0.6451	0.5465
9	B2	336.9525	1.9142	0.2699
10	A1	353.3249	2.0697	0.2068
11	A2	367.7640	0.9971	0.0000
12	A1	392.0084	2.9427	0.0479
13	A1	551.8261	3.1144	4.1015
14	B2	576.2165	2.6074	0.3595
15	B1	580.1767	2.4583	1.1473
16	A2	632.9286	2.8558	0.0000
17	B2	700.1235	4.5266	72.7341
18	B1	747.4769	4.0334	2.0903
19	A1	842.4061	5.7717	86.6780
20	B2	927.4656	6.6103	2.7188
21	A1	1110.3249	9.1672	31.9230
22	B2	1248.5489	11.2093	32.6932
23	A1	1260.9417	11.5674	4.7570
24	A1	1373.5931	13.5157	119.0218
25	B2	1374.7643	13.8325	366.3739
26	A1	1551.2307	17.1239	99.1801
27	B2	1593.9752	18.7827	71.6809

bmk/pyFCFCF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	93.8498	0.1105	0.0000
2	B1	110.3047	0.1559	0.0005
3	A1	181.7484	0.5149	0.0041
4	B1	219.2368	0.4268	3.0234
5	B2	224.2824	0.6623	0.0178
6	B2	319.5394	1.2897	1.5325

7	B1	320.3731	0.8399	0.4060
8	A1	330.0763	1.3972	0.4390
9	A2	378.2960	1.0565	0.0000
10	A1	418.0113	2.0743	0.5656
11	B2	418.7838	1.8972	0.2553
12	A1	588.4401	3.2697	1.6494
13	A1	629.9542	3.8624	1.2322
14	B1	660.8745	3.1889	0.8720
15	A2	706.1242	3.5804	0.0000
16	B2	713.0314	3.9712	0.0521
17	B1	765.4292	4.2356	19.2991
18	B2	823.5757	5.7824	107.0671
19	A1	1101.9748	9.8587	172.5458
20	B2	1140.6815	10.4203	12.3180
21	A1	1185.4495	10.5659	3.5162
22	B2	1299.9915	12.4126	17.5156
23	A1	1481.1719	16.2865	90.5653
24	B2	1483.8048	16.2065	405.0281
25	A1	1503.3451	16.7694	59.1967
26	A1	1630.4831	19.0016	256.8132
27	B2	1660.4179	20.2862	115.6229

bmk/pyFCFCF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	95.4874	0.1144	0.0000
2	B1	111.8977	0.1602	0.0027
3	A1	180.2355	0.5063	0.0000
4	B1	218.1463	0.4224	2.7610
5	B2	222.8634	0.6535	0.0132
6	B2	318.6299	1.2862	1.4169
7	B1	322.7795	0.8538	0.5911
8	A1	329.2444	1.3949	0.3729
9	A2	373.4887	1.0294	0.0000
10	A1	417.6440	2.0654	0.5790
11	B2	417.6887	1.8803	0.2566
12	A1	587.5401	3.2320	1.5121
13	A1	630.5165	3.8936	0.7726
14	B1	666.6890	3.2481	1.1276
15	B2	712.9547	3.9715	0.0067
16	A2	716.5537	3.6889	0.0000
17	B1	785.1487	4.4517	14.6231
18	B2	820.1248	5.7241	99.9377
19	A1	1105.7975	9.8976	153.0757
20	B2	1141.8514	10.4113	8.2611
21	A1	1181.9786	10.5114	2.3566
22	B2	1289.4620	12.2567	17.7049
23	B2	1483.9552	16.2199	382.1092
24	A1	1487.1914	16.3786	103.1463
25	A1	1504.3524	16.8864	36.7609
26	A1	1623.7913	18.8584	246.9372
27	B2	1654.5114	20.1614	126.1772

bmk/pyFCFCF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	95.4380	0.1143	0.0000
2	B1	111.9564	0.1605	0.0022
3	A1	181.5700	0.5137	0.0040
4	B1	218.3022	0.4232	2.4785
5	B2	224.4381	0.6631	0.0076
6	B2	320.2120	1.3002	1.2976
7	B1	323.2071	0.8557	0.5382
8	A1	330.7575	1.4087	0.2985
9	A2	375.9307	1.0432	0.0000
10	A1	418.6705	2.0759	0.5696
11	B2	419.1996	1.8943	0.2436
12	A1	589.8181	3.2630	1.3305
13	A1	631.3842	3.9017	0.7577
14	B1	666.5973	3.2484	0.9153
15	B2	716.4769	4.0124	0.0011
16	A2	717.4283	3.6979	0.0000
17	B1	784.9686	4.4478	15.3691
18	B2	822.7843	5.7608	99.0571
19	A1	1107.5860	9.9304	162.8022
20	B2	1146.4231	10.5384	10.6085
21	A1	1185.3985	10.5804	1.4432
22	B2	1302.6216	12.4741	14.1322
23	A1	1488.2284	16.3978	102.3319
24	B2	1491.0024	16.3775	389.4835
25	A1	1509.5597	16.9764	38.7526
26	A1	1634.5254	19.1010	260.9737
27	B2	1660.5267	20.2616	118.6261

bmk/pyFCFCF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	94.7804	0.1127	0.0000
2	B1	111.1783	0.1581	0.0018
3	A1	181.8719	0.5156	0.0112
4	B1	216.6464	0.4163	2.7709
5	B2	224.9025	0.6663	0.0023
6	B2	318.8843	1.2866	1.3771
7	B1	319.9255	0.8395	0.2932
8	A1	329.3755	1.3925	0.3390
9	A2	371.3734	1.0175	0.0000
10	A1	416.4197	2.0615	0.5929
11	B2	417.7463	1.8873	0.1827
12	A1	587.8355	3.2430	1.5299
13	A1	627.8648	3.8586	0.8501
14	B1	661.0823	3.1931	0.5906
15	A2	710.1925	3.6246	0.0000

16	B2	710.3930	3.9433	0.0431
17	B1	773.6421	4.3228	22.6621
18	B2	817.8178	5.6918	102.3049
19	A1	1101.9157	9.8407	176.9120
20	B2	1141.6709	10.4810	13.6716
21	A1	1179.7745	10.4839	1.3044
22	B2	1312.0957	12.6215	11.9608
23	A1	1483.2145	16.3097	90.7628
24	B2	1491.3729	16.3776	412.8443
25	A1	1510.3624	16.9376	50.7410
26	A1	1642.6629	19.2792	262.5284
27	B2	1664.8611	20.3535	104.0070

bmk/pyFCFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	99.6112	0.1238	0.0000
2	A"	144.3043	0.2284	0.0037
3	A'	200.9469	0.5578	0.0248
4	A"	219.8219	0.4281	4.0919
5	A'	280.1754	0.8705	0.2997
6	A'	319.5967	1.2173	1.1807
7	A"	332.5900	0.8939	0.8714
8	A'	342.2487	1.3008	0.9039
9	A'	415.9502	1.9450	0.2477
10	A"	418.2529	1.3090	1.7402
11	A'	478.3431	2.1597	0.4425
12	A'	602.6224	3.6196	1.0902
13	A'	649.7260	3.9209	4.7364
14	A"	649.9807	3.0869	1.5178
15	A"	698.0256	3.4993	0.1536
16	A'	737.7519	4.2551	0.6794
17	A"	749.0946	4.0591	13.5369
18	A'	932.3702	7.3408	144.1296
19	A'	1110.4544	10.0360	185.7843
20	A'	1153.4174	10.6041	27.2263
21	A'	1291.7901	12.4845	21.0470
22	A'	1317.4356	13.1121	23.5237
23	A'	1484.7249	16.3948	70.6242
24	A'	1503.3031	16.6038	250.3272
25	A'	1559.2430	18.1910	479.1489
26	A'	1653.7397	19.5933	208.5726
27	A'	1684.1955	20.7499	19.0245

bmk/pyFCFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	101.3671	0.1281	0.0022
2	A"	145.7588	0.2331	0.0033
3	A'	199.4586	0.5493	0.0248

4	A"	219.1382	0.4250	3.5236
5	A'	278.1624	0.8578	0.3474
6	A'	318.7864	1.2134	1.0883
7	A"	335.4750	0.9107	0.9776
8	A'	341.6683	1.2971	0.8073
9	A'	415.2084	1.9303	0.2263
10	A"	419.9758	1.3204	1.4524
11	A'	477.4448	2.1498	0.5195
12	A'	604.0919	3.6150	1.2039
13	A'	648.2362	3.9185	3.8307
14	A"	659.5256	3.1845	2.0871
15	A"	717.4515	3.6993	0.7517
16	A'	738.2807	4.2620	0.7931
17	A"	783.2587	4.4255	9.3459
18	A'	932.8872	7.3283	131.2072
19	A'	1114.7369	10.0919	163.3990
20	A'	1154.6788	10.6152	27.1780
21	A'	1284.9971	12.2011	23.1333
22	A'	1317.8556	13.3475	21.3303
23	A'	1490.7203	16.5394	76.3839
24	A'	1503.1422	16.6088	230.5919
25	A'	1560.2345	18.2466	466.0805
26	A'	1647.0546	19.4543	206.9481
27	A'	1678.8239	20.6344	20.3399

bmk/pyFCFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	101.2516	0.1278	0.0017
2	A"	145.3367	0.2318	0.0017
3	A'	200.8205	0.5570	0.0336
4	A"	218.8966	0.4241	3.1432
5	A'	278.8465	0.8619	0.3511
6	A'	320.0995	1.2234	1.0209
7	A"	335.7518	0.9125	0.9308
8	A'	342.9952	1.3080	0.7056
9	A'	416.4967	1.9436	0.2180
10	A"	419.9155	1.3194	1.3665
11	A'	478.4746	2.1612	0.5334
12	A'	605.7929	3.6469	1.0132
13	A'	649.3956	3.9255	3.7483
14	A"	657.7785	3.1676	1.7691
15	A"	715.8012	3.6818	0.5397
16	A'	740.9328	4.2937	0.7128
17	A"	777.6662	4.3642	9.6880
18	A'	934.7565	7.3642	133.7391
19	A'	1116.4430	10.1373	175.3419
20	A'	1158.1829	10.7066	28.0566
21	A'	1294.3426	12.4929	19.4515
22	A'	1321.4982	13.2646	19.3483
23	A'	1491.4344	16.5223	68.8631
24	A'	1508.0007	16.7353	242.1849

25	A'	1564.3265	18.3218	467.2769
26	A'	1657.6611	19.6915	213.5004
27	A'	1685.1042	20.7465	15.7239

bmk/pyFCFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	100.4483	0.1257	0.0016
2	A"	144.5135	0.2291	0.0042
3	A'	201.1127	0.5587	0.0498
4	A"	217.8807	0.4201	3.7606
5	A'	277.0334	0.8508	0.3319
6	A'	318.2725	1.2052	1.1922
7	A"	332.2504	0.8938	0.7164
8	A'	340.9754	1.2952	0.8355
9	A'	414.7237	1.9343	0.2164
10	A"	418.4837	1.3106	1.9847
11	A'	476.8916	2.1462	0.4841
12	A'	603.6619	3.6279	1.1203
13	A'	645.8021	3.8769	4.1433
14	A"	653.5603	3.1264	1.6247
15	A"	711.1493	3.6354	1.3187
16	A'	734.4465	4.2174	0.7220
17	A"	771.5505	4.2947	12.4632
18	A'	929.1502	7.2806	139.1008
19	A'	1110.6272	10.0480	187.1158
20	A'	1152.6134	10.6186	29.1270
21	A'	1293.9985	12.6994	16.6448
22	A'	1324.9024	13.0873	19.6376
23	A'	1486.5104	16.4030	61.9590
24	A'	1508.2785	16.7423	261.8559
25	A'	1565.4582	18.3245	470.7182
26	A'	1664.4495	19.8443	209.9145
27	A'	1689.4217	20.8338	12.4907

bmk/pyFFCFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	120.5997	0.1589	0.0000
2	B1	124.0357	0.1885	0.0499
3	B2	200.5138	0.5678	0.0152
4	B1	214.5640	0.4025	3.8079
5	A1	284.9826	0.9299	1.0423
6	B2	313.8850	1.0677	0.3979
7	A1	337.6629	1.3913	1.3463
8	B1	340.7933	0.9534	0.9768
9	A1	436.9063	2.0335	0.0030
10	A2	455.1018	1.5432	0.0000
11	B2	468.7232	2.0749	0.0566
12	A1	554.4200	3.1843	1.7213

13	B1	601.3240	2.6379	9.6744
14	A2	699.5469	3.5133	0.0000
15	A1	712.0934	4.6465	8.8970
16	B2	733.4863	4.1878	0.0390
17	B1	738.6327	3.9441	3.8073
18	A1	951.0989	7.3604	136.4729
19	B2	998.9985	8.5725	151.5941
20	B2	1214.0890	11.5746	1.9716
21	A1	1292.1137	12.6776	59.7708
22	B2	1300.6276	12.5494	47.5853
23	A1	1485.4042	16.5684	3.6945
24	A1	1508.3716	16.5662	103.7991
25	B2	1541.1933	17.7422	778.4133
26	A1	1659.5707	19.7537	126.1872
27	B2	1673.3324	20.5652	7.2966

bmk/pyFFCFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	121.6245	0.1616	0.0000
2	B1	126.2836	0.1956	0.0803
3	B2	199.5240	0.5620	0.0087
4	B1	214.4837	0.4017	3.2108
5	A1	283.4045	0.9184	1.1006
6	B2	312.9491	1.0610	0.4128
7	A1	337.1219	1.3912	1.1143
8	B1	343.5301	0.9694	0.9934
9	A1	435.9355	2.0193	0.0029
10	A2	455.8503	1.5484	0.0000
11	B2	466.7295	2.0531	0.0514
12	A1	555.0791	3.1871	2.0099
13	B1	606.2450	2.6865	9.2462
14	A1	712.0420	4.6418	6.8841
15	A2	719.9365	3.7224	0.0000
16	B2	734.9574	4.2050	0.2343
17	B1	776.8662	4.3548	2.8013
18	A1	948.3264	7.3141	127.3434
19	B2	1003.1966	8.6272	132.9431
20	B2	1214.8886	11.4461	5.3119
21	B2	1293.1271	12.5797	45.4595
22	A1	1295.4108	12.7396	56.1689
23	A1	1489.1522	16.6842	0.2131
24	A1	1509.4893	16.5902	110.0850
25	B2	1543.0855	17.8036	748.3188
26	A1	1653.6872	19.6389	116.3186
27	B2	1668.8707	20.4702	8.6629

bmk/pyFFCFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	121.6296	0.1616	0.0000
2	B1	126.3324	0.1958	0.0781
3	B2	200.9417	0.5703	0.0032
4	B1	214.1875	0.4007	2.8491
5	A1	284.3554	0.9245	1.0775
6	B2	314.1085	1.0689	0.3558
7	A1	338.3878	1.4018	1.0251
8	B1	343.2553	0.9678	0.9470
9	A1	436.9982	2.0300	0.0001
10	A2	456.1435	1.5505	0.0000
11	B2	468.0469	2.0668	0.0629
12	A1	556.0841	3.2022	1.8935
13	B1	607.2022	2.6952	9.3704
14	A1	713.1129	4.6594	6.7111
15	A2	717.7863	3.7004	0.0000
16	B2	737.9126	4.2400	0.1594
17	B1	771.8818	4.2987	2.0920
18	A1	950.4046	7.3468	129.2060
19	B2	1005.2036	8.6795	141.6042
20	B2	1220.4766	11.6735	3.2550
21	A1	1296.9345	12.7758	61.0160
22	B2	1302.9705	12.6400	43.1270
23	A1	1489.6100	16.6626	3.8634
24	A1	1513.7697	16.6936	100.1332
25	B2	1547.1922	17.8904	760.7063
26	A1	1665.1957	19.8939	121.7029
27	B2	1673.6746	20.5452	4.8540

bmk/pyFFCFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	120.4904	0.1585	0.0000
2	B1	125.3899	0.1927	0.0796
3	B2	201.0414	0.5709	0.0000
4	B1	212.7564	0.3952	3.4762
5	A1	282.8291	0.9143	1.0064
6	B2	311.9909	1.0547	0.4584
7	A1	336.4584	1.3853	1.2217
8	B1	340.3945	0.9523	0.8926
9	A1	435.5444	2.0220	0.0052
10	A2	455.0260	1.5426	0.0000
11	B2	466.8146	2.0565	0.0627
12	A1	554.2070	3.1802	1.7710
13	B1	598.8324	2.6205	11.8587
14	A1	709.1326	4.6079	7.8298
15	A2	714.6135	3.6680	0.0000
16	B2	731.2110	4.1626	0.0415
17	B1	766.0085	4.2346	1.9309
18	A1	945.9524	7.2783	132.8699
19	B2	1000.3859	8.6080	151.4078
20	B2	1217.7602	11.7167	1.4609
21	A1	1289.3746	12.6377	60.7174

22	B2	1311.6677	12.7038	42.8099
23	A1	1486.6419	16.5551	7.8607
24	A1	1513.0185	16.6951	91.6356
25	B2	1547.7250	17.9024	781.9575
26	A1	1671.5002	20.0292	125.8245
27	B2	1678.4563	20.6401	2.7916

bmk/pyFFFFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	122.9952	0.1653	0.0000
2	B1	161.8930	0.2839	0.0003
3	B1	221.8498	0.4349	5.4744
4	B2	275.6920	0.8428	0.0556
5	A1	277.0680	0.8388	0.8161
6	B2	324.1129	1.1215	1.0077
7	A1	353.3133	1.2888	1.7914
8	B1	358.9568	1.0437	3.8524
9	A2	444.2254	1.4708	0.0000
10	B2	468.5191	2.0800	0.1044
11	A1	486.9610	2.2132	0.2196
12	A1	607.7589	3.7640	0.0488
13	B1	637.4564	2.9700	2.5559
14	A2	691.6185	3.4349	0.0000
15	A1	711.6281	4.6120	5.8896
16	B1	728.3917	3.8446	8.0480
17	B2	756.1427	4.4722	0.0074
18	B2	1020.7558	8.8823	200.5250
19	A1	1124.2827	10.3568	243.5955
20	B2	1221.5934	11.8218	2.1075
21	B2	1315.7565	12.7749	28.2783
22	A1	1349.8915	14.0438	24.5427
23	A1	1492.9512	16.4797	34.6721
24	B2	1552.5623	18.0356	744.7781
25	A1	1587.2528	18.7509	184.0449
26	A1	1673.9271	20.0515	117.5868
27	B2	1699.4332	21.0906	6.0875

bmk/pyFFFFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	124.2892	0.1687	0.0000
2	B1	163.8499	0.2910	0.0002
3	B1	221.5395	0.4331	4.5097
4	B2	273.5712	0.8294	0.0577
5	A1	275.2640	0.8275	0.9097
6	B2	323.4151	1.1162	0.9565
7	A1	352.9000	1.2851	1.6162
8	B1	362.3904	1.0655	3.4503
9	A2	446.8134	1.4882	0.0000

10	B2	466.6016	2.0596	0.1051
11	A1	486.8277	2.2089	0.2725
12	A1	610.0208	3.7869	0.0587
13	B1	653.9107	3.1401	3.7976
14	A1	711.3706	4.6076	4.5671
15	A2	718.9756	3.7124	0.0000
16	B2	758.5200	4.5012	0.1024
17	B1	781.8621	4.4057	5.3017
18	B2	1025.6865	8.9517	181.7722
19	A1	1129.7782	10.4524	225.6154
20	B2	1224.1002	11.7790	4.3796
21	B2	1307.3078	12.7266	26.9309
22	A1	1356.3052	14.1908	23.2796
23	A1	1498.7841	16.6101	37.1404
24	B2	1554.6365	18.0992	729.7743
25	A1	1587.4938	18.7881	183.0634
26	A1	1668.5295	19.9387	111.0689
27	B2	1694.8228	20.9903	6.0796

bmk/pyFFFFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	123.8098	0.1674	0.0000
2	B1	162.9641	0.2877	0.0005
3	B1	220.9097	0.4305	3.9917
4	B2	273.8919	0.8314	0.0619
5	A1	275.7867	0.8306	0.9310
6	B2	324.5095	1.1238	0.9057
7	A1	354.0335	1.2937	1.4684
8	B1	361.2752	1.0593	3.2087
9	A2	446.1673	1.4840	0.0000
10	B2	467.6850	2.0711	0.1128
11	A1	487.7562	2.2195	0.3010
12	A1	610.9836	3.8043	0.0479
13	B1	650.7774	3.1083	3.3164
14	A1	712.6277	4.6248	4.4881
15	A2	715.0857	3.6730	0.0000
16	B2	761.0631	4.5333	0.0603
17	B1	771.5957	4.2945	5.1934
18	B2	1027.0839	8.9925	190.6579
19	A1	1130.6843	10.4764	236.1891
20	B2	1227.5006	11.9424	2.7122
21	B2	1317.8136	12.8337	23.0441
22	A1	1354.4840	14.1455	23.9223
23	A1	1497.9283	16.5885	35.9925
24	B2	1558.2301	18.1684	729.7277
25	A1	1592.3521	18.8797	175.4341
26	A1	1679.6593	20.1889	119.5984
27	B2	1700.8697	21.0993	3.5824

bmk/pyFFFFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	122.6588	0.1643	0.0000
2	B1	162.1204	0.2846	0.0000
3	B1	220.6913	0.4301	5.0646
4	B2	271.9130	0.8196	0.0565
5	A1	273.9527	0.8198	0.9098
6	B2	322.2865	1.1087	1.1585
7	A1	351.8186	1.2776	1.7672
8	B1	359.0058	1.0459	3.6737
9	A2	446.1249	1.4833	0.0000
10	B2	466.6183	2.0621	0.0971
11	A1	486.0641	2.2040	0.2275
12	A1	608.7472	3.7804	0.0263
13	B1	647.6343	3.0789	3.7073
14	A1	708.9996	4.5775	5.0628
15	A2	712.9470	3.6511	0.0000
16	B2	753.4399	4.4406	0.0184
17	B1	769.5285	4.2684	5.6092
18	B2	1020.9607	8.8993	198.2515
19	A1	1124.1111	10.3627	242.3964
20	B2	1223.4947	11.9181	1.3463
21	B2	1326.5693	12.9418	22.2116
22	A1	1346.7039	13.9888	23.8449
23	A1	1492.7416	16.4735	31.9911
24	B2	1557.5430	18.1467	740.8993
25	A1	1593.6935	18.8873	177.2773
26	A1	1685.6556	20.3232	119.5555
27	B2	1704.7697	21.1846	2.7402

bmk/pyFFHFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	119.4156	0.1560	0.0000
2	B1	210.0244	0.3489	4.2789
3	A1	286.1439	0.8743	0.7739
4	B1	305.4265	0.4583	1.0482
5	B2	307.7755	0.9917	0.3116
6	A1	367.9753	1.2778	3.1270
7	B2	460.5817	1.7902	0.1197
8	A2	469.9813	1.6453	0.0000
9	B1	494.7156	0.6394	0.8482
10	A1	518.6391	2.3344	2.2288
11	B2	673.5270	1.5902	2.9795
12	A2	705.8618	3.5753	0.0000
13	A1	706.4818	4.4363	15.4363
14	B1	736.9193	2.9474	11.0967
15	A1	762.2283	3.2390	11.9536
16	B1	906.7941	0.6648	35.3217
17	B2	932.9787	2.6069	113.0125
18	B2	1199.5118	2.2461	51.0211

19	B2	1215.8139	2.5682	11.7447
20	A1	1265.7180	10.4434	195.0745
21	B2	1305.5409	9.4725	102.6963
22	A1	1463.0869	14.5556	1.3602
23	A1	1497.4281	15.8225	64.0759
24	B2	1555.0329	11.1513	770.4143
25	A1	1671.9988	19.0415	30.2213
26	B2	1687.1942	15.2849	0.4025
27	A1	3223.5957	6.7022	10.3166

bmk/pyFFHFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	120.7545	0.1594	0.0000
2	B1	210.6558	0.3526	3.4664
3	A1	284.8735	0.8660	0.8211
4	B2	307.0715	0.9866	0.2456
5	B1	308.7482	0.4661	1.0402
6	A1	368.1586	1.2780	2.7259
7	B2	458.8602	1.7689	0.0783
8	A2	471.0935	1.6531	0.0000
9	B1	499.5558	0.6379	0.7696
10	A1	519.0899	2.3294	2.4118
11	B2	674.9920	1.5890	2.9166
12	A1	708.3060	4.4943	12.7708
13	A2	728.9086	3.8134	0.0000
14	A1	762.5503	3.2331	12.5015
15	B1	766.6964	2.3654	13.3036
16	B1	925.6707	0.7363	26.5554
17	B2	935.9485	2.5894	96.5747
18	B2	1206.8273	2.2666	55.6195
19	B2	1214.7673	2.7474	3.7410
20	A1	1271.6462	10.5050	178.4501
21	B2	1297.5834	8.1647	106.2499
22	A1	1466.1634	14.5466	3.3278
23	A1	1501.2532	16.0936	65.2188
24	B2	1557.7626	11.1511	757.9023
25	A1	1665.7657	18.9652	28.8068
26	B2	1683.1348	14.9659	0.4575
27	A1	3212.7210	6.6539	7.8994

bmk/pyFFHFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	120.5319	0.1588	0.0000
2	B1	210.1713	0.3510	3.0400
3	A1	285.7131	0.8707	0.8236
4	B2	307.9749	0.9921	0.2236
5	B1	308.1092	0.4654	1.0253
6	A1	369.1516	1.2862	2.5188

7	B2	460.1869	1.7803	0.0747
8	A2	470.8091	1.6512	0.0000
9	B1	497.6502	0.6378	0.6594
10	A1	519.6815	2.3346	2.4053
11	B2	676.7672	1.6022	2.8359
12	A1	708.8275	4.4899	12.9427
13	A2	725.7465	3.7807	0.0000
14	B1	762.6026	2.4885	11.6691
15	A1	764.8857	3.2633	12.8299
16	B1	920.9658	0.7175	29.4019
17	B2	938.4134	2.6342	102.3493
18	B2	1207.6073	2.5068	52.0773
19	B2	1222.3463	2.4126	9.5737
20	A1	1273.1933	10.5601	186.2453
21	B2	1307.0151	9.0071	101.5587
22	A1	1468.6173	14.6584	0.6691
23	A1	1501.5218	15.9431	65.0601
24	B2	1560.8249	11.3614	753.3737
25	A1	1676.6525	19.1785	30.5268
26	B2	1689.5241	14.8241	1.9728
27	A1	3236.1759	6.7523	7.9729

bmk/pyFFHFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	119.4195	0.1559	0.0000
2	B1	208.9967	0.3475	3.9200
3	A1	283.7832	0.8595	0.7967
4	B2	305.7687	0.9770	0.3589
5	B1	306.6656	0.4634	1.0744
6	A1	366.7104	1.2689	2.9762
7	B2	458.7602	1.7680	0.1021
8	A2	469.9602	1.6449	0.0000
9	B1	494.2714	0.6309	0.7977
10	A1	518.1485	2.3258	2.1464
11	B2	670.8428	1.5904	2.6619
12	A1	704.1758	4.4156	13.9062
13	A2	722.5179	3.7473	0.0000
14	B1	757.6801	2.4109	13.0379
15	A1	763.8942	3.2626	12.6731
16	B1	919.9965	0.7173	29.7702
17	B2	933.9730	2.6097	111.7329
18	B2	1199.6302	2.2911	49.3573
19	B2	1220.2822	2.4734	14.6281
20	A1	1265.0665	10.4718	194.7206
21	B2	1315.8038	10.1071	90.5733
22	A1	1467.0169	14.6746	0.1018
23	A1	1497.5591	15.6617	59.6869
24	B2	1558.8474	11.5628	767.8858
25	A1	1684.2519	19.3006	30.4313
26	B2	1691.7207	15.1534	2.2700
27	A1	3245.9734	6.7964	8.7655

bmk/pyFHFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	132.8010	0.1738	0.1376
2	A"	216.5156	0.3737	4.7532
3	A"	267.2858	0.3034	1.2505
4	A'	277.7005	0.8451	0.2322
5	A'	325.4569	1.0716	1.2879
6	A'	360.2159	1.2544	1.8109
7	A"	394.9142	0.9554	1.0332
8	A'	469.8600	1.8253	0.4320
9	A'	538.5724	1.9130	2.9805
10	A'	611.2566	3.7373	0.0448
11	A"	640.6602	1.3516	5.8465
12	A'	682.2807	1.7057	3.3249
13	A"	693.6285	2.1555	0.0188
14	A"	746.7105	2.2079	2.6921
15	A'	817.1244	3.8484	39.8897
16	A"	857.0787	0.6656	43.6980
17	A'	1046.1841	2.3370	74.3102
18	A'	1117.9345	8.2383	156.5762
19	A'	1195.9265	1.6620	119.9778
20	A'	1282.4176	9.5575	25.6471
21	A'	1330.0539	8.7912	24.0109
22	A'	1464.0423	13.6249	101.1421
23	A'	1500.8680	13.6625	106.7712
24	A'	1569.5350	11.3178	485.4475
25	A'	1666.0296	15.9302	300.6406
26	A'	1691.7814	19.6297	44.5923
27	A'	3239.6303	6.7742	12.5229

bmk/pyFHFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	133.8589	0.1764	0.1118
2	A"	216.6681	0.3774	3.9010
3	A"	269.9105	0.3070	1.3289
4	A'	275.8453	0.8333	0.2646
5	A'	324.8864	1.0665	1.1419
6	A'	360.4460	1.2544	1.4767
7	A"	396.2814	0.9720	0.9724
8	A'	469.2963	1.8205	0.4315
9	A'	537.1001	1.9025	2.6129
10	A'	613.8027	3.7709	0.0108
11	A"	650.3327	1.3269	6.4865
12	A'	683.6141	1.6984	3.6301
13	A"	708.5471	1.9539	0.0098
14	A"	774.4668	2.0082	0.5351
15	A'	818.1241	3.8561	34.4514

16	A''	871.4323	0.7522	38.7758
17	A'	1047.9121	2.2982	63.1722
18	A'	1123.3458	8.2494	139.2255
19	A'	1202.5505	1.7067	121.7805
20	A'	1280.3306	10.8892	20.1323
21	A'	1327.2212	7.9942	28.7714
22	A'	1468.6431	14.0114	111.6223
23	A'	1504.6282	13.6194	90.9656
24	A'	1571.3457	11.2980	479.5867
25	A'	1660.6782	15.5868	294.2146
26	A'	1686.7054	19.5052	43.4337
27	A'	3228.5603	6.7249	9.3677

bmk/pyFHFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	133.5816	0.1756	0.1014
2	A''	216.1784	0.3758	3.4712
3	A''	269.0134	0.3060	1.3250
4	A'	276.4412	0.8369	0.2726
5	A'	326.0708	1.0740	1.1043
6	A'	361.6383	1.2636	1.3746
7	A''	395.3417	0.9673	0.8419
8	A'	470.3258	1.8326	0.4316
9	A'	538.5496	1.9117	2.4666
10	A'	614.5734	3.7882	0.0112
11	A''	648.9922	1.3532	5.9458
12	A'	685.6179	1.7104	3.4825
13	A''	706.9528	1.9725	0.0000
14	A''	769.2727	2.1205	0.8573
15	A'	819.7943	3.8850	35.6833
16	A''	865.4021	0.7195	39.6974
17	A'	1050.7287	2.3427	68.8196
18	A'	1125.7353	8.4013	146.0875
19	A'	1204.8768	1.7017	118.0754
20	A'	1286.7078	9.9703	23.1289
21	A'	1333.2125	8.6210	26.2911
22	A'	1472.6318	13.9191	101.7416
23	A'	1505.0500	13.6892	97.4896
24	A'	1575.3915	11.3114	477.0809
25	A'	1671.0531	15.7831	301.7819
26	A'	1693.3581	19.5088	38.3149
27	A'	3252.1947	6.8246	9.5579

bmk/pyFHFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	132.8547	0.1738	0.1301
2	A''	215.8329	0.3752	4.4239
3	A''	267.5283	0.3039	1.3578

4	A'	274.5797	0.8260	0.2698
5	A'	323.5703	1.0573	1.3618
6	A'	359.0232	1.2456	1.7250
7	A''	394.6821	0.9555	0.9628
8	A'	468.8722	1.8155	0.4058
9	A'	537.0923	1.9000	2.6357
10	A'	612.0342	3.7621	0.0331
11	A''	645.5240	1.3666	6.2228
12	A'	679.6521	1.7038	3.1589
13	A''	702.9902	1.9563	0.0120
14	A''	767.4064	2.1283	0.9393
15	A'	816.2393	3.8322	38.1840
16	A''	867.9947	0.7173	42.2475
17	A'	1047.1968	2.3687	76.9782
18	A'	1119.2103	8.2938	155.4359
19	A'	1196.8368	1.6492	114.0543
20	A'	1285.4764	8.7684	26.7694
21	A'	1337.3007	9.7202	19.8675
22	A'	1468.0861	13.4828	91.9381
23	A'	1502.5104	13.7863	114.5475
24	A'	1574.6040	11.4277	484.0487
25	A'	1676.5000	16.2473	300.9856
26	A'	1697.9239	19.6400	35.2434
27	A'	3262.4475	6.8708	10.6009

bmk/pyHHHHH_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	385.0119	0.2251	0.0000
2	B1	420.3767	0.3911	4.2865
3	A1	615.9102	1.5870	4.1551
4	B2	671.9756	1.6839	0.3943
5	B1	724.5978	0.4425	71.1017
6	B1	768.6493	0.7643	15.0479
7	A2	908.7096	0.6071	0.0000
8	B1	969.5083	0.7383	0.0098
9	A2	1012.9836	0.8842	0.0000
10	A1	1016.3574	4.4189	3.8395
11	B1	1021.6564	0.7915	0.0195
12	A1	1045.4586	2.8352	8.2345
13	B2	1077.0282	1.2291	0.0000
14	A1	1100.7709	1.2012	4.3422
15	B2	1166.8282	1.0136	3.3066
16	A1	1255.0089	1.2087	4.7902
17	B2	1272.3836	4.1901	0.3228
18	B2	1390.8560	1.3674	0.0806
19	B2	1479.4765	2.5868	25.8588
20	A1	1523.7300	2.7454	4.0759
21	A1	1632.6439	7.8040	24.1919
22	B2	1635.7551	9.3368	10.4732
23	B2	3161.5589	6.4116	14.9035
24	A1	3163.2197	6.4314	0.9426

25	A1	3179.1689	6.4940	2.5525
26	B2	3195.6103	6.5851	8.2948
27	A1	3202.7570	6.6474	1.2258

bmk/pyHHHHH_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	386.5042	0.2239	0.0000
2	B1	422.3673	0.3904	4.1208
3	A1	613.6369	1.5719	4.7392
4	B2	670.1465	1.6706	0.2228
5	B1	730.5527	0.4366	65.2386
6	B1	777.0744	0.7808	11.2332
7	A2	914.6224	0.6154	0.0000
8	B1	980.9136	0.7586	0.0239
9	A1	1016.1255	4.4059	3.1796
10	A2	1029.2209	0.9189	0.0000
11	B1	1031.8405	0.8303	0.0128
12	A1	1045.7885	2.7553	9.2251
13	B2	1075.0913	1.2386	0.1165
14	A1	1101.2020	1.2214	2.5316
15	B2	1161.1661	1.0488	3.9777
16	A1	1254.7635	1.2222	4.3806
17	B2	1267.4298	3.6232	0.4739
18	B2	1396.2954	1.3788	0.2031
19	B2	1481.7715	2.5789	23.5205
20	A1	1528.5104	2.7386	3.3508
21	A1	1628.7473	7.5562	23.7115
22	B2	1634.0488	9.1508	10.8721
23	B2	3152.9758	6.3760	16.1124
24	A1	3154.8440	6.3991	1.3752
25	A1	3172.0005	6.4617	2.8045
26	B2	3187.8199	6.5507	10.5892
27	A1	3194.8827	6.6105	1.9683

bmk/pyHHHHH_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	388.0441	0.2255	0.0000
2	B1	423.6336	0.3950	3.9411
3	A1	616.0107	1.5888	4.8763
4	B2	673.2257	1.6891	0.2983
5	B1	731.6640	0.4311	69.0975
6	B1	779.9724	0.8016	11.4786
7	A2	918.5969	0.6204	0.0000
8	B1	983.7157	0.7644	0.0266
9	A1	1019.9523	4.4609	4.9634
10	A2	1032.7864	0.9263	0.0000
11	B1	1045.4291	0.8523	0.0017
12	A1	1051.2748	2.8232	8.6615

13	B2	1082.5020	1.2441	0.0226
14	A1	1105.1240	1.2344	3.1863
15	B2	1171.7002	1.0331	3.3816
16	A1	1257.9300	1.2167	3.9669
17	B2	1275.8805	4.0924	0.2342
18	B2	1400.2399	1.3862	0.1998
19	B2	1488.4068	2.6324	25.4063
20	A1	1532.8109	2.7389	3.4103
21	A1	1639.8845	7.7835	24.4457
22	B2	1641.8106	9.1209	9.9540
23	B2	3174.3384	6.4632	16.1440
24	A1	3176.2731	6.4871	1.7693
25	A1	3194.9486	6.5560	2.7985
26	B2	3211.1722	6.6478	9.6221
27	A1	3218.2877	6.7093	1.6808

bmk/pyHHHHH_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	386.5056	0.2254	0.0000
2	B1	420.7049	0.3924	4.2419
3	A1	615.5271	1.5839	4.1905
4	B2	671.5592	1.6784	0.4183
5	B1	726.0156	0.4280	70.9966
6	B1	774.2798	0.7942	11.5495
7	A2	911.7769	0.6110	0.0000
8	B1	975.1314	0.7478	0.0215
9	A1	1016.8644	4.4350	5.5561
10	A2	1022.8367	0.9047	0.0000
11	B1	1034.7850	0.8272	0.0431
12	A1	1050.3218	2.9114	6.5808
13	B2	1083.5265	1.2251	0.0013
14	A1	1103.5223	1.2005	4.7990
15	B2	1171.7012	0.9857	3.1019
16	A1	1255.9693	1.2003	4.2527
17	B2	1278.7515	4.8521	0.3168
18	B2	1392.3016	1.3699	0.1138
19	B2	1483.1061	2.6453	25.4896
20	A1	1525.9169	2.7515	3.3050
21	B2	1642.4146	9.4230	10.0974
22	A1	1642.9768	8.1393	24.0393
23	B2	3182.3755	6.4969	15.1311
24	A1	3184.1379	6.5177	1.8902
25	A1	3201.6359	6.5860	3.1714
26	B2	3217.3679	6.6761	10.0841
27	A1	3224.5714	6.7391	1.6054

camb3lyp/pyCCCCC_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	59.4435	0.0711	0.0000
2	B1	81.7577	0.1332	0.0175
3	B1	150.8322	0.2142	0.0165
4	A1	208.1318	0.8402	0.0691
5	B2	220.5187	0.8801	0.3196
6	A1	223.1611	0.8458	0.0537
7	B2	230.6035	1.0922	0.0006
8	B1	289.5965	0.6666	0.9364
9	B2	338.8160	1.9536	0.2996
10	A1	356.4784	2.1436	0.1358
11	A2	373.8829	1.0310	0.0000
12	A1	393.5076	2.9913	0.1222
13	A1	556.8733	3.1671	6.7889
14	B2	594.7839	2.8037	0.9581
15	B1	596.2947	2.6020	1.5453
16	A2	652.6110	3.0367	0.0000
17	B2	697.6703	4.4501	86.3812
18	B1	772.8702	4.2983	0.2128
19	A1	844.6038	5.7592	89.9172
20	B2	918.5799	6.4579	3.4624
21	A1	1121.4539	9.3269	33.3949
22	B2	1246.9275	11.2094	28.1098
23	A1	1260.0629	11.5247	4.3415
24	B2	1386.8995	14.0675	411.4215
25	A1	1389.3411	13.8209	121.8414
26	A1	1580.6352	17.7806	106.4313
27	B2	1611.7553	19.1413	68.4612

camb3lyp/pyCCCCC_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	61.1981	0.0753	0.0000
2	B1	83.6110	0.1390	0.0116
3	B1	151.7605	0.2168	0.0240
4	A1	205.3166	0.8297	0.0320
5	B2	217.8438	0.8595	0.2961
6	A1	220.4138	0.8151	0.0252
7	B2	225.4541	1.0438	0.0008
8	B1	292.5816	0.6810	0.8753
9	B2	338.7585	1.9531	0.3086
10	A1	356.8834	2.1508	0.1167
11	A2	377.2951	1.0500	0.0000
12	A1	393.6698	2.9947	0.1497
13	A1	556.9001	3.1684	5.9649
14	B2	592.1952	2.7810	0.5267
15	B1	603.6275	2.6653	1.4111
16	A2	665.8514	3.1616	0.0000
17	B2	697.4985	4.4439	80.2940
18	B1	792.4769	4.5222	1.5874
19	A1	844.7364	5.7606	84.4735
20	B2	916.8784	6.4343	3.3284
21	A1	1120.4536	9.3119	30.8947

22	B2	1243.0689	11.1531	27.2415
23	A1	1259.9372	11.5126	5.2757
24	B2	1384.4944	14.0118	379.5811
25	A1	1385.8569	13.7507	106.2210
26	A1	1576.3712	17.6805	98.3847
27	B2	1605.0998	18.9685	63.4296

camb3lyp/pyCCCCC_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	61.4168	0.0758	0.0000
2	B1	83.9577	0.1400	0.0138
3	B1	152.5480	0.2191	0.0032
4	A1	206.2580	0.8387	0.0440
5	B2	218.9497	0.8683	0.2648
6	A1	221.5974	0.8231	0.0224
7	B2	226.2196	1.0508	0.0004
8	B1	293.6836	0.6863	0.8225
9	B2	339.9005	1.9634	0.3190
10	A1	358.0703	2.1603	0.1380
11	A2	379.7939	1.0641	0.0000
12	A1	395.4519	3.0187	0.1404
13	A1	559.4720	3.1959	5.7292
14	B2	595.5954	2.8147	0.6851
15	B1	606.5417	2.6913	1.3713
16	A2	669.3466	3.1953	0.0000
17	B2	702.1169	4.5001	80.1446
18	B1	794.0541	4.5397	1.5316
19	A1	848.4057	5.8163	87.2799
20	B2	921.8870	6.5096	2.8479
21	A1	1124.6539	9.3866	31.5850
22	B2	1245.4744	11.1929	28.9956
23	A1	1262.0373	11.5534	4.8286
24	B2	1386.1741	14.0440	378.2039
25	A1	1387.9789	13.7929	108.4611
26	A1	1576.7791	17.6902	102.5914
27	B2	1607.3282	19.0305	62.1813

camb3lyp/pyCCCCC_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	59.9705	0.0723	0.0000
2	B1	81.8768	0.1333	0.0156
3	B1	149.9822	0.2118	0.0004
4	A1	206.6813	0.8288	0.0460
5	B2	219.0572	0.8686	0.1797
6	A1	221.2769	0.8317	0.0124
7	B2	228.7773	1.0750	0.0011
8	B1	288.8341	0.6631	0.5939
9	B2	336.5653	1.9358	0.3682

10	A1	354.1147	2.1243	0.1269
11	A2	373.7581	1.0302	0.0000
12	A1	390.0833	2.9482	0.1281
13	A1	551.7110	3.1098	7.3240
14	B2	590.5949	2.7689	1.5358
15	B1	593.0897	2.5708	1.2264
16	A2	651.3322	3.0251	0.0000
17	B2	690.6782	4.3538	87.6486
18	B1	772.2895	4.2991	1.9003
19	A1	838.0082	5.6613	92.8125
20	B2	911.5537	6.3479	2.9639
21	A1	1113.2157	9.1856	35.1421
22	B2	1250.4649	11.2705	26.1420
23	A1	1256.4825	11.4468	3.9356
24	B2	1384.1219	14.0062	398.9439
25	A1	1386.1341	13.7529	116.7389
26	A1	1581.1728	17.7898	107.2491
27	B2	1610.6681	19.1179	66.0180

camb3lyp/pyFCFCF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	94.2799	0.1118	0.0000
2	B1	111.4871	0.1597	0.0005
3	A1	186.9617	0.5457	0.0226
4	B1	217.6095	0.4216	3.3070
5	B2	228.9981	0.6940	0.0341
6	B2	318.1095	1.2761	1.1475
7	B1	322.1755	0.8471	0.5552
8	A1	328.9135	1.3785	0.3976
9	A2	385.4847	1.0978	0.0000
10	A1	415.2491	2.0866	0.6001
11	B2	417.5869	1.9056	0.1527
12	A1	592.6842	3.3512	1.7473
13	A1	626.2882	3.8023	2.5793
14	B1	666.7380	3.2511	1.5898
15	B2	713.8864	3.9850	0.4046
16	A2	716.4842	3.6831	0.0000
17	B1	789.2524	4.4901	16.8237
18	B2	812.2680	5.6074	114.8766
19	A1	1092.0520	9.7551	181.3200
20	B2	1121.7773	10.1495	22.5696
21	A1	1178.2077	10.3815	7.8310
22	B2	1305.4975	12.4440	14.8345
23	A1	1462.8744	15.8968	47.4518
24	B2	1486.0637	16.2403	441.7331
25	A1	1502.9055	16.5169	101.6620
26	A1	1660.5589	19.6840	223.6781
27	B2	1681.8079	20.6940	89.6717

camb3lyp/pyFCFCF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	95.6200	0.1150	0.0000
2	B1	112.7174	0.1631	0.0015
3	A1	185.2806	0.5359	0.0065
4	B1	215.9305	0.4148	2.9161
5	B2	227.7236	0.6859	0.0258
6	B2	318.3738	1.2811	1.1045
7	B1	324.2955	0.8595	0.7042
8	A1	329.0993	1.3825	0.3350
9	A2	379.7577	1.0651	0.0000
10	A1	415.8270	2.0914	0.5770
11	B2	417.7030	1.9014	0.1763
12	A1	593.5413	3.3344	1.5794
13	A1	628.0757	3.8482	1.7873
14	B1	669.7264	3.2807	1.5310
15	B2	715.0310	3.9994	0.1026
16	A2	725.0338	3.7729	0.0000
17	B1	804.5272	4.6647	13.5856
18	B2	811.1580	5.5844	107.0287
19	A1	1097.7828	9.8396	163.8716
20	B2	1126.1612	10.2363	18.6111
21	A1	1177.2521	10.3736	5.6656
22	B2	1300.4187	12.3640	12.9984
23	A1	1467.9809	15.9891	54.7101
24	B2	1487.4430	16.2747	419.1957
25	A1	1502.5157	16.5511	80.9406
26	A1	1656.5241	19.5898	215.3103
27	B2	1675.9460	20.5404	90.9951

camb3lyp/pyFCFCF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	95.4803	0.1147	0.0000
2	B1	112.5798	0.1628	0.0000
3	A1	186.9813	0.5457	0.0030
4	B1	216.5348	0.4173	2.5666
5	B2	229.5971	0.6975	0.0207
6	B2	319.6022	1.2903	1.0589
7	B1	325.2769	0.8641	0.6438
8	A1	330.2690	1.3904	0.2885
9	A2	382.6829	1.0818	0.0000
10	A1	416.9479	2.1022	0.5672
11	B2	418.6075	1.9094	0.1757
12	A1	594.5602	3.3574	1.3952
13	A1	629.1358	3.8503	1.7396
14	B1	669.9623	3.2834	1.2564
15	B2	717.2717	4.0248	0.1256
16	A2	725.9649	3.7828	0.0000
17	B1	803.6892	4.6548	12.5812
18	B2	815.2687	5.6450	105.3480

19	A1	1099.7099	9.8737	166.0101
20	B2	1129.6885	10.2903	17.0459
21	A1	1181.3185	10.4438	5.8728
22	B2	1304.1143	12.4353	13.8210
23	A1	1472.9589	16.1141	52.4424
24	B2	1491.0974	16.3548	409.9693
25	A1	1504.7634	16.5917	88.1016
26	A1	1658.1812	19.6322	221.6431
27	B2	1679.6891	20.6436	93.9774

camb3lyp/pyFCFCF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	94.4474	0.1122	0.0000
2	B1	111.4737	0.1594	0.0009
3	A1	186.7907	0.5448	0.0002
4	B1	214.8891	0.4105	2.9105
5	B2	229.6688	0.6981	0.0124
6	B2	317.7440	1.2754	1.0438
7	B1	321.0575	0.8429	0.3523
8	A1	328.2182	1.3762	0.2833
9	A2	376.8534	1.0485	0.0000
10	A1	413.4428	2.0706	0.6378
11	B2	416.1277	1.8914	0.0910
12	A1	591.4029	3.3061	1.7043
13	A1	625.3826	3.8133	1.8675
14	B1	664.4046	3.2276	0.9132
15	B2	710.9125	3.9526	0.3237
16	A2	717.4834	3.6960	0.0000
17	B1	791.1128	4.5125	19.8696
18	B2	805.8126	5.5036	109.2991
19	A1	1093.9565	9.7681	178.7177
20	B2	1124.1119	10.2008	19.5230
21	A1	1172.3239	10.2858	5.1745
22	B2	1310.4174	12.5446	11.7969
23	A1	1470.9277	16.0653	52.4064
24	B2	1490.0869	16.3256	429.7351
25	A1	1506.8498	16.6419	90.9092
26	A1	1663.0464	19.7409	226.8824
27	B2	1681.2938	20.6845	86.4344

camb3lyp/pyFCFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	99.8863	0.1247	0.0000
2	A''	143.5726	0.2266	0.0079
3	A'	205.8302	0.5874	0.0228
4	A''	217.1585	0.4185	4.3453
5	A'	278.0202	0.8573	0.2669
6	A'	317.3895	1.1950	0.9098

7	A''	333.5097	0.8990	1.0600
8	A'	339.5491	1.2838	0.8226
9	A'	414.1585	1.9534	0.2498
10	A''	418.1097	1.3061	1.4943
11	A'	479.2089	2.1791	0.4334
12	A'	602.9897	3.6762	0.6840
13	A'	646.7607	3.8606	7.3919
14	A''	656.2090	3.1522	2.2222
15	A''	710.2501	3.6209	0.3142
16	A'	734.7569	4.2198	0.7024
17	A''	774.7089	4.3274	11.6604
18	A'	921.3738	7.2028	154.2442
19	A'	1097.6902	9.8576	194.2843
20	A'	1134.8306	10.3132	32.7318
21	A'	1280.2092	12.4973	23.2146
22	A'	1313.3471	12.6592	18.0431
23	A'	1466.0350	15.9359	49.1763
24	A'	1506.2329	16.6118	291.7641
25	A'	1551.6816	17.8683	441.2246
26	A'	1681.9067	20.2114	187.5274
27	A'	1701.5385	21.0964	18.6033

camb3lyp/pyFCFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	101.4556	0.1285	0.0009
2	A''	144.9423	0.2311	0.0066
3	A'	204.4420	0.5793	0.0173
4	A''	216.1840	0.4142	3.6667
5	A'	278.5201	0.8604	0.3080
6	A'	317.8445	1.2019	0.8449
7	A''	336.1666	0.9143	1.1368
8	A'	339.8694	1.2848	0.7106
9	A'	414.4827	1.9520	0.2229
10	A''	418.7484	1.3105	1.2086
11	A'	479.9768	2.1853	0.4970
12	A'	605.4398	3.6925	0.7496
13	A'	647.0290	3.8733	6.1269
14	A''	662.3733	3.2141	2.3899
15	A''	725.4232	3.7780	0.5120
16	A'	736.9433	4.2460	0.6170
17	A''	801.3423	4.6253	9.0284
18	A'	923.4766	7.2216	141.5660
19	A'	1103.2334	9.9458	174.5781
20	A'	1138.7060	10.3954	33.2747
21	A'	1283.0193	12.4924	21.7682
22	A'	1309.7974	12.6796	16.0615
23	A'	1470.3592	16.0222	50.7471
24	A'	1506.6680	16.6254	273.6478
25	A'	1551.9683	17.8977	422.1102
26	A'	1678.3321	20.1317	184.8471
27	A'	1696.7723	20.9674	16.4381

camb3lyp/pyFCFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	101.2548	0.1280	0.0000
2	A"	144.2400	0.2289	0.0025
3	A'	206.1988	0.5894	0.0196
4	A"	216.3591	0.4149	3.2192
5	A'	279.2076	0.8644	0.3058
6	A'	318.6918	1.2066	0.8173
7	A"	336.8238	0.9179	1.0667
8	A'	340.7218	1.2918	0.6383
9	A'	415.4352	1.9609	0.2244
10	A"	419.6403	1.3156	1.0912
11	A'	480.5386	2.1906	0.5119
12	A'	605.9283	3.7022	0.6487
13	A'	648.5425	3.8899	5.8009
14	A"	661.1858	3.2018	1.9886
15	A"	723.7582	3.7607	0.2898
16	A'	738.2497	4.2609	0.5881
17	A"	794.5538	4.5504	8.3457
18	A'	926.0604	7.2648	139.8888
19	A'	1105.2410	9.9810	177.4719
20	A'	1142.3578	10.4529	30.1050
21	A'	1286.4383	12.5610	22.1769
22	A'	1313.3485	12.7462	16.5038
23	A'	1474.9833	16.1330	51.7497
24	A'	1509.7820	16.6851	255.8800
25	A'	1555.2039	17.9790	431.2523
26	A'	1680.7868	20.1902	186.7006
27	A'	1700.2134	21.0648	18.8686

camb3lyp/pyFCFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	100.1365	0.1251	0.0000
2	A"	143.2355	0.2256	0.0042
3	A'	206.1622	0.5890	0.0282
4	A"	215.2924	0.4108	3.9110
5	A'	278.8108	0.8623	0.2756
6	A'	317.0104	1.1949	0.8965
7	A"	332.5546	0.8949	0.8260
8	A'	338.7654	1.2779	0.7088
9	A'	412.6564	1.9395	0.2432
10	A"	417.1229	1.3001	1.7429
11	A'	478.6714	2.1721	0.4920
12	A'	603.4770	3.6677	0.8128
13	A'	644.0077	3.8309	6.4635
14	A"	656.5069	3.1560	1.8666
15	A"	718.3869	3.7064	1.0043

16	A'	732.3193	4.1914	0.6566
17	A''	788.3362	4.4781	11.2408
18	A'	919.1901	7.1505	144.3015
19	A'	1099.7228	9.8851	186.2285
20	A'	1136.5952	10.3538	32.0793
21	A'	1282.1043	12.5495	20.9441
22	A'	1318.7923	12.7799	15.9784
23	A'	1473.2073	16.0920	51.0640
24	A'	1509.3277	16.6843	274.5575
25	A'	1557.7003	18.0304	435.8633
26	A'	1684.7570	20.2873	188.6769
27	A'	1702.6056	21.1137	14.3527

camb3lyp/pyFFCFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	120.2314	0.1581	0.0000
2	B1	124.2747	0.1899	0.0331
3	B2	205.1524	0.5966	0.0403
4	B1	211.7568	0.3924	4.1299
5	A1	283.6449	0.9193	0.8007
6	B2	311.0827	1.0490	0.3233
7	A1	334.5072	1.3660	1.0830
8	B1	339.7043	0.9462	1.0956
9	A1	436.9996	2.0575	0.0659
10	A2	452.6102	1.5255	0.0000
11	B2	468.6424	2.0833	0.0871
12	A1	551.8129	3.1702	1.6918
13	B1	611.6945	2.7346	9.2720
14	A1	710.9483	4.6585	10.6921
15	A2	711.6879	3.6348	0.0000
16	B2	731.7327	4.1671	0.0008
17	B1	763.4998	4.2028	3.3025
18	A1	942.1948	7.2104	140.8670
19	B2	987.5241	8.4453	176.5453
20	B2	1190.3664	11.2741	0.0178
21	A1	1282.0450	12.4782	66.7009
22	B2	1302.4221	12.3979	30.2335
23	A1	1469.7378	16.1560	6.3712
24	A1	1510.9797	16.5373	84.0880
25	B2	1535.5242	17.5190	759.7055
26	B2	1684.7453	20.7642	5.8812
27	A1	1691.8960	20.4529	132.7277

camb3lyp/pyFFCFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	121.3430	0.1610	0.0000
2	B1	126.1890	0.1960	0.0486
3	B2	204.1366	0.5905	0.0316

4	B1	211.4635	0.3908	3.3794
5	A1	283.8830	0.9207	0.8964
6	B2	311.8645	1.0540	0.3297
7	A1	334.6605	1.3691	0.8752
8	B1	341.7456	0.9578	1.0577
9	A1	437.6590	2.0632	0.0487
10	A2	452.6410	1.5258	0.0000
11	B2	468.6622	2.0814	0.0710
12	A1	553.6430	3.1870	1.9163
13	B1	616.0258	2.7762	8.8218
14	A1	712.6355	4.6795	8.5271
15	A2	727.4566	3.7981	0.0000
16	B2	734.2462	4.1968	0.0863
17	B1	794.4253	4.5467	2.7040
18	A1	942.1554	7.2051	131.9887
19	B2	992.6495	8.5285	159.8625
20	B2	1196.4391	11.3682	0.0016
21	A1	1286.1375	12.5624	63.5319
22	B2	1296.9867	12.3339	28.3227
23	A1	1472.3600	16.2096	7.4781
24	A1	1511.4364	16.5607	81.8920
25	B2	1536.6024	17.5507	720.9815
26	B2	1680.1605	20.6411	5.4330
27	A1	1688.5058	20.3763	126.2587

camb3lyp/pyFFCFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	120.9549	0.1599	0.0000
2	B1	126.0938	0.1957	0.0410
3	B2	205.8995	0.6010	0.0232
4	B1	211.6174	0.3915	2.9479
5	A1	284.8449	0.9270	0.8889
6	B2	312.6652	1.0594	0.2877
7	A1	335.5130	1.3737	0.8352
8	B1	341.7822	0.9578	0.9892
9	A1	438.4024	2.0700	0.0276
10	A2	453.8005	1.5337	0.0000
11	B2	469.5041	2.0896	0.0766
12	A1	554.4066	3.1988	1.9024
13	B1	617.5673	2.7900	8.2397
14	A1	713.5590	4.6905	7.9386
15	A2	724.7402	3.7705	0.0000
16	B2	735.5437	4.2117	0.0695
17	B1	788.6496	4.4816	2.0205
18	A1	945.4987	7.2590	132.1554
19	B2	994.5031	8.5568	158.2209
20	B2	1199.9801	11.4300	0.0886
21	A1	1289.8104	12.6321	63.6842
22	B2	1300.5979	12.4045	29.1385
23	A1	1476.2286	16.3073	5.9486
24	A1	1513.7287	16.6051	83.0699

25	B2	1540.8758	17.6435	716.5336
26	B2	1682.6111	20.7153	6.1375
27	A1	1691.5957	20.4531	127.5567

camb3lyp/pyFFCFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	119.5849	0.1563	0.0000
2	B1	124.7573	0.1914	0.0395
3	B2	205.8057	0.6002	0.0074
4	B1	210.0374	0.3855	3.6226
5	A1	284.2330	0.9239	0.8227
6	B2	311.5042	1.0519	0.3272
7	A1	333.5085	1.3600	0.9114
8	B1	338.3419	0.9393	0.9111
9	A1	435.5288	2.0458	0.0808
10	A2	451.9202	1.5207	0.0000
11	B2	467.6850	2.0723	0.0857
12	A1	551.6280	3.1588	1.9231
13	B1	607.4103	2.6978	11.0900
14	A1	709.8175	4.6392	8.9911
15	A2	721.4872	3.7370	0.0000
16	B2	729.8015	4.1454	0.0070
17	B1	782.7009	4.4153	1.7190
18	A1	937.4641	7.1303	135.4451
19	B2	989.9387	8.4794	165.4592
20	B2	1196.5567	11.3932	0.0160
21	A1	1282.0386	12.4848	63.0772
22	B2	1308.0456	12.5186	28.8080
23	A1	1475.7919	16.2865	5.9287
24	A1	1513.3716	16.6069	83.4482
25	B2	1542.0941	17.6841	744.8090
26	B2	1686.2014	20.7907	3.9480
27	A1	1695.1040	20.5355	129.5712

camb3lyp/pyFFFFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	122.1964	0.1633	0.0000
2	B1	160.3997	0.2790	0.0043
3	B1	217.9697	0.4199	5.7276
4	B2	273.0811	0.8274	0.0506
5	A1	274.8782	0.8272	0.7000
6	B2	321.1803	1.1018	0.8558
7	A1	349.4742	1.2620	1.6453
8	B1	356.1206	1.0273	3.7496
9	A2	440.7077	1.4469	0.0000
10	B2	467.3760	2.0768	0.1560
11	A1	487.1479	2.2234	0.1731
12	A1	605.6164	3.7714	0.0058

13	B1	645.5557	3.0544	3.3829
14	A2	704.7665	3.5650	0.0000
15	A1	712.2238	4.6333	7.4144
16	B2	751.0443	4.4129	0.0112
17	B1	756.9794	4.1356	6.8122
18	B2	1006.2382	8.6951	219.3922
19	A1	1109.1559	10.1220	246.1222
20	B2	1195.9561	11.4293	0.1103
21	B2	1317.1697	12.6742	19.0010
22	A1	1326.7327	13.4948	29.9965
23	A1	1477.0857	16.1197	18.7380
24	B2	1546.2739	17.8088	727.8884
25	A1	1580.6921	18.4299	165.9753
26	A1	1701.2208	20.6547	122.6673
27	B2	1714.4321	21.3840	5.5354

camb3lyp/pyFFFFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	123.4541	0.1666	0.0000
2	B1	161.9771	0.2848	0.0010
3	B1	217.6560	0.4181	4.6254
4	B2	273.9635	0.8326	0.0501
5	A1	275.2846	0.8295	0.7878
6	B2	321.9205	1.1066	0.7828
7	A1	349.7677	1.2637	1.4110
8	B1	359.0660	1.0453	3.3213
9	A2	442.0751	1.4561	0.0000
10	B2	467.5129	2.0765	0.1480
11	A1	488.5402	2.2343	0.2378
12	A1	608.5651	3.8071	0.0101
13	B1	656.2544	3.1630	3.8258
14	A1	713.4508	4.6502	5.8709
15	A2	726.2365	3.7853	0.0000
16	B2	754.3225	4.4531	0.0092
17	B1	798.8910	4.5948	5.3188
18	B2	1011.7587	8.7845	203.2455
19	A1	1115.0489	10.2266	230.6279
20	B2	1201.4926	11.5248	0.3295
21	B2	1311.9987	12.6033	16.9812
22	A1	1331.7811	13.6069	27.8965
23	A1	1479.8236	16.1676	21.7412
24	B2	1547.4458	17.8375	701.1542
25	A1	1581.0906	18.4607	157.8275
26	A1	1698.2578	20.5864	117.4017
27	B2	1710.0041	21.2663	4.5655

camb3lyp/pyFFFFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	122.8155	0.1648	0.0000
2	B1	160.9286	0.2809	0.0001
3	B1	217.4640	0.4173	4.0562
4	B2	274.4246	0.8354	0.0539
5	A1	275.7921	0.8324	0.7976
6	B2	322.3866	1.1096	0.7534
7	A1	350.2710	1.2675	1.3111
8	B1	358.5916	1.0426	3.0479
9	A2	442.4800	1.4588	0.0000
10	B2	468.1751	2.0826	0.1522
11	A1	488.7201	2.2359	0.2810
12	A1	608.9394	3.8107	0.0142
13	B1	653.7270	3.1364	3.2151
14	A1	714.3318	4.6607	5.5475
15	A2	722.5311	3.7477	0.0000
16	B2	754.8456	4.4588	0.0077
17	B1	786.5681	4.4595	4.7435
18	B2	1013.3235	8.8108	199.5487
19	A1	1116.9792	10.2605	230.7345
20	B2	1204.9984	11.5903	0.5349
21	B2	1315.6978	12.6742	17.5335
22	A1	1334.6816	13.6669	28.5133
23	A1	1484.2695	16.2697	21.8779
24	B2	1551.8789	17.9402	689.3824
25	A1	1583.8382	18.5267	154.9540
26	A1	1700.9818	20.6544	119.6194
27	B2	1713.3183	21.3556	5.1779

camb3lyp/pyFFFFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	121.4665	0.1612	0.0000
2	B1	159.9953	0.2776	0.0015
3	B1	217.0049	0.4160	5.2306
4	B2	273.9881	0.8328	0.0536
5	A1	275.3519	0.8299	0.7570
6	B2	320.8978	1.0997	0.9166
7	A1	348.5000	1.2547	1.5372
8	B1	355.6688	1.0257	3.5361
9	A2	441.5397	1.4523	0.0000
10	B2	466.5278	2.0672	0.1454
11	A1	487.0286	2.2197	0.2110
12	A1	606.6743	3.7818	0.0052
13	B1	649.9892	3.1014	3.6653
14	A1	710.8957	4.6139	6.0445
15	A2	719.8574	3.7202	0.0000
16	B2	748.9411	4.3877	0.0002
17	B1	785.8767	4.4477	5.1742
18	B2	1008.3777	8.7271	205.1548
19	A1	1111.6441	10.1640	235.6225
20	B2	1201.7972	11.5465	0.2148
21	B2	1322.3826	12.7849	16.9617

22	A1	1329.3870	13.5683	28.0709
23	A1	1482.5832	16.2352	20.3802
24	B2	1552.0802	17.9507	707.0532
25	A1	1586.7573	18.5925	159.8357
26	A1	1704.6431	20.7402	120.8062
27	B2	1715.9779	21.4169	3.9297

camb3lyp/pyFFHFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	118.9014	0.1547	0.0000
2	B1	206.8640	0.3408	4.5862
3	A1	283.5107	0.8611	0.6905
4	B1	302.7023	0.4488	1.0927
5	B2	304.8988	0.9745	0.2337
6	A1	364.1473	1.2517	3.0266
7	B2	461.0884	1.8054	0.0705
8	A2	466.1458	1.6178	0.0000
9	B1	495.5401	0.6224	0.6308
10	A1	517.8504	2.3457	1.7465
11	B2	669.0955	1.5751	2.8691
12	A1	702.0358	4.3387	18.3787
13	A2	716.2473	3.6799	0.0000
14	B1	751.8525	2.6093	13.2772
15	A1	769.0925	3.3542	10.8057
16	B1	917.8513	0.7060	30.6125
17	B2	926.7144	2.7466	136.1103
18	B2	1176.1033	3.8640	24.6192
19	B2	1208.3035	1.6313	41.5132
20	A1	1258.7273	10.4651	202.7295
21	B2	1308.2548	10.2561	79.8239
22	A1	1451.4712	14.5587	0.3935
23	A1	1494.9399	15.0424	46.3112
24	B2	1549.9372	11.1620	755.2638
25	A1	1701.3217	19.6043	30.3450
26	B2	1703.5911	15.4824	1.1862
27	A1	3236.8192	6.7579	5.9902

camb3lyp/pyFFHFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	120.2858	0.1583	0.0000
2	B1	207.4430	0.3447	3.6500
3	A1	284.0830	0.8645	0.7392
4	B1	305.4256	0.4553	1.0719
5	B2	305.9966	0.9817	0.1767
6	A1	364.9164	1.2563	2.5574
7	B2	461.2912	1.8069	0.0523
8	A2	466.9667	1.6235	0.0000
9	B1	500.9033	0.6224	0.5690

10	A1	519.9161	2.3611	1.9752
11	B2	672.7730	1.5860	2.8360
12	A1	704.8552	4.3983	15.8057
13	A2	734.4533	3.8693	0.0000
14	A1	771.4066	3.3681	11.3568
15	B1	775.3568	2.1601	15.0068
16	B2	931.0220	2.7434	121.9022
17	B1	936.3413	0.7806	24.0047
18	B2	1183.1104	3.8939	26.3124
19	B2	1212.5640	1.6867	34.2525
20	A1	1265.4378	10.5853	186.4567
21	B2	1303.2362	9.4283	80.0282
22	A1	1454.7540	14.5914	0.6873
23	A1	1496.0941	15.1576	48.0588
24	B2	1551.6672	11.2062	732.3017
25	A1	1698.8856	19.5600	29.7808
26	B2	1700.2744	15.0594	1.9980
27	A1	3235.0961	6.7470	5.0260

camb3lyp/pyFFHFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	119.8838	0.1572	0.0000
2	B1	207.3515	0.3439	3.2175
3	A1	284.7224	0.8681	0.7452
4	B1	304.8812	0.4537	1.0726
5	B2	306.4635	0.9844	0.1680
6	A1	365.2801	1.2594	2.4055
7	B2	462.0516	1.8124	0.0516
8	A2	467.6318	1.6282	0.0000
9	B1	499.5194	0.6247	0.4392
10	A1	520.2766	2.3635	2.0262
11	B2	673.3819	1.5890	2.8109
12	A1	705.8338	4.4060	15.2242
13	A2	732.0725	3.8449	0.0000
14	B1	771.6102	2.3024	12.5753
15	A1	772.1601	3.3747	11.4378
16	B1	928.7095	0.7524	26.0623
17	B2	932.5218	2.7364	118.5960
18	B2	1186.7480	3.6632	28.3954
19	B2	1215.1910	1.7413	29.8860
20	A1	1268.8986	10.6273	187.0904
21	B2	1306.9333	9.6126	81.8710
22	A1	1458.2465	14.6145	0.5894
23	A1	1500.0712	15.3124	47.7612
24	B2	1556.4442	11.2815	719.5219
25	A1	1701.2781	19.6221	30.7548
26	B2	1703.7604	15.1715	1.7484
27	A1	3239.8130	6.7670	4.7413

camb3lyp/pyFFHFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	118.4363	0.1534	0.0000
2	B1	205.8253	0.3391	4.1440
3	A1	283.8308	0.8629	0.7141
4	B1	303.0351	0.4504	1.1154
5	B2	305.3046	0.9775	0.2478
6	A1	363.1016	1.2439	2.7654
7	B2	460.2901	1.7980	0.0671
8	A2	465.7805	1.6150	0.0000
9	B1	495.1493	0.6145	0.5588
10	A1	518.1965	2.3454	1.7738
11	B2	668.4609	1.5857	2.6632
12	A1	701.8765	4.3534	15.7706
13	A2	727.8311	3.8008	0.0000
14	B1	766.2534	2.1945	14.3160
15	A1	769.1581	3.3489	11.4183
16	B1	926.7961	0.7541	27.2440
17	B2	928.1916	2.7213	126.5847
18	B2	1181.7560	3.4581	26.1776
19	B2	1212.0478	1.7221	33.4679
20	A1	1260.3788	10.4975	194.7313
21	B2	1314.3407	10.3656	72.5152
22	A1	1457.8268	14.6215	0.4871
23	A1	1497.8794	15.1597	45.7144
24	B2	1554.9426	11.4998	740.2523
25	B2	1704.1168	15.5077	1.9737
26	A1	1705.6711	19.7170	30.2249
27	A1	3243.3562	6.7853	6.9461

camb3lyp/pyFHFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	132.0970	0.1727	0.1526
2	A''	213.6061	0.3689	4.8905
3	A''	265.8706	0.2973	1.2438
4	A'	275.4851	0.8333	0.1982
5	A'	322.4942	1.0554	1.1416
6	A'	355.7767	1.2283	1.7202
7	A''	392.0591	0.9399	1.0276
8	A'	471.0803	1.8489	0.5024
9	A'	541.0348	1.9119	3.2172
10	A'	608.3567	3.7533	0.0717
11	A''	642.6623	1.2740	6.4499
12	A'	676.3563	1.6993	3.0140
13	A''	698.0982	1.9899	0.0061
14	A''	761.6136	2.1011	1.2492
15	A'	816.2925	3.8551	46.9243
16	A''	869.9555	0.7292	41.7365
17	A'	1046.8986	2.6328	90.6098
18	A'	1102.1977	8.3337	171.6384

19	A'	1180.6070	1.5757	99.8313
20	A'	1271.0854	7.2545	36.9788
21	A'	1328.4545	9.9687	15.9830
22	A'	1450.2567	12.6342	58.7638
23	A'	1497.1405	14.0989	163.4817
24	A'	1565.8213	10.5870	445.1368
25	A'	1692.2101	17.0846	285.5031
26	A'	1709.1348	19.6022	51.8382
27	A'	3253.0968	6.8308	7.5176

camb3lyp/pyFHFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	133.1127	0.1753	0.1229
2	A"	213.7326	0.3724	3.9242
3	A"	268.5378	0.3010	1.3124
4	A'	276.1232	0.8368	0.2291
5	A'	323.3232	1.0603	0.9793
6	A'	356.6500	1.2344	1.3544
7	A"	393.0459	0.9541	0.9433
8	A'	471.6379	1.8557	0.4821
9	A'	541.2603	1.9149	2.7768
10	A'	611.4573	3.7934	0.0289
11	A"	650.1051	1.2637	6.6759
12	A'	679.5673	1.7082	3.2409
13	A"	709.2038	1.8622	0.0121
14	A"	784.4408	1.9003	0.2185
15	A'	818.5338	3.8771	41.5081
16	A"	885.1913	0.8200	37.8019
17	A'	1049.7519	2.5877	80.7521
18	A'	1108.7037	8.3970	156.3692
19	A'	1187.3410	1.6180	100.0851
20	A'	1274.4951	7.8038	31.9644
21	A'	1325.0453	9.2654	18.9301
22	A'	1455.8034	12.8730	60.3111
23	A'	1497.6867	14.0317	151.0692
24	A'	1567.3383	10.5517	434.5958
25	A'	1689.3179	16.8407	274.1242
26	A'	1705.2614	19.3335	49.7083
27	A'	3251.9472	6.8224	6.2067

camb3lyp/pyFHFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	132.6178	0.1740	0.1094
2	A"	213.4822	0.3703	3.5135
3	A"	267.8017	0.3005	1.3057
4	A'	276.6057	0.8397	0.2330
5	A'	323.8841	1.0636	0.9631
6	A'	357.2562	1.2386	1.2903

7	A''	392.7858	0.9531	0.7874
8	A'	472.0805	1.8576	0.4689
9	A'	541.8994	1.9206	2.5800
10	A'	611.9845	3.7977	0.0244
11	A''	649.3838	1.2890	6.0050
12	A'	680.1224	1.7093	3.1388
13	A''	708.4460	1.8871	0.0001
14	A''	778.3171	2.0239	0.3805
15	A'	819.6237	3.8857	40.6854
16	A''	876.2509	0.7740	37.0985
17	A'	1051.4599	2.5537	79.1277
18	A'	1111.5695	8.4681	153.2332
19	A'	1190.2111	1.6269	97.4164
20	A'	1277.5147	7.9276	32.2466
21	A'	1329.0105	9.3864	19.3542
22	A'	1460.4090	13.1366	59.2160
23	A'	1501.8770	14.0578	141.2322
24	A'	1571.0549	10.6555	431.9729
25	A'	1692.2109	16.8729	278.2466
26	A'	1708.3811	19.4379	51.3434
27	A'	3256.5584	6.8417	5.9241

camb3lyp/pyFHFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	131.6555	0.1715	0.1388
2	A''	212.9200	0.3691	4.5183
3	A''	265.9897	0.2975	1.3534
4	A'	276.1017	0.8368	0.2203
5	A'	322.1616	1.0535	1.1508
6	A'	354.9650	1.2231	1.5722
7	A''	391.3230	0.9372	0.9054
8	A'	470.6735	1.8459	0.4805
9	A'	540.0880	1.9063	2.7184
10	A'	609.5662	3.7680	0.0610
11	A''	645.3403	1.2865	6.4935
12	A'	675.2250	1.7075	2.8963
13	A''	703.6261	1.8604	0.0066
14	A''	776.5477	1.9902	0.3234
15	A'	815.9697	3.8387	42.7461
16	A''	878.3360	0.7782	41.0763
17	A'	1047.4711	2.5892	86.8044
18	A'	1105.6983	8.3583	160.6456
19	A'	1184.7086	1.5772	93.1623
20	A'	1274.8105	7.3481	33.5019
21	A'	1332.8328	10.2559	15.1567
22	A'	1457.3743	12.8613	61.4338
23	A'	1500.7925	14.0898	147.9623
24	A'	1570.4378	10.8939	444.9437
25	A'	1694.6974	17.1938	281.4091
26	A'	1710.9188	19.6238	47.8370
27	A'	3259.9621	6.8599	8.5411

camb3lyp/pyHHHHH_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	390.4284	0.2302	0.0000
2	B1	424.4205	0.3949	4.1853
3	A1	622.5531	1.6262	3.6991
4	B2	676.9124	1.7137	0.3311
5	B1	725.1353	0.4231	70.2716
6	B1	771.6981	0.7921	11.8980
7	A2	909.2167	0.6079	0.0000
8	B1	975.2896	0.7519	0.0034
9	A2	1022.6064	0.9041	0.0000
10	A1	1029.3365	4.4612	6.1835
11	B1	1033.0039	0.8290	0.0320
12	A1	1063.3947	3.0461	4.7745
13	B2	1092.5718	1.2027	0.0115
14	A1	1107.1135	1.1836	6.2696
15	B2	1172.7039	0.9710	3.1582
16	A1	1254.4692	1.1696	5.0478
17	B2	1284.1460	5.1695	0.0727
18	B2	1393.7023	1.3708	0.0711
19	B2	1490.4741	2.7756	28.9547
20	A1	1531.3871	2.8680	2.9973
21	B2	1658.5481	9.9790	13.0178
22	A1	1663.8100	8.9080	26.8440
23	B2	3173.3955	6.4588	23.8062
24	A1	3175.6177	6.4827	2.4829
25	A1	3194.8368	6.5551	4.4586
26	B2	3211.6472	6.6512	17.8020
27	A1	3219.0470	6.7143	4.2192

camb3lyp/pyHHHHH_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	393.1424	0.2310	0.0000
2	B1	427.6453	0.3977	3.9948
3	A1	623.0751	1.6279	4.4818
4	B2	677.2890	1.7131	0.1909
5	B1	730.7103	0.4184	65.0925
6	B1	780.6536	0.8121	8.6305
7	A2	915.8736	0.6169	0.0000
8	B1	984.6724	0.7694	0.0026
9	A1	1030.7859	4.4172	6.5673
10	A2	1036.3252	0.9339	0.0000
11	B1	1046.8996	0.8723	0.0421
12	A1	1067.8548	2.9653	5.6316
13	B2	1094.5325	1.2101	0.0211
14	A1	1109.4789	1.2153	3.9880
15	B2	1172.0215	0.9869	3.5377

16	A1	1254.5597	1.1762	4.1825
17	B2	1282.0732	4.8223	0.1270
18	B2	1399.2461	1.3837	0.1845
19	B2	1495.1745	2.7962	27.8779
20	A1	1537.1165	2.8646	2.6572
21	B2	1659.1863	9.7520	12.5909
22	A1	1663.8948	8.7568	26.3741
23	B2	3171.7888	6.4515	23.0154
24	A1	3174.1923	6.4785	2.6874
25	A1	3195.5450	6.5553	4.0011
26	B2	3212.1374	6.6504	16.9808
27	A1	3219.5837	6.7128	4.2053

camb3lyp/pyHHHHH_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	393.8849	0.2315	0.0000
2	B1	428.2345	0.3997	3.8769
3	A1	623.6740	1.6328	4.7175
4	B2	678.6582	1.7218	0.2547
5	B1	730.7437	0.4134	67.2828
6	B1	782.0729	0.8289	7.9808
7	A2	916.2897	0.6174	0.0000
8	B1	984.3114	0.7712	0.0015
9	A1	1032.2508	4.4422	7.2419
10	A2	1035.9337	0.9343	0.0000
11	B1	1048.6527	0.8740	0.0249
12	A1	1068.7542	2.9726	5.9735
13	B2	1095.8509	1.2131	0.0139
14	A1	1110.8056	1.2152	3.9804
15	B2	1174.8259	0.9894	3.3057
16	A1	1256.5885	1.1793	3.9091
17	B2	1285.3181	4.8864	0.0650
18	B2	1400.7306	1.3862	0.1506
19	B2	1497.9400	2.8053	29.0031
20	A1	1539.3517	2.8785	3.3224
21	B2	1662.0767	9.8213	12.1636
22	A1	1666.4134	8.7904	26.8747
23	B2	3174.9979	6.4643	24.4795
24	A1	3177.5276	6.4926	3.7358
25	A1	3199.5072	6.5715	4.4291
26	B2	3216.1959	6.6671	17.5913
27	A1	3223.5653	6.7300	4.2110

camb3lyp/pyHHHHH_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	391.8016	0.2302	0.0000
2	B1	425.0418	0.3952	4.1788
3	A1	622.2358	1.6239	3.9383

4	B2	675.8180	1.7065	0.3947
5	B1	725.3394	0.4103	73.9681
6	B1	776.4201	0.8153	9.5592
7	A2	910.3080	0.6092	0.0000
8	B1	976.8934	0.7569	0.0027
9	A1	1027.5710	4.4122	6.9762
10	A2	1028.4532	0.9183	0.0000
11	B1	1041.2405	0.8580	0.0881
12	A1	1065.2595	3.0293	4.8582
13	B2	1093.4635	1.1964	0.0467
14	A1	1107.1572	1.1843	6.2366
15	B2	1173.2679	0.9538	3.0830
16	A1	1253.5029	1.1635	4.3655
17	B2	1286.6762	5.6145	0.1524
18	B2	1391.3331	1.3663	0.0901
19	B2	1489.3515	2.7937	30.1795
20	A1	1529.5142	2.8742	3.7743
21	B2	1658.7546	10.1001	11.8329
22	A1	1665.1209	9.0870	26.3518
23	B2	3180.7611	6.4892	19.0138
24	A1	3182.7924	6.5129	2.5822
25	A1	3202.8805	6.5876	3.8555
26	B2	3218.9876	6.6816	13.4821
27	A1	3226.2182	6.7451	2.8231

m062x/pyCCCCC_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	60.3240	0.0731	0.0000
2	B1	82.9780	0.1372	0.0226
3	B1	149.5768	0.2104	0.0049
4	A1	209.5639	0.8515	0.0717
5	B2	221.3260	0.8867	0.2878
6	A1	222.7124	0.8406	0.0481
7	B2	230.9904	1.0954	0.0000
8	B1	285.3041	0.6477	0.8989
9	B2	337.8361	1.9258	0.2384
10	A1	354.9884	2.1004	0.1309
11	A2	370.0003	1.0098	0.0000
12	A1	393.7876	2.9814	0.0960
13	A1	557.0952	3.1724	6.0264
14	B1	581.6288	2.4702	1.4140
15	B2	591.1547	2.7574	0.5142
16	A2	633.6137	2.8632	0.0000
17	B2	701.1443	4.5184	84.2044
18	B1	743.2316	3.9852	0.1907
19	A1	844.4587	5.7786	90.2290
20	B2	919.9038	6.5012	3.8271
21	A1	1113.4040	9.2007	33.0054
22	B2	1245.4121	11.1879	26.7777
23	A1	1259.3223	11.5400	4.6745
24	B2	1386.8964	14.0829	422.0387

25	A1	1392.0063	13.8823	127.3828
26	A1	1582.4743	17.8259	105.2414
27	B2	1610.9057	19.0949	63.8867

m062x/pyCCCCC_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	61.9411	0.0771	0.0000
2	B1	84.3393	0.1413	0.0162
3	B1	150.9066	0.2143	0.0052
4	A1	207.2120	0.8394	0.0322
5	B2	219.0438	0.8690	0.2484
6	A1	220.4440	0.8178	0.0155
7	B2	227.0904	1.0583	0.0001
8	B1	290.5765	0.6725	0.7981
9	B2	337.6097	1.9199	0.2443
10	A1	355.2809	2.1010	0.1161
11	A2	375.6246	1.0408	0.0000
12	A1	394.0990	2.9851	0.1109
13	A1	557.0055	3.1729	5.0232
14	B2	587.3179	2.7213	0.1891
15	B1	596.2091	2.5987	1.3347
16	A2	657.2079	3.0806	0.0000
17	B2	701.6670	4.5255	77.6888
18	B1	781.1599	4.3968	1.5044
19	A1	844.5302	5.7843	84.9898
20	B2	918.5946	6.4879	3.6799
21	A1	1110.4864	9.1567	30.3611
22	B2	1239.6675	11.1018	25.7399
23	A1	1258.9703	11.5271	5.5164
24	B2	1384.0780	14.0192	392.6531
25	A1	1387.4269	13.7907	110.3013
26	A1	1576.9676	17.6961	98.0263
27	B2	1602.8415	18.8842	58.7666

m062x/pyCCCCC_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	62.1443	0.0776	0.0000
2	B1	84.7572	0.1426	0.0179
3	B1	151.3406	0.2156	0.0001
4	A1	207.8703	0.8461	0.0388
5	B2	219.9230	0.8760	0.2274
6	A1	221.4268	0.8242	0.0135
7	B2	227.7635	1.0646	0.0002
8	B1	291.4075	0.6765	0.7301
9	B2	338.5635	1.9298	0.2607
10	A1	356.3479	2.1113	0.1271
11	A2	377.7138	1.0525	0.0000
12	A1	395.5152	3.0045	0.1107

13	A1	559.1303	3.1956	5.0300
14	B2	590.4699	2.7528	0.3522
15	B1	598.4330	2.6188	1.3217
16	A2	659.9897	3.1071	0.0000
17	B2	705.2777	4.5680	77.9125
18	B1	782.1613	4.4070	1.4756
19	A1	847.6877	5.8313	87.5394
20	B2	922.9861	6.5518	3.2316
21	A1	1114.6142	9.2280	30.6428
22	B2	1239.8866	11.1026	27.1549
23	A1	1260.6925	11.5597	4.8995
24	B2	1385.5847	14.0471	394.9946
25	A1	1389.3847	13.8294	113.6189
26	A1	1577.1974	17.7011	102.2482
27	B2	1605.1132	18.9489	57.8007

m062x/pyCCCCC_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	60.9620	0.0747	0.0000
2	B1	82.8678	0.1363	0.0194
3	B1	149.0696	0.2092	0.0011
4	A1	207.3340	0.8340	0.0373
5	B2	219.2438	0.8702	0.1566
6	A1	220.6650	0.8250	0.0097
7	B2	228.6459	1.0734	0.0004
8	B1	286.4815	0.6532	0.5010
9	B2	335.4909	1.9059	0.2921
10	A1	352.6964	2.0816	0.1105
11	A2	371.3459	1.0170	0.0000
12	A1	390.4719	2.9394	0.0939
13	A1	551.9079	3.1148	6.5057
14	B1	584.3549	2.4944	1.1176
15	B2	586.0781	2.7134	0.9349
16	A2	640.8156	2.9287	0.0000
17	B2	694.3990	4.4271	84.7558
18	B1	757.7577	4.1415	1.8667
19	A1	838.0655	5.6844	92.1055
20	B2	913.3776	6.3992	3.3412
21	A1	1104.9413	9.0569	33.9414
22	B2	1247.7989	11.2287	24.9125
23	A1	1255.8521	11.4636	4.0086
24	B2	1383.5255	14.0112	410.9985
25	A1	1388.7437	13.8130	121.7976
26	A1	1582.7337	17.8290	106.1148
27	B2	1609.3602	19.0567	59.9993

m062x/pyFCFCF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	95.2788	0.1141	0.0000
2	B1	112.0139	0.1610	0.0047
3	A1	184.5763	0.5309	0.0243
4	B1	217.6648	0.4209	3.1597
5	B2	226.7344	0.6797	0.0364
6	B2	317.9994	1.2774	1.3837
7	B1	319.7707	0.8370	0.4190
8	A1	329.8638	1.3938	0.5262
9	A2	383.7764	1.0878	0.0000
10	A1	415.4553	2.0610	0.6235
11	B2	417.2120	1.8892	0.1210
12	A1	592.4679	3.3342	2.0262
13	A1	626.7911	3.8118	2.0227
14	B1	663.1970	3.2142	1.2759
15	A2	708.7786	3.6063	0.0000
16	B2	712.0053	3.9606	0.2005
17	B1	775.7012	4.3421	17.3685
18	B2	816.7980	5.6770	110.7580
19	A1	1103.2165	9.9206	175.7662
20	B2	1138.7187	10.4660	16.6292
21	A1	1182.0304	10.4939	4.0178
22	B2	1304.8504	12.4629	11.8829
23	A1	1481.6201	16.3624	55.5788
24	B2	1499.2188	16.5445	439.3408
25	A1	1519.5993	16.9555	91.7059
26	A1	1667.9486	19.8632	230.9144
27	B2	1686.1435	20.8023	95.1167

m062x/pyFCFCF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	96.8154	0.1179	0.0000
2	B1	113.5538	0.1654	0.0004
3	A1	183.2158	0.5232	0.0093
4	B1	216.1838	0.4151	2.9249
5	B2	225.7491	0.6734	0.0281
6	B2	318.4698	1.2830	1.4061
7	B1	323.1264	0.8551	0.6075
8	A1	329.9631	1.3935	0.4825
9	A2	378.9555	1.0604	0.0000
10	A1	415.8587	2.0655	0.5740
11	B2	417.0924	1.8834	0.1691
12	A1	592.5489	3.3221	1.7042
13	A1	627.0465	3.8311	1.3964
14	B1	667.1827	3.2543	1.3139
15	B2	712.2520	3.9645	0.0157
16	A2	720.8798	3.7317	0.0000
17	B1	796.2696	4.5727	13.7040
18	B2	816.9250	5.6792	103.6212
19	A1	1104.6248	9.9333	160.1291
20	B2	1139.2006	10.4796	14.3414
21	A1	1180.8398	10.4860	2.9872

22	B2	1298.4253	12.3531	10.6864
23	A1	1480.9385	16.3247	59.0603
24	B2	1498.9549	16.5444	420.1398
25	A1	1516.2732	16.9060	75.1605
26	A1	1663.4560	19.7550	219.7887
27	B2	1679.8796	20.6315	93.2961

m062x/pyFCFCF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	96.4868	0.1171	0.0000
2	B1	113.3818	0.1650	0.0018
3	A1	183.7394	0.5261	0.0037
4	B1	216.4645	0.4164	2.5493
5	B2	225.9142	0.6747	0.0238
6	B2	318.5034	1.2821	1.2905
7	B1	323.5100	0.8565	0.5220
8	A1	330.3331	1.3944	0.4003
9	A2	381.5242	1.0750	0.0000
10	A1	416.7125	2.0751	0.5431
11	B2	417.7113	1.8901	0.1670
12	A1	593.4120	3.3388	1.5628
13	A1	627.8262	3.8332	1.3764
14	B1	666.3727	3.2468	0.9972
15	B2	713.9161	3.9829	0.0369
16	A2	720.8616	3.7316	0.0000
17	B1	793.8163	4.5444	13.5302
18	B2	820.1356	5.7260	102.3176
19	A1	1106.5656	9.9658	162.7955
20	B2	1142.8079	10.5299	13.1858
21	A1	1184.4823	10.5486	2.9187
22	B2	1299.4127	12.3792	11.7033
23	A1	1486.1261	16.4514	58.9539
24	B2	1502.0613	16.6129	416.8282
25	A1	1518.6101	16.9585	81.0850
26	A1	1664.1113	19.7734	229.4581
27	B2	1682.8134	20.7170	97.0433

m062x/pyFCFCF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	95.3947	0.1144	0.0000
2	B1	111.8741	0.1604	0.0034
3	A1	183.2232	0.5232	0.0002
4	B1	215.0301	0.4103	2.7835
5	B2	225.4494	0.6720	0.0133
6	B2	316.0754	1.2632	1.3007
7	B1	319.4788	0.8368	0.2534
8	A1	328.1503	1.3812	0.4026
9	A2	375.4704	1.0405	0.0000

10	A1	413.4468	2.0454	0.6356
11	B2	415.3436	1.8730	0.0703
12	A1	590.3252	3.2855	1.9117
13	A1	625.1356	3.8093	1.4559
14	B1	660.6060	3.1892	0.6691
15	B2	708.2021	3.9184	0.1419
16	A2	712.3642	3.6455	0.0000
17	B1	780.4283	4.3951	20.2577
18	B2	810.0181	5.5720	104.8126
19	A1	1102.6089	9.8837	171.9787
20	B2	1138.9622	10.4728	14.4631
21	A1	1176.1650	10.4025	2.0932
22	B2	1307.8829	12.5248	9.9471
23	A1	1487.1985	16.4776	59.1337
24	B2	1501.6689	16.5993	433.1271
25	A1	1521.9725	17.0411	84.6174
26	A1	1669.5461	19.9006	234.8998
27	B2	1684.5792	20.7692	91.0319

m062x/pyFCFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	100.3218	0.1258	0.0003
2	A"	144.3407	0.2285	0.0034
3	A'	204.5912	0.5800	0.0245
4	A"	217.2192	0.4181	4.1760
5	A'	275.4236	0.8410	0.2698
6	A'	317.5300	1.1952	1.1158
7	A"	331.1398	0.8880	0.8589
8	A'	341.0349	1.2972	1.0215
9	A'	414.0628	1.9358	0.2454
10	A"	417.0407	1.3001	1.6178
11	A'	476.9529	2.1502	0.3630
12	A'	604.8110	3.6819	0.8815
13	A'	647.5212	3.8689	6.7627
14	A"	650.6260	3.0950	1.6998
15	A"	701.2112	3.5310	0.2362
16	A'	733.1605	4.1987	0.7994
17	A"	758.4884	4.1555	12.3641
18	A'	929.1294	7.3051	144.6961
19	A'	1110.3673	10.0733	186.9989
20	A'	1151.1590	10.6163	28.4070
21	A'	1293.8211	12.6090	18.4445
22	A'	1316.6350	12.9668	17.5954
23	A'	1485.3187	16.4155	55.4190
24	A'	1519.9070	16.9487	283.7925
25	A'	1572.0915	18.4016	451.4410
26	A'	1689.9863	20.4300	194.9265
27	A'	1710.3957	21.2974	13.3124

m062x/pyFCFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	102.1719	0.1304	0.0001
2	A''	145.6507	0.2329	0.0029
3	A'	203.3016	0.5725	0.0192
4	A''	216.3876	0.4146	3.7114
5	A'	276.1318	0.8452	0.3120
6	A'	318.1392	1.2023	1.0764
7	A''	334.9207	0.9091	1.0265
8	A'	341.1686	1.2966	0.9093
9	A'	414.1995	1.9331	0.2201
10	A''	419.4527	1.3154	1.3349
11	A'	477.1946	2.1522	0.4272
12	A'	605.9959	3.6912	0.8398
13	A'	646.7478	3.8679	5.4571
14	A''	660.3923	3.1934	2.1827
15	A''	721.7595	3.7418	0.5839
16	A'	734.7910	4.2186	0.7346
17	A''	793.6795	4.5402	9.0366
18	A'	930.0550	7.3139	134.5556
19	A'	1111.9477	10.0968	170.5703
20	A'	1151.5116	10.6312	28.7609
21	A'	1290.7819	12.4497	17.3188
22	A'	1313.2569	13.0270	16.0879
23	A'	1484.5540	16.3844	53.5805
24	A'	1518.5655	16.9187	268.9110
25	A'	1569.3539	18.3473	431.8294
26	A'	1686.1188	20.3402	190.5883
27	A'	1705.1853	21.1523	11.1019

m062x/pyFCFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	101.9049	0.1296	0.0000
2	A''	144.9268	0.2307	0.0008
3	A'	203.7563	0.5754	0.0206
4	A''	216.7003	0.4158	3.2413
5	A'	275.8712	0.8435	0.3053
6	A'	318.1672	1.2008	0.9968
7	A''	335.1220	0.9102	0.9359
8	A'	341.5314	1.2991	0.7878
9	A'	414.8996	1.9408	0.2118
10	A''	420.2458	1.3198	1.2628
11	A'	477.7237	2.1574	0.4353
12	A'	606.4458	3.6987	0.7518
13	A'	647.9206	3.8804	5.2319
14	A''	658.4233	3.1738	1.7768
15	A''	719.7122	3.7206	0.4226
16	A'	735.8197	4.2299	0.7090
17	A''	786.5451	4.4616	8.7145
18	A'	932.3169	7.3504	133.5195

19	A'	1113.9604	10.1302	173.6427
20	A'	1155.1794	10.6851	26.3378
21	A'	1292.9326	12.4426	17.7557
22	A'	1315.7235	13.1329	16.7786
23	A'	1489.3590	16.4996	55.3317
24	A'	1521.0973	16.9701	257.3420
25	A'	1572.5620	18.4313	445.9767
26	A'	1687.3283	20.3684	195.3248
27	A'	1707.5625	21.2269	12.3679

m062x/pyFCFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	100.8411	0.1269	0.0001
2	A"	143.8455	0.2271	0.0016
3	A'	203.2723	0.5725	0.0280
4	A"	216.0475	0.4131	3.7785
5	A'	274.9517	0.8383	0.2812
6	A'	316.1964	1.1881	1.1163
7	A"	331.0940	0.8888	0.6764
8	A'	339.6236	1.2851	0.8921
9	A'	412.2271	1.9200	0.2342
10	A"	417.7314	1.3044	1.8467
11	A'	475.8222	2.1387	0.4067
12	A'	604.2939	3.6634	0.9998
13	A'	643.9235	3.8289	5.8751
14	A"	653.5039	3.1258	1.6060
15	A"	713.7758	3.6611	1.1123
16	A'	730.2289	4.1649	0.7707
17	A"	778.2082	4.3668	11.3518
18	A'	925.4611	7.2310	135.3450
19	A'	1110.1687	10.0624	178.8077
20	A'	1150.4765	10.6047	27.6135
21	A'	1293.9383	12.6365	16.3110
22	A'	1319.7156	13.0277	17.0054
23	A'	1490.1293	16.5211	56.3215
24	A'	1521.3897	16.9877	273.3225
25	A'	1575.7811	18.5054	448.9312
26	A'	1690.8103	20.4640	194.7780
27	A'	1710.0073	21.2789	10.6018

m062x/pyFFCFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	121.4639	0.1612	0.0000
2	B1	124.8480	0.1913	0.0357
3	B2	203.1260	0.5846	0.0345
4	B1	211.9363	0.3927	3.8921
5	A1	281.6008	0.9062	0.8593
6	B2	310.5453	1.0450	0.3929

7	A1	336.1082	1.3802	1.3252
8	B1	339.5221	0.9474	0.9970
9	A1	436.0062	2.0297	0.0775
10	A2	453.1029	1.5290	0.0000
11	B2	467.0217	2.0616	0.0544
12	A1	553.3201	3.1810	1.8650
13	B1	604.4595	2.6664	9.2177
14	A2	702.9470	3.5476	0.0000
15	A1	712.8245	4.6654	10.5225
16	B2	729.9868	4.1461	0.0158
17	B1	747.1607	4.0311	3.5635
18	A1	947.2624	7.2960	137.6181
19	B2	1000.3354	8.6431	158.2936
20	B2	1214.5812	11.6970	0.1200
21	A1	1292.3289	12.7062	60.4319
22	B2	1301.9630	12.4738	31.4148
23	A1	1489.9556	16.6461	7.8466
24	A1	1526.5448	16.9383	92.1532
25	B2	1555.1914	18.0330	767.7516
26	B2	1695.3318	21.0016	3.5863
27	A1	1699.0489	20.6488	129.3664

m062x/pyFFCFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	122.2000	0.1632	0.0000
2	B1	126.9349	0.1981	0.0488
3	B2	202.3813	0.5802	0.0264
4	B1	211.7927	0.3918	3.3439
5	A1	282.1091	0.9089	0.9643
6	B2	311.2758	1.0498	0.4000
7	A1	336.0923	1.3810	1.1424
8	B1	341.9481	0.9608	1.0001
9	A1	436.4125	2.0327	0.0505
10	A2	454.1744	1.5363	0.0000
11	B2	466.5519	2.0564	0.0483
12	A1	554.2651	3.1926	1.9900
13	B1	612.2169	2.7404	9.1191
14	A1	712.4154	4.6602	8.1933
15	A2	724.0934	3.7646	0.0000
16	B2	731.9994	4.1701	0.1349
17	B1	787.8332	4.4745	2.7405
18	A1	947.2705	7.2964	129.5253
19	B2	1002.1550	8.6745	145.8192
20	B2	1215.2046	11.6773	0.2292
21	A1	1291.7787	12.7007	58.7849
22	B2	1295.3898	12.3934	28.5304
23	A1	1488.3839	16.5955	9.3149
24	A1	1524.7563	16.9079	87.3889
25	B2	1553.7202	17.9966	728.1483
26	B2	1689.5462	20.8475	3.3574
27	A1	1695.5276	20.5631	124.4000

m062x/pyFFCFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	121.9033	0.1623	0.0000
2	B1	126.7010	0.1974	0.0452
3	B2	202.8374	0.5831	0.0179
4	B1	211.9544	0.3926	2.8962
5	A1	282.0189	0.9083	0.9351
6	B2	311.1818	1.0490	0.3279
7	A1	336.4972	1.3824	1.0380
8	B1	341.6907	0.9589	0.9157
9	A1	437.0148	2.0392	0.0329
10	A2	455.3958	1.5446	0.0000
11	B2	467.2317	2.0632	0.0561
12	A1	554.9533	3.2015	1.9253
13	B1	612.2274	2.7404	8.9540
14	A1	713.1313	4.6682	7.8395
15	A2	721.5757	3.7389	0.0000
16	B2	733.1541	4.1831	0.0999
17	B1	781.3016	4.4012	1.9342
18	A1	950.0334	7.3403	129.6681
19	B2	1004.1348	8.7033	144.7443
20	B2	1218.8381	11.7185	0.7200
21	A1	1295.6955	12.7732	58.8639
22	B2	1296.3716	12.4366	30.6180
23	A1	1492.2535	16.6941	7.6039
24	A1	1526.8427	16.9520	90.4064
25	B2	1557.7459	18.0895	736.0962
26	B2	1691.3931	20.9068	3.6724
27	A1	1697.2322	20.6084	125.2294

m062x/pyFFCFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	120.5864	0.1588	0.0000
2	B1	125.5959	0.1938	0.0440
3	B2	202.5570	0.5814	0.0044
4	B1	211.0183	0.3889	3.4187
5	A1	280.7405	0.9013	0.8738
6	B2	309.7963	1.0398	0.4141
7	A1	334.5702	1.3694	1.1308
8	B1	338.7794	0.9433	0.8196
9	A1	434.1636	2.0158	0.0953
10	A2	453.5244	1.5317	0.0000
11	B2	465.2635	2.0443	0.0553
12	A1	552.5878	3.1640	1.9913
13	B1	601.9640	2.6481	11.3473
14	A1	710.2020	4.6265	8.9960
15	A2	717.1525	3.6938	0.0000

16	B2	727.6818	4.1204	0.0221
17	B1	773.0464	4.3102	1.7655
18	A1	941.7067	7.2034	131.4774
19	B2	1000.7470	8.6422	147.9574
20	B2	1217.9130	11.7512	0.4189
21	A1	1290.2013	12.6694	57.1326
22	B2	1305.4010	12.5603	31.4666
23	A1	1493.8694	16.7276	7.0109
24	A1	1526.8316	16.9597	92.6374
25	B2	1559.5299	18.1489	760.0736
26	B2	1695.4734	20.9999	2.1233
27	A1	1700.4130	20.6891	126.4296

m062x/pyFFFFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	123.4967	0.1666	0.0000
2	B1	161.2276	0.2815	0.0012
3	B1	218.7651	0.4226	5.6058
4	B2	270.0719	0.8089	0.0584
5	A1	272.8665	0.8139	0.7155
6	B2	321.4182	1.1031	1.0428
7	A1	351.5026	1.2757	1.9658
8	B1	355.4644	1.0253	3.6716
9	A2	441.1012	1.4496	0.0000
10	B2	466.0290	2.0585	0.1026
11	A1	484.8339	2.1958	0.1359
12	A1	608.2162	3.7851	0.0146
13	B1	639.1213	2.9880	2.6956
14	A2	694.9071	3.4678	0.0000
15	A1	714.8372	4.6543	6.8985
16	B1	738.0240	3.9406	7.3075
17	B2	749.8601	4.3945	0.0154
18	B2	1019.3101	8.9078	201.6671
19	A1	1122.8622	10.3625	238.5200
20	B2	1220.7837	11.8936	0.3848
21	B2	1316.3830	12.7167	17.8879
22	A1	1347.2527	13.9722	25.0791
23	A1	1496.3704	16.5895	23.3220
24	B2	1565.1834	18.2972	735.3897
25	A1	1602.5315	19.0055	169.1076
26	A1	1711.1557	20.9106	120.8303
27	B2	1725.4611	21.6467	3.6701

m062x/pyFFFFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	124.5933	0.1696	0.0000
2	B1	162.9919	0.2881	0.0000
3	B1	218.6118	0.4216	4.7525

4	B2	271.4439	0.8170	0.0594
5	A1	273.5802	0.8181	0.8047
6	B2	322.2097	1.1083	0.9690
7	A1	351.4763	1.2754	1.7230
8	B1	359.2476	1.0478	3.4070
9	A2	443.8926	1.4681	0.0000
10	B2	465.7907	2.0558	0.1071
11	A1	485.5636	2.2011	0.1976
12	A1	609.8075	3.8065	0.0214
13	B1	655.0280	3.1500	3.6969
14	A1	714.1445	4.6476	5.3987
15	A2	723.3710	3.7570	0.0000
16	B2	752.8649	4.4318	0.0769
17	B1	792.1383	4.5199	5.3063
18	B2	1021.8782	8.9496	189.1581
19	A1	1125.0356	10.4031	225.0307
20	B2	1221.3829	11.8857	0.6698
21	B2	1310.1717	12.6294	15.7959
22	A1	1346.9273	13.9703	23.5567
23	A1	1494.9168	16.5427	24.8510
24	B2	1564.2188	18.2699	708.0200
25	A1	1600.2539	18.9598	159.8708
26	A1	1708.0340	20.8335	116.0159
27	B2	1720.6458	21.5156	2.8796

m062x/pyFFFFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	123.9007	0.1677	0.0000
2	B1	161.9187	0.2841	0.0002
3	B1	218.5327	0.4214	4.1481
4	B2	271.1063	0.8150	0.0637
5	A1	273.4552	0.8173	0.7955
6	B2	322.0779	1.1073	0.8947
7	A1	351.6883	1.2769	1.5539
8	B1	358.5341	1.0434	3.1358
9	A2	444.5374	1.4725	0.0000
10	B2	466.2930	2.0606	0.1146
11	A1	485.8213	2.2035	0.2189
12	A1	610.1166	3.8089	0.0223
13	B1	651.9250	3.1183	3.1580
14	A1	714.7891	4.6547	5.1681
15	A2	719.5290	3.7179	0.0000
16	B2	753.1427	4.4342	0.0670
17	B1	780.6648	4.3941	4.7881
18	B2	1023.4227	8.9740	186.8135
19	A1	1126.8408	10.4334	225.8874
20	B2	1224.9072	11.9376	1.0432
21	B2	1310.9233	12.6573	16.9433
22	A1	1350.5063	14.0448	23.9079
23	A1	1499.0334	16.6368	25.4869
24	B2	1568.0073	18.3618	707.4917

25	A1	1602.7137	19.0252	160.9315
26	A1	1709.2007	20.8654	118.8690
27	B2	1722.6460	21.5748	3.1110

m062x/pyFFFFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	122.5994	0.1641	0.0000
2	B1	160.8674	0.2804	0.0000
3	B1	218.5788	0.4218	5.1184
4	B2	270.2518	0.8099	0.0600
5	A1	272.6293	0.8124	0.7633
6	B2	320.5621	1.0971	1.1260
7	A1	350.1482	1.2657	1.8402
8	B1	355.8599	1.0282	3.4651
9	A2	443.7024	1.4667	0.0000
10	B2	464.5044	2.0436	0.0935
11	A1	484.1779	2.1878	0.1535
12	A1	608.2666	3.7838	0.0101
13	B1	647.7617	3.0792	3.4724
14	A1	712.1277	4.6168	5.6978
15	A2	715.8617	3.6807	0.0000
16	B2	747.4432	4.3662	0.0316
17	B1	776.4596	4.3440	5.1954
18	B2	1019.5153	8.9049	188.3301
19	A1	1123.0741	10.3629	227.2486
20	B2	1223.5716	11.9409	0.5788
21	B2	1319.0341	12.7842	17.1586
22	A1	1347.3001	13.9907	23.7234
23	A1	1499.7349	16.6599	24.2822
24	B2	1568.5803	18.3856	721.2919
25	A1	1605.9083	19.1011	166.9066
26	A1	1712.2624	20.9424	118.4823
27	B2	1724.8571	21.6328	2.4461

m062x/pyFFHFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	119.8640	0.1571	0.0000
2	B1	207.2785	0.3415	4.3025
3	A1	282.3774	0.8514	0.6827
4	B1	304.0668	0.4562	1.0004
5	B2	304.2091	0.9661	0.3129
6	A1	366.1488	1.2662	3.4366
7	B2	459.2936	1.7723	0.1003
8	A2	466.8152	1.6225	0.0000
9	B1	489.7406	0.6193	0.7564
10	A1	515.8437	2.2965	1.8178
11	B2	667.5911	1.5594	2.7997
12	A1	703.8218	4.3046	17.1784

13	A2	707.3656	3.5908	0.0000
14	B1	741.7533	2.8874	11.1183
15	A1	769.5171	3.3800	9.4805
16	B1	906.9932	0.6702	33.7353
17	B2	935.6804	2.5384	118.6272
18	B2	1190.5362	1.7025	52.1429
19	B2	1215.0966	3.6632	6.0298
20	A1	1267.8054	10.5730	190.7111
21	B2	1306.6064	10.0439	76.5728
22	A1	1473.6999	15.1032	0.1078
23	A1	1510.2921	15.4785	53.9417
24	B2	1565.7049	12.3985	771.1468
25	A1	1708.4208	19.8603	30.0505
26	B2	1711.9475	15.9541	1.7446
27	A1	3245.0785	6.7923	7.7810

m062x/pyFFHFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	121.0409	0.1602	0.0000
2	B1	207.9874	0.3460	3.6053
3	A1	282.9563	0.8548	0.7505
4	B2	305.2062	0.9723	0.2426
5	B1	306.9578	0.4623	1.0069
6	A1	366.4619	1.2680	2.9826
7	B2	459.0094	1.7715	0.0709
8	A2	468.7068	1.6357	0.0000
9	B1	497.2059	0.6200	0.7123
10	A1	517.0066	2.3059	2.0579
11	B2	670.9802	1.5649	2.7665
12	A1	704.5223	4.3413	14.7010
13	A2	732.1041	3.8461	0.0000
14	A1	770.5060	3.3813	10.2279
15	B1	772.7069	2.2715	13.9629
16	B1	928.8734	0.7545	25.3003
17	B2	937.4424	2.5439	108.3671
18	B2	1192.5385	1.7156	50.7329
19	B2	1215.5307	3.7775	3.7006
20	A1	1269.6218	10.6334	177.1891
21	B2	1300.3315	9.3413	74.0275
22	A1	1473.0504	15.0742	0.4150
23	A1	1508.5780	15.4693	53.4704
24	B2	1564.9508	12.4070	748.4069
25	A1	1706.0133	19.8031	29.7853
26	B2	1707.0984	15.6544	2.4220
27	A1	3242.8731	6.7795	6.0877

m062x/pyFFHFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	120.6082	0.1591	0.0000
2	B1	207.8675	0.3451	3.1681
3	A1	282.9327	0.8548	0.7371
4	B2	304.9984	0.9713	0.2117
5	B1	306.1319	0.4603	0.9964
6	A1	366.6882	1.2698	2.7416
7	B2	459.6320	1.7777	0.0677
8	A2	469.3289	1.6402	0.0000
9	B1	495.3820	0.6223	0.5849
10	A1	517.5046	2.3104	2.0384
11	B2	671.5166	1.5728	2.6946
12	A1	705.3257	4.3494	14.3759
13	A2	729.0795	3.8149	0.0000
14	B1	768.4410	2.4184	11.6980
15	A1	771.3566	3.3875	10.3011
16	B1	921.8504	0.7284	26.9143
17	B2	939.0565	2.5556	106.1319
18	B2	1196.8910	1.6899	51.2701
19	B2	1219.1444	4.0025	2.1443
20	A1	1273.0429	10.6674	178.4078
21	B2	1301.7454	9.2848	78.5626
22	A1	1476.4319	15.1036	0.2404
23	A1	1512.2946	15.6233	54.6760
24	B2	1569.3645	12.4284	744.7608
25	A1	1707.0825	19.8350	30.5269
26	B2	1710.1018	15.6855	2.3222
27	A1	3247.2428	6.7979	5.3619

m062x/pyFFHFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	119.2684	0.1555	0.0000
2	B1	206.9240	0.3416	3.9141
3	A1	281.6920	0.8472	0.7001
4	B2	303.6549	0.9625	0.3387
5	B1	304.7240	0.4579	1.0342
6	A1	364.7381	1.2561	3.1527
7	B2	457.6396	1.7587	0.0981
8	A2	467.8458	1.6295	0.0000
9	B1	490.7349	0.6138	0.6118
10	A1	515.8681	2.2945	1.7759
11	B2	666.4883	1.5671	2.5544
12	A1	702.2398	4.3061	14.8677
13	A2	724.1963	3.7646	0.0000
14	B1	761.4735	2.3378	13.2221
15	A1	768.4194	3.3622	9.9861
16	B1	920.3936	0.7268	29.4761
17	B2	935.5079	2.5373	110.8788
18	B2	1192.9125	1.6591	48.4254
19	B2	1218.5043	3.8795	3.9757
20	A1	1267.1987	10.5762	184.3849
21	B2	1310.5688	10.0732	72.0527

22	A1	1477.5633	15.0976	0.0698
23	A1	1511.2784	15.5512	53.2003
24	B2	1568.7727	12.6192	762.6847
25	B2	1710.6854	15.9645	2.5796
26	A1	1711.0581	19.9364	29.7264
27	A1	3252.0535	6.8216	8.1610

m062x/pyFHFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	132.8076	0.1745	0.1324
2	A"	213.9276	0.3682	4.7578
3	A"	265.5109	0.2999	1.1852
4	A'	273.1292	0.8180	0.2057
5	A'	322.6137	1.0510	1.3626
6	A'	357.9093	1.2405	1.9801
7	A"	391.8389	0.9366	0.9776
8	A'	468.7500	1.8119	0.3992
9	A'	537.5936	1.8800	3.0440
10	A'	610.8956	3.7644	0.0438
11	A"	639.6512	1.3255	5.7251
12	A'	675.3395	1.6879	3.1095
13	A"	693.0558	2.0662	0.0064
14	A"	750.6350	2.1467	1.9792
15	A'	819.6370	3.8137	40.8387
16	A"	860.8109	0.6855	42.8971
17	A'	1050.1550	2.2075	74.6159
18	A'	1116.9453	8.2603	157.4001
19	A'	1184.0869	1.6359	113.8225
20	A'	1284.5366	9.4807	19.8141
21	A'	1330.1632	9.5055	18.1535
22	A'	1468.6627	13.3081	73.8876
23	A'	1511.4193	14.3415	145.3006
24	A'	1581.4680	11.8883	472.1310
25	A'	1698.9132	17.4674	288.4291
26	A'	1718.3101	19.9949	44.5810
27	A'	3263.5137	6.8747	10.0455

m062x/pyFHFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	133.7974	0.1771	0.1098
2	A"	214.1085	0.3721	4.0218
3	A"	268.3560	0.3038	1.2680
4	A'	274.0028	0.8229	0.2357
5	A'	323.3990	1.0556	1.1962
6	A'	358.3549	1.2439	1.6165
7	A"	393.7568	0.9548	0.9579
8	A'	468.7827	1.8144	0.3997
9	A'	537.0461	1.8798	2.6752

10	A'	612.4109	3.7904	0.0120
11	A"	649.8460	1.3045	6.3478
12	A'	678.0376	1.6888	3.3261
13	A"	708.2788	1.8884	0.0085
14	A"	780.1304	1.9502	0.3504
15	A'	819.9465	3.8256	36.7186
16	A"	877.3099	0.7823	38.2281
17	A'	1050.6735	2.2161	69.0896
18	A'	1119.4420	8.2606	145.1195
19	A'	1186.7318	1.6527	110.8740
20	A'	1283.0947	9.9332	16.5978
21	A'	1325.6192	9.0035	20.1834
22	A'	1469.5719	13.3540	69.7667
23	A'	1509.2215	14.2592	139.0047
24	A'	1580.1596	11.7905	460.7658
25	A'	1695.5474	17.2696	276.4892
26	A'	1713.8027	19.8310	41.5450
27	A'	3262.0611	6.8651	7.7946

m062x/pyFHFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	133.4177	0.1761	0.1005
2	A"	213.9247	0.3700	3.6079
3	A"	267.5273	0.3032	1.2573
4	A'	273.7473	0.8214	0.2330
5	A'	323.5292	1.0565	1.1316
6	A'	358.7146	1.2461	1.4905
7	A"	393.5976	0.9514	0.8033
8	A'	469.1936	1.8178	0.3966
9	A'	537.6875	1.8858	2.5285
10	A'	612.8136	3.7931	0.0106
11	A"	648.4611	1.3368	5.6699
12	A'	678.4335	1.6935	3.1955
13	A"	706.6236	1.9101	0.0000
14	A"	774.4678	2.0956	0.5693
15	A'	820.8383	3.8353	36.1702
16	A"	871.0332	0.7416	37.0125
17	A'	1052.2743	2.2103	68.4613
18	A'	1122.2945	8.3723	143.2146
19	A'	1190.5710	1.6617	109.8150
20	A'	1285.7980	10.2246	16.4002
21	A'	1327.7364	8.8997	21.9727
22	A'	1474.0934	13.5760	70.7713
23	A'	1512.9174	14.2717	131.3547
24	A'	1583.6733	11.8708	462.6256
25	A'	1697.2715	17.2368	282.0279
26	A'	1715.9591	19.8697	42.4223
27	A'	3266.3031	6.8829	6.9298

m062x/pyFHFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	132.4695	0.1737	0.1247
2	A''	213.7513	0.3687	4.4551
3	A''	265.8535	0.3012	1.2914
4	A'	272.8624	0.8162	0.2264
5	A'	321.7612	1.0453	1.3824
6	A'	356.6896	1.2317	1.8271
7	A''	392.2946	0.9383	0.8454
8	A'	467.6464	1.8020	0.3803
9	A'	536.0614	1.8713	2.6098
10	A'	611.1204	3.7674	0.0410
11	A''	644.7127	1.3480	6.1990
12	A'	673.5448	1.6896	2.9523
13	A''	702.0474	1.8992	0.0017
14	A''	771.1280	2.0951	0.5648
15	A'	817.9320	3.7942	37.3297
16	A''	872.0082	0.7356	42.0093
17	A'	1049.6469	2.2163	73.0367
18	A'	1117.9917	8.2788	147.8367
19	A'	1186.4892	1.6230	104.9488
20	A'	1286.2620	9.4695	18.3494
21	A'	1332.2214	9.7386	17.6971
22	A'	1473.0482	13.4363	77.0677
23	A'	1513.4838	14.3384	137.0119
24	A'	1584.0359	12.0579	471.8380
25	A'	1699.5816	17.5306	284.8159
26	A'	1718.5456	20.0134	40.6719
27	A'	3271.2402	6.9075	10.3467

m062x/pyHHHHH_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	383.4585	0.2250	0.0000
2	B1	415.9705	0.3829	3.9288
3	A1	612.6562	1.5635	3.4359
4	B2	668.7126	1.6664	0.3685
5	B1	720.8023	0.4459	68.1064
6	B1	764.5075	0.7330	16.5683
7	A2	908.4419	0.6069	0.0000
8	B1	971.6453	0.7395	0.0142
9	A2	1017.3279	0.8878	0.0000
10	A1	1021.4132	4.4557	6.6447
11	B1	1025.4435	0.8010	0.0264
12	A1	1056.1902	3.2731	2.3322
13	B2	1089.7319	1.1858	0.0000
14	A1	1102.9527	1.1215	6.8826
15	B2	1165.6924	0.9559	2.8358
16	A1	1252.2154	1.1671	4.6969
17	B2	1278.6767	5.1991	0.0803
18	B2	1384.5350	1.3524	0.0148

19	B2	1484.1449	2.7628	28.2988
20	A1	1526.4744	2.8873	3.2355
21	B2	1657.2882	10.2395	13.3443
22	A1	1663.5612	9.0477	25.8282
23	B2	3188.3745	6.5200	21.0364
24	A1	3190.3848	6.5413	1.9395
25	A1	3208.5658	6.6115	4.0404
26	B2	3226.4140	6.7125	12.3224
27	A1	3232.6575	6.7708	2.3791

m062x/pyHHHHH_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	386.3540	0.2249	0.0000
2	B1	419.2936	0.3843	3.7977
3	A1	612.3374	1.5602	4.3110
4	B2	668.3905	1.6610	0.2089
5	B1	726.2491	0.4284	63.1769
6	B1	774.7232	0.7747	10.7360
7	A2	913.7480	0.6142	0.0000
8	B1	981.8407	0.7610	0.0209
9	A1	1020.8608	4.3875	7.4318
10	A2	1032.5611	0.9225	0.0000
11	B1	1037.0058	0.8446	0.0280
12	A1	1060.2645	3.2578	2.8110
13	B2	1090.6849	1.1843	0.0995
14	A1	1103.3666	1.1323	4.6117
15	B2	1162.1692	0.9628	3.2363
16	A1	1250.1548	1.1686	3.8770
17	B2	1273.3067	4.8862	0.1587
18	B2	1386.9618	1.3578	0.0459
19	B2	1485.9848	2.7893	27.1149
20	A1	1529.0186	2.8794	2.7547
21	B2	1655.6895	10.1067	13.5716
22	A1	1661.8118	8.9819	25.8766
23	B2	3185.6747	6.5076	21.5008
24	A1	3187.8792	6.5319	2.4971
25	A1	3207.5186	6.6044	4.1905
26	B2	3225.4644	6.7060	13.7712
27	A1	3231.8313	6.7642	2.8357

m062x/pyHHHHH_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	387.6875	0.2263	0.0000
2	B1	420.3972	0.3888	3.7274
3	A1	613.3993	1.5694	4.2601
4	B2	670.0814	1.6727	0.2696
5	B1	726.7372	0.4213	64.3703
6	B1	776.1648	0.7994	9.8287

7	A2	915.7028	0.6167	0.0000
8	B1	982.2410	0.7625	0.0081
9	A1	1022.1901	4.4108	7.8632
10	A2	1033.5269	0.9248	0.0000
11	B1	1043.6635	0.8533	0.0105
12	A1	1061.0571	3.2527	2.8319
13	B2	1092.3998	1.1909	0.0762
14	A1	1105.2805	1.1383	4.7457
15	B2	1166.0756	0.9741	2.9939
16	A1	1252.5040	1.1713	3.7034
17	B2	1275.2928	4.7988	0.0962
18	B2	1389.3239	1.3621	0.0457
19	B2	1489.3283	2.7952	28.0508
20	A1	1531.7517	2.8924	3.1629
21	B2	1658.8823	10.1339	13.0054
22	A1	1664.5484	8.9852	26.0826
23	B2	3188.0814	6.5170	23.0826
24	A1	3190.3164	6.5418	3.2894
25	A1	3210.7294	6.6172	4.6323
26	B2	3228.7741	6.7196	14.9395
27	A1	3235.2504	6.7789	3.1128

m062x/pyHHHHH_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	385.6511	0.2256	0.0000
2	B1	416.9052	0.3842	3.9574
3	A1	612.1873	1.5607	3.5246
4	B2	667.2740	1.6573	0.4307
5	B1	722.5508	0.4262	73.3488
6	B1	771.3973	0.7690	13.5700
7	A2	909.6968	0.6085	0.0000
8	B1	975.1994	0.7492	0.0340
9	A1	1018.4614	4.4028	7.0777
10	A2	1025.2441	0.9063	0.0000
11	B1	1035.0213	0.8348	0.0453
12	A1	1058.0142	3.2771	2.3385
13	B2	1090.2684	1.1784	0.0124
14	A1	1102.5864	1.1183	7.2071
15	B2	1165.6293	0.9409	2.8311
16	A1	1250.4516	1.1587	4.2241
17	B2	1279.0343	5.5533	0.1940
18	B2	1380.7572	1.3449	0.0236
19	B2	1481.7657	2.7771	29.5942
20	A1	1523.7386	2.8945	4.0675
21	B2	1656.5491	10.3665	12.1523
22	A1	1664.1889	9.2268	25.2929
23	B2	3194.5997	6.5458	17.7653
24	A1	3196.3154	6.5656	2.1561
25	A1	3215.3919	6.6393	3.8264
26	B2	3232.9514	6.7398	10.9573
27	A1	3239.3253	6.7997	1.9138

mn15/pyCCCCC_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	60.9463	0.0746	0.0000
2	B1	82.2469	0.1348	0.0154
3	B1	148.6991	0.2080	0.0532
4	A1	205.5535	0.8205	0.0485
5	B2	217.6359	0.8568	0.2817
6	A1	219.8295	0.8171	0.0294
7	B2	227.0224	1.0577	0.0000
8	B1	283.6912	0.6407	1.0863
9	B2	333.4251	1.8516	0.1945
10	A1	350.5289	2.0113	0.2150
11	A2	366.2862	0.9898	0.0000
12	A1	393.0255	2.9568	0.0734
13	A1	553.0769	3.1267	5.2428
14	B1	577.0934	2.4320	1.5770
15	B2	583.6360	2.6811	0.4637
16	A2	632.4858	2.8537	0.0000
17	B2	703.6443	4.5656	89.2971
18	B1	742.9589	3.9813	0.1509
19	A1	840.0362	5.7605	96.9413
20	B2	916.8699	6.5010	3.7852
21	A1	1104.9782	9.0792	33.4999
22	A1	1261.8251	11.6029	3.7865
23	B2	1265.5778	11.5272	34.3124
24	A1	1388.9623	13.8271	125.7091
25	B2	1389.2561	14.1344	424.4589
26	A1	1578.9940	17.7424	107.1971
27	B2	1610.8029	19.1260	64.9398

mn15/pyCCCCC_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	63.5434	0.0810	0.0000
2	B1	85.8750	0.1461	0.0117
3	B1	152.0222	0.2177	0.0659
4	A1	201.4652	0.8029	0.0181
5	B2	213.5128	0.8252	0.2488
6	A1	215.8692	0.7750	0.0076
7	B2	220.0191	0.9932	0.0004
8	B1	292.3581	0.6816	1.0177
9	B2	332.8123	1.8331	0.1711
10	A1	350.8304	2.0014	0.2161
11	A2	377.2964	1.0504	0.0000
12	A1	394.5062	2.9734	0.0809
13	A1	554.0588	3.1409	4.0020
14	B2	577.1678	2.6179	0.0983
15	B1	595.7605	2.5977	1.5388

16	A2	661.1053	3.1183	0.0000
17	B2	706.8214	4.6144	80.6371
18	B1	788.7689	4.4764	1.5231
19	A1	842.5306	5.8088	90.2950
20	B2	917.9124	6.5361	3.5013
21	A1	1102.7127	9.0541	30.8281
22	B2	1261.2711	11.4684	31.3487
23	A1	1267.8309	11.7116	4.8307
24	A1	1388.5581	13.8228	107.9988
25	B2	1389.5494	14.1377	395.7613
26	A1	1575.0877	17.6495	99.4488
27	B2	1604.2664	18.9429	57.9204

mn15/pyCCCCC_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	62.3672	0.0781	0.0000
2	B1	85.0799	0.1433	0.0133
3	B1	150.7951	0.2143	0.0228
4	A1	202.4328	0.8114	0.0285
5	B2	215.0263	0.8372	0.1984
6	A1	217.3731	0.7862	0.0029
7	B2	221.0802	1.0026	0.0002
8	B1	289.5914	0.6687	0.9026
9	B2	333.9336	1.8516	0.1923
10	A1	351.6124	2.0171	0.2290
11	A2	375.0317	1.0379	0.0000
12	A1	395.0562	2.9834	0.0856
13	A1	555.4756	3.1531	4.1086
14	B2	582.1791	2.6698	0.2318
15	B1	596.5701	2.6047	1.4702
16	A2	659.9408	3.1074	0.0000
17	B2	708.7730	4.6280	80.8032
18	B1	782.7029	4.4084	1.6518
19	A1	844.5245	5.8320	93.0725
20	B2	921.5890	6.5791	3.0932
21	A1	1109.0383	9.1536	31.2490
22	A1	1265.2929	11.6630	4.0650
23	B2	1267.4119	11.5710	34.6756
24	A1	1389.0351	13.8303	108.9881
25	B2	1389.2526	14.1285	387.1186
26	A1	1577.5755	17.7067	102.9771
27	B2	1608.0875	19.0494	57.7813

mn15/pyCCCCC_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	60.2394	0.0729	0.0000
2	B1	82.1421	0.1339	0.0151
3	B1	147.7317	0.2055	0.0132

4	A1	203.4961	0.8054	0.0278
5	B2	215.5186	0.8403	0.1245
6	A1	217.4272	0.7985	0.0005
7	B2	224.5520	1.0350	0.0001
8	B1	283.6469	0.6406	0.6380
9	B2	330.8543	1.8316	0.2506
10	A1	347.9545	1.9915	0.1942
11	A2	367.2037	0.9947	0.0000
12	A1	389.4185	2.9137	0.0821
13	A1	547.2367	3.0628	5.6853
14	B1	578.1153	2.4420	1.2615
15	B2	578.1958	2.6336	0.8070
16	A2	636.0140	2.8857	0.0000
17	B2	695.2830	4.4545	89.8270
18	B1	752.0664	4.0784	2.1256
19	A1	831.8380	5.6398	98.9596
20	B2	908.2485	6.3661	3.2005
21	A1	1095.3613	8.9147	34.9862
22	A1	1256.9473	11.4972	3.1820
23	B2	1268.9426	11.5845	32.8929
24	A1	1385.0681	13.7445	118.9624
25	B2	1385.7478	14.0572	407.0718
26	A1	1579.6944	17.7551	108.0929
27	B2	1610.2099	19.1174	62.4810

mn15/pyFCFCF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	93.5194	0.1100	0.0000
2	B1	110.9714	0.1580	0.0004
3	A1	182.9686	0.5215	0.0087
4	B1	214.7293	0.4104	3.3832
5	B2	223.6676	0.6615	0.0345
6	B2	313.1256	1.2365	1.1735
7	B1	317.1779	0.8221	0.5949
8	A1	323.9597	1.3331	0.4253
9	A2	380.4295	1.0693	0.0000
10	B2	410.2720	1.8170	0.0674
11	A1	410.4557	1.9944	0.8293
12	A1	586.0777	3.2527	1.9448
13	A1	615.2209	3.7093	1.1607
14	B1	656.1537	3.1481	1.4683
15	B2	703.8483	3.8696	0.1837
16	A2	704.6593	3.5643	0.0000
17	B1	773.1935	4.3126	16.2527
18	B2	814.7559	5.6657	113.2963
19	A1	1095.3829	9.7856	185.6873
20	B2	1131.9505	10.3912	18.3547
21	A1	1174.2466	10.3873	3.8186
22	B2	1319.0657	12.6927	14.5996
23	A1	1475.7777	16.2422	56.9075
24	B2	1496.1852	16.4799	463.0142

25	A1	1512.8197	16.8271	96.0128
26	A1	1658.9261	19.6454	231.6718
27	B2	1679.8857	20.6819	93.0484

mn15/pyFCFCF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	95.8380	0.1156	0.0000
2	B1	113.2258	0.1643	0.0051
3	A1	179.7208	0.5029	0.0010
4	B1	213.5510	0.4057	3.1351
5	B2	220.5272	0.6425	0.0266
6	B2	312.0052	1.2290	1.2039
7	B1	320.4883	0.8407	0.7949
8	A1	323.2363	1.3236	0.3834
9	A2	376.9170	1.0493	0.0000
10	B2	408.6004	1.7938	0.0955
11	A1	410.4056	1.9920	0.7693
12	A1	586.0663	3.2320	1.6385
13	A1	616.0941	3.7479	0.5652
14	B1	659.7547	3.1845	1.6230
15	B2	701.1011	3.8393	0.0020
16	A2	715.9509	3.6813	0.0000
17	B1	796.1802	4.5682	12.9700
18	B2	816.1622	5.6921	104.0783
19	A1	1100.5595	9.8556	165.9412
20	B2	1137.0219	10.4887	14.0570
21	A1	1178.0804	10.4769	2.6818
22	B2	1309.0249	12.5247	12.6673
23	A1	1481.3122	16.3291	69.3430
24	B2	1498.6171	16.5527	445.1287
25	A1	1514.1855	16.9229	70.7811
26	A1	1652.7677	19.5014	220.7376
27	B2	1672.4460	20.4744	90.5743

mn15/pyFCFCF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	94.7109	0.1128	0.0000
2	B1	112.2333	0.1615	0.0011
3	A1	181.6498	0.5138	0.0002
4	B1	213.5752	0.4061	2.7144
5	B2	222.4653	0.6542	0.0174
6	B2	313.1596	1.2385	1.1073
7	B1	320.0853	0.8376	0.7110
8	A1	324.1395	1.3328	0.3141
9	A2	378.5322	1.0587	0.0000
10	B2	410.1718	1.8098	0.0891
11	A1	411.2213	2.0010	0.7504
12	A1	586.7040	3.2488	1.4807

13	A1	617.1141	3.7438	0.6316
14	B1	659.5401	3.1835	1.3600
15	B2	704.1714	3.8750	0.0154
16	A2	715.4884	3.6765	0.0000
17	B1	790.3419	4.5008	12.8466
18	B2	817.2842	5.7025	102.5890
19	A1	1101.2753	9.8660	170.0798
20	B2	1139.6100	10.5257	13.6236
21	A1	1178.4973	10.4758	2.4951
22	B2	1318.4195	12.6963	13.9156
23	A1	1485.9195	16.4583	64.4491
24	B2	1501.5611	16.6088	431.7352
25	A1	1514.8320	16.9191	81.5816
26	A1	1657.1141	19.6084	230.0618
27	B2	1678.9020	20.6596	99.1409

mn15/pyFCFCF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	93.2417	0.1093	0.0000
2	B1	110.5724	0.1567	0.0004
3	A1	182.7549	0.5204	0.0046
4	B1	211.1651	0.3961	3.1223
5	B2	224.4025	0.6659	0.0078
6	B2	312.2886	1.2320	1.0903
7	B1	315.2477	0.8140	0.3749
8	A1	322.7643	1.3259	0.3084
9	A2	370.5128	1.0136	0.0000
10	B2	408.1484	1.7976	0.0347
11	A1	408.2319	1.9770	0.8256
12	A1	582.9516	3.1892	1.8530
13	A1	614.1087	3.7186	0.7360
14	B1	650.7085	3.0961	0.8660
15	B2	699.8025	3.8255	0.1216
16	A2	704.0157	3.5610	0.0000
17	B1	772.5233	4.3049	20.1496
18	B2	806.1172	5.5332	107.4118
19	A1	1094.7223	9.7430	182.7490
20	B2	1132.2974	10.4007	16.1919
21	A1	1166.9766	10.2745	1.6221
22	B2	1322.7240	12.7698	12.1337
23	A1	1481.6496	16.3614	60.9631
24	B2	1498.7877	16.5338	451.2435
25	A1	1514.7971	16.9048	86.8419
26	A1	1660.5667	19.6838	235.6600
27	B2	1679.3379	20.6774	91.7937

mn15/pyFCFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A"	99.1505	0.1227	0.0002
2	A"	142.2777	0.2224	0.0102
3	A'	201.0881	0.5607	0.0286
4	A"	214.7491	0.4093	4.3840
5	A'	267.2876	0.7915	0.3056
6	A'	312.7858	1.1516	1.0231
7	A"	328.8431	0.8741	1.0933
8	A'	335.3685	1.2556	0.9777
9	A'	407.9043	1.8643	0.3051
10	A"	414.7567	1.2862	1.5497
11	A'	465.9357	2.0442	0.4654
12	A'	599.3433	3.6229	0.7411
13	A'	636.4443	3.7474	5.7259
14	A"	646.3330	3.0571	2.0729
15	A"	698.6587	3.5057	0.2946
16	A'	725.3855	4.1100	0.6224
17	A"	757.8154	4.1449	11.4358
18	A'	924.8704	7.2394	146.9732
19	A'	1102.8460	9.9522	195.5493
20	A'	1144.0958	10.5268	29.8997
21	A'	1287.8487	12.7499	20.3789
22	A'	1325.7833	12.8923	19.3156
23	A'	1479.3639	16.2909	55.2847
24	A'	1514.5586	16.8311	288.8000
25	A'	1566.9646	18.3056	482.8816
26	A'	1679.8163	20.1847	196.7265
27	A'	1701.6883	21.1168	13.1833

mn15/pyFCFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	101.4368	0.1282	0.0015
2	A"	143.9141	0.2279	0.0086
3	A'	198.1753	0.5443	0.0246
4	A"	214.3610	0.4074	3.8597
5	A'	267.5715	0.7933	0.3548
6	A'	312.5149	1.1523	0.9967
7	A"	332.5343	0.8952	1.2707
8	A'	334.8074	1.2469	0.8769
9	A'	406.8028	1.8455	0.2498
10	A"	417.2618	1.3016	1.2606
11	A'	464.2638	2.0286	0.5377
12	A'	601.7929	3.6452	0.7771
13	A'	635.1315	3.7428	4.3583
14	A"	653.5160	3.1298	2.5547
15	A"	717.3471	3.6970	0.5997
16	A'	724.2942	4.0984	0.6496
17	A"	794.2828	4.5435	8.4849
18	A'	927.9008	7.2816	133.8211
19	A'	1108.2504	10.0411	175.9293
20	A'	1148.7359	10.6214	27.7581
21	A'	1290.7697	12.7041	18.9788

22	A'	1317.1345	12.8651	17.1131
23	A'	1484.4022	16.3902	58.1225
24	A'	1516.0512	16.8831	280.4465
25	A'	1567.2658	18.3379	454.2426
26	A'	1673.6223	20.0423	192.1312
27	A'	1695.1736	20.9391	10.2162

mn15/pyFCFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	100.3682	0.1256	0.0004
2	A"	142.6537	0.2238	0.0046
3	A'	200.0671	0.5549	0.0316
4	A"	213.7202	0.4051	3.3858
5	A'	267.9556	0.7954	0.3461
6	A'	313.2210	1.1576	0.9332
7	A"	331.8269	0.8914	1.1719
8	A'	335.5853	1.2535	0.7697
9	A'	408.1338	1.8611	0.2565
10	A"	415.8478	1.2924	1.1777
11	A'	465.5998	2.0407	0.5482
12	A'	601.5739	3.6421	0.7100
13	A'	636.7804	3.7597	4.2368
14	A"	651.0391	3.1055	2.1174
15	A"	714.0601	3.6631	0.3497
16	A'	725.9978	4.1181	0.6133
17	A"	781.1293	4.3978	8.4334
18	A'	928.4770	7.2878	133.3252
19	A'	1109.0521	10.0522	180.4222
20	A'	1151.1520	10.6521	26.1937
21	A'	1294.6385	12.8348	19.4736
22	A'	1325.6654	12.9687	18.0220
23	A'	1488.4910	16.4958	58.3100
24	A'	1518.1488	16.9147	257.0868
25	A'	1570.5466	18.4166	474.3270
26	A'	1679.0025	20.1730	196.9590
27	A'	1700.8954	21.1043	13.6498

mn15/pyFCFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	98.8438	0.1217	0.0002
2	A"	141.0378	0.2187	0.0073
3	A'	201.5951	0.5631	0.0483
4	A"	212.0076	0.3982	4.1647
5	A'	269.7676	0.8067	0.3076
6	A'	312.6243	1.1558	1.0240
7	A"	326.8455	0.8650	0.8703
8	A'	334.4053	1.2449	0.8612
9	A'	405.8720	1.8463	0.2929

10	A''	411.8299	1.2680	1.8404
11	A'	464.6054	2.0314	0.5118
12	A'	599.2705	3.6086	0.9241
13	A'	632.2786	3.7036	4.9901
14	A''	643.7693	3.0354	1.8885
15	A''	705.8537	3.5809	1.1567
16	A'	722.0570	4.0717	0.6233
17	A''	770.8076	4.2826	11.1331
18	A'	920.5855	7.1541	138.2880
19	A'	1102.9040	9.9462	188.3505
20	A'	1143.5486	10.5186	29.5029
21	A'	1288.3833	12.7722	18.6364
22	A'	1329.6157	12.9850	17.6623
23	A'	1484.5971	16.4037	55.6953
24	A'	1516.2712	16.8726	272.6811
25	A'	1571.0074	18.4161	481.7448
26	A'	1681.5138	20.2345	197.6861
27	A'	1702.2663	21.1294	10.9688

mn15/pyFFCFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	118.7393	0.1540	0.0000
2	B1	123.8419	0.1885	0.0406
3	B2	200.6097	0.5708	0.0257
4	B1	209.2659	0.3834	4.1557
5	A1	274.3302	0.8558	0.8553
6	B2	304.6037	1.0047	0.4303
7	A1	331.7470	1.3424	1.3183
8	B1	336.7703	0.9303	1.1891
9	A1	429.0486	1.9486	0.0329
10	A2	448.7986	1.5005	0.0000
11	B2	456.2996	1.9613	0.0407
12	A1	546.5455	3.1194	2.2087
13	B1	603.2856	2.6592	9.0368
14	A2	701.0717	3.5294	0.0000
15	A1	702.3989	4.5264	8.2817
16	B2	722.5035	4.0611	0.0159
17	B1	748.5300	4.0423	3.4193
18	A1	943.7972	7.2720	143.9763
19	B2	995.1068	8.5498	162.2318
20	B2	1208.5636	11.6898	0.0063
21	A1	1279.2809	12.4819	66.2708
22	B2	1316.0573	12.6607	32.5543
23	A1	1484.7000	16.5187	9.9622
24	A1	1517.8087	16.7698	99.9815
25	B2	1551.7728	17.9510	797.0379
26	B2	1687.4871	20.8438	4.4903
27	A1	1689.1258	20.4112	130.3344

mn15/pyFFCFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	119.4445	0.1558	0.0000
2	B1	126.3057	0.1965	0.0568
3	B2	198.2097	0.5571	0.0213
4	B1	209.1332	0.3823	3.5267
5	A1	273.7228	0.8514	0.9975
6	B2	304.6077	1.0044	0.4552
7	A1	331.1544	1.3359	1.1424
8	B1	338.6116	0.9409	1.1932
9	A1	428.9946	1.9448	0.0089
10	A2	449.5032	1.5053	0.0000
11	B2	452.7429	1.9270	0.0274
12	A1	548.2435	3.1412	2.4112
13	B1	606.2174	2.6887	8.9278
14	A1	702.0634	4.5210	6.1839
15	A2	719.3185	3.7164	0.0000
16	B2	721.3719	4.0487	0.1588
17	B1	786.4889	4.4564	2.7193
18	A1	946.2199	7.3137	134.0326
19	B2	999.4586	8.6186	143.9034
20	B2	1213.7392	11.7606	0.0460
21	A1	1283.7253	12.5765	62.7806
22	B2	1304.9883	12.5115	29.6732
23	A1	1488.4842	16.5848	12.8278
24	A1	1519.6714	16.8385	96.0061
25	B2	1552.3430	17.9782	757.8723
26	B2	1681.1340	20.6709	3.8187
27	A1	1683.4919	20.2835	123.1772

mn15/pyFFCFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	119.0632	0.1548	0.0000
2	B1	125.5838	0.1942	0.0482
3	B2	200.2440	0.5688	0.0112
4	B1	208.6527	0.3807	3.0893
5	A1	274.2619	0.8550	0.9813
6	B2	305.4557	1.0099	0.3842
7	A1	331.8602	1.3417	1.0601
8	B1	337.9657	0.9371	1.1113
9	A1	429.3875	1.9500	0.0047
10	A2	449.4393	1.5049	0.0000
11	B2	455.2773	1.9511	0.0309
12	A1	548.5493	3.1430	2.3740
13	B1	608.0638	2.7052	8.7026
14	A1	703.4525	4.5370	5.9531
15	A2	716.4320	3.6870	0.0000
16	B2	723.5370	4.0739	0.1351
17	B1	776.0600	4.3395	2.0047
18	A1	946.4387	7.3145	133.7212

19	B2	1000.4608	8.6310	145.3175
20	B2	1218.2013	11.8466	0.1626
21	A1	1286.2021	12.6172	64.2424
22	B2	1314.4497	12.6753	31.5651
23	A1	1491.6717	16.6837	9.1179
24	A1	1520.3461	16.8369	99.4601
25	B2	1557.1520	18.0779	760.2392
26	B2	1685.7510	20.8113	5.3300
27	A1	1689.3527	20.4273	124.6550

mn15/pyFFCFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.0777	0.1496	0.0000
2	B1	123.5569	0.1878	0.0498
3	B2	201.6530	0.5765	0.0006
4	B1	206.5556	0.3728	3.8468
5	A1	275.4116	0.8635	0.8954
6	B2	305.7844	1.0124	0.4459
7	A1	330.5574	1.3345	1.1405
8	B1	333.6906	0.9143	0.9838
9	A1	427.0036	1.9333	0.0449
10	A2	446.1216	1.4825	0.0000
11	B2	454.3116	1.9426	0.0399
12	A1	546.1586	3.1056	2.3937
13	B1	594.5843	2.5851	11.4030
14	A1	699.7042	4.4881	7.0175
15	A2	709.7884	3.6194	0.0000
16	B2	719.7807	4.0305	0.0322
17	B1	765.6195	4.2264	1.7109
18	A1	936.6116	7.1541	137.3171
19	B2	995.8087	8.5557	153.5445
20	B2	1212.7206	11.7644	0.0490
21	A1	1277.7074	12.4556	63.7500
22	B2	1320.0336	12.7556	31.6771
23	A1	1488.5111	16.6005	8.4698
24	A1	1518.3430	16.7925	99.9632
25	B2	1556.8208	18.0763	787.1483
26	B2	1688.6806	20.8722	3.4397
27	A1	1691.2125	20.4689	127.0931

mn15/pyFFFFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	120.5828	0.1588	0.0000
2	B1	158.8480	0.2730	0.0039
3	B1	216.0469	0.4129	5.7401
4	B2	261.4992	0.7576	0.0525
5	A1	264.6255	0.7642	0.7889
6	B2	316.2655	1.0678	1.0633

7	A1	346.1753	1.2362	2.0084
8	B1	353.1592	1.0104	3.9400
9	A2	437.9742	1.4296	0.0000
10	B2	455.5995	1.9615	0.0754
11	A1	473.1563	2.0840	0.2721
12	A1	601.6709	3.6958	0.0209
13	B1	635.7757	2.9607	3.1139
14	A2	692.9530	3.4489	0.0000
15	A1	704.5380	4.5239	5.3229
16	B1	739.0764	3.9481	6.8318
17	B2	742.6025	4.3094	0.0070
18	B2	1014.0314	8.8129	204.1427
19	A1	1115.7196	10.2426	246.3376
20	B2	1213.5967	11.8339	0.1514
21	B2	1329.0097	12.9025	20.9840
22	A1	1334.3684	13.7450	26.4030
23	A1	1489.3415	16.4367	26.3576
24	B2	1561.6862	18.2210	767.7723
25	A1	1595.0872	18.8575	184.2730
26	A1	1699.6055	20.6346	119.9291
27	B2	1715.0374	21.4210	3.4141

mn15/pyFFFFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	121.3673	0.1608	0.0000
2	B1	160.4692	0.2790	0.0009
3	B1	215.9524	0.4121	4.7834
4	B2	262.7680	0.7646	0.0503
5	A1	264.9635	0.7658	0.8907
6	B2	316.5925	1.0696	0.9978
7	A1	345.6115	1.2316	1.7663
8	B1	355.6567	1.0258	3.5967
9	A2	440.0375	1.4432	0.0000
10	B2	452.3916	1.9310	0.0649
11	A1	472.2573	2.0732	0.3588
12	A1	604.1826	3.7250	0.0334
13	B1	648.1044	3.0862	4.0415
14	A1	704.0401	4.5194	3.8791
15	A2	718.1792	3.7046	0.0000
16	B2	742.7625	4.3116	0.0946
17	B1	791.2711	4.5072	5.0392
18	B2	1018.8790	8.8904	185.9168
19	A1	1121.0740	10.3371	229.0179
20	B2	1218.1385	11.9062	0.5218
21	B2	1317.7415	12.7316	18.5366
22	A1	1338.6559	13.8492	24.5045
23	A1	1492.7494	16.5015	30.3316
24	B2	1562.3736	18.2454	741.1189
25	A1	1595.4717	18.8917	175.9001
26	A1	1693.6924	20.4978	112.8786
27	B2	1708.4289	21.2458	2.3440

mn15/pyFFFFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	120.6253	0.1588	0.0000
2	B1	158.8953	0.2733	0.0004
3	B1	215.1030	0.4088	4.2390
4	B2	263.0757	0.7666	0.0530
5	A1	265.1093	0.7665	0.9038
6	B2	317.0721	1.0727	0.9383
7	A1	346.1740	1.2361	1.6207
8	B1	354.1975	1.0177	3.3176
9	A2	438.6261	1.4340	0.0000
10	B2	454.6272	1.9519	0.0698
11	A1	472.9951	2.0805	0.3981
12	A1	604.2419	3.7250	0.0391
13	B1	644.0556	3.0453	3.4120
14	A1	705.1540	4.5320	3.8231
15	A2	713.4684	3.6569	0.0000
16	B2	743.5049	4.3207	0.0857
17	B1	773.1142	4.3086	4.7683
18	B2	1019.4274	8.8979	185.8346
19	A1	1121.9002	10.3490	231.5270
20	B2	1222.3188	11.9872	0.7200
21	B2	1327.4510	12.9054	19.7957
22	A1	1341.6491	13.9068	25.1423
23	A1	1496.6222	16.5940	30.3494
24	B2	1567.3025	18.3559	735.4685
25	A1	1597.9816	18.9517	176.0095
26	A1	1699.3318	20.6372	116.4513
27	B2	1714.0946	21.4036	3.3757

mn15/pyFFFFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	118.8165	0.1541	0.0000
2	B1	157.3685	0.2680	0.0020
3	B1	214.1640	0.4053	5.5331
4	B2	265.1273	0.7786	0.0517
5	A1	266.6500	0.7757	0.8470
6	B2	316.8070	1.0712	1.1429
7	A1	345.2246	1.2292	1.9021
8	B1	350.6769	0.9977	3.7543
9	A2	436.4492	1.4195	0.0000
10	B2	453.7865	1.9447	0.0693
11	A1	472.2766	2.0740	0.2947
12	A1	602.3055	3.7022	0.0158
13	B1	638.1573	2.9904	3.7954
14	A1	701.6623	4.4862	4.3241
15	A2	708.3284	3.6047	0.0000

16	B2	739.7331	4.2756	0.0291
17	B1	769.2458	4.2627	5.0135
18	B2	1014.5039	8.8165	192.9002
19	A1	1116.1155	10.2472	236.8193
20	B2	1217.1786	11.9009	0.3181
21	B2	1332.3719	12.9829	19.4535
22	A1	1334.9935	13.7753	25.3036
23	A1	1493.0850	16.5145	27.2586
24	B2	1566.1547	18.3289	751.5668
25	A1	1598.7239	18.9576	180.1111
26	A1	1701.6684	20.6887	118.5159
27	B2	1715.8502	21.4437	2.5991

mn15/pyFFHFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.0537	0.1498	0.0000
2	B1	204.6630	0.3330	4.5001
3	A1	274.9502	0.8053	0.7511
4	B2	297.8839	0.9207	0.3317
5	B1	299.8899	0.4394	1.0343
6	A1	360.9917	1.2311	3.4906
7	B2	448.1922	1.6739	0.1023
8	A2	462.5243	1.5932	0.0000
9	B1	486.8670	0.6065	0.7987
10	A1	504.6473	2.1742	2.1177
11	B2	659.1334	1.4933	2.6093
12	A1	693.1312	4.1591	14.8559
13	A2	705.1775	3.5694	0.0000
14	B1	738.2914	2.6751	11.9502
15	A1	759.9759	3.3203	9.6677
16	B1	906.5263	0.6798	31.2839
17	B2	928.6816	2.4103	117.7290
18	B2	1178.5804	1.6071	57.7009
19	B2	1208.2836	3.8874	8.2816
20	A1	1253.3458	10.4053	202.9910
21	B2	1319.7136	11.3288	76.4326
22	A1	1467.6936	14.8622	0.0356
23	A1	1499.6816	15.3716	57.2472
24	B2	1561.8872	12.5246	801.5668
25	A1	1697.2210	19.6790	30.1571
26	B2	1703.0508	16.2008	1.3829
27	A1	3254.8795	6.8293	3.3308

mn15/pyFFHFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	118.1832	0.1527	0.0000
2	B1	205.3237	0.3368	3.6656
3	A1	274.8722	0.8043	0.8258

4	B2	298.4638	0.9226	0.2720
5	B1	302.7944	0.4496	1.0062
6	A1	360.6028	1.2276	3.0135
7	B2	444.9930	1.6474	0.0795
8	A2	464.0394	1.6037	0.0000
9	B1	492.7024	0.6125	0.8420
10	A1	505.0118	2.1684	2.4159
11	B2	659.8812	1.4866	2.5363
12	A1	693.8644	4.1888	12.2608
13	A2	726.9974	3.7939	0.0000
14	A1	761.6113	3.3364	10.0917
15	B1	767.4329	2.1006	14.5634
16	B1	926.4490	0.7607	23.1816
17	B2	931.6593	2.3621	102.6787
18	B2	1181.8952	1.5097	57.3817
19	B2	1211.9898	5.0248	2.1579
20	A1	1258.7916	10.5115	185.5894
21	B2	1309.0760	10.4682	73.1369
22	A1	1471.9977	14.8680	0.0556
23	A1	1500.8811	15.5458	59.2227
24	B2	1563.1913	12.7622	780.5449
25	A1	1692.3009	19.6025	29.3418
26	B2	1697.2389	15.7693	2.5826
27	A1	3248.3798	6.7970	2.2127

mn15/pyFFHFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.6878	0.1514	0.0000
2	B1	204.3695	0.3331	3.2464
3	A1	275.2234	0.8062	0.8301
4	B2	298.8110	0.9258	0.2462
5	B1	301.8395	0.4467	1.0013
6	A1	361.1912	1.2322	2.8136
7	B2	447.4212	1.6666	0.0823
8	A2	463.5613	1.6005	0.0000
9	B1	489.5921	0.6078	0.6788
10	A1	505.8550	2.1782	2.4413
11	B2	661.3761	1.5089	2.5053
12	A1	695.6234	4.2127	12.2010
13	A2	723.6786	3.7598	0.0000
14	B1	759.5179	2.2789	12.2365
15	A1	761.9612	3.3330	10.3224
16	B1	915.3314	0.7239	26.2110
17	B2	932.6782	2.3962	102.1269
18	B2	1187.0170	1.5508	57.6806
19	B2	1217.5803	4.6289	2.7652
20	A1	1262.3350	10.5320	188.4309
21	B2	1318.4526	10.9788	76.9010
22	A1	1474.3334	14.8629	0.0908
23	A1	1504.9196	15.6903	59.4491
24	B2	1568.4570	12.6243	772.5503

25	A1	1697.5632	19.7081	30.7068
26	B2	1703.2299	16.0222	1.5842
27	A1	3257.4454	6.8382	2.2660

mn15/pyFFHFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	115.7402	0.1464	0.0000
2	B1	202.5886	0.3280	4.2557
3	A1	275.9750	0.8110	0.7754
4	B1	299.2494	0.4396	1.0117
5	B2	299.3831	0.9316	0.3548
6	A1	359.7443	1.2222	3.2186
7	B2	446.5328	1.6659	0.0931
8	A2	460.4880	1.5790	0.0000
9	B1	483.9223	0.5962	0.7942
10	A1	504.9190	2.1714	2.1406
11	B2	658.7602	1.5170	2.3596
12	A1	691.7018	4.1663	12.8419
13	A2	716.7018	3.6881	0.0000
14	B1	751.1022	2.1639	13.6541
15	A1	758.8534	3.3057	10.3627
16	B1	909.4474	0.7180	27.1129
17	B2	929.4597	2.4169	111.1230
18	B2	1181.6887	1.5689	54.5300
19	B2	1212.8654	4.1128	5.8756
20	A1	1254.0002	10.4236	196.6839
21	B2	1324.6741	11.3687	71.1990
22	A1	1471.4464	14.8403	0.0298
23	A1	1501.6082	15.4777	56.4383
24	B2	1566.1202	12.7379	790.3030
25	A1	1700.5358	19.7583	30.2143
26	B2	1703.7775	16.2560	1.8110
27	A1	3257.5193	6.8410	3.5857

mn15/pyFHFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	130.3404	0.1674	0.1496
2	A''	211.4094	0.3593	4.8641
3	A''	261.1120	0.2879	1.1381
4	A'	265.4622	0.7711	0.2309
5	A'	316.6774	1.0063	1.3572
6	A'	352.1268	1.1941	2.0608
7	A''	389.4165	0.9239	1.1260
8	A'	457.5947	1.7100	0.3299
9	A'	524.0144	1.7896	2.2666
10	A'	603.7817	3.6964	0.0026
11	A''	632.4272	1.2382	5.8464
12	A'	665.9176	1.6023	2.8923

13	A''	687.5063	1.9976	0.0173
14	A''	748.3583	2.1814	1.7701
15	A'	810.4017	3.7246	37.8153
16	A''	861.5971	0.6966	40.3573
17	A'	1039.3712	2.0797	76.0941
18	A'	1109.2387	7.9971	162.6569
19	A'	1174.1718	1.6372	121.2934
20	A'	1277.3388	8.6561	25.1905
21	A'	1338.7504	10.9893	14.5892
22	A'	1461.5110	13.2648	76.7014
23	A'	1504.1989	14.0077	135.1804
24	A'	1575.2060	12.2227	505.6916
25	A'	1687.9835	17.3923	295.6203
26	A'	1708.6512	19.8720	43.6087
27	A'	3270.8402	6.9025	4.3824

mn15/pyFHFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	130.9685	0.1687	0.1238
2	A''	211.7479	0.3636	4.0361
3	A''	263.8249	0.2919	1.2233
4	A'	266.1599	0.7744	0.2681
5	A'	316.8157	1.0047	1.1902
6	A'	351.6601	1.1896	1.6523
7	A''	390.1845	0.9364	1.0868
8	A'	455.4323	1.6947	0.3448
9	A'	521.0229	1.7673	1.8731
10	A'	606.2646	3.7287	0.0091
11	A''	641.6416	1.2441	6.3534
12	A'	666.3159	1.5948	3.0646
13	A''	699.8322	1.8187	0.0575
14	A''	775.9897	1.8985	0.2407
15	A'	811.0129	3.7150	32.4893
16	A''	876.6020	0.7958	36.0698
17	A'	1039.8909	1.9904	65.1529
18	A'	1114.7810	7.9399	144.8830
19	A'	1178.0347	1.6940	120.8818
20	A'	1279.6126	9.4880	20.0894
21	A'	1329.7078	10.1868	16.5365
22	A'	1467.3213	13.5611	82.6705
23	A'	1504.3308	13.9677	121.2743
24	A'	1575.9571	12.3787	495.4161
25	A'	1681.9321	17.0976	284.5303
26	A'	1702.3749	19.6744	38.8981
27	A'	3263.4322	6.8663	2.8977

mn15/pyFHFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A"	130.3759	0.1673	0.1111
2	A"	210.8957	0.3601	3.6004
3	A"	262.1916	0.2902	1.1903
4	A'	266.1443	0.7745	0.2692
5	A'	317.4110	1.0091	1.1402
6	A'	352.5786	1.1969	1.5672
7	A"	388.8368	0.9316	0.9370
8	A'	456.8508	1.7048	0.3406
9	A'	522.8466	1.7835	1.7953
10	A'	606.4737	3.7267	0.0049
11	A"	639.6279	1.2575	5.7584
12	A'	667.4816	1.6116	3.0285
13	A"	698.2346	1.8259	0.0130
14	A"	766.3627	2.0940	0.5869
15	A'	812.0327	3.7329	32.8643
16	A"	863.0462	0.7361	36.2596
17	A'	1042.0551	2.0288	66.9444
18	A'	1117.0868	8.1364	144.6115
19	A'	1182.7087	1.6808	116.9164
20	A'	1284.2720	9.2541	22.6362
21	A'	1338.7763	10.6393	16.7381
22	A'	1471.2353	13.7338	78.5333
23	A'	1508.8623	13.9687	115.5360
24	A'	1580.0777	12.3613	495.6929
25	A'	1687.9361	17.2275	290.0549
26	A'	1708.0704	19.8160	42.2863
27	A'	3272.8738	6.9091	2.9894

mn15/pyFHFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	128.9310	0.1638	0.1411
2	A"	209.7866	0.3566	4.6993
3	A"	260.2321	0.2867	1.1989
4	A'	267.7860	0.7843	0.2520
5	A'	316.9868	1.0094	1.3544
6	A'	351.1670	1.1888	1.8941
7	A"	386.3346	0.9131	1.0470
8	A'	456.4951	1.7075	0.3262
9	A'	522.2127	1.7826	1.9716
10	A'	604.6065	3.7049	0.0033
11	A"	633.5072	1.2558	6.1504
12	A'	664.7559	1.6220	2.7786
13	A"	691.7083	1.7976	0.0295
14	A"	761.7836	2.0370	0.5001
15	A'	808.6884	3.7057	34.8213
16	A"	861.9910	0.7328	39.5428
17	A'	1039.8801	2.1017	75.6143
18	A'	1110.7518	8.0558	153.2594
19	A'	1177.6053	1.6171	112.3391
20	A'	1279.7006	8.6809	23.7242
21	A'	1341.8210	11.1724	14.4500

22	A'	1466.7917	13.4442	76.9481
23	A'	1506.6428	14.0107	125.7242
24	A'	1578.6031	12.4190	503.4217
25	A'	1689.7574	17.4266	292.8550
26	A'	1709.9189	19.8825	40.9609
27	A'	3273.9881	6.9163	4.6061

mn15/pyHHHHH_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	378.3464	0.2192	0.0000
2	B1	411.5670	0.3745	3.9164
3	A1	594.3420	1.4753	3.7862
4	B2	651.9949	1.5875	0.3676
5	B1	711.1776	0.4265	62.8420
6	B1	756.3168	0.7169	14.6155
7	A2	895.6172	0.5894	0.0000
8	B1	960.3163	0.7285	0.0040
9	A1	1004.5816	4.3037	7.6137
10	A2	1006.2895	0.8689	0.0000
11	B1	1020.9483	0.8008	0.0299
12	A1	1046.1655	3.3198	1.1948
13	B2	1081.1698	1.1426	0.0046
14	A1	1092.3948	1.0714	6.8231
15	B2	1153.0816	0.8865	2.4264
16	A1	1237.3877	1.1284	4.5506
17	B2	1293.6019	6.8628	0.0998
18	B2	1370.6002	1.3261	0.0151
19	B2	1472.1640	2.7766	26.1192
20	A1	1512.2117	2.9043	2.3159
21	B2	1648.2938	10.6262	14.2434
22	A1	1652.6215	9.3506	26.1542
23	B2	3189.6415	6.5209	30.1764
24	A1	3191.9626	6.5432	4.8170
25	A1	3210.9079	6.6166	6.7571
26	B2	3227.8602	6.7169	26.1871
27	A1	3235.5451	6.7823	6.4782

mn15/pyHHHHH_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	382.0173	0.2202	0.0000
2	B1	417.5255	0.3835	3.9517
3	A1	592.1967	1.4583	4.6534
4	B2	648.9437	1.5663	0.2244
5	B1	724.0593	0.4322	58.0924
6	B1	769.6863	0.7364	11.2424
7	A2	908.3113	0.6067	0.0000
8	B1	974.7931	0.7515	0.0011
9	A1	1004.4156	4.2489	8.3935

10	A2	1025.6071	0.9095	0.0000
11	B1	1037.1054	0.8490	0.0276
12	A1	1050.7455	3.2860	1.6659
13	B2	1079.9834	1.1324	0.1381
14	A1	1092.0731	1.0731	4.5878
15	B2	1145.3727	0.8842	2.6531
16	A1	1233.4051	1.1313	3.8672
17	B2	1287.8737	6.4784	0.2124
18	B2	1370.8031	1.3280	0.0740
19	B2	1472.7097	2.8048	25.0034
20	A1	1514.7600	2.9132	1.9823
21	B2	1646.5604	10.4625	14.0401
22	A1	1649.2683	9.2451	25.6138
23	B2	3183.9404	6.4960	29.9153
24	A1	3186.1213	6.5199	5.5964
25	A1	3206.5300	6.5945	6.2410
26	B2	3221.9529	6.6891	27.9893
27	A1	3230.2666	6.7553	7.3066

mn15/pyHHHHH_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	381.9398	0.2192	0.0000
2	B1	415.4781	0.3785	3.7685
3	A1	593.7463	1.4703	4.8081
4	B2	652.4774	1.5869	0.2938
5	B1	718.8049	0.4157	61.7206
6	B1	767.8348	0.7550	10.4817
7	A2	904.1862	0.6009	0.0000
8	B1	970.4176	0.7473	0.0038
9	A1	1007.2042	4.2787	9.0882
10	A2	1023.2259	0.9080	0.0000
11	B1	1040.2445	0.8566	0.0132
12	A1	1051.5680	3.2923	1.7624
13	B2	1083.6100	1.1458	0.0887
14	A1	1095.1308	1.0855	4.8638
15	B2	1154.3227	0.8907	2.4449
16	A1	1237.4378	1.1301	3.5545
17	B2	1295.4100	6.7977	0.1327
18	B2	1373.6478	1.3328	0.0718
19	B2	1477.3728	2.8044	25.4877
20	A1	1517.6797	2.9212	2.4235
21	B2	1651.5481	10.6206	13.7939
22	A1	1654.4544	9.3540	25.8169
23	B2	3192.7142	6.5331	30.5716
24	A1	3195.1056	6.5569	6.3506
25	A1	3215.2255	6.6333	6.9610
26	B2	3231.5210	6.7311	28.1218
27	A1	3239.5774	6.7990	7.0559

mn15/pyHHHHH_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	379.9085	0.2190	0.0000
2	B1	411.8344	0.3758	3.8853
3	A1	594.0225	1.4741	3.9470
4	B2	650.7564	1.5800	0.4140
5	B1	710.3024	0.4046	67.3999
6	B1	759.4802	0.7633	11.0318
7	A2	894.1039	0.5873	0.0000
8	B1	958.5228	0.7250	0.0073
9	A1	1002.6078	4.2702	7.9918
10	A2	1010.5158	0.8809	0.0000
11	B1	1023.5269	0.8168	0.0699
12	A1	1049.1564	3.3125	1.3671
13	B2	1082.7390	1.1388	0.0000
14	A1	1093.4282	1.0740	6.8106
15	B2	1154.5887	0.8805	2.4069
16	A1	1236.7429	1.1220	4.0065
17	B2	1296.8091	7.2151	0.1706
18	B2	1368.3830	1.3228	0.0270
19	B2	1471.3933	2.7949	26.1821
20	A1	1510.7950	2.9124	2.6136
21	B2	1649.2370	10.7546	13.3584
22	A1	1654.2002	9.5293	25.4477
23	B2	3192.5697	6.5338	25.4342
24	A1	3194.7242	6.5557	5.0347
25	A1	3214.6343	6.6318	6.0426
26	B2	3230.6014	6.7288	22.3535
27	A1	3238.2432	6.7952	5.2504

o3lyp/pyCCCCC_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	54.2441	0.0591	0.0000
2	B1	77.5726	0.1198	0.0162
3	B1	149.3956	0.2105	0.0001
4	A1	202.6488	0.8051	0.0694
5	B2	214.9747	0.8379	0.3915
6	A1	218.1188	0.8011	0.0813
7	B2	224.7989	1.0367	0.0025
8	B1	284.6812	0.6434	0.5836
9	B2	329.5526	1.8454	0.3628
10	A1	345.7802	2.0038	0.1307
11	A2	368.7875	1.0034	0.0000
12	A1	382.7761	2.8212	0.2160
13	A1	539.8541	2.9763	8.0485
14	B1	577.0621	2.4384	1.2293
15	B2	582.2645	2.6860	1.7582
16	A2	629.1818	2.8232	0.0000
17	B2	679.6524	4.2229	102.5966
18	B1	735.6612	3.8914	0.1453

19	A1	819.3548	5.4422	98.5928
20	B2	887.2274	6.0313	3.4238
21	A1	1076.5161	8.5883	35.2396
22	A1	1221.2476	10.8361	3.0077
23	B2	1289.3210	11.8518	85.4158
24	A1	1346.8180	12.9853	135.2358
25	B2	1348.4291	13.3687	381.9433
26	A1	1526.9988	16.5941	97.5463
27	B2	1563.7411	18.1250	61.6483

o3lyp/pyCCCCC_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	56.0377	0.0631	0.0000
2	B1	79.3582	0.1251	0.0112
3	B1	149.5332	0.2108	0.0023
4	A1	198.2273	0.7829	0.0348
5	B2	211.0289	0.8086	0.3686
6	A1	214.3209	0.7632	0.0537
7	B2	217.4803	0.9695	0.0048
8	B1	285.6252	0.6485	0.6162
9	B2	328.7846	1.8335	0.3637
10	A1	345.3820	1.9972	0.1263
11	A2	370.0270	1.0103	0.0000
12	A1	382.6399	2.8163	0.2356
13	A1	539.1372	2.9694	6.4501
14	B2	578.1361	2.6483	1.0782
15	B1	579.4202	2.4559	1.1422
16	A2	639.0589	2.9130	0.0000
17	B2	679.4800	4.2188	92.5868
18	B1	747.9101	4.0274	1.1638
19	A1	818.7250	5.4388	91.4487
20	B2	885.2080	6.0095	3.3235
21	A1	1073.9996	8.5528	32.0812
22	A1	1218.8717	10.7866	4.3856
23	B2	1283.1826	11.7594	69.1331
24	A1	1340.0691	12.8560	117.9291
25	B2	1341.6321	13.2273	357.2297
26	A1	1518.5084	16.4062	89.3255
27	B2	1551.7606	17.8258	55.6536

o3lyp/pyCCCCC_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	56.1357	0.0633	0.0000
2	B1	79.6336	0.1259	0.0136
3	B1	150.2362	0.2129	0.0038
4	A1	199.1597	0.7907	0.0494
5	B2	212.1074	0.8170	0.3301
6	A1	215.5004	0.7716	0.0502

7	B2	218.1848	0.9758	0.0033
8	B1	286.5505	0.6528	0.5987
9	B2	330.1358	1.8466	0.3712
10	A1	346.8538	2.0109	0.1468
11	A2	372.4395	1.0236	0.0000
12	A1	384.4945	2.8407	0.2201
13	A1	541.7876	2.9973	6.0962
14	B2	581.4309	2.6808	1.2236
15	B1	581.9515	2.4771	1.0636
16	A2	641.9747	2.9400	0.0000
17	B2	684.2341	4.2741	91.6023
18	B1	750.3457	4.0541	0.9538
19	A1	822.4907	5.4930	93.1665
20	B2	890.2729	6.0820	2.8754
21	A1	1079.3317	8.6418	32.2104
22	A1	1221.5446	10.8355	4.0405
23	B2	1284.1175	11.7720	73.7320
24	A1	1342.3333	12.8988	120.1163
25	B2	1343.4220	13.2610	349.5589
26	A1	1518.7968	16.4129	91.9339
27	B2	1553.9499	17.8858	54.0376

o3lyp/pyCCCCC_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	54.4953	0.0597	0.0000
2	B1	77.3497	0.1189	0.0149
3	B1	148.0042	0.2065	0.0207
4	A1	201.6355	0.7953	0.0598
5	B2	213.9348	0.8302	0.2665
6	A1	216.3560	0.7903	0.0327
7	B2	223.4395	1.0244	0.0018
8	B1	282.0790	0.6318	0.3379
9	B2	326.9554	1.8245	0.4387
10	A1	342.9503	1.9788	0.1383
11	A2	366.8565	0.9928	0.0000
12	A1	378.9569	2.7738	0.2299
13	A1	533.9732	2.9127	8.4543
14	B1	569.6104	2.3699	0.8668
15	B2	577.7008	2.6495	2.5519
16	A2	624.5395	2.7821	0.0000
17	B2	671.8655	4.1172	103.5272
18	B1	729.1299	3.8339	1.1478
19	A1	811.6689	5.3334	101.9570
20	B2	878.8374	5.9059	2.8618
21	A1	1067.2113	8.4352	36.9434
22	A1	1216.2981	10.7358	2.6777
23	B2	1290.2420	11.8602	88.0329
24	A1	1341.5310	12.8792	132.8808
25	B2	1342.9119	13.2598	365.8721
26	A1	1525.3594	16.5575	97.0029
27	B2	1559.7368	18.0377	58.7784

o3lyp/pyFCFCF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	88.8322	0.0992	0.0000
2	B1	107.9229	0.1502	0.0041
3	A1	185.9125	0.5395	0.0122
4	B1	214.1498	0.4078	2.3268
5	B2	228.3882	0.6900	0.0384
6	B2	314.2968	1.2527	0.6289
7	B1	315.6402	0.8117	0.4045
8	A1	321.9790	1.3313	0.1561
9	A2	380.7273	1.0712	0.0000
10	A1	407.1765	1.9821	0.7226
11	B2	408.3748	1.8116	0.0663
12	A1	575.7993	3.1417	1.7186
13	A1	610.2072	3.6372	2.3562
14	B1	644.4414	3.0390	1.4549
15	A2	691.7307	3.4335	0.0000
16	B2	702.3823	3.8609	0.7064
17	B1	751.0937	4.0658	13.3428
18	B2	791.0628	5.3135	125.0264
19	A1	1065.0584	9.2632	187.0488
20	B2	1093.8622	9.6989	21.9088
21	A1	1138.5755	9.7125	6.1796
22	B2	1349.8822	13.2117	13.7230
23	A1	1425.7152	15.1139	44.7607
24	B2	1446.7214	15.3789	454.7933
25	A1	1465.7409	15.7326	104.4120
26	A1	1613.2668	18.5769	200.1203
27	B2	1634.5020	19.6384	69.5810

o3lyp/pyFCFCF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	89.6062	0.1009	0.0000
2	B1	108.4768	0.1516	0.0000
3	A1	183.5111	0.5255	0.0022
4	B1	211.6008	0.3978	2.0735
5	B2	226.2788	0.6767	0.0318
6	B2	313.6165	1.2500	0.6484
7	B1	315.8390	0.8139	0.5367
8	A1	321.3293	1.3279	0.1231
9	A2	372.2347	1.0235	0.0000
10	A1	406.8251	1.9751	0.6868
11	B2	407.4599	1.7969	0.0993
12	A1	574.9170	3.1093	1.4782
13	A1	610.9017	3.6676	1.4962
14	B1	642.4960	3.0199	1.2488
15	A2	694.5842	3.4635	0.0000

16	B2	701.5618	3.8526	0.2533
17	B1	758.8338	4.1507	10.8898
18	B2	788.8834	5.2803	115.2660
19	A1	1068.4229	9.2928	168.7475
20	B2	1096.6620	9.7599	17.8895
21	A1	1135.4866	9.6811	3.4916
22	B2	1340.2606	13.0466	9.7012
23	A1	1428.7927	15.1598	54.4568
24	B2	1445.1465	15.3457	427.8073
25	A1	1462.7313	15.7201	81.4044
26	A1	1605.3000	18.3964	193.8595
27	B2	1623.9670	19.3753	71.9297

o3lyp/pyFCFCF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	89.5258	0.1008	0.0000
2	B1	108.3671	0.1513	0.0021
3	A1	185.5858	0.5374	0.0007
4	B1	212.4759	0.4015	1.7944
5	B2	228.6907	0.6916	0.0251
6	B2	315.2038	1.2618	0.6241
7	B1	317.3918	0.8212	0.5362
8	A1	322.8544	1.3383	0.1019
9	A2	375.8786	1.0439	0.0000
10	A1	408.1236	1.9884	0.6834
11	B2	408.4806	1.8059	0.1014
12	A1	576.2163	3.1327	1.2981
13	A1	612.1354	3.6738	1.4079
14	B1	644.1138	3.0357	1.0964
15	A2	697.0688	3.4883	0.0000
16	B2	703.9687	3.8794	0.2517
17	B1	762.6776	4.1922	8.8882
18	B2	793.1935	5.3417	112.2366
19	A1	1070.8382	9.3369	166.2361
20	B2	1100.3884	9.8156	15.4435
21	A1	1140.2029	9.7548	4.0110
22	B2	1342.7523	13.0937	10.6961
23	A1	1434.9351	15.3024	53.1816
24	B2	1448.7763	15.4232	413.6770
25	A1	1465.4832	15.7750	85.8370
26	A1	1607.0183	18.4396	196.8175
27	B2	1627.6658	19.4779	73.5390

o3lyp/pyFCFCF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	88.5356	0.0985	0.0000
2	B1	107.4346	0.1486	0.0082
3	A1	186.8645	0.5452	0.0000

4	B1	210.7990	0.3945	1.8909
5	B2	230.5806	0.7035	0.0195
6	B1	313.1982	0.8008	0.2217
7	B2	314.6431	1.2587	0.5181
8	A1	321.7235	1.3344	0.0716
9	A2	369.4453	1.0078	0.0000
10	A1	405.0408	1.9609	0.7760
11	B2	406.7816	1.7951	0.0306
12	A1	573.7510	3.0927	1.5926
13	A1	609.0786	3.6419	1.6462
14	B1	639.4208	2.9895	0.6543
15	A2	688.6754	3.4063	0.0000
16	B2	699.1452	3.8268	0.6419
17	B1	748.7422	4.0436	14.9435
18	B2	783.6481	5.1978	119.0082
19	A1	1065.7742	9.2408	181.8560
20	B2	1095.3211	9.7327	17.4503
21	A1	1131.9079	9.6163	3.1323
22	B2	1351.5356	13.2607	8.0989
23	A1	1433.6967	15.2714	52.6093
24	B2	1448.5338	15.4093	443.0541
25	A1	1468.6467	15.8443	91.3715
26	A1	1613.9541	18.5926	201.5900
27	B2	1630.4672	19.5432	65.4266

o3lyp/pyFCFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	94.7555	0.1120	0.0004
2	A"	138.1958	0.2105	0.0008
3	A'	204.8309	0.5811	0.0245
4	A"	213.8800	0.4058	3.1249
5	A'	279.0005	0.8641	0.2437
6	A'	314.6013	1.1884	0.5252
7	A"	327.4438	0.8655	0.8234
8	A'	334.6582	1.2378	0.5427
9	A'	405.5585	1.8573	0.2590
10	A"	411.8799	1.2676	1.2498
11	A'	466.8422	2.0664	0.4828
12	A'	588.0323	3.4794	0.7724
13	A'	629.4739	3.6767	7.5924
14	A"	635.4956	2.9589	2.1190
15	A"	688.1535	3.4002	0.5175
16	A'	723.1427	4.0895	0.5084
17	A"	741.6092	3.9627	8.6696
18	A'	898.8291	6.8374	160.0430
19	A'	1070.8263	9.3842	192.5420
20	A'	1105.0957	9.8162	36.4625
21	A'	1245.4751	11.9242	23.1800
22	A'	1358.7068	13.3888	19.3408
23	A'	1429.0993	15.1553	46.0643
24	A'	1466.8187	15.7533	299.4694

25	A'	1514.2142	17.0407	443.1645
26	A'	1635.2984	19.1147	169.5321
27	A'	1655.2220	20.0134	10.7802

o3lyp/pyFCFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	95.7839	0.1144	0.0001
2	A"	138.9706	0.2129	0.0008
3	A'	202.6494	0.5686	0.0219
4	A"	211.9118	0.3979	2.6166
5	A'	278.7884	0.8628	0.2897
6	A'	314.2356	1.1894	0.5017
7	A"	327.9252	0.8691	0.8907
8	A'	334.2521	1.2325	0.4698
9	A'	404.8671	1.8449	0.2242
10	A"	409.3335	1.2522	0.9746
11	A'	466.1352	2.0584	0.5648
12	A'	589.1251	3.4755	0.8871
13	A'	628.3420	3.6768	6.0352
14	A"	635.3039	2.9573	2.0011
15	A"	695.0661	3.4692	0.4831
16	A'	723.2643	4.0917	0.3539
17	A"	755.6796	4.1137	7.0742
18	A'	899.4106	6.8311	145.4859
19	A'	1074.3710	9.4343	171.2329
20	A'	1107.4410	9.8740	37.7454
21	A'	1247.8460	11.9870	21.2870
22	A'	1349.2388	13.2295	14.5867
23	A'	1431.3344	15.1954	49.3048
24	A'	1464.2250	15.7026	279.4043
25	A'	1512.0240	17.0179	422.3704
26	A'	1627.7298	18.9486	167.8645
27	A'	1646.1658	19.7789	8.8632

o3lyp/pyFCFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	95.6577	0.1140	0.0001
2	A"	138.3828	0.2112	0.0000
3	A'	204.8486	0.5811	0.0237
4	A"	212.3592	0.3997	2.2490
5	A'	279.9419	0.8696	0.2851
6	A'	315.3143	1.1955	0.4886
7	A"	329.2121	0.8759	0.8801
8	A'	335.2871	1.2411	0.4199
9	A'	405.9544	1.8551	0.2260
10	A"	411.4621	1.2648	0.8378
11	A'	466.9887	2.0660	0.5793
12	A'	589.8452	3.4881	0.7778

13	A'	630.0715	3.6956	5.6187
14	A''	635.7411	2.9609	1.7124
15	A''	695.0239	3.4686	0.2201
16	A'	724.6339	4.1069	0.3272
17	A''	753.4275	4.0918	5.8581
18	A'	902.3965	6.8797	141.2019
19	A'	1076.8583	9.4757	169.7754
20	A'	1111.4296	9.9342	32.9790
21	A'	1252.1670	12.0676	21.0591
22	A'	1351.8879	13.2816	15.5074
23	A'	1437.0389	15.3255	51.1494
24	A'	1467.4516	15.7639	259.5995
25	A'	1515.8236	17.1118	422.7815
26	A'	1630.2950	19.0081	167.9228
27	A'	1649.5309	19.8746	10.0650

o3lyp/pyFCFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	94.6214	0.1115	0.0010
2	A''	137.5872	0.2087	0.0000
3	A'	206.3778	0.5894	0.0342
4	A''	211.2581	0.3954	2.6301
5	A'	281.1239	0.8775	0.2478
6	A'	314.7292	1.1946	0.4683
7	A''	324.8693	0.8530	0.5849
8	A'	334.2617	1.2342	0.4303
9	A'	403.8350	1.8403	0.2717
10	A''	408.2211	1.2452	1.4353
11	A'	466.0359	2.0564	0.5727
12	A'	587.9123	3.4606	0.9476
13	A'	626.4290	3.6470	6.5554
14	A''	631.7413	2.9226	1.4333
15	A''	690.1105	3.4215	0.9493
16	A'	720.4430	4.0590	0.4113
17	A''	747.0193	4.0218	8.0831
18	A'	895.8688	6.7709	147.8949
19	A'	1072.1330	9.3948	179.6766
20	A'	1106.3146	9.8475	35.4274
21	A'	1247.5422	11.9880	21.0338
22	A'	1360.6343	13.4449	14.1738
23	A'	1436.1426	15.3026	51.1948
24	A'	1468.1167	15.7878	284.9036
25	A'	1518.9726	17.1744	429.1952
26	A'	1635.8952	19.1475	168.0511
27	A'	1653.4685	19.9475	7.5361

o3lyp/pyFFCFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	113.6710	0.1413	0.0000
2	B1	119.7648	0.1767	0.0251
3	B2	205.0617	0.5956	0.0318
4	B1	208.6433	0.3812	2.9110
5	A1	282.0067	0.9103	0.6765
6	B2	310.6499	1.0460	0.2231
7	A1	330.3257	1.3316	0.6833
8	B1	333.6086	0.9112	0.8498
9	A1	427.0916	1.9521	0.0522
10	A2	443.9233	1.4679	0.0000
11	B2	456.6026	1.9772	0.0742
12	A1	538.8214	3.0269	1.6345
13	B1	592.3257	2.5656	8.2031
14	A2	690.5004	3.4222	0.0000
15	A1	692.3674	4.4145	9.9194
16	B2	720.3147	4.0395	0.0050
17	B1	732.4206	3.8658	2.2617
18	A1	917.4819	6.8459	145.9906
19	B2	966.3034	8.0857	178.5265
20	B2	1162.7139	10.8310	0.7413
21	A1	1243.1692	11.7447	63.8303
22	B2	1351.9986	13.2325	27.4220
23	A1	1432.3769	15.3610	4.0579
24	A1	1471.3971	15.6801	92.6126
25	B2	1496.8276	16.6602	767.7211
26	B2	1640.5779	19.7507	3.7854
27	A1	1643.0841	19.2963	122.7640

o3lyp/pyFFCFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	114.3119	0.1428	0.0000
2	B1	121.0518	0.1807	0.0364
3	B2	203.2960	0.5852	0.0262
4	B1	207.2964	0.3758	2.3565
5	A1	281.4272	0.9066	0.8075
6	B2	310.8598	1.0471	0.2319
7	A1	329.7392	1.3277	0.5417
8	B1	333.2252	0.9095	0.8342
9	A1	426.4846	1.9439	0.0220
10	A2	441.1407	1.4496	0.0000
11	B2	455.2076	1.9621	0.0599
12	A1	539.5612	3.0319	1.8911
13	B1	590.8059	2.5530	7.5563
14	A1	692.2448	4.4103	7.6825
15	A2	697.5704	3.4929	0.0000
16	B2	720.8420	4.0463	0.0310
17	B1	749.1709	4.0445	1.9898
18	A1	915.8308	6.8195	136.0259
19	B2	970.0142	8.1412	159.3406
20	B2	1167.9424	10.9327	0.5992
21	A1	1244.6179	11.7798	60.5614

22	B2	1341.9711	13.0626	23.8062
23	A1	1432.9660	15.3717	5.3321
24	A1	1468.9413	15.6453	88.8635
25	B2	1495.1945	16.6329	727.6650
26	B2	1631.6321	19.5215	3.2307
27	A1	1635.5552	19.1279	116.2367

o3lyp/pyFFCFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	113.8813	0.1417	0.0000
2	B1	121.0975	0.1808	0.0323
3	B2	205.4895	0.5980	0.0185
4	B1	207.7921	0.3779	2.0054
5	A1	282.9039	0.9163	0.7934
6	B2	312.0057	1.0549	0.2081
7	A1	330.7355	1.3332	0.5150
8	B1	333.8888	0.9127	0.8091
9	A1	427.4465	1.9528	0.0081
10	A2	443.4094	1.4646	0.0000
11	B2	456.3629	1.9728	0.0610
12	A1	540.4429	3.0447	1.9162
13	B1	594.4449	2.5851	6.6535
14	A1	693.5960	4.4269	6.9340
15	A2	696.0447	3.4784	0.0000
16	B2	722.1892	4.0615	0.0286
17	B1	748.2063	4.0339	1.4295
18	A1	919.3918	6.8741	134.1768
19	B2	972.1934	8.1732	153.5129
20	B2	1172.2994	11.0080	0.3036
21	A1	1249.3914	11.8658	58.2379
22	B2	1344.7362	13.1183	23.7074
23	A1	1437.7594	15.4866	3.8504
24	A1	1471.5406	15.6952	90.8475
25	B2	1499.8730	16.7334	712.0745
26	B2	1634.2208	19.5990	3.7483
27	A1	1638.7719	19.2069	116.2002

o3lyp/pyFFCFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	112.6497	0.1387	0.0000
2	B1	119.9240	0.1772	0.0249
3	B1	206.1368	0.3716	2.3775
4	B2	206.9747	0.6064	0.0065
5	A1	283.8830	0.9244	0.6958
6	B2	312.1251	1.0563	0.1950
7	A1	329.5473	1.3265	0.5031
8	B1	330.3898	0.8944	0.6632
9	A1	425.3900	1.9367	0.0562

10	A2	440.9895	1.4483	0.0000
11	B2	455.5470	1.9651	0.0737
12	A1	538.0028	3.0092	1.9359
13	B1	584.0953	2.4940	9.1964
14	A1	690.8891	4.3907	7.9302
15	A2	693.6632	3.4548	0.0000
16	B2	718.2343	4.0168	0.0004
17	B1	742.3606	3.9732	1.0436
18	A1	911.9677	6.7556	139.8995
19	B2	968.3185	8.1098	162.8134
20	B2	1168.6050	10.9484	0.3641
21	A1	1242.6334	11.7404	57.9863
22	B2	1354.0409	13.2861	24.4091
23	A1	1438.2844	15.4872	3.7290
24	A1	1472.3400	15.7185	94.3090
25	B2	1501.6970	16.7886	746.0630
26	B2	1639.2737	19.7025	1.7199
27	A1	1644.0302	19.3267	119.1005

o3lyp/pyFFFFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	115.8216	0.1466	0.0000
2	B1	154.8674	0.2599	0.0004
3	B1	214.7027	0.4078	4.1673
4	A1	274.5156	0.8235	0.6538
5	B2	275.8943	0.8437	0.0430
6	B2	319.7630	1.0920	0.5983
7	A1	345.3018	1.2313	1.2317
8	B1	350.1529	0.9924	2.9892
9	A2	434.3194	1.4057	0.0000
10	B2	455.7487	1.9753	0.1235
11	A1	474.8250	2.1112	0.2091
12	A1	591.6791	3.5942	0.0004
13	B1	627.7657	2.8932	3.3886
14	A2	685.4407	3.3725	0.0000
15	A1	692.9038	4.3892	6.6881
16	B1	729.9752	3.8400	4.6994
17	B2	739.7948	4.2849	0.1069
18	B2	984.5569	8.3228	221.8845
19	A1	1082.7419	9.6520	245.0998
20	B2	1167.0223	10.9346	0.0177
21	A1	1289.0860	12.7537	29.2794
22	B2	1367.2394	13.5590	18.7059
23	A1	1440.0664	15.3229	17.1413
24	B2	1507.9611	16.9520	732.6495
25	A1	1541.8617	17.5498	171.1068
26	A1	1655.2952	19.5530	110.0498
27	B2	1669.0227	20.3083	3.0179

o3lyp/pyFFFFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	116.5619	0.1485	0.0000
2	B1	155.8293	0.2634	0.0000
3	B1	213.2744	0.4018	3.3064
4	A1	274.2049	0.8214	0.7590
5	B2	276.0821	0.8445	0.0442
6	B2	319.7803	1.0917	0.5532
7	A1	344.8111	1.2273	1.0470
8	B1	350.2870	0.9941	2.6124
9	A2	431.7969	1.3895	0.0000
10	B2	454.4934	1.9622	0.1143
11	A1	474.6097	2.1066	0.3002
12	A1	593.4926	3.6137	0.0027
13	B1	629.4704	2.9107	3.2629
14	A1	692.2486	4.3811	5.0800
15	A2	696.0101	3.4773	0.0000
16	B2	740.9583	4.2995	0.0138
17	B1	753.0210	4.0827	4.0325
18	B2	988.7197	8.3860	203.5627
19	A1	1086.9675	9.7242	229.2649
20	B2	1171.4447	11.0242	0.0045
21	A1	1291.6683	12.8198	26.9439
22	B2	1357.3982	13.3884	14.8712
23	A1	1440.5286	15.3215	21.0015
24	B2	1506.2718	16.9141	704.0159
25	A1	1539.9515	17.5353	161.6745
26	A1	1648.4157	19.3958	104.7937
27	B2	1660.3985	20.0892	2.2386

o3lyp/pyFFFFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	116.0032	0.1470	0.0000
2	B1	154.9428	0.2602	0.0008
3	B1	213.3723	0.4022	2.8217
4	A1	275.0181	0.8262	0.7560
5	B2	276.8624	0.8494	0.0462
6	B2	320.3606	1.0956	0.5337
7	A1	345.3901	1.2315	0.9640
8	B1	350.6373	0.9959	2.4055
9	A2	433.5107	1.4007	0.0000
10	B2	455.3712	1.9699	0.1131
11	A1	475.0265	2.1101	0.3507
12	A1	594.0917	3.6201	0.0068
13	B1	628.5588	2.9002	2.7128
14	A1	693.5309	4.3968	4.6453
15	A2	693.7919	3.4560	0.0000
16	B2	741.4382	4.3045	0.0120
17	B1	744.9197	4.0002	3.2833
18	B2	990.6676	8.4176	194.6913

19	A1	1089.4842	9.7665	223.7516
20	B2	1175.7639	11.1025	0.0475
21	A1	1295.6238	12.8995	26.8384
22	B2	1360.2963	13.4453	15.3469
23	A1	1445.9970	15.4402	21.8988
24	B2	1511.0562	17.0240	682.4358
25	A1	1543.1815	17.6132	156.5025
26	A1	1651.1933	19.4643	105.1967
27	B2	1663.6348	20.1758	2.6751

o3lyp/pyFFFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	114.7785	0.1439	0.0000
2	B1	154.2429	0.2578	0.0000
3	B1	212.8477	0.4005	3.6091
4	A1	276.0294	0.8325	0.6957
5	B2	277.9217	0.8560	0.0487
6	B2	319.9162	1.0929	0.5982
7	A1	344.4685	1.2252	1.0747
8	B1	347.5776	0.9788	2.6990
9	A2	431.9578	1.3903	0.0000
10	B2	454.7573	1.9643	0.1161
11	A1	474.2924	2.1035	0.2682
12	A1	592.3374	3.5984	0.0005
13	B1	625.5550	2.8730	2.9420
14	A1	691.1598	4.3648	5.1631
15	A2	691.9668	3.4380	0.0000
16	B2	737.4070	4.2571	0.0550
17	B1	745.4326	4.0021	3.5076
18	B2	986.5510	8.3491	202.0522
19	A1	1085.1113	9.6890	229.9187
20	B2	1172.7321	11.0516	0.0001
21	A1	1291.7006	12.8271	26.7230
22	B2	1368.8020	13.6039	14.9255
23	A1	1445.3903	15.4301	20.2560
24	B2	1511.8195	17.0470	705.6508
25	A1	1546.9651	17.6935	164.0707
26	A1	1656.5813	19.5878	106.9013
27	B2	1667.7417	20.2664	1.5011

o3lyp/pyFFHFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	112.3448	0.1381	0.0000
2	B1	202.5815	0.3240	3.4175
3	A1	282.1400	0.8507	0.6407
4	B1	295.7322	0.4299	0.9383
5	B2	304.5497	0.9739	0.1451
6	A1	359.5304	1.2215	2.3352

7	B2	449.7266	1.7333	0.0632
8	A2	459.1557	1.5701	0.0000
9	B1	483.4293	0.6087	0.4681
10	A1	506.1247	2.2367	1.6926
11	B2	662.0455	1.5928	2.2306
12	A1	685.2212	4.1675	16.8276
13	A2	695.9777	3.4749	0.0000
14	B1	721.2844	2.4560	10.7013
15	A1	747.1349	3.1535	11.2291
16	B1	883.8580	0.6462	29.2537
17	B2	908.7412	2.7807	138.9552
18	B2	1150.0618	4.8184	15.7817
19	B2	1194.0857	1.3933	72.1043
20	A1	1221.6808	9.9309	204.8748
21	B2	1358.2464	13.1564	78.8311
22	A1	1415.7442	13.9324	0.6482
23	A1	1459.0005	14.2695	45.1633
24	B2	1513.1812	10.3227	740.1044
25	A1	1654.4418	18.5578	24.0063
26	B2	1661.6397	14.6346	2.5054
27	A1	3223.9129	6.6979	3.3965

o3lyp/pyFFHFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	113.2487	0.1403	0.0000
2	B1	202.3563	0.3259	2.6717
3	A1	282.0047	0.8494	0.6980
4	B1	296.8397	0.4330	0.9307
5	B2	304.9837	0.9764	0.1098
6	A1	359.4074	1.2199	1.9473
7	B2	448.4720	1.7199	0.0495
8	A2	457.3507	1.5579	0.0000
9	B1	485.1870	0.6040	0.4073
10	A1	506.6922	2.2351	1.9480
11	B2	663.9396	1.5946	2.2119
12	A1	686.4353	4.2092	13.9016
13	A2	705.1842	3.5673	0.0000
14	B1	736.3630	2.1345	11.6292
15	A1	747.4697	3.1501	11.8377
16	B1	895.0661	0.6895	24.6324
17	B2	911.4448	2.7387	122.7020
18	B2	1155.5053	4.5961	18.1313
19	B2	1196.1997	1.4369	64.0108
20	A1	1225.9139	10.0097	188.3932
21	B2	1348.2431	12.8141	71.0077
22	A1	1417.2913	13.9324	1.0802
23	A1	1457.0985	14.3251	47.3048
24	B2	1511.4441	10.3979	720.0833
25	A1	1648.1519	18.4366	23.7764
26	B2	1653.7145	14.1828	3.7230
27	A1	3213.3956	6.6505	2.9142

o3lyp/pyFFHFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	112.9482	0.1395	0.0000
2	B1	202.5688	0.3261	2.3092
3	A1	282.9216	0.8546	0.6961
4	B1	296.5633	0.4311	0.9259
5	B2	305.6807	0.9802	0.1091
6	A1	359.8276	1.2235	1.8054
7	B2	449.5294	1.7272	0.0471
8	A2	459.0201	1.5693	0.0000
9	B1	484.6929	0.6070	0.3353
10	A1	507.2372	2.2396	2.0070
11	B2	664.4836	1.5946	2.1561
12	A1	687.9199	4.2243	13.0523
13	A2	704.5551	3.5616	0.0000
14	B1	735.3596	2.2416	9.2782
15	A1	748.5421	3.1595	11.6656
16	B1	890.0270	0.6732	24.9240
17	B2	913.2076	2.7251	115.9131
18	B2	1160.0735	4.2918	19.7682
19	B2	1198.7645	1.4799	56.8687
20	A1	1230.5804	10.0680	183.9517
21	B2	1351.2077	12.8782	71.7349
22	A1	1421.9903	13.9617	0.9092
23	A1	1461.5618	14.5003	47.5317
24	B2	1516.6570	10.5027	698.1111
25	A1	1650.7654	18.5100	24.5076
26	B2	1657.0223	14.2997	3.3646
27	A1	3215.6101	6.6596	2.3130

o3lyp/pyFFHFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	111.5036	0.1360	0.0000
2	B1	200.9696	0.3216	2.9148
3	A1	283.4124	0.8581	0.6590
4	B1	294.8193	0.4285	0.9695
5	B2	305.6604	0.9820	0.1358
6	A1	358.4154	1.2134	2.0179
7	B2	448.8501	1.7259	0.0614
8	A2	456.8431	1.5541	0.0000
9	B1	480.6135	0.5956	0.3291
10	A1	505.7600	2.2300	1.6840
11	B2	661.4003	1.6096	2.0673
12	A1	684.8433	4.1822	13.6825
13	A2	700.7025	3.5231	0.0000
14	B1	730.8876	2.1205	10.5627
15	A1	746.5628	3.1407	11.6120

16	B1	885.4138	0.6720	28.4387
17	B2	909.9977	2.7586	126.4271
18	B2	1156.0554	4.6021	15.5656
19	B2	1198.0849	1.4192	60.3419
20	A1	1223.0200	9.9544	193.7368
21	B2	1360.8519	13.1353	67.8307
22	A1	1422.0534	13.9824	0.6708
23	A1	1460.6173	14.3792	46.3445
24	B2	1515.8927	10.6075	722.5157
25	A1	1656.8147	18.6383	23.5501
26	B2	1659.0050	14.5313	4.1864
27	A1	3227.3230	6.7116	5.4798

o3lyp/pyFHFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	126.0676	0.1561	0.1194
2	A"	209.3151	0.3481	3.7905
3	A"	258.0442	0.2833	1.1070
4	A'	276.1772	0.8355	0.1741
5	A'	320.5589	1.0440	0.8473
6	A'	351.8384	1.2007	1.3378
7	A"	385.6186	0.9133	0.7828
8	A'	459.8274	1.7706	0.4453
9	A'	526.9243	1.8391	3.0832
10	A'	594.5105	3.5905	0.0781
11	A"	626.5659	1.2728	6.0772
12	A'	668.1182	1.6865	2.4341
13	A"	679.8766	1.8721	0.0100
14	A"	736.0000	2.2147	1.0742
15	A'	797.3227	3.7222	44.8966
16	A"	836.7249	0.6461	36.1382
17	A'	1025.6376	2.7643	99.3402
18	A'	1075.3775	7.9587	173.8888
19	A'	1160.9868	1.5183	90.1921
20	A'	1244.2556	5.3928	46.7141
21	A'	1369.2163	13.2724	9.5176
22	A'	1414.9653	11.4903	53.1921
23	A'	1461.4196	13.5566	177.8234
24	A'	1528.1740	9.9511	431.3543
25	A'	1648.2488	15.8820	264.6676
26	A'	1665.8770	18.6540	42.6478
27	A'	3237.3077	6.7595	3.4771

o3lyp/pyFHFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	126.5964	0.1574	0.0975
2	A"	208.7921	0.3511	2.9713
3	A"	259.4744	0.2838	1.1893

4	A'	276.1348	0.8346	0.2108
5	A'	320.6218	1.0433	0.7324
6	A'	351.8419	1.2002	1.0410
7	A''	383.6727	0.9137	0.7034
8	A'	458.9132	1.7625	0.4245
9	A'	525.2411	1.8283	2.5637
10	A'	596.5060	3.6140	0.0331
11	A''	628.6201	1.2753	5.9664
12	A'	669.4569	1.6862	2.6149
13	A''	685.0900	1.7640	0.0001
14	A''	748.0939	1.9747	0.3534
15	A'	797.6876	3.7195	39.0260
16	A''	846.3682	0.6985	33.7659
17	A'	1026.3158	2.6606	87.8351
18	A'	1080.1529	7.9726	157.8393
19	A'	1165.0418	1.5520	90.9942
20	A'	1247.1411	5.5697	43.0605
21	A'	1359.4964	12.8958	9.9024
22	A'	1418.2093	11.7188	56.2779
23	A'	1459.1459	13.4408	163.2441
24	A'	1526.6125	9.9806	420.9613
25	A'	1641.4613	15.5666	253.1998
26	A'	1657.7672	18.3517	39.5154
27	A'	3227.2457	6.7138	2.8272

o3lyp/pyFHFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	126.1583	0.1562	0.0849
2	A''	208.6577	0.3486	2.6367
3	A''	258.9277	0.2838	1.1706
4	A'	276.9899	0.8398	0.2131
5	A'	321.2636	1.0469	0.7200
6	A'	352.4723	1.2043	0.9863
7	A''	384.3802	0.9173	0.5966
8	A'	459.5829	1.7653	0.4027
9	A'	526.1498	1.8361	2.3105
10	A'	597.2471	3.6212	0.0206
11	A''	628.8661	1.3008	5.1690
12	A'	669.9217	1.6848	2.4889
13	A''	685.3280	1.8184	0.0042
14	A''	744.2500	2.1084	0.4813
15	A'	799.2018	3.7302	37.4085
16	A''	839.8870	0.6654	31.4961
17	A'	1028.3909	2.6194	83.2960
18	A'	1083.5443	8.0361	150.6902
19	A'	1168.1812	1.5569	87.4779
20	A'	1250.8871	5.7546	41.2814
21	A'	1362.7960	12.8870	10.3107
22	A'	1423.9709	12.0426	57.0846
23	A'	1463.8843	13.4445	149.1143
24	A'	1530.7793	10.1054	414.3116

25	A'	1644.3834	15.6142	253.0181
26	A'	1660.9354	18.4534	40.6803
27	A'	3229.7161	6.7236	2.2531

o3lyp/pyFHFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	125.3310	0.1541	0.1099
2	A"	208.2258	0.3486	3.2838
3	A"	257.3854	0.2815	1.2146
4	A'	277.9191	0.8457	0.1906
5	A'	320.6649	1.0455	0.8171
6	A'	351.0232	1.1963	1.1640
7	A"	382.5599	0.9015	0.6326
8	A'	459.3148	1.7682	0.4196
9	A'	525.4675	1.8313	2.4181
10	A'	595.3384	3.5983	0.0659
11	A"	625.7565	1.2892	5.7408
12	A'	666.9035	1.7007	2.2628
13	A"	681.7049	1.7774	0.0074
14	A"	743.8356	2.0236	0.2876
15	A'	796.5834	3.7016	39.7308
16	A"	840.4687	0.6748	37.4254
17	A'	1025.7960	2.7290	93.1266
18	A'	1078.6587	7.9733	159.8323
19	A'	1165.7415	1.5230	81.4213
20	A'	1247.8871	5.4384	41.5340
21	A'	1370.1233	13.3151	9.1906
22	A'	1421.9493	11.7277	59.9587
23	A'	1463.9042	13.5167	159.6445
24	A'	1531.3671	10.2014	427.1606
25	A'	1648.4077	15.9629	258.2174
26	A'	1664.9174	18.6089	37.7789
27	A'	3241.3704	6.7760	5.5872

o3lyp/pyHHHHH_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	371.6796	0.2071	0.0000
2	B1	409.2671	0.3725	3.6539
3	A1	606.3039	1.5409	3.3648
4	B2	661.0274	1.6326	0.2943
5	B1	708.2847	0.3977	66.4409
6	B1	752.6696	0.8242	9.8998
7	A2	886.4174	0.5777	0.0000
8	B1	946.2849	0.7014	0.0451
9	A2	985.8604	0.8440	0.0000
10	B1	994.6659	0.7446	0.0001
11	A1	1003.3130	4.2469	5.5579
12	A1	1040.0414	3.1282	3.5582

13	B2	1073.8801	1.1844	0.0012
14	A1	1088.9643	1.1414	6.1455
15	B2	1164.9387	0.8822	2.1042
16	A1	1237.5711	1.1513	4.3354
17	B2	1313.4268	8.6252	0.0785
18	B2	1369.5874	1.3278	0.0000
19	B2	1460.9026	2.6358	25.4659
20	A1	1501.1963	2.6720	2.3063
21	B2	1618.3265	9.2058	10.7213
22	A1	1622.8255	8.2547	22.8567
23	B2	3146.9577	6.3458	31.3702
24	A1	3149.0456	6.3698	4.7148
25	A1	3173.5013	6.4598	4.7292
26	B2	3190.2129	6.5584	26.9037
27	A1	3198.3088	6.6264	7.9037

o3lyp/pyHHHHH_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	373.8046	0.2073	0.0000
2	B1	411.6331	0.3746	3.4941
3	A1	604.4233	1.5280	4.1187
4	B2	658.7786	1.6174	0.1720
5	B1	712.5943	0.3898	62.6246
6	B1	759.9433	0.8526	6.8047
7	A2	892.1662	0.5854	0.0000
8	B1	954.0262	0.7146	0.0208
9	A2	998.9375	0.8716	0.0000
10	A1	1001.7122	4.1828	5.9041
11	B1	1012.4886	0.7901	0.0073
12	A1	1041.9309	3.0574	4.4951
13	B2	1072.5123	1.1828	0.0448
14	A1	1087.8066	1.1560	4.2551
15	B2	1160.8151	0.8802	2.2554
16	A1	1234.1294	1.1521	3.5435
17	B2	1305.7269	8.3189	0.0306
18	B2	1370.7482	1.3307	0.0159
19	B2	1460.8365	2.6467	24.9371
20	A1	1502.2877	2.6588	2.2591
21	B2	1614.1160	8.9703	10.1193
22	A1	1618.3058	8.0988	22.3604
23	B2	3137.1390	6.3052	29.4283
24	A1	3139.3921	6.3314	4.8028
25	A1	3165.6999	6.4257	4.1531
26	B2	3182.1316	6.5227	24.9736
27	A1	3190.4258	6.5905	7.3758

o3lyp/pyHHHHH_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	373.7245	0.2072	0.0000
2	B1	411.4972	0.3752	3.3769
3	A1	605.3298	1.5356	4.3807
4	B2	660.6576	1.6291	0.2302
5	B1	711.4603	0.3829	60.5426
6	B1	760.4661	0.8786	5.3148
7	A2	890.5803	0.5832	0.0000
8	B1	950.8638	0.7128	0.0178
9	A2	996.0130	0.8667	0.0000
10	A1	1003.8544	4.2134	6.5242
11	B1	1005.7395	0.7758	0.0008
12	A1	1043.8828	3.0643	4.9077
13	B2	1074.6440	1.1890	0.0542
14	A1	1090.0609	1.1603	3.8314
15	B2	1164.3711	0.8860	2.0943
16	A1	1237.2986	1.1578	3.1059
17	B2	1308.5568	8.3631	0.0664
18	B2	1373.9118	1.3357	0.0135
19	B2	1464.5916	2.6552	25.8846
20	A1	1505.8403	2.6716	3.0139
21	B2	1617.5491	9.0298	9.6945
22	A1	1621.0999	8.1266	22.7504
23	B2	3137.6980	6.3066	31.6556
24	A1	3140.1504	6.3346	6.7632
25	A1	3167.0533	6.4304	5.0240
26	B2	3184.1007	6.5302	27.0425
27	A1	3192.3922	6.5990	7.7891

o3lyp/pyHHHHH_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	372.0940	0.2056	0.0000
2	B1	409.3567	0.3699	3.5196
3	A1	605.6978	1.5393	3.4859
4	B2	659.2611	1.6240	0.4007
5	B1	707.1041	0.3818	75.1343
6	B1	757.0021	0.8531	8.5149
7	A2	886.7844	0.5780	0.0000
8	B1	946.2739	0.7044	0.0687
9	A2	992.2086	0.8596	0.0000
10	A1	1001.2255	4.2222	5.8803
11	B1	1003.6419	0.7758	0.0157
12	A1	1041.3470	3.1158	3.8297
13	B2	1073.9405	1.1819	0.0551
14	A1	1088.3696	1.1422	6.5485
15	B2	1165.0568	0.8774	1.9553
16	A1	1236.9166	1.1449	3.5811
17	B2	1313.4295	8.8199	0.0094
18	B2	1367.0873	1.3234	0.0025
19	B2	1458.2117	2.6395	28.7858
20	A1	1498.4141	2.6669	4.0875
21	B2	1615.9220	9.2424	8.5282

22	A1	1622.0176	8.3778	22.4459
23	B2	3153.4457	6.3719	20.9269
24	A1	3155.2327	6.3945	3.6024
25	A1	3179.0585	6.4821	3.6556
26	B2	3195.5654	6.5803	16.5878
27	A1	3203.5528	6.6488	4.0853

pbe0/pyCCCCC_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	58.1506	0.0679	0.0000
2	B1	81.4060	0.1318	0.0191
3	B1	149.5474	0.2106	0.0005
4	A1	206.5569	0.8377	0.0729
5	B2	218.9923	0.8674	0.3442
6	A1	221.7636	0.8241	0.0777
7	B2	227.3413	1.0609	0.0001
8	B1	286.2810	0.6520	0.6791
9	B2	337.6891	1.9202	0.2782
10	A1	355.2209	2.0950	0.1668
11	A2	369.4819	1.0071	0.0000
12	A1	395.5256	3.0075	0.1392
13	A1	556.3252	3.1639	6.1260
14	B1	582.4349	2.4808	1.2865
15	B2	590.9592	2.7555	0.8277
16	A2	635.9692	2.8848	0.0000
17	B2	702.9004	4.5440	91.7105
18	B1	743.3823	3.9799	0.1466
19	A1	844.6993	5.7984	94.6609
20	B2	918.0079	6.4848	3.7288
21	A1	1110.1373	9.1521	32.7521
22	A1	1259.9962	11.5432	4.1029
23	B2	1302.7027	12.1546	55.4662
24	B2	1381.9263	14.0256	409.4841
25	A1	1383.8225	13.7160	131.4693
26	A1	1569.1266	17.5219	105.0668
27	B2	1602.0448	18.9512	60.9736

pbe0/pyCCCCC_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	60.2270	0.0728	0.0000
2	B1	83.6447	0.1388	0.0129
3	B1	150.0939	0.2121	0.0013
4	A1	202.2919	0.8167	0.0329
5	B2	215.2533	0.8387	0.3151
6	A1	218.2287	0.7874	0.0423
7	B2	220.0689	0.9939	0.0000
8	B1	288.7074	0.6640	0.6751
9	B2	337.2134	1.9123	0.2800

10	A1	355.1846	2.0926	0.1542
11	A2	372.8600	1.0257	0.0000
12	A1	395.6590	3.0084	0.1594
13	A1	555.9678	3.1617	4.9831
14	B2	587.1886	2.7217	0.4004
15	B1	590.4716	2.5499	1.1918
16	A2	652.1778	3.0340	0.0000
17	B2	703.1586	4.5437	83.2655
18	B1	769.0408	4.2601	1.3101
19	A1	844.6723	5.8020	87.6061
20	B2	916.4882	6.4680	3.5964
21	A1	1108.5841	9.1304	29.6347
22	A1	1258.8566	11.5138	5.3558
23	B2	1297.2983	12.0750	46.8288
24	B2	1376.6995	13.9113	378.2802
25	A1	1378.6818	13.6145	113.2250
26	A1	1562.3618	17.3667	95.8311
27	B2	1592.0092	18.6905	54.9891

pbe0/pyCCCCC_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	60.3923	0.0732	0.0000
2	B1	83.9318	0.1397	0.0152
3	B1	150.8066	0.2142	0.0039
4	A1	203.1005	0.8238	0.0454
5	B2	216.2629	0.8467	0.2829
6	A1	219.3728	0.7955	0.0387
7	B2	220.7654	1.0002	0.0000
8	B1	289.6715	0.6685	0.6140
9	B2	338.3815	1.9237	0.2937
10	A1	356.4449	2.1043	0.1752
11	A2	375.2009	1.0388	0.0000
12	A1	397.3229	3.0309	0.1564
13	A1	558.3865	3.1876	4.8359
14	B2	590.5214	2.7546	0.5480
15	B1	593.1741	2.5733	1.1496
16	A2	655.0974	3.0616	0.0000
17	B2	707.4120	4.5953	83.2162
18	B1	770.7889	4.2795	1.2659
19	A1	848.1937	5.8547	90.4519
20	B2	921.2415	6.5386	3.1409
21	A1	1113.2372	9.2110	30.1720
22	A1	1260.8891	11.5528	4.9392
23	B2	1298.3062	12.0878	50.7438
24	B2	1378.2312	13.9411	375.5311
25	A1	1380.4651	13.6494	116.1432
26	A1	1562.1518	17.3625	99.7566
27	B2	1593.9118	18.7472	54.2887

pbe0/pyCCCCC_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	58.6886	0.0692	0.0000
2	B1	81.5416	0.1320	0.0167
3	B1	148.7373	0.2083	0.0171
4	A1	205.0600	0.8256	0.0538
5	B2	217.5159	0.8560	0.2002
6	A1	219.7674	0.8098	0.0240
7	B2	225.4783	1.0437	0.0003
8	B1	285.3864	0.6479	0.3816
9	B2	335.1225	1.8993	0.3537
10	A1	352.5111	2.0715	0.1574
11	A2	369.9450	1.0095	0.0000
12	A1	391.7343	2.9594	0.1525
13	A1	550.5422	3.0999	6.6969
14	B1	580.5155	2.4618	0.9631
15	B2	586.4166	2.7174	1.3701
16	A2	637.6021	2.8998	0.0000
17	B2	695.0645	4.4362	93.5274
18	B1	748.9729	4.0460	1.5646
19	A1	837.0498	5.6859	97.9659
20	B2	909.7133	6.3556	3.1392
21	A1	1100.8054	8.9931	34.4809
22	A1	1255.0883	11.4399	3.6221
23	B2	1303.8327	12.1686	55.3270
24	B2	1377.0570	13.9247	396.8055
25	A1	1379.0539	13.6166	128.4903
26	A1	1567.8266	17.4915	105.1823
27	B2	1599.0058	18.8856	58.4265

pbe0/pyFCFCF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	92.6485	0.1079	0.0000
2	B1	110.8573	0.1580	0.0044
3	A1	185.7727	0.5380	0.0178
4	B1	216.8082	0.4179	2.4526
5	B2	227.0717	0.6818	0.0408
6	B2	317.2037	1.2699	0.9239
7	B1	319.9506	0.8360	0.3785
8	A1	327.8400	1.3685	0.2739
9	A2	383.7371	1.0880	0.0000
10	A1	415.5003	2.0670	0.6325
11	B2	416.2643	1.8814	0.1213
12	A1	590.3264	3.3110	1.6635
13	A1	624.1089	3.8005	1.9738
14	B1	657.3789	3.1602	1.2890
15	A2	705.7098	3.5744	0.0000
16	B2	712.3163	3.9677	0.3945
17	B1	768.2732	4.2573	15.4312
18	B2	814.7716	5.6554	117.3632

19	A1	1092.5516	9.7458	182.1788
20	B2	1125.9261	10.2772	19.4492
21	A1	1172.0957	10.3098	5.7571
22	B2	1359.1426	13.4224	13.8060
23	A1	1468.3202	16.0339	52.2407
24	B2	1485.4145	16.2307	454.0274
25	A1	1504.6086	16.6044	98.3794
26	A1	1653.4240	19.5145	217.7692
27	B2	1674.1944	20.5618	81.0223

pbe0/pyFCFCF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	93.8018	0.1106	0.0000
2	B1	111.8607	0.1606	0.0000
3	A1	183.4742	0.5246	0.0032
4	B1	214.4919	0.4088	2.2097
5	B2	225.1317	0.6697	0.0305
6	B2	316.8714	1.2700	0.9279
7	B1	321.1130	0.8435	0.5364
8	A1	327.5425	1.3682	0.2309
9	A2	375.9557	1.0439	0.0000
10	A1	415.4625	2.0636	0.6055
11	B2	415.6068	1.8690	0.1578
12	A1	589.9514	3.2828	1.4448
13	A1	625.1886	3.8364	1.2452
14	B1	658.7639	3.1742	1.2635
15	B2	712.1611	3.9673	0.0820
16	A2	712.8611	3.6490	0.0000
17	B1	783.1415	4.4221	12.1755
18	B2	813.0850	5.6268	108.1959
19	A1	1096.8034	9.7933	163.0326
20	B2	1129.4051	10.3502	15.5432
21	A1	1170.0979	10.2933	3.4379
22	B2	1350.7675	13.2775	10.6020
23	A1	1472.0762	16.0876	63.4553
24	B2	1484.9352	16.2250	428.1639
25	A1	1503.1553	16.6349	72.8131
26	A1	1646.8147	19.3614	210.7728
27	B2	1665.0064	20.3252	83.3355

pbe0/pyFCFCF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	93.6270	0.1102	0.0000
2	B1	111.6881	0.1602	0.0012
3	A1	185.2974	0.5351	0.0012
4	B1	215.1798	0.4116	1.9317
5	B2	227.2160	0.6825	0.0254
6	B2	318.2289	1.2802	0.8839

7	B1	322.1453	0.8483	0.4862
8	A1	328.7602	1.3763	0.1949
9	A2	378.8205	1.0601	0.0000
10	B2	416.5029	1.8772	0.1591
11	A1	416.5750	2.0751	0.5940
12	A1	591.0596	3.3056	1.2858
13	A1	626.1544	3.8388	1.2321
14	B1	659.5262	3.1818	1.0288
15	A2	713.8605	3.6593	0.0000
16	B2	714.2285	3.9905	0.1035
17	B1	782.7768	4.4181	11.3698
18	B2	816.9724	5.6845	106.7831
19	A1	1098.4757	9.8262	164.7223
20	B2	1132.3493	10.3931	14.2256
21	A1	1174.1189	10.3577	3.8983
22	B2	1353.1972	13.3242	11.8266
23	A1	1476.8990	16.2069	62.1366
24	B2	1488.0476	16.2928	419.2114
25	A1	1504.8883	16.6641	79.3941
26	A1	1647.8977	19.3904	216.7138
27	B2	1668.4332	20.4228	86.1447

pbe0/pyFCFCF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	92.6112	0.1078	0.0000
2	B1	110.6461	0.1571	0.0046
3	A1	186.1934	0.5406	0.0000
4	B1	213.7484	0.4056	2.1042
5	B2	228.6397	0.6913	0.0167
6	B2	317.1381	1.2721	0.8223
7	B1	318.4517	0.8300	0.2160
8	A1	327.3058	1.3685	0.1734
9	A2	373.4463	1.0296	0.0000
10	A1	413.4197	2.0475	0.6801
11	B2	414.4978	1.8638	0.0671
12	A1	588.1512	3.2579	1.5875
13	A1	623.0734	3.8074	1.3937
14	B1	654.6976	3.1338	0.6631
15	A2	706.3367	3.5838	0.0000
16	B2	709.1399	3.9331	0.3221
17	B1	771.0321	4.2887	18.0978
18	B2	807.2106	5.5351	112.1567
19	A1	1093.3594	9.7278	178.3765
20	B2	1127.3158	10.3086	15.9509
21	A1	1165.3865	10.2065	3.0886
22	B2	1361.1940	13.4744	9.9018
23	A1	1476.0942	16.1915	60.0447
24	B2	1487.8854	16.2811	444.6774
25	A1	1507.9594	16.7286	85.9088
26	A1	1654.2228	19.5338	221.4297
27	B2	1671.2817	20.4962	77.9971

pbe0/pyFCFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	98.3461	0.1207	0.0004
2	A''	142.1284	0.2222	0.0013
3	A'	204.2601	0.5784	0.0250
4	A''	216.6768	0.4163	3.3157
5	A'	275.9323	0.8442	0.2690
6	A'	317.3586	1.1943	0.7524
7	A''	331.6190	0.8888	0.7924
8	A'	339.4998	1.2809	0.6753
9	A'	413.4946	1.9310	0.2388
10	A''	416.5418	1.2970	1.3810
11	A'	475.1371	2.1367	0.4528
12	A'	602.4233	3.6588	0.6982
13	A'	644.1554	3.8441	6.6247
14	A''	647.4088	3.0678	1.8872
15	A''	699.6300	3.5147	0.2978
16	A'	733.6122	4.2078	0.5873
17	A''	754.0163	4.1021	10.5848
18	A'	922.9820	7.2178	152.8243
19	A'	1099.0317	9.8862	193.4417
20	A'	1137.5405	10.3981	30.7092
21	A'	1281.1541	12.6328	21.9093
22	A'	1366.6572	13.5789	18.4297
23	A'	1470.8196	16.0637	51.9836
24	A'	1505.1259	16.6016	296.3166
25	A'	1554.5764	17.9780	450.2277
26	A'	1675.4454	20.0669	183.2128
27	A'	1695.7520	20.9816	13.1625

pbe0/pyFCFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	99.7424	0.1241	0.0003
2	A''	143.2379	0.2258	0.0012
3	A'	202.2703	0.5669	0.0198
4	A''	215.1226	0.4099	2.7932
5	A'	276.4311	0.8473	0.3141
6	A'	317.4676	1.1992	0.7151
7	A''	333.3148	0.8990	0.8912
8	A'	339.4412	1.2779	0.5879
9	A'	413.1033	1.9213	0.2097
10	A''	416.2402	1.2957	1.1027
11	A'	474.8549	2.1327	0.5259
12	A'	604.0198	3.6629	0.7869
13	A'	643.4391	3.8474	5.2822
14	A''	652.1122	3.1155	2.0796
15	A''	714.0486	3.6621	0.5513

16	A'	734.5950	4.2203	0.4918
17	A''	780.9009	4.3937	7.9048
18	A'	924.1753	7.2210	138.8511
19	A'	1103.4683	9.9538	172.2242
20	A'	1140.3743	10.4622	31.1066
21	A'	1284.5441	12.7104	20.1328
22	A'	1358.3426	13.4431	14.8597
23	A'	1473.9027	16.1217	54.0918
24	A'	1503.6295	16.5789	279.8863
25	A'	1553.4322	17.9784	427.6329
26	A'	1669.0377	19.9249	181.4403
27	A'	1688.0256	20.7750	10.6977

pbe0/pyFCFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	99.4940	0.1234	0.0000
2	A''	142.5390	0.2237	0.0001
3	A'	204.1867	0.5778	0.0224
4	A''	215.4255	0.4111	2.4524
5	A'	277.5604	0.8541	0.3109
6	A'	318.4019	1.2049	0.6874
7	A''	334.0562	0.9030	0.8371
8	A'	340.3000	1.2848	0.5239
9	A'	414.0240	1.9302	0.2118
10	A''	417.4004	1.3024	1.0238
11	A'	475.5746	2.1395	0.5427
12	A'	604.4842	3.6728	0.6801
13	A'	644.9091	3.8633	5.0350
14	A''	651.5237	3.1091	1.7420
15	A''	712.7901	3.6492	0.3492
16	A'	735.7602	4.2334	0.4682
17	A''	775.0495	4.3313	7.3246
18	A'	926.5839	7.2625	137.5578
19	A'	1105.1323	9.9822	174.7625
20	A'	1143.5122	10.5100	28.2785
21	A'	1287.5838	12.7666	20.3780
22	A'	1360.8760	13.4929	15.9402
23	A'	1478.2676	16.2262	55.8952
24	A'	1506.2527	16.6270	262.9200
25	A'	1556.3421	18.0513	436.4660
26	A'	1671.0660	19.9718	183.6466
27	A'	1691.0172	20.8642	12.3277

pbe0/pyFCFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	98.4307	0.1207	0.0003
2	A''	141.6320	0.2207	0.0003
3	A'	205.3410	0.5841	0.0323

4	A''	214.5117	0.4075	2.9262
5	A'	278.1492	0.8581	0.2742
6	A'	317.4058	1.1992	0.7227
7	A''	330.2007	0.8824	0.5836
8	A'	338.9515	1.2757	0.5662
9	A'	411.7027	1.9137	0.2369
10	A''	414.9163	1.2871	1.6194
11	A'	474.2603	2.1263	0.5246
12	A'	602.3807	3.6414	0.8652
13	A'	640.9735	3.8113	5.8022
14	A''	647.5060	3.0702	1.5428
15	A''	708.1002	3.6029	1.0967
16	A'	731.0547	4.1783	0.5294
17	A''	769.5171	4.2683	9.8553
18	A'	919.8803	7.1479	142.7425
19	A'	1100.3541	9.8984	183.3998
20	A'	1138.3515	10.4194	30.1204
21	A'	1283.0903	12.6932	20.1071
22	A'	1368.9136	13.6395	15.1872
23	A'	1477.7237	16.2142	55.7382
24	A'	1506.9599	16.6502	283.6483
25	A'	1559.7059	18.1226	443.3709
26	A'	1676.1371	20.0991	183.8564
27	A'	1694.7048	20.9417	9.4677

pbe0/pyFFCFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.8756	0.1518	0.0000
2	B1	123.2827	0.1869	0.0288
3	B2	204.0856	0.5904	0.0353
4	B1	211.1782	0.3902	3.0817
5	A1	281.1442	0.9017	0.7654
6	B2	310.6280	1.0451	0.2755
7	A1	335.3984	1.3704	0.9387
8	B1	338.7883	0.9413	0.8583
9	A1	435.4196	2.0272	0.0236
10	A2	450.6486	1.5128	0.0000
11	B2	464.5333	2.0420	0.0634
12	A1	551.7365	3.1766	1.7002
13	B1	603.1997	2.6583	8.6142
14	A2	701.5607	3.5334	0.0000
15	A1	707.9609	4.6092	9.2417
16	B2	730.5585	4.1546	0.0000
17	B1	743.9076	3.9922	2.8749
18	A1	943.5517	7.2523	144.4897
19	B2	990.4663	8.4876	169.2019
20	B2	1198.1325	11.5103	0.3921
21	A1	1276.8942	12.4015	63.4646
22	B2	1358.9817	13.4050	29.6029
23	A1	1473.6931	16.2607	5.8068
24	A1	1509.5767	16.5316	94.5383

25	B2	1537.8424	17.6020	775.3109
26	B2	1680.9839	20.7029	4.2664
27	A1	1684.3247	20.2822	129.4284

pbe0/pyFFCFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	118.7272	0.1540	0.0000
2	B1	125.0159	0.1924	0.0442
3	B2	202.4876	0.5810	0.0262
4	B1	210.2908	0.3864	2.4959
5	A1	281.1348	0.9017	0.8888
6	B2	311.3790	1.0499	0.2897
7	A1	335.1591	1.3696	0.7576
8	B1	339.8079	0.9474	0.8501
9	A1	435.2069	2.0230	0.0084
10	A2	449.7690	1.5071	0.0000
11	B2	463.5430	2.0307	0.0494
12	A1	552.8790	3.1862	1.9433
13	B1	605.1859	2.6788	8.0983
14	A1	708.4529	4.6134	7.1477
15	A2	716.6429	3.6874	0.0000
16	B2	731.9937	4.1721	0.0726
17	B1	774.2003	4.3200	2.3178
18	A1	942.3955	7.2314	134.1150
19	B2	994.7162	8.5534	150.7844
20	B2	1204.1824	11.6238	0.2665
21	A1	1279.3274	12.4537	59.8712
22	B2	1349.8877	13.2549	26.7899
23	A1	1475.0563	16.2856	7.3103
24	A1	1508.4310	16.5268	91.3117
25	B2	1537.1538	17.5984	735.7078
26	B2	1673.5550	20.5057	3.5389
27	A1	1678.0024	20.1394	121.8827

pbe0/pyFFCFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	118.2973	0.1529	0.0000
2	B1	124.8676	0.1920	0.0390
3	B2	204.4616	0.5926	0.0194
4	B1	210.6098	0.3878	2.1754
5	A1	282.4448	0.9103	0.8799
6	B2	312.3848	1.0567	0.2525
7	A1	335.9756	1.3740	0.7176
8	B1	340.0109	0.9481	0.7964
9	A1	435.9900	2.0306	0.0018
10	A2	451.2805	1.5173	0.0000
11	B2	464.4926	2.0398	0.0544
12	A1	553.5989	3.1974	1.9252

13	B1	606.9634	2.6944	7.6944
14	A1	709.4175	4.6256	6.6542
15	A2	714.5123	3.6662	0.0000
16	B2	733.1593	4.1854	0.0560
17	B1	769.5470	4.2690	1.7000
18	A1	945.5246	7.2815	134.3880
19	B2	996.1762	8.5753	149.5441
20	B2	1207.0635	11.6731	0.0861
21	A1	1282.9348	12.5199	59.8607
22	B2	1352.4409	13.3057	27.5233
23	A1	1478.6883	16.3786	5.5092
24	A1	1510.2584	16.5581	93.1814
25	B2	1540.9834	17.6799	732.7371
26	B2	1675.5446	20.5711	4.1702
27	A1	1680.7173	20.2071	123.2595

pbe0/pyFFCFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	116.9965	0.1495	0.0000
2	B1	123.6084	0.1880	0.0344
3	B2	205.5424	0.5986	0.0053
4	B1	209.1687	0.3823	2.6426
5	A1	282.7780	0.9137	0.7904
6	B2	311.9826	1.0544	0.2718
7	A1	334.5378	1.3652	0.7542
8	B1	336.8670	0.9314	0.6901
9	A1	433.5983	2.0114	0.0328
10	A2	449.3135	1.5037	0.0000
11	B2	463.2599	2.0280	0.0629
12	A1	551.1915	3.1608	1.9629
13	B1	597.6612	2.6112	10.2849
14	A1	706.3204	4.5828	7.6431
15	A2	711.7787	3.6385	0.0000
16	B2	728.6260	4.1331	0.0027
17	B1	764.4250	4.2135	1.3542
18	A1	937.6252	7.1526	138.9768
19	B2	992.4303	8.5118	157.0311
20	B2	1203.9250	11.6260	0.1307
21	A1	1276.2252	12.3936	58.9199
22	B2	1361.3080	13.4644	28.0539
23	A1	1479.5331	16.3883	5.2192
24	A1	1510.7982	16.5770	96.0154
25	B2	1543.1617	17.7439	763.4499
26	B2	1680.4308	20.6784	2.3254
27	A1	1685.4151	20.3180	126.1356

pbe0/pyFFFFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	119.9592	0.1572	0.0000
2	B1	159.0296	0.2739	0.0005
3	B1	217.7980	0.4193	4.4723
4	B2	271.4791	0.8170	0.0491
5	A1	272.8514	0.8136	0.6998
6	B2	321.6582	1.1047	0.7533
7	A1	350.1393	1.2659	1.4505
8	B1	355.3085	1.0228	3.1689
9	A2	439.5461	1.4398	0.0000
10	B2	463.7459	2.0409	0.1123
11	A1	483.1088	2.1816	0.2234
12	A1	605.3693	3.7580	0.0052
13	B1	637.0619	2.9735	2.9362
14	A2	694.5674	3.4638	0.0000
15	A1	708.8814	4.5872	6.3149
16	B1	736.2086	3.9150	6.0848
17	B2	750.5657	4.4081	0.0173
18	B2	1009.3728	8.7432	212.5490
19	A1	1110.8236	10.1546	244.0843
20	B2	1202.3494	11.6198	0.0017
21	A1	1325.4223	13.5050	28.1519
22	B2	1373.3028	13.7059	19.3552
23	A1	1480.4651	16.2064	21.0142
24	B2	1548.2235	17.8813	740.4313
25	A1	1582.4635	18.5104	172.5486
26	A1	1695.7266	20.5264	116.8365
27	B2	1709.7720	21.2945	3.8434

pbe0/pyFFFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	120.9888	0.1599	0.0000
2	B1	160.4030	0.2789	0.0000
3	B1	216.9916	0.4157	3.5388
4	B2	272.5212	0.8230	0.0497
5	A1	273.2578	0.8158	0.7991
6	B2	322.2215	1.1082	0.6948
7	A1	350.0506	1.2648	1.2401
8	B1	357.3900	1.0359	2.8064
9	A2	440.0109	1.4430	0.0000
10	B2	462.9124	2.0316	0.1041
11	A1	483.4004	2.1818	0.3045
12	A1	607.5685	3.7832	0.0105
13	B1	646.6662	3.0717	3.4423
14	A1	708.8521	4.5872	4.8227
15	A2	715.6863	3.6775	0.0000
16	B2	752.7484	4.4353	0.0065
17	B1	779.2087	4.3721	4.5623
18	B2	1014.1032	8.8170	194.7631
19	A1	1115.6795	10.2390	227.2141
20	B2	1207.4686	11.7198	0.0680
21	A1	1329.2136	13.5955	25.7457

22	B2	1364.4503	13.5540	16.3267
23	A1	1481.7121	16.2222	24.8577
24	B2	1547.4169	17.8662	713.2663
25	A1	1581.5615	18.5176	164.2549
26	A1	1689.9864	20.3937	110.8843
27	B2	1702.3708	21.1017	2.8127

pbe0/pyFFFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	120.2961	0.1581	0.0000
2	B1	159.3354	0.2751	0.0007
3	B1	216.9840	0.4156	3.1189
4	B2	273.4530	0.8287	0.0525
5	A1	274.1095	0.8208	0.8061
6	B2	322.7767	1.1119	0.6652
7	A1	350.5204	1.2684	1.1459
8	B1	357.1928	1.0346	2.6100
9	A2	440.8445	1.4485	0.0000
10	B2	463.6175	2.0381	0.1102
11	A1	483.7217	2.1848	0.3493
12	A1	607.9003	3.7868	0.0146
13	B1	644.8708	3.0525	2.9404
14	A1	709.7560	4.5985	4.5634
15	A2	712.4752	3.6454	0.0000
16	B2	753.1368	4.4393	0.0044
17	B1	768.4063	4.2567	4.0344
18	B2	1015.3102	8.8373	191.6827
19	A1	1117.2916	10.2669	227.3631
20	B2	1210.3021	11.7718	0.1650
21	A1	1331.8402	13.6481	26.4284
22	B2	1367.1741	13.6073	17.0769
23	A1	1485.8793	16.3158	25.2521
24	B2	1551.4395	17.9595	702.7106
25	A1	1584.0338	18.5770	161.8985
26	A1	1692.2438	20.4505	112.7870
27	B2	1705.2178	21.1803	3.2649

pbe0/pyFFFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	119.0154	0.1547	0.0000
2	B1	158.5114	0.2722	0.0000
3	B1	216.6068	0.4145	4.0256
4	B2	273.9716	0.8319	0.0524
5	A1	274.5739	0.8238	0.7503
6	B2	321.9455	1.1066	0.7916
7	A1	349.3486	1.2599	1.3268
8	B1	354.3723	1.0185	2.9444
9	A2	439.8146	1.4414	0.0000

10	B2	462.5641	2.0282	0.1044
11	A1	482.6161	2.1743	0.2655
12	A1	606.0952	3.7636	0.0042
13	B1	641.6580	3.0228	3.2376
14	A1	706.9918	4.5603	5.0524
15	A2	710.4556	3.6250	0.0000
16	B2	748.4077	4.3825	0.0020
17	B1	768.1325	4.2501	4.3420
18	B2	1011.1518	8.7666	197.1676
19	A1	1112.8630	10.1866	232.1354
20	B2	1207.7225	11.7309	0.0363
21	A1	1327.7725	13.5742	26.2274
22	B2	1375.1952	13.7552	16.8926
23	A1	1485.6860	16.3161	23.4276
24	B2	1552.5675	17.9924	722.6693
25	A1	1587.8131	18.6605	168.3986
26	A1	1696.9841	20.5625	114.1844
27	B2	1709.0237	21.2702	2.2609

pbe0/pyFFHFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	116.3207	0.1480	0.0000
2	B1	206.1372	0.3371	3.5658
3	A1	281.8854	0.8487	0.6643
4	B1	301.5338	0.4462	1.0029
5	B2	304.4586	0.9684	0.2060
6	A1	364.9665	1.2582	2.6589
7	B2	456.9120	1.7603	0.0878
8	A2	465.3538	1.6128	0.0000
9	B1	490.1853	0.6217	0.4790
10	A1	514.8307	2.2968	1.8281
11	B2	669.2217	1.5766	2.5506
12	A1	699.9854	4.3140	16.2707
13	A2	706.6379	3.5829	0.0000
14	B1	735.5678	2.6984	11.1045
15	A1	764.1109	3.3150	10.5981
16	B1	896.8311	0.6607	31.8101
17	B2	928.2692	2.6352	128.3161
18	B2	1177.8358	2.5417	37.1909
19	B2	1209.6756	2.0088	37.8474
20	A1	1253.0455	10.4020	201.7984
21	B2	1363.1006	12.9912	75.9229
22	A1	1455.7572	14.6047	0.0958
23	A1	1494.6039	15.1489	50.0573
24	B2	1550.9371	11.6103	767.4493
25	A1	1694.1473	19.5080	27.3802
26	B2	1699.1435	15.8048	1.6756
27	A1	3239.4442	6.7661	4.9628

pbe0/pyFFHFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.5165	0.1510	0.0000
2	B1	206.3305	0.3401	2.7737
3	A1	282.3486	0.8511	0.7213
4	B1	303.8050	0.4513	0.9952
5	B2	305.5055	0.9748	0.1579
6	A1	365.2405	1.2595	2.2252
7	B2	456.0801	1.7516	0.0677
8	A2	465.3813	1.6130	0.0000
9	B1	494.1637	0.6171	0.4230
10	A1	515.8902	2.3005	2.0793
11	B2	671.9294	1.5799	2.5201
12	A1	701.7945	4.3637	13.5964
13	A2	724.6681	3.7682	0.0000
14	B1	759.6266	2.1725	13.1699
15	A1	765.0114	3.3163	11.1274
16	B1	914.9261	0.7322	25.0497
17	B2	931.4002	2.6061	112.7381
18	B2	1183.4371	2.3663	40.8495
19	B2	1213.4832	2.1980	29.3243
20	A1	1258.2821	10.4946	184.2610
21	B2	1354.0229	12.5924	70.7097
22	A1	1458.0843	14.6198	0.2352
23	A1	1493.9938	15.2369	52.5266
24	B2	1550.3875	11.6882	746.4995
25	A1	1689.0256	19.4114	26.8696
26	B2	1692.4987	15.3741	2.7628
27	A1	3232.1668	6.7319	4.0682

pbe0/pyFFHFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.0867	0.1499	0.0000
2	B1	206.3168	0.3395	2.4623
3	A1	283.2206	0.8562	0.7274
4	B1	303.2635	0.4499	0.9882
5	B2	306.1828	0.9790	0.1495
6	A1	365.5448	1.2621	2.0884
7	B2	456.9540	1.7592	0.0651
8	A2	466.3299	1.6197	0.0000
9	B1	493.1865	0.6196	0.3462
10	A1	516.3406	2.3046	2.1267
11	B2	672.4958	1.5841	2.4825
12	A1	702.7760	4.3725	13.1609
13	A2	722.6473	3.7477	0.0000
14	B1	756.5145	2.3073	10.9786
15	A1	765.7753	3.3230	11.1809
16	B1	907.3888	0.7074	26.5491
17	B2	932.6583	2.6063	110.2539
18	B2	1186.2907	2.2920	41.7427

19	B2	1216.2350	2.2838	25.6936
20	A1	1261.5341	10.5346	185.1573
21	B2	1356.8525	12.6639	73.2731
22	A1	1461.2351	14.6273	0.1556
23	A1	1497.6869	15.3880	52.3545
24	B2	1554.7983	11.7381	734.2488
25	A1	1691.0763	19.4671	27.8357
26	B2	1695.5462	15.4712	2.4536
27	A1	3235.8142	6.7473	3.7920

pbe0/pyFFHFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	115.6662	0.1463	0.0000
2	B1	204.9072	0.3353	3.1616
3	A1	283.1921	0.8563	0.6840
4	B1	301.6803	0.4470	1.0277
5	B2	305.7763	0.9778	0.2108
6	A1	363.9272	1.2505	2.3804
7	B2	455.8385	1.7533	0.0836
8	A2	464.5699	1.6071	0.0000
9	B1	489.1931	0.6095	0.3670
10	A1	514.8569	2.2929	1.8328
11	B2	668.8207	1.5931	2.3590
12	A1	699.4235	4.3265	13.7128
13	A2	718.8789	3.7092	0.0000
14	B1	751.6243	2.1890	12.5469
15	A1	763.3610	3.3013	11.1026
16	B1	905.3775	0.7098	28.8582
17	B2	929.4613	2.6213	118.7373
18	B2	1182.9198	2.3679	36.8064
19	B2	1214.1003	2.1443	29.6028
20	A1	1254.2043	10.4251	193.3648
21	B2	1366.1053	12.9799	68.6118
22	A1	1461.7846	14.6370	0.0640
23	A1	1496.7430	15.2801	50.5802
24	B2	1554.5310	11.9055	756.4107
25	A1	1696.4469	19.5868	27.1671
26	B2	1697.4845	15.7454	2.8762
27	A1	3243.3532	6.7822	6.2396

pbe0/pyFHFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	129.9879	0.1663	0.1228
2	A''	212.7067	0.3621	3.9212
3	A''	263.0396	0.2938	1.1790
4	A'	273.5993	0.8202	0.1968
5	A'	322.6951	1.0526	1.0298
6	A'	356.7974	1.2315	1.5297

7	A''	390.7783	0.9386	0.8177
8	A'	467.2238	1.8037	0.4215
9	A'	535.3882	1.8774	2.7591
10	A'	608.3463	3.7510	0.0499
11	A''	636.8286	1.2875	6.1385
12	A'	675.9625	1.6836	2.7478
13	A''	691.1405	1.9657	0.0032
14	A''	747.4013	2.1989	1.4520
15	A'	814.3326	3.8123	42.2357
16	A''	849.7424	0.6735	39.9415
17	A'	1045.1098	2.4120	85.7762
18	A'	1104.3469	8.2042	167.2248
19	A'	1177.3379	1.5796	104.9661
20	A'	1274.5958	7.0346	34.6666
21	A'	1377.9652	12.9106	10.2781
22	A'	1453.5529	12.7707	69.5617
23	A'	1497.8598	14.0685	152.2599
24	A'	1565.4209	11.2258	463.6002
25	A'	1686.0671	17.0486	282.3974
26	A'	1704.6135	19.6676	45.4814
27	A'	3254.7188	6.8358	5.7042

pbe0/pyFHFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	130.7552	0.1682	0.0979
2	A''	212.5839	0.3659	3.0826
3	A''	265.1722	0.2959	1.2633
4	A'	274.2882	0.8238	0.2318
5	A'	323.2145	1.0549	0.8874
6	A'	357.1785	1.2338	1.1934
7	A''	390.8977	0.9478	0.7526
8	A'	466.7184	1.8000	0.4068
9	A'	534.2852	1.8712	2.3313
10	A'	610.6995	3.7801	0.0161
11	A''	643.3057	1.2710	6.4445
12	A'	678.0896	1.6848	2.9583
13	A''	701.4314	1.8042	0.0001
14	A''	769.9754	1.9450	0.2210
15	A'	815.2734	3.8193	36.7373
16	A''	864.0136	0.7604	36.4209
17	A'	1046.2693	2.3465	75.1265
18	A'	1109.7840	8.2162	150.6388
19	A'	1182.5096	1.6189	104.4093
20	A'	1278.4537	7.3086	31.3064
21	A'	1369.4573	12.5195	10.6463
22	A'	1457.8865	12.9995	73.6660
23	A'	1496.5349	13.9711	139.0713
24	A'	1564.9957	11.2456	452.6030
25	A'	1680.3450	16.7610	270.4559
26	A'	1697.8200	19.4008	41.7941
27	A'	3248.0939	6.8041	4.5394

pbe0/pyFHFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	130.2406	0.1669	0.0882
2	A"	212.3595	0.3634	2.7966
3	A"	264.4759	0.2956	1.2494
4	A'	275.1698	0.8291	0.2343
5	A'	323.8604	1.0590	0.8671
6	A'	357.7174	1.2376	1.1340
7	A"	390.9772	0.9486	0.6427
8	A'	467.2927	1.8039	0.4038
9	A'	535.0698	1.8783	2.1724
10	A'	611.1376	3.7841	0.0114
11	A"	642.7893	1.2920	5.7790
12	A'	678.6064	1.6868	2.8505
13	A"	700.9738	1.8430	0.0072
14	A"	764.7393	2.0856	0.3973
15	A'	816.3511	3.8287	36.2500
16	A"	855.9671	0.7193	35.3255
17	A'	1047.8453	2.3320	74.0881
18	A'	1112.1300	8.2873	148.1622
19	A'	1185.1410	1.6256	101.6223
20	A'	1281.1063	7.4273	31.7235
21	A'	1372.5299	12.5375	11.3665
22	A'	1462.0643	13.2299	72.7866
23	A'	1500.4612	13.9857	129.8142
24	A'	1568.3994	11.3256	450.3897
25	A'	1682.7985	16.7894	273.9728
26	A'	1700.5563	19.4913	43.1057
27	A'	3251.8136	6.8196	4.2833

pbe0/pyFHFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	129.3643	0.1646	0.1135
2	A"	211.9510	0.3629	3.5503
3	A"	262.9282	0.2933	1.2846
4	A'	275.5798	0.8318	0.2157
5	A'	322.8594	1.0546	1.0205
6	A'	356.0271	1.2272	1.3734
7	A"	389.5333	0.9338	0.6977
8	A'	466.5729	1.8015	0.4043
9	A'	534.0247	1.8711	2.2814
10	A'	609.2634	3.7601	0.0453
11	A"	639.4851	1.2905	6.3276
12	A'	674.9411	1.6972	2.6084
13	A"	696.9958	1.8159	0.0036
14	A"	763.6502	2.0370	0.2801
15	A'	813.4454	3.7955	38.1449

16	A''	857.9552	0.7254	40.3539
17	A'	1045.3159	2.3981	82.2888
18	A'	1107.2565	8.2173	155.8325
19	A'	1181.7723	1.5780	96.5363
20	A'	1278.0437	7.1437	31.2979
21	A'	1379.4068	13.0011	9.9438
22	A'	1460.2223	12.9796	76.0786
23	A'	1500.7302	14.0537	138.0273
24	A'	1569.1229	11.4881	462.6061
25	A'	1686.4416	17.1041	278.3134
26	A'	1704.2903	19.6447	40.7801
27	A'	3259.3425	6.8549	7.0566

pbe0/pyHHHHH_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	379.2747	0.2171	0.0000
2	B1	415.3128	0.3817	3.8249
3	A1	612.6914	1.5590	3.5091
4	B2	668.3352	1.6595	0.3531
5	B1	716.8347	0.4094	71.5014
6	B1	763.1210	0.8283	11.1862
7	A2	898.3036	0.5934	0.0000
8	B1	960.6109	0.7250	0.0275
9	A2	1003.3908	0.8710	0.0000
10	B1	1011.2844	0.7746	0.0075
11	A1	1020.2628	4.3845	6.4520
12	A1	1057.2658	3.1531	3.3173
13	B2	1086.8633	1.1774	0.0253
14	A1	1101.2439	1.1325	6.8114
15	B2	1169.6198	0.8925	2.3274
16	A1	1248.7561	1.1618	4.6642
17	B2	1325.4284	8.3026	0.0062
18	B2	1379.3109	1.3486	0.0071
19	B2	1478.6224	2.7575	27.7477
20	A1	1519.4957	2.8637	3.0757
21	B2	1649.5326	10.1941	12.1170
22	A1	1654.2223	9.0289	25.0706
23	B2	3170.9162	6.4457	26.3875
24	A1	3173.1211	6.4702	3.3214
25	A1	3195.2530	6.5520	4.3831
26	B2	3212.4186	6.6530	19.6147
27	A1	3219.8368	6.7187	4.9661

pbe0/pyHHHHH_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	381.5294	0.2169	0.0000
2	B1	417.5857	0.3824	3.6178
3	A1	611.4521	1.5496	4.2828

4	B2	666.9763	1.6487	0.2067
5	B1	721.4460	0.3999	66.3680
6	B1	771.3743	0.8540	7.4458
7	A2	903.8863	0.6010	0.0000
8	B1	969.5538	0.7418	0.0204
9	A2	1017.8632	0.9027	0.0000
10	A1	1019.8827	4.3194	6.9046
11	B1	1027.2661	0.8233	0.0152
12	A1	1060.2640	3.0840	4.1253
13	B2	1086.6393	1.1777	0.0098
14	A1	1101.2041	1.1497	4.5043
15	B2	1166.4241	0.8927	2.5098
16	A1	1246.5044	1.1650	3.7164
17	B2	1319.1889	7.9967	0.0318
18	B2	1382.0067	1.3544	0.0471
19	B2	1480.1441	2.7728	27.0230
20	A1	1522.2052	2.8534	2.9477
21	B2	1646.9787	9.9824	11.5765
22	A1	1651.2024	8.8845	24.4919
23	B2	3164.2353	6.4174	25.6719
24	A1	3166.6329	6.4448	3.5893
25	A1	3190.8428	6.5312	3.9953
26	B2	3207.7666	6.6309	19.1698
27	A1	3215.3202	6.6965	5.0266

pbe0/pyHHHHH_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	382.2508	0.2175	0.0000
2	B1	418.4054	0.3852	3.5602
3	A1	612.3428	1.5564	4.4803
4	B2	668.6207	1.6589	0.2690
5	B1	721.3204	0.3939	67.1642
6	B1	773.0078	0.8795	6.4447
7	A2	904.0390	0.6011	0.0000
8	B1	968.5864	0.7427	0.0168
9	A2	1017.1024	0.9022	0.0000
10	A1	1021.5568	4.3428	7.6089
11	B1	1028.2403	0.8226	0.0039
12	A1	1061.5057	3.0837	4.4149
13	B2	1088.1804	1.1821	0.0047
14	A1	1102.8360	1.1529	4.4755
15	B2	1169.3777	0.8974	2.3845
16	A1	1248.7825	1.1689	3.4882
17	B2	1321.8938	8.0219	0.0106
18	B2	1384.0664	1.3579	0.0359
19	B2	1483.1160	2.7801	27.9586
20	A1	1524.6990	2.8650	3.5430
21	B2	1649.7406	10.0358	11.2298
22	A1	1653.4176	8.9037	24.9999
23	B2	3166.6554	6.4269	26.9365
24	A1	3169.1773	6.4557	4.6779

25	A1	3193.9601	6.5437	4.4053
26	B2	3211.1144	6.6444	19.6660
27	A1	3218.5979	6.7104	5.0165

pbe0/pyHHHHH_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	380.5866	0.2166	0.0000
2	B1	415.6763	0.3808	3.7480
3	A1	612.0908	1.5570	3.6449
4	B2	666.6122	1.6503	0.4216
5	B1	716.0995	0.3918	77.8547
6	B1	768.3300	0.8608	8.8015
7	A2	898.2136	0.5932	0.0000
8	B1	961.6370	0.7302	0.0491
9	A2	1009.8340	0.8870	0.0000
10	A1	1017.8807	4.3455	6.8949
11	B1	1020.9923	0.8088	0.0333
12	A1	1058.6517	3.1426	3.4885
13	B2	1086.9690	1.1730	0.0894
14	A1	1100.7286	1.1317	6.9914
15	B2	1169.1612	0.8862	2.2525
16	A1	1247.8342	1.1565	4.0390
17	B2	1326.0253	8.5217	0.0353
18	B2	1376.8916	1.3453	0.0117
19	B2	1476.5005	2.7671	29.4999
20	A1	1517.2294	2.8625	4.1721
21	B2	1647.8050	10.2528	10.6359
22	A1	1653.8758	9.1646	24.5315
23	B2	3176.4376	6.4683	20.3460
24	A1	3178.5108	6.4926	3.1457
25	A1	3201.0526	6.5753	3.6851
26	B2	3217.7114	6.6747	14.3473
27	A1	3225.0750	6.7413	3.1646

pbe/pyCCCCC_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	53.0595	0.0566	0.0000
2	B1	77.0147	0.1180	0.0164
3	B1	141.5617	0.1887	0.0119
4	A1	198.2115	0.7709	0.1008
5	B2	210.4561	0.8020	0.4180
6	A1	213.3826	0.7641	0.1166
7	B2	218.9166	0.9833	0.0013
8	B1	271.9707	0.5882	0.4709
9	B2	322.9777	1.7734	0.4260
10	A1	338.9604	1.9200	0.1606
11	A2	350.6816	0.9072	0.0000
12	A1	376.3541	2.7336	0.2830

13	A1	527.1158	2.8447	7.7974
14	B1	548.1306	2.1966	0.9985
15	B2	566.7083	2.5447	2.5424
16	A2	597.8259	2.5489	0.0000
17	B2	664.8084	4.0440	107.7330
18	B1	693.1060	3.4616	0.0646
19	A1	802.8504	5.2330	98.2423
20	B2	864.4185	5.7248	3.6211
21	A1	1049.0278	8.1558	33.7480
22	A1	1197.1581	10.4010	3.7138
23	B2	1282.9822	11.6766	192.5665
24	A1	1313.7953	12.3559	129.5202
25	B2	1317.2495	12.8330	284.9553
26	A1	1486.5580	15.7190	94.9493
27	B2	1519.1561	17.0882	53.3221

pbe/pyCCCCC_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	55.5955	0.0621	0.0000
2	B1	79.6367	0.1258	0.0114
3	B1	142.6747	0.1916	0.0008
4	A1	193.9102	0.7504	0.0459
5	B2	206.7135	0.7749	0.3844
6	A1	209.9114	0.7293	0.0798
7	B2	211.5255	0.9172	0.0033
8	B1	275.6280	0.6051	0.5075
9	B2	322.7390	1.7671	0.4154
10	A1	339.1870	1.9202	0.1457
11	A2	355.8137	0.9341	0.0000
12	A1	377.0205	2.7406	0.2921
13	A1	527.4707	2.8499	6.2164
14	B1	559.1938	2.2883	1.0103
15	B2	563.3495	2.5155	1.6639
16	A2	617.9868	2.7240	0.0000
17	B2	666.0576	4.0562	96.9465
18	B1	722.8583	3.7621	0.9167
19	A1	803.6925	5.2487	90.3321
20	B2	864.1544	5.7275	3.5026
21	A1	1048.8878	8.1582	30.3130
22	A1	1196.5162	10.3823	5.0948
23	B2	1279.8385	11.6299	150.6521
24	A1	1309.2071	12.2703	109.6344
25	B2	1311.0607	12.7219	280.1881
26	A1	1480.2675	15.5820	86.5559
27	B2	1509.2501	16.8373	47.2787

pbe/pyCCCCC_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	55.6881	0.0622	0.0000
2	B1	79.9201	0.1266	0.0143
3	B1	143.3724	0.1936	0.0213
4	A1	194.8301	0.7584	0.0615
5	B2	207.8444	0.7834	0.3333
6	A1	211.1826	0.7378	0.0713
7	B2	212.1683	0.9228	0.0020
8	B1	276.4286	0.6088	0.4620
9	B2	324.1950	1.7805	0.4218
10	A1	340.7225	1.9333	0.1673
11	A2	358.1376	0.9465	0.0000
12	A1	379.0724	2.7669	0.2802
13	A1	530.3841	2.8796	5.8735
14	B1	561.8799	2.3101	0.9458
15	B2	567.1089	2.5511	1.8625
16	A2	621.2012	2.7528	0.0000
17	B2	671.3956	4.1184	95.4783
18	B1	724.5783	3.7804	0.8057
19	A1	808.0916	5.3115	92.4564
20	B2	870.1624	5.8119	3.0242
21	A1	1054.5500	8.2513	30.3958
22	A1	1199.1193	10.4301	4.6972
23	B2	1280.8723	11.6459	162.1982
24	A1	1311.5943	12.3149	111.4046
25	B2	1313.7251	12.7683	264.9677
26	A1	1480.8690	15.5952	89.8079
27	B2	1511.9518	16.9091	46.1638

pbe/pyCCCCC_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	53.8077	0.0582	0.0000
2	B1	77.3552	0.1188	0.0152
3	B1	140.8557	0.1868	0.0593
4	A1	196.8721	0.7597	0.0806
5	B2	209.2341	0.7931	0.2639
6	A1	211.5976	0.7527	0.0466
7	B2	217.3365	0.9691	0.0014
8	B1	271.6688	0.5870	0.2286
9	B2	320.5336	1.7545	0.5078
10	A1	336.3524	1.8978	0.1610
11	A2	351.9880	0.9139	0.0000
12	A1	372.7742	2.6897	0.3056
13	A1	521.5865	2.7866	8.3755
14	B1	548.2993	2.1969	0.7680
15	B2	562.4504	2.5125	3.5469
16	A2	602.0287	2.5850	0.0000
17	B2	657.5907	3.9464	108.9945
18	B1	700.9114	3.5429	1.0336
19	A1	795.7045	5.1339	101.8301
20	B2	856.6884	5.6114	2.9557
21	A1	1040.2710	8.0148	35.5344

22	A1	1193.0822	10.3186	3.1982
23	B2	1284.3808	11.6961	219.3236
24	A1	1309.8080	12.2767	125.2618
25	B2	1314.4879	12.7774	243.4882
26	A1	1486.1559	15.7086	94.7379
27	B2	1516.9183	17.0433	51.0236

pbe/pyFCFCF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	86.1195	0.0934	0.0000
2	B1	105.0407	0.1418	0.0091
3	A1	179.3976	0.5020	0.0202
4	B1	204.4564	0.3716	1.9704
5	B2	218.9568	0.6346	0.0563
6	B2	304.0879	1.1674	0.5105
7	B1	305.0306	0.7596	0.2519
8	A1	312.5231	1.2410	0.1095
9	A2	364.4814	0.9817	0.0000
10	A1	397.3994	1.9027	0.7127
11	B2	398.6451	1.7333	0.0633
12	A1	564.5614	3.0260	1.5780
13	A1	593.1464	3.4535	2.3493
14	B1	615.9735	2.7762	1.2148
15	A2	660.8507	3.1326	0.0000
16	B2	680.6760	3.6258	0.9759
17	B1	715.7625	3.6935	11.1399
18	B2	772.5686	5.0801	127.8962
19	A1	1034.7627	8.7575	184.4950
20	B2	1058.4735	9.0847	23.2692
21	A1	1107.9925	9.1941	7.4220
22	B2	1342.4349	13.0384	11.9081
23	A1	1383.2364	14.1761	45.2673
24	B2	1401.4076	14.4370	458.6336
25	A1	1424.1847	14.8452	92.7394
26	A1	1567.6972	17.5344	176.8282
27	B2	1585.6126	18.4670	48.7495

pbe/pyFCFCF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	87.5626	0.0965	0.0000
2	B1	106.3763	0.1452	0.0007
3	A1	176.9573	0.4883	0.0060
4	B1	202.7475	0.3654	1.8337
5	B2	216.6882	0.6210	0.0471
6	B2	303.5019	1.1652	0.5427
7	B1	306.8862	0.7699	0.4014
8	A1	312.2189	1.2398	0.0956
9	A2	359.1414	0.9529	0.0000

10	A1	397.4947	1.9014	0.6770
11	B2	398.1229	1.7225	0.0917
12	A1	564.7367	3.0020	1.4014
13	A1	594.8481	3.4988	1.4877
14	B1	617.7955	2.7933	1.1791
15	A2	669.2871	3.2144	0.0000
16	B2	680.2283	3.6219	0.4142
17	B1	732.6673	3.8679	8.8568
18	B2	771.6152	5.0631	117.4130
19	A1	1039.8526	8.8185	167.2767
20	B2	1063.0549	9.1786	19.8600
21	A1	1106.9869	9.1966	4.3319
22	B2	1334.8165	12.9211	6.0664
23	A1	1387.7215	14.2466	54.6205
24	B2	1401.8639	14.4375	433.6293
25	A1	1423.8148	14.8893	69.6193
26	A1	1562.2829	17.4149	171.9010
27	B2	1577.3253	18.2594	51.0937

pbe/pyFCFCF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	87.3110	0.0960	0.0000
2	B1	106.1375	0.1447	0.0045
3	A1	179.0305	0.4997	0.0024
4	B1	203.4227	0.3680	1.4966
5	B2	219.0300	0.6349	0.0375
6	B2	305.1279	1.1769	0.5168
7	B1	308.0274	0.7751	0.3691
8	A1	313.7572	1.2499	0.0749
9	A2	362.3162	0.9701	0.0000
10	A1	398.8759	1.9147	0.6534
11	B2	399.3120	1.7326	0.0934
12	A1	566.0751	3.0287	1.1970
13	A1	596.1546	3.5017	1.4533
14	B1	618.7607	2.8024	0.9502
15	A2	670.8740	3.2299	0.0000
16	B2	682.8253	3.6500	0.4232
17	B1	732.4707	3.8660	7.5583
18	B2	776.4919	5.1316	114.3764
19	A1	1042.3368	8.8623	166.5352
20	B2	1067.4096	9.2438	17.4350
21	A1	1112.0014	9.2749	4.8083
22	B2	1338.2096	12.9787	8.1569
23	A1	1393.9407	14.3880	53.4954
24	B2	1405.7940	14.5231	419.2858
25	A1	1426.3720	14.9382	74.2466
26	A1	1564.2798	17.4633	176.3224
27	B2	1581.7346	18.3776	53.4362

pbe/pyFCFCF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	86.1780	0.0935	0.0000
2	B1	105.0020	0.1415	0.0120
3	A1	179.9555	0.5052	0.0001
4	B1	201.5548	0.3607	1.6095
5	B2	220.6152	0.6444	0.0290
6	B1	303.7774	0.7549	0.1247
7	B2	304.1840	1.1708	0.4389
8	A1	312.1528	1.2423	0.0499
9	A2	355.6494	0.9340	0.0000
10	A1	395.3900	1.8840	0.7742
11	B2	397.0455	1.7174	0.0244
12	A1	562.7288	2.9762	1.5622
13	A1	592.2661	3.4654	1.6670
14	B1	613.3221	2.7516	0.6056
15	A2	661.9401	3.1457	0.0000
16	B2	677.6728	3.5951	0.8749
17	B1	718.8490	3.7261	13.5579
18	B2	765.5571	4.9721	122.4004
19	A1	1036.3663	8.7520	181.7973
20	B2	1061.1032	9.1406	19.2175
21	A1	1101.9718	9.1125	3.7766
22	B2	1345.4811	13.1231	4.9256
23	A1	1391.1370	14.3284	52.0340
24	B2	1404.2306	14.4764	450.7548
25	A1	1427.9001	14.9676	80.6855
26	A1	1569.4039	17.5718	179.5653
27	B2	1583.3437	18.4146	45.8837

pbe/pyFCFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	91.6341	0.1047	0.0015
2	A''	134.0627	0.1980	0.0007
3	A'	197.0100	0.5384	0.0289
4	A''	204.0217	0.3690	2.6852
5	A'	266.1399	0.7857	0.2496
6	A'	304.0961	1.0985	0.4306
7	A''	315.4947	0.8043	0.5556
8	A'	323.8229	1.1630	0.4311
9	A''	394.9695	1.1661	1.1032
10	A'	395.8214	1.7781	0.2650
11	A'	455.3180	1.9677	0.5054
12	A'	575.2035	3.3502	0.5151
13	A''	607.3530	2.7022	1.7935
14	A'	612.5051	3.4797	7.7259
15	A''	656.5314	3.0935	0.3409
16	A'	700.5186	3.8382	0.5522
17	A''	703.3285	3.5663	7.4087
18	A'	874.8833	6.4928	161.8881

19	A'	1040.1223	8.8584	186.6172
20	A'	1070.1793	9.2113	38.6386
21	A'	1207.3002	11.1955	22.9188
22	A'	1350.9944	13.2088	17.2597
23	A'	1385.9485	14.2196	43.4111
24	A'	1421.4023	14.8009	330.8887
25	A'	1468.0387	15.9952	386.0386
26	A'	1588.3303	18.0190	148.8345
27	A'	1604.6389	18.8029	7.0312

pbe/pyFCFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	93.3193	0.1085	0.0000
2	A"	135.5437	0.2025	0.0009
3	A'	194.7607	0.5260	0.0229
4	A"	202.9340	0.3648	2.3286
5	A'	266.3018	0.7867	0.2936
6	A'	303.9643	1.1008	0.4253
7	A"	317.7875	0.8172	0.6807
8	A'	323.7361	1.1600	0.3896
9	A"	395.1328	1.1671	0.8837
10	A'	395.5562	1.7702	0.2278
11	A'	455.2143	1.9650	0.5767
12	A'	577.4835	3.3612	0.6316
13	A"	611.3707	2.7400	1.8671
14	A'	612.2950	3.4893	6.2343
15	A"	670.5310	3.2274	0.4621
16	A'	701.0955	3.8453	0.3345
17	A"	730.2003	3.8396	5.6412
18	A'	876.8855	6.5082	147.4321
19	A'	1045.2060	8.9348	166.4209
20	A'	1074.2670	9.2999	40.6305
21	A'	1211.6832	11.2958	20.8354
22	A'	1343.5335	13.0935	10.5193
23	A'	1389.7603	14.2869	46.5691
24	A'	1421.1344	14.7960	312.6457
25	A'	1468.1780	16.0225	366.8311
26	A'	1583.3242	17.9158	147.3276
27	A'	1597.9928	18.6262	5.5555

pbe/pyFCFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	92.9862	0.1077	0.0004
2	A"	134.6774	0.2000	0.0000
3	A'	196.9285	0.5378	0.0239
4	A"	203.1263	0.3655	1.9053
5	A'	267.4438	0.7932	0.2902
6	A'	305.1156	1.1074	0.4100

7	A''	318.5579	0.8213	0.6351
8	A'	324.8380	1.1686	0.3366
9	A''	396.3276	1.1737	0.7659
10	A'	396.7607	1.7810	0.2241
11	A'	456.0843	1.9727	0.5774
12	A'	578.0647	3.3718	0.5246
13	A''	610.7290	2.7333	1.5148
14	A'	614.2028	3.5094	5.7855
15	A''	669.0983	3.2137	0.2241
16	A'	702.6710	3.8625	0.3175
17	A''	723.0231	3.7680	4.8511
18	A'	880.0395	6.5585	143.8444
19	A'	1047.8471	8.9796	167.9187
20	A'	1078.6418	9.3634	35.1699
21	A'	1216.0121	11.3755	20.6634
22	A'	1347.0753	13.1573	12.4402
23	A'	1395.4308	14.4142	48.0242
24	A'	1424.5635	14.8598	289.8271
25	A'	1471.8178	16.1118	373.2099
26	A'	1586.2751	17.9793	148.9665
27	A'	1601.8625	18.7353	6.6770

pbe/pyFCFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	91.8124	0.1049	0.0016
2	A''	133.7582	0.1972	0.0000
3	A'	198.1630	0.5443	0.0346
4	A''	201.8715	0.3608	2.2940
5	A'	268.1251	0.7977	0.2569
6	A'	304.1798	1.1033	0.4154
7	A''	314.1731	0.7990	0.3949
8	A'	323.4192	1.1593	0.3583
9	A''	392.8752	1.1536	1.3248
10	A'	394.1416	1.7621	0.2797
11	A'	454.4893	1.9579	0.5868
12	A'	575.5355	3.3381	0.6950
13	A''	606.2042	2.6922	1.3226
14	A'	609.4701	3.4497	6.8742
15	A''	663.6780	3.1634	0.9426
16	A'	698.0798	3.8114	0.4376
17	A''	716.7534	3.7018	7.0951
18	A'	872.4332	6.4349	150.9563
19	A'	1042.1461	8.8820	176.1229
20	A'	1072.3773	9.2610	38.4611
21	A'	1210.0489	11.2731	20.8411
22	A'	1354.1799	13.2942	10.4733
23	A'	1393.0042	14.3601	47.6805
24	A'	1423.6369	14.8469	316.8958
25	A'	1473.3868	16.1365	378.7438
26	A'	1589.9519	18.0715	148.3768
27	A'	1604.2185	18.7714	5.1700

pbe/pyFFCFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	109.3103	0.1307	0.0000
2	B1	116.7605	0.1679	0.0168
3	B2	197.4200	0.5528	0.0419
4	B1	198.5576	0.3448	2.4747
5	A1	270.4226	0.8334	0.6442
6	B2	298.4202	0.9646	0.1742
7	A1	320.3592	1.2486	0.6506
8	B1	321.0559	0.8448	0.5860
9	A1	417.5446	1.8718	0.0148
10	A2	425.6360	1.3494	0.0000
11	B2	445.0765	1.8812	0.0716
12	A1	525.9828	2.8994	1.4115
13	B1	568.1118	2.3601	7.1519
14	A2	658.5822	3.1120	0.0000
15	A1	673.4120	4.1841	9.6795
16	B1	693.1922	3.4645	1.9618
17	B2	697.6898	3.7896	0.0529
18	A1	896.4061	6.5436	145.1560
19	B2	937.7207	7.6288	180.3061
20	B2	1124.7386	10.1379	1.4203
21	A1	1205.8823	11.0506	61.3067
22	B2	1346.7315	13.1048	18.5655
23	A1	1388.8689	14.3945	5.5811
24	A1	1428.5907	14.7821	83.0712
25	B2	1447.5430	15.5687	741.7926
26	B2	1590.4797	18.5589	2.2809
27	A1	1595.8076	18.1890	116.7674

pbe/pyFFCFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	110.6005	0.1338	0.0000
2	B1	118.6966	0.1738	0.0295
3	B2	195.5142	0.5420	0.0343
4	B1	197.9413	0.3422	2.0626
5	A1	270.1830	0.8320	0.7643
6	B2	298.9289	0.9677	0.1923
7	A1	320.0989	1.2473	0.5390
8	B1	322.1494	0.8509	0.6183
9	A1	417.5703	1.8697	0.0033
10	A2	425.4882	1.3485	0.0000
11	B2	444.1820	1.8705	0.0563
12	A1	527.6005	2.9140	1.6211
13	B1	570.3654	2.3811	6.8956
14	A2	673.2026	3.2521	0.0000
15	A1	674.6732	4.1978	7.6644

16	B2	698.7170	3.8016	0.0006
17	B1	723.8505	3.7745	1.5342
18	A1	896.2127	6.5388	134.8972
19	B2	942.8653	7.7068	162.1085
20	B2	1131.8771	10.2768	1.3347
21	A1	1209.4283	11.1232	58.7367
22	B2	1338.8014	12.9764	14.4961
23	A1	1391.2387	14.4378	7.5297
24	A1	1428.4915	14.7994	77.9796
25	B2	1448.1226	15.5868	705.2277
26	B2	1584.0111	18.3888	1.7409
27	A1	1590.8580	18.0827	109.4356

pbe/pyFFCFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	110.0198	0.1323	0.0000
2	B1	118.4827	0.1731	0.0263
3	B2	197.6594	0.5541	0.0240
4	B1	198.2036	0.3432	1.6635
5	A1	271.6010	0.8408	0.7571
6	B2	300.1034	0.9753	0.1669
7	A1	321.1356	1.2530	0.5035
8	B1	322.2852	0.8514	0.5688
9	A1	418.5696	1.8783	0.0000
10	A2	426.9897	1.3581	0.0000
11	B2	445.3972	1.8816	0.0553
12	A1	528.5297	2.9273	1.5974
13	B1	572.5678	2.3994	6.1849
14	A2	670.5255	3.2272	0.0000
15	A1	675.9272	4.2121	6.9708
16	B2	700.3066	3.8191	0.0001
17	B1	718.1715	3.7164	1.0144
18	A1	900.1262	6.5983	133.7830
19	B2	945.0955	7.7385	157.4416
20	B2	1136.5782	10.3575	0.8670
21	A1	1214.1801	11.2075	57.3595
22	B2	1342.4027	13.0442	15.0004
23	A1	1396.0499	14.5523	5.9141
24	A1	1430.8818	14.8420	79.2888
25	B2	1452.8964	15.6854	694.4191
26	B2	1586.9330	18.4744	2.2121
27	A1	1594.5058	18.1687	110.0911

pbe/pyFFCFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	108.6454	0.1290	0.0000
2	B1	117.2040	0.1693	0.0198
3	B1	196.4544	0.3370	2.0395

4	B2	198.9042	0.5609	0.0084
5	A1	272.0151	0.8444	0.6695
6	B2	299.7633	0.9735	0.1752
7	B1	318.7245	0.8334	0.4536
8	A1	319.6396	1.2447	0.5077
9	A1	415.9292	1.8578	0.0236
10	A2	424.1445	1.3397	0.0000
11	B2	443.9776	1.8691	0.0728
12	A1	525.5431	2.8861	1.6713
13	B1	562.0055	2.3103	8.7154
14	A2	667.4422	3.1977	0.0000
15	A1	672.1286	4.1635	8.0068
16	B2	695.9134	3.7708	0.0292
17	B1	712.2850	3.6572	0.7263
18	A1	891.3608	6.4623	139.5618
19	B2	940.5476	7.6664	166.7855
20	B2	1131.7594	10.2742	0.9101
21	A1	1206.3004	11.0663	56.6921
22	B2	1349.9107	13.1817	15.2136
23	A1	1394.8320	14.5158	5.4502
24	A1	1430.5011	14.8403	83.5007
25	B2	1452.9958	15.6996	727.1276
26	B2	1590.4992	18.5429	0.8498
27	A1	1597.6651	18.2377	113.6292

pbe/pyFFFFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	111.2876	0.1354	0.0000
2	B1	150.3275	0.2448	0.0010
3	B1	204.7445	0.3703	3.6514
4	B2	262.4051	0.7633	0.0393
5	A1	262.4288	0.7529	0.6422
6	B2	308.3213	1.0150	0.4960
7	A1	333.9567	1.1513	1.0766
8	B1	337.2803	0.9214	2.3656
9	A2	416.2014	1.2908	0.0000
10	B2	444.2309	1.8789	0.1165
11	A1	462.9243	2.0078	0.2612
12	A1	577.3371	3.4313	0.0046
13	B1	599.5868	2.6380	2.8650
14	A2	652.7672	3.0575	0.0000
15	A1	674.3212	4.1624	6.3922
16	B1	688.0905	3.4154	4.0349
17	B2	716.3731	4.0178	0.2463
18	B2	955.3435	7.8493	221.1810
19	A1	1051.7548	9.1147	237.4847
20	B2	1128.4666	10.2220	0.1523
21	A1	1248.4153	11.9527	28.6162
22	B2	1359.8207	13.3933	14.0343
23	A1	1395.4106	14.3576	15.6951
24	B2	1457.8055	15.8323	707.2325

25	A1	1494.9890	16.4873	158.1881
26	A1	1607.2887	18.4245	101.1568
27	B2	1617.4178	19.0701	1.9578

pbe/pyFFFFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	112.6738	0.1388	0.0000
2	B1	151.9695	0.2504	0.0001
3	B1	204.2193	0.3680	2.9701
4	A1	262.5853	0.7536	0.7374
5	B2	263.0023	0.7665	0.0406
6	B2	308.6317	1.0167	0.4702
7	A1	333.8455	1.1501	0.9391
8	B1	339.1524	0.9327	2.1603
9	A2	416.6824	1.2938	0.0000
10	B2	443.5256	1.8705	0.1042
11	A1	463.4150	2.0094	0.3415
12	A1	580.1424	3.4626	0.0011
13	B1	606.2400	2.7013	3.0278
14	A2	671.9930	3.2403	0.0000
15	A1	675.0326	4.1717	4.9703
16	B2	717.9715	4.0366	0.0725
17	B1	728.2162	3.8169	3.1479
18	B2	960.7437	7.9323	204.3611
19	A1	1057.2794	9.2083	223.1088
20	B2	1134.6173	10.3436	0.0543
21	A1	1253.0361	12.0547	26.3305
22	B2	1352.1009	13.2678	9.4493
23	A1	1397.5937	14.3917	19.1333
24	B2	1458.3433	15.8382	681.8221
25	A1	1495.5644	16.5259	148.9111
26	A1	1603.0907	18.3318	96.3443
27	B2	1611.3060	18.9134	1.2769

pbe/pyFFFFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	111.8548	0.1367	0.0000
2	B1	150.6477	0.2459	0.0004
3	B1	203.9961	0.3671	2.4345
4	A1	263.4445	0.7584	0.7409
5	B2	263.8770	0.7717	0.0422
6	B2	309.3368	1.0213	0.4476
7	A1	334.5051	1.1548	0.8462
8	B1	338.7562	0.9306	1.9257
9	A2	417.2623	1.2975	0.0000
10	B2	444.4593	1.8788	0.1008
11	A1	463.7972	2.0127	0.3886
12	A1	580.6137	3.4669	0.0001

13	B1	603.9716	2.6785	2.4590
14	A2	668.0287	3.2032	0.0000
15	A1	676.1759	4.1847	4.5889
16	B1	714.3638	3.6789	2.5975
17	B2	718.6854	4.0443	0.0711
18	B2	962.7022	7.9629	197.1321
19	A1	1059.7413	9.2487	220.1896
20	B2	1139.1105	10.4235	0.0067
21	A1	1256.8067	12.1285	26.5034
22	B2	1355.9885	13.3405	10.4814
23	A1	1402.8895	14.5048	19.5849
24	B2	1463.1622	15.9461	664.0350
25	A1	1498.6220	16.5973	144.9072
26	A1	1606.2606	18.4071	97.6437
27	B2	1615.0088	19.0095	1.6606

pbe/pyFFFFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	110.4701	0.1334	0.0000
2	B1	149.8994	0.2434	0.0001
3	B1	203.4017	0.3653	3.2352
4	A1	263.9214	0.7613	0.6916
5	B2	264.5244	0.7755	0.0433
6	B2	308.5536	1.0164	0.5428
7	A1	333.2937	1.1465	0.9863
8	B1	335.5773	0.9134	2.2060
9	A2	415.4251	1.2858	0.0000
10	B2	443.1579	1.8675	0.1098
11	A1	462.4080	2.0006	0.3003
12	A1	578.2655	3.4388	0.0050
13	B1	600.4809	2.6484	2.7469
14	A2	665.6867	3.1810	0.0000
15	A1	672.7716	4.1407	5.0847
16	B2	714.2553	3.9938	0.1482
17	B1	714.7987	3.6794	2.8776
18	B2	957.9206	7.8858	204.3665
19	A1	1054.6192	9.1604	225.5360
20	B2	1134.9870	10.3509	0.0676
21	A1	1251.5885	12.0350	26.2855
22	B2	1362.6478	13.4663	9.8348
23	A1	1400.8199	14.4643	17.9826
24	B2	1462.2986	15.9311	687.3318
25	A1	1500.6873	16.6373	152.2398
26	A1	1609.4384	18.4769	99.5113
27	B2	1617.3755	19.0587	0.8437

pbe/pyFFHFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	107.7990	0.1272	0.0000
2	B1	194.3141	0.3012	3.0021
3	A1	271.2171	0.7872	0.6215
4	B1	284.9824	0.4008	0.8900
5	B2	292.7732	0.8976	0.1112
6	A1	348.5875	1.1469	2.1034
7	B2	438.7075	1.6393	0.0644
8	A2	441.7755	1.4532	0.0000
9	B1	466.5601	0.5735	0.2609
10	A1	493.0813	2.1300	1.6514
11	B2	640.6018	1.4815	1.9376
12	A2	665.3432	3.1745	0.0000
13	A1	665.9199	3.9381	16.6530
14	B1	686.5024	2.3582	8.8907
15	A1	731.7033	3.0401	10.9715
16	B1	844.6444	0.5813	30.4169
17	B2	882.1837	2.5968	140.3760
18	B2	1110.3607	4.3309	16.0736
19	B2	1157.1518	1.3280	78.1309
20	A1	1186.6077	9.4052	198.7818
21	B2	1350.5816	13.1722	75.7843
22	A1	1374.5572	13.1720	1.2557
23	A1	1416.1538	13.3552	37.2944
24	B2	1463.2474	9.5287	704.6627
25	A1	1608.0835	17.4789	20.0163
26	B2	1609.4689	13.8580	3.2085
27	A1	3153.0290	6.4028	4.1833

pbe/pyFFHFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	109.3891	0.1310	0.0000
2	B1	194.7113	0.3044	2.3910
3	A1	271.4773	0.7884	0.6731
4	B1	287.4794	0.4077	0.8824
5	B2	293.5622	0.9019	0.0851
6	A1	348.8303	1.1478	1.7898
7	B2	437.9545	1.6293	0.0522
8	A2	442.3620	1.4571	0.0000
9	B1	470.4377	0.5708	0.2646
10	A1	494.3679	2.1344	1.8796
11	B2	642.7923	1.4828	1.9259
12	A1	668.4422	3.9904	14.0770
13	A2	682.4547	3.3400	0.0000
14	B1	711.9273	1.9117	10.8506
15	A1	733.3139	3.0498	11.5393
16	B1	863.3960	0.6456	24.4014
17	B2	886.0780	2.5572	124.5703
18	B2	1117.3584	4.0886	18.7005
19	B2	1160.5878	1.3799	70.9333
20	A1	1192.6999	9.5095	182.9859
21	B2	1342.9848	13.0046	63.1571

22	A1	1378.0799	13.2284	1.9897
23	A1	1416.1922	13.4243	38.8070
24	B2	1463.5460	9.6399	691.3440
25	B2	1604.1039	13.4475	4.7968
26	A1	1604.4571	17.4150	19.7449
27	A1	3146.6971	6.3737	3.4780

pbe/pyFFHFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	108.8777	0.1297	0.0000
2	B1	194.6043	0.3035	1.9766
3	A1	272.4589	0.7938	0.6760
4	B1	286.7100	0.4054	0.8730
5	B2	294.3750	0.9067	0.0841
6	A1	349.3726	1.1519	1.6365
7	B2	439.0683	1.6379	0.0522
8	A2	443.2210	1.4628	0.0000
9	B1	468.8338	0.5735	0.1828
10	A1	494.9113	2.1387	1.9312
11	B2	643.7124	1.4881	1.8832
12	A1	669.7942	4.0034	13.3486
13	A2	680.3289	3.3199	0.0000
14	B1	707.7428	2.0804	8.3234
15	A1	734.2252	3.0565	11.5057
16	B1	853.5735	0.6158	25.8333
17	B2	887.8931	2.5509	118.8159
18	B2	1122.1409	3.8663	20.2092
19	B2	1163.9101	1.4185	64.2015
20	A1	1197.2497	9.5651	180.7298
21	B2	1346.7699	13.0864	65.8305
22	A1	1382.5441	13.2525	1.7794
23	A1	1420.4879	13.5893	38.7512
24	B2	1468.9142	9.7165	671.7485
25	A1	1607.3368	17.4867	20.5533
26	B2	1608.0328	13.5703	4.2665
27	A1	3151.5781	6.3938	3.1039

pbe/pyFFHFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	107.2762	0.1259	0.0000
2	B1	193.0115	0.2993	2.5995
3	A1	272.4730	0.7943	0.6414
4	B1	284.9625	0.4020	0.9147
5	B2	294.0423	0.9063	0.1219
6	A1	347.6951	1.1405	1.8725
7	B2	437.7676	1.6322	0.0583
8	A2	440.8215	1.4467	0.0000
9	B1	464.6895	0.5616	0.1960

10	A1	492.9776	2.1245	1.6443
11	B2	640.2313	1.4977	1.7755
12	A1	665.6677	3.9496	13.9514
13	A2	675.8122	3.2764	0.0000
14	B1	702.4430	1.9255	9.8842
15	A1	731.5190	3.0333	11.4225
16	B1	850.9529	0.6202	28.1492
17	B2	884.0978	2.5751	128.9087
18	B2	1117.2350	4.0779	16.6320
19	B2	1161.5940	1.3622	67.1844
20	A1	1188.8150	9.4421	189.5892
21	B2	1354.7437	13.2473	62.8678
22	A1	1381.1545	13.2579	1.5217
23	A1	1418.5227	13.4455	37.7372
24	B2	1466.6568	9.7885	695.6745
25	B2	1608.5611	13.7776	5.0359
26	A1	1611.3700	17.5654	19.6809
27	A1	3157.5271	6.4211	5.7518

pbe/pyFHFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	121.4399	0.1439	0.1225
2	A"	200.8206	0.3259	3.2774
3	A"	249.5894	0.2630	1.1426
4	A'	263.7342	0.7622	0.1708
5	A'	309.2563	0.9695	0.7504
6	A'	340.8624	1.1254	1.2292
7	A"	370.0506	0.8492	0.5852
8	A'	448.8515	1.6739	0.4403
9	A'	513.6892	1.7446	2.9981
10	A'	579.8659	3.4401	0.0775
11	A"	601.2129	1.1951	5.8677
12	A'	646.9437	1.5771	1.9794
13	A"	652.7440	1.8045	0.0023
14	A"	701.8410	2.0725	0.9519
15	A'	777.2201	3.5182	45.5504
16	A"	803.9310	0.5830	34.5295
17	A'	997.1357	2.6384	98.3396
18	A'	1043.2957	7.3188	174.6507
19	A'	1122.1479	1.4332	85.7738
20	A'	1207.8316	4.9407	45.0185
21	A'	1355.5788	13.2889	13.2648
22	A'	1375.6891	10.7300	46.8142
23	A'	1417.4987	12.9286	183.2544
24	A'	1480.7894	9.2781	399.3445
25	A'	1600.9756	14.9687	243.4452
26	A'	1616.4980	17.6853	36.7282
27	A'	3164.1017	6.4532	3.6249

pbe/pyFHFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	122.5910	0.1467	0.0997
2	A''	201.1470	0.3311	2.6312
3	A''	252.1164	0.2657	1.2162
4	A'	264.1193	0.7639	0.2035
5	A'	309.5331	0.9700	0.6608
6	A'	341.1116	1.1265	0.9706
7	A''	370.1692	0.8558	0.5668
8	A'	448.4811	1.6699	0.4177
9	A'	512.7467	1.7377	2.5237
10	A'	582.7851	3.4736	0.0403
11	A''	607.1087	1.1972	5.9618
12	A'	648.5634	1.5771	2.1878
13	A''	662.5989	1.6419	0.0082
14	A''	723.7041	1.8235	0.1163
15	A'	778.8554	3.5237	39.8864
16	A''	819.2276	0.6562	31.6656
17	A'	999.0914	2.5249	87.1182
18	A'	1049.4768	7.3523	159.3260
19	A'	1127.2400	1.4699	88.1174
20	A'	1212.4994	5.1305	41.3703
21	A'	1348.9423	13.2845	11.0653
22	A'	1379.5050	10.8104	51.2697
23	A'	1417.1718	12.8616	169.0556
24	A'	1481.5774	9.3670	390.9961
25	A'	1596.8152	14.7144	232.7760
26	A'	1610.8508	17.4322	33.6206
27	A'	3157.9498	6.4246	2.8064

pbe/pyFHFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	121.9110	0.1450	0.0850
2	A''	200.6898	0.3275	2.2455
3	A''	251.1528	0.2654	1.1999
4	A'	265.0077	0.7691	0.2074
5	A'	310.3392	0.9748	0.6421
6	A'	341.8985	1.1319	0.9048
7	A''	370.0561	0.8566	0.4474
8	A'	449.1851	1.6740	0.3931
9	A'	513.7176	1.7458	2.3026
10	A'	583.4440	3.4788	0.0284
11	A''	606.3247	1.2209	5.1557
12	A'	649.3981	1.5807	2.0959
13	A''	661.8845	1.6990	0.0248
14	A''	716.5456	2.0157	0.2855
15	A'	780.2313	3.5344	38.5233
16	A''	808.6475	0.6097	30.2586
17	A'	1001.3076	2.4848	83.5463
18	A'	1053.0080	7.4484	153.5848

19	A'	1130.7672	1.4771	84.8749
20	A'	1216.2849	5.2611	40.3819
21	A'	1353.4406	13.3501	10.2628
22	A'	1384.8125	11.0898	52.6935
23	A'	1421.9260	12.8692	155.2937
24	A'	1485.5995	9.4670	387.2214
25	A'	1600.1489	14.7677	234.2842
26	A'	1614.4455	17.5283	35.2673
27	A'	3162.8080	6.4445	2.4951

pbe/pyFHFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	120.9307	0.1426	0.1116
2	A"	200.1587	0.3272	2.8990
3	A"	249.5093	0.2626	1.2454
4	A'	265.5108	0.7722	0.1891
5	A'	309.4183	0.9713	0.7608
6	A'	340.2316	1.1223	1.1027
7	A"	368.0037	0.8406	0.4940
8	A'	448.2684	1.6720	0.4143
9	A'	512.3648	1.7378	2.4600
10	A'	580.9778	3.4506	0.0710
11	A"	602.6994	1.2062	5.7512
12	A'	645.9872	1.5911	1.8729
13	A"	657.7511	1.6524	0.0246
14	A"	715.5315	1.9060	0.1553
15	A'	776.7605	3.5024	40.7053
16	A"	810.3032	0.6226	35.3030
17	A'	997.8402	2.5844	92.5820
18	A'	1047.3601	7.3634	162.2379
19	A'	1127.3736	1.4416	79.6497
20	A'	1211.9293	5.0083	40.2927
21	A'	1358.1506	13.4081	13.8462
22	A'	1382.6963	10.9205	50.3982
23	A'	1420.5295	12.9213	167.4374
24	A'	1484.8230	9.5441	398.1202
25	A'	1602.3321	15.0301	240.0983
26	A'	1616.7573	17.6526	32.3041
27	A'	3169.0061	6.4731	5.1327

pbe/pyHHHHH_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	355.1518	0.1873	0.0000
2	B1	396.3132	0.3495	3.5462
3	A1	594.2348	1.4722	3.2547
4	B2	647.1338	1.5587	0.3242
5	B1	688.9585	0.3558	69.8617
6	B1	732.2097	0.8909	6.6203

7	A2	860.8490	0.5449	0.0000
8	B1	915.1022	0.6557	0.0603
9	A2	952.1139	0.7916	0.0000
10	B1	962.4791	0.6906	0.0012
11	A1	981.5213	3.9533	5.7214
12	A1	1022.5351	2.9628	3.7186
13	B2	1049.1105	1.1195	0.0064
14	A1	1064.0003	1.0958	6.1185
15	B2	1137.5770	0.8274	1.7501
16	A1	1207.0304	1.0975	4.0419
17	B2	1296.4291	9.4629	0.3927
18	B2	1333.8274	1.2595	0.0154
19	B2	1424.6853	2.5479	23.7488
20	A1	1460.8124	2.5356	1.9535
21	B2	1574.9647	8.8072	9.1618
22	A1	1578.8154	7.9738	20.5029
23	B2	3075.9704	6.0596	30.7065
24	A1	3078.3161	6.0864	4.4521
25	A1	3104.0604	6.1758	3.1551
26	B2	3118.5056	6.2625	25.9776
27	A1	3127.1246	6.3324	8.3023

pbe/pyHHHHH_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	358.1713	0.1880	0.0000
2	B1	399.2173	0.3513	3.3944
3	A1	593.2064	1.4638	3.9869
4	B2	645.7558	1.5478	0.1910
5	B1	694.8473	0.3529	64.1338
6	B1	741.5279	0.9052	4.2006
7	A2	868.7396	0.5552	0.0000
8	B1	925.6221	0.6721	0.0275
9	A2	968.6562	0.8254	0.0000
10	A1	981.3588	3.8896	6.0761
11	B1	982.9252	0.7436	0.0004
12	A1	1025.8252	2.8877	4.5376
13	B2	1049.0314	1.1182	0.0189
14	A1	1064.2577	1.1143	4.0694
15	B2	1134.3463	0.8255	1.8429
16	A1	1204.5737	1.1000	3.2738
17	B2	1290.7663	9.2009	0.2876
18	B2	1336.3045	1.2655	0.0001
19	B2	1426.3407	2.5704	22.8939
20	A1	1463.7245	2.5334	1.7192
21	B2	1573.3096	8.6110	8.7143
22	A1	1576.8676	7.8560	20.0580
23	B2	3070.2682	6.0363	29.6205
24	A1	3072.7166	6.0650	4.6155
25	A1	3100.4979	6.1596	2.7547
26	B2	3114.4631	6.2439	25.0674
27	A1	3123.2818	6.3135	8.1983

pbe/pyHHHHH_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	358.3188	0.1878	0.0000
2	B1	399.6508	0.3527	3.2846
3	A1	594.1627	1.4709	4.2257
4	B2	647.7118	1.5592	0.2526
5	B1	693.7741	0.3473	64.3143
6	B1	742.8135	0.9299	3.4367
7	A2	867.9928	0.5541	0.0000
8	B1	923.7268	0.6720	0.0263
9	A2	967.1692	0.8242	0.0000
10	B1	981.9203	0.7408	0.0027
11	A1	983.3904	3.9187	6.7804
12	A1	1027.3608	2.8910	5.0015
13	B2	1051.0350	1.1237	0.0115
14	A1	1066.3027	1.1173	3.8656
15	B2	1137.8941	0.8303	1.7320
16	A1	1207.4469	1.1043	2.9500
17	B2	1294.8389	9.3002	0.3492
18	B2	1338.9174	1.2700	0.0003
19	B2	1429.9108	2.5767	23.7885
20	A1	1466.8043	2.5472	2.3270
21	B2	1576.8793	8.6880	8.4140
22	A1	1579.8655	7.8971	20.6237
23	B2	3073.6127	6.0493	30.8294
24	A1	3076.2357	6.0794	6.1559
25	A1	3104.6536	6.1760	3.1957
26	B2	3118.9513	6.2618	25.5526
27	A1	3127.6870	6.3322	8.1552

pbe/pyHHHHH_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	356.1980	0.1863	0.0000
2	B1	396.8451	0.3481	3.4376
3	A1	593.8361	1.4713	3.3413
4	B2	645.5783	1.5504	0.4184
5	B1	687.3672	0.3425	76.9360
6	B1	737.3333	0.9169	4.9733
7	A2	861.0266	0.5451	0.0000
8	B1	915.7480	0.6584	0.0822
9	A2	959.3559	0.8092	0.0000
10	B1	973.5792	0.7261	0.0027
11	A1	979.6212	3.9246	6.1158
12	A1	1024.1989	2.9513	3.8776
13	B2	1049.6307	1.1164	0.0789
14	A1	1063.9303	1.0971	6.2850
15	B2	1137.6168	0.8242	1.6126

16	A1	1206.6524	1.0925	3.3471
17	B2	1298.1115	9.3953	0.2488
18	B2	1331.9610	1.2590	0.0089
19	B2	1423.4887	2.5641	25.9143
20	A1	1459.2754	2.5367	3.0362
21	B2	1574.4635	8.8579	7.5418
22	A1	1579.7116	8.0998	20.1889
23	B2	3083.0972	6.0885	21.8645
24	A1	3085.2052	6.1145	3.8365
25	A1	3111.1367	6.2038	2.5803
26	B2	3124.8622	6.2882	17.4083
27	A1	3133.1759	6.3578	5.0222

pw91/pyCCCCC_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	53.2208	0.0569	0.0000
2	B1	77.1399	0.1185	0.0161
3	B1	142.2410	0.1905	0.0106
4	A1	197.1286	0.7633	0.1032
5	B2	209.2974	0.7936	0.4137
6	A1	212.2380	0.7560	0.1159
7	B2	217.8461	0.9736	0.0020
8	B1	273.1293	0.5929	0.4787
9	B2	322.1643	1.7694	0.4445
10	A1	337.5685	1.9122	0.1585
11	A2	351.8686	0.9133	0.0000
12	A1	373.8125	2.6955	0.2878
13	A1	524.9048	2.8189	8.0373
14	B1	550.3968	2.2152	1.0076
15	B2	565.4899	2.5368	2.7913
16	A2	600.0490	2.5676	0.0000
17	B2	660.9887	3.9909	107.8911
18	B1	696.2029	3.4920	0.0624
19	A1	799.3577	5.1815	97.9751
20	B2	860.3854	5.6642	3.6482
21	A1	1045.7834	8.1000	34.5768
22	A1	1190.9744	10.2949	3.3147
23	B2	1279.1037	11.6079	180.4865
24	A1	1310.5446	12.2943	128.2514
25	B2	1314.3557	12.7700	293.4990
26	A1	1484.2590	15.6713	94.5111
27	B2	1517.2037	17.0517	55.2436

pw91/pyCCCCC_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	55.7617	0.0625	0.0000
2	B1	79.7023	0.1261	0.0113
3	B1	143.3029	0.1933	0.0002

4	A1	192.9414	0.7434	0.0462
5	B2	205.6628	0.7675	0.3828
6	A1	208.9043	0.7227	0.0784
7	B2	210.6603	0.9096	0.0045
8	B1	276.7140	0.6096	0.5221
9	B2	322.0627	1.7653	0.4394
10	A1	337.8785	1.9146	0.1410
11	A2	356.9184	0.9398	0.0000
12	A1	374.5003	2.7024	0.3006
13	A1	525.3990	2.8254	6.4762
14	B1	561.0836	2.3038	1.0369
15	B2	562.4837	2.5111	1.8882
16	A2	619.6609	2.7386	0.0000
17	B2	662.2575	4.0025	97.4275
18	B1	725.1387	3.7859	0.9455
19	A1	800.3820	5.1986	90.3173
20	B2	860.1984	5.6669	3.5531
21	A1	1045.9358	8.1065	31.3279
22	A1	1190.6235	10.2813	4.6982
23	B2	1276.6257	11.5745	141.2890
24	A1	1306.7102	12.2229	108.8524
25	B2	1309.0666	12.6748	287.1019
26	A1	1478.9001	15.5541	86.2592
27	B2	1508.2417	16.8221	49.2153

pw91/pyCCCCC_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	55.8892	0.0627	0.0000
2	B1	80.0131	0.1270	0.0141
3	B1	144.0411	0.1954	0.0193
4	A1	193.8968	0.7516	0.0620
5	B2	206.8064	0.7761	0.3335
6	A1	210.1651	0.7311	0.0703
7	B2	211.3316	0.9154	0.0027
8	B1	277.5570	0.6135	0.4679
9	B2	323.4975	1.7781	0.4430
10	A1	339.3780	1.9270	0.1622
11	A2	359.2797	0.9525	0.0000
12	A1	376.5371	2.7282	0.2885
13	A1	528.3202	2.8550	6.1358
14	B1	563.7318	2.3254	0.9604
15	B2	566.1725	2.5458	2.0880
16	A2	622.8960	2.7677	0.0000
17	B2	667.6550	4.0655	95.9997
18	B1	726.7058	3.8026	0.8310
19	A1	804.8185	5.2618	92.5349
20	B2	866.2684	5.7520	3.0687
21	A1	1051.5496	8.1988	31.4285
22	A1	1193.1958	10.3285	4.3669
23	B2	1277.7562	11.5915	153.5754
24	A1	1309.0478	12.2666	110.6934

25	B2	1311.6108	12.7205	271.5204
26	A1	1479.4535	15.5664	89.6583
27	B2	1510.8336	16.8907	47.8557

pw91/pyCCCCC_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	53.9782	0.0586	0.0000
2	B1	77.4271	0.1191	0.0150
3	B1	141.5052	0.1886	0.0542
4	A1	195.7746	0.7523	0.0808
5	B2	208.0536	0.7846	0.2620
6	A1	210.4573	0.7444	0.0455
7	B2	216.2289	0.9591	0.0019
8	B1	272.8113	0.5916	0.2364
9	B2	319.7657	1.7511	0.5318
10	A1	335.0171	1.8906	0.1588
11	A2	353.1481	0.9199	0.0000
12	A1	370.2887	2.6530	0.3120
13	A1	519.4598	2.7619	8.6309
14	B1	550.3265	2.2133	0.7841
15	B2	561.2779	2.5054	3.8827
16	A2	603.9390	2.6012	0.0000
17	B2	653.8666	3.8943	109.1709
18	B1	703.3530	3.5674	1.0494
19	A1	792.3787	5.0848	101.7817
20	B2	852.8002	5.5532	2.9957
21	A1	1037.1907	7.9624	36.5774
22	A1	1187.3252	10.2200	2.9464
23	B2	1281.1057	11.6367	205.6885
24	A1	1306.9916	12.2235	124.3443
25	B2	1312.0093	12.7244	254.1971
26	A1	1484.2273	15.6686	94.4288
27	B2	1515.4851	17.0185	53.0505

pw91/pyFCFCF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	86.4176	0.0940	0.0000
2	B1	105.3634	0.1427	0.0106
3	A1	178.6010	0.4977	0.0218
4	B1	205.1388	0.3742	2.0712
5	B2	218.2834	0.6306	0.0550
6	B2	303.7232	1.1658	0.5139
7	B1	305.9369	0.7638	0.2588
8	A1	311.9929	1.2411	0.1076
9	A2	365.6602	0.9881	0.0000
10	A1	396.8323	1.8960	0.7431
11	B2	398.5435	1.7333	0.0537
12	A1	563.3725	3.0096	1.6129

13	A1	592.5568	3.4430	2.4205
14	B1	617.8518	2.7933	1.2634
15	A2	662.6622	3.1495	0.0000
16	B2	681.1253	3.6313	1.0518
17	B1	719.0443	3.7269	11.2954
18	B2	769.9140	5.0376	127.6622
19	A1	1034.5046	8.7537	185.4664
20	B2	1057.3134	9.0655	24.3237
21	A1	1106.2451	9.1603	7.4218
22	B2	1339.4346	12.9819	11.8566
23	A1	1379.0995	14.1008	43.3286
24	B2	1399.8591	14.4022	456.9842
25	A1	1421.9124	14.7942	93.9916
26	A1	1566.7074	17.5131	176.9364
27	B2	1584.4049	18.4423	49.5928

pw91/pyFCFCF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	87.8509	0.0972	0.0000
2	B1	106.7022	0.1462	0.0008
3	A1	176.2511	0.4845	0.0059
4	B1	203.3100	0.3674	1.9269
5	B2	216.1854	0.6181	0.0456
6	B2	303.2888	1.1648	0.5415
7	B1	307.8058	0.7743	0.4176
8	A1	311.7898	1.2410	0.0908
9	A2	360.2003	0.9585	0.0000
10	A1	397.0445	1.8961	0.7111
11	B2	398.1771	1.7242	0.0795
12	A1	563.7463	2.9885	1.4166
13	A1	594.3510	3.4884	1.5344
14	B1	619.5223	2.8089	1.2086
15	A2	671.0406	3.2310	0.0000
16	B2	680.9879	3.6306	0.4637
17	B1	735.1535	3.8941	8.9185
18	B2	769.0105	5.0210	117.5761
19	A1	1039.7781	8.8181	168.6441
20	B2	1062.0801	9.1619	20.7583
21	A1	1105.5187	9.1666	4.3903
22	B2	1332.4698	12.8767	6.1472
23	A1	1384.1405	14.1851	51.8529
24	B2	1400.9449	14.4151	431.1988
25	A1	1421.8793	14.8404	71.7220
26	A1	1562.0293	17.4098	171.9753
27	B2	1576.9482	18.2547	52.0143

pw91/pyFCFCF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	87.5944	0.0966	0.0000
2	B1	106.4267	0.1455	0.0052
3	A1	178.3124	0.4959	0.0025
4	B1	204.0975	0.3704	1.5621
5	B2	218.5169	0.6318	0.0369
6	B2	304.9282	1.1767	0.5189
7	B1	308.9235	0.7793	0.3802
8	A1	313.3718	1.2517	0.0714
9	A2	363.4282	0.9760	0.0000
10	A1	398.4336	1.9090	0.6869
11	B2	399.3499	1.7340	0.0808
12	A1	565.0079	3.0143	1.2110
13	A1	595.7089	3.4916	1.4923
14	B1	620.5578	2.8186	0.9663
15	A2	672.7763	3.2480	0.0000
16	B2	683.6352	3.6592	0.4673
17	B1	735.2282	3.8952	7.6732
18	B2	773.9491	5.0903	114.6851
19	A1	1042.3665	8.8633	167.6610
20	B2	1066.6014	9.2299	18.0755
21	A1	1110.5129	9.2449	4.8846
22	B2	1335.9152	12.9358	8.1631
23	A1	1390.4748	14.3295	50.6467
24	B2	1404.8676	14.5005	416.6145
25	A1	1424.5158	14.8914	76.3136
26	A1	1563.9700	17.4572	176.3281
27	B2	1581.2892	18.3713	54.1653

pw91/pyFCFCF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	86.4047	0.0940	0.0000
2	B1	105.2543	0.1422	0.0134
3	A1	179.1111	0.5006	0.0001
4	B1	202.2467	0.3633	1.6867
5	B2	219.9255	0.6402	0.0282
6	B2	303.8592	1.1696	0.4425
7	B1	304.6694	0.7590	0.1320
8	A1	311.6345	1.2427	0.0465
9	A2	356.8847	0.9405	0.0000
10	A1	394.8612	1.8775	0.8122
11	B2	396.9716	1.7177	0.0183
12	A1	561.6401	2.9618	1.5593
13	A1	591.7214	3.4547	1.6861
14	B1	615.2822	2.7691	0.6294
15	A2	663.9058	3.1642	0.0000
16	B2	678.1971	3.6012	0.9407
17	B1	721.8067	3.7567	13.6362
18	B2	762.9547	4.9310	122.3918
19	A1	1036.2962	8.7505	182.8443
20	B2	1060.2369	9.1260	19.8528
21	A1	1100.3406	9.0816	3.7766

22	B2	1342.9780	13.0756	4.9720
23	A1	1387.7051	14.2684	49.8421
24	B2	1403.2076	14.4521	447.3200
25	A1	1425.8158	14.9185	82.0790
26	A1	1568.6903	17.5565	179.4963
27	B2	1582.6284	18.4026	46.5753

pw91/pyFCFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	91.9150	0.1054	0.0018
2	A"	134.4534	0.1992	0.0008
3	A'	196.3160	0.5345	0.0287
4	A"	204.6139	0.3713	2.8209
5	A'	266.2378	0.7863	0.2487
6	A'	303.8505	1.0995	0.4370
7	A"	316.3665	0.8086	0.5739
8	A'	323.6762	1.1614	0.4412
9	A'	395.6251	1.7772	0.2816
10	A"	395.8095	1.1710	1.1321
11	A'	455.6303	1.9703	0.5121
12	A'	574.2642	3.3342	0.5613
13	A"	609.1150	2.7181	1.8447
14	A'	612.1293	3.4747	7.9296
15	A"	658.4649	3.1116	0.3741
16	A'	701.2243	3.8459	0.5606
17	A"	706.7340	3.6003	7.4877
18	A'	873.8518	6.4731	161.8849
19	A'	1039.8292	8.8517	185.9658
20	A'	1069.1856	9.1964	40.9400
21	A'	1206.6798	11.1812	23.2116
22	A'	1347.9682	13.1515	17.2972
23	A'	1382.7362	14.1585	41.7514
24	A'	1420.1052	14.7714	326.3608
25	A'	1466.5851	15.9645	391.5569
26	A'	1587.4322	18.0007	149.3881
27	A'	1603.6501	18.7798	7.1538

pw91/pyFCFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	93.6326	0.1093	0.0000
2	A"	135.9654	0.2038	0.0011
3	A'	194.1946	0.5228	0.0230
4	A"	203.4884	0.3668	2.4400
5	A'	266.6513	0.7889	0.2950
6	A'	303.8515	1.1030	0.4275
7	A"	318.7438	0.8219	0.7072
8	A'	323.7016	1.1591	0.3955
9	A'	395.5189	1.7712	0.2427

10	A''	396.1129	1.1728	0.8961
11	A'	455.7362	1.9696	0.5916
12	A'	576.6188	3.3462	0.6760
13	A'	612.1364	3.4864	6.4076
14	A''	613.0720	2.7552	1.9024
15	A''	672.3640	3.2449	0.4663
16	A'	702.0909	3.8562	0.3343
17	A''	732.8449	3.8673	5.6983
18	A'	875.9307	6.4899	147.7586
19	A'	1045.0393	8.9301	165.9568
20	A'	1073.4851	9.2881	42.9382
21	A'	1211.3612	11.2854	21.2538
22	A'	1341.1749	13.0489	10.6432
23	A'	1387.0399	14.2360	44.8163
24	A'	1420.4152	14.7772	306.4988
25	A'	1467.1160	15.9986	372.4093
26	A'	1583.1474	17.9139	147.8087
27	A'	1597.7753	18.6213	5.7985

pw91/pyFCFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	93.2860	0.1084	0.0006
2	A''	135.0619	0.2012	0.0000
3	A'	196.3662	0.5347	0.0241
4	A''	203.7930	0.3679	1.9870
5	A'	267.8008	0.7955	0.2930
6	A'	305.0333	1.1099	0.4162
7	A''	319.4700	0.8258	0.6567
8	A'	324.8691	1.1682	0.3444
9	A'	396.7131	1.7816	0.2379
10	A''	397.3483	1.1796	0.7815
11	A'	456.5708	1.9770	0.5913
12	A'	577.1791	3.3562	0.5688
13	A''	612.5004	2.7491	1.5406
14	A'	614.0757	3.5069	5.9444
15	A''	671.0425	3.2322	0.2287
16	A'	703.7382	3.8742	0.3168
17	A''	725.9298	3.7983	4.9313
18	A'	879.1748	6.5412	144.0889
19	A'	1047.8335	8.9775	167.3877
20	A'	1078.0178	9.3541	37.0073
21	A'	1215.8901	11.3698	21.0526
22	A'	1344.7569	13.1140	12.5107
23	A'	1392.8764	14.3672	46.2142
24	A'	1423.8576	14.8415	283.5405
25	A'	1470.8775	16.0912	378.1083
26	A'	1586.0612	17.9765	149.4189
27	A'	1601.5888	18.7294	6.8312

pw91/pyFCFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	92.0493	0.1055	0.0020
2	A"	134.0797	0.1982	0.0000
3	A'	197.4530	0.5403	0.0350
4	A"	202.5483	0.3633	2.3883
5	A'	268.4100	0.7995	0.2595
6	A'	304.0105	1.1053	0.4218
7	A"	315.0916	0.8034	0.4143
8	A'	323.3331	1.1578	0.3667
9	A"	393.9765	1.1600	1.3420
10	A'	393.9800	1.7615	0.3006
11	A'	454.8531	1.9610	0.6047
12	A'	574.6315	3.3224	0.7462
13	A"	608.1116	2.7091	1.3539
14	A'	609.2342	3.4462	6.9972
15	A"	665.6896	3.1823	0.9489
16	A'	698.9053	3.8203	0.4368
17	A"	719.7765	3.7329	7.1641
18	A'	871.5041	6.4169	150.8790
19	A'	1042.0463	8.8782	175.3078
20	A'	1071.6929	9.2512	40.4275
21	A'	1209.8464	11.2667	21.1728
22	A'	1351.7240	13.2478	10.6029
23	A'	1390.4301	14.3119	46.0095
24	A'	1422.7917	14.8260	309.5872
25	A'	1472.3474	16.1150	383.6598
26	A'	1589.3973	18.0613	148.6293
27	A'	1603.7266	18.7605	5.3894

pw91/pyFFCFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	109.7817	0.1318	0.0000
2	B1	117.0412	0.1688	0.0153
3	B2	196.7135	0.5487	0.0428
4	B1	199.0925	0.3466	2.6057
5	A1	270.3660	0.8337	0.6543
6	B2	298.4121	0.9646	0.1820
7	A1	320.0472	1.2478	0.6515
8	B1	321.7904	0.8485	0.6036
9	A1	417.4521	1.8717	0.0231
10	A2	426.3212	1.3537	0.0000
11	B2	445.6062	1.8858	0.0719
12	A1	524.8502	2.8826	1.4744
13	B1	569.8084	2.3744	7.2873
14	A2	660.5882	3.1309	0.0000
15	A1	673.6327	4.1873	9.8617
16	B1	696.1970	3.4942	1.9762
17	B2	698.3833	3.7970	0.0542
18	A1	894.3085	6.5075	144.4414

19	B2	937.6069	7.6265	181.3892
20	B2	1123.8053	10.1189	1.4470
21	A1	1205.4449	11.0407	62.2268
22	B2	1343.5121	13.0440	18.4854
23	A1	1386.2632	14.3474	5.2059
24	A1	1426.9405	14.7461	82.4217
25	B2	1446.3673	15.5415	742.8415
26	B2	1589.3553	18.5349	2.5261
27	A1	1594.7318	18.1652	117.1060

pw91/pyFFCFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	111.0840	0.1349	0.0000
2	B1	119.0484	0.1748	0.0282
3	B2	194.9782	0.5389	0.0339
4	B1	198.5354	0.3443	2.1709
5	A1	270.3486	0.8337	0.7765
6	B2	299.1046	0.9689	0.1995
7	A1	319.8603	1.2471	0.5323
8	B1	322.9776	0.8550	0.6414
9	A1	417.6598	1.8717	0.0077
10	A2	426.3451	1.3539	0.0000
11	B2	444.9449	1.8774	0.0580
12	A1	526.5817	2.8982	1.6933
13	B1	572.2115	2.3967	6.9779
14	A2	675.0829	3.2701	0.0000
15	A1	675.1143	4.2041	7.7911
16	B2	699.7146	3.8124	0.0005
17	B1	726.5766	3.8028	1.5586
18	A1	894.2577	6.5041	134.5101
19	B2	942.8644	7.7068	163.4188
20	B2	1131.0694	10.2586	1.3378
21	A1	1209.4609	11.1211	59.8020
22	B2	1336.2531	12.9284	14.5298
23	A1	1389.0296	14.3998	6.9726
24	A1	1427.3526	14.7714	77.4307
25	B2	1447.5291	15.5710	704.3492
26	B2	1583.6856	18.3837	2.0023
27	A1	1590.4930	18.0747	109.9445

pw91/pyFFCFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	110.4556	0.1334	0.0000
2	B1	118.8002	0.1741	0.0244
3	B2	197.1009	0.5509	0.0241
4	B1	198.8770	0.3456	1.7424
5	A1	271.7793	0.8427	0.7720
6	B2	300.3114	0.9767	0.1774

7	A1	320.9803	1.2535	0.4970
8	B1	323.0496	0.8551	0.5879
9	A1	418.6224	1.8796	0.0007
10	A2	427.8761	1.3637	0.0000
11	B2	446.1198	1.8881	0.0565
12	A1	527.5118	2.9114	1.6785
13	B1	574.3726	2.4146	6.2653
14	A2	672.4923	3.2459	0.0000
15	A1	676.3788	4.2182	7.0555
16	B2	701.3777	3.8308	0.0001
17	B1	720.9995	3.7457	1.0424
18	A1	898.2224	6.5643	133.4883
19	B2	945.2302	7.7404	158.2615
20	B2	1136.0736	10.3451	0.8610
21	A1	1214.2920	11.2073	58.2122
22	B2	1339.8994	12.9977	14.9750
23	A1	1394.0006	14.5179	5.4169
24	A1	1429.8165	14.8163	78.8437
25	B2	1452.3809	15.6717	692.2286
26	B2	1586.5873	18.4686	2.4809
27	A1	1594.0664	18.1594	110.7349

pw91/pyFFCFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	109.0141	0.1299	0.0000
2	B1	117.4656	0.1701	0.0178
3	B1	197.1412	0.3394	2.1282
4	B2	198.2209	0.5569	0.0084
5	A1	272.0918	0.8457	0.6864
6	B2	299.8952	0.9744	0.1856
7	A1	319.3853	1.2443	0.5028
8	B1	319.4659	0.8370	0.4703
9	A1	415.8563	1.8580	0.0323
10	A2	425.0945	1.3457	0.0000
11	B2	444.5635	1.8743	0.0739
12	A1	524.5154	2.8703	1.7575
13	B1	563.9604	2.3264	8.8051
14	A2	669.5166	3.2174	0.0000
15	A1	672.5040	4.1685	8.0638
16	B2	696.7384	3.7796	0.0288
17	B1	715.2154	3.6872	0.7551
18	A1	889.3685	6.4276	139.0647
19	B2	940.6057	7.6670	167.2767
20	B2	1131.2423	10.2620	0.9040
21	A1	1206.2364	11.0634	57.4928
22	B2	1347.2828	13.1324	15.1772
23	A1	1392.7605	14.4801	5.0427
24	A1	1429.2675	14.8121	82.9223
25	B2	1452.4322	15.6851	724.0538
26	B2	1589.8934	18.5317	1.0129
27	A1	1596.9153	18.2214	114.2285

pw91/pyFFFFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	111.6914	0.1364	0.0000
2	B1	150.7075	0.2461	0.0015
3	B1	205.2436	0.3722	3.8347
4	A1	262.5282	0.7535	0.6455
5	B2	262.5728	0.7643	0.0382
6	B2	308.3265	1.0151	0.5132
7	A1	334.0220	1.1518	1.1078
8	B1	338.0186	0.9253	2.4368
9	A2	416.9554	1.2954	0.0000
10	B2	444.7783	1.8837	0.1199
11	A1	463.3103	2.0114	0.2569
12	A1	576.8749	3.4246	0.0035
13	B1	601.4243	2.6547	2.9608
14	A2	654.7437	3.0759	0.0000
15	A1	674.6607	4.1669	6.5033
16	B1	691.6008	3.4496	4.0644
17	B2	717.2648	4.0281	0.2606
18	B2	955.4719	7.8504	222.5122
19	A1	1051.8003	9.1158	238.1831
20	B2	1127.8165	10.2080	0.1646
21	A1	1248.3161	11.9478	28.9825
22	B2	1356.8457	13.3369	14.0055
23	A1	1393.1569	14.3147	14.9962
24	B2	1457.0415	15.8149	708.4546
25	A1	1493.9353	16.4635	158.3674
26	A1	1606.5000	18.4068	101.6352
27	B2	1616.5897	19.0505	2.0458

pw91/pyFFFFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	113.1175	0.1399	0.0000
2	B1	152.4254	0.2520	0.0002
3	B1	204.7498	0.3700	3.1044
4	A1	262.9187	0.7556	0.7450
5	B2	263.4507	0.7692	0.0398
6	B2	308.7896	1.0178	0.4841
7	A1	333.9974	1.1512	0.9592
8	B1	340.0621	0.9375	2.2233
9	A2	417.6236	1.2997	0.0000
10	B2	444.3102	1.8776	0.1081
11	A1	464.0510	2.0154	0.3420
12	A1	579.7712	3.4573	0.0007
13	B1	608.0500	2.7176	3.0857
14	A2	673.9873	3.2593	0.0000
15	A1	675.6193	4.1795	5.0462

16	B2	719.1376	4.0500	0.0804
17	B1	731.0917	3.8468	3.1837
18	B2	960.9521	7.9352	205.9226
19	A1	1057.4626	9.2117	224.0623
20	B2	1134.1068	10.3307	0.0578
21	A1	1253.3304	12.0558	26.8561
22	B2	1349.7942	13.2244	9.4784
23	A1	1395.8720	14.3595	18.3344
24	B2	1458.1396	15.8319	681.0846
25	A1	1494.8134	16.5068	148.5706
26	A1	1603.0236	18.3303	96.8589
27	B2	1611.2297	18.9119	1.3965

pw91/pyFFFFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	112.2602	0.1378	0.0000
2	B1	151.0576	0.2473	0.0003
3	B1	204.6346	0.3695	2.5380
4	A1	263.7979	0.7605	0.7510
5	B2	264.3178	0.7743	0.0414
6	B2	309.5255	1.0225	0.4672
7	A1	334.7417	1.1565	0.8683
8	B1	339.5761	0.9348	1.9829
9	A2	418.2247	1.3035	0.0000
10	B2	445.2080	1.8854	0.1037
11	A1	464.3815	2.0182	0.3887
12	A1	580.2553	3.4615	0.0000
13	B1	605.7284	2.6941	2.5006
14	A2	670.0021	3.2219	0.0000
15	A1	676.7820	4.1925	4.6386
16	B1	717.3811	3.7099	2.6479
17	B2	719.9365	4.0586	0.0768
18	B2	963.0648	7.9680	198.1625
19	A1	1060.1047	9.2550	220.7877
20	B2	1138.9212	10.4168	0.0073
21	A1	1257.3030	12.1345	26.9520
22	B2	1353.7112	13.2981	10.4743
23	A1	1401.3667	14.4770	18.8323
24	B2	1463.0509	15.9422	662.1061
25	A1	1497.9652	16.5812	144.3673
26	A1	1606.1373	18.4047	98.1057
27	B2	1614.8802	19.0068	1.7781

pw91/pyFFFFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	110.8058	0.1342	0.0000
2	B1	150.2278	0.2445	0.0002
3	B1	204.0438	0.3676	3.3503

4	A1	264.2091	0.7631	0.7016
5	B2	264.9278	0.7780	0.0423
6	B2	308.6881	1.0173	0.5644
7	A1	333.4271	1.1475	1.0104
8	B1	336.4090	0.9176	2.2687
9	A2	416.4703	1.2923	0.0000
10	B2	443.7785	1.8729	0.1124
11	A1	462.8678	2.0048	0.3043
12	A1	577.8668	3.4329	0.0036
13	B1	602.3844	2.6652	2.7978
14	A2	667.7323	3.2003	0.0000
15	A1	673.2910	4.1474	5.1048
16	B2	715.3063	4.0057	0.1550
17	B1	717.8861	3.7111	2.9296
18	B2	958.2368	7.8901	205.0643
19	A1	1054.9227	9.1656	225.9120
20	B2	1134.7788	10.3443	0.0692
21	A1	1251.9931	12.0399	26.6444
22	B2	1360.2896	13.4220	9.8611
23	A1	1399.1820	14.4334	17.4053
24	B2	1462.1574	15.9271	684.4826
25	A1	1499.9670	16.6208	151.5068
26	A1	1609.0355	18.4680	99.9152
27	B2	1617.0479	19.0516	0.9133

pw91/pyFFHFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	108.2588	0.1283	0.0000
2	B1	194.7476	0.3023	3.1576
3	A1	271.2960	0.7878	0.6287
4	B1	285.5579	0.4025	0.8954
5	B2	292.8271	0.8982	0.1180
6	A1	348.6935	1.1475	2.1626
7	B2	439.3311	1.6456	0.0626
8	A2	442.3263	1.4568	0.0000
9	B1	468.1204	0.5778	0.2834
10	A1	493.1181	2.1345	1.6420
11	B2	641.1531	1.4829	1.9540
12	A1	666.4466	3.9465	16.8891
13	A2	667.0297	3.1905	0.0000
14	B1	689.0208	2.3636	9.0792
15	A1	731.6660	3.0354	11.0345
16	B1	848.3902	0.5869	30.2281
17	B2	882.3175	2.6237	141.4440
18	B2	1110.2517	4.6702	14.3080
19	B2	1159.2167	1.3086	82.2263
20	A1	1187.0525	9.4113	199.5768
21	B2	1347.6325	13.1126	74.0052
22	A1	1372.5032	13.1703	1.3480
23	A1	1415.1168	13.3113	36.5376
24	B2	1462.8735	9.3827	705.1108

25	A1	1607.5141	17.4612	20.1834
26	B2	1608.6366	13.7223	3.2022
27	A1	3157.6674	6.4212	4.0220

pw91/pyFFHFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	109.8773	0.1322	0.0000
2	B1	195.2237	0.3060	2.5062
3	A1	271.7513	0.7902	0.6806
4	B1	288.1156	0.4094	0.8864
5	B2	293.8170	0.9039	0.0904
6	A1	349.0280	1.1490	1.8295
7	B2	438.8420	1.6385	0.0501
8	A2	443.1524	1.4623	0.0000
9	B1	472.2974	0.5757	0.2913
10	A1	494.6512	2.1418	1.8746
11	B2	643.6893	1.4870	1.9455
12	A1	669.1513	4.0007	14.2632
13	A2	684.2773	3.3576	0.0000
14	B1	714.3110	1.9233	10.9203
15	A1	733.5618	3.0470	11.6339
16	B1	867.3405	0.6515	24.3284
17	B2	886.4210	2.5918	125.9417
18	B2	1117.5459	4.4811	16.4071
19	B2	1163.0261	1.3510	75.2490
20	A1	1193.6016	9.5212	184.1607
21	B2	1340.7085	12.9462	62.2457
22	A1	1376.2930	13.2303	2.1606
23	A1	1415.7747	13.3927	38.0072
24	B2	1463.8679	9.4948	689.2879
25	B2	1604.2067	13.3054	4.8228
26	A1	1604.5721	17.4098	19.8927
27	A1	3152.2066	6.3957	3.6047

pw91/pyFFHFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	109.3282	0.1308	0.0000
2	B1	195.1726	0.3051	2.0703
3	A1	272.7534	0.7957	0.6839
4	B1	287.2985	0.4072	0.8804
5	B2	294.6458	0.9087	0.0923
6	A1	349.6358	1.1536	1.6739
7	B2	439.9049	1.6466	0.0502
8	A2	444.0754	1.4685	0.0000
9	B1	470.6443	0.5775	0.2003
10	A1	495.1713	2.1455	1.9269
11	B2	644.6544	1.4915	1.9013
12	A1	670.5516	4.0141	13.4634

13	A2	682.1682	3.3376	0.0000
14	B1	710.3100	2.0889	8.4319
15	A1	734.4128	3.0531	11.5831
16	B1	857.5496	0.6221	25.5982
17	B2	888.3473	2.5824	119.7119
18	B2	1122.7167	4.2163	18.0207
19	B2	1166.1985	1.3877	67.9249
20	A1	1198.3015	9.5793	181.6091
21	B2	1344.5715	13.0311	64.6367
22	A1	1381.0049	13.2620	1.9590
23	A1	1420.1626	13.5595	38.0252
24	B2	1469.2788	9.5872	668.8652
25	A1	1607.4150	17.4818	20.7600
26	B2	1608.1239	13.4349	4.3089
27	A1	3157.1382	6.4161	3.2073

pw91/pyFFHFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	107.6518	0.1268	0.0000
2	B1	193.5765	0.3008	2.6995
3	A1	272.6837	0.7956	0.6485
4	B1	285.4898	0.4033	0.9225
5	B2	294.2477	0.9080	0.1319
6	A1	347.8484	1.1414	1.9138
7	B2	438.4687	1.6400	0.0567
8	A2	441.7286	1.4526	0.0000
9	B1	466.5782	0.5657	0.2106
10	A1	493.1497	2.1300	1.6407
11	B2	641.0497	1.5023	1.7921
12	A1	666.3268	3.9586	14.0013
13	A2	677.7152	3.2946	0.0000
14	B1	705.0290	1.9368	10.0150
15	A1	731.6148	3.0295	11.4764
16	B1	855.4490	0.6273	28.2805
17	B2	884.4932	2.6069	129.7280
18	B2	1117.7923	4.4478	14.5705
19	B2	1164.1455	1.3360	70.4848
20	A1	1189.7046	9.4530	190.4179
21	B2	1352.5079	13.1947	61.3205
22	A1	1379.5924	13.2678	1.6979
23	A1	1418.0187	13.4133	37.1587
24	B2	1466.9657	9.6565	692.1004
25	B2	1608.4233	13.6393	5.1083
26	A1	1611.2083	17.5556	19.8467
27	A1	3163.1335	6.4436	6.0506

pw91/pyFHFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A"	121.8594	0.1450	0.1272
2	A"	201.3858	0.3277	3.4418
3	A"	250.3094	0.2643	1.1422
4	A'	263.8864	0.7632	0.1707
5	A'	309.2588	0.9699	0.7667
6	A'	340.9020	1.1258	1.2675
7	A"	370.8462	0.8534	0.6139
8	A'	449.2917	1.6782	0.4440
9	A'	514.2341	1.7488	3.0636
10	A'	579.2770	3.4316	0.0747
11	A"	602.5167	1.2033	5.8885
12	A'	647.5311	1.5790	1.9875
13	A"	654.2068	1.8169	0.0003
14	A"	704.3825	2.0870	0.9591
15	A'	777.5252	3.5293	46.0709
16	A"	807.8983	0.5881	34.5229
17	A'	997.5270	2.6959	99.5181
18	A'	1043.2051	7.3503	176.0065
19	A'	1123.7735	1.4471	84.6522
20	A'	1208.0935	4.8119	47.4312
21	A'	1352.9039	13.2589	12.0712
22	A'	1373.4479	10.5723	43.5435
23	A'	1416.3972	12.9137	187.0241
24	A'	1480.4107	9.1282	398.1633
25	A'	1600.4305	14.8800	243.9755
26	A'	1615.7406	17.6519	36.9999
27	A'	3168.5976	6.4712	3.4765

pw91/pyFHFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	123.0660	0.1479	0.1032
2	A"	201.7354	0.3331	2.7521
3	A"	252.9509	0.2673	1.2160
4	A'	264.5166	0.7664	0.2056
5	A'	309.7084	0.9717	0.6725
6	A'	341.2659	1.1278	0.9935
7	A"	371.1624	0.8606	0.5926
8	A'	449.1667	1.6768	0.4233
9	A'	513.6079	1.7442	2.5706
10	A'	582.2787	3.4663	0.0371
11	A"	608.5553	1.2069	5.9489
12	A'	649.4706	1.5814	2.2000
13	A"	664.1916	1.6578	0.0045
14	A"	726.0940	1.8348	0.1266
15	A'	779.4201	3.5385	40.4494
16	A"	823.1715	0.6611	31.6654
17	A'	999.8911	2.5903	88.6630
18	A'	1049.5569	7.3988	160.7582
19	A'	1129.3050	1.4830	86.6500
20	A'	1213.0668	4.9892	43.9880
21	A'	1346.8733	13.2408	10.6094

22	A'	1377.8614	10.6855	46.4437
23	A'	1416.6477	12.8669	173.0986
24	A'	1481.7561	9.2042	388.5127
25	A'	1597.0544	14.6287	233.2110
26	A'	1610.8480	17.3927	34.2210
27	A'	3163.3620	6.4464	2.9393

pw91/pyFHFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	122.3682	0.1462	0.0880
2	A"	201.3584	0.3297	2.3422
3	A"	251.9742	0.2669	1.1997
4	A'	265.3937	0.7715	0.2112
5	A'	310.5431	0.9766	0.6587
6	A'	342.1337	1.1337	0.9292
7	A"	371.0414	0.8609	0.4684
8	A'	449.8294	1.6804	0.3948
9	A'	514.5503	1.7521	2.3362
10	A'	582.9706	3.4715	0.0254
11	A"	607.8218	1.2299	5.1364
12	A'	650.3576	1.5843	2.1069
13	A"	663.5581	1.7140	0.0185
14	A"	719.1102	2.0223	0.3007
15	A'	780.8231	3.5489	38.9185
16	A"	812.7201	0.6155	30.1931
17	A'	1002.1856	2.5406	84.6585
18	A'	1053.2804	7.4905	154.5851
19	A'	1132.8728	1.4899	83.6324
20	A'	1217.0051	5.1359	42.5899
21	A'	1351.4454	13.3024	9.9151
22	A'	1383.4195	10.9827	48.0247
23	A'	1421.4670	12.8747	158.8079
24	A'	1485.8405	9.3209	384.1941
25	A'	1600.3757	14.6843	234.4644
26	A'	1614.4366	17.4887	35.8256
27	A'	3168.2520	6.4664	2.6067

pw91/pyFHFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	121.3155	0.1437	0.1149
2	A"	200.8322	0.3292	3.0092
3	A"	250.2715	0.2640	1.2489
4	A'	265.8363	0.7742	0.1925
5	A'	309.5636	0.9727	0.7789
6	A'	340.3652	1.1234	1.1308
7	A"	369.0427	0.8447	0.5132
8	A'	448.7849	1.6776	0.4144
9	A'	513.0443	1.7432	2.4681

10	A'	580.4613	3.4429	0.0664
11	A''	604.2732	1.2147	5.7498
12	A'	646.8027	1.5954	1.8779
13	A''	659.4643	1.6690	0.0178
14	A''	718.1466	1.9181	0.1663
15	A'	777.2672	3.5154	41.0102
16	A''	814.9358	0.6290	35.5295
17	A'	998.5960	2.6426	93.7657
18	A'	1047.5481	7.4032	163.1153
19	A'	1129.6294	1.4569	77.9793
20	A'	1212.6800	4.8692	42.5176
21	A'	1356.1459	13.3858	12.7458
22	A'	1381.2215	10.7949	46.5665
23	A'	1419.9301	12.9153	170.1494
24	A'	1484.9659	9.3985	395.2482
25	A'	1602.2841	14.9387	240.3063
26	A'	1616.5265	17.6204	32.5808
27	A'	3174.5467	6.4956	5.4652

pw91/pyHHHHH_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	356.9849	0.1894	0.0000
2	B1	398.1322	0.3524	3.6201
3	A1	595.1723	1.4809	3.2824
4	B2	648.3380	1.5673	0.3161
5	B1	691.9122	0.3644	69.0408
6	B1	734.0846	0.8651	7.6568
7	A2	864.3447	0.5493	0.0000
8	B1	918.6801	0.6602	0.0592
9	A2	956.1051	0.7980	0.0000
10	B1	966.6254	0.6979	0.0010
11	A1	982.2620	3.9708	5.5305
12	A1	1021.8729	2.9614	3.9764
13	B2	1050.0353	1.1303	0.0019
14	A1	1065.1034	1.1088	6.0746
15	B2	1140.1268	0.8335	1.8061
16	A1	1208.8372	1.1029	4.1384
17	B2	1293.5903	9.4374	0.3864
18	B2	1338.3958	1.2659	0.0072
19	B2	1427.2695	2.5388	23.7431
20	A1	1463.3138	2.5169	1.8506
21	B2	1574.8084	8.6655	9.1584
22	A1	1578.4400	7.8520	20.6170
23	B2	3081.1229	6.0796	31.5977
24	A1	3083.5585	6.1067	4.5805
25	A1	3108.7211	6.1943	3.2554
26	B2	3122.8499	6.2794	27.4723
27	A1	3131.5179	6.3492	8.8886

pw91/pyHHHHH_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	360.0848	0.1902	0.0000
2	B1	401.1504	0.3545	3.4430
3	A1	594.6497	1.4752	4.0423
4	B2	647.5075	1.5591	0.1867
5	B1	697.6750	0.3589	63.2641
6	B1	743.5850	0.8898	4.6639
7	A2	871.7380	0.5590	0.0000
8	B1	928.7396	0.6767	0.0254
9	A2	971.9789	0.8308	0.0000
10	A1	982.6935	3.9117	5.9285
11	B1	986.6077	0.7504	0.0007
12	A1	1025.6276	2.8892	4.8530
13	B2	1050.4774	1.1302	0.0261
14	A1	1065.8682	1.1292	4.0371
15	B2	1137.5246	0.8330	1.8928
16	A1	1206.8847	1.1065	3.3531
17	B2	1288.5960	9.1209	0.2943
18	B2	1341.5906	1.2740	0.0019
19	B2	1429.7501	2.5648	23.0311
20	A1	1467.1560	2.5176	1.6820
21	B2	1574.1135	8.4618	8.5875
22	A1	1577.4948	7.7316	20.1584
23	B2	3076.4276	6.0605	29.3677
24	A1	3078.9931	6.0898	4.5008
25	A1	3106.2022	6.1825	2.6957
26	B2	3119.8997	6.2654	25.0163
27	A1	3128.7449	6.3347	8.1577

pw91/pyHHHHH_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	360.3435	0.1900	0.0000
2	B1	401.6284	0.3561	3.3289
3	A1	595.4375	1.4810	4.2582
4	B2	649.2959	1.5693	0.2495
5	B1	696.5135	0.3523	63.3052
6	B1	744.7652	0.9192	3.6687
7	A2	870.7395	0.5576	0.0000
8	B1	926.5786	0.6762	0.0218
9	A2	970.1937	0.8291	0.0000
10	A1	984.5939	3.9407	6.5942
11	B1	984.8537	0.7458	0.0017
12	A1	1027.0017	2.8939	5.3102
13	B2	1052.2820	1.1345	0.0164
14	A1	1067.6708	1.1301	3.8422
15	B2	1140.6597	0.8370	1.7667
16	A1	1209.4908	1.1101	3.0019
17	B2	1292.7969	9.2259	0.3483
18	B2	1343.7684	1.2777	0.0003

19	B2	1433.0606	2.5718	23.9611
20	A1	1469.9529	2.5327	2.3091
21	B2	1577.6509	8.5520	8.2536
22	A1	1580.4692	7.7831	20.7674
23	B2	3079.8436	6.0737	30.3934
24	A1	3082.5577	6.1044	5.9991
25	A1	3110.4022	6.1991	3.1259
26	B2	3124.4131	6.2834	25.1509
27	A1	3133.1552	6.3535	7.9816

pw91/pyHHHHH_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	358.1551	0.1884	0.0000
2	B1	398.8328	0.3513	3.4926
3	A1	595.0161	1.4810	3.3684
4	B2	647.0303	1.5600	0.4238
5	B1	690.4734	0.3483	76.9876
6	B1	739.4001	0.9021	5.5632
7	A2	864.4299	0.5493	0.0000
8	B1	919.2791	0.6637	0.0805
9	A2	963.3102	0.8157	0.0000
10	B1	977.7754	0.7339	0.0026
11	A1	980.7707	3.9439	6.0105
12	A1	1023.8615	2.9520	4.1471
13	B2	1050.9276	1.1277	0.0817
14	A1	1065.3420	1.1106	6.3367
15	B2	1140.6199	0.8306	1.6353
16	A1	1208.8270	1.0987	3.3830
17	B2	1295.9701	9.4667	0.2318
18	B2	1336.8765	1.2653	0.0029
19	B2	1426.5510	2.5566	26.3876
20	A1	1462.2742	2.5199	3.1170
21	B2	1575.0231	8.7171	7.2883
22	A1	1580.0541	7.9768	20.3156
23	B2	3089.6584	6.1145	21.2606
24	A1	3091.8358	6.1409	3.6298
25	A1	3117.1223	6.2280	2.5054
26	B2	3130.5940	6.3109	16.7037
27	A1	3138.8083	6.3797	4.7613

revtpss/pyCCCCC_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	55.1838	0.0612	0.0000
2	B1	78.9552	0.1240	0.0167
3	B1	142.8962	0.1921	0.0017
4	A1	196.3485	0.7602	0.0880
5	B2	208.5569	0.7876	0.3832
6	A1	211.5217	0.7476	0.0923

7	B2	216.3134	0.9599	0.0004
8	B1	274.0073	0.5976	0.5769
9	B2	322.9330	1.7674	0.3226
10	A1	338.4390	1.9140	0.1900
11	A2	353.1454	0.9199	0.0000
12	A1	376.7222	2.7322	0.2108
13	A1	528.5043	2.8581	7.9711
14	B1	549.0077	2.2041	1.0189
15	B2	562.9332	2.5078	1.8943
16	A2	598.1624	2.5517	0.0000
17	B2	665.7553	4.0633	105.6412
18	B1	693.6909	3.4659	0.0375
19	A1	802.0506	5.2240	101.1683
20	B2	863.8243	5.7258	3.4354
21	A1	1050.5772	8.1785	35.8754
22	A1	1196.5188	10.3990	5.4688
23	B2	1287.7571	11.8140	96.7108
24	B2	1316.4391	12.8283	379.3592
25	A1	1319.7729	12.4750	124.1192
26	A1	1501.7746	16.0411	100.4512
27	B2	1521.4358	17.0411	41.5829

revtpss/pyCCCCC_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	57.5139	0.0664	0.0000
2	B1	81.4080	0.1314	0.0114
3	B1	143.5847	0.1940	0.0016
4	A1	192.2228	0.7391	0.0395
5	B2	205.1211	0.7627	0.3598
6	A1	208.3540	0.7172	0.0539
7	B2	209.3724	0.8991	0.0006
8	B1	277.1072	0.6122	0.5864
9	B2	323.0686	1.7664	0.3226
10	A1	338.7413	1.9152	0.1756
11	A2	357.2868	0.9417	0.0000
12	A1	377.5038	2.7408	0.2290
13	A1	528.8898	2.8641	6.3688
14	B1	558.4108	2.2808	1.0041
15	B2	559.9626	2.4833	1.2060
16	A2	615.5884	2.7029	0.0000
17	B2	667.2025	4.0760	95.5248
18	B1	718.9134	3.7223	0.9706
19	A1	802.7797	5.2386	93.4936
20	B2	863.5160	5.7258	3.4476
21	A1	1050.6893	8.1831	32.4594
22	A1	1196.5696	10.3921	6.8177
23	B2	1284.5943	11.8016	58.0967
24	B2	1312.1106	12.7125	372.8978
25	A1	1316.4039	12.4115	104.6989
26	A1	1497.6362	15.9487	90.9625
27	B2	1513.7147	16.8414	37.3338

revtpss/pyCCCCC_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	57.6784	0.0668	0.0000
2	B1	81.7240	0.1323	0.0136
3	B1	144.3817	0.1962	0.0026
4	A1	193.0529	0.7460	0.0517
5	B2	206.1387	0.7704	0.3123
6	A1	209.5358	0.7252	0.0449
7	B2	210.0559	0.9048	0.0005
8	B1	278.0870	0.6167	0.5371
9	B2	324.2990	1.7777	0.3386
10	A1	340.1097	1.9271	0.1931
11	A2	359.6796	0.9545	0.0000
12	A1	379.2638	2.7632	0.2250
13	A1	531.4507	2.8902	6.2271
14	B1	561.0410	2.3024	0.9936
15	B2	563.5082	2.5164	1.4501
16	A2	618.5461	2.7293	0.0000
17	B2	671.8310	4.1302	95.3566
18	B1	720.6308	3.7400	1.0066
19	A1	806.6049	5.2934	96.6846
20	B2	868.9408	5.8018	2.9599
21	A1	1055.6931	8.2653	32.9232
22	A1	1198.7882	10.4327	6.3911
23	B2	1284.7394	11.7900	69.6870
24	B2	1313.9347	12.7560	361.8859
25	A1	1317.8680	12.4391	107.0806
26	A1	1496.7140	15.9292	95.2649
27	B2	1515.0794	16.8830	36.7903

revtpss/pyCCCCC_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	55.7904	0.0625	0.0000
2	B1	79.1366	0.1243	0.0146
3	B1	142.2177	0.1903	0.0208
4	A1	194.9104	0.7492	0.0665
5	B2	207.1936	0.7777	0.2384
6	A1	209.6415	0.7349	0.0315
7	B2	214.5898	0.9447	0.0008
8	B1	273.5305	0.5956	0.3082
9	B2	320.5913	1.7504	0.4070
10	A1	335.8565	1.8922	0.1846
11	A2	354.0709	0.9246	0.0000
12	A1	373.1764	2.6903	0.2350
13	A1	522.9224	2.7995	8.6381
14	B1	548.2173	2.1952	0.7857
15	B2	558.8833	2.4766	2.7933

16	A2	600.5040	2.5719	0.0000
17	B2	658.2271	3.9633	107.6486
18	B1	698.0071	3.5145	1.1491
19	A1	794.6642	5.1213	105.2058
20	B2	855.9799	5.6095	2.8645
21	A1	1042.1358	8.0410	38.1286
22	A1	1192.9467	10.3248	4.7415
23	B2	1290.0511	11.8341	117.8917
24	B2	1313.3618	12.7803	346.1507
25	A1	1315.9707	12.3982	121.9301
26	A1	1501.5859	16.0362	100.1677
27	B2	1519.7132	17.0135	40.5103

revtpss/pyFCFCF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	88.5342	0.0986	0.0000
2	B1	107.0998	0.1472	0.0048
3	A1	175.0877	0.4774	0.0115
4	B1	206.4332	0.3788	2.1699
5	B2	213.1765	0.6009	0.0485
6	B2	300.2144	1.1382	0.5653
7	B1	306.9468	0.7703	0.2682
8	A1	310.5443	1.2277	0.1212
9	A2	366.3398	0.9915	0.0000
10	A1	397.9101	1.9038	0.7630
11	B2	399.5907	1.7390	0.0557
12	A1	564.2054	3.0112	1.7739
13	A1	596.1085	3.4979	2.2315
14	B1	618.2833	2.7964	1.1904
15	A2	660.7945	3.1328	0.0000
16	B2	678.3023	3.6024	0.9012
17	B1	711.7775	3.6527	11.4080
18	B2	771.8673	5.0679	126.0279
19	A1	1037.8890	8.8167	188.8307
20	B2	1062.1007	9.1666	23.5766
21	A1	1110.8742	9.2428	7.3824
22	B2	1342.3142	13.0888	2.7072
23	A1	1384.4191	14.2152	48.5356
24	B2	1409.4909	14.5993	471.4822
25	A1	1432.3305	15.0131	92.2490
26	A1	1584.2578	17.9059	181.9443
27	B2	1593.3464	18.5656	42.4118

revtpss/pyFCFCF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	89.8415	0.1016	0.0000
2	B1	108.3271	0.1503	0.0000
3	A1	172.6567	0.4641	0.0013

4	B1	204.4387	0.3713	2.0186
5	B2	211.1458	0.5890	0.0395
6	B2	300.1498	1.1403	0.5977
7	B1	308.6093	0.7799	0.4233
8	A1	310.4982	1.2295	0.1035
9	A2	359.4407	0.9541	0.0000
10	A1	398.2946	1.9044	0.7384
11	B2	399.6341	1.7335	0.0801
12	A1	564.4357	2.9901	1.5395
13	A1	597.9175	3.5427	1.3917
14	B1	620.0030	2.8122	1.1014
15	A2	669.5561	3.2180	0.0000
16	B2	678.9019	3.6103	0.3798
17	B1	727.9723	3.8196	9.0066
18	B2	770.8206	5.0480	116.1541
19	A1	1043.4778	8.8874	171.5644
20	B2	1067.0802	9.2664	20.1859
21	A1	1109.9768	9.2458	4.4013
22	B2	1334.5861	12.9630	0.9990
23	A1	1390.0437	14.3146	56.0960
24	B2	1411.4556	14.6338	443.4632
25	A1	1432.7916	15.0672	71.3892
26	A1	1580.4673	17.8216	176.0271
27	B2	1586.7654	18.4008	45.2285

revtpss/pyFCFCF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	89.6364	0.1011	0.0000
2	B1	108.1302	0.1499	0.0006
3	A1	174.4987	0.4740	0.0000
4	B1	205.1224	0.3739	1.7195
5	B2	213.2031	0.6008	0.0309
6	B2	301.5101	1.1500	0.5699
7	B1	309.6671	0.7847	0.3986
8	A1	311.7724	1.2376	0.0801
9	A2	362.3922	0.9701	0.0000
10	A1	399.4748	1.9156	0.7212
11	B2	400.4403	1.7403	0.0808
12	A1	565.5578	3.0117	1.3770
13	A1	598.7915	3.5438	1.3713
14	B1	620.6673	2.8184	0.8878
15	A2	670.5048	3.2274	0.0000
16	B2	681.0474	3.6327	0.4018
17	B1	727.1900	3.8117	8.3093
18	B2	775.0896	5.1087	114.7671
19	A1	1045.4663	8.9236	173.1089
20	B2	1070.8751	9.3236	18.2177
21	A1	1114.5669	9.3170	4.9156
22	B2	1336.6292	12.9926	2.0586
23	A1	1395.2143	14.4320	55.7105
24	B2	1414.4928	14.7055	434.0212

25	A1	1434.3272	15.0966	76.0153
26	A1	1580.7783	17.8320	181.5772
27	B2	1589.6448	18.4817	47.4848

revtpss/pyFCFCF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	88.4261	0.0984	0.0000
2	B1	106.9142	0.1465	0.0050
3	A1	175.7768	0.4813	0.0016
4	B1	203.6012	0.3679	1.8606
5	B2	215.2146	0.6125	0.0217
6	B2	300.6467	1.1444	0.4912
7	B1	305.6903	0.7656	0.1463
8	A1	310.3702	1.2315	0.0555
9	A2	356.4820	0.9380	0.0000
10	A1	396.0766	1.8856	0.8418
11	B2	398.0616	1.7238	0.0188
12	A1	562.2869	2.9615	1.7277
13	A1	595.5881	3.5126	1.5430
14	B1	616.0689	2.7751	0.5567
15	A2	662.8758	3.1556	0.0000
16	B2	676.0837	3.5794	0.8054
17	B1	715.4596	3.6920	13.8800
18	B2	764.4132	4.9534	121.4135
19	A1	1040.4397	8.8277	186.9201
20	B2	1065.4510	9.2354	19.5985
21	A1	1104.9597	9.1613	3.8594
22	B2	1345.1334	13.1630	0.5600
23	A1	1393.8104	14.4052	54.3956
24	B2	1413.5592	14.6672	460.7026
25	A1	1436.4828	15.1405	83.6767
26	A1	1586.2392	17.9509	184.2999
27	B2	1591.6460	18.5350	40.5793

revtpss/pyFCFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	93.9556	0.1101	0.0007
2	A''	136.5266	0.2051	0.0019
3	A'	191.9107	0.5110	0.0284
4	A''	205.8923	0.3757	2.9346
5	A'	257.5722	0.7354	0.2670
6	A'	300.7856	1.0697	0.4911
7	A''	317.4113	0.8152	0.5843
8	A'	322.5208	1.1572	0.4652
9	A''	395.9870	1.1720	1.1136
10	A'	396.6283	1.7840	0.2816
11	A'	455.5165	1.9682	0.5093
12	A'	576.2756	3.3455	0.7577

13	A''	608.3372	2.7097	1.6748
14	A'	614.8373	3.5192	7.5675
15	A''	653.7187	3.0675	0.1552
16	A''	695.7304	3.4913	7.9378
17	A'	698.9591	3.8237	0.5673
18	A'	876.3241	6.5131	160.8009
19	A'	1043.2151	8.9198	192.1751
20	A'	1073.4074	9.2831	38.2092
21	A'	1209.6481	11.2402	22.8712
22	A'	1350.3563	13.2504	5.6990
23	A'	1388.0553	14.2704	43.3134
24	A'	1429.7465	14.9800	356.5791
25	A'	1475.4556	16.1350	371.6593
26	A'	1604.7209	18.4196	149.9410
27	A'	1614.5691	18.9362	6.8965

revtpss/pyFCFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	95.5682	0.1138	0.0003
2	A''	137.9216	0.2094	0.0024
3	A'	189.8462	0.4998	0.0251
4	A''	204.7768	0.3713	2.5372
5	A'	259.1489	0.7446	0.3181
6	A'	301.4732	1.0797	0.4818
7	A''	319.7711	0.8283	0.7065
8	A'	322.9297	1.1562	0.4196
9	A''	396.4357	1.1750	0.9106
10	A'	396.8512	1.7809	0.2462
11	A'	455.7572	1.9685	0.5917
12	A'	578.6568	3.3569	0.8800
13	A''	613.1411	2.7549	1.7830
14	A'	614.8095	3.5324	6.0492
15	A''	670.1002	3.2241	0.4270
16	A'	700.7144	3.8440	0.3713
17	A''	724.5766	3.7815	5.8271
18	A'	878.4055	6.5293	147.0218
19	A'	1048.7294	9.0051	172.3195
20	A'	1077.7102	9.3730	39.9937
21	A'	1214.4681	11.3471	21.0386
22	A'	1342.6219	13.1241	3.0924
23	A'	1393.0608	14.3642	45.5678
24	A'	1431.0119	15.0047	333.3332
25	A'	1476.4264	16.1795	355.9104
26	A'	1600.8332	18.3585	143.4363
27	A'	1609.9347	18.7929	10.2375

revtpss/pyFCFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A"	95.2427	0.1129	0.0000
2	A"	137.1201	0.2071	0.0003
3	A'	191.7943	0.5102	0.0297
4	A"	205.0388	0.3722	2.1600
5	A'	260.3114	0.7512	0.3169
6	A'	302.4104	1.0852	0.4689
7	A"	320.4914	0.8320	0.6768
8	A'	323.8164	1.1627	0.3679
9	A"	397.6579	1.1818	0.8197
10	A'	397.7215	1.7884	0.2442
11	A'	456.3840	1.9742	0.6013
12	A'	579.1620	3.3674	0.7604
13	A"	612.3013	2.7463	1.4668
14	A'	616.1974	3.5461	5.7509
15	A"	668.2286	3.2061	0.2197
16	A'	701.8523	3.8558	0.3602
17	A"	717.3809	3.7102	5.3772
18	A'	881.1016	6.5730	145.4671
19	A'	1050.8539	9.0416	175.7551
20	A'	1081.4768	9.4284	35.4374
21	A'	1218.1623	11.4144	21.0966
22	A'	1344.7268	13.1584	4.3449
23	A'	1397.7812	14.4701	46.8010
24	A'	1433.5302	15.0530	312.3682
25	A'	1478.9247	16.2454	367.0390
26	A'	1602.3672	18.3746	150.6966
27	A'	1612.0141	18.8746	6.3407

revtpss/pyFCFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	94.0143	0.1100	0.0005
2	A"	136.0877	0.2039	0.0006
3	A'	193.4597	0.5188	0.0423
4	A"	204.0923	0.3686	2.5884
5	A'	261.5442	0.7587	0.2785
6	A'	301.6782	1.0825	0.4749
7	A"	316.3950	0.8110	0.4315
8	A'	322.6161	1.1549	0.3914
9	A"	394.8354	1.1654	1.3614
10	A'	395.0737	1.7688	0.3037
11	A'	454.8717	1.9597	0.6035
12	A'	576.8412	3.3328	1.0124
13	A"	608.7229	2.7137	1.2809
14	A'	612.0672	3.4948	6.7081
15	A"	664.0042	3.1673	0.9075
16	A'	697.4961	3.8070	0.4656
17	A"	712.7483	3.6610	7.3908
18	A'	874.1488	6.4586	150.8687
19	A'	1046.1310	8.9596	182.5304
20	A'	1076.1069	9.3413	38.3436
21	A'	1213.0550	11.3306	21.2053

22	A'	1353.4337	13.3280	3.0545
23	A'	1396.6653	14.4464	47.0696
24	A'	1433.2297	15.0493	336.1866
25	A'	1481.3778	16.2922	372.5042
26	A'	1605.9288	18.4921	140.1023
27	A'	1615.3462	18.9134	14.9278

revtpss/pyFFCFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	112.0816	0.1373	0.0000
2	B1	118.8459	0.1737	0.0240
3	B2	192.0259	0.5231	0.0354
4	B1	200.1477	0.3501	2.7157
5	A1	263.1945	0.7879	0.6827
6	B2	293.3884	0.9319	0.1994
7	A1	319.6435	1.2435	0.7078
8	B1	323.7118	0.8605	0.6521
9	A1	418.4926	1.8799	0.0188
10	A2	427.2939	1.3596	0.0000
11	B2	445.1422	1.8790	0.0529
12	A1	526.1367	2.9001	1.6674
13	B1	568.3114	2.3605	6.9739
14	A2	655.0597	3.0795	0.0000
15	A1	677.1559	4.2324	9.8370
16	B1	684.7704	3.3814	2.1666
17	B2	695.9024	3.7721	0.0309
18	A1	897.1964	6.5573	147.7233
19	B2	940.0959	7.6683	180.2146
20	B2	1127.2832	10.2027	1.1237
21	A1	1209.2697	11.1146	62.9626
22	B2	1345.7221	13.1297	8.7524
23	A1	1391.8352	14.4607	8.2994
24	A1	1437.7892	14.9824	77.4553
25	B2	1454.8015	15.7171	750.5458
26	B2	1597.5180	18.6503	0.3732
27	A1	1613.5979	18.5921	121.3310

revtpss/pyFFCFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	113.1755	0.1400	0.0000
2	B1	120.8436	0.1799	0.0392
3	B2	190.4253	0.5142	0.0282
4	B1	199.6199	0.3478	2.2533
5	A1	263.8584	0.7922	0.8275
6	B2	295.1011	0.9425	0.2223
7	A1	319.8055	1.2454	0.5783
8	B1	325.2625	0.8689	0.6759
9	A1	418.7755	1.8804	0.0051

10	A2	427.4023	1.3604	0.0000
11	B2	444.8616	1.8742	0.0392
12	A1	527.8924	2.9157	1.9104
13	B1	570.4696	2.3809	6.7612
14	A2	671.9080	3.2401	0.0000
15	A1	678.6777	4.2501	7.7392
16	B2	698.1877	3.7980	0.0074
17	B1	718.0341	3.7148	1.6577
18	A1	896.7666	6.5489	137.6575
19	B2	945.4540	7.7510	162.6654
20	B2	1134.9335	10.3475	1.0459
21	A1	1213.2497	11.1947	60.7298
22	B2	1337.4976	12.9928	7.0062
23	A1	1395.3407	14.5285	10.2684
24	A1	1438.3872	15.0108	73.2828
25	B2	1456.7649	15.7630	712.3109
26	B2	1592.8595	18.5269	0.2405
27	A1	1610.0303	18.5161	113.3145

revtpss/pyFFCFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	112.6009	0.1386	0.0000
2	B1	120.6362	0.1793	0.0360
3	B2	192.4514	0.5254	0.0177
4	B1	199.9583	0.3491	1.8985
5	A1	265.2052	0.8004	0.8240
6	B2	296.0720	0.9487	0.1965
7	A1	320.6396	1.2496	0.5426
8	B1	325.4397	0.8695	0.6437
9	A1	419.5326	1.8869	0.0005
10	A2	428.9998	1.3707	0.0000
11	B2	445.6952	1.8820	0.0430
12	A1	528.6997	2.9273	1.8936
13	B1	571.9365	2.3930	6.3219
14	A2	669.1441	3.2143	0.0000
15	A1	679.5301	4.2599	7.1690
16	B2	699.3476	3.8103	0.0032
17	B1	712.1457	3.6550	1.1651
18	A1	900.2231	6.6016	137.9867
19	B2	947.3427	7.7782	160.4864
20	B2	1138.7489	10.4133	0.6352
21	A1	1217.3941	11.2685	60.3238
22	B2	1339.5306	13.0295	7.7081
23	A1	1399.3684	14.6237	8.8487
24	A1	1439.7461	15.0339	74.5463
25	B2	1460.6703	15.8461	707.4842
26	B2	1594.2666	18.5753	0.3981
27	A1	1611.9788	18.5637	114.6313

revtpss/pyFFCFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	111.1689	0.1350	0.0000
2	B1	119.2407	0.1750	0.0278
3	B2	194.0915	0.5341	0.0046
4	B1	198.5668	0.3441	2.3172
5	A1	266.0348	0.8066	0.7252
6	B2	296.0425	0.9489	0.2059
7	A1	319.3537	1.2429	0.5500
8	B1	322.1938	0.8529	0.5297
9	A1	416.8189	1.8655	0.0308
10	A2	426.7243	1.3558	0.0000
11	B2	444.2413	1.8685	0.0549
12	A1	526.1685	2.8902	1.9937
13	B1	562.7364	2.3152	8.6158
14	A2	667.0939	3.1950	0.0000
15	A1	676.4402	4.2186	8.1448
16	B2	695.1475	3.7640	0.0137
17	B1	708.0732	3.6145	0.8643
18	A1	891.7787	6.4698	142.7714
19	B2	943.6585	7.7186	167.8081
20	B2	1135.0507	10.3528	0.6706
21	A1	1210.4423	11.1449	59.0525
22	B2	1348.8793	13.2018	7.6913
23	A1	1399.4764	14.6207	7.8213
24	A1	1439.7869	15.0393	79.4679
25	B2	1461.3661	15.8728	737.3128
26	B2	1598.4866	18.6661	0.0120
27	A1	1615.5583	18.6451	118.3554

revtpss/pyFFFFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	113.9306	0.1419	0.0000
2	B1	152.8654	0.2530	0.0017
3	B1	206.4973	0.3763	3.9648
4	B2	253.0353	0.7094	0.0374
5	A1	254.9635	0.7097	0.6863
6	B2	305.2552	0.9948	0.5628
7	A1	333.4567	1.1479	1.1714
8	B1	339.1182	0.9329	2.4535
9	A2	416.9235	1.2950	0.0000
10	B2	444.7440	1.8814	0.0913
11	A1	463.5629	2.0129	0.2697
12	A1	579.5363	3.4540	0.0000
13	B1	598.4391	2.6244	2.4957
14	A2	648.2931	3.0166	0.0000
15	B1	675.2881	3.2939	4.5492
16	A1	677.6966	4.2089	6.6211
17	B2	715.0607	4.0050	0.1875
18	B2	958.0620	7.8946	221.1442

19	A1	1054.4986	9.1694	242.7696
20	B2	1130.9008	10.2846	0.1209
21	A1	1250.7329	11.9918	29.2162
22	B2	1358.4514	13.4189	4.4921
23	A1	1397.9521	14.4299	16.1200
24	B2	1464.6254	15.9543	713.0684
25	A1	1505.0474	16.6984	155.7386
26	A1	1624.8291	18.8263	104.3157
27	B2	1627.3829	19.2420	0.4289

revtpss/pyFFFFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	115.2270	0.1452	0.0000
2	B1	154.5505	0.2588	0.0002
3	B1	206.1517	0.3747	3.2037
4	B2	255.5013	0.7230	0.0383
5	A1	256.3932	0.7174	0.8011
6	B2	306.6916	1.0038	0.5326
7	A1	333.9193	1.1507	1.0181
8	B1	341.8726	0.9489	2.2541
9	A2	418.1059	1.3025	0.0000
10	B2	444.7059	1.8794	0.0808
11	A1	464.3019	2.0169	0.3628
12	A1	582.5468	3.4884	0.0011
13	B1	607.5621	2.7124	2.9415
14	A2	670.9698	3.2310	0.0000
15	A1	678.6526	4.2222	5.1290
16	B2	718.0082	4.0395	0.0440
17	B1	721.8186	3.7505	3.2920
18	B2	963.7394	7.9824	205.3403
19	A1	1060.2233	9.2675	228.5776
20	B2	1137.4158	10.4094	0.0345
21	A1	1255.8462	12.1009	27.1766
22	B2	1350.3640	13.2816	2.8442
23	A1	1401.4943	14.4919	19.4289
24	B2	1466.6761	15.9934	685.6555
25	A1	1506.3039	16.7493	147.9485
26	A1	1622.0849	18.7663	98.6513
27	B2	1622.8819	19.1279	0.1909

revtpss/pyFFFFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	114.3668	0.1429	0.0000
2	B1	153.2707	0.2544	0.0001
3	B1	206.1184	0.3746	2.7247
4	B2	256.4583	0.7285	0.0404
5	A1	257.3001	0.7224	0.8122
6	B2	307.2281	1.0072	0.5189

7	A1	334.3948	1.1540	0.9358
8	B1	341.5754	0.9472	2.0760
9	A2	418.9201	1.3076	0.0000
10	B2	445.2276	1.8840	0.0837
11	A1	464.4785	2.0183	0.4061
12	A1	582.8984	3.4916	0.0029
13	B1	605.2311	2.6889	2.4457
14	A2	666.6957	3.1910	0.0000
15	A1	679.4448	4.2314	4.8140
16	B1	708.3861	3.6178	2.9023
17	B2	718.2847	4.0415	0.0444
18	B2	965.3139	8.0080	201.0987
19	A1	1062.2010	9.3002	228.2478
20	B2	1140.9911	10.4737	0.0013
21	A1	1258.9328	12.1611	27.7326
22	B2	1352.7023	13.3229	3.5818
23	A1	1405.7969	14.5839	19.7977
24	B2	1470.4942	16.0826	673.4238
25	A1	1508.2914	16.7973	145.2853
26	A1	1623.5251	18.8021	100.2163
27	B2	1625.0585	19.1871	0.3226

revtpss/pyFFFFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	112.9520	0.1394	0.0000
2	B1	152.3894	0.2515	0.0004
3	B1	205.7810	0.3736	3.5736
4	B2	257.7318	0.7358	0.0405
5	A1	258.3056	0.7283	0.7497
6	B2	306.7162	1.0042	0.6175
7	A1	333.4253	1.1474	1.0832
8	B1	338.6035	0.9310	2.3485
9	A2	417.6812	1.2996	0.0000
10	B2	443.9117	1.8719	0.0855
11	A1	463.2311	2.0069	0.3159
12	A1	580.9667	3.4675	0.0000
13	B1	602.6947	2.6673	2.7045
14	A2	665.4993	3.1798	0.0000
15	A1	676.6797	4.1941	5.2819
16	B1	710.1912	3.6323	3.0889
17	B2	714.1053	3.9936	0.1036
18	B2	961.4382	7.9447	206.0541
19	A1	1058.1020	9.2290	231.9869
20	B2	1138.0146	10.4247	0.0448
21	A1	1254.5209	12.0854	27.4589
22	B2	1361.3215	13.4870	3.1229
23	A1	1405.1584	14.5751	18.3562
24	B2	1470.3894	16.0834	693.8555
25	A1	1511.1422	16.8573	152.5740
26	A1	1627.1276	18.8842	101.6506
27	B2	1627.9612	19.2542	0.0634

revtpss/pyFFHFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	110.5927	0.1338	0.0000
2	B1	196.2020	0.3068	3.2600
3	A1	264.8434	0.7488	0.6902
4	B2	287.1650	0.8578	0.1521
5	B1	289.1621	0.4153	0.9216
6	A1	348.3561	1.1460	2.3189
7	B2	437.1453	1.5988	0.0999
8	A2	442.8018	1.4596	0.0000
9	B1	465.8959	0.5923	0.3651
10	A1	492.7805	2.1293	1.7042
11	B2	638.0982	1.5017	2.0091
12	A2	661.4056	3.1377	0.0000
13	A1	670.8255	4.0329	16.7633
14	B1	680.0536	2.5927	7.6028
15	A1	733.8581	3.0518	12.2498
16	B1	865.6683	0.5934	29.8176
17	B2	884.5089	2.7564	142.1043
18	B2	1112.8776	5.8071	10.6980
19	B2	1181.4318	1.3035	96.2857
20	A1	1192.2032	9.5243	200.2362
21	B2	1350.0250	13.0557	44.8508
22	A1	1378.8341	13.3321	2.8450
23	A1	1423.0899	13.3272	35.1129
24	B2	1470.8088	9.1804	707.7098
25	B2	1617.7525	12.9100	6.6830
26	A1	1628.5108	17.8963	22.5389
27	A1	3183.6294	6.5283	1.5750

revtpss/pyFFHFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	112.0858	0.1375	0.0000
2	B1	196.8103	0.3108	2.5802
3	A1	266.0763	0.7552	0.7566
4	B2	289.1307	0.8689	0.1200
5	B1	292.0155	0.4218	0.9150
6	A1	348.9644	1.1497	1.9727
7	B2	437.0172	1.5945	0.0821
8	A2	443.8638	1.4667	0.0000
9	B1	471.0043	0.5901	0.3627
10	A1	494.4130	2.1372	1.9355
11	B2	641.4743	1.5068	2.0204
12	A1	673.5565	4.0878	14.0744
13	A2	681.7268	3.3333	0.0000
14	B1	710.1023	2.1684	9.2400
15	A1	735.8537	3.0645	12.9049

16	B1	885.2174	0.6534	24.3975
17	B2	888.6964	2.7221	126.7402
18	B2	1120.3880	5.6061	12.7059
19	B2	1184.3049	1.3366	88.7208
20	A1	1198.9912	9.6354	185.0734
21	B2	1341.8351	12.7669	38.8503
22	A1	1383.2916	13.3936	3.7636
23	A1	1423.9922	13.4151	37.0039
24	B2	1472.6077	9.3590	691.1018
25	B2	1614.0547	12.5587	8.5862
26	A1	1626.1086	17.8604	22.0733
27	A1	3178.2911	6.5036	1.3889

revtpss/pyFFHFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	111.5099	0.1360	0.0000
2	B1	196.7040	0.3098	2.2174
3	A1	266.9620	0.7600	0.7651
4	B2	289.7861	0.8727	0.1204
5	B1	291.3153	0.4202	0.9119
6	A1	349.2644	1.1522	1.8369
7	B2	437.7702	1.6016	0.0774
8	A2	444.8073	1.4730	0.0000
9	B1	469.3932	0.5930	0.2928
10	A1	494.7853	2.1392	1.9961
11	B2	641.9988	1.5103	1.9718
12	A1	674.4482	4.0947	13.5305
13	A2	678.8057	3.3055	0.0000
14	B1	705.1471	2.3330	7.2693
15	A1	736.5235	3.0707	12.9306
16	B1	875.1708	0.6262	25.3446
17	B2	890.3868	2.7176	122.9082
18	B2	1124.5783	5.4628	13.6472
19	B2	1186.4174	1.3513	83.1740
20	A1	1202.6986	9.6840	184.9944
21	B2	1344.1907	12.8275	41.8620
22	A1	1386.9445	13.4095	3.5092
23	A1	1427.0703	13.5515	36.9188
24	B2	1476.8742	9.4423	676.8644
25	B2	1616.7499	12.6209	8.1159
26	A1	1627.2701	17.8981	22.9645
27	A1	3179.6899	6.5089	1.0955

revtpss/pyFFHFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	109.9174	0.1322	0.0000
2	B1	195.4407	0.3063	2.8951
3	A1	267.4477	0.7632	0.7138

4	B1	289.6574	0.4170	0.9561
5	B2	289.8824	0.8753	0.1667
6	A1	347.8411	1.1425	2.0807
7	B2	436.5150	1.5972	0.0905
8	A2	443.2078	1.4621	0.0000
9	B1	465.9170	0.5809	0.2888
10	A1	493.2996	2.1275	1.7152
11	B2	638.9143	1.5231	1.8449
12	A1	671.0390	4.0475	14.0436
13	A2	675.5488	3.2744	0.0000
14	B1	701.5371	2.1738	8.5362
15	A1	733.9215	3.0489	12.6810
16	B1	875.3847	0.6340	27.7933
17	B2	887.3812	2.7436	131.5829
18	B2	1120.7262	5.6404	11.0599
19	B2	1186.1762	1.3186	84.8209
20	A1	1195.1108	9.5781	193.1039
21	B2	1354.0690	13.0681	37.6434
22	A1	1386.8696	13.4413	2.9924
23	A1	1426.2327	13.4368	36.0144
24	B2	1475.6252	9.4918	698.9406
25	B2	1617.6019	12.8952	8.7190
26	A1	1631.8602	17.9973	22.2816
27	A1	3189.2926	6.5509	2.6676

revtpss/pyFHFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	124.1892	0.1507	0.1310
2	A"	202.8023	0.3331	3.5687
3	A"	252.1657	0.2702	1.1607
4	A'	255.6132	0.7152	0.1888
5	A'	305.5006	0.9389	0.8469
6	A'	339.8357	1.1130	1.3754
7	A"	371.9291	0.8657	0.6219
8	A'	447.7234	1.6447	0.3980
9	A'	513.0239	1.7323	2.7806
10	A'	581.8064	3.4552	0.0607
11	A"	602.9750	1.3325	4.9571
12	A'	644.6484	1.6009	2.1300
13	A"	652.0639	1.9833	0.0049
14	A"	695.8736	2.2619	1.9286
15	A'	779.8361	3.5671	46.7002
16	A"	818.7295	0.5648	33.3463
17	A'	1001.8493	3.0387	104.8254
18	A'	1047.1765	7.6849	176.7737
19	A'	1138.0963	1.5852	74.3039
20	A'	1215.6232	3.9540	65.8076
21	A'	1353.0770	13.2910	13.5475
22	A'	1380.2207	10.2022	30.8372
23	A'	1424.2153	13.1874	208.6804
24	A'	1492.6556	8.4870	381.5524

25	A'	1618.2417	15.0979	239.8630
26	A'	1627.6086	17.6538	31.5993
27	A'	3194.2587	6.5773	1.3416

revtpss/pyFHFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	125.2653	0.1534	0.1053
2	A"	203.3043	0.3386	2.8516
3	A"	254.8621	0.2729	1.2349
4	A'	257.4365	0.7248	0.2279
5	A'	306.6629	0.9445	0.7448
6	A'	340.5633	1.1175	1.0915
7	A"	372.8013	0.8765	0.6098
8	A'	447.7731	1.6439	0.3746
9	A'	512.4964	1.7309	2.3116
10	A'	584.9163	3.4923	0.0268
11	A"	610.2615	1.3369	5.2093
12	A'	647.2746	1.6027	2.3717
13	A"	664.4646	1.7952	0.0002
14	A"	722.1312	2.0842	0.5761
15	A'	781.8898	3.5777	41.1314
16	A"	834.1252	0.6248	31.0026
17	A'	1004.6708	2.9192	93.7393
18	A'	1053.7080	7.7523	161.8130
19	A'	1143.0660	1.6093	77.5297
20	A'	1220.4189	4.1361	61.0932
21	A'	1346.1713	13.2568	11.9646
22	A'	1385.1461	10.3574	35.6965
23	A'	1425.3157	13.1350	193.3914
24	A'	1494.3074	8.5584	375.3745
25	A'	1615.3016	14.9531	225.8254
26	A'	1623.5565	17.3289	32.3453
27	A'	3189.1610	6.5534	1.0606

revtpss/pyFHFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	124.5967	0.1517	0.0926
2	A"	202.9321	0.3355	2.5141
3	A"	253.8865	0.2724	1.2251
4	A'	258.3308	0.7299	0.2342
5	A'	307.3199	0.9486	0.7347
6	A'	341.1125	1.1210	1.0321
7	A"	372.8550	0.8772	0.5082
8	A'	448.2376	1.6467	0.3657
9	A'	513.1283	1.7371	2.1638
10	A'	585.4060	3.4964	0.0188
11	A"	609.1586	1.3563	4.5173
12	A'	647.7410	1.6040	2.2793

13	A"	663.2952	1.8624	0.0036
14	A"	714.5983	2.2636	0.8836
15	A'	782.9845	3.5858	40.2480
16	A"	824.2485	0.5889	29.5279
17	A'	1006.6327	2.8740	91.3755
18	A'	1056.6572	7.8163	157.8377
19	A'	1145.9763	1.6074	75.9794
20	A'	1223.1975	4.2492	60.0427
21	A'	1349.1505	13.2890	10.9617
22	A'	1389.3561	10.6265	37.2764
23	A'	1428.9304	13.1245	181.1367
24	A'	1497.2185	8.6502	374.1444
25	A'	1617.0116	14.9331	229.7391
26	A'	1625.6407	17.4084	32.5432
27	A'	3190.7837	6.5595	0.8084

revtpss/pyFHFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	123.5848	0.1493	0.1209
2	A"	202.5819	0.3352	3.2328
3	A"	252.3811	0.2700	1.2722
4	A'	259.3620	0.7359	0.2125
5	A'	306.7449	0.9478	0.8568
6	A'	339.7063	1.1135	1.2414
7	A"	371.2796	0.8623	0.5478
8	A'	447.4074	1.6461	0.3755
9	A'	511.9468	1.7295	2.2777
10	A'	583.4372	3.4720	0.0552
11	A"	606.4906	1.3425	5.0404
12	A'	644.7363	1.6177	2.0307
13	A"	660.1683	1.8118	0.0029
14	A"	715.0829	2.1565	0.6462
15	A'	780.1355	3.5592	42.0675
16	A"	828.1474	0.6031	34.3628
17	A'	1003.7766	2.9797	99.4566
18	A'	1051.7945	7.7405	165.2986
19	A'	1143.9623	1.5933	69.8007
20	A'	1220.2988	3.9965	60.3182
21	A'	1356.0937	13.4053	13.8535
22	A'	1388.1572	10.4408	36.2263
23	A'	1428.8247	13.1959	193.2329
24	A'	1497.0492	8.7309	383.2287
25	A'	1619.8674	15.2325	233.9343
26	A'	1628.7180	17.6170	30.5127
27	A'	3201.0977	6.6049	2.3614

revtpss/pyHHHHH_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	361.5808	0.1985	0.0000
2	B1	399.8300	0.3614	3.5331
3	A1	590.2775	1.4401	3.4094
4	B2	645.3975	1.5424	0.3161
5	B1	701.5996	0.4257	58.5259
6	B1	740.4936	0.7343	14.8441
7	A2	883.5460	0.5738	0.0000
8	B1	937.9727	0.6770	0.0514
9	A2	974.9594	0.8194	0.0000
10	B1	986.0480	0.7153	0.0001
11	A1	989.1976	4.0993	4.7193
12	A1	1029.1070	3.1401	4.0065
13	B2	1062.7873	1.2016	0.0611
14	A1	1078.4362	1.1789	5.0227
15	B2	1158.0543	0.8700	1.7083
16	A1	1227.9091	1.1487	3.9744
17	B2	1294.7564	9.1589	0.2440
18	B2	1368.9550	1.3249	0.0967
19	B2	1451.2144	2.5828	24.0936
20	A1	1494.0181	2.4968	1.4844
21	B2	1593.4980	7.9282	8.6151
22	A1	1602.7596	7.5861	21.0205
23	B2	3107.2419	6.1804	32.3537
24	A1	3108.7223	6.1962	7.8620
25	A1	3127.2215	6.2730	7.9085
26	B2	3141.5642	6.3581	47.1699
27	A1	3151.5829	6.4319	13.5897

revtpss/pyHHHHH_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	364.4786	0.1985	0.0000
2	B1	402.5806	0.3616	3.3583
3	A1	589.1633	1.4299	4.1276
4	B2	645.1183	1.5352	0.1891
5	B1	707.6368	0.4021	56.9068
6	B1	749.8719	0.7997	9.0524
7	A2	889.9483	0.5824	0.0000
8	B1	947.6938	0.6963	0.0238
9	A1	990.3421	4.0466	5.0453
10	A2	990.3596	0.8531	0.0000
11	B1	1002.9949	0.7636	0.0037
12	A1	1033.3033	3.0494	4.8107
13	B2	1062.9394	1.1983	0.2136
14	A1	1078.7258	1.1970	3.1535
15	B2	1154.7031	0.8688	1.8128
16	A1	1226.0733	1.1541	3.2259
17	B2	1289.5239	8.8540	0.1646
18	B2	1371.4220	1.3324	0.1632
19	B2	1453.4606	2.6081	23.7242
20	A1	1497.2522	2.5006	1.4312
21	B2	1592.7785	7.7857	8.1166

22	A1	1601.9129	7.4887	20.5934
23	B2	3103.5707	6.1656	30.7848
24	A1	3105.3709	6.1853	7.7906
25	A1	3125.4962	6.2638	6.3076
26	B2	3139.4571	6.3475	42.8497
27	A1	3149.5045	6.4207	12.8569

revtpss/pyHHHHH_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	364.9396	0.1989	0.0000
2	B1	403.1768	0.3647	3.3311
3	A1	589.7955	1.4346	4.3306
4	B2	646.6400	1.5444	0.2413
5	B1	707.0879	0.3921	57.2698
6	B1	750.9794	0.8406	7.2792
7	A2	889.7038	0.5820	0.0000
8	B1	946.0442	0.6952	0.0156
9	A2	988.8040	0.8509	0.0000
10	A1	991.8092	4.0713	5.6332
11	B1	1003.5249	0.7602	0.0001
12	A1	1033.9491	3.0483	5.2764
13	B2	1063.8577	1.1996	0.1828
14	A1	1079.7293	1.1964	3.0384
15	B2	1156.7090	0.8723	1.7178
16	A1	1227.4044	1.1567	2.9698
17	B2	1291.8738	8.8747	0.2076
18	B2	1372.5503	1.3341	0.1484
19	B2	1455.5691	2.6145	24.3753
20	A1	1498.7866	2.5106	1.7740
21	B2	1594.8993	7.8254	7.8562
22	A1	1603.4244	7.5025	21.2843
23	B2	3104.1424	6.1675	32.4508
24	A1	3106.1313	6.1890	9.6580
25	A1	3126.9152	6.2685	7.0323
26	B2	3141.1206	6.3536	43.5418
27	A1	3151.1178	6.4273	12.7983

revtpss/pyHHHHH_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	363.0911	0.1979	0.0000
2	B1	400.6080	0.3602	3.4670
3	A1	589.7133	1.4371	3.4763
4	B2	644.2065	1.5347	0.3939
5	B1	702.2176	0.3917	66.9642
6	B1	746.9076	0.8146	10.3566
7	A2	884.7075	0.5752	0.0000
8	B1	940.6234	0.6858	0.0691
9	A2	983.7566	0.8399	0.0000

10	A1	988.3053	4.0830	5.1968
11	B1	998.9385	0.7533	0.0092
12	A1	1030.9622	3.1364	4.0376
13	B2	1063.4374	1.1974	0.0100
14	A1	1078.5880	1.1764	5.1029
15	B2	1157.5063	0.8641	1.5985
16	A1	1228.0990	1.1460	3.3230
17	B2	1296.9540	9.4278	0.1368
18	B2	1367.4406	1.3218	0.0950
19	B2	1450.2531	2.5973	25.9442
20	A1	1492.6701	2.4984	2.3586
21	B2	1592.9436	8.0182	7.3125
22	A1	1603.5497	7.7240	20.7851
23	B2	3115.1878	6.2123	25.3106
24	A1	3116.6545	6.2292	7.2910
25	A1	3136.0417	6.3070	6.5873
26	B2	3150.0429	6.3918	34.7250
27	A1	3159.7161	6.4653	9.3883

wb97xd/pyCCCCC_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	58.8720	0.0697	0.0000
2	B1	81.2651	0.1315	0.0177
3	B1	150.9862	0.2147	0.0079
4	A1	206.6798	0.8326	0.0704
5	B2	218.7730	0.8671	0.3123
6	A1	220.8355	0.8248	0.0494
7	B2	228.0937	1.0682	0.0001
8	B1	287.9587	0.6591	0.8805
9	B2	336.4971	1.9260	0.3040
10	A1	353.4574	2.1082	0.1316
11	A2	372.4181	1.0229	0.0000
12	A1	389.8756	2.9296	0.1261
13	A1	552.2886	3.1134	7.1841
14	B1	588.2526	2.5302	1.4057
15	B2	591.4417	2.7724	1.0282
16	A2	642.3609	2.9425	0.0000
17	B2	692.7151	4.3855	88.5105
18	B1	755.8588	4.1139	0.1560
19	A1	837.3862	5.6633	91.6992
20	B2	910.4377	6.3470	3.4764
21	A1	1108.8919	9.1149	34.7543
22	A1	1249.9526	11.3503	4.2969
23	B2	1257.5734	11.3794	34.6757
24	B2	1380.7737	13.9562	412.8064
25	A1	1382.7147	13.6913	126.2298
26	A1	1576.7536	17.6958	105.4314
27	B2	1610.2257	19.1202	67.7425

wb97xd/pyCCCCC_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	60.3722	0.0732	0.0000
2	B1	82.7984	0.1362	0.0118
3	B1	151.8631	0.2172	0.0143
4	A1	203.4291	0.8167	0.0306
5	B2	215.9221	0.8453	0.2883
6	A1	218.5824	0.7998	0.0203
7	B2	223.7752	1.0279	0.0018
8	B1	291.3084	0.6751	0.7818
9	B2	336.1163	1.9205	0.3090
10	A1	353.5475	2.1104	0.1112
11	A2	376.9108	1.0478	0.0000
12	A1	389.9029	2.9297	0.1478
13	A1	551.9977	3.1116	6.1990
14	B2	588.1654	2.7432	0.5488
15	B1	598.1912	2.6167	1.2555
16	A2	659.4448	3.1013	0.0000
17	B2	692.3676	4.3776	81.4473
18	B1	781.7360	4.4010	1.4209
19	A1	836.9970	5.6597	85.1183
20	B2	908.0753	6.3160	3.4671
21	A1	1107.3155	9.0910	31.7246
22	A1	1248.9127	11.3224	5.2444
23	B2	1252.0357	11.2984	30.8468
24	B2	1377.3348	13.8798	383.8621
25	A1	1378.5981	13.6093	109.6898
26	A1	1572.2118	17.5884	97.3932
27	B2	1602.0188	18.9018	61.4741

wb97xd/pyCCCCC_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	60.7146	0.0741	0.0000
2	B1	83.2203	0.1375	0.0137
3	B1	152.6967	0.2197	0.0013
4	A1	204.1298	0.8240	0.0408
5	B2	216.8185	0.8526	0.2579
6	A1	219.7401	0.8073	0.0185
7	B2	224.5071	1.0343	0.0020
8	B1	292.4581	0.6806	0.7316
9	B2	337.1870	1.9303	0.3249
10	A1	354.6591	2.1198	0.1273
11	A2	379.3762	1.0617	0.0000
12	A1	391.5052	2.9511	0.1462
13	A1	554.3855	3.1368	6.1425
14	B2	591.1411	2.7727	0.7555
15	B1	601.5484	2.6465	1.2776
16	A2	662.9847	3.1350	0.0000
17	B2	696.5004	4.4272	82.0385
18	B1	784.2540	4.4289	1.4691

19	A1	840.3713	5.7096	88.6082
20	B2	912.2733	6.3786	2.9906
21	A1	1111.0413	9.1560	32.8353
22	A1	1250.9363	11.3612	4.7211
23	B2	1253.2464	11.3113	34.6859
24	B2	1378.4920	13.9006	381.4105
25	A1	1380.1472	13.6396	113.1109
26	A1	1571.3002	17.5700	101.5349
27	B2	1604.1617	18.9729	62.1613

wb97xd/pyCCCCC_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	59.3031	0.0707	0.0000
2	B1	81.2820	0.1314	0.0151
3	B1	150.4399	0.2132	0.0001
4	A1	205.4594	0.8232	0.0406
5	B2	217.5313	0.8576	0.1697
6	A1	218.9645	0.8108	0.0089
7	B2	226.0069	1.0485	0.0001
8	B1	287.9471	0.6590	0.5220
9	B2	334.4198	1.9069	0.3775
10	A1	351.4919	2.0887	0.1188
11	A2	373.7137	1.0300	0.0000
12	A1	387.3024	2.8978	0.1303
13	A1	548.1543	3.0681	7.6250
14	B2	587.4033	2.7366	1.5404
15	B1	588.1807	2.5275	1.1118
16	A2	645.2232	2.9689	0.0000
17	B2	687.7354	4.3197	89.6998
18	B1	762.2954	4.1896	1.8439
19	A1	832.8137	5.5977	94.5646
20	B2	905.6902	6.2742	3.0116
21	A1	1102.5929	9.0093	36.3190
22	A1	1248.3349	11.3112	3.8252
23	B2	1260.2365	11.4219	33.5227
24	B2	1378.8170	13.9128	400.4980
25	A1	1380.9129	13.6522	122.8038
26	A1	1577.3173	17.7071	105.6735
27	B2	1609.9699	19.1234	66.1696

wb97xd/pyFCFCF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	92.8797	0.1084	0.0000
2	B1	110.5219	0.1571	0.0015
3	A1	186.2893	0.5415	0.0122
4	B1	218.2169	0.4236	2.7088
5	B2	229.1424	0.6942	0.0282
6	B2	318.4198	1.2847	1.0337

7	B1	320.2103	0.8366	0.4844
8	A1	328.5262	1.3896	0.3029
9	A2	385.2259	1.0961	0.0000
10	A1	414.3289	2.0582	0.6284
11	B2	416.4584	1.8873	0.1269
12	A1	588.3798	3.2836	1.9317
13	A1	624.1585	3.7858	2.4560
14	B1	664.6746	3.2302	1.4160
15	A2	712.1192	3.6399	0.0000
16	B2	714.6561	3.9958	0.4318
17	B1	778.0138	4.3649	16.6214
18	B2	806.9807	5.5247	116.6068
19	A1	1089.7655	9.7019	183.7411
20	B2	1120.4236	10.1437	21.7941
21	A1	1169.1895	10.2331	6.2458
22	B2	1316.9805	12.6490	14.8139
23	A1	1458.8787	15.8327	49.1857
24	B2	1482.9917	16.1752	445.4698
25	A1	1500.4030	16.4817	103.8054
26	A1	1657.6762	19.6184	227.4287
27	B2	1679.4919	20.6577	92.3846

wb97xd/pyFCFCF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	94.2237	0.1116	0.0000
2	B1	111.7344	0.1604	0.0014
3	A1	184.6939	0.5322	0.0010
4	B1	216.5974	0.4171	2.2903
5	B2	227.9941	0.6866	0.0193
6	B2	318.8682	1.2922	0.9991
7	B1	322.3043	0.8488	0.6510
8	A1	328.8461	1.3968	0.2447
9	A2	379.0416	1.0608	0.0000
10	A1	414.8682	2.0588	0.6078
11	B2	416.4393	1.8800	0.1438
12	A1	588.7608	3.2590	1.7201
13	A1	626.1211	3.8348	1.5918
14	B1	668.5455	3.2686	1.3408
15	B2	715.8885	4.0115	0.1059
16	A2	721.9725	3.7432	0.0000
17	B1	795.0316	4.5566	12.9665
18	B2	805.4971	5.4953	107.0876
19	A1	1096.2618	9.7855	163.4261
20	B2	1126.4122	10.2611	17.1664
21	A1	1168.1621	10.2356	3.3594
22	B2	1309.2040	12.5252	11.5342
23	A1	1465.1020	15.9461	59.5315
24	B2	1484.4070	16.2138	425.1295
25	A1	1500.7490	16.5539	77.6278
26	A1	1652.9144	19.5068	223.1148
27	B2	1671.1720	20.4364	94.2685

wb97xd/pyFCFCF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	93.9792	0.1110	0.0000
2	B1	111.5320	0.1600	0.0000
3	A1	186.3399	0.5417	0.0000
4	B1	217.1609	0.4194	2.0655
5	B2	229.8554	0.6982	0.0140
6	B2	320.0668	1.3012	0.9517
7	B1	323.2216	0.8530	0.5885
8	A1	329.8513	1.4033	0.2015
9	A2	381.7579	1.0763	0.0000
10	A1	415.8035	2.0684	0.5964
11	B2	417.0767	1.8857	0.1417
12	A1	589.4594	3.2783	1.5530
13	A1	626.8179	3.8325	1.5900
14	B1	669.1246	3.2745	1.1062
15	B2	717.4802	4.0294	0.1457
16	A2	722.9389	3.7532	0.0000
17	B1	794.8350	4.5544	13.1330
18	B2	808.8678	5.5452	106.6623
19	A1	1097.3393	9.8095	167.4561
20	B2	1128.3256	10.2834	16.1525
21	A1	1171.2436	10.2822	3.9933
22	B2	1311.7474	12.5718	13.6948
23	A1	1469.3548	16.0585	56.4780
24	B2	1486.7683	16.2640	415.3282
25	A1	1501.3056	16.5489	88.1129
26	A1	1652.9052	19.5110	230.2973
27	B2	1674.7079	20.5454	99.5785

wb97xd/pyFCFCF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	93.0181	0.1087	0.0000
2	B1	110.5876	0.1572	0.0005
3	A1	186.6996	0.5440	0.0031
4	B1	215.9144	0.4141	2.3572
5	B2	230.6648	0.7033	0.0054
6	B2	318.7994	1.2903	0.9447
7	B1	319.5366	0.8346	0.3160
8	A1	328.4215	1.3928	0.1992
9	A2	376.5818	1.0467	0.0000
10	A1	413.0351	2.0439	0.6696
11	B2	415.0842	1.8720	0.0685
12	A1	587.3287	3.2461	1.8242
13	A1	623.9665	3.8010	1.7182
14	B1	663.9420	3.2224	0.7637
15	B2	712.4012	3.9705	0.3132

16	A2	715.4362	3.6769	0.0000
17	B1	783.3244	4.4258	20.1394
18	B2	802.0512	5.4459	110.9649
19	A1	1092.8639	9.7289	180.5534
20	B2	1124.5508	10.2230	18.3133
21	A1	1165.1925	10.1776	3.6351
22	B2	1320.1768	12.7207	12.2084
23	A1	1469.3085	16.0595	54.7760
24	B2	1487.6237	16.2749	435.1636
25	A1	1505.2428	16.6316	94.6220
26	A1	1659.5502	19.6629	234.4218
27	B2	1678.8374	20.6546	92.1480

wb97xd/pyFCFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	98.7405	0.1217	0.0001
2	A"	142.2276	0.2226	0.0023
3	A'	205.4769	0.5847	0.0196
4	A"	218.2284	0.4226	3.6111
5	A'	280.9950	0.8762	0.2593
6	A'	318.5779	1.2154	0.8143
7	A"	332.2266	0.8916	0.9559
8	A'	340.5811	1.2865	0.7164
9	A'	413.1032	1.9323	0.2397
10	A"	418.6025	1.3092	1.4401
11	A'	477.2448	2.1600	0.4338
12	A'	600.0445	3.6229	0.8816
13	A'	643.8166	3.8324	7.4109
14	A"	652.8615	3.1187	1.9324
15	A"	704.1403	3.5601	0.2065
16	A'	735.3214	4.2274	0.6381
17	A"	761.5798	4.1847	11.6487
18	A'	917.9621	7.1341	154.5797
19	A'	1095.6632	9.8185	195.2558
20	A'	1132.5820	10.2874	33.8213
21	A'	1276.7225	12.4793	22.5319
22	A'	1324.1744	12.8229	19.3075
23	A'	1462.3014	15.8737	48.9391
24	A'	1502.4903	16.5369	291.6802
25	A'	1549.3626	17.8324	453.7050
26	A'	1678.4030	20.1330	190.4144
27	A'	1699.1869	21.0544	18.7998

wb97xd/pyFCFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	100.3890	0.1257	0.0013
2	A"	143.7563	0.2275	0.0016
3	A'	204.3215	0.5778	0.0177

4	A"	217.4375	0.4190	2.8881
5	A'	282.1697	0.8836	0.3037
6	A'	319.4338	1.2276	0.7543
7	A"	335.1665	0.9084	1.0482
8	A'	341.3128	1.2894	0.6172
9	A'	413.3855	1.9285	0.2050
10	A"	420.5692	1.3223	1.1485
11	A'	477.7975	2.1631	0.5000
12	A'	602.3501	3.6308	0.9965
13	A'	644.1361	3.8498	5.9935
14	A"	661.1007	3.2015	2.1680
15	A"	722.3861	3.7484	0.5424
16	A'	738.1975	4.2619	0.5427
17	A"	792.2514	4.5215	8.4137
18	A'	920.3768	7.1524	139.3919
19	A'	1102.2310	9.9219	171.9123
20	A'	1137.8813	10.3974	34.5827
21	A'	1281.7370	12.5392	20.1798
22	A'	1317.9434	12.7842	16.0655
23	A'	1467.6476	15.9846	50.7718
24	A'	1502.8200	16.5586	278.2496
25	A'	1550.5037	17.8887	434.3584
26	A'	1673.9525	20.0389	191.3305
27	A'	1692.8604	20.8726	14.1709

wb97xd/pyFCFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	100.0802	0.1249	0.0002
2	A"	142.9433	0.2250	0.0003
3	A'	206.0793	0.5879	0.0238
4	A"	217.6649	0.4199	2.6158
5	A'	283.4293	0.8913	0.3053
6	A'	320.3135	1.2334	0.7380
7	A"	335.7592	0.9115	0.9930
8	A'	342.0722	1.2951	0.5553
9	A'	414.0926	1.9351	0.2077
10	A"	421.2350	1.3259	1.1090
11	A'	478.2296	2.1673	0.5215
12	A'	602.4530	3.6373	0.8774
13	A'	645.3086	3.8614	5.7902
14	A"	660.2417	3.1923	1.8574
15	A"	721.1502	3.7354	0.3885
16	A'	739.1493	4.2725	0.5286
17	A"	787.1531	4.4665	8.4094
18	A'	922.2109	7.1846	139.7391
19	A'	1103.3099	9.9405	176.9360
20	A'	1140.0073	10.4258	32.1401
21	A'	1283.8396	12.5803	21.3486
22	A'	1320.5006	12.8268	17.8513
23	A'	1471.6472	16.0827	52.4942
24	A'	1505.0473	16.5934	257.4973

25	A'	1552.4751	17.9387	449.4037
26	A'	1674.9203	20.0610	194.0029
27	A'	1695.7185	20.9674	17.6042

wb97xd/pyFCFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	98.9865	0.1222	0.0000
2	A"	141.9212	0.2217	0.0010
3	A'	206.5564	0.5904	0.0377
4	A"	216.8929	0.4168	3.2143
5	A'	283.4867	0.8921	0.2743
6	A'	319.0667	1.2241	0.8161
7	A"	331.9429	0.8910	0.7611
8	A'	340.5796	1.2846	0.6281
9	A'	411.8691	1.9187	0.2316
10	A"	419.1541	1.3131	1.7062
11	A'	476.7791	2.1530	0.4997
12	A'	600.7531	3.6148	1.0464
13	A'	641.9185	3.8152	6.3823
14	A"	655.9790	3.1505	1.6984
15	A"	716.2277	3.6860	1.0881
16	A'	733.9673	4.2111	0.5881
17	A"	781.0025	4.3960	11.1355
18	A'	916.8411	7.0974	144.6315
19	A'	1099.0585	9.8692	186.9169
20	A'	1135.8990	10.3528	32.9052
21	A'	1280.5678	12.5623	20.5770
22	A'	1328.1320	12.9270	17.8700
23	A'	1471.7553	16.0849	52.3231
24	A'	1506.3804	16.6290	275.1049
25	A'	1556.3370	18.0205	454.2634
26	A'	1680.3089	20.1922	194.1033
27	A'	1700.1220	21.0741	15.0595

wb97xd/pyFFCFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	118.6421	0.1539	0.0000
2	B1	123.1237	0.1864	0.0339
3	B2	205.2092	0.5964	0.0283
4	B1	212.9884	0.3972	3.4288
5	A1	285.1061	0.9316	0.8019
6	B2	313.6290	1.0662	0.2890
7	A1	335.3186	1.3748	0.8827
8	B1	339.2165	0.9431	1.0328
9	A1	435.3718	2.0349	0.0793
10	A2	454.4340	1.5381	0.0000
11	B2	466.7910	2.0653	0.0843
12	A1	549.4311	3.1348	1.8002

13	B1	607.0575	2.6919	8.7733
14	A2	705.5192	3.5731	0.0000
15	A1	708.1565	4.6165	10.7023
16	B2	732.9945	4.1828	0.0018
17	B1	750.6925	4.0646	3.1936
18	A1	936.0506	7.1129	142.1065
19	B2	986.4328	8.4198	175.9287
20	B2	1190.3863	11.2983	0.0184
21	A1	1276.1790	12.3728	67.1161
22	B2	1313.9816	12.5946	35.0649
23	A1	1466.4491	16.1055	6.2260
24	A1	1507.5784	16.4704	88.1038
25	B2	1533.6889	17.4928	770.7791
26	B2	1684.1151	20.7605	5.3716
27	A1	1687.8067	20.3614	131.0457

wb97xd/pyFFCFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	119.8334	0.1569	0.0000
2	B1	125.1542	0.1928	0.0557
3	B2	204.2504	0.5905	0.0187
4	B1	212.9916	0.3968	2.6389
5	A1	285.8814	0.9369	0.9009
6	B2	315.0891	1.0759	0.3079
7	A1	335.7493	1.3806	0.6685
8	B1	341.8138	0.9579	0.9966
9	A1	435.9475	2.0374	0.0593
10	A2	455.3767	1.5447	0.0000
11	B2	466.5843	2.0606	0.0675
12	A1	551.1878	3.1489	2.0415
13	B1	611.9410	2.7386	8.2689
14	A1	709.9875	4.6381	8.3661
15	A2	724.5572	3.7693	0.0000
16	B2	735.8694	4.2170	0.1057
17	B1	785.6577	4.4476	2.4456
18	A1	935.6417	7.1017	131.3143
19	B2	992.8152	8.5201	155.3373
20	B2	1198.9096	11.4371	0.0079
21	A1	1281.1272	12.4731	62.3229
22	B2	1305.6329	12.4858	32.8381
23	A1	1469.5970	16.1702	8.1093
24	A1	1508.3491	16.5149	86.0683
25	B2	1534.9334	17.5420	737.0211
26	B2	1678.1647	20.5903	3.8840
27	A1	1682.8608	20.2509	124.0616

wb97xd/pyFFCFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	119.3437	0.1556	0.0000
2	B1	124.9926	0.1923	0.0485
3	B2	206.0585	0.6011	0.0115
4	B1	213.2181	0.3978	2.3779
5	A1	287.1823	0.9458	0.9017
6	B2	316.1523	1.0832	0.2758
7	A1	336.4604	1.3838	0.6336
8	B1	341.8487	0.9576	0.9505
9	A1	436.4468	2.0424	0.0417
10	A2	456.3387	1.5513	0.0000
11	B2	467.1710	2.0666	0.0776
12	A1	551.6769	3.1575	2.0434
13	B1	613.2198	2.7498	8.2441
14	A1	710.5822	4.6451	7.9019
15	A2	722.5639	3.7490	0.0000
16	B2	736.6183	4.2253	0.0791
17	B1	781.2095	4.3983	1.9038
18	A1	938.1990	7.1427	132.6520
19	B2	993.6532	8.5314	156.1204
20	B2	1200.5026	11.4603	0.1282
21	A1	1283.7187	12.5206	64.1070
22	B2	1308.0385	12.5305	35.3318
23	A1	1473.0432	16.2624	5.7588
24	A1	1509.1212	16.5177	88.6271
25	B2	1538.0825	17.6053	735.9091
26	B2	1679.9885	20.6614	5.2150
27	A1	1684.2932	20.2883	126.0538

wb97xd/pyFFCFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.9171	0.1519	0.0000
2	B1	123.7164	0.1883	0.0458
3	B2	206.5250	0.6037	0.0010
4	B1	211.9249	0.3928	2.9706
5	A1	286.9584	0.9454	0.8363
6	B2	315.3989	1.0784	0.3181
7	A1	334.9819	1.3732	0.7204
8	B1	338.8308	0.9414	0.8767
9	A1	434.0497	2.0222	0.0937
10	A2	454.9440	1.5415	0.0000
11	B2	465.8079	2.0536	0.0824
12	A1	549.8970	3.1310	2.0421
13	B1	604.0062	2.6667	10.7654
14	A1	707.4803	4.6020	8.9400
15	A2	719.3444	3.7161	0.0000
16	B2	731.8940	4.1703	0.0106
17	B1	775.4259	4.3346	1.6406
18	A1	932.5631	7.0536	136.7534
19	B2	990.0538	8.4710	163.7111
20	B2	1198.2334	11.4427	0.0395
21	A1	1277.8983	12.4129	63.4010

22	B2	1317.3252	12.6797	36.2122
23	A1	1474.5776	16.2884	5.3262
24	A1	1510.3123	16.5481	89.9647
25	B2	1541.0728	17.6836	762.1767
26	B2	1685.8966	20.8014	3.7066
27	A1	1689.4341	20.4104	128.1636

wb97xd/pyFFFFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	120.7118	0.1592	0.0000
2	B1	158.9663	0.2739	0.0007
3	B1	219.3027	0.4254	4.8171
4	B2	277.0540	0.8512	0.0506
5	A1	277.5292	0.8423	0.6871
6	B2	323.5465	1.1181	0.7798
7	A1	351.0418	1.2732	1.4798
8	B1	355.7253	1.0245	3.5232
9	A2	442.1256	1.4565	0.0000
10	B2	465.6341	2.0604	0.1449
11	A1	485.2704	2.2058	0.1607
12	A1	603.4620	3.7373	0.0081
13	B1	640.4856	3.0037	2.8883
14	A2	697.5888	3.4939	0.0000
15	A1	709.2887	4.5928	7.3178
16	B1	741.3681	3.9710	6.7834
17	B2	752.6149	4.4335	0.0182
18	B2	1005.6114	8.6758	220.1858
19	A1	1107.4162	10.0891	248.1799
20	B2	1195.3212	11.4379	0.0875
21	A1	1322.7147	13.4241	30.1392
22	B2	1329.0109	12.8814	21.2686
23	A1	1473.6250	16.0598	19.2132
24	B2	1544.1332	17.7714	736.9364
25	A1	1577.6816	18.3766	171.6911
26	A1	1697.9250	20.5791	122.3894
27	B2	1712.5108	21.3493	5.1662

wb97xd/pyFFFFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	122.1694	0.1631	0.0000
2	B1	160.9304	0.2809	0.0002
3	B1	219.2721	0.4248	3.6311
4	A1	278.5954	0.8485	0.7812
5	B2	278.7076	0.8611	0.0506
6	B2	324.8236	1.1265	0.7197
7	A1	351.7156	1.2776	1.2389
8	B1	359.6197	1.0482	3.0796
9	A2	445.2305	1.4772	0.0000

10	B2	465.6048	2.0581	0.1340
11	A1	486.5046	2.2146	0.2200
12	A1	606.5464	3.7720	0.0117
13	B1	654.7898	3.1489	3.5460
14	A1	710.5395	4.6097	5.6470
15	A2	723.4157	3.7574	0.0000
16	B2	756.3314	4.4792	0.0086
17	B1	790.2650	4.4961	4.8164
18	B2	1012.4141	8.7837	200.3923
19	A1	1114.3251	10.2093	229.6694
20	B2	1202.9887	11.5735	0.3268
21	B2	1320.7915	12.7606	18.2397
22	A1	1329.8358	13.5835	26.7685
23	A1	1476.4271	16.1102	23.3792
24	B2	1544.9165	17.7990	715.3548
25	A1	1578.7598	18.4354	164.5432
26	A1	1693.6284	20.4810	117.2700
27	B2	1706.2909	21.1785	3.4187

wb97xd/pyFFFFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	121.3584	0.1609	0.0000
2	B1	159.7281	0.2766	0.0008
3	B1	219.2187	0.4246	3.3045
4	A1	279.5524	0.8543	0.8077
5	B2	279.8988	0.8685	0.0543
6	B2	325.3899	1.1304	0.7153
7	A1	352.1061	1.2806	1.1684
8	B1	359.0593	1.0448	2.9320
9	A2	445.4635	1.4788	0.0000
10	B2	465.9978	2.0619	0.1456
11	A1	486.4526	2.2141	0.2593
12	A1	606.5203	3.7714	0.0171
13	B1	652.6876	3.1266	3.1272
14	A1	711.0760	4.6160	5.4093
15	A2	720.1075	3.7238	0.0000
16	B2	756.3813	4.4788	0.0059
17	B1	780.5884	4.3913	4.5959
18	B2	1012.9623	8.7926	199.8090
19	A1	1115.2093	10.2246	232.6096
20	B2	1204.6033	11.6010	0.5598
21	B2	1323.4417	12.8079	20.2472
22	A1	1331.3178	13.6123	28.3835
23	A1	1480.6453	16.2055	23.4387
24	B2	1548.4012	17.8790	706.3592
25	A1	1579.8531	18.4596	163.8899
26	A1	1694.5348	20.5063	119.2275
27	B2	1708.7485	21.2565	4.5004

wb97xd/pyFFFFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	119.9819	0.1572	0.0000
2	B1	158.7691	0.2732	0.0000
3	B1	219.0348	0.4242	4.3250
4	A1	279.5668	0.8545	0.7672
5	B2	279.9176	0.8687	0.0529
6	B2	324.2875	1.1230	0.8778
7	A1	350.7658	1.2708	1.3937
8	B1	356.5321	1.0301	3.3566
9	A2	444.9852	1.4753	0.0000
10	B2	464.8182	2.0507	0.1322
11	A1	485.2263	2.2024	0.1995
12	A1	604.9047	3.7511	0.0074
13	B1	649.2324	3.0940	3.4710
14	A1	708.3818	4.5783	5.9255
15	A2	717.6437	3.6987	0.0000
16	B2	751.3340	4.4174	0.0007
17	B1	778.8567	4.3690	4.9928
18	B2	1008.9035	8.7249	205.5199
19	A1	1111.0238	10.1496	237.6757
20	B2	1202.5044	11.5763	0.2287
21	A1	1327.3004	13.5393	28.3700
22	B2	1331.8585	12.9511	20.5202
23	A1	1481.1857	16.2213	21.6967
24	B2	1550.3786	17.9293	722.2607
25	A1	1583.8689	18.5486	169.3523
26	A1	1699.7371	20.6300	120.2395
27	B2	1713.4516	21.3755	3.8244

wb97xd/pyFFHFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.3545	0.1506	0.0000
2	B1	207.3889	0.3403	3.8974
3	A1	285.6301	0.8725	0.6782
4	B1	301.9522	0.4473	1.0795
5	B2	307.7050	0.9949	0.2027
6	A1	365.6542	1.2631	2.7602
7	B2	459.4859	1.8015	0.0649
8	A2	468.1892	1.6323	0.0000
9	B1	492.5810	0.6259	0.5654
10	A1	516.4389	2.3295	1.7116
11	B2	672.0755	1.6160	2.7025
12	A1	700.3871	4.3319	17.9643
13	A2	710.1978	3.6189	0.0000
14	B1	741.9384	2.7430	11.6892
15	A1	763.9581	3.2989	10.9856
16	B1	909.2036	0.6800	32.0291
17	B2	926.8133	2.7934	136.2124
18	B2	1176.2001	3.9717	24.1300

19	B2	1210.8274	1.5910	44.4753
20	A1	1253.6232	10.3933	205.4255
21	B2	1320.1712	10.9487	86.3430
22	A1	1448.4249	14.5304	0.4642
23	A1	1491.2992	14.9455	48.4395
24	B2	1548.2019	11.0812	760.6974
25	A1	1697.1172	19.5359	29.5973
26	B2	1703.3214	15.4460	1.3583
27	A1	3236.7620	6.7575	4.0157

wb97xd/pyFFHFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	118.8735	0.1545	0.0000
2	B1	208.2640	0.3453	2.8900
3	A1	286.7651	0.8789	0.7245
4	B1	305.3921	0.4550	1.0720
5	B2	309.4840	1.0064	0.1558
6	A1	366.8257	1.2705	2.2712
7	B2	459.5523	1.8010	0.0462
8	A2	470.0403	1.6454	0.0000
9	B1	498.6899	0.6241	0.4743
10	A1	518.4029	2.3411	1.9056
11	B2	676.7326	1.6283	2.6653
12	A1	703.5751	4.3992	14.9973
13	A2	732.1230	3.8462	0.0000
14	A1	765.7224	3.3058	11.3941
15	B1	769.5191	2.2203	13.5849
16	B1	930.4422	0.7603	24.8412
17	B2	932.0846	2.7778	118.7685
18	B2	1185.5025	3.7913	27.5413
19	B2	1216.1732	1.6844	35.1177
20	A1	1261.5731	10.5215	186.4176
21	B2	1312.4860	10.1100	83.6615
22	A1	1452.8564	14.6308	0.9161
23	A1	1492.8517	15.0617	51.8629
24	B2	1549.6134	11.2362	744.3762
25	A1	1693.8276	19.4737	28.7899
26	B2	1698.7290	14.9361	3.0118
27	A1	3236.7937	6.7540	3.1334

wb97xd/pyFFHFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	118.3144	0.1531	0.0000
2	B1	208.0825	0.3440	2.6451
3	A1	287.7078	0.8845	0.7377
4	B1	304.6338	0.4531	1.0670
5	B2	310.2641	1.0118	0.1547
6	A1	367.0439	1.2726	2.1661

7	B2	460.1473	1.8083	0.0432
8	A2	470.4661	1.6485	0.0000
9	B1	497.6131	0.6252	0.4160
10	A1	518.7072	2.3437	1.9700
11	B2	677.3192	1.6357	2.6279
12	A1	704.1526	4.3995	14.6593
13	A2	729.5731	3.8198	0.0000
14	A1	766.0520	3.3091	11.4558
15	B1	766.5346	2.3323	11.9724
16	B1	922.5877	0.7364	26.5242
17	B2	932.9116	2.7809	117.6975
18	B2	1187.7189	3.7250	28.4755
19	B2	1217.9279	1.7010	32.3287
20	A1	1263.9798	10.5525	190.6632
21	B2	1315.3533	10.2333	88.9108
22	A1	1455.5062	14.6071	0.5943
23	A1	1496.1409	15.2237	51.6966
24	B2	1553.7837	11.2226	733.6641
25	A1	1694.6985	19.5007	30.0462
26	B2	1701.5518	15.0836	2.2505
27	A1	3240.0434	6.7677	3.4825

wb97xd/pyFFHFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	116.8965	0.1494	0.0000
2	B1	206.8706	0.3401	3.4555
3	A1	287.2381	0.8820	0.7017
4	B1	303.1071	0.4504	1.0965
5	B2	309.4799	1.0074	0.2331
6	A1	365.2476	1.2599	2.5129
7	B2	458.8677	1.7999	0.0594
8	A2	469.2058	1.6393	0.0000
9	B1	493.5540	0.6164	0.4978
10	A1	517.3082	2.3315	1.7439
11	B2	673.0289	1.6377	2.4630
12	A1	700.6859	4.3500	15.2481
13	A2	725.7262	3.7801	0.0000
14	B1	761.4602	2.2511	13.4931
15	A1	763.9383	3.2920	11.4323
16	B1	921.2412	0.7368	28.7474
17	B2	929.7408	2.7873	126.1000
18	B2	1184.0658	3.6619	25.3039
19	B2	1216.1397	1.6621	35.8140
20	A1	1256.8573	10.4436	198.9616
21	B2	1324.5854	10.8780	82.5500
22	A1	1456.4299	14.6150	0.3552
23	A1	1495.6726	15.1326	49.5583
24	B2	1554.2394	11.3936	752.5878
25	A1	1700.2699	19.6329	29.5133
26	B2	1704.1739	15.4607	2.1962
27	A1	3247.4867	6.8024	5.3465

wb97xd/pyFHFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	130.5980	0.1686	0.1294
2	A"	213.9754	0.3648	4.2590
3	A"	264.0066	0.2963	1.2197
4	A'	278.4771	0.8505	0.1915
5	A'	324.7330	1.0716	1.0485
6	A'	357.7364	1.2431	1.5602
7	A"	392.5727	0.9389	0.8956
8	A'	469.3561	1.8453	0.4781
9	A'	538.7313	1.9073	3.2176
10	A'	606.6348	3.7246	0.0733
11	A"	641.0197	1.3132	6.0931
12	A'	678.8790	1.7310	2.9289
13	A"	694.4568	2.0054	0.0027
14	A"	751.5993	2.1586	1.5867
15	A'	813.3941	3.8521	45.6645
16	A"	859.8231	0.6923	41.6660
17	A'	1046.0533	2.6791	93.1134
18	A'	1100.5697	8.3485	172.5392
19	A'	1181.6422	1.5677	98.6009
20	A'	1269.4858	6.7466	39.6057
21	A'	1338.7490	10.7752	15.6597
22	A'	1447.0910	12.5022	57.6368
23	A'	1493.5065	14.0068	166.7007
24	A'	1563.2491	10.5390	450.4148
25	A'	1688.8525	16.9620	286.6093
26	A'	1706.8680	19.4859	52.7174
27	A'	3252.8000	6.8299	5.2321

wb97xd/pyFHFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	131.8333	0.1717	0.0984
2	A"	214.3838	0.3701	3.2052
3	A"	266.9468	0.3001	1.3261
4	A'	279.8454	0.8583	0.2264
5	A'	326.0124	1.0791	0.8959
6	A'	358.9746	1.2515	1.1899
7	A"	394.9252	0.9581	0.8068
8	A'	469.6649	1.8489	0.4421
9	A'	538.6713	1.9089	2.7081
10	A'	609.9507	3.7638	0.0303
11	A"	650.5007	1.2975	6.4459
12	A'	682.8552	1.7405	3.1396
13	A"	707.9652	1.8490	0.0017
14	A"	778.7168	1.9607	0.2293
15	A'	815.7125	3.8750	39.1401

16	A"	877.7685	0.7886	37.3682
17	A'	1049.3267	2.6113	80.8800
18	A'	1108.5687	8.4153	154.8999
19	A'	1189.7351	1.6128	99.8945
20	A'	1274.8257	7.3226	32.9823
21	A'	1332.3912	9.9967	18.1896
22	A'	1454.1594	12.7812	60.7490
23	A'	1493.7455	13.9625	155.3814
24	A'	1565.0607	10.5689	443.8659
25	A'	1684.7263	16.7169	275.0755
26	A'	1701.7314	19.1062	50.6129
27	A'	3253.6882	6.8297	4.0471

wb97xd/pyFHFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	131.2197	0.1701	0.0901
2	A"	214.1306	0.3677	2.9821
3	A"	266.1409	0.2994	1.3135
4	A'	280.8890	0.8647	0.2355
5	A'	326.6996	1.0840	0.8944
6	A'	359.4873	1.2554	1.1468
7	A"	394.5286	0.9555	0.7143
8	A'	470.0565	1.8530	0.4443
9	A'	539.1960	1.9147	2.5679
10	A'	610.0929	3.7639	0.0265
11	A"	649.6486	1.3099	5.9377
12	A'	683.2973	1.7432	3.0499
13	A"	707.3341	1.8724	0.0012
14	A"	774.0315	2.0395	0.3944
15	A'	816.4002	3.8816	39.0674
16	A"	869.2645	0.7553	37.1845
17	A'	1050.6055	2.5923	80.7655
18	A'	1110.1351	8.4698	154.3302
19	A'	1191.6121	1.6152	97.9710
20	A'	1276.5587	7.4190	34.6352
21	A'	1335.7584	10.0486	19.2214
22	A'	1457.4704	13.0402	60.6281
23	A'	1497.6945	13.9628	145.5748
24	A'	1567.6039	10.6216	442.5703
25	A'	1686.3703	16.7042	282.0078
26	A'	1704.0785	19.2633	51.7450
27	A'	3257.0979	6.8441	4.5116

wb97xd/pyFHFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	130.2666	0.1676	0.1165
2	A"	213.7966	0.3667	3.8645
3	A"	264.5441	0.2971	1.3272

4	A'	280.8044	0.8644	0.2221
5	A'	325.4114	1.0768	1.0774
6	A'	357.5716	1.2426	1.4197
7	A''	393.4411	0.9423	0.8109
8	A'	469.0761	1.8462	0.4461
9	A'	538.0381	1.9063	2.6865
10	A'	608.3347	3.7426	0.0628
11	A''	646.0730	1.3152	6.3648
12	A'	678.9699	1.7479	2.7951
13	A''	703.0760	1.8546	0.0007
14	A''	772.0903	2.0365	0.3800
15	A'	813.6246	3.8461	41.2012
16	A''	871.2908	0.7540	41.8708
17	A'	1048.0825	2.6491	89.1225
18	A'	1105.3028	8.3941	161.7689
19	A'	1187.9168	1.5722	93.1051
20	A'	1274.5274	6.9502	35.6495
21	A'	1341.8384	10.8243	16.2478
22	A'	1455.9098	12.8119	63.6297
23	A'	1498.4725	14.0118	151.3313
24	A'	1568.6475	10.8241	453.7189
25	A'	1690.4010	17.0319	285.0603
26	A'	1708.4648	19.4877	49.7498
27	A'	3264.3544	6.8785	6.7437

wb97xd/pyHHHHH_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	386.2357	0.2257	0.0000
2	B1	420.1939	0.3889	4.0170
3	A1	618.6966	1.6069	3.5512
4	B2	673.4221	1.6989	0.3433
5	B1	722.7394	0.4272	71.0788
6	B1	768.1411	0.7807	13.5671
7	A2	907.2267	0.6052	0.0000
8	B1	971.5123	0.7416	0.0097
9	A2	1017.2507	0.8938	0.0000
10	A1	1023.5264	4.4524	5.7917
11	B1	1028.1252	0.8142	0.0235
12	A1	1056.9904	3.1187	4.2932
13	B2	1089.9890	1.2057	0.0241
14	A1	1104.5994	1.1706	6.7695
15	B2	1174.8609	0.9573	3.0220
16	A1	1254.0847	1.1666	4.9510
17	B2	1294.1319	5.6726	0.0986
18	B2	1388.0190	1.3608	0.0463
19	B2	1484.9872	2.7301	28.2472
20	A1	1526.3602	2.8385	3.0071
21	B2	1656.1333	9.9454	12.9590
22	A1	1661.3405	8.8062	26.1974
23	B2	3170.3981	6.4461	26.5666
24	A1	3172.4832	6.4680	3.5752

25	A1	3192.6292	6.5446	5.5691
26	B2	3210.2705	6.6467	21.5907
27	A1	3218.1257	6.7129	5.3464

wb97xd/pyHHHHH_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	388.5134	0.2261	0.0000
2	B1	422.7981	0.3905	3.7897
3	A1	618.2363	1.6023	4.1613
4	B2	673.1526	1.6938	0.1961
5	B1	727.8307	0.4193	65.6206
6	B1	776.6305	0.8055	9.6784
7	A2	912.6190	0.6125	0.0000
8	B1	980.4549	0.7596	0.0169
9	A1	1023.9653	4.3948	6.0726
10	A2	1030.2399	0.9218	0.0000
11	B1	1039.4020	0.8521	0.0290
12	A1	1061.1393	3.0681	4.9367
13	B2	1091.6174	1.2140	0.0129
14	A1	1106.3547	1.1988	4.5103
15	B2	1173.8471	0.9711	3.3734
16	A1	1254.0733	1.1731	4.0365
17	B2	1289.0585	5.2689	0.1480
18	B2	1393.7344	1.3732	0.1321
19	B2	1488.7929	2.7465	27.5726
20	A1	1531.3978	2.8231	2.8017
21	B2	1655.3769	9.6924	12.3154
22	A1	1660.4994	8.6507	25.6011
23	B2	3171.4855	6.4499	26.0959
24	A1	3173.8409	6.4754	3.7049
25	A1	3196.1922	6.5564	4.9466
26	B2	3213.5812	6.6575	20.8762
27	A1	3221.4283	6.7228	5.4609

wb97xd/pyHHHHH_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	389.4403	0.2268	0.0000
2	B1	423.7089	0.3935	3.7259
3	A1	619.0215	1.6080	4.4224
4	B2	674.5372	1.7027	0.2544
5	B1	727.7459	0.4123	67.3361
6	B1	778.4738	0.8291	8.5182
7	A2	913.4798	0.6136	0.0000
8	B1	980.7357	0.7624	0.0085
9	A1	1025.5819	4.4227	6.7903
10	A2	1030.5004	0.9236	0.0000
11	B1	1043.7487	0.8578	0.0181
12	A1	1061.8936	3.0548	5.4205

13	B2	1092.4751	1.2158	0.0030
14	A1	1107.3686	1.1982	4.5722
15	B2	1176.1616	0.9749	3.1841
16	A1	1255.7129	1.1760	3.8623
17	B2	1292.5343	5.2897	0.0987
18	B2	1394.4416	1.3742	0.1067
19	B2	1490.9260	2.7520	28.6591
20	A1	1533.0136	2.8404	3.4221
21	B2	1657.6333	9.7682	11.9943
22	A1	1661.8106	8.6637	26.2000
23	B2	3173.9671	6.4602	25.6548
24	A1	3176.3440	6.4867	4.2660
25	A1	3199.4363	6.5699	4.8146
26	B2	3216.9575	6.6712	18.6869
27	A1	3224.6374	6.7365	4.5686

wb97xd/pyHHHHH_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	387.5540	0.2259	0.0000
2	B1	420.6944	0.3897	3.9492
3	A1	618.5937	1.6073	3.7069
4	B2	672.3920	1.6931	0.3906
5	B1	723.0125	0.4108	75.0487
6	B1	773.4527	0.8141	10.4088
7	A2	907.3908	0.6053	0.0000
8	B1	973.7699	0.7493	0.0169
9	A1	1021.9691	4.4182	6.4735
10	A2	1023.0436	0.9074	0.0000
11	B1	1035.0141	0.8391	0.0663
12	A1	1059.0869	3.1199	4.3127
13	B2	1091.3864	1.2041	0.0641
14	A1	1105.2451	1.1708	6.8784
15	B2	1176.1301	0.9493	2.9989
16	A1	1254.6761	1.1646	4.3455
17	B2	1295.7742	5.9388	0.1676
18	B2	1387.2680	1.3596	0.0444
19	B2	1484.5289	2.7415	29.3859
20	A1	1525.7123	2.8439	3.8839
21	B2	1656.2582	10.0398	11.8703
22	A1	1662.3978	8.9391	25.6402
23	B2	3182.0162	6.4943	21.2291
24	A1	3184.1103	6.5176	3.3911
25	A1	3205.6612	6.5976	4.3327
26	B2	3222.5058	6.6970	15.1982
27	A1	3230.1068	6.7632	3.3100

x3lyp/pyCCCCC_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	57.0200	0.0654	0.0000
2	B1	79.4374	0.1258	0.0168
3	B1	148.0980	0.2065	0.0036
4	A1	203.7097	0.8060	0.0836
5	B2	215.8312	0.8442	0.3600
6	A1	218.5483	0.8118	0.0731
7	B2	226.0868	1.0496	0.0017
8	B1	283.7308	0.6393	0.7458
9	B2	331.3011	1.8864	0.3952
10	A1	347.5977	2.0597	0.1131
11	A2	365.3955	0.9846	0.0000
12	A1	381.4813	2.8166	0.1941
13	A1	540.5039	2.9835	8.6724
14	B1	579.6265	2.4576	1.3460
15	B2	582.8069	2.7049	2.2466
16	A2	631.8492	2.8463	0.0000
17	B2	674.4421	4.1340	97.4120
18	B1	740.9365	3.9533	0.1815
19	A1	819.7241	5.4093	94.1798
20	B2	886.7525	5.9924	3.6158
21	A1	1086.2570	8.7339	36.0511
22	A1	1220.7175	10.8050	3.8237
23	B2	1259.6146	11.3847	38.9338
24	B2	1347.5003	13.3098	412.8213
25	A1	1349.6718	13.0364	126.3466
26	A1	1533.1500	16.7271	102.1835
27	B2	1563.5944	18.0542	64.1117

x3lyp/pyCCCCC_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	59.0315	0.0701	0.0000
2	A"	81.5128	0.1322	0.0115
3	A"	149.4597	0.2103	0.0099
4	A'	201.0345	0.7965	0.0401
5	A'	213.3548	0.8257	0.3402
6	A'	216.0319	0.7840	0.0434
7	A'	221.1238	1.0038	0.0024
8	A"	287.5340	0.6572	0.7226
9	A'	331.4215	1.8878	0.4014
10	A'	348.0907	2.0681	0.0958
11	A"	370.2373	1.0110	0.0000
12	A'	381.8571	2.8213	0.2219
13	A'	540.8727	2.9880	7.5332
14	A'	580.9694	2.6902	1.5511
15	A"	589.5364	2.5426	1.2736
16	A"	649.2289	3.0053	0.0000
17	A'	674.8068	4.1329	89.9668
18	A"	766.3710	4.2294	1.3413
19	A'	820.2224	5.4159	88.0658
20	A'	885.6794	5.9785	3.4893
21	A'	1086.0035	8.7318	33.2069

22	A'	1220.1042	10.7853	4.7803
23	A'	1256.7284	11.3484	34.3837
24	A'	1344.8818	13.2486	377.9748
25	A'	1346.2013	12.9688	109.0446
26	A'	1528.8262	16.6292	93.8524
27	A'	1557.0148	17.8890	59.2739

x3lyp/pyCCCCC_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	59.1878	0.0704	0.0000
2	B1	81.8207	0.1331	0.0140
3	B1	150.1445	0.2123	0.0000
4	A1	201.9922	0.8053	0.0529
5	B2	214.4565	0.8343	0.3065
6	A1	217.2147	0.7919	0.0396
7	B2	221.8655	1.0105	0.0015
8	B1	288.4068	0.6614	0.6823
9	B2	332.6597	1.8987	0.4061
10	A1	349.4362	2.0791	0.1151
11	A2	372.4572	1.0233	0.0000
12	A1	383.7655	2.8464	0.2095
13	A1	543.6142	3.0167	7.2417
14	B2	584.4403	2.7240	1.7778
15	B1	591.9892	2.5638	1.2322
16	A2	652.0963	3.0323	0.0000
17	B2	679.7347	4.1911	89.5102
18	B1	767.4820	4.2417	1.2496
19	A1	824.0416	5.4721	90.7252
20	B2	890.9185	6.0545	2.9933
21	A1	1090.6375	8.8112	33.7370
22	A1	1222.4819	10.8296	4.3713
23	B2	1258.4956	11.3755	37.3314
24	B2	1346.7012	13.2841	374.6742
25	A1	1348.4939	13.0129	111.1325
26	A1	1529.2279	16.6385	97.7347
27	B2	1559.2148	17.9484	57.6876

x3lyp/pyCCCCC_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	57.7294	0.0670	0.0000
2	B1	79.7250	0.1265	0.0155
3	B1	147.3960	0.2045	0.0044
4	A1	202.4103	0.7949	0.0605
5	B2	214.5868	0.8348	0.2263
6	A1	216.8454	0.8006	0.0253
7	B2	224.5443	1.0354	0.0019
8	B1	283.3621	0.6377	0.4401
9	B2	328.9444	1.8687	0.4743

10	A1	345.0889	2.0395	0.1093
11	A2	366.1367	0.9885	0.0000
12	A1	377.8867	2.7727	0.2046
13	A1	535.0721	2.9247	9.3363
14	B1	578.4516	2.4452	1.0477
15	B2	578.6634	2.6735	3.2611
16	A2	633.7116	2.8632	0.0000
17	B2	667.1368	4.0332	98.3844
18	B1	745.3399	4.0055	1.5554
19	A1	812.8567	5.3103	97.1757
20	B2	879.3783	5.8806	3.0620
21	A1	1077.9441	8.5957	37.8915
22	A1	1216.7800	10.7230	3.4216
23	B2	1263.1478	11.4455	36.9281
24	B2	1344.4581	13.2462	400.0135
25	A1	1346.2346	12.9662	121.1162
26	A1	1533.6337	16.7351	102.6159
27	B2	1562.2338	18.0256	61.7843

x3lyp/pyFCFCF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	91.8316	0.1061	0.0000
2	B1	109.2831	0.1535	0.0029
3	A1	184.4078	0.5311	0.0226
4	B1	214.6400	0.4098	3.0118
5	B2	226.4343	0.6784	0.0390
6	B2	313.8466	1.2479	0.8769
7	B1	317.6103	0.8231	0.4495
8	A1	323.2011	1.3450	0.2529
9	A2	378.7548	1.0598	0.0000
10	A1	408.0321	2.0118	0.7498
11	B2	411.4042	1.8518	0.0583
12	A1	580.4451	3.1958	1.8009
13	A1	615.5843	3.6825	2.8791
14	B1	650.2339	3.0923	1.4749
15	A2	697.3328	3.4881	0.0000
16	B2	704.4369	3.8852	0.8439
17	B1	762.6001	4.1927	14.7094
18	B2	789.0969	5.2668	123.2496
19	A1	1069.2764	9.3472	186.2617
20	B2	1095.5156	9.7033	23.2084
21	A1	1144.7972	9.7851	7.8325
22	B2	1318.5977	12.6521	11.0179
23	A1	1428.2888	15.1437	46.7117
24	B2	1449.3968	15.4312	443.5877
25	A1	1467.2999	15.7463	95.8261
26	A1	1619.3188	18.7157	208.7162
27	B2	1636.8170	19.6366	72.5555

x3lyp/pyFCFCF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	93.1912	0.1092	0.0000
2	B1	110.5918	0.1571	0.0001
3	A1	182.8592	0.5222	0.0070
4	B1	213.1261	0.4039	2.6643
5	B2	225.2458	0.6709	0.0313
6	B2	314.1875	1.2534	0.8478
7	B1	319.7778	0.8353	0.5944
8	A1	323.4890	1.3501	0.2094
9	A2	374.0090	1.0332	0.0000
10	A1	408.7317	2.0172	0.7151
11	B2	411.7799	1.8501	0.0774
12	A1	581.4570	3.1819	1.6291
13	A1	617.8918	3.7324	2.0287
14	B1	653.2321	3.1213	1.4002
15	B2	705.9944	3.9039	0.3716
16	A2	706.4421	3.5811	0.0000
17	B1	779.1646	4.3756	11.9984
18	B2	788.2315	5.2471	114.7648
19	A1	1075.5375	9.4344	169.3117
20	B2	1100.8170	9.8077	19.5681
21	A1	1144.2726	9.7891	5.0204
22	B2	1313.9153	12.5790	8.9077
23	A1	1434.2066	15.2515	54.0849
24	B2	1451.5003	15.4773	418.1559
25	A1	1467.6281	15.7980	75.0692
26	A1	1615.9100	18.6390	202.3195
27	B2	1631.5872	19.5037	75.8763

x3lyp/pyFCFCF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	93.0337	0.1089	0.0000
2	B1	110.4172	0.1567	0.0013
3	A1	184.7069	0.5328	0.0034
4	B1	213.6600	0.4061	2.3452
5	B2	227.3215	0.6837	0.0251
6	B2	315.5302	1.2632	0.8149
7	B1	320.7530	0.8398	0.5490
8	A1	324.7809	1.3583	0.1784
9	A2	376.7862	1.0488	0.0000
10	A1	409.9274	2.0292	0.6978
11	B2	412.6892	1.8579	0.0783
12	A1	582.5347	3.2048	1.4385
13	A1	618.9260	3.7347	1.9761
14	B1	653.3949	3.1232	1.1496
15	A2	707.1455	3.5884	0.0000
16	B2	708.1737	3.9284	0.3975
17	B1	778.1505	4.3642	10.8754
18	B2	792.6125	5.3101	112.6398

19	A1	1077.5239	9.4704	170.7682
20	B2	1104.3052	9.8606	17.8807
21	A1	1148.5540	9.8595	5.3748
22	B2	1316.9721	12.6360	9.9645
23	A1	1439.3540	15.3768	52.0601
24	B2	1454.9669	15.5528	408.7951
25	A1	1469.9257	15.8388	81.7918
26	A1	1617.4531	18.6780	207.5467
27	B2	1635.2281	19.6021	77.8933

x3lyp/pyFCFCF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	92.0248	0.1065	0.0000
2	B1	109.3243	0.1534	0.0048
3	A1	184.4314	0.5314	0.0005
4	B1	211.8803	0.3989	2.5903
5	B2	227.3008	0.6837	0.0170
6	B2	313.6332	1.2489	0.7677
7	B1	316.4665	0.8187	0.2619
8	A1	322.6142	1.3449	0.1585
9	A2	370.5723	1.0138	0.0000
10	A1	406.1542	1.9941	0.7995
11	B2	410.0392	1.8385	0.0212
12	A1	579.2919	3.1539	1.7606
13	A1	614.7926	3.6936	2.1307
14	B1	647.8961	3.0691	0.7781
15	A2	698.5470	3.5028	0.0000
16	B2	701.5575	3.8547	0.7688
17	B1	765.5211	4.2260	17.7189
18	B2	782.3583	5.1605	117.5594
19	A1	1071.2902	9.3551	184.3905
20	B2	1098.0732	9.7588	20.0045
21	A1	1138.9074	9.6981	4.4131
22	B2	1323.1837	12.7508	7.4957
23	A1	1436.2352	15.3023	52.9542
24	B2	1453.2016	15.5072	432.9474
25	A1	1471.2545	15.8737	84.1064
26	A1	1621.9361	18.7743	211.6738
27	B2	1635.7905	19.6124	69.3807

x3lyp/pyFCFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	97.4266	0.1186	0.0004
2	A''	140.9438	0.2185	0.0048
3	A'	203.3250	0.5728	0.0253
4	A''	214.2760	0.4073	3.9762
5	A'	277.0885	0.8520	0.2652
6	A'	313.5939	1.1782	0.7386

7	A''	328.6804	0.8727	0.8970
8	A'	334.9305	1.2458	0.6862
9	A'	407.8390	1.8958	0.2940
10	A''	411.2446	1.2639	1.4073
11	A'	473.1478	2.1273	0.4893
12	A'	591.5770	3.5230	0.8270
13	A'	635.1901	3.7300	8.4254
14	A''	641.1270	3.0096	2.1439
15	A''	692.9954	3.4466	0.4065
16	A'	725.6590	4.1181	0.6259
17	A''	750.2906	4.0586	10.0225
18	A'	900.4123	6.8627	159.9616
19	A'	1074.9534	9.4499	192.8434
20	A'	1107.9775	9.8476	38.0277
21	A'	1252.1379	12.0107	23.9037
22	A'	1326.6496	12.8170	14.6021
23	A'	1432.0701	15.1970	47.1486
24	A'	1469.7518	15.8075	291.4956
25	A'	1516.2940	17.0653	432.9505
26	A'	1641.5513	19.2589	176.7841
27	A'	1658.4997	20.0454	11.2091

x3lyp/pyFCFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	99.0409	0.1225	0.0002
2	A''	142.4031	0.2231	0.0043
3	A'	202.0168	0.5653	0.0196
4	A''	213.3041	0.4032	3.3567
5	A'	277.4756	0.8544	0.3061
6	A'	314.0541	1.1851	0.6823
7	A''	331.3063	0.8877	0.9876
8	A'	335.3601	1.2477	0.5997
9	A'	408.3604	1.8964	0.2563
10	A''	411.6523	1.2665	1.1206
11	A'	474.1601	2.1353	0.5546
12	A'	594.1621	3.5370	0.9317
13	A'	635.9759	3.7508	7.0385
14	A''	646.5129	3.0623	2.2228
15	A''	707.4922	3.5928	0.5264
16	A'	728.1514	4.1474	0.4835
17	A''	776.5585	4.3438	7.8931
18	A'	902.9181	6.8859	146.8858
19	A'	1081.0149	9.5448	172.7057
20	A'	1112.7991	9.9485	39.7239
21	A'	1257.1280	12.1135	22.2179
22	A'	1322.2114	12.7572	12.0660
23	A'	1437.2243	15.2999	48.7056
24	A'	1470.8641	15.8344	270.6362
25	A'	1517.4688	17.1151	415.8143
26	A'	1638.7444	19.2012	175.4199
27	A'	1654.5590	19.9382	9.7828

x3lyp/pyFCFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	98.8149	0.1219	0.0001
2	A"	141.6805	0.2209	0.0012
3	A'	203.9400	0.5762	0.0218
4	A"	213.4134	0.4036	2.9488
5	A'	278.3197	0.8593	0.3048
6	A'	314.9786	1.1898	0.6665
7	A"	331.9262	0.8911	0.9335
8	A'	336.2539	1.2551	0.5399
9	A'	409.3359	1.9054	0.2549
10	A"	412.5363	1.2715	1.0139
11	A'	474.7378	2.1406	0.5619
12	A'	594.7028	3.5483	0.7980
13	A'	637.4832	3.7666	6.6545
14	A"	645.3041	3.0500	1.8542
15	A"	705.5327	3.5729	0.2934
16	A'	729.3825	4.1613	0.4627
17	A"	769.4613	4.2680	7.1598
18	A'	905.6695	6.9312	144.7513
19	A'	1083.1169	9.5814	175.4476
20	A'	1116.4107	10.0035	35.7948
21	A'	1260.5708	12.1789	22.2837
22	A'	1325.2778	12.8156	12.9697
23	A'	1441.9755	15.4112	50.1980
24	A'	1473.8655	15.8910	253.7367
25	A'	1520.6901	17.1945	422.5866
26	A'	1641.1741	19.2552	177.0757
27	A'	1657.7617	20.0299	11.2312

x3lyp/pyFCFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	97.7138	0.1192	0.0007
2	A"	140.7124	0.2178	0.0021
3	A'	203.8081	0.5752	0.0304
4	A"	212.2241	0.3991	3.5244
5	A'	277.8844	0.8570	0.2746
6	A'	313.2517	1.1791	0.7116
7	A"	327.5608	0.8679	0.6756
8	A'	334.2454	1.2408	0.5901
9	A'	406.3436	1.8818	0.3117
10	A"	409.6448	1.2540	1.6473
11	A'	472.7576	2.1213	0.5586
12	A'	592.0948	3.5123	0.9977
13	A'	632.6077	3.7042	7.4586
14	A"	640.6440	3.0054	1.6685
15	A"	700.1605	3.5202	1.0333

16	A'	723.2799	4.0908	0.5564
17	A''	763.4437	4.2001	9.8123
18	A'	898.2234	6.8099	149.6847
19	A'	1077.1629	9.4789	183.9253
20	A'	1110.0368	9.8953	38.1282
21	A'	1254.5154	12.0783	21.7437
22	A'	1331.5798	12.9268	11.4656
23	A'	1439.1673	15.3460	49.5848
24	A'	1472.6190	15.8746	276.6842
25	A'	1522.2467	17.2228	426.1182
26	A'	1644.2880	19.3366	176.5001
27	A'	1659.3047	20.0461	8.5178

x3lyp/pyFFCFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.3187	0.1505	0.0000
2	B1	121.8309	0.1826	0.0251
3	B2	203.1660	0.5847	0.0395
4	B1	208.6941	0.3810	3.7306
5	A1	281.5830	0.9082	0.7600
6	B2	308.7993	1.0338	0.3176
7	A1	329.8322	1.3323	0.8479
8	B1	334.5962	0.9176	0.9302
9	A1	430.4879	2.0011	0.1190
10	A2	443.6232	1.4656	0.0000
11	B2	462.6997	2.0340	0.0801
12	A1	541.4411	3.0436	1.8072
13	B1	598.5529	2.6187	8.7509
14	A2	694.9711	3.4653	0.0000
15	A1	699.5906	4.5153	11.0569
16	B2	722.7999	4.0672	0.0047
17	B1	739.8856	3.9472	2.8674
18	A1	918.1149	6.8303	144.6024
19	B2	968.3115	8.1244	181.6023
20	B2	1164.8963	10.8358	0.4565
21	A1	1252.9268	11.9067	64.7627
22	B2	1319.3859	12.6541	21.9167
23	A1	1434.3293	15.3878	4.6466
24	A1	1475.0296	15.7469	85.3450
25	B2	1499.3134	16.6967	754.3583
26	B2	1642.7509	19.7540	4.0427
27	A1	1650.0739	19.4561	130.4415

x3lyp/pyFFCFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	118.5904	0.1538	0.0000
2	B1	123.7735	0.1887	0.0386
3	B2	202.1490	0.5787	0.0314

4	B1	208.3211	0.3792	3.0502
5	A1	281.8262	0.9095	0.8521
6	B2	309.5937	1.0389	0.3233
7	A1	330.0511	1.3362	0.6725
8	B1	336.2774	0.9270	0.9085
9	A1	431.2960	2.0077	0.0900
10	A2	443.5305	1.4651	0.0000
11	B2	463.0411	2.0347	0.0645
12	A1	543.4481	3.0613	2.0411
13	B1	602.5332	2.6560	8.3369
14	A1	701.7998	4.5424	8.9192
15	A2	709.9345	3.6165	0.0000
16	B2	725.6249	4.1001	0.0352
17	B1	769.9609	4.2717	2.3403
18	A1	918.3561	6.8294	135.3893
19	B2	974.1663	8.2175	164.6618
20	B2	1172.3630	10.9726	0.3448
21	A1	1257.6393	12.0011	61.9454
22	B2	1314.2016	12.5791	20.0280
23	A1	1437.6320	15.4585	5.4010
24	A1	1476.2063	15.7847	82.2786
25	B2	1501.3112	16.7470	716.4307
26	B2	1638.8265	19.6496	3.8002
27	A1	1647.4748	19.4009	123.6246

x3lyp/pyFFCFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	118.1423	0.1526	0.0000
2	B1	123.6392	0.1883	0.0328
3	B2	204.0648	0.5900	0.0229
4	B1	208.4410	0.3798	2.6586
5	A1	282.9662	0.9169	0.8450
6	B2	310.5195	1.0451	0.2885
7	A1	330.9571	1.3408	0.6474
8	B1	336.2678	0.9267	0.8546
9	A1	432.1057	2.0150	0.0590
10	A2	444.6631	1.4726	0.0000
11	B2	463.8749	2.0427	0.0674
12	A1	544.2147	3.0734	2.0188
13	B1	604.0732	2.6695	7.7533
14	A1	702.7455	4.5535	8.2466
15	A2	706.8229	3.5856	0.0000
16	B2	726.8608	4.1141	0.0260
17	B1	763.9057	4.2055	1.6994
18	A1	921.8803	6.8848	135.2161
19	B2	976.0654	8.2458	162.3413
20	B2	1175.9946	11.0364	0.1267
21	A1	1261.4870	12.0723	61.7767
22	B2	1317.3142	12.6393	20.5465
23	A1	1441.5592	15.5544	4.0834
24	A1	1478.5646	15.8301	83.6756

25	B2	1505.4820	16.8358	710.8005
26	B2	1641.0645	19.7170	4.3487
27	A1	1650.5346	19.4753	124.5909

x3lyp/pyFFCFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	116.7893	0.1491	0.0000
2	B1	122.3825	0.1843	0.0281
3	B2	203.8939	0.5887	0.0082
4	B1	206.7321	0.3734	3.2181
5	A1	282.3190	0.9139	0.7735
6	B2	309.3198	1.0374	0.3171
7	A1	328.8836	1.3270	0.6890
8	B1	332.7281	0.9081	0.7521
9	A1	429.0551	1.9891	0.1426
10	A2	442.4642	1.4578	0.0000
11	B2	461.9857	2.0250	0.0789
12	A1	541.2036	3.0315	2.0680
13	B1	593.7843	2.5780	10.4847
14	A1	698.7591	4.5001	9.2834
15	A2	703.6580	3.5538	0.0000
16	B2	720.9455	4.0467	0.0004
17	B1	758.2994	4.1451	1.3784
18	A1	913.3367	6.7513	139.2082
19	B2	971.0949	8.1639	169.9417
20	B2	1171.5212	10.9661	0.1943
21	A1	1253.0132	11.9154	61.0161
22	B2	1324.4987	12.7639	19.9688
23	A1	1440.4057	15.5158	4.4065
24	A1	1477.4289	15.8164	84.8614
25	B2	1505.6081	16.8523	740.3129
26	B2	1643.7780	19.7652	2.2299
27	A1	1653.2583	19.5363	127.3001

x3lyp/pyFFFFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	119.3496	0.1558	0.0000
2	B1	157.7615	0.2699	0.0035
3	B1	215.1414	0.4091	5.2637
4	B2	272.8623	0.8261	0.0441
5	A1	273.4860	0.8188	0.7000
6	B2	318.2827	1.0820	0.7950
7	A1	345.3074	1.2323	1.4875
8	B1	351.2385	0.9989	3.3829
9	A2	433.4391	1.3997	0.0000
10	B2	461.7989	2.0310	0.1419
11	A1	481.6741	2.1770	0.1790
12	A1	595.3557	3.6456	0.0035

13	B1	632.5529	2.9343	3.3919
14	A2	689.0824	3.4072	0.0000
15	A1	700.5213	4.4877	7.6483
16	B1	735.1360	3.8987	5.7587
17	B2	742.2636	4.3135	0.0846
18	B2	987.2819	8.3714	225.0724
19	A1	1087.2441	9.7263	247.0931
20	B2	1170.1807	10.9621	0.0002
21	A1	1297.6720	12.8945	30.2566
22	B2	1333.7342	12.9496	14.3958
23	A1	1443.2162	15.3752	17.6519
24	B2	1510.5398	16.9907	720.0127
25	A1	1545.5252	17.6159	161.4136
26	A1	1661.8213	19.7047	116.5001
27	B2	1672.7136	20.3567	3.3335

x3lyp/pyFFFFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	120.7384	0.1594	0.0000
2	B1	159.3951	0.2757	0.0009
3	B1	214.6332	0.4066	4.2446
4	B2	273.5130	0.8298	0.0447
5	A1	273.8114	0.8206	0.7857
6	B2	318.9963	1.0865	0.7280
7	A1	345.6969	1.2347	1.2762
8	B1	353.5735	1.0132	2.9842
9	A2	434.1078	1.4041	0.0000
10	B2	462.2714	2.0334	0.1317
11	A1	483.2922	2.1896	0.2434
12	A1	598.5868	3.6833	0.0067
13	B1	641.1698	3.0198	3.6226
14	A1	702.2375	4.5106	6.1161
15	A2	708.9129	3.6060	0.0000
16	B2	745.7462	4.3555	0.0074
17	B1	774.5725	4.3193	4.6062
18	B2	993.4471	8.4699	209.0858
19	A1	1093.7735	9.8404	232.4168
20	B2	1176.9241	11.0896	0.0429
21	A1	1303.4395	13.0192	28.0791
22	B2	1328.8933	12.8765	12.2528
23	A1	1446.8039	15.4412	20.5253
24	B2	1512.6521	17.0378	693.4977
25	A1	1546.8456	17.6687	152.8394
26	A1	1659.7780	19.6599	111.9083
27	B2	1669.1524	20.2627	2.7008

x3lyp/pyFFFFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A2	120.0491	0.1576	0.0000
2	B1	158.3025	0.2718	0.0000
3	B1	214.3924	0.4056	3.7257
4	B2	274.0892	0.8334	0.0476
5	A1	274.4081	0.8241	0.7962
6	B2	319.4808	1.0897	0.7068
7	A1	346.1964	1.2384	1.1892
8	B1	353.1001	1.0105	2.7495
9	A2	434.5003	1.4067	0.0000
10	B2	462.8830	2.0390	0.1338
11	A1	483.4476	2.1908	0.2866
12	A1	598.9778	3.6871	0.0101
13	B1	638.5895	2.9931	3.0416
14	A1	703.1318	4.5212	5.7451
15	A2	704.7491	3.5646	0.0000
16	B2	746.1705	4.3599	0.0079
17	B1	761.7765	4.1833	4.0284
18	B2	995.0592	8.4965	204.4063
19	A1	1095.7775	9.8749	231.7420
20	B2	1180.4709	11.1554	0.1258
21	A1	1306.3972	13.0795	28.5707
22	B2	1332.1098	12.9380	12.8369
23	A1	1451.3707	15.5430	20.9002
24	B2	1516.9404	17.1361	680.7458
25	A1	1549.5793	17.7335	149.7170
26	A1	1662.3777	19.7236	113.7068
27	B2	1672.2276	20.3436	3.1045

x3lyp/pyFFFFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	118.7028	0.1540	0.0000
2	B1	157.4501	0.2688	0.0014
3	B1	213.8230	0.4039	4.7728
4	B2	273.5998	0.8304	0.0475
5	A1	273.9477	0.8215	0.7545
6	B2	317.9763	1.0798	0.8516
7	A1	344.3983	1.2255	1.3866
8	B1	350.0691	0.9934	3.1613
9	A2	433.2260	1.3982	0.0000
10	B2	461.1615	2.0231	0.1320
11	A1	481.6548	2.1740	0.2181
12	A1	596.5189	3.6567	0.0029
13	B1	634.8743	2.9592	3.4017
14	A1	699.4669	4.4719	6.2343
15	A2	702.2126	3.5392	0.0000
16	B2	740.1635	4.2886	0.0371
17	B1	761.5391	4.1766	4.3910
18	B2	989.7849	8.4091	210.1719
19	A1	1090.1040	9.7741	236.5147
20	B2	1176.4084	11.0877	0.0177
21	A1	1300.5041	12.9706	28.0495

22	B2	1338.4814	13.0529	11.8868
23	A1	1448.5914	15.4850	19.6502
24	B2	1515.9875	17.1197	700.0130
25	A1	1551.7069	17.7798	155.3368
26	A1	1665.2035	19.7872	114.6941
27	B2	1673.8650	20.3761	1.9655

x3lyp/pyFFHFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	116.0244	0.1474	0.0000
2	B1	203.7269	0.3300	4.2428
3	A1	281.5582	0.8495	0.6902
4	B1	298.0942	0.4384	1.0049
5	B2	302.7565	0.9623	0.2248
6	A1	359.6755	1.2215	2.7845
7	B2	455.6504	1.7738	0.0671
8	A2	458.1222	1.5627	0.0000
9	B1	488.9876	0.6159	0.5647
10	A1	511.4956	2.3056	1.6796
11	B2	662.4491	1.5734	2.4941
12	A1	692.1831	4.2566	18.7064
13	A2	700.1357	3.5153	0.0000
14	B1	730.2014	2.5758	11.5258
15	A1	755.6037	3.2177	11.6539
16	B1	898.3369	0.6665	30.4108
17	B2	910.8369	2.8285	141.7507
18	B2	1152.5907	5.3774	14.4109
19	B2	1200.1395	1.3984	71.7025
20	A1	1233.8881	10.0830	202.6127
21	B2	1324.8991	11.8842	65.6164
22	A1	1418.1222	13.9586	1.0026
23	A1	1462.6633	14.3551	43.3291
24	B2	1516.0634	10.0956	733.5666
25	A1	1662.2361	18.7071	27.2439
26	B2	1663.2671	14.1358	2.8332
27	A1	3219.8587	6.6814	4.3650

x3lyp/pyFFHFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.5552	0.1513	0.0000
2	B1	204.2241	0.3337	3.3676
3	A1	282.1258	0.8529	0.7322
4	B1	300.6625	0.4449	0.9921
5	B2	303.8350	0.9692	0.1713
6	A1	360.5771	1.2268	2.3477
7	B2	456.1418	1.7762	0.0517
8	A2	458.8130	1.5674	0.0000
9	B1	494.0354	0.6154	0.5051

10	A1	513.7404	2.3219	1.8977
11	B2	666.3452	1.5843	2.4793
12	A1	695.5484	4.3224	16.0653
13	A2	717.4648	3.6914	0.0000
14	B1	754.5351	2.1546	13.1884
15	A1	758.1941	3.2330	12.2418
16	B2	915.6615	2.8155	126.9820
17	B1	916.6209	0.7334	24.3830
18	B2	1160.5061	5.3511	16.1305
19	B2	1205.0634	1.4364	65.2447
20	A1	1241.2031	10.2086	186.8346
21	B2	1319.9130	11.4336	63.8221
22	A1	1422.1161	14.0064	1.4778
23	A1	1464.5148	14.4823	44.8938
24	B2	1518.4941	10.1838	711.9164
25	A1	1660.6140	18.6816	26.8264
26	B2	1660.7921	13.7403	3.9910
27	A1	3218.1900	6.6711	3.6716

x3lyp/pyFFHFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	117.1167	0.1501	0.0000
2	B1	204.0822	0.3328	2.9692
3	A1	282.8569	0.8570	0.7393
4	B1	299.9541	0.4428	0.9868
5	B2	304.4018	0.9725	0.1676
6	A1	360.9247	1.2297	2.2141
7	B2	456.8795	1.7816	0.0513
8	A2	459.4362	1.5718	0.0000
9	B1	492.4600	0.6175	0.4038
10	A1	514.0581	2.3237	1.9460
11	B2	666.8581	1.5866	2.4443
12	A1	696.5440	4.3303	15.4162
13	A2	714.7589	3.6643	0.0000
14	B1	750.2522	2.3046	10.7686
15	A1	758.9479	3.2399	12.2685
16	B1	908.3316	0.7056	26.2142
17	B2	917.2106	2.8074	122.9775
18	B2	1164.4946	5.1599	17.3589
19	B2	1207.3956	1.4583	60.1266
20	A1	1244.7945	10.2538	186.7541
21	B2	1323.1223	11.5401	65.7888
22	A1	1425.8819	14.0334	1.3305
23	A1	1468.4315	14.6313	44.8241
24	B2	1523.1421	10.2651	698.5224
25	A1	1662.9321	18.7416	27.7542
26	B2	1664.0319	13.8371	3.7000
27	A1	3222.6652	6.6898	3.3817

x3lyp/pyFFHFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	115.6393	0.1463	0.0000
2	B1	202.5269	0.3282	3.8037
3	A1	281.9688	0.8519	0.7121
4	B1	298.1551	0.4395	1.0396
5	B2	303.1713	0.9653	0.2379
6	A1	358.7037	1.2142	2.5371
7	B2	455.0607	1.7669	0.0646
8	A2	457.3670	1.5573	0.0000
9	B1	488.1656	0.6069	0.4730
10	A1	511.7756	2.3047	1.6947
11	B2	661.8150	1.5839	2.3106
12	A1	692.2858	4.2736	15.9491
13	A2	710.4767	3.6209	0.0000
14	B1	745.1249	2.1747	12.3480
15	A1	755.9245	3.2147	12.2459
16	B1	906.4773	0.7087	27.4967
17	B2	912.5920	2.7968	131.5281
18	B2	1158.9314	5.0237	15.3567
19	B2	1203.5436	1.4300	62.1698
20	A1	1235.6784	10.1168	194.4458
21	B2	1330.5356	11.9302	57.8065
22	A1	1424.7272	14.0415	1.2209
23	A1	1465.3318	14.4519	43.0711
24	B2	1520.4754	10.4355	720.9208
25	B2	1663.2294	14.1303	4.2354
26	A1	1666.6893	18.8205	27.0074
27	A1	3226.6380	6.7095	5.5261

x3lyp/pyFHFFF_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A''	129.4825	0.1655	0.1452
2	A''	210.7949	0.3587	4.5812
3	A''	262.0976	0.2900	1.1915
4	A'	274.4163	0.8267	0.1947
5	A'	319.4254	1.0371	1.0575
6	A'	351.5869	1.2002	1.6039
7	A''	386.2863	0.9198	0.9229
8	A'	465.8041	1.8172	0.4962
9	A'	534.8646	1.8805	3.3765
10	A'	598.1547	3.6260	0.1023
11	A''	630.2100	1.2751	6.1706
12	A'	669.2447	1.6853	2.6931
13	A''	684.1229	1.9684	0.0131
14	A''	743.0231	2.1931	1.4048
15	A'	803.1633	3.7803	48.8141
16	A''	851.8613	0.6695	38.4539
17	A'	1030.4596	2.8863	98.8833
18	A'	1080.0879	8.1225	175.7321

19	A'	1167.0513	1.5581	88.7009
20	A'	1250.3976	5.4126	51.2146
21	A'	1338.5492	11.7592	9.9314
22	A'	1419.3103	11.6589	51.3149
23	A'	1464.2767	13.5746	173.6793
24	A'	1532.7943	9.5417	420.5216
25	A'	1654.0640	15.8758	270.8508
26	A'	1668.9418	18.5663	44.5833
27	A'	3233.8074	6.7444	4.8683

x3lyp/pyFHFFF_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	130.6212	0.1685	0.1175
2	A"	211.0040	0.3631	3.6619
3	A"	264.7694	0.2933	1.2694
4	A'	274.9327	0.8295	0.2254
5	A'	320.2445	1.0418	0.9103
6	A'	352.5456	1.2067	1.2617
7	A"	386.6757	0.9299	0.8394
8	A'	466.6128	1.8248	0.4718
9	A'	535.3459	1.8846	2.9117
10	A'	601.5642	3.6678	0.0501
11	A"	637.0445	1.2725	6.3248
12	A'	672.6128	1.6947	2.9201
13	A"	694.7759	1.8354	0.0069
14	A"	764.9979	1.9594	0.3276
15	A'	805.8958	3.8029	43.2971
16	A"	867.0955	0.7481	35.3572
17	A'	1033.8587	2.8130	88.3085
18	A'	1087.2835	8.1983	160.8638
19	A'	1174.0764	1.5998	90.2886
20	A'	1255.7000	5.6416	47.4871
21	A'	1334.2531	11.3371	11.3354
22	A'	1425.5295	11.9389	52.6088
23	A'	1465.6283	13.5207	159.8279
24	A'	1535.0817	9.5567	411.1783
25	A'	1652.1127	15.6589	259.7943
26	A'	1665.8832	18.2688	43.7125
27	A'	3232.5710	6.7359	3.9428

x3lyp/pyFHFFF_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	130.0765	0.1670	0.1045
2	A"	210.6250	0.3603	3.2954
3	A"	263.9434	0.2928	1.2561
4	A'	275.5570	0.8333	0.2302
5	A'	320.8149	1.0452	0.9013
6	A'	353.1290	1.2107	1.2090

7	A"	386.4188	0.9294	0.7074
8	A'	467.0533	1.8268	0.4547
9	A'	535.9435	1.8900	2.6867
10	A'	602.0972	3.6725	0.0426
11	A"	636.0879	1.2958	5.6063
12	A'	673.0884	1.6954	2.8149
13	A"	693.7376	1.8774	0.0000
14	A"	758.2803	2.1071	0.5347
15	A'	807.0257	3.8113	42.2503
16	A"	857.7844	0.7043	34.3287
17	A'	1035.6475	2.7735	86.0379
18	A'	1090.1986	8.2599	157.1566
19	A'	1176.9505	1.6046	87.8295
20	A'	1258.5613	5.7811	46.8757
21	A'	1337.8161	11.3651	11.7790
22	A'	1430.2348	12.2201	52.6619
23	A'	1469.7906	13.5354	149.1140
24	A'	1538.6843	9.6594	408.5722
25	A'	1654.8780	15.6874	262.8393
26	A'	1668.8294	18.3668	44.8967
27	A'	3236.9497	6.7541	3.6723

x3lyp/pyFHFFF_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A"	129.1125	0.1645	0.1339
2	A"	210.0644	0.3595	4.1859
3	A"	262.1509	0.2898	1.3121
4	A'	275.0193	0.8302	0.2161
5	A'	319.0981	1.0352	1.0692
6	A'	350.8149	1.1954	1.4662
7	A"	384.7218	0.9132	0.7928
8	A'	465.5663	1.8148	0.4699
9	A'	534.0309	1.8750	2.8274
10	A'	599.4446	3.6415	0.0894
11	A"	632.2170	1.2909	6.0857
12	A'	668.1101	1.6940	2.5616
13	A"	689.1458	1.8401	0.0022
14	A"	756.7618	2.0422	0.4190
15	A'	803.1375	3.7638	44.3505
16	A"	860.0216	0.7126	38.5365
17	A'	1031.1862	2.8242	93.9605
18	A'	1083.9799	8.1472	164.6950
19	A'	1171.3004	1.5609	83.3939
20	A'	1254.2056	5.5048	46.2251
21	A'	1342.4826	11.9851	9.4569
22	A'	1426.4597	11.8772	54.7850
23	A'	1467.7418	13.5550	157.6584
24	A'	1537.1264	9.8390	421.8194
25	A'	1656.4301	16.0111	266.3777
26	A'	1670.3810	18.5644	40.8612
27	A'	3240.9116	6.7741	6.0915

x3lyp/pyHHHHH_bs1

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	382.6017	0.2209	0.0000
2	B1	418.2806	0.3869	4.0274
3	A1	617.1147	1.6030	3.6427
4	B2	670.4881	1.6841	0.3002
5	B1	716.1421	0.4171	67.7030
6	B1	759.6235	0.7885	12.0159
7	A2	895.2639	0.5891	0.0000
8	B1	956.8823	0.7191	0.0245
9	A2	999.7033	0.8644	0.0000
10	B1	1008.8506	0.7728	0.0081
11	A1	1012.9897	4.2894	4.9034
12	A1	1048.7686	2.9536	6.1714
13	B2	1078.2708	1.2150	0.0024
14	A1	1094.7351	1.2150	5.3092
15	B2	1170.9262	0.9277	2.5068
16	A1	1243.4596	1.1683	4.7104
17	B2	1287.0052	6.6598	0.0215
18	B2	1385.6269	1.3553	0.0504
19	B2	1472.6579	2.6455	27.0524
20	A1	1513.1544	2.6560	2.5176
21	B2	1622.3186	8.7905	10.5237
22	A1	1627.8702	7.9787	24.2135
23	B2	3151.8780	6.3659	27.2937
24	A1	3154.1712	6.3909	3.8086
25	A1	3174.0293	6.4647	4.9454
26	B2	3189.5370	6.5542	24.7450
27	A1	3197.4294	6.6199	6.6348

x3lyp/pyHHHHH_bs2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	386.1803	0.2220	0.0000
2	B1	422.0849	0.3897	3.8492
3	A1	617.7126	1.6048	4.4102
4	B2	671.0335	1.6842	0.1686
5	B1	722.9646	0.4096	63.7607
6	B1	769.7457	0.8179	8.3782
7	A2	903.7610	0.6005	0.0000
8	B1	968.2051	0.7391	0.0131
9	A1	1014.5665	4.2637	5.1470
10	A2	1016.4816	0.9004	0.0000
11	B1	1028.4222	0.8279	0.0164
12	A1	1052.9604	2.8604	7.0819
13	B2	1080.2020	1.2221	0.0665
14	A1	1097.1654	1.2494	3.3222
15	B2	1170.7386	0.9369	2.7380

16	A1	1243.5917	1.1754	3.9425
17	B2	1284.9922	6.3224	0.0039
18	B2	1391.2522	1.3687	0.1474
19	B2	1477.4371	2.6687	25.8518
20	A1	1519.0536	2.6575	2.1466
21	B2	1623.4646	8.5838	10.1359
22	A1	1628.5411	7.8501	23.6980
23	B2	3150.9445	6.3616	26.1881
24	A1	3153.4219	6.3896	3.9544
25	A1	3175.2619	6.4674	4.3255
26	B2	3190.5008	6.5557	23.1226
27	A1	3198.3836	6.6202	6.4109

x3lyp/pyHHHHH_bs3

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	386.6086	0.2223	0.0000
2	B1	422.5298	0.3918	3.7520
3	A1	618.2951	1.6096	4.6372
4	B2	672.3933	1.6927	0.2327
5	B1	722.3788	0.4023	65.3327
6	B1	770.7393	0.8428	7.3423
7	A2	903.1596	0.5996	0.0000
8	B1	966.6289	0.7391	0.0125
9	A2	1014.9121	0.8984	0.0000
10	A1	1016.1919	4.2885	5.7035
11	B1	1027.3204	0.8235	0.0027
12	A1	1054.0248	2.8709	7.5640
13	B2	1081.6160	1.2250	0.0605
14	A1	1098.5916	1.2482	3.1900
15	B2	1173.3423	0.9409	2.5681
16	A1	1245.7489	1.1791	3.6332
17	B2	1288.0148	6.3532	0.0221
18	B2	1392.9146	1.3715	0.1195
19	B2	1480.3024	2.6785	27.0872
20	A1	1521.4191	2.6716	2.8294
21	B2	1626.4177	8.6448	9.6675
22	A1	1631.1078	7.8824	24.3372
23	B2	3153.7904	6.3728	27.7296
24	A1	3156.3954	6.4020	5.2763
25	A1	3178.8137	6.4817	4.8429
26	B2	3194.2462	6.5709	23.9215
27	A1	3202.0586	6.6360	6.4605

x3lyp/pyHHHHH_bs4

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A2	384.3003	0.2205	0.0000
2	B1	419.3321	0.3864	4.0132
3	A1	616.8613	1.6010	3.8333

4	B2	669.4634	1.6772	0.3771
5	B1	716.4545	0.3982	73.6089
6	B1	765.2349	0.8279	9.1765
7	A2	897.1084	0.5915	0.0000
8	B1	959.1678	0.7253	0.0296
9	A2	1007.6161	0.8835	0.0000
10	A1	1011.7412	4.2637	5.6083
11	B1	1020.7650	0.8114	0.0387
12	A1	1050.3479	2.9364	6.1931
13	B2	1079.2448	1.2096	0.0063
14	A1	1094.8940	1.2158	5.2954
15	B2	1171.3061	0.9161	2.3969
16	A1	1242.9963	1.1623	3.9971
17	B2	1289.5531	7.1538	0.0001
18	B2	1383.4417	1.3510	0.0643
19	B2	1471.5418	2.6605	28.6857
20	A1	1511.2564	2.6589	3.4139
21	B2	1622.3138	8.9026	9.1856
22	A1	1629.1615	8.1491	23.8720
23	B2	3160.0058	6.3991	21.0149
24	A1	3162.0752	6.4236	3.6202
25	A1	3182.5691	6.4990	4.2058
26	B2	3197.4782	6.5869	18.1283
27	A1	3205.1599	6.6528	4.3808

2 Benchmark

Table SI.A.1. Performance of the different DFT functionals coupled with the four selected triple- ζ basis sets with respect to the experimental FT-IR vibrational wavenumbers, evaluated in terms of standard deviation (σ , in cm^{-1}) and least-square linear regression parameters, *viz.* intercept (a_0 , in cm^{-1}), slope (a_1) and regression coefficient (R^2).

functional	basis set	σ	a_0	a_1	R^2
APF[D]	BS1	30.08	8.19	1.01424	0.99907
	BS2	30.44	9.81	1.01303	0.99906
	BS3	29.32	6.92	1.01565	0.99916
	BS4	34.70	14.49	1.01058	0.99872
B3LYP[GD3BJ]	BS1	26.50	11.56	1.00538	0.99907
	BS2	27.37	10.82	1.00785	0.99910
	BS3	24.34	5.72	1.01288	0.99942
	BS4	36.04	12.97	1.00932	0.99822
B3P86	BS1	28.27	4.97	1.01615	0.99917
	BS2	29.62	7.15	1.01589	0.99915
	BS3	28.40	5.65	1.01636	0.99923
	BS4	32.20	9.45	1.01380	0.99883
BLYP	BS1	58.65	36.64	1.00426	0.99632
	BS2	60.70	39.98	1.00367	0.99622
	BS3	61.66	39.49	1.00457	0.99609
	BS4	59.45	35.11	1.00727	0.99631
BMK	BS1	29.97	5.76	1.01834	0.99920
	BS2	30.30	8.78	1.01489	0.99911
	BS3	32.23	6.87	1.01935	0.99907
	BS4	32.15	6.19	1.01932	0.99905
CAM-B3LYP[GD3BJ]	BS1	31.41	1.75	1.02477	0.99927
	BS2	32.85	3.81	1.02342	0.99916
	BS3	33.18	3.38	1.02422	0.99914
	BS4	32.45	2.31	1.02456	0.99915
M06-2X	BS1	33.95	1.37	1.02662	0.99910
	BS2	34.81	3.02	1.02585	0.99905
	BS3	35.31	2.93	1.02609	0.99905
	BS4	35.12	1.58	1.02716	0.99901

MN15	BS1	35.01	11.60	1.01579	0.99887
	BS2	37.81	17.31	1.01304	0.99880
	BS3	37.00	10.48	1.01936	0.99884
	BS4	37.70	14.61	1.01493	0.99872
O3LYP	BS1	36.23	20.10	1.00112	0.99817
	BS2	39.77	21.77	1.00087	0.99774
	BS3	30.44	16.13	1.00274	0.99877
	BS4	40.48	21.45	1.00285	0.99779
PBE[GD3BJ]	BS1	67.56	48.98	0.99480	0.99497
	BS2	68.68	47.55	0.99975	0.99510
	BS3	69.91	48.02	0.99960	0.99485
	BS4	68.55	45.89	0.99999	0.99419
PBE0[GD3BJ]	BS1	30.61	1.34	1.02319	0.99921
	BS2	31.77	4.95	1.02103	0.99917
	BS3	31.95	6.17	1.01982	0.99913
	BS4	30.88	0.38	1.02416	0.99919
PW91	BS1	67.99	46.46	0.99854	0.99415
	BS2	66.68	45.25	1.00038	0.99535
	BS3	64.42	43.29	1.00093	0.99502
	BS4	67.95	46.71	0.99800	0.99411
RevTPSS	BS1	66.51	45.48	0.99736	0.99445
	BS2	61.80	41.61	0.99989	0.99530
	BS3	62.85	41.87	1.00033	0.99523
	BS4	64.53	40.16	1.00134	0.99470
wB97X[GD2]	BS1	30.95	2.31	1.02312	0.99922
	BS2	32.19	5.85	1.02109	0.99919
	BS3	31.90	4.42	1.02203	0.99917
	BS4	31.95	2.00	1.02404	0.99916
X3LYP	BS1	28.27	12.95	1.00617	0.99903
	BS2	29.50	11.47	1.00989	0.99906
	BS3	29.09	8.87	1.01185	0.99905
	BS4	37.18	13.80	1.01051	0.99826

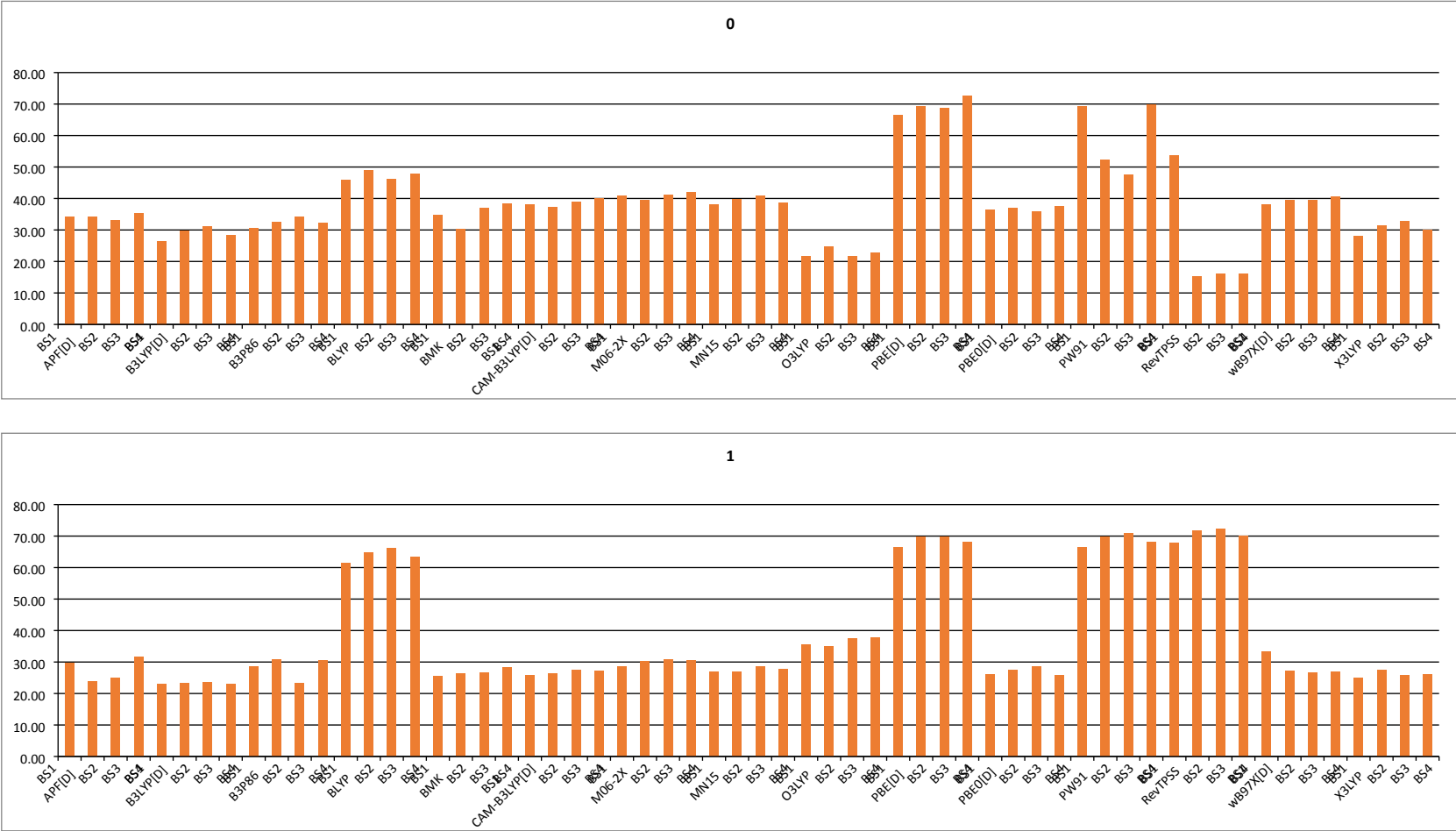
Table SI.A.1 Comparison between experimental and calculated IR and Raman frequencies (in cm^{-1}) and relative intensities of the 7 RNMs.

RNM	Vibrational Frequency (cm^{-1})				IR Intensity (Relative to the maximum)			Raman Activity (Relative to the maximum)	
	Experimental IR	Experimental Raman	Calculated harmonic	Calculated anharmonic	Experimental	Calculated harmonic	Calculated Anharmonic	Experimental	Calculated
0	RNM ₁	602	612	619 613 +300	0.26	0.19	0.22	0.10	0.11
	RNM ₂	699	662	672	1.00	0.01	0.01	0.15	0.15
	RNM ₃	990	1000	1016	0.19	0.25	0.00	1.00	0.83
	RNM ₄	1029	1039	1056	0.18	0.32	0.29	0.84	1.00
	RNM ₅	N/A	-	1287	-	0.00	0.00	-	0.07
	RNM ₆	1574	1582	1623	0.12	0.39	0.46	0.17	0.23
	RNM ₇	1581	1600	1628	0.23	1.00	1.00	0.12	0.35
1	RNM ₁	-	277	275	-	0.00	0.02	0.27	0.01
	RNM ₁ (2)	-	478	484	-	0.00	0.00	0.46	0.30
	RNM ₂	-	460	463	-	0.00	0.00	0.46	0.27
	RNM ₂ (2)	1170	1160	1177	-	0.00	0.00	0.09	0.16
	RNM ₃	693	697	702	0.20	0.05	0.06	0.38	0.57
	RNM ₃ (2)	1285	1287	1303	0.47	0.25	0.22	0.10	0.06
	RNM ₄	618	595	599	0.33	0.0	0.00	1.00	1.00
	RNM ₄ (2)	1285	1287	1303	0.47	0.25	0.22	0.10	0.06
	RNM ₅	1295	-	1332	0.13	0.11	0.18	-	0.19
	RNM ₆	1634	1654	1666	0.26	0.02	0.00	0.08	0.37
	RNM ₇	1645	1626	1657	1.00	1	1.00	0.06	0.16
	RNM ₁	-	354	351	-	0.00	0.00	0.42	0.19
	RNM ₁ (2)	817	825	827	1.00	0.93	1.00	0.09	0.02
	RNM ₂	-	337	333	-	0.00	0.00	0.26	0.09
2	RNM ₂ (2)	887	-	893	0.13	0.03	0.03	-	0.2
	RNM ₃	-	-	-	-	-	-	-	-
	RNM ₃ (2)	1085	1091	1094	0.58	0.34	0.23	0.10	0.00
	RNM ₄	-	392	386	-	0.00	0.00	1.00	0.30
	RNM ₄ (2)	1085	1091	1094	0.58	0.34	0.23	0.10	0.11
	RNM ₅	1223	1230	1259	0.28	0.38	0.35	0.09	0.63
	RNM ₆	1505	1547	1555	0.65	0.57	0.18	0.13	1.00
	RNM ₇	1498	1522	1525	0.27	1.00	0.93	0.42	0.33

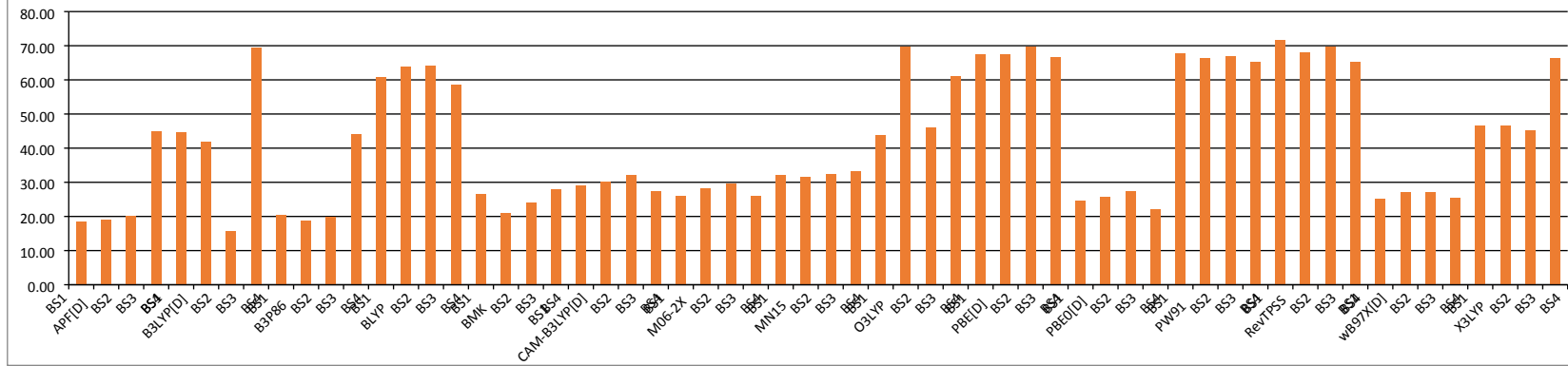
3	RNM ₁	-	408	410	406	-	0.00	0.00	0.67	0.17
	RNM ₁ (2)	575	576	584	577	0.25	0.01	0.01	1.00	0.75
	RNM ₂	-	410	413	409	-	0.00	0.00	0.67	0.15
	RNM ₂ (2)	1088	1088	1101	1080	0.39	0.90	0.13	0.05	0.03
	RNM ₃									
	RNM ₃ (2)	1142	1149	1148	1129	0.39	0.03	0.04	0.09	0.14
	RNM ₅	1271	1270	1316	1288	0.19	0.05	0.06	0.11	0.37
	RNM ₆	1603	1615	1630	1584	1.00	0.36	0.29	0.13	1.00
	RNM ₇	1594	1586	1612	1572	0.47	1.00	1.00	0.09	0.28
4	RNM ₁	-	334	336	333	-	0.00	0.56	0.39	0.06
	RNM ₁ (2)									
	RNM ₂	-	401	409	404	-	0.00	0.00	0.91	0.23
	RNM ₂ (2)	-	470	475	472	-	0.00	0.00	0.41	0.20
	RNM ₃									
	RNM ₃ (2)	1239	-	1258	1234	0.23	0.13	0.20	-	0.28
	RNM ₄	586	588	596	589	0.15	0.00	0.01	1.00	1.00
	RNM ₄ (2)									
5	RNM ₅	1303	-	1324	1299	0.13	0.07	0.09	-	0.28
	RNM ₆	1625	-	1652	1607	1.00	0.06	0.13	-	0.66
	RNM ₇	1606	-	1636	1589	0.26	1.00	1.0	-	0.46
	RNM ₁	-	285	284	282	-	0.01	0.04	0.12	0.01
	RNM ₁ (2)	-	432	432	427	-	0.00	0.00	0.38	0.20
	RNM ₁ (3)	538	540	546	540	0.21	0.02	0.02	1.00	1.00
	RNM ₂	-	460	464	459	-	0.00	0.00	0.38	0.25
	RNM ₂ (2)	-	-	1173	1150	-	0.00	0.00	-	0.25
5	RNM ₃	697	697	702	695	0.52	0.07	0.00	0.37	0.54
	RNM ₃ (2)	1237	-	1260	1239	0.79	0.49	0.57	-	0.02
	RNM ₄									
	RNM ₄ (2)	1269	-	1260	1239	0.79	0.49	0.57	-	0.02
	RNM ₅	1314	-	1317	1296	0.10	0.15	0.20	-	0.58
	RNM ₆	1611	-	1635	1588	0.10	0.03	0.01	-	0.19
	RNM ₇	1631	-	1646	1622	1.00	1.00	1.00	-	0.49
	RNM ₁									
	RNM ₁ (2)									
	RNM ₂	-	463	467	462	-	0.00	0.00	0.26	0.26
	RNM ₂ (2)	528	527	536	531	0.19	0.01	0.02	0.22	0.31

6	RNM ₃	795	797	806	796	0.94	0.17	0.23	0.26	0.78
	RNM ₃ (2)									
	RNM ₄	597	599	603	597	0.03	0.00	0.00	1.00	1.00
	RNM ₄ '	1405	-	1430	1401	0.69	0.23	0.37	-	0.40
	RNM ₅	1295	-	1337	1308	0.14	0.04	0.04	-	0.13
	RNM ₆	1631	-	1650	1603	1.00	1.00	1.00	-	0.27
	RNM ₇	1652	-	1663	1620	0.11	0.17	0.15	-	0.44
7	RNM ₁	-	305	283	281	-	0.00	0.00	0.13	0.02
	RNM ₁ (2)	-	507	515	509	-	0.01	0.02	0.26	0.42
	RNM ₁ (3)	742	743	759	748	0.62	0.03	0.14	0.45	1.00
	RNM ₂	-	451	457	452	-	0.00	0.00	0.05	0.15
	RNM ₂ (2)	1138	1142	1161	1134	0.14	0.09	0.34	0.06	0.14
	RNM ₃	692	696	696	689	0.56	0.08	0.09	1.00	0.05
	RNM ₃ (2)	1240	1230	1243	1209	0.23	1.00	1.00	0.05	0.01
	RNM ₄	693	693	696	689	0.03	0.08	0.09	0.03	0.05
	RNM ₄ (2)	1226	1230	1243	1209	1.00	1.00	1.00	0.06	0.01
	RNM ₅	1273	1287	1323	1297	0.33	0.34	0.68	0.04	0.09
	RNM ₆	1638	1628	1659	1613	0.21	0.02	0.04	0.03	0.32
	RNM ₇	1645	1647	1658	1628	0.05	0.15	0.03	0.05	0.08

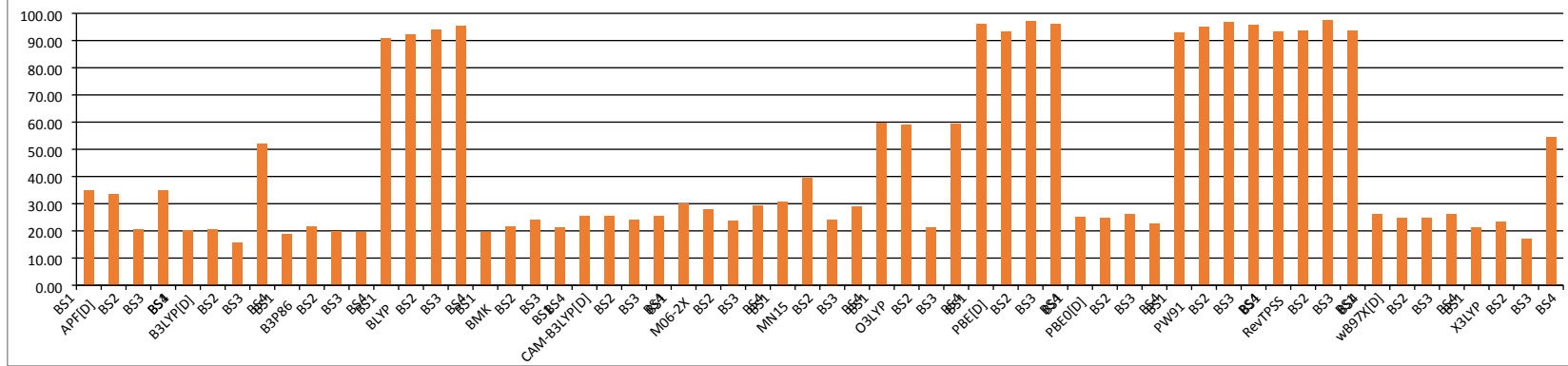
Figure SI.A.1. Standard deviations

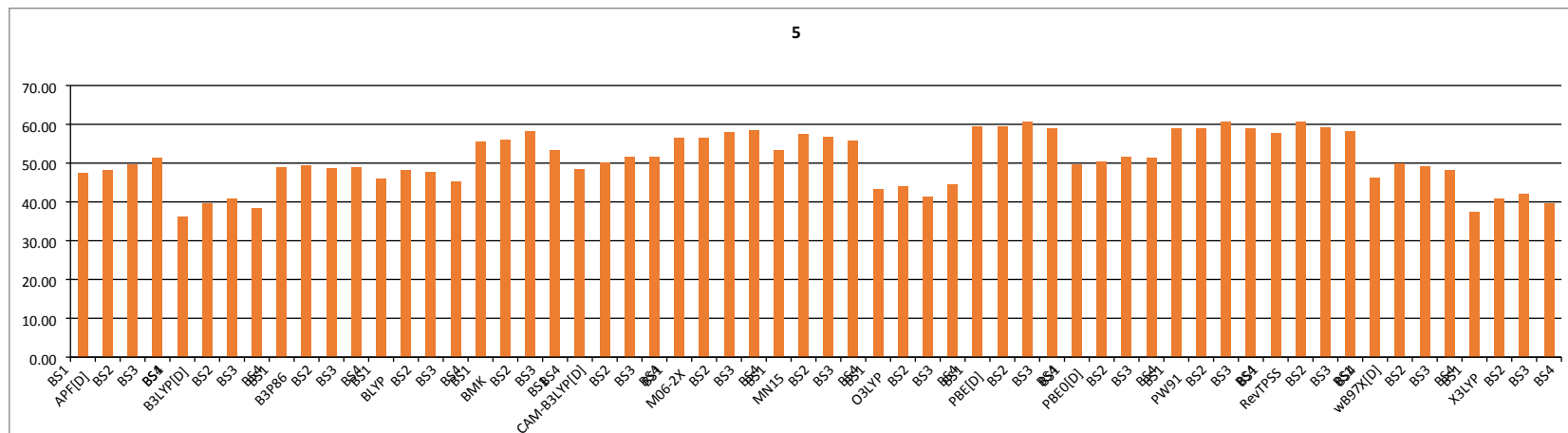
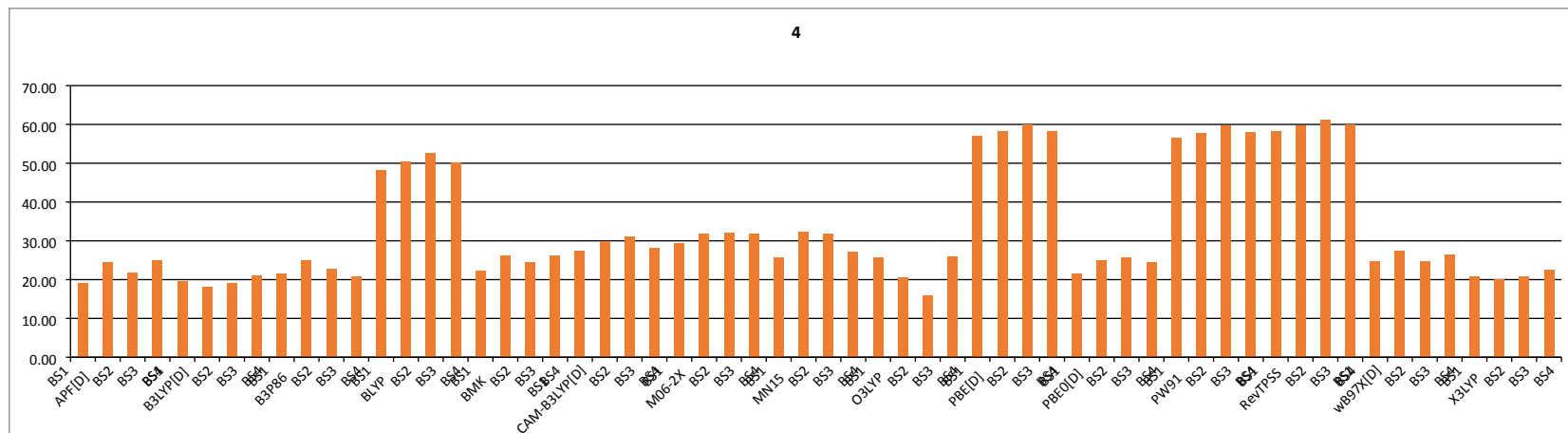


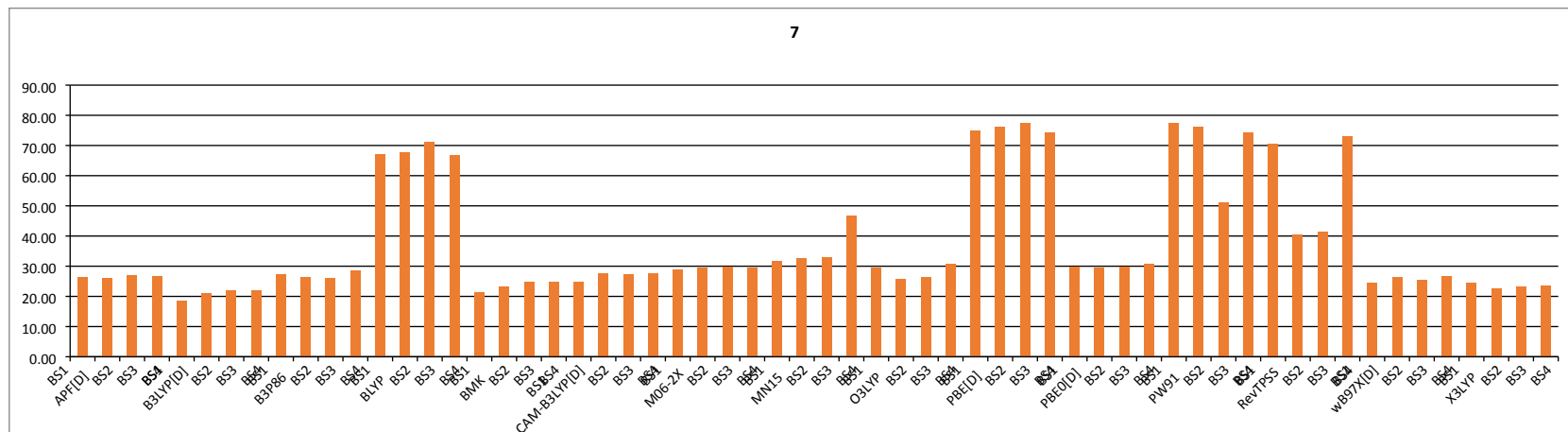
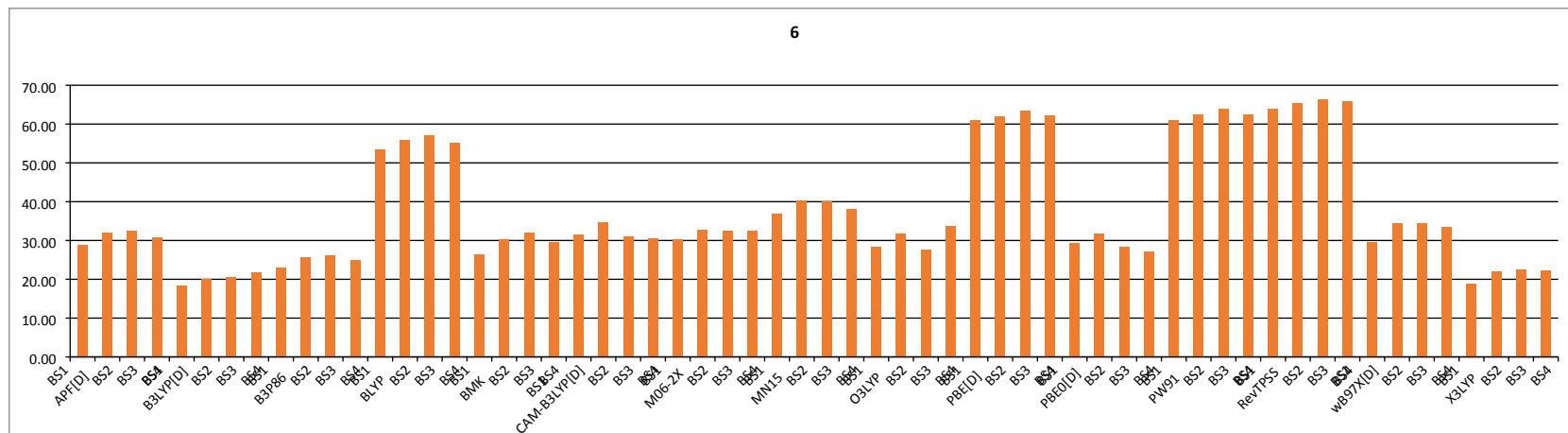
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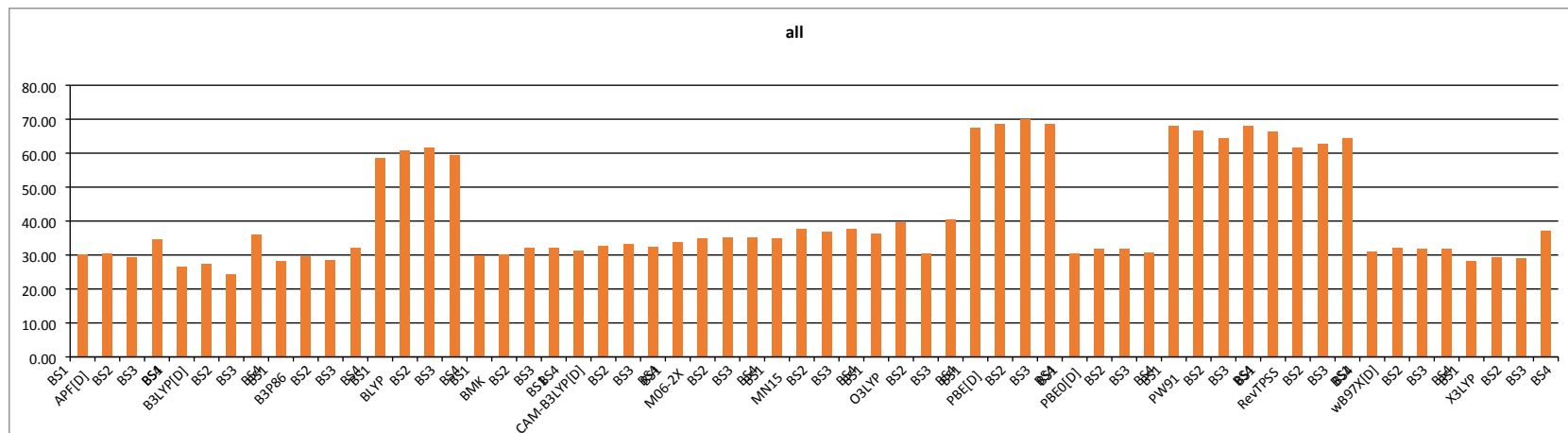
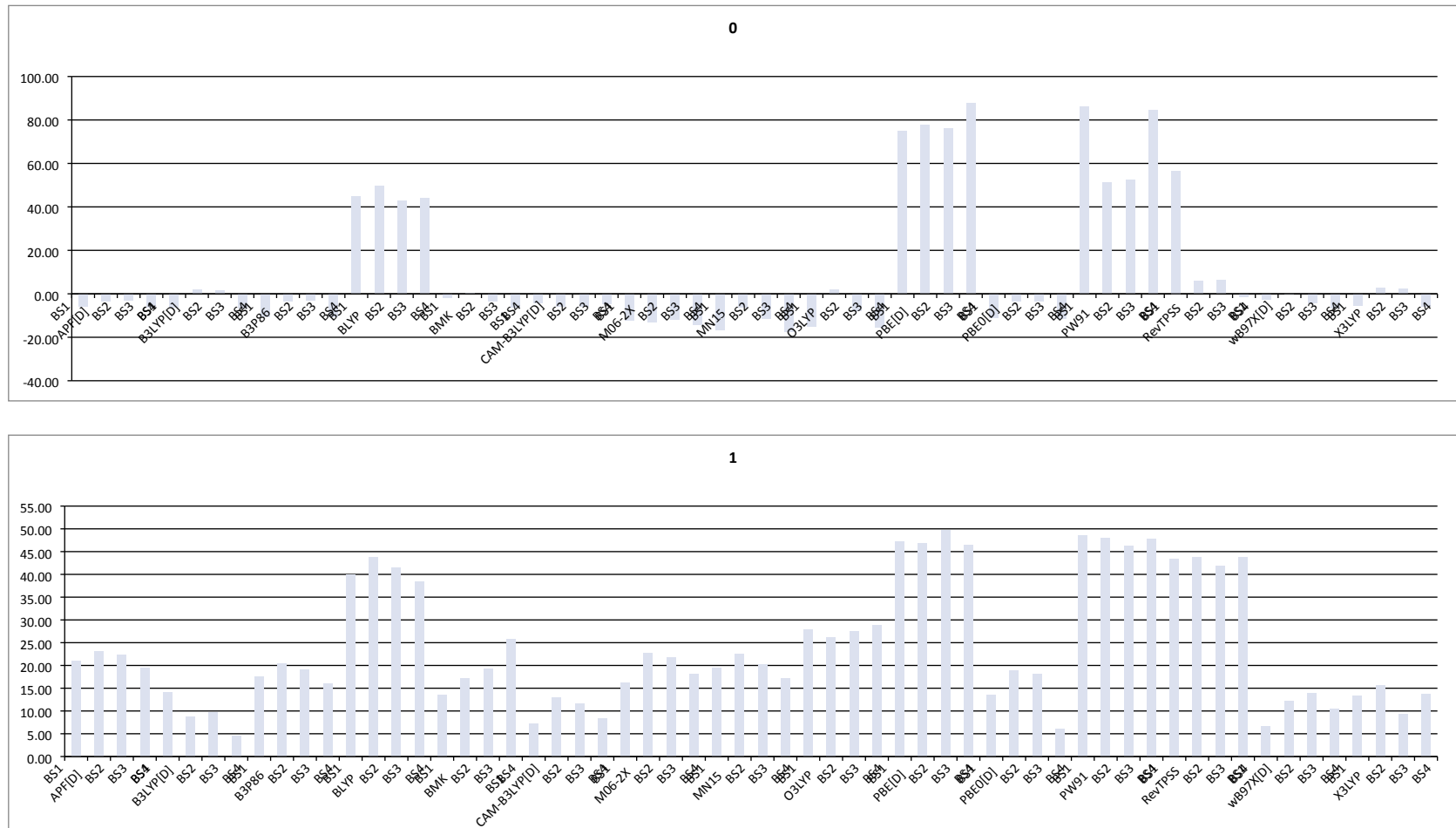
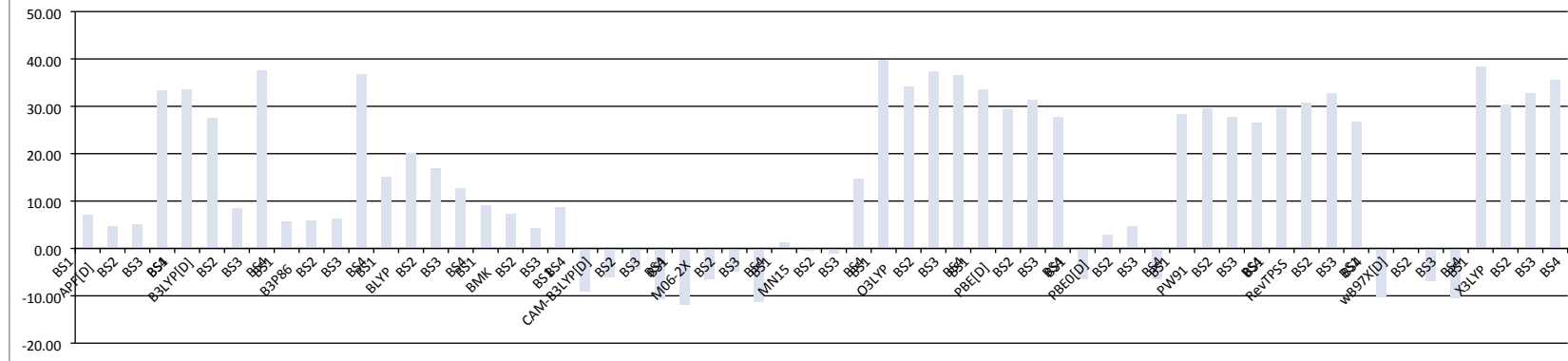


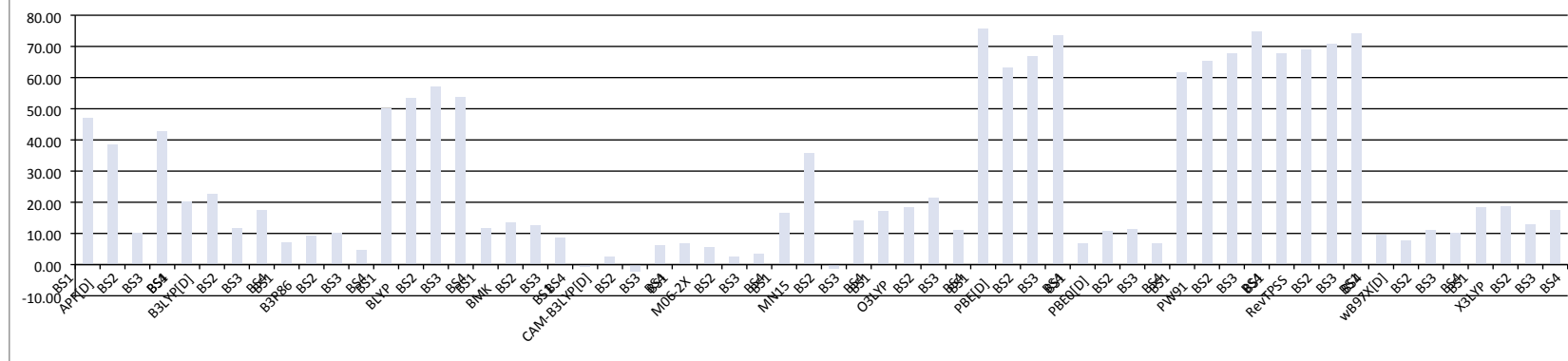
Figure SI.A.2. Intercepts



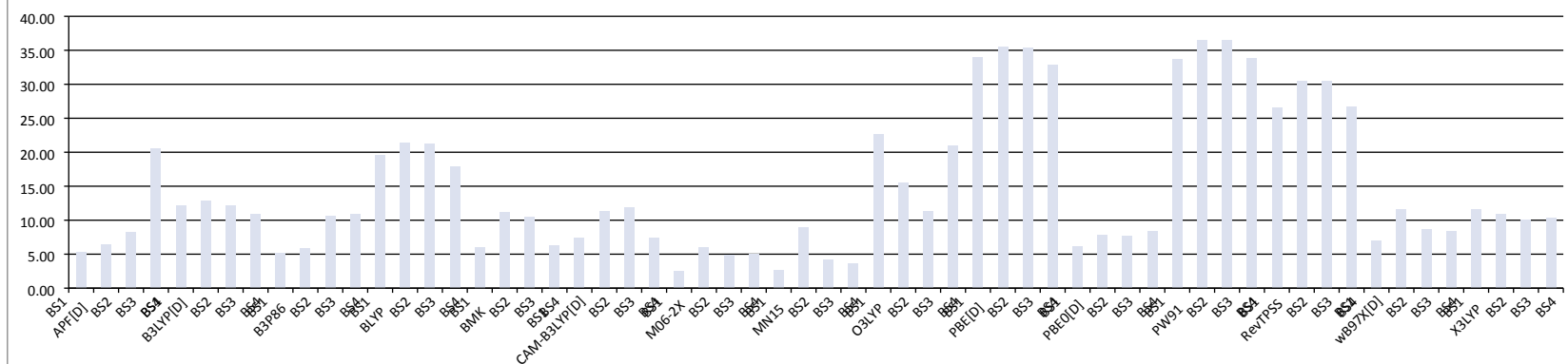
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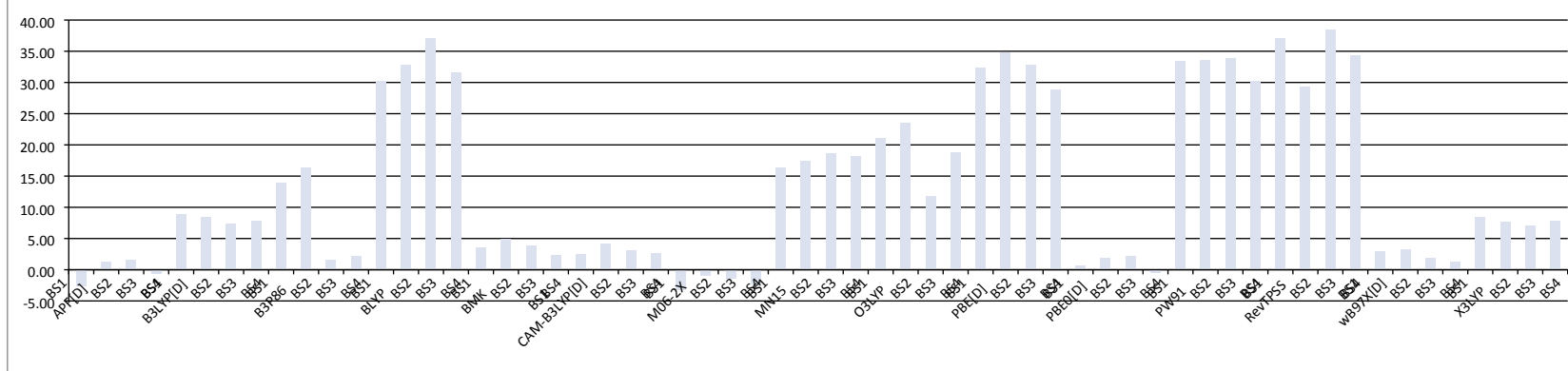
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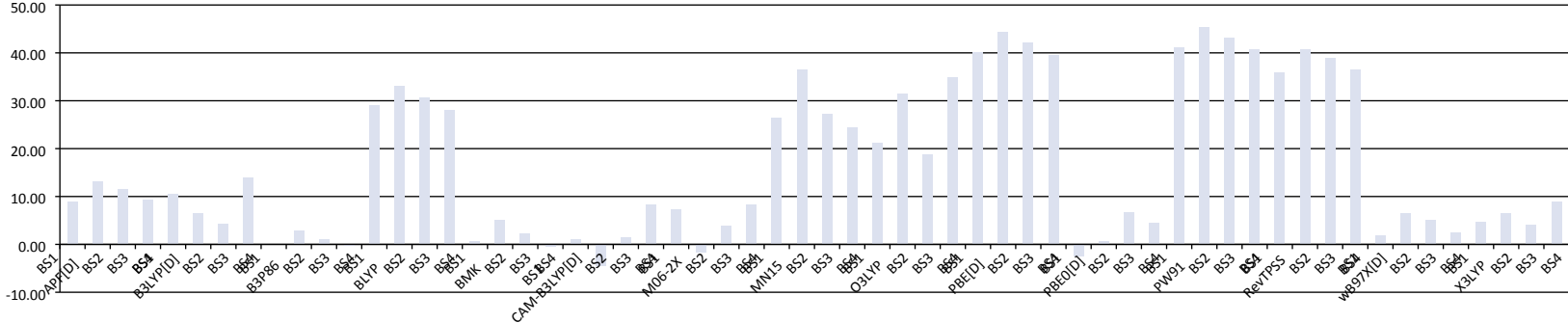
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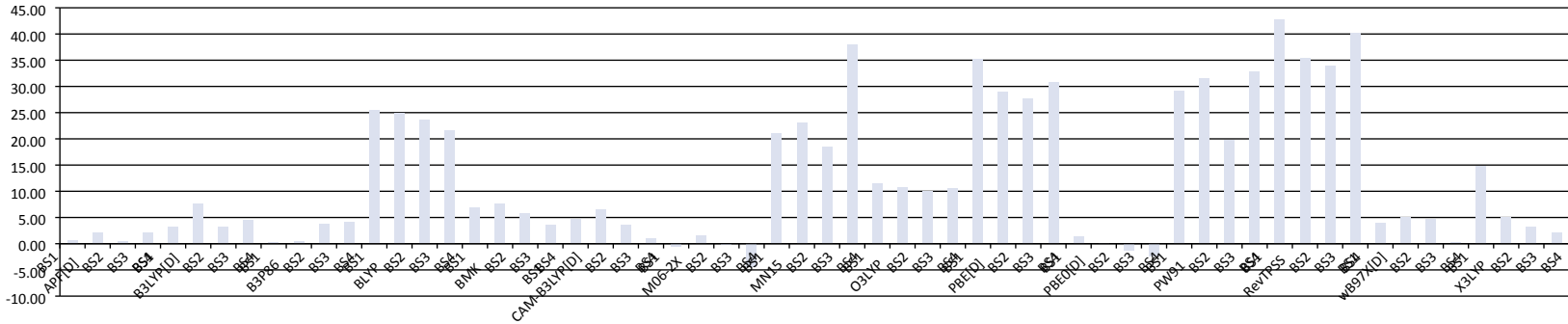
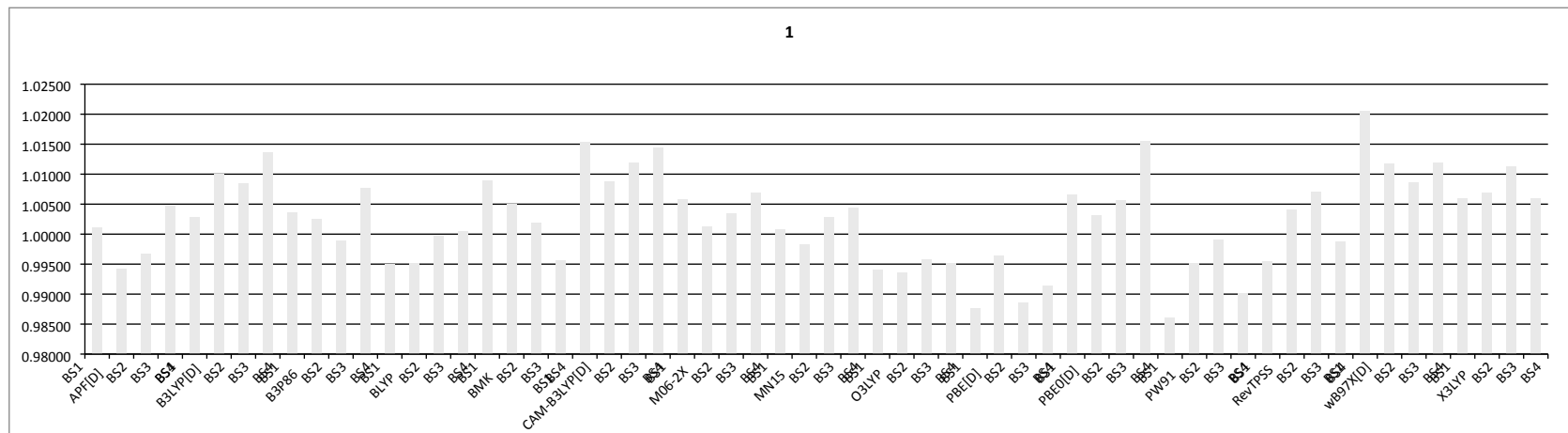
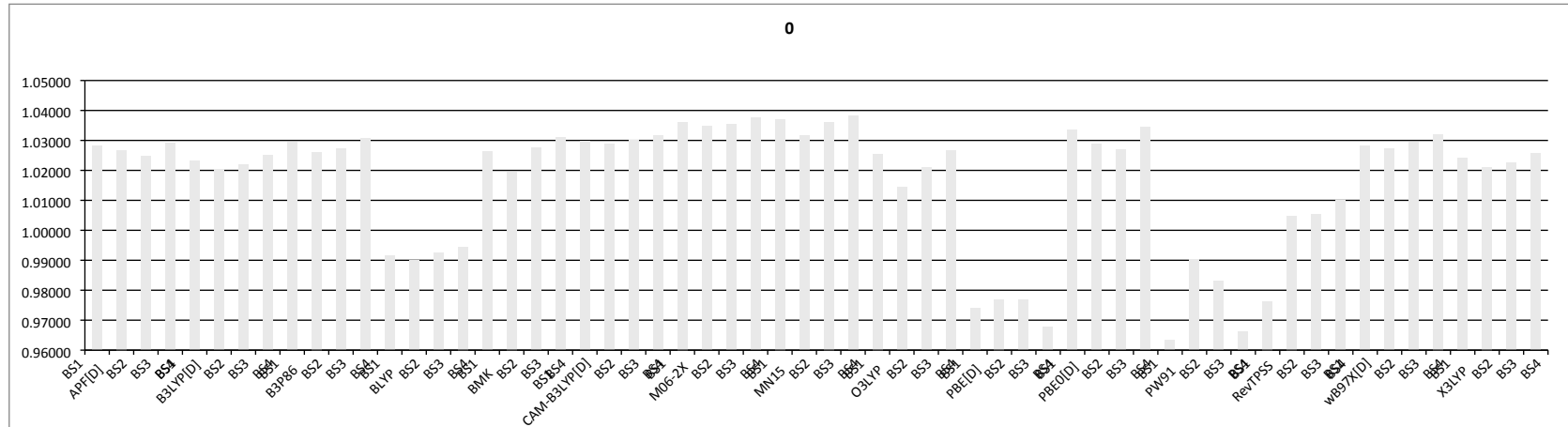
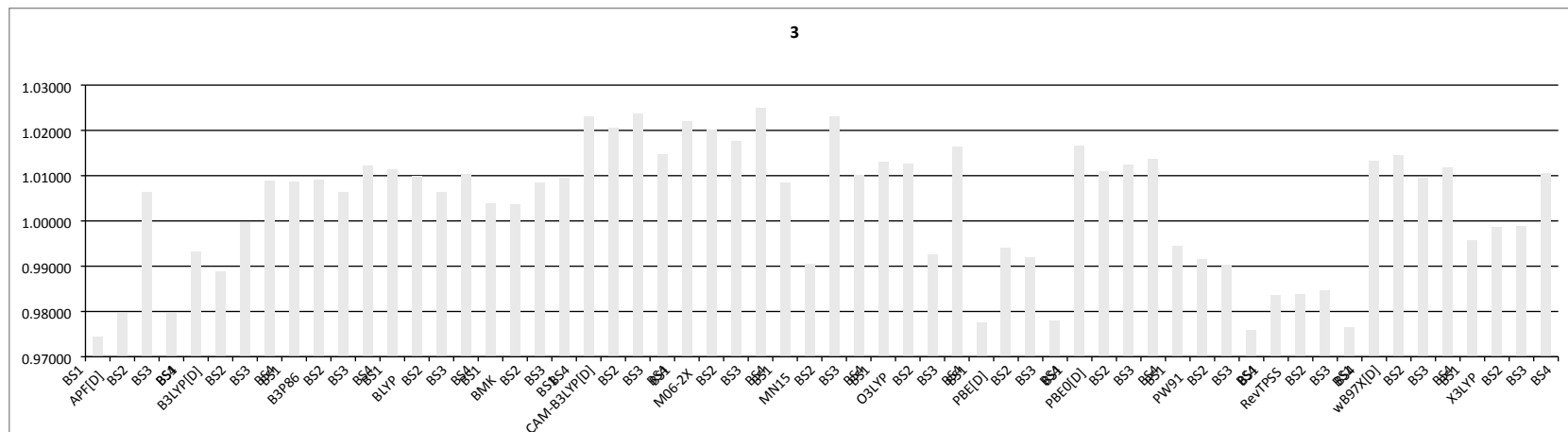
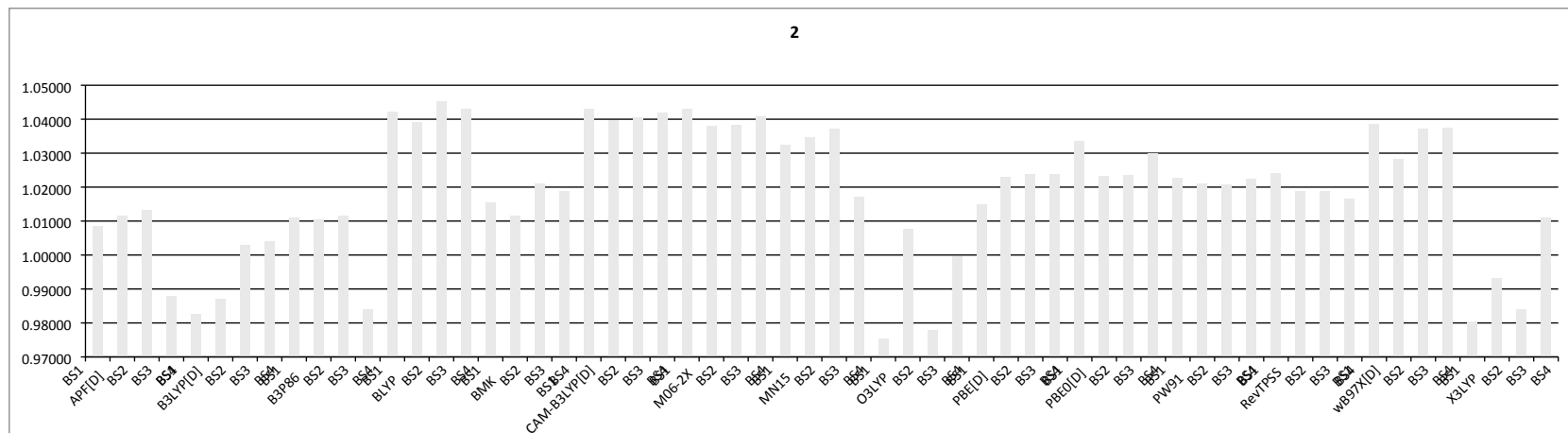
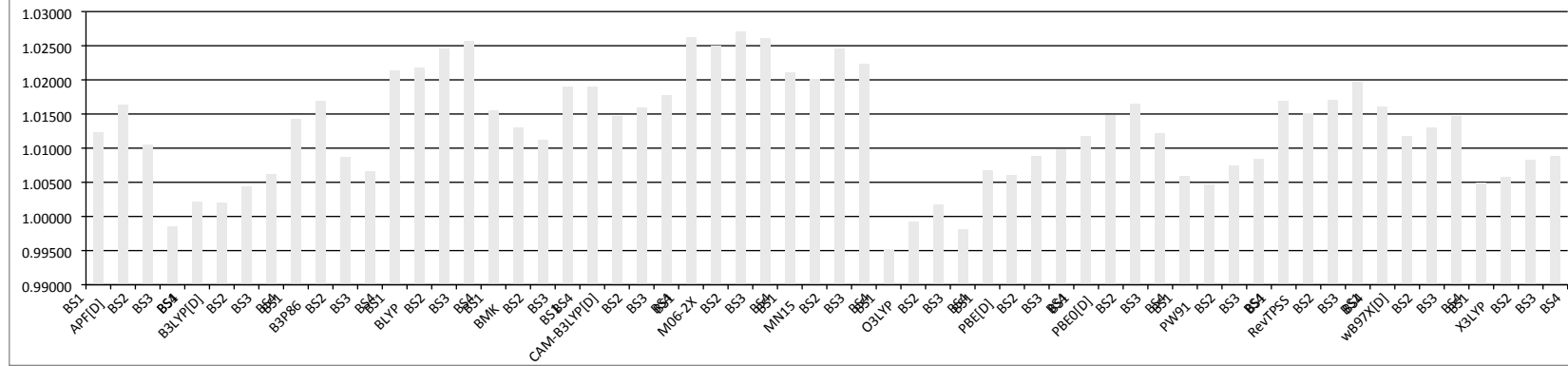


Figure SI.A.3. Slopes

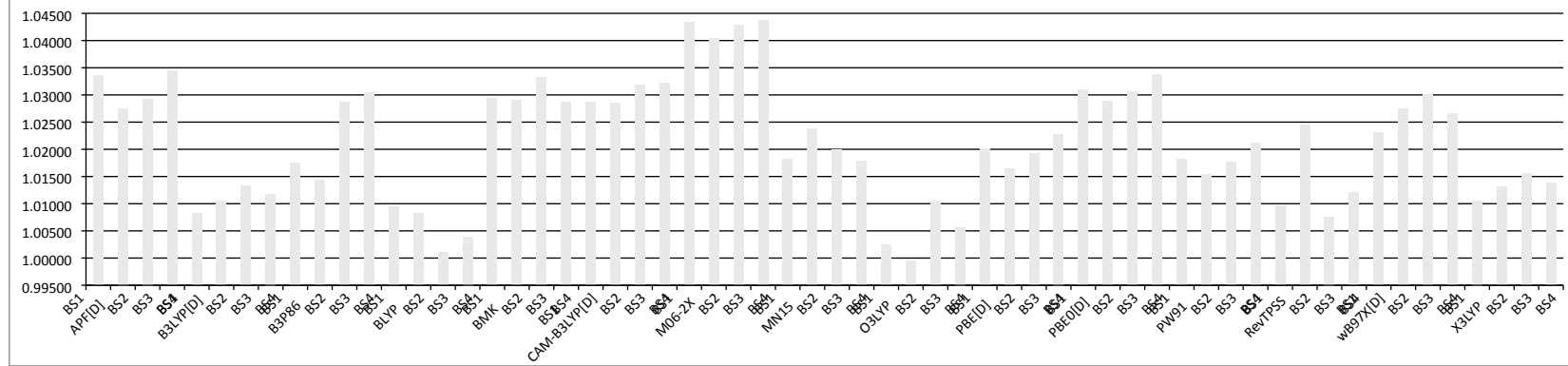




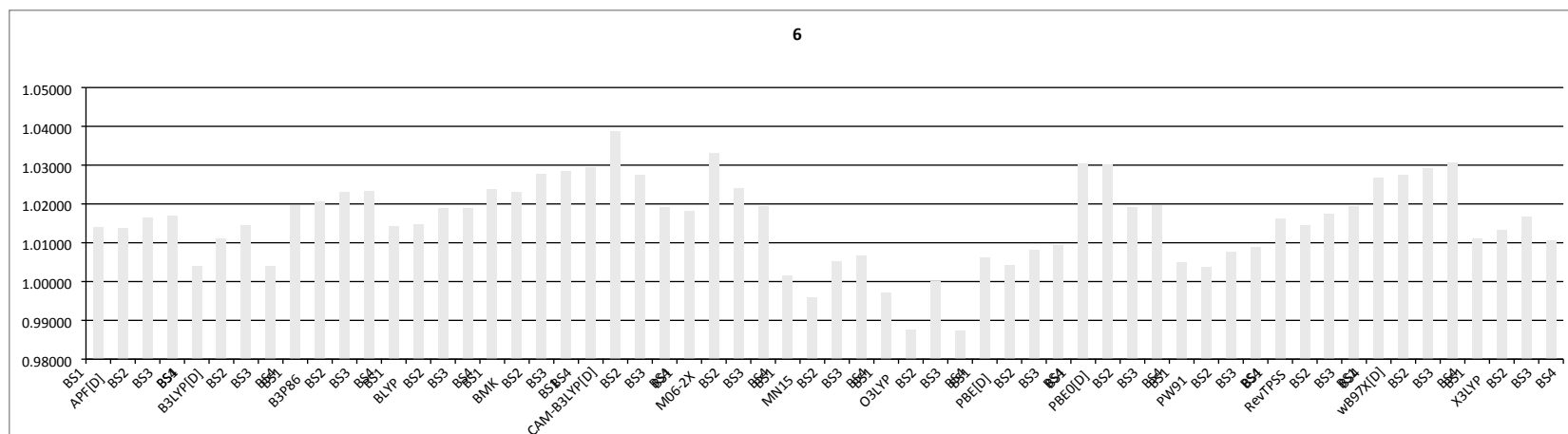
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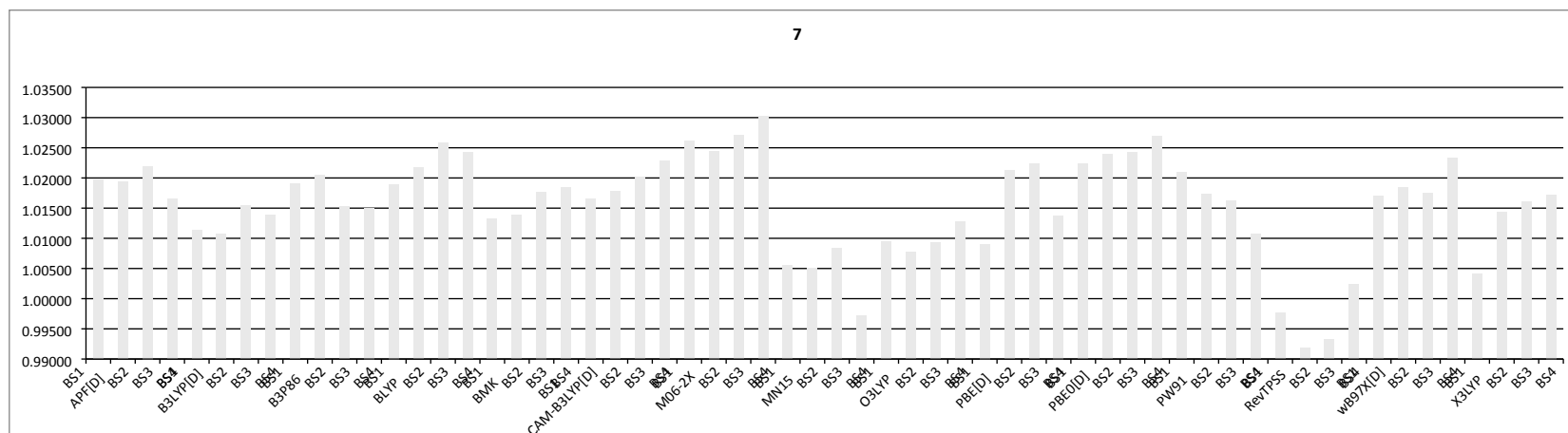
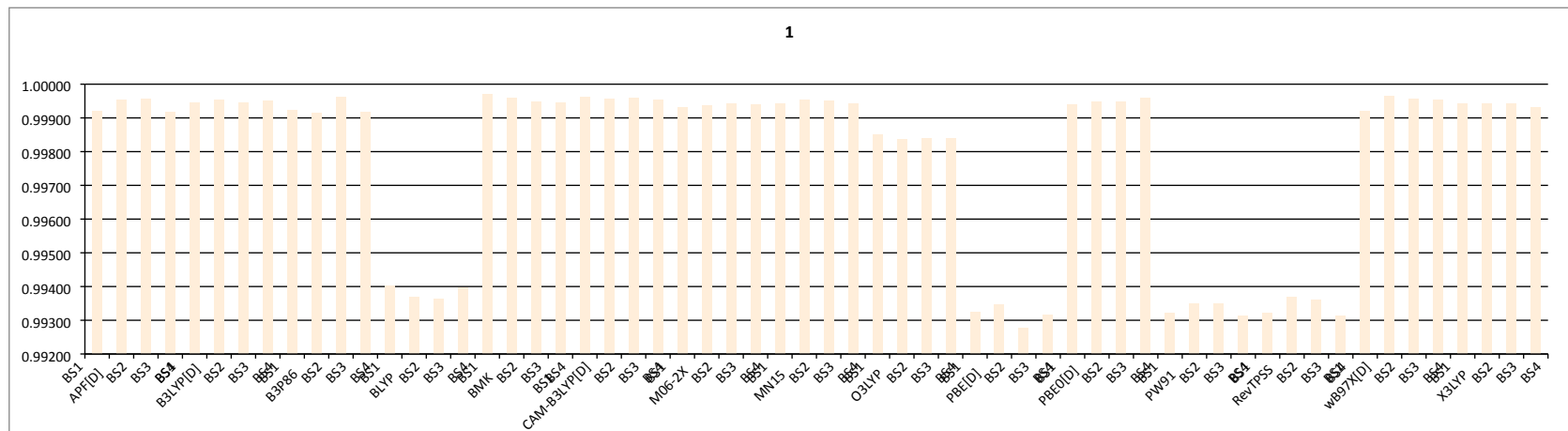
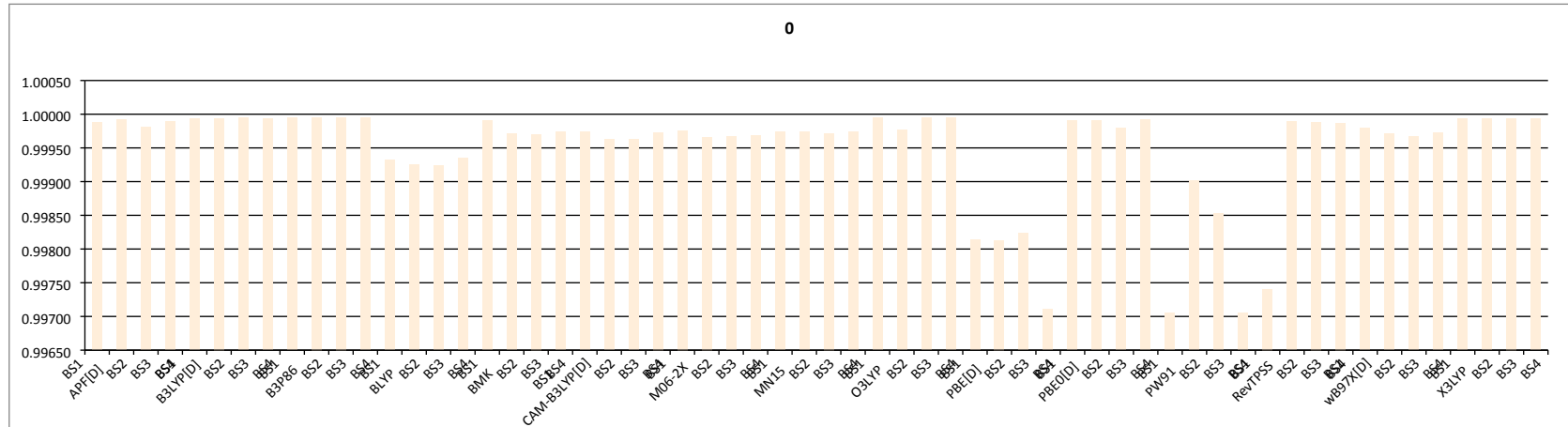
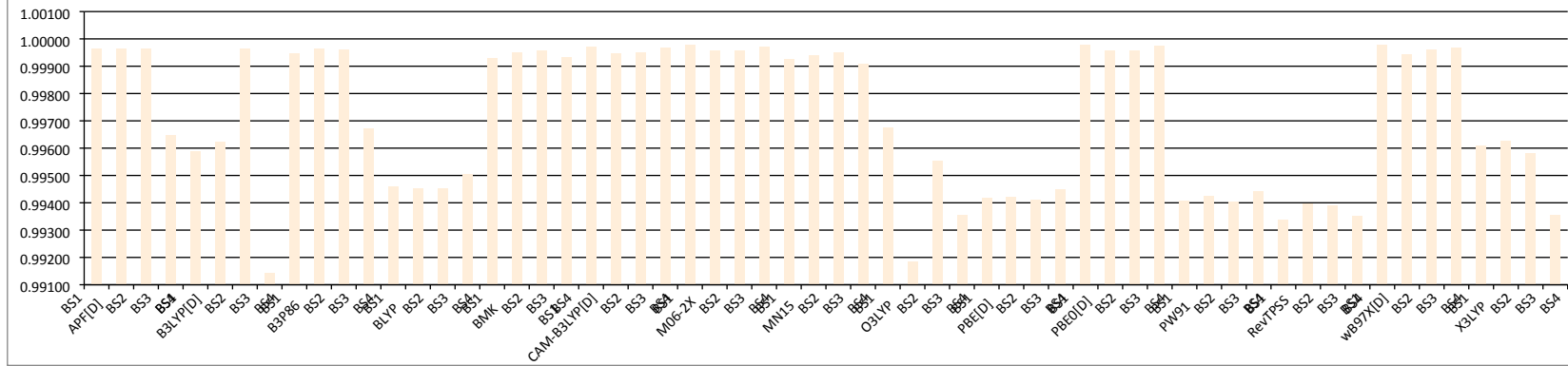


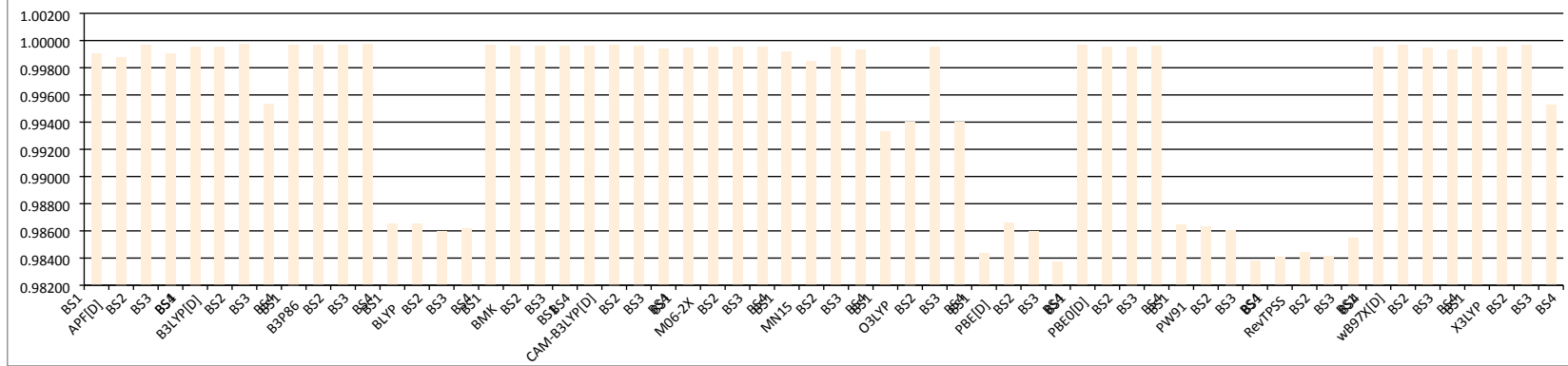
Figure SI.A.4. Regression coefficients

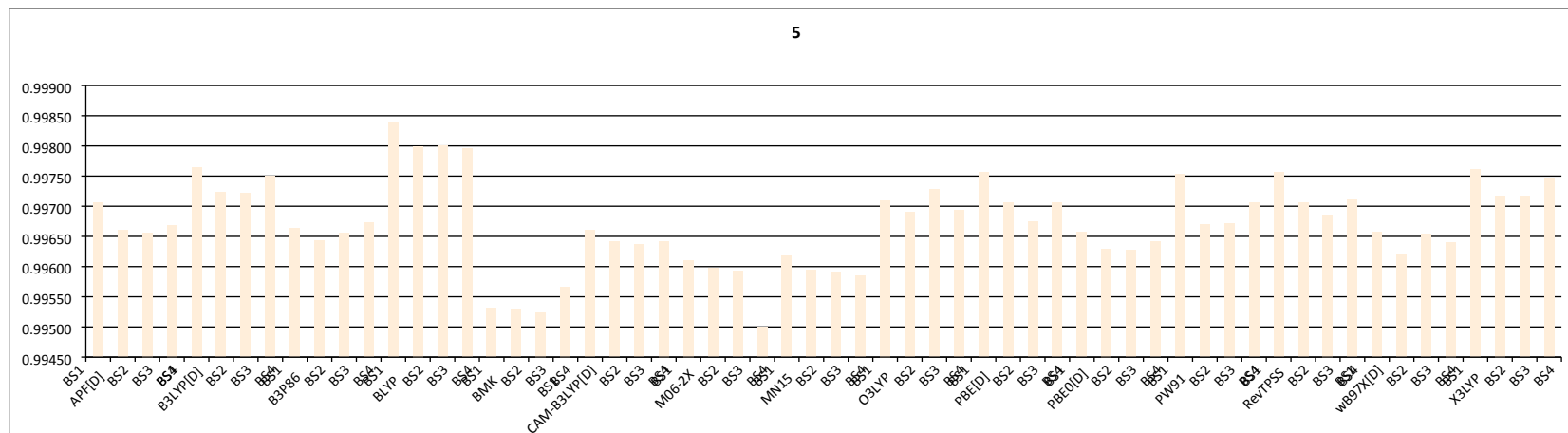
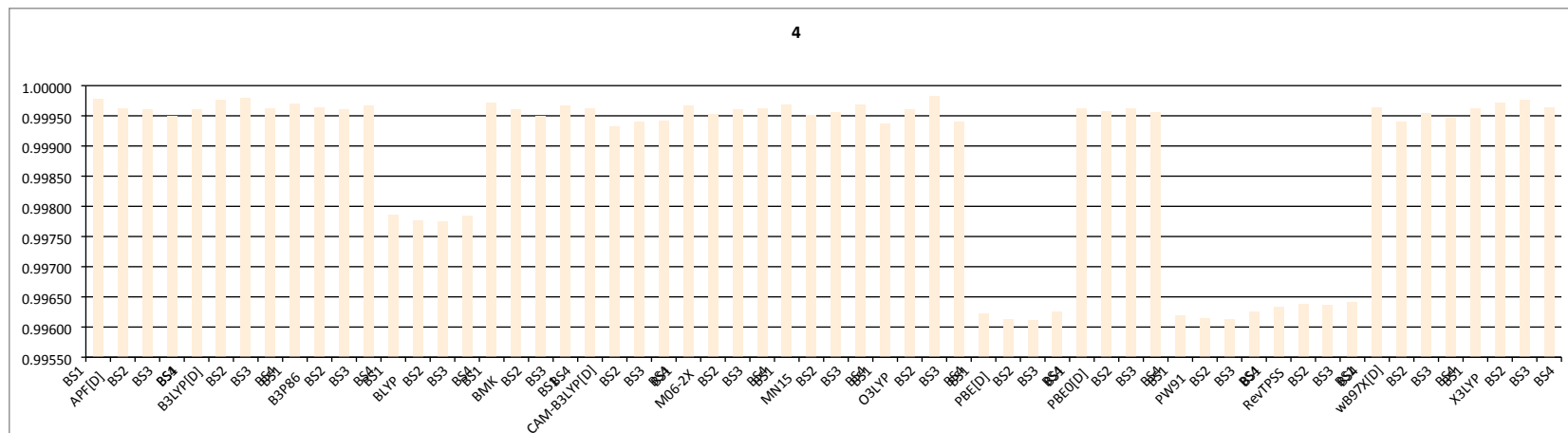


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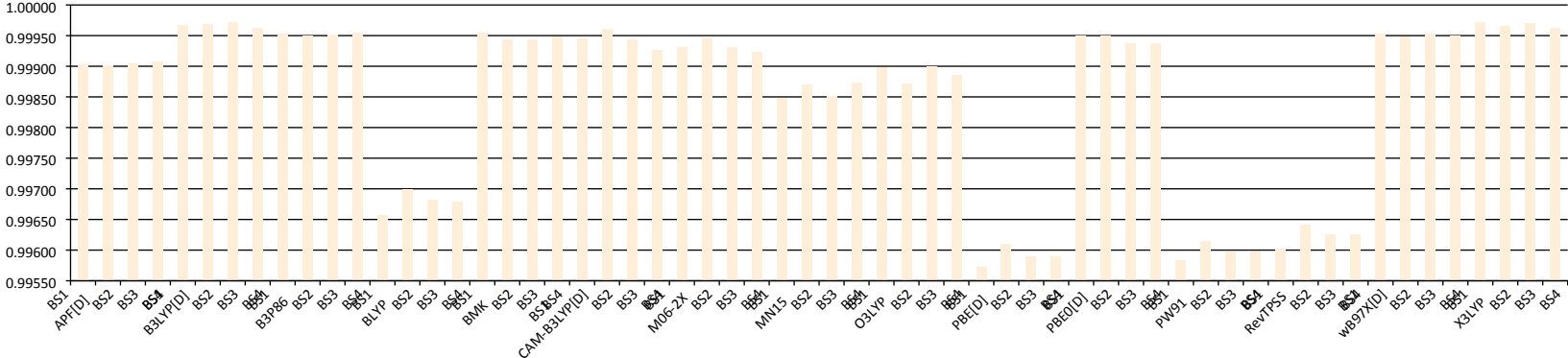


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